List of changes in the software package BREMS

Below is the list of changes for each version of the software package BREMS (available from https://web.vu.lt/ff/a.poskus/brems/ or https://www.researchgate.net/publication/332171944_BREMS) up to the current version (1.5.8.9).

1.1.0 (2017-09-27):

1. A new command-line argument ("R_atom") has been inserted into the set of the command-line arguments of S_integral.exe (source code file "S_integral.f90"). It is equal to the "atomic radius", defined as the value of the radial coordinate r where the interaction potential $V(r)$ becomes zero, i.e., is "truncated". If this command-line argument is zero or negative, then the interaction potential will not be truncated. Although the results obtained in the latter case may be more accurate (provided that the absolute value of the command-line argument "Q_last" is small enough), the computation time may become prohibitively long if the electron energy is greater than 1 MeV and the decrease of the screening function is very slow. Besides, it is usually possible to achieve a negligibly small difference between the results obtained with R_atom = 0 and with R_atom > 0 by a judicious choice of the value of R_atom. It should be much greater than the typical distance from the nucleus to the point where the interaction event occurs. The latter distance is approximately equal to the inverse of the minimum momentum transfer, which is equal to $q_{\min} = p_1 - p_2 - k$. For example, if $1 / q_{\min}$ is of the order of 10, then the value R_atom = 500 should be sufficient to achieve acceptable accuracy.

   Notes: **1)** If this command-line argument is positive, then the phase correction integrals (Q_1 and Q_2) are calculated only for $r <$ R_atom. Since $V(r) = 0$ for $r \geq$ R_atom, the upper bound of the phase correction integrals is equal to R_atom rather than to ∞. At $r \geq$ R_atom, $Q_{1,2} = 0$. **2)** Even if the wave function has not attained the asymptotic form at $r =$ R_atom, the Hamming's algorithm is terminated anyway. In such a case, the phase shift and the normalization factor are calculated on the basis of the values of g_κ and f_κ at the first point satisfying the condition $r \geq$ R_atom, and the corresponding uncertainties (range widths) are set to zero. **3)** If r0_min < R_atom, then, as it follows from the previous two notes, the point of transition to analytical integration (r_0) cannot exceed R_atom. Consequently, at electron energies greater than 1 MeV, the judicious choice of R_atom (see above) usually results in a significant reduction of r_0. Since a decr of r_0 may cause an increase of the precision level needed to compute the analytical integrals to an acceptable accuracy (and hence a significant increase of the time of the analytical integration), it may be advantageous specify a value of r0_min greater than R_atom (or to increase R_atom) when the electron energy is greater than 1 MeV (see the description of the command-line argument "pr_transition2").
2. Added two variables for output to the *S* integral data file: the above-mentioned atomic radius and the maximum number of steps of the numerical quadrature ("nPoints"). This change required modifying the files "Read_S_int2.f90", "fileSize.f90", "Read_S_integrals.f90" and "Bremsstrahlung.f90". The corresponding executables (Read_S_integrals.exe and Bremsstrahlung.exe) have been re-compiled. The current version number of the *S* integral data file has been increased to 3.
3. Updated the user manual.

1.1.1 (2017-09-28):

1. An inconsistent calculation of the uncertainties of the *S* integrals in the case of truncated point-Coulomb potential (with R_atom ≠ 0) has been fixed. Before this fix, the mentioned uncertainties were calculated in the same way as for the exact (non-truncated) point-Coulomb potential (with R_atom = 0). After this fix, the mentioned uncertainties are calculated in the same way as for the screened potentials, because truncation of the potential is, in fact, a special case of screening of the nucleus (when the screening negative charge forms a spherical shell of zero thickness).
2. An interpretation of a negative value of the command-line argument "R_atom" of S_integral.exe has been changed. Previously, it was interpreted in the same way as the zero value. Now, it is interpreted as the opposite of the factor that must be used for multiplying the inverse minimum momentum transfer in order to calculate the value of R_atom. In the latter case, the value of "r_min", which is controlled by the command-line argument "pr_transition2", doubles up as the minimum allowed value of R_atom (i.e., if the calculated value of R_atom is less than r0_min, then R_atom is set equal to r0_min).
3. Updated the user manual.

1.1.2 (2017-09-30):

1. Fixed a bug in S_integral.f90 that caused incorrect re-calculation of the number of wave functions that have not attained the asymptotic form yet after reducing κ_{max} in the case of the zero photon energy.
2. Added an option in S_integral.f90 to "round up" the value of r_0 (the point of transition from the numerical integration to the analytical integration), i.e., to extend the region of the numerical integration up to the value of the radial coordinate equal to 10^n, $2 \cdot 10^n$ or $5 \cdot 10^n$ in relativistic units, where n is an integer number. In order to select this option, the value of the command-line argument "pr_incr" must be specified with the minus sign. This option is useful for creating a library of cross sections for multiple chemical elements, because the integral from r_0 to ∞ (the "analytical" integral) is expressed as a linear combination of four integrals, and each of the latter four integrals depends only on r_0, T_1 and k (but not on the atomic number Z). Thus, if the values of r_0, T_1 and k are exactly the same for different Z, then it will be possible to reuse the values of the mentioned four integrals and thus to skip the stage of the analytical integration for some combinations of Z, T_1 and k (in such a case, a change of Z would require only to recalculate the coefficients of the mentioned linear combination, which depend on the phase shifts).
3. Updated the user manual.

1.2.0 (2017-10-04):

1. Added an option to create a file with the integrals of the products of three spherical Bessel functions and r^2 from r_0 to ∞ (the integrals S_{11}, S_{12}, S_{21} and S_{22}, defined in Section 1.2 of the user manual). Unless changed by the user, the name of this file is formed by combining the prefix "S_integrals_" and the values of the incident electron energy (T_1), bremsstrahlung photon energy (k), the lower bound of the integrals (r_0) and the suffix "_a". Consequently, this file will be called the "_a" file. This option is selected by setting the command-line argument "iTestRun" of S_integral.exe equal to −2. Added an option to calculate the second part of the S_1 and S_2 integrals by combining the values of the S_{ij} integrals ($i, j = 1, 2$) loaded from an existing "_a" file (each S_1 or S_2 integral from r_0 to ∞ is equal to a linear combination of the four corresponding S_{ij} integrals, with coefficients depending on the phase shifts, which are determined at the stage of the numerical solution of the radial Dirac equations). This option is selected by setting the command-line argument "iTestRun" of S_integral.exe equal to 2 or −1 (in the first case, the "test" numerical integration will be performed, and in the second case it will not be performed). Since this option can be selected only when $k \neq 0$, the name of the existing "_a" file is defined using the last three command-line arguments, which in the case $k = 0$ are used to define the name of the phase shift data file.
2. Updated the user manual.

1.3.0 (2017-10-15):

1. Added an option to "skip" some of the values of κ_2 when calculating the S integrals and the cross sections. The terms corresponding to the missing partial waves in the expressions of the single- and double differential cross sections are obtained by logarithmic cubic spline interpolation (see Section 1.3 in the updated user manual for details). This option is controlled by three additional command-line arguments inserted after the arguments controlling the limits of κ_2 (those command-line arguments are used by the programs S_integral.exe, Bremsstrahlung.exe and Read_S_integrals.exe). This option makes it possible to decrease the processing time by a factor of 5 or more when the electron energy is of the order of 1 MeV.
2. Updated the user manual.

1.3.1 (2017-11-02):

1. If the test integration has been performed, then the overall range of variation of the phase shift is obtained by combining its ranges of variation corresponding to the original integration and to the test integration (previously, only the range of variation during the original integration was taken into account). As a result, the overall uncertainty of the phase shift is typically greater than in the previous version of S_integral.exe at least by a factor of 2, and it is no longer zero when the interaction potential is truncated before the wave functions attain the asymptotic form.

2. The *S* integral data files now include the normalization factors and the uncertainties (ranges of variation) of the phase shifts and of the normalization factors.
3. If the radial range of the numerical integration was extended by "rounding up" the value of the transition point r_0, then both the original and the rounded values of r_0 are now stored in the *S* integral data file (the previous version of S_integral.exe stored only the rounded value of r_0).
4. The mentioned additional data in the *S* integral data files are loaded by S_integral.exe when the numerical integrals are being re-used. In addition, those data are displayed by Read_S_integrals.exe.
5. Rearranged several columns in the file "system_parms.txt" and inserted three columns in the file "err_test.txt" (both those files are updated by Bremsstrahlung.exe).
6. Fixed several minor bugs.
7. Updated the user manual.

1.3.2 (2017-11-05):

1. Fixed a bug that caused a failure to decrease Kmax(2) after a decrease of Kmax(1) when a zero value of the photon energy k had been specified on the command line of S_integral.exe (when $k = 0$, Kmax(2) should always be equal to Kmax(1)). Because of this bug, the infinite series in the expressions of the differential cross sections were truncated at a value of κ greater than Kmax(1), and the values of the differential cross sections calculated by Bremsstrahlung.exe were incorrect.
2. Fixed a bug that caused the zero value of the uncertainty of the phase shift when the interaction potential was truncated at a certain value of the radial coordinate.
3. Fixed a bug that caused the error message "Incorrect set of test integrals", which could appear at the stage of the analytical integration from r_0 to ∞ when the largest negative values of κ_1 or κ_2 were greater in absolute value than the largest positive values of κ_1 or κ_2.

1.3.3 (2017-11-08):

1. A better method of dealing with the accumulation of errors due to uncertainties of the *S* integrals when calculating the cross sections has been implemented. Instead of excluding the *S* integrals with relative uncertainties greater than 100 % in Bremsstrahlung.exe (as it was done in the previous version), the errors of cross sections are checked in the next stage of the calculation by Brems_fit.exe. This is done by comparing the "original" and "test" cross sections calculated by Bremsstrahlung.exe. If it is determined that the relative errors of the single- or double differential cross sections are greater than the user-specified maximum relative error, then the maximum value of κ_{max} is reduced. The mentioned maximum relative error is specified using an additional command-line argument of Brems_fit.exe.
2. Two of the output files of Brems_fit.exe ("CS_fitted.txt" and "CS_parms.txt") now include three columns with the original and reduced values of κ_{max} (column headers "kmax0" and "kmax", respectively) and the value of the maximum relative error ("MaxRelErr"), which is used as the criterion for the mentioned decrease of the maximum value of κ_{max}.
3. Fixed a bug in Brems_fit.exe, which caused incorrect update of the range of variation of the single- or double differential cross section as a function of κ_{max} after decreasing the lower limit of the fitting range. This could cause an apparent "lockup" of the program or incorrect results of the fitting.
4. Modified the calculation of the relative error of cross sections, which is used to determine if the maximum value of κ_{max} should be reduced in Brems_fit.exe. Now, it is defined as the "scaled" absolute error, i.e., the absolute difference of the "original" and "test" cross sections divided by the maximum value of the "original" cross section in the specified range of values of κ_{max}.

1.3.4 (2017-11-09):

1. Fixed an error in S_integral.f90, which in rare cases (at values of Z close to 90 or greater) caused incorrect values of the steps of the numerical algorithms used to solve the system of differential equations and to perform the Newton-Cotes quadrature during the "test" integration. Because of this error, incorrect values of the test numerical integrals could be obtained.

2. Modified the calculation of the maximum relative error of cross sections, which is written to the file "err_test.txt" by Bremsstrahlung.exe. Now, it is defined as the "scaled" maximum absolute error, i.e., the maximum absolute difference of the "original" and "test" cross sections divided by the maximum value of the "original" cross section in the specified range of values of κ_{max} (this change mirrors the corresponding change done to Brems_fit.f90 in the previous update).

1.3.5 (2017-11-17):

1. Added an option to smooth the fitted angular distribution in Brems_fit.exe. This allows eliminating occasional large peaks that sometimes appear in the fitted dependence of the double differential cross section (DCS) on the photon emission angle (θ) due to the fitting errors when the DCS is relatively far from saturation as a function of κ_{max}. This option is controlled by an additional command-line argument, which indicates the maximum interval between adjacent inflection points (i.e., the points where the second derivative of DCS(θ) changes sign). If two inflection points separated by an interval less than or equal to the specified maximum value are found and if the relative change of the DCS immediately before or after such a point exceeds the corresponding relative change of the original (unfitted) DCS by more than 20 %, then the program will attempt to remove one or both of the mentioned inflection points by smoothing the DCS as a function of θ.
2. During the calculation of the analytical integrals (from r_0 to ∞), S_integral.exe now displays the percentage of the calculated terms at 10-second intervals.
3. Corrected the user manual.

1.3.6 (2017-11-25):

1. Added the option to use two values of the increment of the emission angle θ in two angular ranges. This option is controlled by two additional arguments of Bremsstrahlung.exe and Brems_fit.exe. The integration of the DCS is done in those two ranges independently, using the 10^{th}-order Newton-Cotes formula. Consequently, it is recommended to set the number of angular integration steps in each of those two ranges to a multiple of 10.
2. Changed the meaning of a negative value of "interval_max" in Brems_fit.exe: now the sign of this command-line argument indicates the number of smoothing cycles. The minus sign indicates one smoothing cycle, and a positive value indicates additional smoothing cycles.
3. The maximum value of κ_{max} (the variable "sz" in the files "S_integral.f90", "Bremsstrahlung.f90" and "Read_S_integrals.f90") has been increased from 160 to 300. However, the recommended upper limit of κ_{max} for calculation of cross sections is approximately 160 when $k \neq 0$, and 220 when $k \to 0$ (at larger values of κ_{max}, the calculation time and the memory requirements would become prohibitive).
4. Added an option to skip the nonlinear fitting in Brems_fit.exe if the file with the fitted DCS already exists. This option is controlled by an additional command-line argument "iCalculate".
5. Changed the effect of setting the command-line argument "iCalculate" of Bremsstrahlung.exe to zero: if this command-line argument is 0 and if the cross section data files already exist, then Bremsstrahlung.exe quits without updating any files. In addition, this command-line argument is now allowed to be equal to –1. The meaning of this value is the same as the meaning of the value 0 in the previous version, i.e., if the cross section data files already exist, then only the file with the shape functions is re-created (the cross section data, which are needed for calculating the shape functions, are loaded from the existing files).
6. When Brems_fit.exe determines that the fitted DCS has to be extrapolated into the angular range $160° < \theta \leq 180°$ and that the quadratic extrapolation gives a better fit than the third-degree extrapolation, the original fitted DCS is no longer replaced in the angular range $150° \leq \theta \leq 160°$ by the extrapolated DCS. I.e., the mentioned replacement is done only in the range $160° < \theta \leq 180°$ (as in the case when the third-degree extrapolation gives a better fit than the quadratic extrapolation).
7. The values of the numerical integrals of the DCS and their deviations from the corresponding values of the CS are now written to the output file of Bremsstrahlung.exe along with the values of cross sections for each κ_{max}.

8. If the file with the 3j coefficients is too small, then Bremsstrahlung.exe no longer recreates it "from scratch". Instead, the missing data are appended to it. The 3j coefficients are now stored in multiple files with the maximum size equal to approximately 2 GB (rather than in a single file as in the previous version).
9. Updated the user manual.

2017-11-28**:**

10. Fixed a bug in Bremsstrahlung.exe that caused a memory allocation error when the total size of the files with the 3j coefficients was greater than 2 GB, i.e., when κ_{max} was greater than 198 (this change involved a reduction of the maximum size of the file "3j.dat" to approximately 1.977 GB).

2017-11-29**:**

11. Modified Bremsstrahlung.exe so as to prevent the program from updating the file with the 3j coefficients after another instance of Bremsstrahlung.exe opened the same file for update (this is achieved by creating a temporary "lock" file in the current folder).

2017-11-30**:**

12. Optimized the preliminary stage of the analytical integration from r_0 to ∞ (including the calculation of the coefficients of the explicit formulas for the spherical Bessel functions). As a result, the total time of the analytical integration has decreased. When $\kappa_{max} = 200$, the processing time has decreased by approximately 3 min on a computer with an Intel Core i7-4930K processor.
13. Modified the smoothing procedure in Brems_fit.f90. Now, the function that is being smoothed is the logarithm of the ratio of the fitted DCS and the original (unfitted) DCS (in the previous version, it was the logarithm of the fitted DCS). With the newer method of smoothing, a large relative difference between the fitted CS and the angular integral of the smoothed fitted DCS (in excess of 10 %) is much less likely when the incident electron energy is of the order of 1 MeV.

2017-12-01**:**

14. Changed the calculation of the variable "extrap" in Brems_fit.f90 (this variable indicates if the original fitted values of the DCS at values of $\theta > 160°$ should be replaced with the values obtained by extrapolation of the angular dependence of the fitted DCS from smaller angles). Now, its value is determined from the shape of the angular dependence of the fitted DCS before the smoothing (previously, its value was determined from the shape of the smoothed fitted DCS). This change has an effect only when smoothing of the fitted DCS is requested.
15. A more stringent requirement for the shape of the fitted function DCS(θ) at $\theta > 160°$ is now used when determining whether the angular extrapolation should be applied: in addition to the requirement that the function DCS(θ) must be monotonous, the absolute value of its first derivative is required to decrease monotonously in the mentioned angular range. If any of those requirements is not satisfied, the original fitted values of the DCS at $\theta > 160°$ will be replaced with the values obtained by extrapolation of the angular dependence of the fitted DCS from smaller angles.

2017-12-08**:**

16. Fixed an error in the subroutine "simplex" (incorrect array bounds in the declarations). This error could cause a crash of Brems_fit.exe or S_integral.exe, if those executables were created using a Fortran compiler other than the compiler used for compiling the executables included in the distribution package of BREMS.
17. Fixed an error in the subroutine "R" in file "Bremsstrahlung.f90" (in declaration of the length of the array FL). This error could cause a failure to compile Bremsstrahlung.exe using a Fortran compiler other than the compiler used for compiling the executables included in the distribution package of BREMS.
18. If the interaction potential is truncated (i.e., if the command-line argument "R_atom" of S_integral.exe is non-zero), then the ratio of the current value of the radial coordinate and the truncation radius is now displayed every 5 seconds during the numerical integration.

1.4.0 (2017-12-10):

1. The architecture of BREMS has been modified significantly. Instead of three separate executable files, now there is a single main program (file "Brems.f90"), which calls subroutines "S_integrals", "Bremsstrahlung" and "Brems_fit", which perform the three stages of the calculation.
2. The method of entering parameter values has been improved. Each parameter of the calculation process may be either specified as a command-line argument, or loaded from a user-specified file (the "parameter file"). The parameter values are specified using the format "<parameter_name>=<parameter_value>". If a parameter value is not specified on the command line or in the parameter file, then a default value will be used. There are 63 parameters in total, allowing great flexibility in the process of calculating the single- and double differential cross sections, in the amount of additional data (such as error estimates) calculated by the program, and in the number of files created (such as the files with intermediate data).
3. The Fortran-90 statements that previously relied on non-standard Fortran extensions have been modified in order to make them compatible with other Fortran compilers (such as GNU Fortran).
4. In addition to the Windows executables, the BREMS distribution package now includes the Linux executables (compiled using the GNU Fortran compiler on Debian GNU/Linux). They are in the subfolder "Linux_executables".
5. Updated the user manual.

2017-12-11**:**

6. Fixed a bug in Brems.f90 that caused incorrect value of the ratio of the photon and electron energies.
7. Fixed a bug in Brems.f90 that caused unnecessary modification of parameter k2_breakpoint1 if the value of parameter lmax_MP has been explicitly specified by the user.
8. Added the BREMS parameter file "Brems_defaults.inp" with the default values of all parameters for the case when 10 keV $\leq T_1 <$ 100 keV and $k \neq 0.1$.
9. Corrected the user manual.

2017-12-12**:**

10. Added one more column in the file "CS_fitted.txt". The last column contains the relative difference of the previous two numbers on the same line, i.e., the relative deviation of the numerical integral of the fitted DCS from the value of c_∞ returned by the fitting procedure.

2017-12-13**:**

11. Fixed a bug in Brems.f90, which caused incorrect interpretation of the names of the data files in stage 3 (i.e., in the subroutine Brems_fit), when those names were not formed in the default manner (i.e., when prefix='.').

2017-12-15**:**

12. During the calculation of the cross sections in stage 2 (in subroutine "Bremsstrahlung"), the intermediate values of the single- and double differential cross sections are written every 5 seconds to the temporary files (their names are formed by appending the suffix "_tmp" to the original filenames). If the calculation is interrupted, the temporary files may be used instead of the final files as the input files for stage 3.

1.4.1 (2017-12-27):

1. The precision level used for calculating the sine and cosine integrals si(x) and ci(x) in subroutine SICI_MP has been increased from 2000 to 4000 digits. The precision level used for calculating the higher-order trigonometric integrals (denoted I_1 and I_2 in Section 1.2 of the user manual) and the coefficients of the spherical Bessel functions has been increased from 1000 to 2000 digits.
2. The method of estimating the accumulated rounding error in subroutine SICI_MP has been improved.
3. The I_1 and I_2 trigonometric integrals (defined in Section 1.2 of the user manual) are now calculated using the explicit formulas instead of the recurrence relations. This allows decreasing the accumulated rounding error. The estimate of this error is used to determine if the precision level specified by the user can be achieved. If it is not so, the program quits with an error message.

4. The calculation of the default values of κ_{1max} and κ_{2max} (parameters Kmax1 and Kmax2, respectively) has been improved. Those default values are calculated by interpolation between 32 tabulated values corresponding to 8 values of T_1 (10 eV, 100 eV, 1 keV, 10 keV, 100 keV, 1 MeV, 3 MeV, 10 MeV) and 4 values of k / T_1 (0, 0.1, 0.4, 0.95). The interpolation with respect to T_1 is linear-log (logarithmic in T_1), and the interpolation with respect to k / T_1 is linear-linear. The mentioned tabulated values corresponding to $T_1 = 1$ MeV, 3 MeV and 10 MeV depend on the chosen accuracy level defined by parameter "accuracy_level_1MeV" of the main program.
5. One more file has been added to the set of output files of stage 3 (subroutine Brems_fit). It contains the data of the original DCS and the fitted DCS only (possibly after the polynomial extrapolation of the angular dependence of the DCS). Its name starts with "DCS_fitted_". The name of file that had the mentioned name in the previous version has been changed by replacing "fitted" with "alt" (meaning "alternatives"). In the header of column 3 of the latter file, "fitted" has been replaced with "fitted0".
6. Fixed a bug that prevented the breakpoints of κ_2 to be set automatically when the parameter "accuracy_level_1MeV" was non-zero.
7. The command line of Read_S_integrals.exe has been simplified and made more compatible with Brems.exe. The command-line arguments of Read_S_integrals.exe must be specified in the same way as for Brems.exe, i.e., using the format "<parameter_name>=<parameter_value>". Up to 21 command-line arguments may be specified. The names, meanings and default values of most of them are the same as of the corresponding parameters of Brems.exe.
8. Updated the user manual.

2017-12-28**:**

9. Fixed a bug that caused a crash of the Linux executable of BREMS with a message about a "segmentation fault" or a "syntax error in literal string" in the stage of calculating the trigonometric integrals. This bug has been fixed by decreasing the number of significant digits in the Euler's constant (returned by function "GammaConstant()") from 7721 to 4000.
10. Changed the name of parameter "accuracy_level_1MeV" to "accuracy_level", because it now affects the default values of parameters "tol_A", "tol_delta" and "Q_last" at all energies. In addition, "accuracy_level" may now be assigned negative values −1 and −2. If accuracy_level is positive, then only the parameters that have not been explicitly specified by the user will be assigned the values corresponding to the given accuracy level. If the accuracy level is specified with the minus sign, then the values of sixteen control parameters will be reset, even if those parameters have been explicitly specified by the user.

2017-12-29**:**

11. Added parameter "nErrMax" to the set of parameters used in stage 3 (in the subroutine Brems_fit). It is used to specify the maximum allowed number of consecutive irrecoverable error points in the angular dependence of the fitted DCS. The values of the fitted DCS corresponding to nErr ≤ nErrMax consecutive values of θ where the original fitting failed are calculated by log-linear interpolation between the two closest values of θ where the fitting was successful (this is done before the smoothing of the fitted DCS). If nErrMax = 0, then the fitting procedure will be terminated after the first irrecoverable error. The default value of this parameter is 1.
12. When polynomial extrapolation of the angular dependence of the fitted DCS is applied, the values of the fitted DCS are replaced by those obtained by calculating the polynomial not only in the range $\theta > 160°$, but also in the range used for optimizing the polynomial coefficients, i.e., $150° \le \theta \le 160°$.

2017-12-30**:**

13. Now, if an error occurs during fitting of the DCS (followed by an increase of the variable "tol_range" and a restart of the fitting process as explained in the description of parameter "tol_range_max" of the subroutine Brems_fit), then the CS is not fitted again (only the DCS is fitted repeatedly).

2018-01-04**:**

14. A zero value of "sign" of the dependence of the DCS on κ_{max} (as defined in the description of parameter "tol_range_max" of the subroutine Brems_fit) is no longer treated as an error when it occurs after a DCS with sign −1 or before a DCS with sign +1, because the resulting "dips" or peaks in the angular dependence of the fitted DCS are usually eliminated by smoothing (however, if a sequence of DCS with sign 0 is simultaneously after a DCS with sign −1 and before a DCS with sign +1, this is still treated as an error).
15. Breakpoints of κ_2 may now be defined independently of the definition of the limits of κ_1. This change affects only the behavior of subroutine S_integrals, but not subroutine Bremsstrahlung (the latter behaves as before, i.e., requires κ_1 to be defined in terms of $|\kappa_1|$, which must start from 1).
16. Updated the user manual.

2018-01-05**:**

17. Fixed a bug in Brems.f90 that caused a failure to read a user-specified value of parameter "prefix_fit" (used by subroutine Brems_fit in stage 3) when parameter "firstStage" was equal to 3.

2018-01-07**:**

18. The suitability of a dependence of CS or DCS on κ_{max} for fitting is now determined using more stringent criteria: not only is this dependence required to be monotonous, but its curvature is required to be consistent with a tendency to saturation, i.e., the change of the CS or DCS in the first half of the fitting interval must be greater than its change in the second half of the fitting interval.

1.4.2 (2018-01-16):

1. The errors of the cross sections due to uncertainties of the *S* integrals and the errors due to truncation of the sum with respect to *l* have been separated from each other in stage 2 (subroutine Bremsstrahlung). This is achieved by calculating two sets of test cross sections (instead of one set as in the previous version). Each one of those two sets reflects the influence of one of the mentioned two factors only (file name suffixes are "_test" and "_test2", respectively). Accordingly, two more columns have been added to the file "err_test.txt".
2. In accord with the change described above, subroutine Brems_fit (in stage 3) now allows two independent tolerances of the error of the cross sections: the one corresponding to the uncertainties of the *S* integrals (parameter "maxRelErr"), and the one corresponding to the truncation with respect to *l* (new parameter "maxRelErr2").
3. In the current version of BREMS, stage 2 is terminated if it is determined that the range of variation of the CS and the DCS for last 8 – 40 values of κ_{max} and for all values of the angle θ is less than 0.1% (the interval of κ_{max} used for this test depends on the current value of κ_{max} and is the same as the nonlinear fitting interval used in stage 3).
4. The parameter "fitMode" used by subroutine Brems_fit (in stage 3) can now be equal to −1 and 2 (in addition to 0 and 1, which were the only allowed values of this parameter in the previous version). If fitMode = –1, then the nonlinear fitting of the DCS as a function of κ_{max} will be skipped for all values of the angle θ and the fitted DCS will be replaced with the original DCS (this replacement may be followed by the polynomial extrapolation of the angular dependence at $\theta > 160°$). The difference between fitMode = 1 and fitMode = 2 is only in treatment of irrecoverable errors when nErrMax > 0. If fitMode = 1, then in the case of an irrecoverable error the fitted DCS will be replaced with the original DCS. If fitMode = 2, then in the case of an irrecoverable error the fitted DCS will be replaced with the log-linearly interpolated value (this corresponded to fitMode = 1 in the previous version of BREMS).
5. Now, the Wigner 3j coefficients are calculated (or loaded from files) in subroutine Bremsstrahlung only for the needed values of l_2 (previously, the entire set of 3j coefficients corresponding to a given value of $\max(|\kappa_1|_{max}, |\kappa_2|_{max})$ was calculated or loaded from files before calculating the *R* factors). This change has decreased the memory requirements approximately by half when $\max(|\kappa_1|_{max}, |\kappa_2|_{max}) > 160$) and Kmin1 = Kmin2 = 1 and isAbs_K1 = isAbs_K2 = 1. In addition, this change has decreased the memory

requirements when $\min(|\kappa_1|, |\kappa_2|) > 81$, because then the 3j coefficients corresponding to $l_2 < \min(|\kappa_1|, |\kappa_2|) - 1$ are not calculated or loaded from files.

6. Instead of a small number of large 3j files (as in the previous version of BREMS), a separate file is now used for each value of $l_2 > 80$. Those files are loaded (or created) during the calculation of the R factors when a given value of l_2 becomes needed for the first time. All 3j files are in a separate subfolder "3j"; file names have the format "3j_⟨l_2⟩.dat". The 3j coefficients are stored in a single one-dimensional array, which is re-allocated every time when a new value of l_2 becomes needed or when the previous value of l_2 becomes unnecessary. The starting position for each value of l_2 in this array is stored in a separate index array.
7. The file "CS.txt" (one of the output files of stage 2) is now updated after each calculation of the cross sections in stage 2 (previously, it was updated only when the condition Kmin1 = Kmin2 = 1 and isAbs_K1 = isAbs_K2 = 1 was not satisfied). The information in the file "CS.txt" is now more detailed: it includes all the columns from the file "system_parms.txt", plus "Kmin1", "Kmin2", "isAbs_K1", "isAbs_K2", "lmin", "CS", "DCS_integral", "rel_diff".
8. The file "system_parms.txt" (one of the output files of stage 2) is now updated only when Kmin1 = Kmin2 = 1 and isAbs_K1 = isAbs_K2 = 1 (previously, it was updated after each calculation of the cross sections in stage 2).
9. Several columns have been added to some of the output files in stages 2 and 3.
10. The additional file name suffix defined by the parameter "suffix2" is now appended to the names of the files "DCS1.txt" and "ShapeFn1.txt", which are created in stage 2.
11. The checking for a correct curvature of the dependence of the CS or DCS on κ_{max} has been made more precise (previously, an almost linear dependence was occasionally assigned incorrect curvature, resulting in an incorrect fitted value of the CS or DCS).
12. The user manual has been updated.

2018-01-17**:**

13. If the fitted value of the CS or DCS exceeds the original value by a factor greater than 20, or if the difference of the mentioned two values exceeds the range of variation of the CS or DCS in the fitting interval by a factor greater than 200, the program now treats it as an error. This change eliminates incorrect fitted values of the CS or DCS, which were occasionally obtained with the previous version of BREMS when the dependence of the CS or DCS on κ_{max} in the fitting interval was almost linear (in such a case, the fitting results are especially sensitive to errors of the unfitted CS or DCS).

2018-01-18**:**

14. The information in the files "DCS.txt" and "ShapeFn.txt", which are updated in stage 2 when the dependence of the CS and DCS on κ_{max} is not calculated (i.e., when the condition Kmin1 = Kmin2 = 1 and isAbs_K1 = isAbs_K2 = 1 is not satisfied), is now more detailed: the first 16 columns in those files contain the same data as the first 16 columns in the file "CS.txt".
15. The files that were updated in stage 2 by appending a single line (i.e., "CS.txt", "system_parms.txt" and "err_test.txt") are no longer deleted after a successul completion of stage 3 when the parameter "del_CS" is equal to 1.
16. The calculation of the default value of the parameter "lmax_MP" (the alternative value of l_{max} to be used with multiple precision) in the case $l_{min} > 0$ has been improved: now the default value of lmax_MP is calculated on the basis of the difference of parameters "lmax" and "lmin" (previously, only "lmax" was used for this calculation).
17. The default values of parameters "tol_A" and "tol_delta" corresponding to accuracy level 2 have been increased by a factor of 2: "tol_A" has been changed from 10^{-9} to $2 \cdot 10^{-9}$, and "tol_delta" has been changed from -10^{-9} to $-2 \cdot 10^{-9}$.
18. The user manual has been updated.

2018-01-19**:**

19. The number of breakpoints of κ_{max} for determining the interval of κ_{max} to be used for the nonlinear fitting of the CS or DCS as a function of κ_{max} has been increased from 6 to 7: the value of the breakpoint No. 4 has been decreased from 50 to 45, and a breakpoint with the value 60 has been inserted after it (the value of N_{fit} corresponding to the inserted breakpoint is 20).

2018-01-20**:**

20. The maximum allowed ratio of the change of the CS due to extrapolation and the range of variation of the CS in the fitting interval of κ_{max} has been decreased from 200 to 25 (the corresponding maximum allowed ratio for the DCS has not been changed and it is equal to 200).

