ESPResSo – An open source package for simulating coarse-grained models

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ESPResSo[1, 2] is an open-source simulation package for coarse-grained models. The primary simulation approaches are molecular dynamics as well as lattice-Boltzmann hydrodynamics. The package is used in a wide variety of research fields including soft matter, statistical and biological physics and process engineering. Examples for its use include electrophoresis of polymers and colloids, phase equilibria in polyelectrolytes and gels, magnetic soft matter, dynamics of self-propelled bacteria, and agglomeration of soot particles in combustion exhausts.

The strength of the package is its Python interface, controlling an efficient MPI-parallel simulation core. This provides a high degree of flexibility in the simulation process and is particularly useful to develop new simulation techniques. The use of Python makes it easy to get started with the package and allows for a tight integration of the simulations with other Python packages for scientific calculations, plotting and machine learning.

ESPResSo is developed following a transparent process in line with the FAIR principles. The code is hosted on GitHub, additions and changes are peer-reviewed and have to pass automated tests before being merged. More than 100 authors have contributed to the project, so far. We currently pursue four main development goals:

1. coupling ESPResSo to the waLBerla[3] package for stencil methods, to make rapidly prototyped[4] lattice-based schemes, e.g., for the diffusion-advection-reaction equation and for lattice-Boltzmann hydrodynamics available to molecular dynamics simulations in ESPResSo.

2. better support for Monte Carlo schemes, as they are often combined with molecular dynamics, e.g., to model chemical reactions

3. making ESPResSo a development platform for machine-learned potentials, by coupling to established software pakages from that field

4. within the EuroHPC Center of Excellence MultiXScale, improve ESPResSo's scaleability on HPC systems.

References

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