Contribution ID: **435** Type: **Sectional talk**

Optimization and effective usage of quantum-chemistry software on the Govorun supercomputer

Tuesday 8 July 2025 15:00 (15 minutes)

In computational molecular physics, the cornerstone of productive and precise research lies in the deployment of robust and purpose-fit scientific software. To fully exploit the capabilities of modern high-performance computing (HPC) architectures, it is imperative that such software be implemented in an optimized form to achieve maximal computational efficiency and scalability.

In this talk, we highlight our experience with two open-source quantum chemistry packages: DIRAC, a relativistic molecular code co-developed by one of the authors (M.I.) [1], and Quantum ESPRESSO, widely used for periodic DFT simulations [2].

We benchmarked various parallel configurations of DIRAC on the Govorun supercomputer and similarly evaluated Quantum ESPRESSO, including its GPU-enabled version. Test systems included molecule with superheavy element and periodic structure with superheavy addatom, both relevant to our group's current theoretical adsorption research.

Our objective in this talk is to share our practical insights on—how targeted optimization of DIRAC and Quantum ESPRESSO on HPC systems like Govorun can enhance computational performance and support efficient, large-scale simulations in quantum chemistry.

References

(1) Trond Saue, Radovan Bast, André Severo Pereira Gomes, Hans Jørgen Aa. Jensen, Lucas Visscher, Ignacio Agustín Aucar, Roberto Di Remigio, Kenneth G. Dyall, Ephraim Eliav, Elke Fasshauer, Timo Fleig, Loïc Halbert, Erik Donovan Hedegård, Benjamin Helmich-Paris, Miroslav Iliaš, Christoph R. Jacob, Stefan Knecht, Jon K. Laerdahl, Marta L. Vidal, Malaya K. Nayak, Małgorzata Olejniczak, Jógvan Magnus Haugaard Olsen, Markus Pernpointner, Bruno Senjean, Avijit Shee, Ayaki Sunaga, Joost N. P. van Stralen; The DIRAC code for relativistic molecular calculations. J. Chem. Phys. 29 May 2020; 152 (20): 204104. https://doi.org/10.1063/5.0004844

(2) Paolo Giannozzi, Oscar Baseggio, Pietro Bonfà, Davide Brunato, Roberto Car, Ivan Carnimeo, Carlo Cavazzoni, Stefano de Gironcoli, Pietro Delugas, Fabrizio Ferrari Ruffino, Andrea Ferretti, Nicola Marzari, Iurii Timrov, Andrea Urru, Stefano Baroni; Quantum ESPRESSO toward the exascale. J. Chem. Phys. 21 April 2020; 152 (15): 154105. https://doi.org/10.1063/5.0005082

Authors: SEN, Dipayan (Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research); Ms ESAWII, Heba (FLNP); Dr ИЛЬЯШ, Мирослав (BLTP JINR)

Presenter: Dr ИЛЬЯШ, Мирослав (BLTP JINR)

Session Classification: Application software in HTC and HPC