2018-01-21**:**

21. Corrected the values of the two variables "theta_limit_1" and "theta_limit_2" that are displayed and written to the file "CS_parms.txt" in stage 3 (they are displayed as two numbers after "theta_limits =").
22. The BREMS distribution package now includes all ASCII files created by running the Windows batch file "Brems_79_100keV_KS.bat", as well as the file "Screen_output_Z=79_T1=0.1_Ep=0.01.txt" with the complete text that is displayed on the screen during the first call to Brems.exe in the mentioned batch file.
23. The user manual has been corrected.

2018-01-22**:**

24. Explanations of the various parts of the sample screen output contained in the file "Screen_output_Z=79_T1=0.1_Ep=0.01.txt" have been included into the user manual (file "Brems.pdf").

2018-01-26**:**

25. The name of the folder with the tabulated Kohn-Sham potential function data is now constructed by appending the name "V/Kohn-Sham/" to the name of the executable path specified on the command line. Consequently, the subfolder "V" is no longer required to be in the current folder when the Kohn-Sham potential is required (i.e., when IV = 3, which is the default option). If the subfolder "V" is not in the current folder, then it must be in the same folder where the executable file "Brems.exe" is located, and the name of that folder must be specified before the name of the executable file on the command line. For example, if the current folder is "C:\" and the BREMS installation folder is "C:\BREMS\", then the command line must start with "BREMS\Brems.exe" or "C:\BREMS\Brems.exe", even if the folder "C:\BREMS\" is in the system path (defined by the %PATH% environment variable on Windows, or by the $PATH variable on Linux).
26. The batch files and their output files have been moved to the subfolder "Test_runs".
27. The file "README.txt" has been added. This file gives the names and a brief description of the files that make up the distribution package of BREMS and instructions on the installation and execution of the program.

2018-01-29**:**

28. Fixed a bug that caused a reference to the variable p(2) (the momentum of the final electron) before it was initialized, when calculation of analytical integrals only (from r_0 to ∞) was requested ("iTestRun=-2") and the parameter "pr_transition2" was positive.
29. The final kinetic energy of the electron is no longer allowed to be less than 1 eV.

1.4.3 (2018-02-09):

1. The recurrence relations, which are used for calculating the coefficients of the power-series expansion of the radial wave function at small r, are now evaluated using multiple precision arithmetic. This modification has been done in order to eliminate the effects of the accumulation of rounding errors, especially in the case of the lowest electron energies (of the order of 100 eV or less). The maximum number of terms in the power series (variable "nterms_max" in "S_integrals.f90") has been increased

from 50 to 100, and the maximum relative change of the value of the radial wave function caused by adding the last retained term (variable "series_err") has been reduced from 10^{-10} to 10^{-18}.

2. Added the option of doubling the size of the integration step automatically if it is less than $0.05/p_1$ and also less than half of the distance corresponding to a predefined value of the relative decrease of the interaction potential $V(r)$. This change causes a reduction of the time of numerical integration at low energies (especially in the case of the point-Coulomb potential). The mentioned maximum relative decrease of $V(r)$ is specified using a new parameter "delta_V_max" (its default value is 0.01). This parameter is used only outside of the interval of the power-series solution, i.e., when the wave functions corresponding to all values of κ_1 and κ_2 are calculated either by iterative solution of the coupled radial Dirac equations (using the Hamming's modified predictor-corrector method) or by evaluating the asymptotic expressions (in terms of the spherical Bessel functions). If delta_V_max is zero, then the integration step will be fixed outside of the interval of power-series solution. Inside the interval of power-series solution, the size of the integration step is controlled using the parameter "r_incr_max" (see below).
3. A negative value of parameter "r_incr_max" is now interpreted as the opposite of the maximum allowed relative decrease of the screening function (delta_V_series_max) near $r = 0$, which should be used for calculating the initial value of the integration step size and also for its automatic adjustment inside the interval of power-series solution. In this case, the maximum allowed initial value of the integration step (r_incr_max) is initially set to pr_incr_init/p_1, where "pr_incr_init" is the initial value of parameter "pr_incr", and then r_incr_max is doubled or halved iteratively until the optimum value is found. This value of r_incr_max is subsequently used in the same way as in the previous versions of BREMS, i.e., it is used to set the initial value of the integration step size "r_incr": if r_incr (which is initially set to pr_incr_init/p_1) is greater than r_incr_max, then the initial value of r_incr will be set equal to r_incr_max. Afterwards, the value of r_incr may be increased automatically, because this increase is capped only by the value of pr_incr_init/p_1 and (inside the interval of power-series solution) by the value of 0.05*r_transition*iRun, where "r_transition" is the value of the radial coordinate corresponding to the transition from the power-series solution to the Hamming's algorithm, and "iRun" is equal 1 or 2 for the initial or "test" numerical integration, respectively. The mentioned automatic increase of r_incr is controlled by the parameter delta_V_max outside of the interval of power-series solution (see above), or by the value of delta_V_series_max inside the interval of power-series solution (in the latter case, the function whose decrease is being checked is the screening function rather than the interaction potential). If parameter "r_incr_max" is positive, then the integration step will be fixed inside the interval of power-series solution (as in the previous versions of BREMS). The default value of parameter "r_incr_max" is –0.01.
4. The "test integration" is now possible when $k = 0$ (in the previous versions of BREMS, it was possible only when $k \neq 0$). Since the S integrals are not calculated numerically in the case $k = 0$, the option "iTestRun=1" is applied in this case only to the process of solving the coupled radial Dirac equations. I.e., when iTestRun=1, the system of ODEs is solved using two sets of computational tolerances and step sizes. Thus, two sets of phase shifts and normalization factors are obtained. The differences of the corresponding phase shifts and normalization factors in the mentioned two sets are used for estimating their uncertainties.
5. The updates of the average values of the normalization factors A_κ and the phase shifts $\tilde{\delta}_\kappa$ and the calculation of their ranges of variation are now done at two alternating intervals of the radial coordinate r: each odd-numbered update is done after an interval of $(n_1 + 0.5)\pi/p_1$, and each even-numbered update is done after an interval of $(n_2 + 0.5)\pi/p_2$, where n_1 and n_2 are integers, which are chosen so that both those intervals are approximately equal to $50/p_1$. This modification has been done in order to maximize the cancellation of the oscillating term in the normalization factors and the phase shifts, and thus to improve the accuracy of the mentioned average values (the radial period of the mentioned oscillations is equal to π / p).
6. The default value of l_{max} corresponding to accuracy level 2 has been increased from $\max(|\kappa_1|_{max},|\kappa_2|_{max})$ to $\max(|\kappa_1|_{max},|\kappa_2|_{max}) + ¼ \min(|\kappa_1|_{max},|\kappa_2|_{max})$.
7. Added a new parameter "lmax_MP_ratio", which is equal to (lmax_MP – lmin) / (lmax – lmin). If lmax_MP is not specified by the user or if lmax_MP_ratio is non-zero, then the value of lmax_MP will be calculated using the values of lmax and lmax_MP_ratio (if lmax_MP is not specified by the user and

lmax_MP_ratio is zero, then lmax_MP_ratio will be reset to the default value). By default, the value of lmax_MP_ratio is linearly interpolated with respect to k / T_1 from a predefined value at $k / T_1 = 0$ to 1 at $k / T_1 \geq 0.95$. This interpolation has been implemented because it was noticed that in the case of a strongly peaked angular distribution of bremsstrahlung photons the values of the DCS corresponding to large angles ($\theta > 150°$) are especially sensitive to the truncation of the series with respect to l, and this effect becomes more pronounced with increasing k / T_1. If lmax_MP is specified by the user and lmax_MP_ratio is zero, then the user-specified value of lmax_MP will be used. The mentioned predefined value of lmax_MP_ratio at $k / T_1 = 0$ depends on lmax − lmin: (a) when lmax − lmin ≥ 80, it is 1/3; (b) when 40 ≤ lmax − lmin < 80, it is 1/2; (c) when lmax − lmin < 40, it is 1.

8. The tabulated default values of Kmax1 and Kmax2 corresponding to $T_1 = 1$ MeV, 3 MeV and 10 MeV are now dependent on Z when $Z \leq 7$. For $Z = 1$, the mentioned values are automatically increased by 20 (variable "kmax_default_1MeV_plus" in "Brems.f90") in comparison with the original values (array "kmax_default_1MeV") and capped at 220 (variable "kmax_default_1MeV_max"). For $1 < Z < 7$, the mentioned tabulated values are automatically increased by a value obtained by linear interpolation with respect to Z. This modification has been done because it was noticed that the number of partial waves needed to obtain an acceptable accuracy of the final cross sections increases with decreasing Z, and an especially pronounced increase is observed at $Z = 1$ and $Z = 2$.
9. The tabulated default values of Kmax1 and Kmax2 corresponding to $T_1 = 1$ MeV, 3 MeV and 10 MeV (either the original ones or the ones obtained after an additional increase as described above) are automatically rounded to the nearest multiple of 5. If $T_1 > 0.1$ MeV (i.e., in the energy range where the default values of Kmax1 and Kmax2 depend not only on T_1 and k / T_1, but also on Z) and if the value of Kmax1 or Kmax2 has not been specified by the user, then its final (interpolated) value is also rounded to the nearest multiple of 5. This rounding is needed to facilitate reusing the values of the S_{ij} integrals ($i, j = 1, 2$) at default values of parameters, when the method of partial-wave interpolation is applied. In this case, the difference of adjacent retained values of κ_2 is equal to 5, possibly excluding the last two values, whose difference may be less than 5. In order to make the difference of the last two values equal to 5 as well, Kmax2 must be a multiple of 5 (that is why Kmax2 is rounded).
10. The interval of the argument values of spherical Bessel functions where the subroutines SPHJ and SPHY are used has been narrowed to [0, 100] (in the previous versions of BREMS, it was [0, 1000]). In the case of the previous value of the endpoint of this interval, large errors could occur when the value of the increment of $p_1 r$ or $p_2 r$ was equal to $\pi / 2^n$, where n is a positive integer.
11. If the S integrals are calculated using multiple precision (i.e., more than 38 significant digits) and some of the values of κ_2 are "skipped" (for the purpose of the subsequent partial-wave interpolation in stage 2), then the program no longer allocates the memory for storing the unused S_{ij} integrals ($i, j = 1, 2$), which would be needed for calculating only the S integrals corresponding to the skipped values of κ_2.
12. During the process of optimizing the precision level, the comparison of the two values of an S_{ij} integral ($i, j = 1, 2$) calculated at two precision levels is done by calculating their relative difference and checking if its absolute value is less than 10^{-13} (in the previous versions of BREMS, the comparison was done by setting the precision level to 3 machine words and then checking if the compared values are exactly equal to each other). This change sometimes causes a reduction of the optimal precision level (and thus a decrease of the processing time).
13. The time of the numerical integration (from 0 to r_0), the time of the analytical integration (from r_0 to ∞), and the total duration of stage 1 are now written to the binary files with S integral data. If the numerical or analytical integrals were loaded from files, then the corresponding time is copied from the last loaded file with the corresponding data.
14. Four columns with the values of the processing time (in seconds) have been added to the file "CS.txt", which is updated in stage 2. Those are the times of the numerical and analytical integration, duration of stage 2, and the total elapsed time at the end of stage 2. If firstStage = 2 or if stage 1 is skipped due to presence of the files with the S integral data, then the times of the numerical and analytical integration are copied from the last loaded file with the S integral data.
15. The accuracy of the trigonometric integrals (denoted I_1 and I_2 in the user manual) is tested by calculating them at two precision levels and then calculating their relative difference. In addition, the accumulated rounding error is calculated explicitly (as in the previous version of BREMS). The final estimate of the relative uncertainty of the I_1 or I_2 integral is the larger of the two mentioned values.

16. A more accurate estimation of the range of the phase shifts $\tilde{\delta}_\kappa$ has been implemented. Before adding a new value of $\tilde{\delta}_\kappa$ to the set of compared values, the new value is compared with the average value of all "old" phase shifts in the set. In order to minimize the deviation of the new phase shift from the average phase shift, the new phase shift is modifed by adding $2\pi n$, where n is an integer number, which is chosen so as to make the final deviation less than π and greater than $-\pi$.
17. If the testing for errors due to the truncation with respect to l is requested in stage 3 (i.e., if the parameter "maxRelErr2" is positive) and if the decrease of $\kappa_{\max}$ in Brems_fit is such that the reduced value of $\kappa_{\max}$ is less than the value of a new parameter "kmin_fit", this is treated as a terminal error. If there is no additional reduction of $\kappa_{\max}$ in Brems_fit, or if the testing for errors due to the truncation with respect to l is not requested, then this test is not performed. The aim of this test is to reduce the possibility that the testing for errors due to the truncation with respect to l becomes impossible due to an excessive additional reduction of $\kappa_{\max}$ in stage 3. This would happen if $\kappa_{\max}$ becomes less than $l_{\max} / 2$. Since the default initial value of $l_{\max}$ is typically close to the initial value of $\kappa_{\max}$, the default value of parameter "kmin_fit" is defined as ncycles0 / 2, where "ncycles0" is the initial number of cycles in stage 2, i.e., the initial value of max(Kmax1,Kmax2). If the user-specified value of kmin_fit is non-positive, then kmin_fit is reset in the program to ncycles0 / 2 before starting stage 3 (if firstStage = 3, then the value of ncycles0 is read from the first line of the "_CS_…_test2.txt" file, which is created in stage 2 when the parameter "lmax_decr" is negative). If firstStage = 3 and the line with the value of ncycles0 is absent (old format of the "_CS_..._test2.txt" file), then the mentioned test will not be performed (i.e., any reduction of $\kappa_{\max}$ will be allowed in stage 3), unless the user specifies the value of kmin_fit explicitly.
18. One more breakpoint of $K \equiv \max(\max|\kappa_1|, \max|\kappa_2|)$ for defining the range of $\kappa_{\max}$ to be used for fitting in stage 3 has been inserted: this breakpoint is $K = 7$ (the next breakpoint is 13, which was the smallest value of K that was allowed for fitting in the previous versions of BREMS). The corresponding number of points to be used for fitting is $N_{\text{fit}} = 5$.
19. The full path to the 3j data files (i.e., the binary files where the values of the Wigner 3j coefficients are stored) is now constructed by appending the subfolder name "3j/" to the folder name specified on the command line before the name of the executable file "Brems.exe". I.e., if the full name of the executable specified on the command line contains the slash '/' or the backslash '\', then the program will search for the "3j" subfolder in the same folder where the file "Brems.exe" is located. Otherwise, the "3j" subfolder should be in the current folder.
20. If the name of a parameter file is specified on the command line and if the attempt to open this file is not successful, the program now quits with an error message (the previous version of BREMS continued in such a case using the default values of all parameters that were not specified on the command line).
21. Several minor bugs have been fixed.
22. The user manual has been updated.

2018-02-10**:**

23. Parameter "theta_max" has been renamed to "theta_max1" in order to be consistent with the names of the related parameters "theta_max2", "np1" and "np2".

2018-02-22**:**

24. The calculation of the default value of the parameter "lmax_MP_ratio" when lmax – lmin < 80 has been modified in order to prevent the default value of lmax_MP from increasing after lmax is reduced. Now, the value of lmax_MP_ratio is linearly interpolated with respect to lmax – lmin when lmax – lmin < 80. The maximum value of lmax_MP_ratio corresponds to lmax = lmin and is equal to 1. The minimum value of lmax_MP_ratio corresponds to lmax – lmin = 80 and is obtained by linear interpolation with respect to k / T_1, with the maximum value equal to 1 (it corresponds to $k / T_1 \geq 0.95$) and the minimum value equal to 1 / 3 (it corresponds to $k = 0$). Since the default value of lmax_MP is equal to lmin + (lmax – lmin) * lmax_MP_ratio, the mentioned linear interpolation of lmax_MP_ratio with respect to lmax – lmin causes a quadratic dependence of the default value of lmax_MP on lmax – lmin. If this dependence has a maximum at lmax – lmin < 80, then it is additionally "capped" by reducing it to the value corresponding to lmax – lmin = 80.

1.4.4 (2018-03-02):

1. In the case of the Kohn-Sham potential (option "IV=3", which is the default), the cubic spline interpolation of the screening function has been implemented instead of the piecewise-exponential interpolation, excluding the initial interval of the $V(r)$ data table, where the interpolation by a single exponential function is applied. The extrapolation at large r is exponential (as in the previous versions of BREMS). The boundary conditions for the first derivative are obtained from the expressions of the two mentioned exponential functions.
2. When testing the convergence of the Taylor series expansion of the wave function at small r, the values of its first derivative are now taken into account, too.
3. Fixed a minor bug in the subroutine S_integrals, which could cause a relative change of the differential cross sections up to 0.5 % in the case of the Kohn-Sham potential (option "IV=3", which is the default). This bug was caused by usage of a single set of the coefficients of the interpolating function for the screening function during the numerical solution of the coupled radial Dirac equations, even when the starting and ending points of the current cycle of the solution (i.e., the lower and upper bounds of the current step of the Newton-Cotes quadrature) belonged to different intervals of the tabular $V(r)$ data (in such a case, only the coefficients corresponding to the last interval were used, whereas the correct approach requires using the coefficients corresponding to the interval containing the current value of r).
4. Fixed a bug in Read_S_integrals, which sometimed caused incorrect default values of Kmax1, Kmax2, and lmax (i.e., the values used when those parameters were not specified by the user).

2018-03-03**:**

5. The default value of parameter "maxRelErr", which is used by the subroutine "Brems_fit" (in stage 3), has been increased from 0.005 to 0.01.
6. The algorithm of automatic adjustment of the integration step has been improved. Since the criteria of this adjustment inside the interval of power-series solution and outside of that interval are different, the integration step at the point of transition from the power-series solution to the Hamming's modified predictor-corrector algorithm may become larger than the value defined by the parameter "delta_V_max". Since in the previous version of BREMS the integration step was never reduced (it could only be increased), integration errors could occur in such a situation, resulting in an excessive reduction of Kmax1 or Kmax2 (especially at electron energies less than 10 keV). In the current version of BREMS, if the integration step becomes too large, the mentioned criterion corresponding to the interval of the power-series solution is modified so as to prevent the integration step from growing to such a large value, and the process of numerical integration is restarted. ***Note***: The maximum integration step is not set to the optimal value before starting the numerical integration, because the optimal value of the maximum integration step depends on the radial coordinate corresponding to the mentioned transition, which may not be known beforehand.

2018-03-05**:**

7. The default value of parameter "step1", which is used by the subroutine "S_integrals" (in stage 1), has been reduced from 0.002 to 0.001.
8. Fixed a bug that caused a failure to create the subfolder "3j", where the binary files with the Wigner 3j coefficients are placed, when the command line used to start BREMS included the name of the folder where the executable file Brems.exe is located (i.e., when the subfolder "3j" had to be created in the BREMS installation folder rather than in the current folder).

2018-03-07**:**

9. The calculation of the exact phase shift corresponding to the point-Coulomb potential (which is used in the subroutine S_integrals for calculating the asymptotic form of the wave functions in the case "IV=1 iExact=2" and displayed by Read_S_integrals.exe if the file with the S integral data has been created using the option "IV=1") has been simplified and made more accurate. This modification eliminated the possibility of a floating-point overflow, which was previously possible when calculating the mentioned phase shift in the case of large values of κ (if such an overflow occurred, an incorrect value of the phase shift would be obtained).

2018-03-21**:**

10. The automatic reduction of Kmax1 in the subroutine S_integrals in the case of an error during the solution of the coupled radial Dirac equations is now applied when Kmin1=1 and isAbs_K1=1, without any constraints on Kmin2 and isAbs_K2, and the automatic of reduction of Kmax2 requires only that Kmin2=1 and isAbs_K2=2 (previously, all four mentioned conditions had to be satisfied in order to enable the automatic reduction of Kmax1 or Kmax2).
11. The option "iSkip=-3" has been added. It differs from "iSkip=-2" in that an existing complete file with *S* integral data is not overwritten. Instead, a new file with an additional suffix "_1", "_2", etc is created (as in the case "iSkip=0"). If there is no complete file, then the option "iSkip=-3" is equivalent to "iSkip=-2" or "iSkip=2".
12. When $\min(T_1 - k, k) > 100$ keV, the default value of parameter "ndp" is −100. Otherwise, it is −300 (in the previous version of BREMS, the latter value was the only default value of ndp).
13. Parameters "first" and "last" have been added to the set of parameters of Read_S_integrals.exe. They specify the first and last additional suffix in the names of the *S* integral data files to be loaded. The allowed values of those parameters are integer numbers from 0 to 9. "0" means no additional suffix, and a positive value means that the additional suffix is formed by concatenating the underscore and the specified number. The default value of parameter "first" is 0. The default value of "last" is 9.

2018-03-24**:**

14. Fixed a bug in the file "S_integrals.f90" (incorrect array dimensions in the subroutine SBESJ2), which could cause a crash of the program due to an out-of-bounds array index.

2018-03-25**:**

15. Fixed a bug in the file "S_integrals.f90" (usage of an uninitialized variable "fcos" when calculating the uncertainty of the sine and cosine integrals at argument values greater than 4600 in the subroutine SICI_MP). In the Linux version of BREMS, this bug sometimes caused an abnormally long computation of the trigonometric integrals or a termination of the program with the error message "Exponent overflow".
16. In the previous version of BREMS, the sine and cosine integrals (si(x) and ci(x)) were calculated twice for each value of their argument. The redundant second call to the subroutine SICI_MP has been removed. As a result, the time of the analytical integration has decreased.
17. Fixed a bug (a value of an array index exceeding the dimension of that array) in the subroutine SPLINE. This error caused a crash of the Linux version of BREMS when the Kohn-Sham potential was used (i.e., in the case of the option "IV=3", which is the default).

2018-03-27**:**

18. Expanded the user manual with additional information regarding the numerical methods (Section 1.2) and the theory behind the interaction potentials implemented in BREMS (Section 7). Added a description of the test run and the excerpts from the corresponding output files in Section 8.

2018-03-28**:**

19. Inserted the column "max_abs_dev_140-150deg" into the file "CS_parms.txt", which is optionally updated by the subroutine Brems_fit (in stage 3). This column contains the maximum absolute difference between the original fitted DCS and the one obtained from the polynomial equation in the angular range $140° \le \theta < 150°$. This value may be used as an estimate of the absolute error introduced by the angular extrapolation of the fitted scaled DCS in the angular range $160° < \theta \le 180°$.

2018-03-31**:**

20. Recompiled the Linux versions of the executable files "Brems.exe" and "Read_S_integrals.exe" (in the subfolder "Linux_executables") using the optimization option "-O3" of the GNU Fortran compiler. The set of the compiler commands in the file "Linux_executables/Compile.sh" has been updated.

21. Fixed a bug that caused an abnormal termination of the Linux version of BREMS after an automatic reduction of Kmax1 or Kmax2 (this reduction occurs in the case of a certain type of error during the numerical solution of the coupled radial Dirac equations). The program was terminated because of an attempt to allocate an array that was already allocated (such a situation did not cause a fatal error in the Windows version of BREMS, compiled using the PGI Visual Fortran compiler).
22. Fixed a bug that sometimes caused an excessive difference of the original and "test" numerical integrals (due to a small difference of their upper bounds), and hence an overestimation of the uncertainties of the total S integrals (from 0 to ∞).

2018-04-05**:**

23. Fixed an error in the calculation of the phase correction integrals in the case "IV=2" (i.e., when the Thomas-Fermi-Csavinszky potential is used).

1.4.4.1 (2018-04-06):

1. Added the fourth sequence to the version number of BREMS. This sequence is incremented after each minor change of the code, and set to zero after each major modification (when any of the previous three sequences is changed).
2. The complete version number of BREMS is displayed immediately after starting the executable file.
3. Added two parameters "dir_V" and "dir_3j", which are used to specify the names of the folders with the tabular potential function data and the binary 3j coefficient data, respectively. Their default values are "V" and "3j", respectively. If the specified folder name is incomplete, i.e., if it does not start with the forward slash '/' or the backslash '\' and does not contain the colon ':', then it is assumed to be a subfolder either of the BREMS installation folder or of the current folder, depending on whether the path to the BREMS executable file has been specified before its name on the command line or not.
4. Removed the folder "Brems/Linux_executables/V", because the sample Linux bash scripts have been rewritten so as to read the tabular potential data from the files located in the folder "Brems/V" (i.e., from the same files that are used by the Windows sample batch files).

1.4.4.2 (2018-04-08):

1. In order to facilitate inclusion of additional potential functions (corresponding to IV=4, IV=5, etc.), which are defined in tabular format, the statement (condition) "IV.eq.3" in the headers of all existing conditional operators has been replaced with "IV.ge.3", and the assignment of the name of the file with the tabular $V(r)$ data to the variable "fileName" in the subroutine INITIALIZE (in the file "S_integrals.f90") has been placed into the body of the conditional operator with the header "if (IV.eq.3)".
2. Minor changes in the source code: removed the unused variables and most of the obsolescent or non-standard features of Fortran-90 in the declarations of variables.

1.4.4.3 (2018-04-26):

1. Increased the error tolerance for calculating the confluent hypergeometric function (it is used at small values of the radial coordinate when the options "IV=1" and "iExact=1" or "iExact=2" are specified). Previously, the program sometimes quit with an error message because the mentioned error tolerance was too low.
2. The accuracy of the quadruple-precision (QP) and multiple-precision (MP) calculations at the stage of the power-series solution of the coupled radial Dirac equations has been improved by using the QP or MP value of the parameter $\gamma = (\kappa^2 - Z^2\alpha^2)^{1/2}$ in the subroutines "power_solution_QP" and "power_solution_MP" (the name of the corresponding variable in the source code is "gam_QP" or "gam", respectively). Previously, the double-precision value of this parameter was used in the mentioned subroutines, which could cause accumulation of errors and instability at extremely low electron energies (of the order of 100 eV or lower).

1.4.4.4 (2018-04-29):

Fixed a bug that could cause large errors in the values of cross sections calculated at electron energies of the order of 1 keV or lower in the case of the point-Coulomb potential (option "IV=1").

1.4.4.5 (2018-04-30):

1. The accuracy of the quadruple-precision (QP) and multiple-precision (MP) calculations at the stage of the power-series solution of the coupled radial Dirac equations has been further improved (in comparison with the update from v1.4.4.2 to v1.4.4.3) by using the QP or MP value of the ratio of the initial values of the major and minor components of the wave function in the subroutines "power_solution_QP" and "power_solution_MP". Previously, the double-precision value of the mentioned ratio was used in the mentioned subroutines, which could cause accumulation of errors and instability at extremely low electron energies (of the order of 100 eV or lower).
2. The occasional floating-point overflows or underflows during the process of solving the coupled radial Dirac equations at extremely low electron energies (of the order of 100 eV or lower) have been eliminated by using different decimal exponents for the initial value of the function $r^{-\gamma}g$ (needed at the stage of the power-series solution) and for the value of the function g (needed at the stage of the predictor-corrector solution of the coupled radial Dirac equations). ***Note***: The same decimal exponent is used for the minor component of the wave function ($r^{-\gamma}f$ and f, respectively).

1.4.4.6 (2018-05-02):

1. Added the parameter "k2_excl_last", which acts as a "switch" (0 or 1) indicating whether the last value of $|\kappa_2|$ should be excluded from the set of the breakpoints used to calculate the cubic spline coefficients for the partial-wave interpolation. In the case "k2_excl_last=1", the interpolated values between the last two breakpoints of $|\kappa_2|$ are calculated using the same spline coefficients as between the previous two breakpoints. This parameter has been added because it has been noticed that in the case "IV=1" and at low electron energies (of the order of 10 eV or lower) there is a discontinuity at the last value of $|\kappa_2|$ in the dependences of the terms of the CS and DCS on $|\kappa_2|$ (the last term is much less than the smoothly extrapolated value). Consequently, if the last value of $|\kappa_2|$ is not exluded from the calculation of the spline coefficients, the interpolating curve has an oscillatory character between the last several pairs of breakpoints of $|\kappa_2|$, causing large errors in the cross sections. The default value of this parameter is 1 in the case "IV=1", and 0 otherwise.
2. Added the column "k2excl" with the values of the parameter "k2_excl_last" (described above) in the files "CS.txt", "DCS.txt", "ShapeFn.txt", "err_test.txt", and "system_parms.txt", which are updated at stage 2 (by the subroutine "Bremsstrahlung").
3. Three variables in the file "AuxiliaryPrograms\CubicSplineInterpolation\splint.f90", which were previously of the type "REAL", have been declared as "double precision" (the names of those variables are the following: a, b, h). Because of this change, the values of the cross sections calculated using the partial wave interpolation method have changed in the ninth or eighth significant digit.
4. Updated the user manual.

1.4.4.7 (2018-05-03):

1. Fixed a bug that sometimes caused a floating-point overflow in the maximum values of the two components of the wave function (variables "u1_max" and "u2_max" in the file "S_integrals.f90") at the point of the transition from the power-series solution to the Hamming's modified predictor-corrector algorithm.
2. Added the two columns "CS[kmax]" and "CS[k->Inf]" in the file "Errors.txt", which is optionally updated at stage 3 (by the subroutine "Brems_fit"). Those two columns contain the original (unfitted) and the extrapolated (fitted) values of the CS, respectively.
3. Updated the user manual.

1.4.4.8 (2018-05-06):

When the partial-wave interpolation method is applied and the parameter "k2_excl_last" (introduced in v1.4.4.6) is equal to 1, the accuracy of the cross sections has been improved by calculating the values of the last term in the sum by a separate cubic spline interpolation, with the spline coefficients calculated using the exact values of the mentioned term corresponding to the user-specified breakpoints of $|\kappa_2|_{\max}$ (in the previous version, the values of the mentioned term at all values of $|\kappa_2|_{\max}$ excluding the breakpoints were calculated by the same method as the values of all other terms, i.e., by a cubic spline extrapolation from the previous interval of $|\kappa_2|$, with the spline coefficients calculated using the set of terms corresponding to the current value of $|\kappa_2|_{\max}$).

1.4.4.9 (2018-05-19):

Fixed a bug that could in rare cases cause an indeterminate (infinite) value of an S integral after an automatic reduction of $|\kappa_{1,2}|_{\max}$ in the subroutine S_integrals (this error could happen when the value of the radial coordinate corresponding to the mentioned reduction was very close to the truncation radius R_a).

1.4.5.0 (2018-05-27):

1. The default value of parameter "R_atom" (specifying the atomic radius) cannot be less than max(800, 126 / p_2), i.e., either approximately six Bohr radii or twenty periods of the final electron wave function, whichever is greater (in the previous versions, the default minimum value of R_atom was 800). This change improves the accuracy at the low energies and at the default values of the control parameters, especially when $T_2 < 100$ eV.
2. In the current version, the S integrals are normalized and the number of wave functions that have not attained the asymptotic form is decremented at the end of the current integration step (and not at the start of the next step as in the previous versions). This ensures that the value of the radial coordinate corresponding to the transition from the Hamming's modified predictor-corrector algorithm to the analytical calculation of the wave functions (using their asymptotic expressions in terms of the spherical Bessel functions) is exactly equal to the predefined limit R_a, defined by the value of parameter "R_atom" (either the default one or specified by the user). In the previous versions, the mentioned transition point was usually greater than R_a by the magnitude of the last integration step.
3. The values of parameters "R_atom" (specifying the atomic radius) and "pr_transition2" (specifying the lower bound r_0 of the radial integrals to infinity) in the case "iTestRun=-2" (calculation of the integrals from r_0 to ∞ only) are now treated in the same way as in the case when iTestRun > –2 (for example, r_0 is set to max(800, 126 / p_2) when neither of the two mentioned parameters is specified by the user). This facilitates using the options "iTestRun=-2" and "iTestRun=2", because the value of parameter "pr_transition2" is now not required to be explicitly specified by the user when the option "iTestRun=-2" is used.
4. Updated the user manual.

1.4.5.1 (2018-05-28):

1. The final value of the truncation radius of the potential function is now written to the binary file with the S integral data along with the initial value (which is passed as an argument to the subroutine "S_integrals" in stage 1). If the initial value is negative, then the final value (the true truncation radius) is calculated by the subroutine S_integrals (in stage 1), and it is different from the initial value.
2. The program "Read_S_integrals.exe" now displays both the initial value and the final value of the truncation radius of the potential function ("R_atom_init" and "R_atom", respectively). In addition, the table with the phase shift data contains an additional column "difference2", if the last loaded data file corresponds to IV = 1 (unscreened point-Coulomb potential), iExact < 2 (numerical estimation of phase shifts), and R_atom > 0. The values in the column "difference2" are obtained by subtracting the term $\nu \ln(2pR_a)$ from the values of the previous column ("difference").
3. Updated the user manual.

1.4.5.2 (2018-05-29):

1. The value of "difference2" defined in the description of the previous update is now also displayed in the screen output of the subroutine S_integrals when appropriate.
2. The subroutine Read_S_int (file "S_integrals.f90") now checks if the *S* integral data file version number specified in the file does not exceed the maximum supported version number. If this requirement is not satisfied, then the program quits with an error message.

