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Scaling Particle-based Simulations of Plasma Processes to Industrial Applications using HPC

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Significant physical insight into the relevant industrial processes that are related to thin film deposition can be obtained from particle-based numerical simulation tools. Due to their heavy computational demand, however, numerous large-scale technical applications are still infeasible to examine via simulation. Different generic test cases for low-pressure plasma, such as magnetron sputtering or plasma source devices, can bridge the gap between academic desktop-scale and industry-relevant scales. The considered benchmarks serve as demonstrators showing the advantages of high-performance computing for industrial applications. The simulations are performed using the open-source code PICLas (<https://github.com/piclas-framework/piclas>), which is a parallel, three-dimensional PIC-MCC/DSMC solver that is developed cooperatively by the Institute of Space Systems, the Institute of Aerodynamics and Gas Dynamics at the University of Stuttgart and the spin-off boltzplatz. The software is fully parallelized for distributed memory systems via Message Passing Interface (MPI) and optimized to run on modern high-performance computing (HPC) architectures. Domain decomposition is performed using space-filling curves and the sub-domains can be dynamically re-distributed among the available MPI processes during run-time. Important HPC aspects, such as dynamic workload balancing approaches, are highly crucial when efficient simulations are required. With increasing number of processors or high heterogeneity within the simulation domain, workload imbalances can heavily decrease the overall simulation efficiency. This can be encountered by improved algorithms, which detect and reduce workload imbalances. Previously, different strategies have been implemented in PICLas for measuring and re-distributing workloads. In future, these schemes continue to play a critical role, e.g., when complex three-dimensional simulations of industry-relevant applications are considered, where strong workload imbalances are present.

Keywords

PIC-MCC/DSMC

Simulation

HPC