Hybrid Parallelization of Particle-Field Coupled Plasma Simulations based on MPI-3 Shared Memory

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Next-generation plasma thrusters for the aerospace industry are being developed by combining the ongoing efforts in experimental and numerical research and are important for current and future space programs. Due to the complex physical nature of various effects that are observed within electric propulsion systems, such as Hall-effect or high-efficiency multi-stage plasma thrusters, experiments cannot always give the necessary insight that is required to improve these devices. Under this premise, PICLas [1] has been developed with the requirements of a simulation tool that is highly efficient, scalable and physically accurate to cover a wide range of academic and industrial applications in the field of plasma physics and rarefied gas flows. The numerical approximation of Boltzmann's equation is at the core of the tool, which describes chemically reacting rarefied gas and plasma flows in a kinetic manner with the help of statistical mechanics. The coupling of the Particle-In-Cell method with the Monte Carlo Collision or Direct Simulation Monte Carlo Collision method has shown to be an efficient numerical approach to tackle complex plasma flows. The different particle- and field-based methods in PICLas can be used separately or in combination to adequately describe the complex multi-scale physics of problems that are encountered. Due to the computationally challenging task posed by these methods, high-performance computing has enabled the utilization of such tools during the past decades. One of the major bottlenecks that is encountered in particle-field coupled simulations of complex three-dimensional flows are temporal or spatial workload imbalances between the processors that are created by strongly heterogeneous problems. In electric propulsion systems, this can occur when physical phenomena like particle-field instabilities arise, which lead to a strong concentration of simulation particles in specific spatial or temporal regions of the simulation domain. This generates subsequent problems for the domain decomposition of the simulation when domain partitioning is used to equally distribute the workload among the available processors. To tackle this problem in combination with a large number of processors, PICLas offers dynamic load balancing, where the execution times of the relevant algorithms are measured on the fly, sampled and assigned to the corresponding simulation elements. The elements are then assigned to each processor using a space-filling curve, which is divided depending on the workload of each element in order to give each processor an equal share of the total workload. Because current and future CPU-based HPC systems steadily increase the number of physical processors on each compute node, advanced programming models are required for an effective parallelization of existing and future code frameworks. Due to the reduction of per-core random access memory in these systems, PICLas that was originally designed as a purely MPI-based scheme, has incorporated MPI-3 shared-memory approaches to mitigate this problem. Furthermore, this approach allows a communication-free identification of the overlapping regions between different compute nodes, i.e., elements where particles are able to transition from one compute node to another.

References

[1] S. Fasoulas, C.-D. Munz, M. Pfeiffer, J. Beyer, T. Binder, S. Copplestone, A. Mirza, P. Nizenkov, P. Ortwein, and W. Reschke. "Combining particle-in-cell and direct simulation Monte Carlo for the simulation of reactive plasma flows". In: *Physics of Fluids* 31.7 (2019), p. 072006.

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