1.4.5.3 (2018-05-30):

The parameter "pr_transition2" is no longer required to be non-zero when only the calculation of the integrals from r_0 to ∞ (the "analytical" integrals) is requested (option "iTestRun=-2"). Instead, either "R_atom" or "pr_transition2" must be non-zero.

1.4.5.4 (2018-06-29):

Several variables in the file "AuxiliaryPrograms\CubicSplineInterpolation\spline.f90", which were previously of the type "REAL", have been declared as "double precision".

1.4.6.0 (2018-07-18):

1. Added the parameter "method", which allows using the Runge-Kutta method for solution of the coupled radial Dirac equations in stage 1 (subroutine "S_integrals"), instead of the Hamming's modified predictor-corrector method (which is used by default).
2. The smoothing of the CS and DCS with respect to κ_{max} has been added to the beginning of stage 3 (subroutine "Brems_fit"). In the case of a nonlinear fitting error, the program will replace the actual values of the CS or DCS with their moving averages over several consecutive values of κ_{max} and then retry the fitting. If the error occurs again, the averaging period will be increased by 1 until the error does not occur or the maximum averaging period is reached. The maximum averaging period is controlled by the new parameter "avg_period_max_ratio", which is equal to the ratio of the maximum averaging period and the width of the fitting interval (N_{fit}). In the case "avg_period_max_ratio=0", no averaging will be applied. The default value of this parameter is 0.5.
3. A column with the final value of the averaging period ("nAvg") has been inserted in the files "CS_parms.txt" and "DCS_..._parms.txt".
4. The default value of the maximum allowed number of consecutive points where an irrecoverable fitting error occurred in the angular dependence of the DCS (parameter "nErrMax") has been increased from 1 to 6.
5. Two columns with the total number of the values of θ where an irrecoverable error occurred when fitting the dependence of the DCS on κ_{max} ("nErrTot") and the maximum number of consecutive values of θ where an irrecoverable error occurred ("nErr") have been inserted in the files "CS_fitted.txt" and "CS_parms.txt". If the angular extrapolation is necessary, then the irrecoverable fitting errors that occur in the extrapolation range ($\theta > 160°$) are not included in "nErrTot" and "nErr".
6. The interpretation of parameter "kmin_fit" (used in stage 3 by subroutine "Brems_fit") is no longer linked to the parameters "maxRelErr2" and "lmax_decr". Parameter "kmin_fit" is now equal to 1 by default (i.e., any reduction of κ_{max} is allowed in stage 3).
7. The hypergeometric series, which is needed in stage 1 for calculating the limits $\lim_{k\to 0}(kS_1)$ and $\lim_{k\to 0}(kS_2)$, is now calculated using the multiple-precision arithmetic with adaptive precision level (subroutine "Hypergeom" in file "S_integrals.f90") instead of the third-party subroutine "PFQ".
8. The final kinetic energy of the electron T_2 (parameter "T2") may now be specified instead of the photon energy k (parameter "Ep").
9. The minimum allowed value of T_2 has been decreased from 1 eV to 0.1 eV.
10. Updated the user manual.

1.4.6.1 (2018-07-28):

For consistency with the numbering convention used in BREMS, the allowed values of the parameter "method" have been increased by 1, i.e., they are now equal to 1 and 2 (the option "method=1" corresponds to the Hamming's modified predictor-corrector method, and the option "method=2" corresponds to the Runge-Kutta method).

1.4.6.2 (2018-07-30):

Fixed a bug in the subroutine S_integrals, which caused an excessively long "test" numerical integration. This bug was caused by an uninitialized variable, which was referenced periodically during the test integration in order to determine if the estimates of the normalization factors and phase shifts should be updated at the current integration step. As a result, those estimates were updated too frequently (at each step, instead of the predefined intervals). The final results of the calculation were not affected by this bug.

1.4.7.0 (2018-08-05):

1. Added an option of using the power-series solution method for solving the coupled radial Dirac equations ("method=3"). This method is now the default one.
2. A new parameter "nterms_max", which indicates the maximum order in the mentioned power-series expansion of the wave functions, has been added. Its default value is 100.
3. The option "Q_last=0" now indicates that the value of the phase-correction integral Q should be ignored when determining the point of transition to analytical integration (as before, it is always ignored for IV=1 with R_atom=0). "Q_last=0" is the default when the photon energy is zero.
4. The user manual has been updated.

1.4.8.0 (2018-08-12):

1. In the case of zero photon energy (option "Ep=0"), the values of $\lim_{k\to 0}(kS_1)$ and $\lim_{k\to 0}(kS_2)$ are no longer written to the S integral data files in stage 1. Instead, they are calculated "on the fly" when needed (by the subroutine "Bremsstrahlung" in stage 2 or by the program Read_S_integrals.exe) if the option "Ep=0" has been specified by the user. Now, only the values of the phase shifts, normalization factors and the calculation parameters are written to the ".dat" file created in stage 1 when Ep=0.
2. The partial-wave interpolation method is now applied in the case of zero photon energy by default when Kmax2 ≥ 120 (previously, this method was never applied by default when option "Ep=0" was used).
3. The default value of Kmax(1) = Kmax(2) in the case of zero photon energy (Ep=0) and $T_1 > 0.1$ MeV is now calculated differently than in the case Ep≠0. In particular, when Ep=0 and $T_1 > 0.1$ MeV, the default values of Kmax(1,2) corresponding to "accuracy_level=2" are now greater than in the previous versions of BREMS, and those values are now capped at 300 (previosly, they were capped at 220). The default values of Kmax(1,2) corresponding to $Z < 7$, Ep=0, $T_1 > 0.1$ MeV have been increased at both accuracy levels.
4. The stretched-exponential fitting model used for extrapolating the functions CS($\kappa_{\max}$) and DCS($\kappa_{\max}$) has been modified by letting the natural logarithm of the stretching exponent to be a linear function of $\kappa_{\max}$. The slope coefficient of this linear function is the new (fifth) varied parameter, which is denoted h: $(\mathrm{D})\mathrm{CS} = c_\infty \pm \exp(a + b\cdot\kappa_{\max}^{\exp(d+h\kappa_{\max})})$.
5. Parameters "vary_h_CS" and "vary_h_DCS" have been added. They indicate the method of calculating parameter h when fitting the CS or the DCS, respectively: (1) if vary_h_CS(DCS)=0, h will be equal to zero (as in the previous versions of BREMS); (2) if vary_h_CS(DCS) < 0, h will be calculated as the value corresponding to the smallest sum of squared absolute deviations after performing the fitting −vary_h_CS(DCS) times with quasi-random initial values and quasi-random initial increments of parameters d and h; (3) if vary_h_CS(DCS) = 1, h will be calculated by minimizing the absolute difference between the optimal values of c_∞ corresponding to two different fitting intervals – the original one and the alternative one, whose endpoint coincides with the center of the original fitting interval. The latter method is the default one. In the case of a single or multiple four-parameter nonlinear fitting (cases

(1) and (3)), the sum of absolute deviations is minimized. In the case of the five-parameter nonlinear fitting (case (2)), the sum of squared absolute deviations is minimized.

6. Added parameters "fitRange_CS" and "fitRange_DCS", which control the width of the fitting interval when fitting the function CS(κ_{max}) or DCs(κ_{max}), respectively. The number of points (i.e., values of κ_{max}) in the fitting interval (N_{fit}) is calculated as follows:

   (a) if fitRange_CS(DCS) is equal to 1, then $N_{fit} = \frac{K}{8} + 1.5\sqrt{K}$,

   (b) if fitRange_CS(DCS) is equal to 2, then $N_{fit} = \frac{K}{4} + 1.2\sqrt{K}$,

   where $K \equiv \max(\max|\kappa_1|, \max|\kappa_2|)$. The calculated value of N_{fit} is rounded to the nearest integer. The option "fitRange_CS(DCS)=2" corresponds to a wider fitting interval. By default, fitRange_CS(DCS)=2 when vary_h_CS(DCS) is non-zero, and fitRange_CS(DCS)=1 when vary_h_CS(DCS) is zero.

7. Added parameters "tol_corr_CS" and "tol_corr_DCS", which are used to specify the threshold value of the relative correction of the CS or DCS due to nonlinear fitting, respectively, which must be exceeded in order to perform the five-parameter fitting (with parameter h varied). Before performing the five-parameter fitting of CS(κ_{max}) or DCS(κ_{max}) (i.e., optimizing parameter h), the four-parameter fitting with $h = 0$ is performed, and if the relative correction of the CS or DCS due to the fitting is less than parameter "tol_corr_CS" or "tol_corr_DCS" respectively, then the result of the four-parameter fitting is accepted without attempting the five-parameter fitting. The default value of those two parameters is 0.01. ***Note***: The five-parameter fitting is never attempted if the number of points in the fitting interval (N_{fit}) is less than 20.

8. Parameter "tol3" has been added. It is used to specify the tolerance of parameter h of the nonlinear fitting function. The default value of tol3 is 10^{-9}.

9. Parameters "avg_period_min" and "avg_period_max" have been added. They allow setting the minimum and maximum averaging period explicitly, rather than calculating it from the width of the fitting interval (using the parameter "avg_period_max_ratio"). If the partial-wave interpolation is applied, then the default value of avg_period_min is equal to parameter k2_step_last (i.e., the interval between the last two breakpoints of κ_{max} if k2_step_last > k2_step0, or the interval between the first two breakpoints of κ_{max} if k2_step_last = k2_step0). If the partial-wave interpolation is not applied, then the default value of avg_period_min is equal to 5 when $\max(\max|\kappa_1|, \max|\kappa_2|) \geq 80$, or to 1 otherwise.

10. Added parameter "suffix3", which denotes the suffix that is appended in stage 3 to the names of files "DCS_fitted_...", "ShapeFn_fitted_...", "DCS_alt_...", and "DCS_parms_".

11. The average absolute residuals of the nonlinear fitting are now written to the files "CS_parms.txt" and "DCS_parms_....txt".

12. The adaptive extension of the fitting interval in the direction of decreasing κ_{max} is no longer performed in stage 3 (in subroutine "Brems_fit").

13. Updated the user manual.

1.4.8.1 (2018-08-17):

1. The nonlinear fitting model has been modified so that the stretching exponent itself (rather than its natural logarithm) increases linearly with κ_{max}, i.e., the stretching exponent is equal to $d(1 + h\kappa_{max})$. Negative values of the slope coefficient dh are no longer allowed. The parameter d has been redefined as the actual intercept of the stretching exponent, rather than its natural logarithm.

2. The meanings of the signs of parameter "vary_h_CS(DCS)" have been interchanged. The default values of "vary_h_CS" and "vary_h_DCS" are 50 and 5, respectively, for "accuracy_level=1", and 100 and 10 for "accuracy_level=2".

3. The endpoint of the fitting interval is now changed in increments of 1 for several fitting cycles. In each case, the starting point of the interval is recalculated in the usual way, so that the entire interval is shifted in the direction of the decreasing κ_{max} relative to the original interval. By default, the fitting is performed starting with shift -4 and ending with shift 0 (five fitting cycles). The maximum shift is controlled by parameters "shift_k_max" and "shift_k_max_ratio", which are used in the same way as avg_period_max and avg_period_max_ratio: shift_k_max=min(shift_k_max0,idnint(shift_k_max_ratio*n1)). The default

values are “shift_k_max=4” and “shift_k_max_ratio=0.25” (the latter value is the maximum allowed value of shift_k_max_ratio). The number of fittings specified by parameter “vary_h_CS(DCS)” is performed for each shift. The arithmetic average of the optimal values of CS or DCS corresponding to all shifts is used as the optimal fitted CS or fitted DCS. However, the other output data, including the values of “nErr” and “nErrTot” in the file “CS_fitted.txt” and all the data that are output to the files “DCS_alt_...txt”, “DCS_parms_….txt” and “CS_parms.txt” (excluding the column “CS_fitted[k->Inf]”), correspond to the zero shift. The standard deviation of the average fitted CS or DCS over all shifts is used as the estimate of the uncertainty of the fitted CS or DCS. When the fitted DCS integral can be estimated with sufficient accuracy, i.e., when fitMode>0 and the limiting values of θ are 0 and 180° and the maximum angular increment is less than or equal to 1°, then the values of the fitted DCS integral are used, too, when calculating the optimal fitted CS and its standard deviation (i.e., the number of observations of the fitted CS is equal in this case to 2*(shift_k_max+1)).

4. The maximum allowed value of avg_period_max_ratio has been decreased to 0.25.
5. The last two columns in the file “DCS_alt….txt” (corresponding to arrays f1 and f2, respectively, in Brems_fit.f90) have been redefined. f1 is obtained from the original fitted DCS by replacing the values at $\theta \geq 140°$ with those calculated from the polynomial approximation. f2 is obtained by replacing the values at $\theta \geq 160°$ with those calculated from the polynomial approximation, and by replacing the values at $140° < \theta < 160°$ with the weighted average of the original fitted DCS and the polynomial approximation (the weight coefficients are $(160° - \theta) / (20°)$ and $(\theta - 140°) / (20°)$, respectively). When the polynomial angular extrapolation is deemed necessary, the values of f2 are used as the true fitted DCS.
6. The values of parameters vary_h_CS, vary_h_DCS, shift_k_max, and the number of observations of the fitted CS (used for averaging) are written to the file “CS_fitted.txt”.
7. Four columns with the relative corrections, scaled absolute corrections, standard relative deviations, and scaled standard absolute deviations of the fitted DCS and fitted shape function have been added in the files “DCS_fitted_....txt” and “ShapeFn_fitted….txt”. When calculating the “scaled” corrections or standard deviations, the product of $\sin(\theta)$ and the DCS or shape function is divided by the maximum value of the same product.
8. Five columns with the relative correction of the CS, maximum relative correction of the DCS, maximum scaled absolute correction of the DCS, maximum relative correction of the shape function, and maximum scaled absolute correction of the shape function have been added in the file “CS_fitted.txt”.
9. Five columns with the standard relative deviation of the fitted CS, maximum standard relative deviation of the fitted DCS, maximum scaled standard absolute deviation of the fitted DCS, maximum standard relative deviation of the fitted shape function, and maximum scaled standard absolute deviation of the fitted shape function have been added in the files “CS_fitted.txt” and “Errors.txt”.
10. Four columns with the maximum relative difference of the DCS, maximum scaled absolute difference of the DCS, maximum relative difference of the shape function, and maximum scaled absolute difference of the shape function have been added in the file “Errors.txt”. Those differences are calculated relative to the values of the same function corresponding to the maximum (original) value of the endpoint of the range of κ_{max} (i.e., to the “optimal” fitting conditions).
11. The file “Errors.txt” now includes a column with the values of the fitted DCS integrals, and a column with their relative differences.
12. The column “CS_fitted[k->Inf]” of the file “CS_fitted.txt” is now also present in the file “CS_parms.txt”.
13. Updated the user manual.

1.4.8.2 (2018-08-19):

1. Fixed the testing for nonlinear fitting errors in subroutine “Brems_fit” (because of that bug, some types of fitting errors were previously missed in stage 3).
2. Added the relative tolerances of the varied parameters to the set of input parameters of stage 3 (subroutine “Brems_fit”). The corresponding parameters are “rtol1”, “rtol2”, “rtol3” (they are equal to 10^{-9} by default). This change has reduced the possibility of a lock-up in stage 3.
3. Now, only the “shift 0” is required to be successful in stage 3 (previously, all shifts were required to be successful, which could in rare cases cause a failure of the program).

4. The nonlinear fitting errors that occur in the angular extrapolation range ($\theta > 160°$) are no longer counted if the number of points in the fitting interval of κ_{max} is less than 20 (even when the angular extrapolation is not required).
5. Updated the user manual.

1.4.8.3 (2018-08-21):

A more reliable test of the tendency to saturation of the dependence of the CS or DCS on κ_{max} inside the fitting interval has been implemented in stage 3 (file "Brems_fit.f90", subroutine "FitInfo").

1.4.8.4 (2018-08-23):

1. Some of the criteria used for testing if the dependence CS(κ_{max}) or DCS(κ_{max}) is suitable for the nonlinear fitting (i.e., has a tendency to saturation) have been relaxed; smoothing of the dependences CS(κ_{max}) and DCS(κ_{max}) has been implemented in stage 3 (file "Brems_fit.f90", subroutine "FitInfo"). Those modifications have reduced the probability of a nonlinear fitting failure (i.e., a fatal error), especially near the tip of the spectrum when the function DCS(κ_{max}) is frequently oscillatory.
2. Some of the criteria used for testing if the results of the nonlinear fitting are acceptable have been relaxed. Those modifications (similarly to the previously described ones) have reduced the probability of a nonlinear fitting failure, especially near the tip of the spectrum.
3. The fitting errors that occur in the angular extrapolation interval ($\theta > 160°$) are never counted (thus, they cannot cause a fatal error).

1.4.8.5 (2018-08-26):

1. Increased the maximum default value of Kmax1 and Kmax2 from 250 to 300.
2. The default values of parameters "tol_A" and "tol_delta" in the case of zero photon energy ("Ep=0") no longer depend on the accuracy level, and they are equal to $2 \cdot 10^{-9}$ and $-2 \cdot 10^{-9}$, respectively.
3. The final values of the phase correction integrals are no longer taken into account when estimating the uncertainties of the phase shifts in the case of a screened interaction potential and non-zero photon energy.
4. The natural cubic spline (with zero second derivatives at both endpoints of the interpolation interval) is now used in stage 2 for calculation of the double differential cross sections when the partial-wave interpolation method is applied. In the previous versions of BREMS, the second derivative at the starting point of the interpolation interval was not required to be zero. Instead, the first derivative was required to be equal to its finite-difference estimate. The latter boundary condition is still implemented in the current version of BREMS for calculation of the single differential cross sections when the partial-wave interpolation method is applied.
5. Fixed a bug causing a crash in the case of zero photon energy ("Ep=0"), when the calculation was started from stage 2 ("firstStage=2") and the maximum values of $|\kappa_1|$ and $|\kappa_2|$ in the data file were greater than those requested by the user.
6. Updated the program Read_S_integrals to be consistent with the recent modifications of BREMS.

1.4.8.6 (2018-08-27):

1. Fixed a bug in "S_integrals.f90" (subroutines "power_series", "power_series_QP", "power_series_MP"), which could cause a crash if the user-specified values of parameters "Kmax1" and "Kmax2" were not equal to each other and the option "method=3" (which is the default) was used.
2. Corrected the user manual.

1.4.8.7 (2018-08-30):

1. Modified the calculation of the default value of parameter "Kmax2". Now, it is defined as the smaller of these two numbers: the default value of Kmax1 corresponding to the current values of T_1 and k / T_1, and the default value of Kmax1 corresponding to $T_1 = T_2$ and $k = 0$. When $T_2 << T_1$, such definition yields significantly smaller values of Kmax2 than in the previous versions of BREMS (where the default value

of Kmax2 was equal to the default value of Kmax1), and the calculation time is therefore significantly shorter than before. ***Note***: In the case "method=1", the effect of this modification is reduced because of the automatic decrease of Kmax2 in stage 1, which is possible when the option "method=1" is specified.

2. When the partial-wave interpolation method is not applied, the value of parameter "k2_breakpoint1" that is written to the file "CS.txt" in stage 2 is now equal to 0 (previously, it was equal to the initial value of Kmax2).

1.4.8.8 (2018-08-31):

1. Several minor changes of the code (needed to improve compatibility with the Intel Fortran compiler and to eliminate several compiler warnings) have been made.
2. The Windows executables have been recompiled using the Intel Fortran compiler. During the analytical integration (from r_0 to ∞), the current Windows executable Brems.exe is faster than the previous version (which was compiled using the PGI Fortran compiler) by 30 – 70 % when multiple precision or quadruple precision is used, and by 10 – 15 % when double precision is used. No significant differences between the two versions in the durations of numerical integration (from 0 to r_0) and in the durations of stage 2 have been noticed. In stage 3, the current Windows executable Brems.exe is faster by a factor of 2.5 – 3 than the previous version.

1.4.8.9 (2018-09-08):

1. Fixed a bug in the subroutine "power_series_MP" (file "S_integrals.f90"), which could in rare cases cause a crash of the program due to an access violation (this could happen when the two energy values of the electron were enumerated by the mentioned subroutine in the wrong order).
2. The calculation of the default value of parameter Kmax2 has been slightly modified: if it is greater than 80 and the photon energy is non-zero, then Kmax2 is rounded to the nearest multiple of 5.

1.4.8.10 (2018-09-15):

1. The accuracy of multiple-precision calculation of the Taylor series coefficients in the vicinity of $r = 0$ (subroutine "power_series_MP") has been improved. Now, all coefficients are recalculated when it is determined that the current precision level is insufficient and the required precision level is greater than the maximum precision level that was used in the current run (previously, only the additional coefficients were calculated at the new precision level, whereas the other coefficients were not recalculated, which means that their precision was lower).
2. Fixed a bug in the program "Read_S_integrals.exe" (this bug sometimes caused a fatal error if the values of parameters "Kmax1" and "Kmax2" were not specified explicitly on the command line).

1.4.9.0 (2018-09-25):

1. Two of the three angular ranges used for angular polynomial extrapolation ($140° \le \theta < 150°$ and $150° \le \theta \le 160°$) have been replaced by the wider angular ranges $120° \le \theta < 140°$ and $140° \le \theta \le 160°$, respectively.
2. Added the fourth-, fifth- and sixth-order angular polynomials into the set of alternatives for polynomial extrapolation in the angular range $\theta > 160°$ (the optimal degree of the extrapolating polynomial is determined on the basis of the maximum error in the angular range $120° \le \theta < 140°$). Because of this change, three columns with the values of the three additional polynomial coefficients have been inserted into the file "CS_parms.txt", which is optionally updated in stage 3 (by the subroutine "Brems_fit").
3. Modified the calculation of the standard deviation (SD) in the angular extrapolation interval ($\theta > 160°$) when the angular extrapolation is deemed necessary. In such a case, the mentioned SD is obtained by adding in quadrature the standard deviation indicating the degree of variability of the fitted DCS between the "shifts" (i.e., the SD that was output by the previous versions of BREMS), and the angular extrapolation error, which is calculated as a linear function of θ, equal to zero at $\theta = 160°$ and to the maximum value at $\theta = 180°$. The latter maximum value is assumed equal to the maximum absolute error of the extrapolating polynomial in the angular range $120° \le \theta < 140°$.

4. The least-absolute-value fitting has been replaced by the least squares fitting (because the optimal values of the varied parameters in the case of least-absolute-value fitting are more likely to correspond to a local minimum of the sum of absolute deviations, rather than the global minimum).
5. The effect of the option "Q_last=0", when it is used together with "R_atom=0" and non-zero photon energy, has been modified. This option now indicates that the truncation radius of the potential function must be determined "dynamically", based on the magnitudes of the ranges of variation of the normalization factor "A" and the phase shift "delta" alone. In this case, the truncation radius is equal to the value of the radial coordinate where the mentioned ranges of variation for all values of κ_1 and κ_2 and for both energies of the electron become less than the specified tolerances "tol_A" and "tol_delta", and the asymptotic expressions of the wave functions (in terms of the spherical Bessel functions) are never used for calculating the S integrals before the truncation radius is reached (even if the ranges of variation of the estimates of the normalization factors and phase shifts for a given pair of values of E and κ are less than the corresponding tolerances "tol_A" and "tol_delta"). In the case of zero photon energy, the option "Q_last=0 R_atom=0" also has a slightly different meaning than in the previous version of BREMS. Now, it means that the final values of the normalization factors and the phase shifts must be calculated at the last value of the radial coordinate, using the current values of the phase correction integral Q, and their uncertainties must be reset to zero (previously, the normalization factor and the phase shift corresponding to each value of κ_1 and κ_2 were calculated independently, on the basis of the current uncertainties corresponding to this κ, and the mentioned uncertainties were not reset to zero). Thus, the only difference in comparison with the case of non-zero photon energy is that the current value of Q is used for estimating the phase shift (in the case of non-zero photon energy, Q is reset to zero, which is equivalent to truncation of the interaction potential).
6. If the asymptotic form of the wave function (in terms of the spherical Bessel functions) is not attained before the truncation radius is reached, then the normalization factor and the phase shift are now determined at the truncation radius from the values of the spherical Bessel functions calculated using the explicit expressions and multiple-precision arithmetic. This ensures that the final values of normalization factors and phase shifts are not affected by accumulation of rounding errors (which is possible, for example, in the case of methods based on recurrence relations). If the interaction potential is truncated explicitly (i.e., parameter "R_atom" is non-zero), then, in order to achieve this maximum accuracy, one should use sufficiently small values of parameters "tol_A" and "tol_delta" (for example, 10^{-300}), so that the asymptotic form is not attained before the truncation radius is reached, and the less accurate methods of calculating the spherical Bessel functions are never used for calculating the S integrals (they are used only for calculating the current uncertainties of the normalization factors and the phase shifts, which are displayed periodically during the numerical solution of the coupled radial Dirac equations in stage 1). If the interaction potential is truncated "dynamically" (i.e., parameters "R_atom" and "Q_last" are zero), then the asymptotic expressions of the wave functions (in terms of the spherical Bessel functions) are never used for calculating the S integrals before the truncation radius is reached, so that the mentioned maximum accuracy is always guaranteed.
7. Fixed a bug in the file "Brems_fit.f90" (incorrect lower bound of the index of array "arg" declared in subroutines "SmoothDCS", "SmoothDCS2", and "N_infl").
8. Fixed a bug in the file "S_integrals.f90" causing a crash in the case "Ep=0" when the set of values of κ_2 is not contained entirely inside the set of values of κ_1.
9. Updated the user manual.

1.4.9.1 (2018-09-27):

1. During the power-series solution in the vicinity of $r = 0$ (in stage 1), the values of wave functions obtained at different precision levels are now required to become exactly equal to each other after rounding to double precision (rather than to differ by less than 10^{-10} % as in the previous versions of BREMS).
2. If the calculation process starts from stage 3 (option "firstStage=3"), then the five parameters defining the set of angles ("theta_min", "theta_max1", "np1", "theta_max2", and "np2") are no longer required to be exactly the same as those used in stage 2 (when the input files with the DCS data were created). If neither of these five parameters is explicitly specified by the user, then all angles will be read from the first line of the file with the DCS data. If the calculation process starts from stage 3 and at least one of these five parameters is specified explicitly, then the set of angles will be recalculated, and the program

will attempt to locate the corresponding columns in the input file with the DCS data. If the data for at least one of the angles is not available, then the program will quit with an error message.

3. Eliminated the possibility of a crash due to multiple instances of BREMS attempting to write to the same output file simultaneously.
4. The Windows executables of BREMS and Read_S_integrals have been recompiled using the Intel compiler option "/fp:precise", because absence of this option could make multiple-precision arithmetic operations insufficiently precise. When using BREMS versions 1.4.8.8 – 1.4.9.0, which were compiled without the mentioned option, the smallest S integrals (corresponding to largest values of κ_1, κ_2, and l) sometimes differed from the correct values by more than an order of magnitude (however, the effect of this imprecision on the values of the cross sections was noticed only in the 7^{th} or 8^{th} significant digit). ***Note***: The Windows executables of BREMS v1.4.8.7 and older versions, which were compiled using the PGI Fortran compiler, were not affected by this imprecision.
5. Updated the user manual.

1.4.9.2 (2018-09-28):

1. The format of the header line of the files with the DCS and shape function data created in stage 2 (by subroutine "Bremsstrahlung") has been modified: now, it contains the values of the angle with the maximum precision (18 significant digits). In the previous versions of BREMS, the values of the angle that were included in the header line were rounded to 4 significant digits, which could cause errors or inaccuracies when reading the angles in stage 3 (in subroutine "Brems_fit"). However, for compatibility with the DCS data files created by the older versions of BREMS, the previous format of the header line is also recognized and processed correctly.
2. The Windows executables of BREMS and Read_S_integrals have been recompiled using an additional Intel compiler option "/Qfp-speculation=safe" (in order to further reduce the likelihood of floating-point errors). This is the second non-default floating-point option of the Intel Fortran compiler used (the first one, introduced in BREMS v1.4.9.1, is "/fp:precise").

1.4.9.3 (2018-10-04):

1. The final estimates of the phase shifts and normalization factors (at the truncation radius) are now calculated at the highest precision level of ~4000 significant digits, because the method of adaptive precision level, which was used in the previous version of BREMS for calculating the explicit expressions of the spherical Bessel functions at the truncation radius, is flawed (at argument values less than n, it could yield erroneous values of j_n).
2. Subroutine SBESJY (implementing the Lentz-Thompson algorithm of continued fractions) is no longer used for calculating the spherical Bessel functions during the numerical integration, because it has been noticed that its accuracy is by 2 – 7 orders of magnitude worse than the accuracy of the recursion algorithms, which are implemented in subroutines SPHJ and SPHY. Consequently, the range of the argument values where subroutines SPHJ and SPHY are applied has been extended to 5000 (at larger arguments, the explicit formulas are used, as in the previous versions of BREMS).
3. Added a new parameter "j_QP". It is an integer number 0, 1, or 2, which defines the way the quadruple-precision (QP) arithmetic should be used during the numerical quadrature when calculating the spherical Bessel function of the first kind $j_l(kr)$, which is used as a factor in the integrands of the S integrals. If j_QP=0, then QP will not be used, except when $kr > 5000$ and the required accuracy of the explicit formula cannot be achieved with double precision. If j_QP=1, then, in addition to the above, QP will be used for calculating $j_l(kr)$ at $kr \leq 5000$ (where $j_l(kr)$ is calculated by backward recursion). If j_QP=2, then, in addition to the above, QP will always be used for calculating $j_l(kr)$ at $kr > 5000$. By default, j_QP=0 in the case "accuracy_level=1", and j_QP=2 in the case "accuracy_level=2".

1.4.9.4 (2018-10-08):

1. Fixed a bug, which sometimes caused incorrect values of the phase shifts during the "test" integration in the case of zero photon energy when the option "R_atom=0 Q_last=0" (which is the default when Ep=0) was used.

2. In the case “Ep=0 R_atom=0 Q_last=0”, the final value of the phase correction integral (Q) is now reset to zero (as in the case “Ep≠0 R_atom=0 Q_last=0”). Although this introduces an error into the values of phase shifts (in comparison with the values corresponding to a non-truncated interaction potential), the values of the S integrals and cross sections do not change, because in the case “Ep=0” they depend only on the differences of the phase shifts (so that the mentioned error cancels out).
3. Parameters “tol_A” and “tol_delta” are now allowed to be zero when R_atom≠0.
4. Eliminated the redundant recalculation of spherical Bessel functions, which were calculated earlier during the same step of the numerical integration (in stage 1). This modification has decreased the time of the numerical integration by up to 10 percent (the calculation results have not been affected).
5. Added a new parameter “tol_Nfit”, which specifies the minimum number of values of κ_{max} in the fitting interval (N_{fit}) needed for the five-parameter fitting (with the stretching exponent approximated by a linear function of κ_{max}) to be possible (if N_{fit} is less than tol_Nfit, then the four-parameter fitting with a constant stretching exponent will be performed). The default value of this parameter is 10.
6. Updated the user manual.

1.4.9.5 (2018-10-11):

The Windows executables (“Brems.exe” and “Read_S_integrals.exe”) have been recompiled using static libraries (Intel Fortran compiler option “/libs:static /threads”), because the default compiler option (“/libs:dll /threads”), which was used for compiling the previous versions of BREMS, caused a failure to execute the Windows executables with a message about missing *.dll files, if the Intel Fortran compiler was not installed. The source code has not been modified, apart from a correction of a few typos in messages and comments.

1.4.9.6 (2018-10-14):

In stage 3 (subroutine “Brems_fit”), if the relative range of variation of the CS or DCS for “shift 0” is less than 0.001, then the final CS or DCS is set equal to the value of the unfitted CS or DCS corresponding to shift 0 and to the maximum value of κ_{max}, and the standard deviation is set equal to the range of variation of the CS or DCS in the fitting interval corresponding to shift 0. As an indication of this special case, the values of the mentioned standard deviations are output with the minus sign.

