List of changes in the software package BREMS

Below is the list of changes for each version of the software package BREMS (available for download from http://web.vu.lt/ff/a.poskus/brems/ or http://www.apsoftware.org/BREMS/) up to the current version (1.4.12.9).

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 factor 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 decrease 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 singly and doubly 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 singly or doubly 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 singly or doubly 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 doubly 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 singly- and doubly-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 singly- and doubly-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 factor (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 factor 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 factor 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 factor 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 that 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 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 doubly 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 singly 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, 1e-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 singly and doubly 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 singly 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 doubly 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 κ_{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 doubly 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 $\overline{\kappa_1}$).
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 doubly 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 $l_1 + \overline{l_1}$, 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 singly and doubly differential cross sections of bremsstrahlung. The mentioned inequality is never true in the case of calculation of actual (total) cross sections, because in this case |Kmin2| is always equal to 1.