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

Mathias Winkel
# Contents

List of Figures xiii  
List of Tables xv  
List of Algorithms xvii  

1 Introduction 1  
1.1 Fundamental plasma parameters ................................. 3  
1.2 MAXWELL’s equations and the dielectric function .............. 11  
1.3 LORENTZ plasma and DRUDE model ............................. 13  
1.4 The electron-ion collision frequency ........................... 15  
1.5 Scope of this work .............................................. 19  

2 The N-body problem 21  
2.1 Molecular dynamics from basic principles ....................... 21  
2.2 Numerical considerations – mathematics ........................ 23  
2.2.1 Time discretization and general molecular dynamics .......... 23  
2.2.2 Leap-frog integration ....................................... 24  
2.2.3 Simulation timestep ....................................... 25  
2.3 Technical constraints – computers ................................ 27  
2.4 The N-body problem ........................................... 28  
2.4.1 Direct summation ........................................... 29  
2.4.2 Grid-based approaches ....................................... 29  
2.4.3 Multipole-based approaches ................................. 30  

3 The parallel Barnes-Hut tree code PEPC 37  
3.1 The BARNES-HUT algorithm ..................................... 38  
3.1.1 Tree construction ........................................... 38  
3.1.2 Computation of multipole properties .......................... 38  
3.1.3 Tree traversal and multipole acceptance criterion ........... 41  
3.2 The parallel tree algorithm ...................................... 45  
3.2.1 Allocation of globally unique keys ............................ 46  
3.2.2 Hash table .................................................. 48  
3.2.3 Domain decomposition ....................................... 49
## Contents

3.2.4 Parallel tree construction ........................................... 50
3.2.5 Parallel tree traversal ............................................... 52
3.3 Performance analysis for the pure-MPI tree code PEPC ............... 54
3.4 Other implementations and algorithm variations ....................... 58
3.5 Summary .............................................................. 60

4 Periodic boundary conditions ........................................... 61
4.1 Periodic movement constraint .......................................... 61
4.2 Periodic forces and potential ......................................... 62
4.2.1 Next-neighbor periodicity ......................................... 62
4.2.2 Nearest-image periodicity ......................................... 63
4.2.3 Ewald summation .................................................... 63
4.2.4 FMM-approach for periodic boundary conditions ................. 65
4.2.5 Renormalization approach for the lattice coefficients ............. 70
4.2.6 Near-field .......................................................... 76
4.2.7 Dipole correction .................................................... 76
4.3 Verification of correctness and computational overhead ............... 78
4.4 Summary .............................................................. 81

5 Multi-level parallelism .................................................... 83
5.1 Hybrid parallelization ................................................... 83
5.1.1 An MPI + Pthreads tree traversal .................................. 84
5.1.2 Performance results for the new approach ......................... 90
5.1.3 Intra- and inter-node load balancing ............................. 94
5.2 Branch nodes ........................................................... 95
5.2.1 A-priori branch node estimation .................................. 96
5.2.2 Hierarchical branch node clustering ................................ 96
5.3 Modularity, applications, and further prospects ....................... 98
5.3.1 Modularity and further applications ................................ 98
5.3.2 Projected technical optimizations ................................ 100
5.3.3 Further hybrid parallelism and task-based approaches .......... 100
5.3.4 Additional directions of parallelization ......................... 101
5.4 Summary .............................................................. 102

6 Collective electronic properties in nano clusters ......................... 105
6.1 Introduction ........................................................... 106
6.2 Numerical simulation setup ............................................ 106
6.3 Total momentum autocorrelation function ............................ 109
6.3.1 Dynamical conductivity and its connection to simulation ......... 109
6.3.2 Simulation results ................................................... 112
6.3.3 Analysis and theory for the resonance shift ....................... 116
6.3.4 Conclusions ........................................................ 118
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.

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