1.4.10.0 (2018-10-25):

1. Each successful “shift” (i.e., the processing of the data corresponding to a given interval of values of κ_{max}) now has an associated uncertainty of the CS or DCS. If the fitting was not performed (due to insufficient variation of the CS or DCS inside the fitting interval), then the uncertainty is assumed equal to the range of variation of the CS or DCS inside the fitting interval. If the fitting was performed, then the uncertainty is calculated using the corresponding diagonal element of the variance-covariance matrix. This associated uncertainty contributes to the overall uncertainty. This contribution is calculated as the square root of the sum of squared uncertainties divided by the number of successful shifts, and it is added in quadrature with the uncertainty used in the previous versions of BREMS. Those modifications are applied to the uncertainties of the shape functions, too.
2. Added a new criterion for choosing between the four-parameter fitting (with $h = 0$, where h is the slope coefficient of the stretching exponent) and the five-parameter fitting: it is the magnitude of the uncertainty of the fitted CS or DCS corresponding to each of the mentioned two cases. If at least one of the two least-squares estimates of the CS or DCS is inside the confidence interval of the other estimate, then the estimate corresponding to the smaller uncertainty is preferred, otherwise the estimate obtained by the five-parameter fitting is preferred.
3. The stretching exponent has been redefined as $d + h\kappa_{max}$ (previously, it was defined as $d(1 + h\kappa_{max})$). This has been done in order to eliminate the strong correlation between the optimal values of d and h when d is much less than the linear term in the stretching exponent (the linear term is equal to $h\kappa_{max}$ in the case of the new definition of the stretching exponent, or $dh\kappa_{max}$ in the case of the previous definition).
4. The default value of parameter “tol_corr” has been reduced from 0.01 to 0.001.
5. Added a new parameter “range_ratio_max”, which is the maximum allowed ratio of the ranges of variation of the CS or DCS in two fitting intervals (“shifts”). All shifts where the (absolute) range of

variation exceeded the minimum observed range of variation by a factor greater than "range_ratio_max" are excluded. The default value of this parameter is 10.

6. A column "nObs" with the numbers of observations (i.e., of the shifts that have not been excluded) for each angle has been inserted in the files "DCS_fitted_..." and "ShapeFn_fitted_...". The number in the column "nObs" in the file "CS_fitted.txt" now also is the number of retained shifts only.
7. The angular smoothing is now applied to the relative uncertainties, too. The initial smoothing of the relative uncertainties (in the subroutine SmoothDCS) is performed by applying the same coefficients to the relative uncertainties as to the logarithms of the corresponding ratios of the fitted DCS and the original DCS. The second stage of smoothing of the relative uncertainties (in the subroutine SmoothDCS2, calling the SSP subroutine DSG13) is performed by the same method as the smoothing of the DCS (each smoothing of the DCS is followed by an independent smoothing of the relative uncertainties in the same angular interval). After the smoothing, the original value of the uncertainty will be restored if the fitting has not been performed due to insufficient variation of the DCS in the fitting interval and the value of the uncertainty after the smoothing is less than twice the range of variation of the DCS, whereas the change of the corresponding value of the DCS due to the smoothing is less than the range of variation of the DCS.
8. The check for the necessity of the angular polynomial extrapolation is now performed after the angular smoothing (previously, this was done using the unsmoothed DCS, although the coefficients of the extrapolating polynomial were calculated using the smoothed DCS).
9. Updated the user manual.

1.4.10.1 (2018-11-13):

1. Fixed a bug causing the array "a_log" reallocation error when parameter Kmax1 or Kmax2 is automatically reduced in subroutine S_integrals (such reduction is possible only with "method=1").
2. Subroutine Bremsstrahlung has been modified so that in the case "iCalculate=-1" the values of the angle θ are read from the first line of the existing file with the DCS data (similarly to subroutine Brems_fit).

1.4.10.2 (2018-12-15):

1. Improved calculation of the uncertainties for the error points in the angular dependence of the fitted DCS (previously, those uncertainties were zero, and now they are calculated by interpolation between the values of the uncertainties corresponding to the non-error points).
2. When parameter "R_atom" is non-zero and parameter "method" is equal to 3, the default values of parameters "tol_A" and "tol_delta" are now zero.

1.4.10.3 (2018-12-19):

When determining whether the current "shift" should be excluded from the calculation of the average fitted DCS due to excessive range of variation in comparison with the minimum observed range of variation, only the values of the unfitted CS are used (previously, the values of the unfitted DCS corresponding to the current value of the angle θ were used). Thus, the excluded shifts are now the same for all values of θ (and the same as for the CS). This change sometimes makes the angular dependence of the average fitted DCS smoother and more accurate than that calculated with the previous version of BREMS.

1.4.11.0 (2019-01-12):

1. The maximum allowed absolute value of κ_1 and κ_2, i.e., the maximum number of partial waves used in the expansions of the differential cross sections (parameter "sz" in the source code), has been increased from 300 to 500. This makes it possible to improve the accuracy of the differential cross sections at $T_1 > 3$ MeV. However, the values of Kmax1 and Kmax2 greater than 300 may require a prohibitive amount of RAM for storing the R factors in stage 2 (for example, when Kmax1 = Kmax2 = 500, more than 32 GB of RAM are needed). For this reason, the default values of parameters Kmax1 and Kmax2 corresponding to $T_1 > 3$ MeV have not been increased.
2. The precision level used for calculating the trigonometric integrals in stage 1 has been increased from 2000 to 2500 (this may be needed when the incident electron energy T_1 is greater than 10 MeV).

3. The maximum number in the additional suffix "_<number>", which is automatically appended to the name of the output file with the *S* integral data in stage 1, has been increased from 9 to 999. Added a new parameter "start_suffix", which indicates the starting number in this suffix (its default value is zero, which means absence of the additional suffix).
4. When calculating the uncertainties (standard deviations) of the single- and double differential cross sections ("CS" and "DCS", respectively) in stage 3, the variance of the fitted (D)CS is now used instead of the variance of the average fitted (D)CS. I.e., the corresponding term in the expression of the overall squared uncertainty has been increased by a factor equal to the number of observations (fitting intervals, or "shifts") used to calculate the average (D)CS.
5. A bug that could in rare cases cause indeterminate values ("NaNs") of the DCS (in stage 2) has been fixed. This bug was caused by occasional negative values of the terms in the expression the DCS as a sum with respect to $|\kappa_2|$ (those negative values are possible due to rounding errors when calculating those terms at Kmax1 and Kmax2 greater than the default values). Since the partial-wave interpolation method requires calculation of the logarithm of each term of the mentioned sum, indeterminate values appeared as a result of an attempt to calculate the logarithm of a negative number. In the current verion, the values of the interpolation breakpoints that are less than 10^{-18} of the current value of the sum (including all negative values) are recalculated by an additional cubic spline interpolation between the logarithms of all other breakpoints.

1.4.11.1 (2019-01-14):

The absolute uncertainty of the fitted single differential cross section is now calculated by adding in quadrature the previous estimate (which takes into account only the fitting errors and the differences between the fitting results corresponding to different fitting intervals) and the angular integral of the absolute uncertainty of the fitted double differential cross section. This modification is applied only when the angular interval is from 0° to 180° and the angular grid is sufficiently dense for accurate estimation of the latter integral (i.e., the maximum angular step is not greater than 1°).

1.4.12.0 (2019-02-13):

1. The width of the fitting interval corresponding to fitRange_(D)CS=1 has been re-defined to be exactly half of that corresponding to fitRange_(D)CS=2 (i.e., the smaller of the two widths has been slightly reduced).
2. Added the option "fitRange_(D)CS=3", which indicates that both fitting intervals should be tried, and the fitted (D)CS should be calculated as the average of the least squares estimates corresponding to each of the two fitting intervals. In this case, the calculation of the uncertainty of the fitted (D)CS is modified accordingly. The final estimate of the mentioned uncertainty takes into account both the uncertainties of the least squares estimates of the (D)CS corresponding to each of the two fitting intervals, and the difference of those two least squares estimates of the (D)CS (the exact formula used to estimate the uncertainty is given in the updated user manual). Parameters fitRange_CS and fitRange_DCS must be either both equal to 3, or both different from 3 (they are equal to 3 by default).
3. The values of parameters fitRange_CS and fitRange_DCS are now written to the files "CS_fitted.txt", "CS_parms.txt" and "Errors.txt". The output value "3" indicates that both fitting attempts (corresponding to the two widths of the fitting interval) were successful in shift 0. If one of the two fitting attempts failed in shift 0, or if the user-specified input value of parameter fitRange_(D)CS is less than 3, then the output value is "1" or "2", indicating the interval where the fitting was successful in shift 0.
4. Added new parameters wt_fitRange2_CS and wt_fitRange2_DCS, which have the meaning of the ratio of the weight factors corresponding to the two possible widths of the fitting interval (defined by fitRange_(D)CS = 1 and fitRange_(D)CS = 2). Those weights are used when calculating the average fitted (D)CS and its uncertainty in the case "fitRange_(D)CS=3". When wt_fitRange2_(D)CS < 1, a greater weight is assigned to the fitted (D)CS corresponding to the narrower fitting interval (corresponding to fitRange_(D)CS = 1). The default value of wt_fitRange2_(D)CS is 1, which corresponds to a simple arithmetic average. This parameter has an effect only when fitRange_(D)CS = 3.
5. Added new parameters thr_ratio_h_CS and thr_ratio_h_DCS, which control the condition to perform the comparison of the absolute uncertainties of the fitted (D)CS needed to determine which of the two fitting modes ($h = 0$ or $h > 0$) should be preferred. Parameter thr_ratio_h_(D)CS specifies the threshold value of

the ratio of the absolute difference between the two estimates of the fitted (D)CS and the larger of the two corresponding absolute uncertainties, which must be exceeded in order to use the result corresponding to $h > 0$ unconditionally (i.e., without the additional requirement for the uncertainty corresponding to $h > 0$ to be less than the uncertainty corresponding to $h = 0$). The default value is thr_ratio_h_(D)CS=1, which means that the additional requirement will be applied only when the larger of the two confidence intervals contains the value of the fitted (D)CS corresponding to the other fitting mode. If thr_ratio_h_(D)CS=0, then the result corresponding to $h > 0$ will always be used (i.e., the uncertainties corresponding to $h = 0$ and $h > 0$ will never be compared). If thr_ratio_h_(D)CS is set equal to an extremely large value, then the two uncertainties will always be compared, and the result corresponding to the smaller uncertainty will always be used. This parameter has an effect only when parameter vary_h_(D)CS is non-zero.

6. Parameter "dir_V" has been redefined: now it means not the name of the parent folder, but the name of the actual folder where the ASCII files containing the $V(r)$ data are located. Its default value has been modified accordingly: it is now "V/Kohn-Sham" (previously, it was "V").
7. Memory usage in stage 2 at large values of $\kappa_{\max}$ has been reduced approximately by half.
8. Updated the user manual.

1.4.12.1 (2019-03-19):

The precision level used for calculating the trigonometric integrals in stage 1 has been increased from 2500 to 3000 (this may be needed when $T_1 \geq 10$ MeV and $\kappa_{\max} \geq 300$).

1.4.12.2 (2019-03-24):

1. The requirements that must be satisfied in order to enable the skipping of the values of κ_2 in stage 1 (in order to apply the partial-wave interpolation method in stage 2) have been relaxed: now, the only required option is "isAbs_K2=1" (previously, the option "Kmin2=1" was also required).
2. (2019-03-30) The same modification has been implemented in the program "Read_S_integrals" (its source code is in the file "Read_S_integrals\Read_S_integrals.f90").

1.4.12.3 (2019-04-02):

Fixed a minor bug in the messages that are displayed during the integration from r_0 to infinity (this bug caused incorrect numerical values in some of the messages when the user requested quadruple or multiple precision without optimization of the precision level).

1.4.12.4 (2019-04-06):

Fixed a minor bug in the subroutine "Bremsstrahlung", which prevented loading of more than ten S integral data files in stage 2 (the S integral data files whose sequence numbers were greater than 9 were not loaded).

1.4.12.5 (2019-05-25):

1. The time of calculation of the double differential cross section (DCS) in stage 2 has been shortened by half. This has been achieved by employing the fact that terms of the sum in the expression of the DCS are symmetric with respect to interchange of two summation indices (κ_1 and $\bar{\kappa}_1$).
2. Several redundant lines of code have been removed in the files "Bremsstrahlung.f90" and "Brems_fit.f90".

1.4.12.6 (2019-05-30):

The time of calculation of the double differential cross section (DCS) in stage 2 has been shortened additionally by employing the symmetry with respect to inversion $\theta \to \pi - \theta$. The symmetric and antisymmetric parts of the sum are obtained by adding the terms with even and odd $l_1 + \bar{l}_1$, respectively. For all pairs of θ that are symmetric with respect to $\theta = 90°$, it is sufficient to calculate the symmetric and antisymmetric parts of the DCS for $\theta \leq 90°$ only, whereas the value of the DCS for $\theta > 90°$ can be obtained by subtracting the antisymmetric part from the symmetric part. This causes an additional decrease of the summation time by half when all values of θ can be grouped into pairs of symmetric values (θ and $\pi - \theta$).

1.4.12.7 (2019-06-10):

A minor bug in the file "AuxiliaryPrograms/CubicSplineInterpolation/spline.f90" has beeen fixed. This bug could show up when parameter "k2_excl_last" was set to 1 (by default, this is the case only when parameter "IV" is equal to 1, i.e., when the unscreened Coulomb potential is used). This bug caused an invalid reference to an array (the array subscript was erroneously set to zero, while the smallest allowed value is 1). It did not affect the final results, because the mentioned array element was not used in the calculations (however, the invalid array reference could cause an abnormal termination of the program if it was compiled in debug mode).

1.4.12.8 (2019-06-22):

Fixed a bug in the file "S_integrals.f90", which in rare cases caused a slight difference between the calculated value of the truncation radius of the potential function (parameter R_atom) and the endpoint of the numerical integration range (r_0) when the options "R_atom=0 Q_last=0" were used (those options are the default ones in the case of zero photon energy).

1.4.12.9 (2019-08-23):

Fixed a bug in the file "Bremsstrahlung.f90", which caused incorrect results when |Kmax2| < |Kmin2|. The condition |Kmax2| < |Kmin2| may be satisfied when the aim of the calculation is determining the contribution of a particular subset of partial waves to the single- and double differential cross sections of bremsstrahlung. The mentioned inequality is never true in the case of calculation of the actual (total) cross sections, because in this case |Kmin2| is always equal to 1.

1.5.0.0 (2020-10-13):

Version No. 1.5.0.0 is a major update of BREMS, with numerous improvements and additional capabilities. Because of the improvements of performance, the endpoint of the energy range where BREMS can be applied has been increased from 3 MeV to 10 MeV. Below is a list of some of the most important changes:

1. The calculation of the "numerical" part of S integrals (from 0 to r_0) in stage 1 has been optimized, causing a decrease of the duration of this stage by a factor of 3 – 6 in comparison with the previous version of BREMS (at the same number of S integrals). This improvement is mainly caused by the replacement of multidimensional arrays with one-dimensional arrays in the code of BREMS.
2. An additional method of decreasing the number of S integrals that have to be calculated exactly has been implemented. This method is based on the cubic spline interpolation of the S integrals with respect to l (the orbital quantum number of the emitted photon). When a large number of partial waves is needed (e.g., in the case of a high energy of the outgoing electron), this method makes it possible to decrease the time of calculation of the S integrals additionally by a factor of 5 – 6, without a significant deterioration of the accuracy of the final results.
3. The duration of stage 2 has been reduced significantly by using an alternative expression of the partial-wave double differential cross section (DDCS). This expression is mathematically equivalent to the one that was implemented in the previous versions of BREMS, but requires much less processing time (because it requires triple summation instead of the quadruple summation performed in the previous versions of BREMS). In the case of a large number of partial waves, the duration of stage 2 is thereby reduced by a factor of 3 – 4.
4. The accuracy of fitting the DDCS in stage 3 at electron energies of the order of 1 MeV has been improved using angular spline fitting and extrapolation.
5. Two "special" modes of operation of BREMS have been implemented:
   - calculation of the angular dependence of the approximate DDCS according to the Born approximation (with or without the atomic form factor) or Sommerfeld-Maue approximation (with or without the additive screening correction), and the corresponding single differential cross section (SDCS),
   - fitting of an arbitrary screening function defined in tabular format by a linear combination of up to 200 decaying exponentials (this is a necessary first step before calculation of the atomic form factor and of the approximate DDCS based on the screened Born approximation).

1.5.1.0 (2020-10-17):

1. The default definition of the "objective function", which is minimized during the angular spline fitting in stage 3, has been simplified: it is now equal to the squared rms value of the relative uncertainty of the spline fitting over the entire angular range $0° \le \theta \le 180°$.
2. It is now possible to add more terms to the definition of the mentioned objective function and to specify their weights. The names of the corresponding new parameters are "splineUnc_wt", "splineRes_wt", and "splineDiff_wt". In order to be consistent with this naming, the name of parameter "i_ref_err" has been changed to "i_splineSF".
3. The user manual has been updated.

1.5.1.1 (2020-10-24):

1. Negative values of parameter "splineInt_max_fitted" are now allowed. A negative value of this parameter indicates that the program must use the largest average inter-knot interval (i.e., the smallest number of knots) such that the other adjustable parameters of the spline function approximating the angular dependence of the κ_{max}-fitted DCS can be determined successfully (i.e., there is no angular spline fitting error).
2. The default values of parameters "splineInt_min_fitted" and "splineInt_max_fitted" have been changed to 90 and −180, respectively (in the previous version, those parameters were equal to 180 by default).
3. The user manual has been updated.

1.5.1.2 (2020-10-31):

Fixed a bug causing zero values of the DCS calculated according to the Sommerfeld-Maue approximation, when the user specified a zero or negative value of parameter "tol_change_HG".

1.5.1.3 (2020-11-08):

1. Fixed a bug causing an error during the angular spline fitting in stage 3 when the κ_{max}-fitted DCS at all angles is identical to the original partial-wave DCS (for example, at extremely low energies).
2. The default value of parameter "splineInt_min_fitted" has been reduced from 90 to 30.

1.5.1.4 (2020-11-10):

Fixed a bug which in rare cases caused an error message about "irregular large-angle dependence" of a reference DCS at the beginning of stage 3.

1.5.2.0 (2020-11-13):

1. The option to apply the Elwert factor has been added. This option is controlled by the "switches" "Elwert1" and "Elwert2" (alias "Elwert" for both) indicating whether the DCS calculated according to the Born approximation must be modified by the Elwert factor in the case appr=0 and appr<0, respectively (in the latter case, this factor can be applied only to the additive screening correction). The default value of those two parameters is equal to 1 (i.e., the Elwert factor is applied, except in the case "appr=-1 IV=1" or "appr=-2 IV=1", when this factor is not applicable).
2. The file "CS_Born_SM.txt", which is updated after each calculation of the approximate DCS and CS corresponding to one of the analytical approximations (Born or Sommerfeld-Maue), now includes two additional columns: column "Z_alpha_beta1" with the values of the Coulomb parameter corresponding to the incident electron, and column "Born_DCS_factor" with the values of the Elwert factor or the number 1 if the application of the Elwert factor has been "switched off" by the user (i.e., if parameter "Elwert1" or "Elwert2" has been set to 0).
3. Parameters "suffix_ref1" and "suffix_ref2" (alias "suffix_ref" for both), which are used when forming the names of the files with the data of reference functions No. 1 and No. 2, respectively, have been added. The default value of those two parameters is an empty string.
4. The aliases "name_ref1" and "name_ref2" have been removed.
5. Parameter "relErr_tol" is no longer allowed to be negative or zero, or greater than 0.01.
6. The user manual has been updated.

1.5.2.1 (2020-11-17):

1. Added a new parameter “nd_DCS”, which replaces negative values of parameter “nd_F”. Consequently, the precision level used for calculation of the analytical expression of the DCS in the case of the screened Born approximation can now be specified independently of the precision level used for calculation of the atomic form factor (AFF).
2. The default value of parameter “nd_F” (which indicates the precision level of the AFF) has been reduced from 200 to 38. Since the latter value corresponds to quadruple precision arithmetic (whereas the former value corresponds to multiple precision arithmetic), the time of calculation of the screened DDCS and SDCS by adaptive numerical integration of the analytical TDCS has been reduced by a factor of 3 to 20.
3. The maximum number of integrand function evaluations during the adaptive numerical integration of the analytical TDCS has been reduced by a factor of 100.
4. If an error occurs during the adaptive numerical integration of the analytical TDCS when calculating the reference DCS at the start of stage 3, the current run of BREMS is not terminated any more. Instead, a warning is displayed and the corresponding reference DCS is not used during the further processing.
5. The user manual has been updated.

1.5.2.2 (2020-11-26):

1. Fixed a bug causing an offset of 0.5 in the value of κ_{max} used in the fitting equation when the partial-wave interpolation method is not applied and parameter “avg_period_min_(D)CS” is not specified explicitly.
2. Fixed a bug causing the program to use the original partial-wave DCS instead of its moving average, when the partial-wave interpolation method is not applied and parameter “avg_period_min_DCS” is not specified explicitly.
3. Fixed a bug causing an infinite loop in stage 3 when the κ_{max}-fitting fails both with the angular spline fitting of the partial-wave DCS and without it.

1.5.2.3 (2020-11-27):

1. The initial value of d for the simplex optimization in stage 3 has been reduced from 1 to $e^{-10} \approx 4.5 \cdot 10^{-5}$.
2. The default value of parameters “tol_corr_CS” and “tol_corr_DCS” has been increased from 0.001 to 0.005.
3. The accuracy of the multiple linear regression (performed for the angular spline fitting in stage 3 and for the approximation of an arbitrary screening function by a linear combination of exponentials) has been slightly improved.

1.5.2.4 (2020-12-01):

1. Fixed a bug which caused using the reference function equal to 1 for all combinations of the spline argument type and the logarithm option, excluding the combination of those two parameters corresponding to the first successful angular spline fitting of the original partial-wave DCS or of the κ_{max}-fitted DCS for each type of the reference function requested.
2. Fixed a bug causing the angular spline extrapolation of the κ_{max}-fitted DCS after specifying the option “splineExt_fitted=0” (which must suppress the mentioned extrapolation).

1.5.3.0 (2020-12-03):

1. In the case of $-\cos\theta$ as the spline argument, the first- and second- degree angular polynomial fitting is now allowed, if the current number of knots is equal to the minimum possible value (two). This option is controlled by parameters “minDeg_cos” and “maxDeg_cos” in the case of the angular fitting of the original partial-wave (PW) DCS, or by parameters “minDeg_cos_fitted” and “maxDeg_cos_fitted” in the case of the angular spline fitting of the κ_{max}-fitted DCS. If the first- or second-degree polynomial has been selected as the optimal case, then this is indicated in the output files by the number of knots equal to 0 or 1, respectively. Absence of the polynomial or spline fitting is now indicated by the number of knots equal to −1 (not by 0 as previously).
2. The default value of parameter “splineArg_fitted2” has been increased from 1 to 2.

3. If the κ_{max}-fitting is successful in cycle 1, but fails in cycle 2 (with the number of points greater by a factor of 2 than in cycle 1), then the result corresponding to cycle 1 is accepted (in the previous versions of BREMS, the current "shift" was in such a case excluded from the further analysis).
4. During the κ_{max} fitting after the angular spline fitting of the original PW DCS, the moving average interval is no longer fixed, if its initial value is equal to 1 (in the previous versions of BREMS, the angular spline fitting of the PW DCS always precluded the possibility to increase the moving average interval after a failure of the subsequent κ_{max} fitting).
5. Fixed the bug causing the data in the files "CS_parms.txt" and "DCS_parms_..." to correspond to a "shift" different from shift 0.
6. The user manual has been updated.

1.5.3.1 (2020-12-06):

1. The basis functions of the linear regression when the fitting function is a linear or quadratic polynomial of $-\cos\theta$ have been redefined so that two coefficients of the linear regression have the meaning of the values of the approximating polynomial at the two endpoints, and the third coefficient (in the case of the quadratic polynomial) has the meaning of the first derivative at the first endpoint. This makes the estimates of the uncertainties of the approximate values at the data points (and hence the values of the objective function, which is minimized during the optimization of the endpoint positions) obtained in the case of linear or quadratic polynomial fitting more comparable with those obtained in the case of cubic spline fitting.
2. The initial values of parameter d (the constant term in the stretching exponent used to approximate the dependence of (D)CS on κ_{max}) for the different attempts of the simplex optimization procedure are now equidistant on the logarithmic scale and range from $\exp(-10)$ to 1 (in the previous versions of BREMS, they were quasi-random).
3. The initial value of parameter h (the slope coefficient of the stretching exponent used to approximate the dependence of (D)CS on κ_{max}) for the different attempts of the simplex optimization procedure is now fixed and equal to 10^{-10} (in the previous versions of BREMS, a set of quasi-random initial values of h was used).
4. The user manual has been updated.

1.5.3.2 (2020-12-07):

1. During the angular spline fitting of the κ_{max}-fitted DCS, when choosing between the reference functions No. 1 and 3 or between No. 2 and No. 3 on the basis of their similarity to the κ_{max}-fitted DCS, the standard deviation of the relative difference is used (in the previous versions of BREMS, the average absolute value of the relative difference was used). In the case of default values of the control parameters, this change usually makes the choice of the reference function No. 1 (corresponding to the Born approximation by default) more likely (and the choice of the reference function No. 3 less likely) than in the previous versions of BREMS.
2. In the case of constant stretching exponent in the fitting function used to approximate the dependence of CS or DCS on κ_{max} (i.e., when parameter h is equal to 0), the initial value of parameter d is now equal to $\exp(-5) \approx 0.0067$ (instead of 1).

1.5.3.3 (2020-12-30):

1. Fixed a bug causing incorrect behavior of the program when splineIntRatio_min_fitted[1,2] = = splineIntRatio_max_fitted[1,2].
2. If parameter "split_n" or "split_a" is non-zero, it is no longer possible to load the S integral data from files.

1.5.4.0 (2021-01-13):

1. Added a new method of κ_{max}-fitting, which is the polynomial regression with the argument of the polynomial defined as $x = \exp(-a\kappa_{max}^{d})$, where $d = 0.5$, and a is determined by least squares. The polynomial approximation is by default applied only when the relative correction of the (D)CS by the stretched exponential approximation (with $h = 0$) is positive and greater than 0.2. The mentioned threshold value of the relative correction is controlled by the new parameters "polyn_thr_CS" and "polyn_DCS" (alias "polyn_thr" for both). The maximum degree of the polynomial is by default equal to 6 when fitting the CS, and 4 when fitting the DCS. It is controlled by the new parameters "maxDeg_CS" and "maxDeg_DCS" (alias "maxDeg" for both).
2. Parameter h (the slope coefficient of the stretching exponent) during the κ_{max}-fitting is now by default allowed to be non-zero only when fitting the dependence of CS on κ_{max}. In addition, the number of fitting attempts with h among the varied parameters has been reduced by a factor of 5. When fitting the DCS, $h = 0$. Those changes, in conjunction with the mentioned polynomial fitting, allow to improve the performance during the κ_{max}-fitting in stage 3, while achieving a similar or better fitting accuracy as with the previous version of BREMS (especially in the case of large positive corrections of the CS or DCS).
3. Added parameters "simple_exp_CS" and "simple_exp_DCS" (alias "simple_exp" for both), which indicate that the dependence of (D)CS on κ_{max} may be approximated by a simple exponential (which is a special case of the stretched exponential, with the stretching exponent equal to 1). This option is applied either in the region of increase with κ_{max} (simple_exp=1), or in the region of decrease with κ_{max} (simple_exp=2), or both (simple_exp=3), if the reduced sum of squared residuals corresponding to the simple exponential approximation does not exceed the reduced sum of squared residuals corresponding to the stretched exponential approximation by a predefined fraction, which is specified using the new parameters "simple_exp_thr_CS" and "simple_exp_thr_DCS" (alias "simple_exp_thr" for both).
4. The terms of the objective function (OF), which is minimized during optimization of the angular spline-fitting parameters, are no longer allowed to have arbitrary weights. The weights can now be equal only to 1 or 0 (i.e., a term is either included or not).
5. Added parameters "splineUnc_wt_fitted" and "splineRes_wt_fitted", which allow to define the OF used during the angular spline fitting of the κ_{max}-fitted DCS independently of the OF used during the angular spline fitting of the original partial-wave DCS ("PW DCS"). The default values of those parameters are the same as those of "splineUnc_wt" and "splineRes_wt", i.e., 1 and 0, respectively.
6. Added parameters "nSplineKnots_max" and "nSplineKnots_max_fitted" (alias "n_spl_knots_max" for both), which can be used to impose an additional limitation on the maximum number of spline knots during the angular spline fitting of the PW DCS or κ_{max}-fitted DCS, respectively. The default value of those parameters is 62, which is equivalent to absence of the additional limitation (because the minimum allowed value of parameters "splineInt_min" and "splineInt_min_fitted" is 3, corresponding to 61 knots).
7. Added parameters "geomAvg" and "geomAvg_fitted" (alias "geom_avg" for both), indicating whether the OF must be defined as the arithmetic average ("geomAvg=0") or as the geometric average ("geomAvg=1"). This parameter has no effect if only one type of relative deviation is used in the definition of the OF. The default value of those parameters is equal to 1 (indicating geometric average).
8. Added parameters "mainDevType" and "mainDevType_fitted" (alias "main_dev_type" for both) indicating the type of relative deviation that must determine the value of the OF when two or more types of relative deviation are included in the definition of the OF. Since the value of the arithmetic average is determined by the largest of the terms used to calculate it, the values of all other terms (corresponding to the other types of relative deviation) are set equal to the value of the "main" relative deviation if they are greater than it and the option "geomAvg[_fitted]=0" is used. Since the value of the geometric average is determined by the smallest of the factors used to calculate it, the values of all other factors (corresponding to the other types of relative deviation) are set equal to the value of the "main" relative deviation if they are less than it and the option "geomAvg[_fitted]=1" is used. When mainDevType[_fitted]=0, all included types of relative deviation are treated equally when calculating the OF. This parameter is ignored when only one type of relative deviation is used in the definition of the OF (for example, in the case of the default definition of the OF). The allowed values of parameter "mainDevType_fitted" are all integer numbers from 0 to 5, with the positive values corresponding to the relative deviations δ_{diff}, δ_{unc}, δ_{res}, δ_{CS}, and δ_{SF} (in the same order). The allowed values of parameter "mainDevType" are the same, excluding the values 1 and 5. The default value of those parameters is 2.

9. When calculating the rms value of the relative uncertainty (needed for calculation of the OF during the angular spline fitting of the DCS), the points belonging to the small-angle range $0° \le \theta < \theta_{min}$ are no longer taken into account (because they are irrelevant for the large-angle extrapolation, which is the main purpose of the angular spline fitting).
10. Added an option to determine spline knots on the basis of the second derivative (curvature) of the dependence of the DCS on the angle θ. This option is activated by specifying a negative value of parameter splineIntRatio_min1 in the case of the angular spline fitting of the original PW DCS, or of parameter splineIntRatio_min_fitted1 in the case of the angular spline fitting of the κ_{max}-fitted DCS. If splineIntRatio_min[_fitted]1<0, then a larger absolute value of the second derivative corresponds to a larger knot density (smaller inter-knot intervals). This provides a unique value of each knot, so that no iterative optimization is needed. The knots are found in this case by projecting uniformly spaced points onto a density function, which is proportional to the cumulative integral of the square root of the absolute value of the second derivative of the spline-smoothed DCS. The absolute value of splineIntRatio_min[_fitted]1 is interpreted in this case as the minimum number of points inside one inter-knot interval to be used for the mentioned spline smoothing of the DCS (which is needed for construction of the mentioned density function).
11. The default method of constructing the angular spline-fitting interval of the PW DCS has been modified: now its starting point θ_{min} (parameter "spline_theta_min") is fixed at 10° by default, whereas the endpoint θ_{max} is selected from a set of six equidistant values (in increments of 2°), with the maximum value determined as in the previous versions (on the basis of the magnitude of the large-angle distortion of the PW DCS).
12. When parameters "splineExt" and "splineExt_fitted" are non-zero, the maximum value of the large-angle endpoint of the angular spline-fitting interval of the κ_{max}-fitted DCS ("spline_theta_max_fitted2") is automatically reset to the value of θ_{max} used for the angular spline fitting of the PW DCS. The default value of the starting point (parameter "spline_theta_min_fitted") is 10°.
13. The default value of parameter "splineExt_fitted" has been changed from 1 to -1, which means that now the angular spline extrapolation of the κ_{max}-fitted DCS is always performed, i.e., it is not replaced by the spline smoothing in the entire angular range $0° \le \theta \le 180°$, even when the angular dependence of the original κ_{max}-fitted DCS does not have any obvious anomalies (such as an extra minimum at large angles).
14. The default value of parameter "splineArg_fitted1" has been increased from 1 to 2. Since parameter "splineArg_fitted2" is also equal to 2 by default, this means that the angular spline fitting of the κ_{max}-fitted DCS is by default performed using only $-\cos\theta$ as the argument of the spline function.
15. The default value of parameter "spline_combine" has been changed from 1 to 2, which means that now only the average of the κ_{max}-fitted DCS (averaged over all κ_{max}-fitting intervals) is spline-fitted by default (in the previous versions of BREMS, the angular spline fitting was by default performed for each κ_{max}-fitting interval separately, whereupon the spline-fitted DCS was averaged over all κ_{max}-fitting intervals).
16. The user manual has been updated.

