ESPResSo++: Extensible Simulation Package for Research on Soft matter

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ESPResSo++ is a free, open-source, parallelized, object-oriented simulation package designed to perform molecular dynamics and Monte Carlo simulations of condensed (soft) matter systems. While still under development, the package is expected to support traditional methods as well as state-of-the-art algorithms such as Green's function and temperature accelerated molecular dynamics, hybrid MC/MD, DPD, lattice Boltzmann simulations, Maggs method, and dipolar P3M. ESPResSo++ will also perform parallel, multiscale simulations of molecular systems where the representation of each molecule (all-atom versus coarse-grained) can be changed on-the-fly (i.e., Adaptive Resolution Scheme or AdResS). The software has been designed to make it simple to add new algorithms as well. This will enable scientists to use ESPResSo++ as a research platform for their own methodological developments, which at the same time allows the software to grow and acquire the most modern methods. The ESPResSo++ kernel has been made efficient by use of advanced C++ programming language features, high-performance storage techniques, and cache optimization. One distinguishing feature of the package is that ESPResSo++ simulations are controlled by a Python script. This approach provides maximal freedom and it makes online analysis and interactive simulations possible. Furthermore, users may take advantage of the many offerings of Python such as the SciPy and NumPy libraries. ESPResSo++ is targeted for a range of machines from single-processor desktop workstations to high-performance supercomputers. It is intended to be used for scientific as well as industrial applications. The software is licensed under the GNU General Public License. Detailed information about the ESPResSo++ project is available online (http://www.espresso-pp.de).