Scaling the hardware zoo: user-side timings of common quantum chemistry routines

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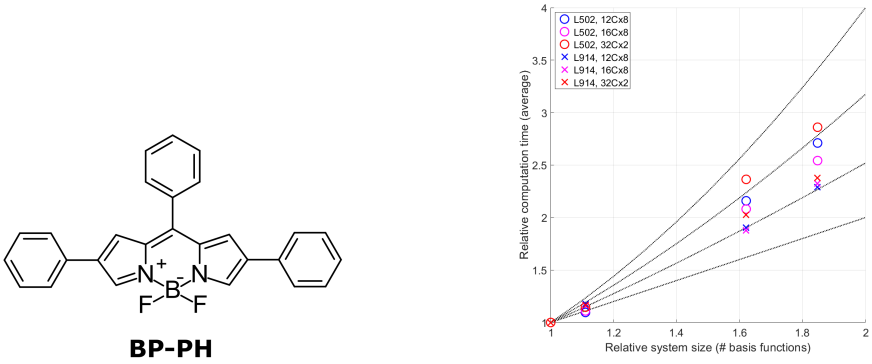

Fig. 1. Effect of system size on the computation times (*right*) for different variants of the BODIPY compound (*e. g. left*).

While using the “latest and greatest” hardware is in many cases preferable for high-performance computations, practical and financial considerations often result in systems that gradually become heterogeneous after expanding or upgrading the equipment. Assessing the performance of different parts of such a system might allow to sustain its “on-paper” capacity by adapting computation jobs and scenarios for the existing configuration.

With that in mind, a recent set of data for study of excited-state reaction paths in photoactive BODIPY derivatives [1,2] (Fig. 1, left) was obtained using different counts and types of computation nodes currently available at the VU HPC Saulėtekis location [3]. The computations consisted of a series of similar compound jobs involving several types of quantum-chemical routines and were performed using *Gaussian16* program package [4].

It was found that previous-generation CPU nodes (accounting for slightly less than 50 % of the available resources), while performing 2–8 times slower (per core) than the most recent hardware, can still supply around 20 % of total capacity for short/ exploratory jobs or 10 % for complex computations. On the other hand, medium-size molecules like BODIPY derivatives do not reach theoretical limits for computational cost scaling, with modeled dependence on basis set size M being less than M^2 (Fig. 1, right).

REFERENCES

[1] S. Toliautas *et al.*, *Chem. Eur. J.* **25**, 10342–10349 (2019).
[2] K. Maleckaitė *et al.*, *Molecules* **27**, 23:1–14 (2022).
[3] *sauletekis.ff.vu.lt/en/info/kontaktai/*.
[4] *Gaussian 16*, Rev. **C.01**, M. J. Frisch *et al.*, Gaussian, Inc., Wallingford CT (2016).