1.5.4.1 (2021-01-18):

1. After the simplex optimization using the stretched exponential approximation during the κ_{max}-fitting (with parameters c, d and h varied independently and parameters a and b determined by linear regression), a second simplex optimization has been added, with parameters b, d and h varied independently and parameters c and a determined by linear regression.
2. The calculation procedure of the confidence interval of parameter c in the case of the stretched exponential approximation has been simplified: since it is calculated as the intercept of a linear fit, its confidence interval is now calculated using the formula corresponding to a two-parameter linear model.
3. If the optimal degree of the approximating polynomial during the κ_{max}-fitting is equal to 1 or 2, then the sum of squared residuals corresponding to the polynomial regression is now compared with the sum of squared residuals corresponding to the stretched exponential regressions (with $h = 0$), and the case with the smaller value of the mentioned sum is selected.
4. The user manual has been updated.

1.5.4.2 (2021-01-25):

1. During the κ_{max}-fitting using the stretched exponential approximation, the second simplex optimization (with parameters b, d and h varied independently and parameters c and a determined by linear regression) has been made more accurate: if there are signs of a floating-point overflow when calculating the sum of squared values of the argument of the linear regression, then the program now switches to using logarithms of the sums needed for the linear regression.
2. The criteria for determining the optimal degree of the approximating polynomial during the κ_{max}-fitting have been modified: 1) the requirement for the magnitude of the relative uncertainty of the zero-degree coefficient (c) of the approximating polynomial has been made more stringent: it is not allowed to become both greater than 5 % and greater than the relative uncertainty corresponding to the degree of the polynomial (M) that is the "best" one among the degrees tested up to that point; 2) if the value of M corresponding to the shortest total length of $M + 2$ longest runs of constant sign of the residuals (M') is less than the maximum degree $M = M_{max}$ of all polynomials satisfying the other criteria, then M' is preferred to M_{max} only when the corresponding total lengths of $M' + 2$ and $M_{max} + 2$ longest runs of constant sign of the residuals are less than $0.5N_{fit}$ and greater than $0.7N_{fit}$, respectively, where N_{fit} is the number of values of κ_{max} in the fitting interval.
3. The default value of parameter "maxDeg_DCS" has been increased from 4 to 6.
4. The user manual has been updated.

1.5.4.3 (2021-01-29):

1. When parameter c (the constant term) of the stretched exponential approximation is determined iteratively (by the simplex method), its absolute tolerance is now calculated by multiplying parameter "tol1" by the absolute range of variation of the original CS or DCS inside the fitting interval of κ_{max} (in previous versions of BREMS, the mentioned absolute tolerance was equal to the value of parameter "tol1"). Without this modification, the default value of tol1 (i.e., 10^{-6}) might be too large, because the saturation value of the DCS is sometimes less than 10^{-4}.
2. The user manual has been updated.

1.5.4.4 (2021-01-30):

If the default option "fitRange_DCS=3" (indicating a combination of two κ_{max}-fitting interval widths) is used and a sequence of irrecoverable κ_{max}-fitting errors of type 1 (irregular shape of the original partial-wave DCS) occurs with the second value of fitting interval width (the larger one), then parameter fitRange_DCS is now automatically reset to 1 and the fitting of the DCS is restarted. This means that only one value of the κ_{max}-fitting interval width is used. In previous versions of BREMS, the behavior of the program in such a situation was the same as in the case of a sequence of irrecoverable κ_{max}-fitting errors of type 2 (failure of the κ_{max}-fitting algorithm), i.e., the program used the results corresponding to the narrower fitting interval as the final result for the current "shift", but this choice did not affect the results for the other shifts (i.e., the wider fitting interval could still be used with the other values of the endpoint of the κ_{max}-fitting interval).

1.5.4.5 (2021-02-01):

1. Reference function No. 3 is no longer used if its angular dependence is irregular and either splineRef_fitted1=-1 or splineRef_fitted2=-1.
2. The user manual has been updated.

1.5.5.0 (2021-05-13):

1. A new method of extrapolation of the truncated partial-wave series (PW DCS) to $\kappa_{max} \to \infty$ at electron energies of the order of a few MeV has been implemented. This method is based on the following empirical observation. If the dependence of the PW DCS on κ_{max} at each value of the photon emission angle θ is expressed as $\mathrm{DCS}(\kappa_{max}) = \mathrm{DCS}(K') + \mu\,(\mathrm{DCS}(K) - \mathrm{DCS}(K'))$, where K' and K are constant and $K' \le \kappa_{max} \le K$, then the factor μ is approximately angle-independent in a wide angular interval. If this property of the PW DCS holds up to $\kappa_{max} \to \infty$, then the problem of calculating the exact theoretical DCS (i.e., the PW DCS corresponding to $\kappa_{max} \to \infty$) is reduced to calculation of the angle-independent "scale factor" μ in the following expression: $\mathrm{DCS}_\mu \equiv \mathrm{DCS}(\kappa_{max} \to \infty) = \mathrm{DCS}(K'') + \mu\,(\mathrm{DCS}(K) - \mathrm{DCS}(K''))$, where K is the maximum value of κ_{max} in the data used for the analysis, whereas K' and K'' are (largely arbitrary) "base" values of κ_{max} (in the updated user manual and in the comments in the source code, DCS_μ is called the "μ-corrected DCS"). The scale factor μ in the latter expression is calculated by minimizing the distortions in the angular dependence of DCS_μ (if the PW DCS is a decreasing function of κ_{max}, then those distortions are located at large angles, and if the PW DCS is an increasing function of κ_{max}, then those distortions are located at small angles).
2. 21 user-adjustable parameters related to the new method mentioned above have been added.
3. The naming of the files with the reference function data has been made more flexible by adding one more naming rule (it is specified by setting parameter "auto_naming_ref1" or "auto_naming_ref2" to 2 and using the new parameters "prefix2_ref1" and "prefix2_ref2").
4. The column number in the file with the reference function data can now be specified using parameters "col_ref1" and "col_ref2".
5. It is now possible to specify the accuracy of a reference function loaded from a file independently of the accuracy of the angular integration of an analytical triply differential cross section. The former is controlled by a new parameter "relErr_tol_ref", while the latter is controlled by parameter "relErr_tol".
6. Added parameter "fn_V", which allows specifying an arbitrary name of the file with the interaction potential data (instead of constructing it from the folder name specified by parameter "dir_V" and the atomic number specified by parameter "Z" or "Z_V").
7. Added parameter "j_file", which allows writing values of the spherical Bessel function $j_l(kr)$ used in the integrands of the S integrals to a file, and subsequently loading values of $j_l(kr)$ from this file (instead of calculating them at each step of the numerical integration). This may improve the performance in stage 1 when the S integrals are calculated for different intervals of $|\kappa_1|$ before merging them into a single dataset. This improvement is achieved by eliminating the overhead caused by redundant recalculations of $j_l(kr)$.
8. The default values of several parameters controlling the angular spline fitting and extrapolation of the PW DCS and κ_{max}-fitted DCS have been changed.
9. Several minor bugs have been fixed.
10. The user manual has been updated.

1.5.5.1 (2021-05-31):

1. The default value of parameter "l_step_incr" has been reduced from 8 to 2. This improves the accuracy of interpolated S integrals when the cubic spline interpolation with respect to l is applied, due to the reduction of intervals between adjacent knots of the spline (the calculation time is increased accordingly).
2. Added the option "fitRef_mu[1,2]=3", which indicates that both reference functions must be tried when calculating the dependent variable of the polynomial fit of the μ-corrected DCS, and the reference function corresponding to the smallest deviation of the polynomial fit from the μ-corrected DCS must be used. The default value of parameters "fitRef_mu1" and "fitRef_mu2" has been set equal to 3.
3. The meaning of nine columns in the file "mu_range.txt" has been changed. Those columns previously contained the ratio of the deviations of the DCS from the reference function after applying the μ-correction and before it. Those columns now contain the maximum relative deviations of the μ-corrected DCS from the original partial-wave DCS corresponding to the maximum value of κ_{max} (i.e., $\kappa_{max} = K$).

4. The negative relative deviations in the file “mu_range.txt” are now calculated by interchanging the two values that are being compared, so that the range of possible values of the negative relative deviations is now unlimited from below (previously, the negative relative deviations could not be less than −1).
5. The file “DCS_mu….txt” now contains an additional column “PW_DCS(K")”, which has been inserted between the columns “PW_DCS(K')” and “PW_DCS(K)”.
6. The μ-correction is now by default disabled when the partial-wave DCS is an increasing function of κ_{max} (which is always the case when the photon energy is zero). This has been achieved by setting the default value of parameter “thr_range_mu1” to 181.
7. Fixed a bug that caused a failure to replace the fitted DCS values with the μ-corrected values when the partial-wave DCS is an increasing function of κ_{max} and the μ-correction is enabled (this bug did not affect updating of the files “mu_range.txt” and “DCS_mu_....txt”).
8. The user manual has been updated.

1.5.5.2 (2021-06-29):

1. The code of “S_integrals.f90” has been optimized for the case of high energies of the outgoing electron, when the cubic spline interpolation of S integrals with respect to l (the orbital quantum number of the emitted photon) is applied, and the number of the calculated S integrals is of the order of 10^6. As a result of this optimization, the duration of numerical integration (from 0 to the cutoff radius) in stage 1 has been in some cases reduced by half or more.
2. Added parameters “update_n” and “prefix_suffix_n”, which control an alternative method of processing the available “_n” data files. If parameter “update” is equal to 1 or 2 and there is no request to read the numerical S integral data from pre-existing “_n” or complete files (i.e., if parameter “iSkip” is not equal to ±2 or −3), or if there are no “_n” or complete files at the indicated location, then the program will attempt to load the numerical integrals from the data files with the names defined by prefix-suffix pairs listed in the file whose name is given by parameter “prefix_suffix_n”. The mentioned data files may be either “_n” files or complete files. If some of the required numerical integrals are missing, then only those integrals will be calculated (unlike in the case “iSkip=±2” or “iSkip=-3”, when the data files must contain *all* needed numerical integrals), and the final “_n” and complete files will contain both the loaded numerical integrals and the calculated numerical integrals.
3. Added an option to calculate the spherical Bessel functions $j_l(kr)$, which are used as a factor in the integrands of the S integrals, by the power-series method (in addition to the default method of backward recursion). This option is controlled by two new parameters “Jtest_interval” and “Jtest_period”.
4. Added parameter “nterms_max_J”, which is used to set the maximum degree of the power-series expansion of the spherical Bessel function $j_l(kr)$, which is used in the integrand of the S integrals. This parameter is used only when the mentioned spherical Bessel function is calculated by the power-series method, rather than by backward recursion (see the description of the previous change). The default value of this parameter is 150.
5. The maximum number of significant digits corresponding to quadruple precision has been reduced from 37 to 30.
6. Parameter “output_mu” is now allowed to be equal to −1 (in addition to 1 and 0). The option “output_mu=-1” indicates that only the files “mu_range.txt” and “DCS_mu_....txt” must be updated in stage 3. In such a case, the κ_{max}-fitting is not performed, and parameter “iFit” has no effect.
7. The user manual has been updated.

1.5.5.3 (2021-07-09):

1. The default value of parameter "Jtest_interval" has been changed from 0 to -1 (corresponding to the power-series method, except at the smallest values of the radial coordinate r, where the backward recursion method is always used), because it has been noticed that the estimate of the spherical Bessel function $j_l(kr)$, which is used in the integrands of the S integrals, is subject to large errors when l and kr are sufficiently large and parameter "Jtest_interval" is set equal to 0. This is because in the case of a sufficiently large l an interval of values of kr exists, where neither the backward recursion method nor the evaluation of the closed-form expression of $j_l(kr)$ at quadruple precision (QP) are capable to provide an accurate estimate of $j_l(kr)$ (i.e., the value of kr is too large for the backward recursion method, but too small for the closed-form evaluation at QP). For example, if $l = 960$, then the endpoints of such an interval are of the order of $kr \sim 10^4$.
2. The default value of parameter "j_QP" is now equal to 2 at both values of parameter "accuracy_level", because the backward recursion algorithm is used only at small r by default (see the description of the previous change), so that there is no point to sacrifice precision for time.
3. Eliminated the error message "*** MPROUN: Exponent overflow", which sometimes appeared during the second part of stage 1, i.e., during the integration from the cutoff radius r_0 to ∞, in the case of sufficiently large values of the electron energy and r_0.
4. Corrected the NLO correction term in the analytical expression of the TDCS corresponding to the Sommerfeld-Maue (SM) approximation by removing its "NNLO" part (with an inconsistent power of Z, higher by one than the remaining part of the NLO correction term), because it was shown (A. Mangiarotti et al, Radiat. Phys. Chem., Vol. 167 (2020) art. No. 108292) that inclusion of the NNLO part of the NLO correction term sometimes causes large errors in the values of the SM DDCS at large angles of photon emission.
5. The user manual has been updated.

1.5.5.4 (2021-07-29):

1. Added parameter "mu", which is used to specify an arbitrary fixed positive value of the scale factor μ. When mu<0, it is optimized (as in the previous versions of BREMS), using |mu| as the initial value. A zero value of mu is not allowed. Setting a positive value of mu is allowed only in the case "output_mu=-1". Default value of this parameter is equal to −1.
2. In the case "check=1", Read_S_integrals now displays the maximum absolute difference in addition to the maximum relative difference, along with the corresponding values of κ_1, κ_2, and l.
3. If interpolation of S integrals with respect to l has been requested, but the errors cannot be estimated (due to absence of the "test" integrals in the available data), then the error estimates of the interpolated values of S integrals, which are displayed by Read_S_integrals, are now equal to -1 (previously, they were equal to 0, which made it impossible to differentiate between the interpolated and non-interpolated S integrals in the data displayed by Read_S_integrals).
4. Fixed a bug in Bremsstrahlung.f90, which caused an access violation at the beginning of stage 2 when the following three conditions were satisfied simultaneously: (a) parameter k12ratio is greater than 1, (b) the maximum value of $|\kappa_2|$ (parameter Kmax2) is automatically reduced to $\max|\kappa_1|$ / k12ratio, (c) the interpolation with respect to $|\kappa_2|$ is not applied, although it would be applied by default using the original value of Kmax2.

1.5.5.5 (2021-08-04):

1. The rules for calculating the default value of parameter "Kmax2", when $T_1 > 100$ keV, have been modified. When $T_1 > 100$ keV, the default value of parameter "k12ratio" (which is defined as $\max(|\kappa_1|) / \max(|\kappa_2|)$) is now typically equal to the integer part of p_1 / p_2 (i.e., the ratio of the initial and final momenta of the electron), if either Kmax1 or Kmax2 is not specified by the user. This change causes a reduction of the default value of Kmax2 when $p_2 / p_1 \leq 0.5$.
2. The five auxiliary $V(r)$ data files ("FitData.txt", "FitData_lo.txt", "FitData_all.txt", "r_spline.txt", "TaylorCoefs.txt") have been moved into subfolder "V/Kohn-Sham/". The name of the folder containing

four of those files (excluding "FitData_all.txt", which is not used by BREMS) can now be specified using the new parameter "dirV_aux".

3. Parameter "dir_V" has been renamed to "dirV", and alias "dir_V" has been added for parameters "dirV" and "dirV_aux". In addition, the meaning of parameter "dirV" has been extended by allowing it to contain not only the folder name, but also an arbitrary initial part of the file name (the same applies to parameter "dirV_aux").
4. The user manual has been updated.

1.5.5.6 (2021-08-19):

1. Calculation of the coefficients of the closed-form expressions of spherical Bessel functions (which is done at the start of stage 1) has been shortened by a factor of up to 4 (by determining the prime factors of the factorials used in the expressions of those coefficients).
2. The multiple precision values of the Bessel functions are no longer recalculated at the end of the "test integration" in stage 1 (instead, their values calculated at the end of the initial integration are used). This change may cause a significant reduction of the duration of stage 1 in the case of large values of κ_1, κ_2 and l.
3. Some two-dimensional arrays, which are represented as symmetric square matrices, have been converted to one-dimensional arrays, causing a reduction of the maximum memory used in stage 1.

1.5.5.7 (2021-08-29):

1. The multiple-precision (MP) values of the spherical Bessel functions $j_{n1}(p_1R_a)$, $y_{n1}(p_1R_a)$, $j_{n2}(p_2R_a)$, $y_{n2}(p_2R_a)$ (for estimation of the final phase shifts and normalization factors at the cutoff radius $r = R_a$) are now calculated using forward recursion at the precision level of 5000 digits. This method is significantly faster than the evaluation of the exact closed-form expressions of the spherical Bessel functions at the same precision level, which was implemented in previous versions of BREMS. Accordingly, the MP calculation of the coefficients of spherical Bessel functions has been moved to the beginning of the subroutine S_int (where the mentioned coefficients are needed in order to perform the integration from r_0 to ∞).
2. The evaluation of the closed-form expressions of the spherical Bessel functions $j_n(pr)$ and $y_n(pr)$ (for estimation of the intermediate phase shifts and normalization factors in the radial range where the wave functions have not attained the asymptotic form yet) has been replaced with forward recursion using quadruple precision (or backward recursion using quadruple precision in the case of $j_n(pr)$, if $pr \le \max(n)$). The calculation of the spherical Bessel function $j_l(kr)$, which is used as a factor in the integrands of the S integrals, has been similarly modified (except when the default method of calculation of $j_l(kr)$, which does not involve recursion, is applied). The definition of parameter "j_QP" has been modified accordingly.
3. The "primary" phase shift (calculated by the subroutine "A_delta"), which is further denoted by δ'_κ, is equal to $\bar{\delta}_\kappa$ when $\kappa > 0$, and equal to $\bar{\delta}_\kappa - \pi/2$ when $\kappa < 0$ (equivalently, equal to δ_κ when κ is positive or even, and equal to $\delta_\kappa + \pi$ when κ is negative and odd). $\bar{\delta}_\kappa$ is calculated from δ'_κ. δ'_κ is used instead of $\bar{\delta}_\kappa$ for calculation of "delta_range". When $\kappa < 0$, δ'_κ is displayed along with $\bar{\delta}_\kappa$. Read_S_integrals.exe now displays values of δ'_κ in an additional column "delta'". δ'_κ is written to the S integral data files instead of $\bar{\delta}_\kappa$.
4. Multiple "in=" directives (i.e., multiple parameter files) are now allowed (both on the command line and in the parameter files).
5. Fixed a bug causing infinities in the file "mu_range.txt" in the case of a μ-fitting failure.
6. The user manual has been updated.

1.5.5.8 (2021-10-06):

1. Added parameter "r0_Kmax_p_min", which is the minimum allowed value of the ratio r_0 / max($|\kappa_{1\max}|/p_1$,$|\kappa_{2\max}|/p_2$), where r_0 is the cutoff radius of the potential function. This parameter has been added in order to ensure numerical stability of the forward recursion used for calculating the values of the spherical Bessel functions corresponding to the argument value $p_1 r_0$ and $p_2 r_0$ (because calculation of $j_n(z)$ with $n > 0$ may be subject to numerical instability if $z < n$). If r_0 is not specified explicitly (using parameter "R_atom"), but is calculated from other parameters, and if the calculated value of r_0 is less than $r_{0\min}$ = r0_Kmax_p_min · max($|\kappa_{2\max}|/p_1$,$|\kappa_{1\max}|/p_2$), then the calculated value of r_0 will be replaced with $r_{0\min}$. The default value of this parameter is equal to 1.1.
2. Added parameter "tol_V", which is the maximum allowed value of the screening function at the cutoff radius $r = r_0$. The corresponding value of the radial coordinate is the minimum allowed value of the cutoff radius of the potential function ($r_{0\min}$). If r_0 is not specified explicitly (using parameter "R_atom"), but is calculated from other parameters, and if the calculated value of r_0 is less than $r_{0\min}$, then the calculated value of r_0 will be replaced with $r_{0\min}$. By default, this parameter is equal to 10^{-10} in the case of zero photon energy, and to 1 in the case of non-zero photon energy (the latter value is equivalent to absence of any constraints, because the corresponding radial coordinate is equal to 0).
3. Fixed a bug that in some cases caused a crash of the program with an error message about "access violation" during the integration from the cutoff radius r_0 to ∞ with a non-default value of parameter Kmin1 or Kmin2 (i.e., when Kmin1 > 1 or Kmin2 > 1).
4. Fixed a bug that caused sub-optimal spline fitting of the angular dependence of the partial-wave DCS or of the $\kappa_{\max}$-fitted DCS when the set of inter-knot intervals was required to form a geometric progression, i.e., when only one of the two parameters ε_1 and ε_2 controlling the knot density was used (for example, by setting parameter "n_splineIntRatio2" or "n_splineIntRatio_fitted2" to zero).
5. The default value of parameter "maxRelErr" has been increased from 0.01 to 0.02.
6. The user manual has been updated.

1.5.5.9 (2021-11-05):

1. Fixed two bugs in the files "Brems_fit.f90" and "Born_SM_appr.f90", which caused runtime errors at the start of stage 3 when using the Linux version of BREMS.
2. Corrected the sample Linux bash script "Linux_executables/Brems_79_100keV_KS.sh".

1.5.6.0 (2022-04-30):

1. A new "special" mode of operation has been implemented: cubic spline fitting and interpolation of the logarithm of the scaled single differential cross section (CS) with respect to the logarithm of the kinetic energy of the incident electron (T_1) for a given atomic number Z and for a fixed value of the ratio k / T_1, where k is the energy of the bremsstrahlung photon, as well as creating the input "grid" data files used for the mentioned spline fitting, which contain values of CS and their uncertainties on a two-dimensional grid defined by a set of values of T_1 and k / T_1. The name of the corresponding subroutine is "Brems_CS_interp". Its source code is in the file "Brems_CS_interp.f90". This mode of operation is controlled by 46 new parameters, and it is turned on or off using parameter "CS_int", which is also used to specify the extent of the calculations in this mode of operation, and to indicate if a successful spline fitting and interpolation must be followed by a "normal" run of BREMS, using the interpolated value of the CS instead of parameter "CS_ref_spline" (this is another new parameter, which is described below).
2. The new subfolder "CS_int" of the distribution package of BREMS contains 100 ASCII files with the spline-fitting grid data, which were created using the option "CS_int=1" (see above) for each value of the atomic number Z from 1 to 100. The range of values of k / T_1 in those files is from 0 to 0.95 (the values from 0 to 0.9 are equidistant, with the increment equal to 0.1), whereas the range of values of T_1 is from 0.1 MeV to 300 MeV (for $k > 0$), or from 0.1 MeV to 100 MeV (for $k = 0$). In the case of non-zero photon energy, the values of the CS were calculated by the partial-wave method at $T_1 \leq 30$ MeV, and by applying the Sommerfeld-Maue (SM) approximation with the next-to-leading order (NLO) correction and the screening correction at $T_1 \geq 50$ MeV. In the case of zero photon energy, all values of the CS in those files were calculated as a weighted integral of the differential cross section of electron elastic

scattering with respect to the electron's scattering angle (if the photon energy is equal to zero, then this method is more efficient then the one implemented in BREMS).

3. Added parameter "CS_ref_spline". If it is positive, then the default value of parameter "splineCS_wt_fitted" is changed from 0 to 1, and the value of CS_ref_spline is used as the "reference CS" for calculation of the additional term in the definition of the objective function (the mentioned term is the rms relative difference between the reference CS and the angular integral of the spline fit of the κ_{max}-fitted DCS). If CS_ref_spline=0 and splineCS_wt_fitted=1 and $T_1 \le$ T1_CS_mode_thr, then CS_ref_spline will be assigned the default value, which is equal to the saturation value of CS as a function of κ_{max} obtained by nonlinear least squares fitting. If splineCS_wt_fitted=0, then CS_ref_spline is not used (in such a case, CS_ref_spline is reset to zero). The value of CS_ref_spline is written to the file "CS_fitted.txt" in a new column with the header "CS_ref_spline" (it has been inserted between the columns "CS_MA[kmax]" and "CS_fitted[k->Inf]"). When $T_1 >$ T1_CS_mode_thr and CS_ref_spline > 0 and splineCS_wt_fitted = 1, the default values of two other parameters are modified, too: the default value of parameter "splineExt_fitted" is changed from -2 to -1, and the default value of parameter "mainDevType_fitted" is changed from 2 to 4. It is also possible to replace CS_ref_spline with the interpolated value returned by subroutine Brems_CS_interp. This is achieved by setting parameter "CS_int" to a value greater than 1. If the mentioned interpolated value of the CS is sufficiently accurate, then the accuracy of the final κ_{max}-fitted DCS may be improved, especially at small angles, which determine the value of the CS when the angular distribution of bremsstrahlung photons is strongly peaked in the forward direction (in such a case, the relative corrections of the DCS due to the κ_{max} fitting at small angles are typically very large, hence the final κ_{max}-fitted DCS may be too inaccurate if the additional information supplied by the value of the CS is not used).
4. Added a group of parameters intended to improve flexibility and accuracy of the "μ-correction". Those parameters are "mode_mu", "maxCorr_mu", "thrCorr_mu", "maxDev_mu", "fitEndOffset_mu_min", "fitEndOffset_mu_max", "n_fitEndOffset_mu", "fitDegree_mu_min2", fitDegree_mu_max2". Parameter "**mode_mu**" (which is equal to 3 by default) is used to specify the method of determining the optimal value of the scale factor μ for each "shift": **(a)** if mode_mu=1, then the values of μ for each shift are optimized by minimizing the deviation of the μ-corrected DCS from the fitting polynomial in the extrapolation range, whereas the degree of the fitting polynomial (fitDegree_mu) and the type of the "reference function" used for the mentioned fitting (fitRef_mu_opt) are the same for all shifts and determined at the start of stage 3 by minimizing the standard deviation of the μ-corrected DCS over different values of the endpoint of the fitting interval, defined in terms of its offset from the first irregularity of the μ-corrected DCS (fitEndOffset_mu), or by minimizing the distortion of the μ-corrected DCS in the extrapolation interval (if only one value of fitEndOffset_mu is used); **(b)** if mode_mu=2, then fitDegree_mu and fitRef_mu_opt are determined at the start of stage 3 (as in the case mode_mu=1), but the values of μ for each shift are determined by averaging the scale ratio $\mu = (\mathrm{DCS}(\kappa_{max}\to\infty, \theta) - \mathrm{DCS}(K', \theta)) \,/\, (\mathrm{DCS}(K, \theta) - \mathrm{DCS}(K', \theta))$ inside the angular interval where the absolute value of the relative correction of the PW DCS due to the κ_{max}-fitting is between the values defined by parameters "maxCorr_mu" and "thrCorr_mu", whose default values are 0.01 and 0.001, respectively, if the maximum absolute deviation of the mentioned scale ratio from its average value inside the mentioned angular interval is less than the value defined by parameter "**maxDev_mu**" (its default value is 0.01). In this case, the polynomial fitting is performed only once for each value of fitEndOffset_mu, in order to calculate the extrapolated μ-corrected DCS corresponding to the mentioned value of μ. If no such angular interval exists, or if its width is less than 20°, or if the number if data points inside this interval is less than 20, then μ is optimized as in the case mode_mu=1 (i.e., the case mode_mu=2 then becomes equivalent to the case mode_mu=1); **(c)** if mode_mu=3, then the values of μ for each shift are determined as in the case mode_mu=2, whereas fitDegree_mu and fitRef_mu_opt are determined for each shift separately by minimizing the standard deviation over different values of fitEndOffset_mu, or the distortion of the μ-corrected DCS in the extrapolation interval (using the previously-determined fixed value of μ). In order to minimize the standard deviation of the μ-corrected DCS over different values of the endpoint of the fitting interval (fitEndOffset_mu), several equidistant values of fitEndOffset_mu are tested. The endpoints of the range of fitEndOffset_mu to be tested are defined by parameters "**fitEndOffset_mu_min**" and "**fitEndOffset_mu_max**" (their default values are 20 and 40, respectively), and the number of values of fitEndOffset_mu is specified using parameter "**n_fitEndOffset_mu**" (its default value is 21). The optimization of the degree of the fitting polynomial

(fitDegree_mu) is performed by testing several values – from the minimum degree defined by parameter "**fitDegree_mu_min2**" (default value 1) to the maximum degree defined by parameter "**fitDegree_mu_max2**" (default value 20) – and selecting the one that corresponds to the least sensitivity of the values of the fitting polynomial in the fitting and extrapolation intervals to the choice of the value of fitEndOffset_mu. The number "2" at the end of the names of the latter two parameters indicates that they must be used only when the PW DCS is a decreasing function of κ_{max}. Otherwise, parameters "**fitDegree_mu_min1**" and "**fitDegree_mu_max1**" are used. However, they are not allowed to be different from each other. I.e., when the PW DCS is an increasing function of κ_{max}, only one value of fitDegree_mu is allowed (it may be specified using the alias "fitDegree_mu1", and it is equal to 3 by default).

5. The maximum allowed value of $\max|\kappa_1|$ or $\max|\kappa_2|$ (parameter Kmax1 or Kmax2, respectively) has been increased from 500 to 999, but the sum $\max|\kappa_1| + \max|\kappa_2|$ cannot be greater than 1000. By default, this modification is applied only in the case $T_1 > 10$ MeV and $T_2 / T_1 \leq 0.03$ (i.e., near the tip of the photon spectrum). In other cases, the default value of Kmax1 is smaller (if $T_1 \leq 10$ MeV, then the previous default values of Kmax1 and Kmax2 are used). This may be overridden by the user, if values of $|\kappa_1|$ or $|\kappa_2|$ greater than 500 are needed.
6. Added parameter "T1_Kmax_mode_thr", which is the threshold value of the kinetic energy of the incident electron T_1 (in MeV) that must be exceeded in order to change the method of calculating the default limiting values of $\max|\kappa_1|$, $\max|\kappa_2|$ and $\max(l)$ in the case of non-zero energy of the photon (k). When $T_1 >$ T1_Kmax_mode_thr and $k \neq 0$, the sum in the expression of the "R factors" (defined by Eq. (1.1.10) of the User Manual) is not truncated by default (i.e., all allowed values of l are used), and the choice of the default values of $\max|\kappa_1|$ and $\max|\kappa_2|$ is based on proximity to the tip of the photon energy spectrum. If $T_1 >$ T1_Kmax_mode_thr and $T_2 / T_1 > 0.03$ (far from the tip), then $\max|\kappa_1|$ and $\max|\kappa_2|$ are chosen so that $\max(|\kappa_1|,|\kappa_2|) \leq 500$, $\max|\kappa_2| \geq 50$, and $\max(l)$ is between 500 and 800. If $T_1 >$ T1_Kmax_mode_thr and $T_2 / T_1 \leq 0.03$ (close to the tip), then $\max|\kappa_1|$ and $\max|\kappa_2|$ are chosen so that $\max|\kappa_1| \geq 500$, $\max|\kappa_2| \geq 30$, and $\max|\kappa_1| + \max|\kappa_2| \leq 1000$. The default value of parameter "T1_Kmax_mode_thr" is equal to 10. The mentioned threshold value of T_2 / T_1 is specified by another new parameter "tip_thr" (see below).
7. Added parameter "tip_thr", which is the threshold value of the ratio T_2 / T_1 that is used to determine if the photon energy is sufficiently close to the tip of the spectrum in order to apply the additional modification of the default values of $\max|\kappa_1|$ and $\max|\kappa_2|$ (see also the description of parameter "T1_Kmax_mode_thr" above). The default value of parameter "tip_thr" is equal to 0.03.
8. Added parameter "T1_CS_mode_thr", which is the threshold value of the kinetic energy of the incident electron T_1 (in MeV) that must be exceeded in order to change the role assigned to the κ_{max}-fitted CS (as compared to the role of the angular integral of the κ_{max}-fitted DCS) when the photon energy is non-zero. At large values of T_2 and non-zero photon energy, the κ_{max} fitting of the CS is not performed, and the final value of the CS is set equal to $\int \mathrm{DCS} d\Omega$, i.e., the angular integral of the final κ_{max}-fitted DCS (at lower energies or in the case of zero photon energy, the final estimate of the CS is the arithmetic average of the κ_{max}-fitted CS and $\int \mathrm{DCS} d\Omega$). The default value of this parameter is equal to 10.
9. The Wigner 3j coefficients with $l_2 + l_1 + l$ equal to an odd number are no longer calculated or stored in the 3j data files, because those coefficients are not used in the expressions of the bremsstrahlung cross sections. As a result, the size of the 3j data files has been reduced approximately by half.
10. The subroutines F3J_QP and F3J_MP, which were previously used to calculate the Wigner 3j coefficients using the extended-precision arithmetic with a fixed number of significant digits (30, 100, or 200), have been replaced by the subroutine F3J_QP_MP, which chooses the optimal precision level dynamically: this choice is based on the degree of cancellation of the terms of the Racah formula. The improvement of accuracy caused by this modification is significant only in the range $81 \leq \max(l_1, l_2) \leq 160$, where the previous versions of BREMS used exclusively quadruple-precision arithmetic (approximately 30 significant digits). The 3j coefficients that are significantly affected by this modification are typically the smallest ones, and their role in the calculation of bremsstrahlung cross sections is negligible.
11. Added an option to update the Wigner 3j coefficients stored in old data files (created by a version of BREMS older than v1.5.6.0). This option is controlled by the new parameters "update_3j_start" and

"update_3j_end". If the program detects an old format of the files with the 3j coefficients corresponding to values of $\max(l_1, l_2)$ in the range update_3j_start $\le \max(l_1, l_2) \le$ update_3j_end, then those 3j coefficients will be recalculated, and the corresponding data files will be recreated. The remaining 3j coefficients will not be recalculated, whereas the corresponding files may be modified or not, depending on another new parameter "update_3j_format" (see below). Default values: update_3j_start=81, update_3j_end=160.

