High-resolution Simulations of Strongly Coupled Coulomb Systems with a Parallel Tree Code

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Plasma systems that can be experimentally studied today are reaching from hot, low-density plasmas of fusion research to cold dense solids that are dominated by quantum-mechanical effects and strong correlations. Their consistent theoretical description requires a multitude of effects to be considered. In particular, strong correlations pose significant difficulties here. Computer simulations provide a tool for bridging between experiments and theory as they do not suffer from these complications.

The experimentally accessible optical and transport properties in plasmas are primarily featured by the electronic subsystem, such as its collective behavior and interaction with the ionic background, i.e. Coulomb collisions. In this work the collisional behavior of warm dense bulk matter and collective effects in nano plasmas are investigated by means of molecular dynamics simulations. To this end, simulation experiments performed earlier on electronic resonances in metallic nano clusters are extended to significantly larger systems. The observed complex resonance structure is analyzed using a newly introduced spatially resolved spectral diagnostic. As a second field of study, the bulk collision frequency as the key parameter for optical and transport properties in warm dense matter is evaluated in a generalized Drude approach for a hydrogen-like plasma. Here, the combined high-field and strong coupling regime that is only scarcely covered by theoretical models is of primary interest.

To solve the underlying N-body problem for both applications, a highly parallel Barnes-Hut tree code is utilized and considerably extended with respect to functionality, versatility, and scalability. With its new excellent scalability to hundred thousands of processors and simulation setups consisting of up to billions of particles and its support for periodic boundary conditions with an efficient and precise real-space approach it delivers highly resolved results and is prepared for further studies on the warm dense matter regime. Here, its unique predictive capabilities can finally be used for connecting to real-world experiments.

This publication was written at the Jülich Supercomputing Centre (JSC) which is an integral part of the Institute for Advanced Simulation (IAS). The IAS combines the Jülich simulation sciences and the supercomputer facility in one organizational unit. It includes those parts of the scientific institutes at Forschungszentrum Jülich which use simulation on supercomputers as their main research methodology.

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