12. Added parameter "update_3j_format", which indicates that the format of the Wigner 3j data files corresponding to the values of $\max(l_1, l_2)$ that are either less than update_3j_start or greater than update_3j_end files must be updated, i.e., the redundant 3j coefficients (which are not needed for the calculation of the bremsstrahlung cross sections) must be removed (causing a decrease of the file size approximately by half). Default value: update_3j_format=0 (i.e., the 3j data files created by a version of BREMS older than v1.5.6.0 are not modified by default).
13. Added a new mode of operation: generation of the files with values of the Wigner 3j coefficients. This mode is turned on by setting the switch "only_3j" to 1. The range of files to be created is defined using parameters "start_3j" and "end_3j". The only parameters used in this mode are those that are relevant to calculation of the Wigner 3j coefficients (those are the parameters whose names contain characters "3j"). The default value of parameter "only_3j" is equal to zero.
14. Added parameters "start_3j" and "end_3j", which are used in conjunction with the new option "only_3j=1" (see above). Those two parameters define the endpoints of the range of $\max(l_1, l_2)$ corresponding to the 3j data files that must be created or updated to the latest format. The default values of those two parameters are equal to 81 and 950, respectively.
15. During the angular spline fitting of the $\kappa_{\max}$-fitted DCS, the second knot-density parameter (ε_2) is by default not used (i.e., the inter-knot intervals form a geometric progression by default), and $\lg(\varepsilon_1)$ is by default varied from −10 to +10 in steps of 1, for a total of 21 test values.
16. The default value of parameter "splineInt_min_fitted" has been reduced from 50 to 10.
17. Added parameter "show_CPU_time", which is a "switch" (1 or 0), indicating whether the displayed execution times must have the meaning of the elapsed CPU time (as in the previous versions of BREMS), or the actual time. The default value of this parameter is equal to 0 (i.e., the actual time is displayed by default). ***Note***: If the screen output of the program has been paused (e.g., by pressing the "Pause" key or by selecting the context menu command "Edit/Mark" in the console window on Windows), then the duration of the paused state of the program is not included in the time displayed after resuming execution of the program, regardless of the value of parameter "show_CPU_time".
18. If the μ fitting is applied and the DCS is a decreasing function of $\kappa_{\max}$, then the default endpoints of the spline-fitting interval ($\theta_{\min}$ and $\theta_{\max}$) to be used for fitting the $\kappa_{\max}$-fitted DCS have been modified as follows: $\theta_{\min}$ is assigned six equidistant values from 0 to the starting point of the interval of constant scale factor μ (parameter "start_angle_mu"), and $\theta_{\max}$ is equal to 180°.
19. Parameter splineExt_fitted is now allowed to be equal to ±2. Those values indicate that the spline extrapolation to small angles must not be performed when the starting angle for the spline fitting of the $\kappa_{\max}$-fitted DCS is greater than 0. If splineExt_fitted is equal to ±1, then the small-angle extrapolation is performed. The default value of splineExt_fitted is equal to -2, i.e., the small-angle extrapolation is not performed by default.
20. The default value of k12ratio has been slightly modified: if $1 < \kappa_{1\max} / \kappa_{2\max} < 2$, then k12ratio is set equal to the *nearest* integer (instead of rounding down to 1).
21. Added parameter "T2_thr_mu" indicating the threshold value of the outgoing electron energy (in MeV), which must be exceeded in order to apply the "μ-correction" by default in stage 3. The default value of this parameter is 0.1 (i.e., the μ-correction will not be applied if $T_2 \le 0.1$ MeV, unless the user specifically requests it).
22. Added parameter "verbosity", which controls output of messages about irrecoverable $\kappa_{\max}$-fitting errors in stage 3. Allowed values: 0 – no messages about irrecoverable $\kappa_{\max}$-fitting errors, except after exceeding the maximum allowed number of such errors, 1 – only messages about irrecoverable kmax-fitting errors that occur at $\theta <$ 0.5 * (180° + |spline_theta_max_thr|), 2 – messages about all irrecoverable $\kappa_{\max}$-fitting errors. The default value of this parameter is equal to 0.

23. All values of parameter “mu” are now allowed. When it is non-zero, the optimization of the scale factor μ is not performed (this is possible only when output_mu=-1).
24. The default value of parameter “spline_combine” has been changed from 1 to 0, which means that the κ_{max}-fitted DCS data for different shifts are by default spline-fitted and extrapolated separately.
25. Parameter “k2_step0” has been renamed to “k2_step_first” (alias “k2_step”).
26. If k12ratio (i.e., the ratio Kmax1 / Kmax2) is greater than 1, then parameters “k2_step_first” and “k2_step_last” are now by default set to 10 starting from Kmax2 = 250 (instead of 300).
27. The condition $|\kappa_2|_{max} > 150$ has been removed from the set of conditions needed in order to apply the interpolation of S integrals with respect to l.
28. When $T_1 > 30$ MeV, the default angular increment at $\theta < 10°$ has been reduced from 0.1° to 0.02° (841 points in total).
29. The maximum number of function evaluations for adaptive quadrature when calculating the analytical Born- or SM-approximation cross sections (variable “nEval_max” in the file “Born_SM_appr.f90”) has been increased by a factor of 10.
30. If the required accuracy of the adaptive quadrature (when calculating the analytical Born- or SM-approximation cross sections) is not achieved due to insufficient number of integrand evaluations (error code 1), then the current values of the integral and its uncertainty are output (rather than terminating the program with an error message).
31. The threshold value of Kmax for applying the moving-average-smoothing by default has been reduced from 80 to 50.
32. The default value of parameter “spline_theta_max_thr” has been changed from -80 to 80.
33. Two rules for reducing the default value of parameter “R_atom” (it was previously equal to -13) at high electron energy and non-zero photon energy have been added: when $T_1 \geq 20$ MeV and $10 \text{ MeV} \leq T_2 < 20$ MeV, the default value of R_atom is -7; when $T_2 \geq 20$ MeV, the default value of R_atom is -4. Thus, the complete specification is the following: **a)** when $T_1 < 1$ MeV, R_atom=-20, **b)** when $1 \text{ MeV} \leq T_1 < 20$ MeV, or $T_1 \geq 20$ MeV and $T_2 < 10$ MeV, R_atom=-13, **c)** when $T_1 \geq 20$ MeV and $10 \text{ MeV} \leq T_2 < 20$ MeV, R_atom=-7, **d)** when $T_2 \geq 20$ MeV, R_atom=-4.
34. In order to improve the accuracy of the angular dependence of the final κ_{max}-fitted DCS near the tip of the photon spectrum at electron energies higher than 3 MeV, the default values of parameters controlling the κ_{max}-fitting when $T_1 > 3$ MeV and $T_2 / T_1 \leq 10^{-4}$ have been modified as follows:
    (a) splineRef0=splineRef1=splineRef2=0 (i.e., the cubic spline fitting of the PW DCS is not performed),
    (b) splineRef_fitted1=0 (unless splineRef_fitted3 has been set to zero),
    (c) fitRange_(D)CS=1,
    (d) spline_theta_max_fitted1=spline_theta_max_fitted2=180,
    (e) splineInt_min_fitted=min(5,splineInt_max_fitted),
    (f) spline_combine=2.
35. The κ_{max}-fitting of the DCS is no longer restarted from the zero angle after an increase of the variable tol_range (which is the threshold value of the relative change of the DCS as a function of κ_{max} inside the fitting interval). The new value of tol_range is applied at the current value of the photon emission angle θ and at all greater angles.
36. The limitation on the number of consecutive κ_{max}-fitting errors (parameter “nErrMax”) is no longer applied inside the angular interval $\theta \geq (180° + |\text{spline\_theta\_max\_thr}|) / 2$.
37. The default value of parameter “maxRelErr” has been increased from 0.02 to 0.05.
38. Several minor bugs have been fixed.
39. The user manual has been updated. In particular, the introduction now includes a more detailed discussion of the method of “μ-correction” (see Section 1.5.4 of the updated User’s Manual).

1.5.6.1 (2022-06-12):

1. The angular dependence of the reference DCS is now always allowed to have a minimum (in previous versions of BREMS, it was allowed only in the case of a sufficiently small range of variation of the DCS as a function of the photon emission angle θ).
2. The angular dependence of the reference DCS is now allowed to have one "abnormal" inflection point (i.e., a change from superlinear decrease to sublinear decrease, or a change from sublinear increase to superlinear increase), or two extremum points (a minimum and a maximum). However, if such an inflection point or a pair of a minimum and a maximum is found during calculation of the reference DCS by adaptive numerical integration of the analytical triple differential cross section, then the program will still attempt to remove it by successive halving of the relative error tolerance for the adaptive quadrature. If this inflection point (or a pair of a minimum and a maximum) cannot be removed after a predefined maximum number of integration attempts, then it will be accepted (unlike in previous versions, which would quit with an error message in such a case). The mentioned maximum number of integration attempts is stored in the internal variable "nAttempts_max" in the file "Born_SM_appr.f90 (at the time of this writing, nAttempts_max = 10).
3. Added parameter "maxRelDev_mu", which is used to apply an additional requirement (in addition to that defined by parameter "maxDev_mu") for fixing the value of the scale ratio μ corresponding to the current "shift" (as opposed to optimization of μ). The meaning of parameter "maxRelDev_mu" is the maximum value of $|(\mu - \mu_{avg}) / (\mu_{avg} - 1)|$, where μ is the scale ratio calculated using the κ_{max}-fitted DCS (i.e., $\mu = (\mathrm{DCS}(\kappa_{max}\to\infty, \theta) - \mathrm{DCS}(K', \theta)) / (\mathrm{DCS}(K, \theta) - \mathrm{DCS}(K', \theta))$) and μ_{avg} is the average μ, calculated inside the angular interval where the absolute value of the relative correction of the DCS due to the κ_{max}-fitting is between the values specified using parameters "maxCorr_mu" and "thrCorr_mu". The default value of parameter maxRelDev_mu is equal to 0.1.
4. The μ-correction is no longer applied in the current shift and in all subsequent shifts if the relative correction of the DCS due to the κ_{max}-fitting is less than the value defined by parameter maxCorr_mu inside the entire angular range where the μ-correction would be applied (i.e., at $\theta \geq \theta_{start}$ if the partial-wave DCS is a decreasing function of κ_{max}, or at $\theta \leq \theta_{end}$ if the partial-wave DCS is an increasing function of κ_{max}).
5. The user manual has been updated.

1.5.6.2 (2022-08-08):

1. In the case mode_mu=2, the value of μ is now extrapolated to $\kappa_{max} \to \infty$ using the stretched-exponential approximation $\mu_{theor}(\kappa_{max}) = (\exp(-\lambda K''^{C}) - \exp(-\lambda \kappa_{max}^{C})) / (\exp(-\lambda K''^{C}) - \exp(-\lambda K^{C}))$ instead of calculating the empirical arithmetic average. The two unknown parameters λ and C are estimated by nonlinear least squares fitting in the range $K'' \leq \kappa_{max} \leq K$, using the set of values of the empirical arithmetic average of $\mu(\kappa_{max}, \theta)$ over the angular interval where the relative change of the DCS due to the initial κ_{max}-fitting is between the values specified by parameters "thrCorr_mu" and "maxCorr_mu". The additional condition for performing this extrapolation (as opposed to optimization of μ by solving the integral equation, which minimizes the difference between the μ-corrected DCS and its polynomial approximation) is controlled by parameter maxDev_mu (parameter maxRelDev_mu has been dropped). In addition, the meaning of maxDev_mu has been changed: now it indicates the maximum allowed deviation of the empirical value of μ from 1 (rather than from the average μ). The default value of maxDev_mu has also been changed accordingly (increased from 0.01 to 0.1). The default minimum value of the relative correction needed for performing this extrapolation (as opposed to optimization of μ by solving the integral equation), which is given by parameter "thrCorr_mu", has been reduced from 0.001 to 0.
2. "splineRef2=0", "splineInt_min=3", "splineInt_max=6", "splineArg1=2", and "splineArg2=2" are now used by default.
3. The case "fitRef_mu=0" is now allowed to be used alongside "fitRef_mu=1" and "fitRef_mu=2" as one of the alternatives chosen on the basis of the balance between the quality of the polynomial fit inside the angular fitting interval and the stability of the polynomial extrapolation (outside the fitting interval) with respect to the different values of the endpoint of the fitting interval. Thus, seven values of fitRef_mu from -2 to 4 are now allowed: values from 0 to 3 have the same meaning as before, -2 and -1 correspond

to two alternatives (0 and 2, or 0 and 1, respectively), and 4 (the default value) corresponds to all three alternatives (0, 1, and 2).

4. The default value of parameter "fitDegree_mu_max2" has been increased from 20 to 30.
5. The default values of parameters "fitEndOffset_mu_max" and "n_fitEndOffset_mu" have been reduced from 40 to 30 and from 21 to 11, respectively (the default value of parameter "fitEndOffset_mu_min" is equal to 20, as in the previous version of BREMS).
6. Added parameter "tol_corr_mu", which is the tolerance of the relative correction of the DCS due to the κ_{max}-fitting. Parameter "tol_corr_mu" is used to increase the maximum endpoint of the angular range (θ'') for fitting of the μ-corrected DCS by a polynomial of cos θ when the partial-wave DCS is a decreasing function of κ_{max} and an irregularity is found in the angular dependence of the μ-corrected DCS. The mentioned increase of the maximum θ'' occurs after locating the angular range where the values of the mentioned relative correction are less than tol_corr_mu. If the endpoint of the latter angular range (θ_{tol}) is greater than the angle corresponding to the mentioned irregularity (θ_{irreg}), then the maximum θ'' is set equal to min(θ_{tol}, θ_{end}), where θ_{end} is the endpoint of the range of constant μ (or the value of parameter "end_angle_mu"). If θ_{tol} is less than θ_{irreg}, but greater than the arithmetic average of θ_{irreg} and the angle that is offset by fitEndOffset_mu_min relative to θ_{irreg} to smaller angles, then the maximum θ'' is set equal to the value that is symmetric to the angle of the irregularity relative to θ_{tol}, unless the value obtained in this way is greater than θ_{end}. I.e., in this case the maximum θ'' is equal to min($2\theta_{tol}-\theta_{irreg}$, θ_{end}). In any case, all smaller values of θ'' are increased by the same amount, so that the intervals between the adjacent values of θ'' do not change. The default value of parameter "tol_corr_mu" is equal to 0.2.
7. Added parameter "kmax_spline", which indicates the value of κ_{max} to be used for the initial spline-fitting of the angular dependence of the partial-wave DCS. The default value of this parameter is equal to -1, which indicates that the mentioned value of κ_{max} must be set equal to the maximum κ_{max} used in stage 3 (as in the previous version of BREMS).
8. Added two parameters "tol_spline" and "tol_spline_fitted", which are used to specify the absolute tolerance of the change of the natural logarithm of the two spline knot-density parameters (denoted ε_1 and ε_2 in the user manual) during their optimization by the simplex method (as a part of the angular spline fitting). Parameter "tol_spline" is used for the spline fitting of the original partial-wave DCS, whereas parameter "tol_spline_fitted" is used for the spline fitting of the κ_{max}-fitted DCS. The default value of parameters "tol_spline" and "tol_spline_fitted" is equal to 10^{-4}.
9. Added parameter "acc_fact", which is the modification factor to be applied to the four parameters controlling the accuracy of the numerical solution of the coupled radial Dirac equations ("pr_incr", "r_incr_max", "step1" and "delta_V_max"). I.e., the default or user-specified values of the mentioned four parameters are additionally multiplied by the mentioned factor, yielding the final values of those four parameters. The default value of parameter "acc_fact" is 1 (i.e., no additional modification is applied).
10. If the initial μ-fitting (which is performed at the start of stage 3) is successful and the optimal reference function used for the μ-fitting is either No. 1 or No. 2 (not No. 0, which means absence of the reference function) and the default or user-specified value of parameter splineRef_fitted1 or splineRef_fitted2 is non-zero, then either splineRef_fitted1 or splineRef_fitted2 is reset to 1 and the remaining three "splineRef_fitted" parameters are reset to zero. I.e., in this case the reference function used for the angular spline fitting is the same one that was used for the μ-fitting.
11. The default values of parameters "splineCS_wt_fitted", "geomAvg_fitted", "mainDevType_fitted" have been changed. The following defaults are now always used: splineCS_wt_fitted=1, geomAvg_fitted=0, mainDevType_fitted=0.
12. In order to change the "CS mode", two conditions are now required: T_1 > T1_CS_mode_thr and T_2 / T_1 > tip_thr (previously, only the former inequality was required). The inequality T_2 / T_1 > tip_thr has also been added to the set of conditions needed in order to change the default value of parameter "splineExt_fitted" from -2 to -1. Thus, the latter set of conditions is now the following: CS_ref_spline > 0, T_1 > T1_CS_mode_thr, T_2 / T_1 > tip_thr, and splineCS_wt_fitted = 1.

13. If the μ-fitting is applied and the partial-wave DCS is a decreasing function of κ_{max}, then the default value of parameter "splineInt_min_fitted" is now changed to min(max(3, θ_{start}/3), splineInt_max_fitted), where θ_{start} is the starting point of the interval of constant scale factor μ (or the value of parameter "start_angle_mu").
14. Parameter "maxCorr_mu" is no longer used to determine if the relative correction is sufficiently large to apply the μ-fitting. Instead, a fixed value of 0.001 (given by variable tol_test(1) in the source code) is used for this purpose. Parameter "maxCorr_mu" is used only for determining the endpoints of the angular range to be used for averaging the scale factor $\mu(\kappa_{max}, \theta)$ when it is determined that the final value of μ must be calculated by stretched-exponential fitting with respect go κ_{max} (rather than by minimizing the difference between the original μ-corrected DCS and its polynomial approximation).
15. If the scale factor μ is determined by iterative minimization of the difference between the μ-corrected DCS and its polynomial approximation, then the final value of μ is no longer allowed to be less than or equal to 1.
16. The cubic spline interpolation of S integrals with respect to l has been made more accurate, particularly when $|\kappa_2| << |\kappa_1|$ (the S integrals corresponding to such pairs of κ_1 and κ_2 are especially important at high energies and close to the tip of the spectrum, i.e., when T_1 is of the order of 10 MeV and $T_2 / T_1 < 0.05$). The following three modifications have been implemented: **(a)** if the second grid point of the $S(l)$ envelope corresponding to a particular pair of κ_1 and κ_2 is an extremum point, or if the absolute value of the first S integral exceeds the absolute values of all remaining S integrals corresponding to the same pair of κ_1 and κ_2 by a factor greater than 5, then the first point of the $S(l)$ envelope is excluded from the further cubic spline interpolation (and from the set of grid points referred to in the description of the next two modifications); **(b)** if the $S(l)$ envelope does not change sign, then the cubic spline interpolation is always performed using a single logarithmic spline segment; **(c)** if the $S(l)$ envelope changes sign and the second grid point of the $S(l)$ envelope is not an extremum point, whereas the ratio of the two maximum absolute values of the $S(l)$ envelope of either sign is greater than 5 or less than 0.2, then a constant term is added to all values of the envelope, such that they all have the same sign and the minimum absolute value becomes equal to the absolute value of the corresponding grid point of the original envelope (i.e., the absolute value of the mentioned offset of the $S(l)$ envelope is equal to twice the smaller one of the two maximum absolute values corresponding to each of the two subsets of grid points with the same sign, and the sign of the offset is opposite to the sign of the corresponding grid point of the original envelope). After that, the interpolation is performed using a single logarithmic spline segment, and then the mentioned constant term is subtracted from the interpolated values, yielding the final interpolated $S(l)$ envelope.
17. The files in the subfolder "CS_int" have been recreated using the latest version of the code.
18. Several minor bugs have been fixed.
19. The user manual has been updated.

1.5.6.3 (2022-08-31):

1. In the case "IV=1" (i.e., the point-Coulomb potential without screening), the default values of Kmax1, Kmax2 and R_atom have been increased by a factor that decreases with increasing T_1, and becomes equal to 1 starting from $T_1 = 100$ keV. The maximum value of the mentioned factor corresponds to $T_1 \leq 100$ eV and is equal to 3 in the case of Kmax, and to 1000 in the case of R_atom. In the case of Kmax, the mentioned decrease is logarithmic (i.e., Kmax is a linear function of $\ln(T_1)$), whereas R_atom is inversely proportional to T_1 when 100 eV $\leq T_1 \leq$ 100 keV.
2. Added an option to calculate the screening correction to the Sommerfeld-Maue (SM) DDCS or SDCS as the difference of the screened and unscreened Born DDCS or SDCS (previously, the screening correction was always taken into account by adding the difference of the screened and unscreened Born TDCS to the SM TDCS corresponding to absence of screening, and then performing the double or triple angular integration). Although both methods are mathematically equivalent, the new method is typically more efficient at low energies (when $T_1 < 10$ keV), whereas the old method is typically more accurate at higher energies. Added parameter "T1_scrCorr_mode_thr" specifying the value of T_1 corresponding to the transition from the new method of calculating the screening correction to the old one. The default value of the mentioned parameter is equal to 10^{-2}. I.e., the new method is applied by default only when $T_1 < 10$ keV.

3. Added parameter “nTries_max_HG”, which indicates the maximum number of precision levels to be tried when calculating the hypergeometric (HG) function. “nTries_max_HG=1” is equivalent to “tol_change_HG=0” (i.e., a single precision level). If nTries_max_HG>1, then a sequence of up to nTries_max_HG or nTries_max_HG−1 consecutive precision levels will be tried during each calculation of the HG function until the relative difference of the estimates of the HG function corresponding to the last two precision levels becomes less than tol_change_HG. The maximum number of precision levels (i.e., nTries_max_HG) will be used every |err_test_int_HG| evaluations of the HG function (starting from evaluation No. 1), and if the relative difference of the estimates of the HG function corresponding to the last two precision levels (No. nTries_max_HG−1 and No. nTries_max_HG) is greater than tol_change_HG, then the program will either terminate the calculation of the DDCS or SDCS with an error message or display a warning, depending on the sign of err_test_in_HG. During the other evaluations (whose sequence numbers are not equal to $1 + n * |\text{err\_test\_int\_HG}|$, where n is an integer number), up to nTries_max_HG−1 consecutive precision levels will be tried, and if the relative difference of the estimates of the HG function corresponding to the last two precision levels is greater than tol_change_HG, then the estimate of the HG function corresponding to the last precision level (No. nTries_max_HG−1) will be used, without any additional actions or messages. The default value of parameter nTries_max_HG is equal to 4.
4. The permanent change of the precision level to be used for calculation of the hypergeometric function has been disabled. When err_test_int_HG < 0, the only difference from the case of positive err_test_int_HG is that the program does not terminate the calculation of the DDCS or SDCS (only a warning is displayed). The default value of parameter “err_test_int_HG” has been changed from −11 to 11.
5. The default value of parameter “tol_change_HG” has been increased from 10^{-11} to 10^{-9}.
6. The memory usage when calculating the hypergeometric function has been reduced significantly (especially in multiple-precision mode). This reduction has been achieved by using dynamic arrays for storing the values of the coefficients of the HG series.
7. Added parameter “x_HG_transform_thr”, which is the threshold value of the argument x of the hypergeometric (HG) function used in the expression of the Sommerfeld-Maue TDCS, which must be exceeded in order to calculate the mentioned HG function as a linear combination of two HG functions with argument equal to $1 - x$ (see Eq. (1.1.43) in the updated user manual). In the previous version of BREMS, this threshold was not user-adjustable, and it was always equal to 0.7 (which is default value of this parameter).
8. The mentioned transformation formula of the hypergeometric function is now applied not only in the case of double or quadruple precision, but also in the case of multiple precision.
9. The mentioned transformation formula of the hypergeometric (HG) function is no longer applied if the absolute value of the resulting estimate of the HG function is less than the absolute value of each of the two terms on the right-hand side of the transformation formula by a factor greater than 10^8. This modification eliminates the cancellation errors, which could have a significant influence on the values of the Sommerfeld-Maue DDCS and on the duration of angular integration of the Sommerfeld-Maue TDCS, especially at low energies.
10. Fixed a bug in numbering of the four parameters “CS_int_colNum_relErr0”, “CS_int_colNum_CS1”, “CS_int_colNum_relErr1”, “CS_int_colNum_CS2” (because of this bug, user-specified values of those parameters were not interpreted correctly by the program).
11. Fixed a bug in calculation of the total relative standard deviations of the shape function. This bug affected the values in columns “SF_maxRelSD” and “SF_maxScaledSD” of the file “CS_fitted.txt”, as well as the values in the last two columns of the file whose name starts with “ShapeFn_fitted_” (after correction of this error, the values in columns “SF_maxRelSD” and “SF_maxScaledSD” of the file “CS_fitted.txt” are equal to the values in columns “DCS_maxRelSD” and “DCS_maxScaledSD”, respectively, whereas the values in the last two columns of the “ShapeFn_fitted_” file are equal to the corresponding values in the file whose name starts with “DCS_fitted_”).
12. The user manual has been updated.

1.5.6.4 (2022-11-10):

1. Added parameter “Zi”, which has the meaning of the ion charge (in units of the elementary charge). The values of the screening potential and screening function in the input data files may also correspond to incomplete screening (i.e., an ion), indicated by an independent parameter “Zi_V”. If Zi_V is nonzero, then the input potential data are “normalized” automatically, so that the initial value of the screening function is 1, and it approaches 0 as $r \to \infty$. This linear transform yields the “normalized” variable part of the screening function (without the constant term, which is equal to Zi_V / Z_V). After that, the actual potential is calculated using the opposite linear transform and the specified value of parameter “Zi” (thus, the ion charge corresponding to the input data is not required to be equal to the charge of the ion that is being modeled). The same linear transform is also applied in the case “IV=2”, if parameter “Zi” is nonzero. The input and output values of the coefficients of the superposition of decaying exponentials (used to approximate the screening function), as well as the coefficients of the Taylor series approximating the screening function near $r = 0$ pertain only to the mentioned “normalized” variable part of the screening function.
2. Fixed three minor bugs in the file “Brems_fit.f90” (corresponding to stage 3 of the calculation).
3. The mentioned improvements in the calculation of bremsstrahlung from ions are reflected in the updated user manual (specifically, in sections 1.2, 4.1, 7.1, 8.1, and 12).

2022-12-03:

4. The endpoint of the energy range where the default value of R_atom is additionally increased in the case of an ion (IV=1 or Zi≠0) has been changed from 100 keV to 1 MeV. The energy range where the factor of the mentioned additional increase is inversely proportional to T_1 is now $100\ \text{eV} \le T_1 \le 1\ \text{MeV}$. Because of this change, the value of the mentioned factor inside the interval $T_1 \le 100\ \text{keV}$ has become greater by a factor of 10 than in the previous version of BREMS.
5. The mentioned additional increase in the case of an ion (IV=1 or Zi≠0) is now applied not only to the default value of R_atom, but also to the default value of pr_transition2.

1.5.6.5 (2022-12-31):

1. Added parameter “R_atom_delta”, which is the “extended” atomic radius, where the phase shifts are determined. This extension may be needed because the phase shifts are determined by matching the exact expression of the free-field wave function (a superposition of two spherical Bessel functions) with the solution of the coupled radial Dirac equations, and because the spherical Bessel functions of the first kind are calculated by forward recursion, which is numerically unstable at small values of the argument. Another possible reason of increasing R_atom_delta over R_atom is a decrease of the minimum precision level needed for the analytical integration from R_atom_delta to $+\infty$ (in this way, the mentioned precision level can be reduced to double precision, causing a reduction of the duration of analytical integration by one or two orders of magnitude). If R_atom_delta > R_atom, then the process of numerical solution of the coupled radial Dirac equations will not be terminated at r = R_atom. Instead, it will be continued up to r = R_atom_delta, using zero interaction potential. Consequently, the spherical Bessel functions inside the radial interval R_atom < r < R_atom_delta will be calculated by solving the mentioned equations rather than by forward recursion. If R_atom_delta is equal to zero (the default value), then it will be reset to r0_Kmax_p_min * max(max$|\kappa_1|/p_1$, max$|\kappa_2|/p_2$), where p_1 and p_2 are the initial and final momenta of the electron (in relativistic units). If R_atom_delta < 0, then it will also be replaced with the mentioned value, but only if the latter is greater than |R_atom_delta|. Otherwise, R_atom_delta will be replaced with |R_atom_delta|.
2. If the angular interval of constant scale factor μ is found, then additional moving-average smoothing of the angular dependence of the normalized partial-wave (PW) DCS is now applied inside the mentioned interval prior to the κ_{max}-fitting or μ-correction. The mentioned normalization is such that the normalized PW DCS, as a function of κ_{max}, always varies from 0 (at $\kappa_{max} = K''$) to 1 (at $\kappa_{max} = K$). If μ is constant, then the values of the normalized PW DCS at a particular value of κ_{max} should be identical for all values of the angle θ that belong to the mentioned angular interval (this justifies the mentioned moving-average smoothing). The moving average period is specified by a new parameter “MA_period_theta_mu”. If this parameter is zero (the default value), then its value will be determined from the absolute value of another new parameter “theta_mu” (in such a case, MA_period_theta_mu will be set equal to the number of points from 180° – |theta_mu| to |theta_mu|). Depending on whether the PW DCS is a decreasing or

increasing function of κ_{max} inside the angular range of constant μ, the mentioned moving average is either "trailing" (i.e., calculated using the current point and previous MA_period_theta_mu − 1 points), or "leading" (i.e., calculated using the current point and next MA_period_theta_mu − 1 points).

3. Added parameter "theta_mu", which is used for determining a fixed value of the scale factor μ when the other methods fail. In such a case, the fixed value of μ is calculated from the value of the κ_{max}-fitted DCS at a specific angle θ, which is specified by parameter "theta_mu". This approach relies on the fact that the values of the PW DCS used for the κ_{max}-fitting are preprocessed by normalizing and averaging over a large number of consecutive values of θ (this number is specified by parameter "MA_period_theta_mu"). Consequently, it is reasonable to expect that the random errors in those values of PW DCS are sufficiently small to ensure a high accuracy of the κ_{max}-fitted DCS, especially if all the values of θ used for the mentioned averaging can be grouped in pairs of values symmetric with respect to 90°. |theta_mu| cannot be less than 90. If theta_mu > 0, then this approach will be applied if the other methods of determining a fixed value of μ fail. If the PW DCS increases with κ_{max}, then the fixed value of μ will be determined at the angle that is symmetrical to the specified value of theta_mu with respect to 90°, i.e., at 180° − theta_mu. For example, if theta_mu is 110 and the PW DCS increases with κ_{max}, then the fixed value of μ will be determined for the angle of 70°. If theta_mu < 0, then this method of determining a fixed value of μ will not be applied (however, |theta_mu| may still be used for determining MA_period_theta_mu, as explained above). Parameter theta_mu cannot be less than 90. Its default value is equal to -110.
4. The polynomial fitting of the κ_{max}-dependence of the PW DCS is now allowed not only when DCS(κ_{max}) is an increasing function, but also when it is a decreasing function. Consequently, two parameters "polyn_thr_DCS1" and "polyn_thr_DCS2" are now used instead of a single parameter "polyn_thr_DCS" (the suffix "1" or "2" corresponds to the increase or decrease of the DCS with κ_{max}, respectively). These two parameters specify the corresponding absolute values of the threshold relative correction. The default values of these two parameters are equal to 0.2 and 10^{10}, respectively. Since the latter value is very large, the polynomial fitting is never performed by default when DCS(κ_{max}) is a decreasing function.
5. Similarly, two parameters "maxDeg_DCS1" and "maxDeg_DCS2" are now used instead of a single parameter "maxDeg_DCS" (these two parameters specify the corresponding maximum degrees of the fitting polynomial). The default value of these two parameters is equal to 6.
6. Added three parameters "minDeg_CS", "minDeg_DCS1", "minDeg_DCS2", which specify the minimum degrees of the fitting polynomial when fitting the dependence of the PW DCS on κ_{max}. The meanings of the suffixes are the same as for the corresponding "maxDeg_..." parameters (see above). The default value of these three parameters is equal to 0.
7. Instead of using the fixed stretching exponent $d = 0.5$ in the argument of the mentioned polynomial fitting, the value of d is now optimized by simplex fitting with a first-degree polynomial.
8. Two alternative values of each of the six parameters polyn_thr_DCS⟨1,2⟩, maxDeg_DCS⟨1,2⟩, and minDeg_DCS⟨1,2⟩ are now used: one value is used inside the interval of constant scale factor μ, and the other one is used outside that interval. This is because the κ_{max}-dependence of the PW DCS inside the mentioned interval is typically smoother than outside it (because of the mentioned additional angular smoothing, controlled by parameter "MA_period_theta_mu"). Consequently, smaller threshold value of the relative correction and larger maximum degree of the fitting polynomial are acceptable. The names of parameters corresponding to the inside of the mentioned interval end with "_mu" (rather than "_DCS"). Thus, six new parameters have been added: "polyn_thr_mu1", "polyn_thr_mu2", "maxDeg_mu1", "maxDeg_mu2", "minDeg_mu1", "minDeg_mu2". The default value of parameter "maxDeg_mu2" is equal 10. The default values of the other five mentioned parameters are the same as of the corresponding parameters whose names end with "_DCS⟨1,2⟩".
9. Added parameters "simple_fit_CS" and "simple_fit_DCS" (alias "simple_fit" for both), which are "switches" (0 or 1) indicating if the stretched-exponential fitting of the dependence CS(κ_{max}) or DCS(κ_{max}), respectively, must be simplified by requiring that the fitted values corresponding to the initial and ending points of the κ_{max}-fitting interval are exactly equal to the corresponding empirical values. This requirement causes a reduction of the number of varied parameters by 2. The default value of these two parameters is 0 (i.e., the mentioned simplification is not applied by default).
10. The default value of parameter "splineArg1" has been changed from 2 to 1.

11. The default value of parameter “splineInt_max” has been changed from 6 to 60.
12. The default value of parameter “tol_0wt” has been changed from 0.25 to 0.4.
13. The default value of parameters “fitRef_mu1” and “fitRef_mu2” has been changed from 4 to -1.
14. The default value of parameter “maxCorr_mu” has been increased from 0.01 to 0.3.
15. The default value of parameter “splineExt_fitted” has been changed from -2 to -1, except when $T_2 / T_1 \le$ tip_thr (then splineExt_fitted is equal to -2 by default).
16. The default value of parameters “theorSD_CS” and “theorSD_DCS” has been changed from 0 to 1.
17. The default value of parameters “wt_Nfit_CS” and “wt_Nfit_DCS” has been changed from 2 to 1.
18. The default value of parameter “fractAvg_DCS” has been changed from 1 to 0.5.
19. Added an option to output the moving average of the original partial-wave DCS. This option is indicated by “MA_file=1”, and the file name suffix is specified using parameters “suffix_MA” and “suffix3a”. The file with the moving average will not be created if the moving average is not used (i.e., if the MA period is equal to 1).
20. Added an option to use cubic spline fitting instead of polynomial fitting of the “μ-corrected” DCS. This option is specified by a negative value of either fitDegree_mu_min⟨1,2⟩ or fitDegree_mu_max⟨1,2⟩. Then fitDegree_mu means the number of inter-knot intervals (it is one less than the number of “knots”, i.e., breakpoints of the piecewise cubic spline function). The knots are equidistant. The spline argument is $-\cos\theta$. In the files “mu_range.txt” and “mu.txt”, the spline fitting is indicated by a negative number in column “fitDegree_mu” (in such a case, the mentioned number is opposite to the number of inter-knot intervals).
21. When the optimal scale factor μ is determined by iterative minimization of the difference $|\mathrm{DCS}_\mu - \mathrm{DCS}_{\mathrm{ext}}|$, the polynomial fitting is performed in two stages: (a) at the first, the fitting polynomial is the simplest possible polynomial of $\cos(\theta)$ (usually – first-degree polynomial, i.e., fitDegree_mu = 1) multiplied by the reference function (i.e., all higher-degree polynomials are rejected in this stage, even if they yield smaller values of the mentioned standard deviation); (b) after that, the fitting is redone using the fixed value of μ determined in the previous stage, and with the maximum degree of the fitting polynomial defined by parameter “fitDegree_mu_max⟨1,2⟩”. In the default case “mode_mu=3”, if μ is known beforehand (either specified by the user, or determined by the program without resorting to the iterative minimization of $|\mathrm{DCS}_\mu - \mathrm{DCS}_{\mathrm{ext}}|$), then the polynomial fitting is done in one stage (with the maximum degree of the fitting polynomial defined by parameter “fitDegree_mu_max⟨1,2⟩”).
22. Added an option “mode_mu=-1” If mode_mu=-1 and a fixed value of the final scale ratio μ is available (either specified by the user or calculated by the program), then the $\kappa_{\max}$-fitted DCS is replaced with the μ-corrected DCS, but the angular polynomial fitting and extrapolation of the μ-corrected DCS is not performed. If a fixed value of the final scale ratio μ is not available or cannot be determined, then the μ-correction is not performed in the current shift and in all subsequent shifts.
23. Added an option “mode_mu=0”. In this case, the only effect of constant μ is the additional moving-average smoothing of the angular dependence of the normalized PW DCS inside the interval of constant μ prior to the $\kappa_{\max}$-fitting, i.e., the further μ-correction is not performed (which also implies that the program does not attempt to determine the scale factor μ). Instead, the $\kappa_{\max}$-fitting by the stretched exponential or polynomial approximation is performed, using the values of the DCS obtained after the mentioned moving-average smoothing. Since this smoothing is always performed prior to the subsequent μ-correction if an angular range with approximately constant μ exists, the option “mode_mu=0” corresponds to the least effect of constant μ on processing of the DCS in comparison with non-zero values of parameter “mode_mu”.
24. When R_atom_max<1 and a radial breakpoint with $\tilde{V}(r) <$ R_atom_max is found, the new value of R_atom_max is now determined by exponential interpolation (instead of setting it to the mentioned breakpoint).
25. The default value of R_atom_max has been changed from 10^4 to 10^{-6}. I.e., R_atom_max will be reset to the value of the radial coordinate where the screening function is equal to 10^{-6}.
26. The default value of parameter “rmax_R_atom_ratio_max” has been increased from 0.07 to 0.1, and the default value of parameter “nTries_rmax” been increased from 51 to 81.

1.5.6.6 (2023-01-19):

1. Added parameter “T2_CS_mode_thr”, which is the threshold value of the kinetic energy of the outgoing electron T_2 (in MeV) that must be exceeded in order to change the role assigned to the κ_{max}-fitted CS (as compared to the role of the angular integral of the κ_{max}-fitted DCS) when the photon energy is non-zero. Thus, two conditions T_1 > T1_CS_mode_thr and T_2 > T2_CS_mode_thr must be satisfied simultaneously in order for the mentioned change to occur. The default value of T2_CS_mode_thr is equal to 3.
2. When the “simple exponential” fit is performed (under the conditions defined by parameters “simple_exp_CS”, “simple_exp_DCS”, “simple_exp_thr_CS”, “simple_exp_thr_DCS”), an arbitrary fixed value of the stretching exponent d is allowed (thus, a more accurate term for this approximation is “fixed-d approximation” rather than “simple exponential”, because the latter term usually implies $d = 1$). The mentioned fixed value of parameter d for the “simple exponential” fit is specified using three new parameters “d_exp_CS”, “d_exp_DCS1”, and “d_exp_DCS2”. The suffix “1” or “2” corresponds to increase or decrease of the partial-wave DCS with κ_{max}, respectively. The default value of the latter three parameters is equal to 1. This is the same value that was used in the earlier versions of BREMS (where the value of d used for the simple exponential fitting was not adjustable by the user).
3. Added three parameters “d_polyn_CS”, “d_polyn_DCS1”, and “d_polyn_DCS2”, which are used to specify the value of the stretching exponent d in the expression of the argument of the fitting polynomial, when d has to be fixed (rather than optimized by least squares for the case of a first-degree polynomial). The suffix “1” or “2” corresponds to increase or decrease of the PW DCS with κ_{max}, respectively. If d_polyn > 0, then the polynomial fitting will always use d = d_polyn and a non-adjustable initial value of the optimized parameter b (a factor in the argument of the exponential defining the argument of the mentioned polynomial). If d_polyn < 0, then the value of d = |d_polyn| and a non-adjustable initial value of b would be used only in the case of a failure of the previous three-, four- or five-parameter stretched-exponential fitting. In other cases, the argument of the polynomial would be set equal to the exponential obtained by the previous stretched-exponential fitting, i.e., to $\exp(b\kappa_{max}^{d+h\kappa_{max}})$. The default value of these three parameters is equal to 0.5 (since this value is positive, the values of b and d are independent of the values obtained in the preceding stretched-exponential fitting, whereas $h = 0$). This is the same value that was used in BREMS v1.5.6.4 and earlier versions (where the value of d used for the polynomial fitting was not adjustable by the user).
4. Instead of one parameter “simple_exp_thr_DCS”, two new parameters “simple_exp_thr_DCS1” and “simple_exp_thr_DCS2” are now used, corresponding to increase or decrease of the PW DCS with κ_{max}, respectively.
5. Added three parameters “d_init_CS”, “d_init_DCS1” and “d_init_DCS2”, which are used to specify the initial value of the stretching exponent d for the four- or five-parameter stretched-exponential fit when vary_h_(D)CS=0 or vary_h_(D)CS=1. If vary_h_(D)CS ≥ 2, then the value of parameter “d_init_(D)CS⟨1,2⟩” means the geometric average of the maximum and minimum initial values of d to be tested (the range of variation of ln(d) is in such a case equal to 10). The suffix “1” or “2” corresponds to increase or decrease of the PW DCS with κ_{max}, respectively. The default value of these three parameters is equal to $e^{-5} = 0.00673794699908547$. This is the same value that was used in the earlier versions of BREMS (where the initial value of d used for the stretched-exponential fitting was not adjustable by the user).
6. Added parameter “polyn_relErr_tol”, which is the maximum allowed relative uncertainty of the zero-degree term (c) obtained by the polynomial κ_{max}-fitting. The default value of this uncertainty is equal to 0.05. This is the same value that was used in the earlier versions of BREMS (where the maximum allowed relative uncertainty of c was not adjustable by the user).
7. The default value of parameter “splineExt_fitted” has been changed from -1 to -2, except when CS_ref_spline > 0 and T_1 > T1_CS_mode_thr and T_2 > T2_CS_mode_thr and T_2 / T_1 > tip_thr and splineCS_wt_fitted = 1. I.e., the change introduced in the previous version (v1.5.6.5) has been reversed, because the subsequent testing has not shown a consistent improvement of accuracy by using splineExt_fitted=-1 when $T_1 \le$ T1_CS_mode_thr or $T_2 \le$ T2_CS_mode_thr.
8. The splitting of the μ-fitting procedure in two stages, which was introduced in version v1.5.6.5, is no longer performed. When the optimal scale factor μ is determined by iterative minimization of the difference $|DCS_\mu - DCS_{ext}|$, the polynomial fitting is now performed as in v1.5.6.4 and older versions of

BREMS, i.e., in a single stage, without applying the limitation of the smallest possible degree of the fitting polynomial. This reversal has been applied because it has been noticed that the mentioned two-stage method of performing the μ-fitting sometimes caused large uncertainties of the final DCS at small angles.

9. The default value of parameter "thr_range_mu2" has been changed from 60 to 120. In addition, the accuracy of μ-fitting has been slightly improved by changing several internal variables.
10. The average theoretical uncertainty (columns "err2_rms" and "err2_max" in file "Data_interm1.txt") is now calculated over all angles from 0° to 180° (previously, the angular interval from 0° to the starting angle θ_{min} of the spline-fitting interval was excluded). This modification causes a reduction of the theoretical uncertainty of the final fitted DCS in the angular range $\theta < \theta_{min}$.
11. The files in subfolder "CS_int" have been regenerated using the most recent versions of the codes.

1.5.6.7 (2023-03-20):

1. The maximum value of $|\kappa_1| + |\kappa_2|$ can now be increased above the default maximum (which is 1000, given by internal variable sz1), with the condition that the maximum value of $|\kappa_2|$ is not increased above 200 (internal variable sz2). The maximum allowed value of $|\kappa_1|$ is now 2000 (internal variable sz). As a result, the size of 3j data files with the names from "3j_801.dat" to "3j_950.dat" has increased (it is now the same as the size of file "3j_800.dat"). Those files will be created in stage 2 if the user specifies the maximum value of $|\kappa_1|$ greater than 800. In addition, files "3j_951.dat", "3j_952.dat", etc (up to the required maximum of $|\kappa_1|$) will be created if they don't exist (all these files are of the same size). This change did not affect the rules of calculating the default maximum values of $|\kappa_1|$ and $|\kappa_2|$ (those rules are the same as in the previous version of BREMS).
2. Added an option to replace the "μ-correction" and angular spline extrapolation with a simpler method of polynomial large-angle extrapolation of the κ_{max}-fitted DCS. This is done by polynomial fitting of the angular dependence of the κ_{max}-fitted DCS over an interval where the absolute value of the negative correction of the partial-wave DCS due to the κ_{max}-fitting is relatively small (less than 30 % in absolute value by default), if the endpoint of the mentioned interval is sufficiently large (at least 160° by default). This large-angle polynomial extrapolation is controlled by 12 new parameters.
3. The rules of modifying the default values of the endpoints of the interval of the angular spline fitting of the κ_{max}-fitted DCS (parameters "spline_theta_fitted_min" and "spline_theta_fitted_max") have been changed. One of the results of this change is that the number of cases when the spline fitting is performed inside the entire interval from 0° to 180° has increased.
4. Both spline-density parameters (denoted ε_1 and ε_2 in Section 1.7 of the user manual) are now used by default during the angular spline fitting of the κ_{max}-fitted DCS (in the previous version of BREMS, only one parameter was used by default). Consequently, the mentioned fitting is now longer, but more accurate (especially at small angles).
5. Added two parameters "splineLastIntRatio_thr" and "splineLastIntRatio_thr_fitted", which indicate the minimum allowed ratio of the width of the last inter-knot interval (ending at θ_{max}) and the width of the large-angle extrapolation interval (i.e., $180° - \theta_{max}$), when performing the angular spline fitting of the original partial-wave DCS and of the κ_{max}-fitted DCS, respectively. The default value of these two parameters is equal to 1 (i.e., the interval between the last two knots of the optimal spline function cannot be narrower than the large-angle extrapolation interval). Larger values of this parameter would improve stability of the large-angle extrapolation, but may cause deterioration of accuracy of the spline fitting at $\theta < \theta_{max}$.
6. The default value of parameter "tip_thr" has been increased from 0.03 to 0.07.
7. Instead of a single parameter "T2_thr_mu", two parameters "T2_thr_mu1" and "T2_thr_mu2" are now used, corresponding to $T_1 \leq$ T1_Kmax_mode_thr and $T_2 >$ T1_Kmax_mode_thr, respectively. Their default values are 1 MeV and 0.1 MeV, respectively.
8. The file "DCS_..._test2.txt", which is one of the output files of stage 2, has now four additional lines at the beginning, indicating the maximum values of $|\kappa_1|$, $|\kappa_2|$ and l_{max}, and the reduced value of l_{max} used for calculation of differential cross sections stored in this file (those four values are preceded by "Kmax1 =", "Kmax2 =", "lmax2 =" , and "l_test =", respectively).

9. The default value of parameter fitRange_DCS has been changed from 3 to 2.
10. The default value of parameter splineRef_fitted1 has been changed from -1 to 1.
11. The default value of parameter splineRef_fitted0 has been changed from 0 to -1. However, if the overall relative correction of the partial-wave DCS due to the κ_{max}-fitting is sufficiently large and the μ-correction is applied, then splineRef_fitted0 will be reset to 0 for the current shift.
12. The default value of parameter "fn_lmax3" has been changed from the empty string to the period ".", and the meaning of this value has been changed: now it means that the values of parameters Kmax12, lmax3 and lmax_decr3, which are specified in the file "DCS_..._test2.txt", must replace the default or user-specified values, unless the mentioned file has the old format. In other cases, parameter "fn_lmax3" is interpreted as in the previous version of BREMS, i.e., an empty string indicates that the default or user-specified values of parameters Kmax12, lmax3 and lmax_decr3 must be used, and any other string is interpreted as the name of the file with the same format as the file "CS.txt", where the mentioned values are located.
13. Added parameters "fitLog_mu1" and "fitLog_mu2", which are integer numbers 0, 1, or 2, indicating if the polynomial fitting must be applied to the logarithm of the ratio of the μ-corrected DCS and the reference function (instead of the actual ratio DCS_μ / DCS_{ref}) when the partial-wave DCS is an increasing function of κ_{max} or a decreasing function of κ_{max}, respectively. If this parameter is equal to 0, then the logarithm will not be used. If this parameter is equal to 1, then only the logarithm will be used. If this parameter is equal to 2, then both approaches will be tried, and the optimal method will be selected using the same criteria that are used for choosing the optimal degree of the fitting polynomial and the optimal reference function. The default value of parameters "fitLog_mu1" and "fitLog_mu2" is equal to 0 (i.e., the logarithm is not used by default). The output files "mu_range.txt" and "mu.txt" now include an additional column "fitLog_mu", which contains "1" or "0", indicating if the logarithm of the μ-corrected DCS was used during the polynomial fitting.
14. The default value of parameter "T2_min_Born" has been reduced from 1 to 0.5, and the default value of "Z_max_Born" has been increased from 1 to 2.
15. The default value of parameter "tol_corr_mu" has been increased from 0.2 to 0.5.
16. The default value of parameter "maxDev_mu" has been reduced from 0.1 to 0.02.
17. Added parameter "CS_int_exclude_large_T1_T2", to be used during cubic spline fitting and interpolation of the logarithm of the scaled single differential cross section with respect to the logarithm of the kinetic energy of the incident electron (this is one of the three "special" modes of operation of BREMS). This parameter is a "switch" (0 or 1), which indicates if the data points corresponding to T_1 > T1_CS_mode_thr and T_2 > T2_CS_mode_thr and T_2 / T_1 > tip_thr must be excluded from the data grid, if the corresponding "CS_int_appr_..." parameter is equal to 1 (i.e., if the input data file is "CS_fitted.txt", created by BREMS in partial-wave mode). In order for a data point to be excluded, the mentioned three inequalities must be satisfied *simultaneously*. The default value of this parameter is 1 (i.e., the data points satisfying those three inequalities are now excluded by default).
18. The files in the subfolder "CS_int" have been recreated using the latest version of the code.
19. The user manual has been updated.

1.5.7.0 (2023-06-26):

1. Added the capability to take into account the size of the nucleus during the calculation of *S* integrals and of the Born-approximation DCS. One of three analytical approximations of the nuclear charge distribution may be chosen: uniform distribution, Helm's uniform-uniform distribution, and the Fermi distribution (the latter is the default). The nuclear charge distribution is integrated with respect to the radial coordinate *r*, resulting in the "finite-nucleus correction" $\Delta\tilde{V}_f(r)$ of the screening function. The overall screening function $\tilde{V}(r)$ is calculated as the sum of the "point-nucleus screening function" $\tilde{V}_p(r)$ (which includes the electron screening effects) and $\Delta\tilde{V}_f(r)$. The point-nucleus screening function $\tilde{V}_p(r)$ is calculated independently of $\Delta\tilde{V}_f(r)$, using the same parameters as in the previous version of BREMS. The finite-nucleus correction $\Delta\tilde{V}_f(r)$ is calculated using six new parameters, which define the radial dependence of the proton density and the set of additional radial breakpoints near $r = 0$.

2. Added parameter “V_scr_0”, which has the meaning of the value of the tabulated screening function at $r = 0$, i.e., $\tilde{V}(0)$. This allows using the tabular interaction potential data that implicitly include the nuclear size effects, eliminating the need to define the finite-nucleus correction separately (using the mentioned six parameters of the nuclear charge distribution). In such a case, the initial radial breakpoints in the input data must correspond to the interior of the nucleus, whereas V_scr_0 must be equal to 0. The only other allowed value of V_scr_0 is 1, which indicates that the tabulated screening function data have the meaning of the mentioned “point-nucleus screening function” $\tilde{V}_{\mathrm{p}}(r)$ (this is the default).

3. Optimized the sequence of arithmetic operations and assignments to elements of the two arrays holding the intermediate values of S_1 and S_2 integrals during the numerical quadrature (i.e., integration from 0 to the cutoff radius r_0). The mentioned numerical quadrature now involves access to only one large double-precision data array at a time, and all elements of this array are modified sequentially (the array index is changed in increments of 1). Because of this optimization, the duration of the numerical quadrature has been reduced. In the case of a large number of S integrals (of the order of 10^6 or greater), the mentioned reduction is especially pronounced and is typically between 50 % and 70 % (that is to say, performance is typically improved by a factor of 2 to 3). This improvement of performance is probably caused by reduced effects of memory latency (i.e., improved caching of the data) and may therefore depend on the hardware and the operating system (the mentioned improvement of performance was measured on two PCs with i7-7700K and i7-4930K processors running Windows 10).

4. An option of linear interpolation of the screening function $\tilde{V}(r)$ at small r has been added (previously, only the exponential interpolation was performed). This option is controlled by the switch “expInterp”. Linear interpolation is indicated by “expInterp=0”. In such a case, the Taylor expansion of $\tilde{V}(r)$ near $r = 0$ has only zero- and first-degree terms. In the case “V_scr_0=0”, only “expInterp=0” is allowed. In the case “V_scr_0=1”, both values of expInterp are allowed, and the default option is “expInterp=1”.

5. Parameter “del_S_int” is no longer used in stage 1 (it is used only in stage 2 now). The default value of “del_S_int” has been changed from 1 to 0 (i.e., the S integral data file is no longer deleted by default after successful completion of stage 2).

6. The default value of parameter “del_S_n” has been changed from 0 to 1. I.e., the “_n” data files, which contain the initial parts of S integrals, obtained by numerical integration from 0 to the cutoff radius r_0, are now deleted by default after successful calculation of the complete S integrals from 0 to ∞, regardless of whether those files were created in the current run of BREMS or in an earlier run. If only a part of the numerical integrals was used to calculate the complete S integrals, then deletion of the “_n” data files would cause loss of some data. In order to avoid this data loss, the option “del_S_n=0” should be used.

7. Values of parameter “appr” equal to 2, 3, and 4 are now allowed when IV = 1 (no electron screening). In those cases, the analytical point-nucleus screening function (a constant equal to 1) will be replaced by a table of values (all of them are equal to 1), and the corresponding radial breakpoints will be calculated in the same way as in the case “IV=2 appr>1”. This is necessary in order to include nuclear size effects in absence of electron screening (if the point-Coulomb approximation is used, then the mentioned additional allowed values of parameter “appr” do not provide any benefits in comparison with the default option “appr=1”).

8. Two parameters “prefix_ref1” and “prefix_ref2” have been replaced with four parameters “prefix_ref_pn1”, “prefix_ref_pn2”, “prefix_ref_fn1”, “prefix_ref_fn2”, where “pn” and “fn” stand for “point nucleus” and “finite nucleus”, respectively. This modification allows using two sets of reference-function data files, which are located in different folders: one corresponding the point-nucleus approximation (with the nuclear form factor equal to 1), and the other one corresponding to the finite-nucleus approximation (with the nuclear form factor calculated as the Fourier transform of the nuclear charge distribution).

9. In the case “del_CS=1”, two files created in stage 2 are no longer deleted (in addition to files “CS.txt” and “CS_2.txt”). Those are the files whose names start with “_CS_” and “DCS_” and do not include the suffix “_test” or “_test2”. In the case “del_CS=2”, those two files are deleted (as in the previous version of BREMS using “del_CS=1”).

10. Three additional columns with values of the ion charge, the type of the nuclear charge distribution, and the mean nuclear radius have been inserted into the files “CS.txt”, “CS_2.txt”, and “CS_Born_SM.txt”.

11. Additional columns with the program version number, modification time ("timestamp") of the BREMS executable, and timestamps of various input and output files have been inserted into the files "CS.txt", "CS_fitted.txt", "CS_Born_SM.txt" and others. This improves traceability of the data over the multiple stages of calculation and multiple files created in each stage.
12. An alternative one-line comment symbol "//" has been added (in addition to "!").
13. Fixed an error in the power-series solution of the coupled radial Dirac equations corresponding to an ion (in subroutine power_series2). This bug did not affect the results corresponding to a bare nucleus (IV=1 or Zi=Z), or to a neutral atom (Zi=0).
14. Fixed a bug that sometimes caused the sum of default values of Kmax1 and Kmax2 to be greater than 1000.
15. There are many other minor improvements and minor bug fixes.
16. The user manual has been updated.

1.5.7.1 (2023-08-29):

1. Fixed an incorrect value of the first derivative at the initial radial breakpoint ($r = r_1$) of the cubic spline function used for interpolation of the finite-nucleus correction $\Delta\tilde{V}_f(r)$ of the screening function. The correct value of this derivative is $(\Delta\tilde{V}_f(r_1)+1)/r_1$, because $\Delta\tilde{V}_f(0) = -1$ (in BREMS v1.5.7.0, it was set equal to $\Delta\tilde{V}_f(r_1)/r_1$). This error caused unphysical oscillations of the interpolating spline function in a small part of the radial range near the center of the nucleus, including the first six radial breakpoints (from $r = r_1$ to approximately $r = r_6 = 6r_1$, i.e., from 0.05 fm to 0.3 fm by default). Because of a rapid decrease of the amplitude of these oscillations with increasing r, the distortions of the mentioned spline function were negligible at $r > r_6$. Since the reduced wavelength of the incident electron is greater than 6.4 fm at $T_1 < 30$ MeV (i.e., much greater than the value of the sixth radial breakpoint, which is equal to 0.3 fm by default), the effect of this error on the DDCS of bremsstrahlung was negligible at $T_1 < 30$ MeV.
2. In the case of the Fermi distribution of nuclear charge ("nuclear_model=3"), the nuclear form factor is now calculated exactly (by numerical quadrature), instead of using the analytical expression corresponding to Helm's uniform-uniform distribution.
3. Calculation of the factor $(F_n(q) - F_e(q))^2 / q^4$ in the expression of the Born-approximation TDCS of bremsstrahlung has been modified in order to make it more accurate at small values of the momentum transfer q. The mentioned factor is now calculated as $[(F_n(q) - 1) / q^2 + (1 - F_e(q)) / q^2]^2$, where the two terms in brackets are calculated independently. The term $(F_n(q) - 1) / q^2$ is finite at $q = 0$. The value of $(F_n(q) - 1) / q^2$ is replaced by the zero-degree term of its power-series expansion when q is less than $5 \times 10^{-7} / R_n$, where R_n is the nuclear radius. In the case of a neutral atom (or a truncated interaction potential), the term $(1 - F_e(q)) / q^2$ is also finite at $q = 0$. In the case of the exact (not truncated) potential for an ion, the term $(1 - F_e(q)) / q^2$ approaches infinity at $q \to 0$ as $(Z_i / Z) / q^2$, where Z_i is the ion charge. Consequently, the scaled DDCS and SDCS for an ion diverge in the soft-photon limit (this is true not only in the case of the Born approximation, but also in the case of the partial-wave approximation).
4. When calculating the SDCS numerically as the triple angular integral of the analytical TDCS corresponding to the Born approximation or the Sommerfeld-Maue approximation with the screening correction, the value of the relative error tolerance is no longer increased by a factor of 10. That is to say, the same error tolerance is now used both when calculating the DDCS (as the double angular integral of the TDCS), and when calculating the SDCS (this error tolerance is given by parameter "relErr_tol"). This modification has been made after noticing that the mentioned additional increase by a factor of 10 in rare cases (at energies greater than 100 MeV) caused the final SDCS to deviate from the correct value by more than 10 % if the default value of parameter "relErr_tol" (10^{-5}) was used (at the time of this writing, only one such case is known: "Z=77 T1=300 Ep=30" with "appr=0", "appr=-1", or "appr=-2").
5. The files in subfolder "CS_int" have been regenerated using the default distribution of nuclear charge (instead of the point nucleus approximation, which was used previously). The absolute value of the relative change of the SDCS caused by replacing the point nucleus with the Fermi distribution of nuclear charge is less than 0.75 % (i.e., 0.0075) at $Z = 1 - 100$, $T_1 \le 30$ MeV, $k / T_1 \le 0.95$.
6. There are several other minor improvements and bug fixes.
7. The user manual has been updated.

1.5.7.2 (2023-10-28):

1. Added parameter “fit_alt”, which is a “switch” (1 or 0) indicating if stage 3 must be redone using the two alternative sets of PW cross sections (stored in files “…_test.txt” and “…_test2.txt”). If this parameter is non-zero, then the relative deviations of the corresponding κ_{max}-fitted (D)CS from the original κ_{max}-fitted (D)CS will be added in quadrature to the other terms composing the total uncertainty of the κ_{max}-fitted (D)CS. If this parameter is equal to 0, then the mentioned two additional terms will not be included (only the terms reflecting the relative change of the PW DCS will be included). In the case “fit_alt=1”, the duration of stage 3 is longer by a factor of approximately 3 than in the case “fit_alt=0”. The default value of parameter “fit_alt” is equal to 1.
2. The user manual has been updated.

1.5.8.0 (2024-02-07):

1. A new method of improving accuracy of the final DDCS at large angles has been implemented. This method is by default applied when $T_1 > 1$ MeV and $k > 0$, and it relies on using a larger ratio $|\kappa_1|_{max} / |\kappa_2|_{max}$ at large angles. That is to say, the partial-wave DCS (defined by a truncated sum, where $|\kappa_1|$ and $|\kappa_2|$ vary from 1 to $|\kappa_1|_{max}$ and $|\kappa_2|_{max}$, respectively), is calculated twice, using both the “original” value of the ratio $n \equiv |\kappa_1|_{max} / |\kappa_2|_{max}$ and a much greater value of the mentioned ratio. After extrapolation of each of these two partial-wave DCS to $\kappa_{max} \to \infty$, the final DCS is constructed by smoothly joining the small-angle part of the κ_{max}-fitted DCS corresponding to the smaller n (the “original” DCS) with the large-angle part of the κ_{max}-fitted DCS corresponding to the larger n (the “alternative” DCS). The alternative PW DCS is calculated using approximately the same or greater value of $\max(|\kappa_1|_{max})$ as the original PW DCS, and a much-reduced value of $\max(|\kappa_2|_{max})$, which is defined as follows: $\max(|\kappa'_2|_{max}) = \min(30, \max(15, \max(|\kappa_2|_{max})/4))$. This means that the reduced value of $\max(|\kappa_2|_{max})$ is always inside the interval $15 \le \max(|\kappa'_2|_{max}) \le 30$. Although the previously-implemented methods of fitting and extrapolation are usually sufficient to achieve accuracy of a few percent or better at all angles, usage of an increased ratio $|\kappa_1|_{max} / |\kappa_2|_{max}$ makes it possible to reduce the uncertainties at large angles to values of the order of 0.1 % or less, because the value of the alternative PW DCS corresponding to the maximum value of $|\kappa_2|_{max}$ (i.e., to the start of the κ_{max}-extrapolation range) is typically within a few percent of the converged value (i.e., the exact value of the DCS) and hence requires minimal additional extrapolation with respect to $|\kappa_2|_{max} = |\kappa_1|_{max} / n$. The alternative κ_{max}-fitted DCS is by default calculated in the angular range $60° \le \theta \le 180°$. This method is controlled by 15 new parameters (five of them are used to calculate the alternative value of $\max(|\kappa_1|_{max})$, and most of the remaining parameters control the mentioned joining of the two κ_{max}-fitted DCS).
2. Added parameter “l_k2_thr”, which is the value of $|\kappa_2|$ that must be exceeded in order to apply the interpolation of S integrals with respect to l. That is to say, the mentioned interpolation is never applied when $|\kappa_2| \le$ l_k2_thr. The default value of this parameter is equal to 30. This parameter has been added after noticing that the interpolation with respect to l sometimes causes a significant bias (up to 20 %) of the final DCS at large angles, if Kmax2 is of the order of 10 and Kmax1 >> Kmax2.
3. Added parameter “tol_test_a”, which indicates the relative error tolerance for analytical integration (from the cutoff radius r_0 to $+\infty$) when optimization of the precision level is performed (i. e., when ndp < 0). The default value of this parameter is 10^{-6}. ***Note***: all versions of BREMS prior to v1.5.8.0 used multiple precision arithmetic with precision of 22–23 significant digits as a substitute for double precision (15–16 significant digits) during optimization of the precision level (i.e., when ndp < 0). Consequently, the mentioned default value of tol_test_a is approximately equivalent to the previous error tolerance of 10^{-13} when optimization of precision level is performed (the current version of BREMS does not substitute multiple precision for double precision during the mentioned optimization).
4. The extrapolating function used for the large-angle polynomial extrapolation in the case of small negative corrections now includes an additional factor equal to a reference function. The sequence number of the mentioned reference function is specified by a new parameter “fitRef_extrap”, which is by default equal to 1 (this value by default corresponds to the screened Born-approximation DCS).
5. The degree L of the extrapolating polynomial used for the large-angle extrapolation in the case of small negative corrections is no longer fixed, but is by default selected from a set of values from 1 to 10

(specified by two new parameters “degree_extrap_min” and “degree_extrap_max”, respectively, which replaced parameter “degree_extrap”). The optimum value of L is determined as follows. If the rms change of extrapolated large-angle DCS (in the extrapolation range) caused by changing L to $L + 1$ is less than the rms difference between the results corresponding to $L - 1$ and L, and each of the mentioned two rms differences is less than the rms difference between the results corresponding to $L - 1$ and $L + 1$, then L is incremented by 1, and the same check is repeated, unless L has reached the maximum allowed value (10 by default), in which case the latter value becomes the final value of L. If the mentioned conditions are not satisfied simultaneously, then the optimal L is set equal to the previous value ($L - 1$).

6. The default value of parameter “tip_thr” has been increased from 0.07 to 0.1.
7. When loading the S integral data from multiple files in stage 2 (subroutine “Bremsstrahlung”), the values of R_atom_delta (the radial coordinate where the phase shifts are calculated and the transition from numerical integration to analytical integration occurs) stored in different files are no longer required to be equal to each other. Only the values of the cutoff radius of the interaction potential (R_atom) and other physical parameters are required to be equal.
8. Reduced memory usage during calculation of the coefficients of the closed-form expressions of spherical Bessel functions at the start of the analytical integration (from r_0 to $+\infty$). In addition, duration of the mentioned calculation has been reduced by using multiple-precision multiplication instead of multiple-precision division.
9. Duration of the analytical integration (from r_0 to $+\infty$) at the lowest precision level (double precision) has been reduced by reducing the frequency of accessing large three-dimensional arrays. At large values of κ_1, κ_2 and l, the mentioned duration has been reduced by more than 30 %.
10. If $T_1 > 3$ MeV and $T_2 / T_1 \leq 10^{-4}$ and splineRef_fitted3 has not been set to zero, then splineRef_fitted0 and splineRef_fitted1 are no longer set to zero by default. The default values of “thrCorr_extrap1” and “thrCorr_extrap2” are also no longer reset to zero when $T_1 > 3$ MeV and $T_2 / T_1 \leq 10^{-4}$. In addition, the default values of parameters “splineFit_wt” and “wt_avg_DCS” have also been modified for the case $T_1 > 3$ MeV and $T_2 / T_1 \leq 10^{-4}$: splineFit_wt=-2, wt_avg_DCS=2.
11. In stage 3, the file with the fitted shape function is no longer created if the starting angle (specified by parameter “theta_min”) is greater than 0.
12. The default value of parameter “tol_0wt” has been increased from 0.4 to 0.5.
13. Parameter “fit_alt” has been renamed to “fit_test”.
14. Since the single forward slash in a list-directed input has a special meaning in Fortran (it signals to skip a line), the double-slash comment symbol “//” has been replaced with a single slash ‘/’, and the input buffer is now emptied before each read, so that the program does not attempt to process the same parameter string twice after a skipped line.
15. The user manual has been updated.

1.5.8.1 (2024-03-05):

1. The default value of parameter “theta_min+” has been reduced from 60 to 30.
2. When determining the angular interval corresponding to transition from the original κ_{max}-fitted DCS to the alternative κ_{max}-fitted DCS (which is calculated using a much smaller value of $|\kappa_2|_{max}$ than the original DCS), the restriction on the maximum allowed ratio of the alternative and original relative corrections (defined by parameter “thr_corrRatio+”) is no longer applied if the absolute value of at least one of the mentioned two relative corrections is less than 0.001.
3. The default value of parameter “thr_corrRatio+” has been increased from 1 to 10.
4. If the case of several “candidate” transition intervals, the one with the smallest absolute value of the ratio of the maximum relative difference between the original and alternative κ_{max}-fitted DCS to the ratio of the maximum and minimum values of the original κ_{max}-fitted DCS is selected (in the previous version of BREMS, the interval with the smallest starting angle was selected).
5. Added parameter “thr_relSD+”, which is used to specify the maximum allowed value of the relative uncertainty (standard deviation) of the alternative κ_{max}-fitted DCS inside the transition interval. The default value of this parameter is equal to 0.03.

6. Added parameter “theta_width_min+”, which is used to specify the minimum allowed width of the transition interval (in degrees). The default value of this parameter is equal to 5.
7. The calculation of the uncertainty of the final κ_{max}-fitted DCS inside the transition interval has been modified: it is now calculated by adding up the uncertainties of the original and alternative DCS in quadrature, with the same weight factors that are used to calculate the final κ_{max}-fitted DCS.
8. Fixed a bug which caused inaccurate values of the alternative partial-wave DCS (and, consequently, of the alternative κ_{max}-fitted DCS). This bug was caused by using incorrect value of parameter “lmax2”, which was equal to the value corresponding to the original DCS (which is not appropriate for calculation of the alternative DCS).
9. When the maximum value of l in the original S integral data file is less than the theoretical maximum ($|\kappa_1|_{max} + |\kappa_2|_{max}$), the additional data file now includes not only the data corresponding to values of $|\kappa_1|$ greater than the original $|\kappa_1|_{max}$, but also the missing data corresponding to $|\kappa_1|$ less than or equal to the original $|\kappa_1|_{max}$ and to values of l greater than the maximum value of l represented in the original data file. That is to say, the minimum value of $|\kappa_1|$ in the additional data file has been reduced in order to include the data corresponding to missing values of l (as a result, there is now some overlap between the two datasets).
10. The large-angle polynomial extrapolation is no longer performed by default when $T_2 / T_1 \leq 0.02$ and $T_1 > 3$ MeV (in previous versions of BREMS, the threshold value of T_2 / T_1 was 10^{-4}).
11. In the case “spline_combine=2” or when the angular spline fitting is not applied to the κ_{max}-fitted DCS, the points corresponding to the values of θ greater than the first error point inside the interval $\theta >$ (180 + |spline_theta_max_thr|) / 2 are no longer assigned zero weights (i.e., these points are no longer removed from further processing).
12. If S_data = 2 and this option is not compatible with the other parameters, then the program quits with an error message (instead of resetting S_data to 1 with a warning message).
13. The user manual has been updated.

1.5.8.2 (2024-03-21):

1. The default value of parameter “thr_corr1+” has been increased from 0.3 to 0.99, and the default value of parameter “thr_corr2+” has been reduced from 0.1 to 0.02.
2. If both the method of μ-correction (at large angles) and the alternative DCS are used, then the large-angle polynomial extrapolation is disabled when fitting the original DCS. In such a case, the parameters controlling the large-angle polynomial extrapolation will be applied only for fitting the alternative DCS.
3. Improved the calculation of the optimal value of the scale factor μ using the κ_{max}-fitted alternative DCS. It is now defined as the median value of the ratio $(DCS_{alt}(\theta) - DCS(K'', \theta)) / (DCS(K, \theta) - DCS(K'', \theta))$, where DCS_{alt} is the κ_{max}-fitted DCS obtained from analysis of the alternative partial-wave DCS (in the previous version of BREMS, μ was calculated as a weighted average, with weight factors defined so as to ensure zero average relative difference between $DCS_{alt}(\theta)$ and the μ-corrected DCS).
4. In order to further enforce simple exponential fitting during analysis of the alternative partial-wave DCS, parameters “simple_exp_thr_DCS1” and “simple_exp_thr_DCS2” have been increased from 1000 to 10^{100}, and additional options polyn_thr_DCS=-1, d_polyn_DCS=-1, and maxDeg_DCS=1 are used when fitting the alternative partial-wave DCS (the latter two options are needed because the polynomial fitting will be attempted in the case of a fitting error during the simple exponential fitting, if the number of points in the fitting interval is not less than tol_Nfit).
5. The threshold absolute value of the relative correction, which must be exceeded by both the original and alternative κ_{max}-fitted DCS in order to apply parameter “thr_corrRatio+”, has been increased from 0.001 to 0.01.
6. The final estimate of the uncertainty (standard deviation) of the κ_{max}-fitted DCS in the transition interval has been increased by adding the absolute deviations of the original and alternative DCS from the final DCS, multiplied by the corresponding weight factors.
7. Negative values of parameters d_exp_CS, d_exp_DCS1, and d_exp_DCS2 are now allowed. If the value of an exponent is specified with the minus sign, then the simple exponential fitting will be performed

using the absolute value of the specified exponent, and if this fitting fails, then the more general four- or five-parameter fitting (with adjustable d) will be performed instead. If the specified value of the exponent is positive, then there will be no second fitting attempt using the four- or five-parameter stretched-exponential fitting function after a failure of the simple three-parameter exponential fitting.

8. The endpoint of the spline-fitting interval of the alternative κ_{max}-fitted DCS is now reset to the maximum value of θ (usually 180°), if the value of parameter extrap_offset+ was not explicitly specified by the user and the relative correction of the alternative PW DCS at large angles is below the thresholds defined by parameters "thrCorr_extrap1", "thrCorr_extrap2", "thrAngle_extrap1", and "thrAngle_extrap2" (similarly to spline fitting of the original κ_{max}-fitted DCS).
9. The angular interval of large-angle polynomial fitting is now allowed to contain error points (i.e., the points where the preceding κ_{max}-fitting failed), with the condition that the relative range of variation of the PW DCS as a function of κ_{max} at the corresponding value of θ does not exceed 1 %. As a result of this change, the value of θ corresponding to the endpoint of the polynomial fitting interval (i.e., the starting point of the large-angle extrapolation interval) has increased if the mentioned error points are present.
10. The default values of parameters thrCorr_extrap1, thrCorr_extrap2, thrAngle_extrap1, and thrAngle_extrap2, which are used for large-angle polynomial fitting of the alternative DCS, are now different from the corresponding values used for large-angle polynomial fitting of the original DCS, and are equal to 0.1, 0.1, 160°, and 160°, respectively. These values are used if none of the mentioned four parameters is specified explicitly. If at least one of the mentioned four parameters is specified by the user, then the default values of parameters that were not specified explicitly are the same as those that are used for large-angle polynomial fitting of the original DCS.
11. The file "Data_interm1+.txt" is no longer deleted automatically in the case "S_data=3". In addition, its format has been modified so that there are no empty lines.
12. Added two new parameters "fitEndOffset_mu0_max" and "fitEndOffset_mu0_min", which are the alternative values of "fitEndOffset_mu_min" and "fitEndOffset_mu_max", to be used when the scale factor μ is not determined by minimizing the angular integral of the difference of the μ-corrected DCS and its polynomial approximation in the extrapolation interval, but is determined by an alternative method (e. g., by averaging the ratio $(\mathrm{DCS}(\kappa_{max} \to \infty, \theta) - \mathrm{DCS}(K'', \theta)) / (\mathrm{DCS}(K, \theta) - \mathrm{DCS}(K'', \theta))$). The default values of these two parameters are equal to 2 and 12, respectively (thus, they are less than the default values of "fitEndOffset_mu_min" and "fitEndOffset_mu_max", which are equal to 20 and 30, respectively).
13. The default value of parameter "theta_width_min+" has been reduced from 5 to 3.
14. The relative error tolerance used during a search for an irregularity in the angular dependence of the μ-corrected DCS (in subroutine Fit_mu) has been increased from 10^{-5} to 10^{-4}.
15. Added parameter "relErr_tol_spl", which is the relative tolerance when checking the angular dependence of a spline-fitted DCS for existence of extra inflection points or extrema. The default value of this parameter is equal to 10^{-4}.
16. The value of parameter fitRef_extrap to be used for the large-angle polynomial extrapolation of the alternative κ_{max}-fitted DCS is now fixed at zero (i.e., a reference function is no longer used for the large-angle polynomial extrapolation of the alternative κ_{max}-fitted DCS).
17. Fixed a bug, which caused incorrect modification of the internal variable tol_range after detecting an irregular shape of the dependence of the partial-wave DCS on κ_{max}. In previous versions of BREMS, tol_range was sometimes erroneously increased above the value of parameter "tol_range_max" (if the default value of "tol_range_max" was used, then this bug affected only the alternative κ_{max}-fitted DCS).
18. Fixed a bug, which caused replacement of user-specified negative values of polyn_thr_DCS1 and polyn_thr_DCS2 by the absolute values (this replacement is no longer applied).
19. Fixed a bug, which sometimes caused the error message about missing S integral data at the start of stage 2 using the alternative dataset, if the value of l_{max} had been reduced automatically in stage 1.
20. Fixed a bug, which caused a failure to change the endpoint of the spline-fitting interval to 180° after detecting a sufficiently small relative correction of the partial-wave DCS at large angle and switching to large-angle polynomial interpolation, if the μ-correction was applied in the previous "shifts".

21. The files in subfolder “CS_int” have been regenerated using the latest version of BREMS.
22. The user manual has been updated.

1.5.8.3 (2024-05-15):

1. Added parameters “devCapType” and “devCapType_fitted”, which are used in conjunction with parameters “mainDevType” and “mainDevType_fitted”, and which can be equal to 1 or 2, indicating the way the secondary deviations must be “capped” when they become greater than the main one (in the case “geomAvg[_fitted]=0”) or less than the main one (in the case “geomAvg[_fitted]=1”). The value of 1 indicates the original method (i.e., setting equal to the main deviation), and the value of 2 indicates the geometric average of the two relative deviations. The default value is 2. The reason of this modification is the following. When the option “geomAvg[_fitted]=0” is used and a particular type of relative deviation is greater then the “main” one, then setting it equal to the main one may prevent it from influencing the final result. If the “main” relative deviation does not affect a particular property significantly, then that property may in such a case be evaluated incorrectly. An example is calculation of the angular integral of the DDCS when the spline-fitting interval starts at a relatively large angle (much greater than the angle corresponding to the maximum value of the product $\sin(\theta) \cdot \mathrm{DDCS}(\theta)$), and the option “mainDevType_fitted=3” is used. In such a case, minimization of the relative residuals (which is a priority in the case of the mentioned option) has little effect on the value of the mentioned integral. If those residuals are significantly less than the relative deviation of the mentioned integral from the “reference” value of SDCS, then the latter deviation will not be used (because it will be always replaced by the rms value of the relative residuals), and the final DDCS at small angles may be incorrect, causing an erroneous estimate of its angular integral. Instead of setting the secondary types of the relative deviation to the “main” one, a better option could be setting them equal to the geometric average of the “main” deviation and the original value of the secondary deviation.
2. The default value of parameter mainDevType_fitted has been changed from 0 to 3.
3. If the alternative CS-fitting mode is required (i.e., $T_1 >$ T1_CS_mode_thr and $T_2 >$ T2_CS_mode_thr and $T_2 / T_1 >$ tip_thr and $k \neq 0$) and splineCS_wt_fitted $\neq 0$, then the “normal” CS-fitting mode is tried first, with parameter CS_ref_spline equal to zero and with a change in the default value of parameter “splineInt_min_fitted” (it is increased from 10 to 20). The alternative CS mode (with CS_ref_spline obtained by interpolation of the dependence ln CS(ln T_1), or specified by the user, or equal to the default value of zero) is applied only in the case of a failure of the “normal” κ_{max}-fitting of CS(κ_{max}), or when the relative change of CS due to the mentioned κ_{max}-fitting is greater than 30 % (new parameter “relCorr_CS_mode_thr”), or when the final relative uncertainty of the CS (after κ_{max}-fitting both the CS and the DCS) is greater than 5 % (if CS_ref_spline = 0) or 1 % (if CS_ref_spline $\neq 0$) (new parameters “relSD_CS_mode_thr1” and “relSD_CS_mode_thr2”, respectively), or when CS_ref_spline $\neq 0$ and the absolute value of the relative deviation of the κ_{max}-fitted value of CS from CS_ref_spline is greater than 2 % (new parameter “relDiff_CS_mode_thr”), or in the case of a failure to join the original κ_{max}-fitted DCS with the alternative κ_{max}-fitted DCS. This rule is applied both when CS_int=0 and CS_int≥2. Added parameter “retry_CS_mode” (default value 1), which makes it possible to quit after one of the mentioned failures (without applying the alternative CS mode). This is achieved by setting retry_CS_mode to 0. It is also possible to apply the alternative CS mode immediately (without a preceding “normal” run) by setting to zero one of the mentioned new parameters “relCorr_CS_mode_thr”, “relSD_CS_mode_thr1” (if CS_ref_spline = 0), “relSD_CS_mode_thr2” (if CS_ref_spline $\neq 0$), or “relDiff_CS_mode_thr” (if CS_ref_spline $\neq 0$).
4. If $T_1 >$ T1_CS_mode_thr and $T_2 >$ T2_CS_mode_thr and $T_2 / T_1 >$ tip_thr and $k \neq 0$ and CS_ref_spline $\neq 0$ and splineCS_wt_fitted $\neq 0$ and the “normal” CS-fitting mode fails or is skipped (see above), then the following defaults are used for the “alternative” CS-fitting mode: “splineInt_min_fitted=20 splineExt_fitted=-1 mainDevType_fitted=4 splineRef_fitted0=0”.
5. The default value of parameter “thr_corr2+” has been increased from 0.02 to 0.03.
6. The default value of parameter “CS_int_spline_wt_thr” been increased from 0.001 to 0.01.
7. The default option “CS_int_exclude_large_T1_T2=1” is no longer applied to entries with nonzero value in column “rel_diff” (i.e., these entries are no longer excluded from the data grid unconditionally, if the values of T_1 and T_2 belong to the exclusion interval and $k \neq 0$). In order to implement this change, parameters “CS_int_header_rel_diff1” and “CS_int_colNum_rel_diff1” have been added (default values

"rel_diff" and 41, respectively). In order to use the previous method (ignoring column "rel_diff"), the option "CS_int_exclude_large_T1_T2=2" must be specified, or, equivalently, parameter "CS_int_colNum_rel_diff1" must be zero and the default option "CS_int_exclude_large_T1_T2=1" must be used.

8. Fixed a bug that sometimes caused the program to erroneously assume that the alternative set of S integrals (corresponding to a greater ratio $|\kappa_1|_{\max} / |\kappa_2|_{\max}$) is entirely contained inside the original set (this bug showed up only when non-default values of parameters Kmax1, Kmax2 and lmax were specified).
9. Several other minor bugs have been fixed.
10. The files in subfolder "CS_int" have been regenerated using the latest version of BREMS.
11. The user manual has been updated.

1.5.8.4 (2024-06-13):

1. In order to take into account a possible bias in the least squares estimate of the (D)CS obtained by fitting the dependence of the partial-wave (D)CS on $\kappa_{\max}$ by a stretched-exponential or polynomial function, the estimate of the standard error (uncertainty) of the (D)CS has been increased by adding in quadrature the correction of the partial-wave (D)CS due to $\kappa_{\max}$-fitting multiplied by the value of the new parameter "err_corr_ratio" (its default value is equal to 0.1).
2. In order to take into account the mentioned uncertainty of the $\kappa_{\max}$-fitted DCS during the angular spline fitting, the errors of the spline values at the knots are now calculated using a modified value of the sum of squared residuals, with an additional term equal to the sum of squared uncertainties (standard errors) of the original $\kappa_{\max}$-fitted DCS in the spline-fitting interval.
3. The default value of parameter "relSD_CS_mode_thr2" has been reduced from 0.01 to 0.005.
4. At the end of stage 2 and stage 3, before updating the final files, a temporary read-only file with the name "write_lock2" or "write_lock3" is opened in the current folder. If another instance of the program attempts to update the same files, it will first check for existence of the mentioned temporary file, and then attempt to delete it if it exists. If the file exists and the delete attempt is not successful, then the program will wait until the mentioned file is deleted by the instance that created it. This modification helps to avoid a crash when two or more instances of BREMS attempt to update the same file simultaneously.
5. The width of several columns in files "CS_fitted.txt", "mu_range.txt" and "mu.txt" has been reduced so as to make the line length less than 1000 characters.
6. The files in subfolder "CS_int" have been regenerated using the latest version of BREMS.
7. The user manual has been updated.

1.5.8.5 (2024-08-13):

1. A newer version of the multiple-precision package (MPFUN2020) has been implemented. Because of this change, multiple-precision calculations became faster by a factor of approximately 1.5.
2. Added parameter "relCorr_spl_theta_CS_mode_thr", which is the minimum allowed value of the relative correction of the DCS in the part of the angular range (preceding θ_{start}, which is the starting angle of the μ-correction interval) that is excluded from the spline-fitting interval when the alternative CS-fitting mode is applied. The default value of this parameter is equal to 0.01. This means that the starting point of the spline-fitting interval will be reduced below θ_{start} by including all points where the relative correction is less than 1 % (negative corrections also satisfy this condition). This modification helps to reduce the uncertainties of the final $\kappa_{\max}$-fitted DCS at small angles when the alternative CS-fitting mode is applied.
3. The default value of parameter thr_corr2+ has been increased from 0.03 to 0.05.
4. When $T_1 > 3$ MeV, the threshold value of T_2 / T_1, which must be exceeded in order to use non-zero default values of parameters "thrCorr_extrap1" and "thrCorr_extrap2", has been reduced from 0.02 to 0.002.
5. When $T_1 \leq 3$ MeV or $T_2 / T_1 > 0.002$, the default value of parameters "thrCorr_extrap1" and "thrCorr_extrap2" used for processing the alternative $\kappa_{\max}$-fitted DCS has been increased from 0.1 to 0.2.

6. Several minor bugs have been fixed.
7. The starting point of the interval of values of T_1 used for generating the files in subfolder "CS_int" has been reduced from 0.1 MeV to 10 eV. The mentioned interval is now 10 eV ≤ T_1 ≤ 300 MeV. The mentioned files have been regenerated using the latest version of BREMS.
8. The user manual has been updated.

1.5.8.6 (2024-11-08):

1. The default value of parameter "mainDevType_fitted" is no longer changed from 3 to 4 in the case of the alternative CS-fitting mode (i.e., the mentioned default value is equal to 3 in all cases). This modification causes a reduction of the uncertainties of the final κ_{max}-fitted DCS at large energies (T_1 > 10 MeV, T_2 > 3 MeV), when the alternative CS-fitting mode is applied by default.
2. The user manual has been updated.

1.5.8.7 (2024-11-15):

1. A minor bug in the expression of the electron wave function near $r = 0$ has been fixed. This bug had an effect only when finite size of the nucleus was taken into account (by default, this happens when T_1 is greater than a threshold value, which decreases with increasing Z and which is approximately equal to 4 MeV for $Z = 1$ and to 0.4 MeV for $Z = 100$). The mentioned bug affected only the initial part of the power-series solution, in the radial range $0 \le r < r_1$, where r_1 is the first available radial breakpoint (by default, $r_1 = 0.05$ fm = $1.2948 \times 10^{-4}\, \lambda\!\!\!^{-}_{e}$, where $\lambda\!\!\!^{-}_{e}$ is the reduced Compton wavelength of the electron). Since the power-series algorithm for solving the coupled radial Dirac equations requires one component of the solution to be finite at $r = 0$ and the other component to be either finite or zero at $r = 0$, the two components of the solution are expressed at $r < r_1$ as $g(r) = r^\gamma \bar{g}(r)$ and $f(r) = r^\gamma \bar{f}(r)$, where γ is defined so as to ensure that $\bar{g}(0)$ and $\bar{f}(0)$ satisfy the mentioned requirement. The resulting value of γ is equal to $\sqrt{\kappa^2 - \alpha^2 Z^2 \tilde{V}_0^2}$, where $\tilde{V}_0$ is the value of the screening function $\tilde{V}(r)$ at $r = 0$. The finite-nucleus and point-nucleus approximations correspond to $\tilde{V}_0 = 0$ and $\tilde{V}_0 = 1$, respectively. The corresponding values of γ are equal to $|\kappa|$ and

$$\gamma = \sqrt{\kappa^2 - \alpha^2 Z^2}\,, \tag{1}$$

respectively. *However, due to a programming error, BREMS v1.5.7.0 to v1.5.8.6 used the latter value of γ in the case of the finite nucleus, too*. In the latter case, the factors before r^n in the power-series expansions of $\bar{g}(r)$ and $\bar{f}(r)$ are given by the recurrence relations

$$\bar{g}_n = \frac{E + 1 + Z\alpha\tilde{V}'}{\kappa + \gamma + n}\bar{f}_{n-1}, \quad \bar{f}_n = \frac{E - 1 + Z\alpha\tilde{V}'}{\kappa - \gamma - n}\bar{g}_{n-1} \quad (n > 0), \tag{2}$$

where $\tilde{V}'$ is the first derivative (i.e., the slope) of $\tilde{V}(r)$ at $r = 0$ (the relativistic units are used in Eq. (2)). Eq. (2) assumes that $\tilde{V}(r)$ is a linear function at $r < r_1$ (if finite size of the nucleus is taken into account, then BREMS calculates the values of $\tilde{V}(r)$ at $r < r_1$ by linear interpolation). If $\kappa > 0$, then $\bar{g}_0 = 0$ and $\bar{f}_0$ is finite (since $\bar{g}_0 = 0$, the actual value of $\bar{f}_0$ does not matter during the power-series solution, because the wave function is eventually normalized by matching it to the known free-space solution), and if $\kappa < 0$, then $\bar{g}_0$ is finite and $\bar{f}_0 = 0$. In the case of the point-nucleus approximation, both $\bar{g}_0$ and $\bar{f}_0$ are finite and the recurrence relations are different from Eq. (2). When $r < r_1 = 0.05$ fm, the zero- and first-degree terms are sufficient to evaluate the solution to an acceptable accuracy. According to Eq. (2), the first-degree coefficients are equal to

$$\bar{g}_1 = \frac{E + 1 + Z\alpha V'}{\kappa + \gamma + 1}\bar{f}_0\,, \quad \bar{f}_1 = \frac{E - 1 + Z\alpha V'}{\kappa - \gamma - 1}\bar{g}_0\,. \tag{3}$$

Thus, the mentioned bug caused the replacement in Eq. (3) of the factor $(\kappa \pm |\kappa| \pm 1)^{-1} = \pm(2|\kappa| + 1)^{-1}$ with the factor $(\kappa \pm \gamma \pm 1)^{-1} = \pm(|\kappa| + \gamma + 1)^{-1}$, where γ is calculated according to Eq. (1). This affected only the smaller of the two components (for example, if $\kappa > 0$, then it is the $g(r)$ component), because the

larger component includes only the even-degree terms (for example, if $\kappa > 0$, then $\bar{g}_0 = 0$ and Eq. (3) yields $\bar{f}_1 = 0$), and hence it is practically constant at small r. At $r < r_1$, the smaller component grows linearly: $\bar{g}(r) \approx \bar{g}_1 r$ (assuming that $\kappa > 0$). According to Eq. (3), $\bar{g}_1 / \bar{f}_0$ is largest when $\kappa = 1$ and $Z = 100$, and it increases with increasing E. However, even when $T = 30$ MeV (i.e., $E \approx 60$), the value of $\bar{g}_1 r_1$ is relatively small (the maximum value of $\bar{g}_1 r_1 / \bar{f}_0$ is approximately equal to 0.005), and it was increased by a factor of at most $3 / (2 + \gamma_{\min}) \approx 1.12$ (i.e., at most by approximately 12%) because of the mentioned bug. At $r > r_1$, the power-series solution algorithm was not affected by this bug, because the power-series expansion is applied at $r > r_1$ to the original components of the wave function (i.e., to $g(r)$ and $f(r)$) rather than to the auxiliary functions $\bar{g}(r) = r^{-\gamma} g(r)$ and $\bar{f}(r) = r^{-\gamma} f(r)$, so that the value of γ is not used. At this stage of the power-series solution (i.e., at $r > r_1$), the values of $g(r_1)$ and $f(r_1)$ are used as the initial condition for solving the coupled radial Dirac equations. Since the change of the mentioned initial condition due to the mentioned bug is relatively small and since the solution is a smooth function of the initial condition, the effect of this bug on the final values of the DDCS was negligible. By testing approximately twenty combinations of Z, T_1 and k (with T_1 varying from 4 MeV to 30 MeV, Z varying from 1 to 100, and k / T_1 varying from 0 to 0.9999), it was determined that the relative change of the final DDCS caused by this bug was typically of the order of 0.0001 (i.e., of the order of 0.01 %) at all values of the photon emission angle from 0 to 180°, and the absolute maximum of the mentioned relative change was approximately 0.0014 (i.e., 0.14 %). However, the largest values of the mentioned relative change (which are approximately equal to 0.001) occur at the largest angles, which are typically characterized by an even greater estimate of the relative uncertainty of the final DDCS, making the mentioned relative change not statistically significant.

2. Fixed a bug, which caused a failure to delete the *S* integral data file with the additional integrals (file name ending with suffix "+") automatically when the non-default option "del_S_int+=1" or "del_S=1" was used.

1.5.8.8 (2025-03-27):

1. Added the option to use an arbitrary prefix (possibly including a folder name) in the names of all output files of stage 2 and stage 3. The corresponding two new parameters are "prefix2" and "prefix3", respectively. Added the option to apply the mentioned prefixes only to the files that are overwritten in each run of BREMS (such as the "DCS….txt" files), but not to the files that are updated by adding one or several lines (such as the files "CS.txt" and "CS_fitted.txt"). The corresponding two new parameters are "use_current_folder2" and "use_current_folder3", respectively. They can be equal to 1 or 0. If use_current_folder[2,3]=1, then the files "CS.txt", "CS_fitted.txt", etc. are always placed in the current folder, i.e., no additional prefix is used in their names (unlike in names of the "DCS….txt" files).
2. The "_CS" file (one of the output files of stage 2) is now opened at the start of stage 2 and kept open during the entire calculation, so that other instances of BREMS cannot access it before stage 2 is finished. Note: this works on Windows, but does not work on Ubuntu running on the Linux subsystem for Windows (even an open file can be overwritten or deleted by another instance of the program).
3. Incorrect size of the *S* integrals data file is now determined more reliably. In particular, if the file size is an odd number of bytes, this means that the file size is incorrect (previously, it was erroneously assumed in such a case that the file version is 0, which corresponds to a multiple of four bytes). A warning message is now displayed when the file size is a multiple of 4 bytes (corresponding to file version 0), because this may be a result of abnormal termination of the program during output of data to the file.
4. The normalization factors and phase shifts corresponding to the "test" numerical *S* integral data (integration from 0 to the cutoff radius r_0, with all numerical tolerances and step sizes greater by a factor of 2) are now stored in the *S* integral data files (in addition to the normalization factors and phase shifts corresponding to the original numerical integration from 0 to r_0).
5. Added a new parameter "_n" of program "Read_S_integrals". It is a "switch" ("0", "1", or "2") indicating which of the three possible types of data must be displayed. "0" indicates the main type of integrals stored in the data file (typically the total integrals from 0 to ∞, unless it is the "_n" file, which contains only the numerical integrals from 0 to r_0), "1" indicates the "original" numerical integrals from 0 to r_0, and "2" indicates the "test" numerical integrals from 0 to r_0. In the latter case, the phase shifts and normalization factors that are displayed also correspond to the "test" numerical integration, unless the

input data file was created by a version of BREMS older than 1.5.8.8, in which case only the phase shifts and normalization factors corresponding to the original numerical integration are available. Parameter "_n" is equal to 0 by default.

6. After an unsuccessful attempt to create a new *S* integral data file (in stage 1) or a new cross section data file (in stage 2), the program now waits for two seconds and then tries again (up to 20 attempts), instead of quitting immediately. This may be useful if the file has to be created on a shared network resource, which has become temporarily unavailable.
7. The user manual has been updated.

1.5.8.9 (2025-06-08):

1. If the partial-wave DDCS is a decreasing function of κ_{max} and the average relative deviation of the μ-corrected DDCS from the original κ_{max}-fitted DDCS over the first 20 points of the angular interval where the scale factor μ is approximately constant is statistically significant at the 95 % confidence level, then the replacement of the original κ_{max}-fitted DDCS with the μ-corrected DDCS is also applied at smaller values of θ, down to the first value of θ where the relative deviation of the μ-corrected DDCS from the κ_{max}-fitted DDCS is either of the opposite sign to the mentioned average value or greater (in absolute value) than the latter. This extension of the mentioned replacement interval is based on the assumption that the μ-corrected DDCS is more accurate than the original κ_{max}-fitted DDCS not only inside the mentioned interval, but also at somewhat smaller angles.
2. If the "alternative CS-fitting mode" is applied (i.e., when the single differential cross section is estimated not by nonlinear fitting of the corresponding partial-wave series as a function of κ_{max}, but by an alternative method) and the starting angle of the spline fitting interval is greater than the starting angle of the interval where the replacement mentioned in the previous paragraph is applied, then the former starting angle is reduced to the latter value.
3. Fixed a bug that caused a failure to restore the initial value of parameter "mu" (indicating a fixed value of the scale factor μ) after its temporary modification during the κ_{max}-fitting of a "test" PW DDCS dataset (the mentioned parameter must by default be equal to zero, which indicates that a fixed value of μ must not be used).
4. Fixed a bug that caused an access violation if the output file "CS_Born_SM.txt" was open at the same time when the program attempted to write to it.