TOWARDS LARGE-SCALE KINETIC SIMULATIONS OF THE PLASMA-MATERIAL INTERFACE

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PI: Davide Curreli[1]
Co-PIs: Rinat Khaziev[1]
Collaborators: Ryan Mokos[2] and Gregory H. Bauer[2]

[1]University of Illinois at Urbana-Champaign
[2]National Center for Supercomputing Applications/University of Illinois at Urbana-Champaign

EXECUTIVE SUMMARY

In the edge region of magnetically-confined plasmas, the interaction of plasmas and material surfaces poses significant challenges to the survivability of plasma-facing components, currently limiting the successful development of commercially-viable nuclear fusion reactors. Taming the plasma-material interface is one of the top priorities of fusion science research in order to achieve a demonstration fusion power plant. When exposed to plasma irradiation, plasma-facing materials exhibit evidence of surface morphology modifications and nanostructuring, with detrimental consequences on the thermo-mechanical integrity of the wall.

We have improved the on-node performance and tested the scalability on Blue Waters of the hPIC code (HPC platform for Plasma-Material Interactions and Nanostructuring), a fully-kinetic platform for kinetic analysis of plasma-material interactions, including both a Boltzmann description of the near-wall plasma and the multi-physics response of the material surface.

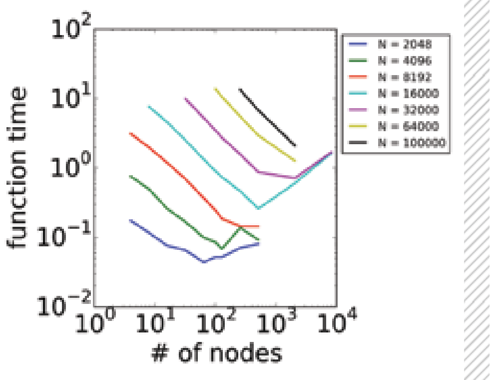

FIGURE 1: Blue Waters scaling of the field module of hPIC with multigrid preconditioner on a square plasma domain of size of NxN. As expected, the scaling deteriorates when small problems are solved at the largest node count.

INTRODUCTION

Understanding the interaction of plasmas with material walls is relevant to the design of the next generation of fusion devices and to industrial processes exploiting plasmas for material manufacturing. In the presence of physical boundaries, plasmas form a near-wall layer, called the plasma sheath, in which the charged particles normally at equilibrium inside the plasma bulk are supersonically accelerated toward the wall. Such acceleration increases the kinetic energy of the particles to levels that might overcome the erosion threshold (sputtering), causing the release of particles from the material wall. The dynamics of this process can be well resolved with electrostatic particle-in-cell (PIC) simulations [1], a well-known numerical method for the solution of the Boltzmann kinetic equation of an ensemble of interacting particles. A typical iteration cycle of a PIC code [2] includes: (1) particle push, during which the particles are moved and their properties (mass, charge) are weighted on the mesh, and (2) the calculation of the electric and magnetic fields from the Maxwell equations and their interpolation at the particles' location. For electrostatic PIC codes it is safe to assume that magnetic field configuration is fixed or quasistatic, and the only equation to solve is the Poisson equation. The major difference between electrostatic PIC (ES-PIC) codes and electromagnetic PIC (EM-PIC) codes is that the latter benefit from the locality of the Maxwell-Faraday and Ampere's equations. Several electromagnetic PIC codes have been developed, showing excellent scalability up to the largest number of nodes on high-performance computing (HPC) systems.

However, existing electrostatic PIC codes are not well supported on HPC systems. Nevertheless, electrostatic PICs are preferable for plasma-material interaction (PMI) problems because they allow less restrictive conditions on the time step and because electromagnetic modes add negligible features in a PMI context. Electrostatic PICs require the solution of an elliptic problem, rather than a set of hyperbolic equations as in electromagnetic PIC codes. In an HPC context, such a difference translates to the need for a more complex communication strategy for ES-PICs. The parallel data partitioning of an ES-PIC code is dictated by the partitioning of the linear solver and by the geometric partitioning of the particle arrays, requiring a different parallelization scheme. The goal of this work was to adapt our electrostatic PIC code hPIC for runs on petascale and exascale supercomputers and to characterize the code's performance at large node numbers.

METHODS & RESULTS

In our implementation of the ES-PIC method we rely on Poisson solvers developed by the FASTMath-SciDAC institute [4], offering a variety of scalable methods for the solution of linear and non-linear algebraic problems. Our code hPIC has been linked to the PETSc library as a back-end. Most of the hPIC development effort has been devoted to improving the on-node performance of each code component and to testing the code on a large number of nodes on Blue Waters. Tests have demonstrated that algebraic multigrid preconditioners with conjugate gradient offer the best solution in terms of parallel performance. Tests were performed on square plasma domains of size *NxN* (with *N* being the number of grid nodes along one dimension). For the largest test case evaluated (*N*=100,000), which corresponds approximately to a plasma domain of 1m² with plasma properties such as those found in the scrape-off layer of fusion devices, the time required to solve the electrostatic problem (Figure 1) was of the order of 2 seconds on 8,192 Blue Waters nodes (262,144 cores). An efficient implementation of the particle parallelization scheme has been adopted, storing the particles along the corresponding field arrays of the Poisson solver, requiring the communication of only those particles no longer associated with the field arrays locally stored at the node level. Tests have shown that this particle communication scheme typically requires less than 1 millisecond on Blue Waters for all cases relevant to our applications, with excellent weak-scaling properties (Figure 2).

WHY BLUE WATERS

Simulations of large plasma volumes at resolutions large enough to resolve the plasma sheath require extensive computational resources, both for node number (more than 1,000 Blue Waters XE nodes) and **in-node memory**. The Blue Waters support staff facilitated fast transition from previous HPC platforms to Blue Waters. Blue Waters offered an excellent environment for code development, both for on-node optimization and testing/profiling, which uniquely contributed to the code optimization at all steps.

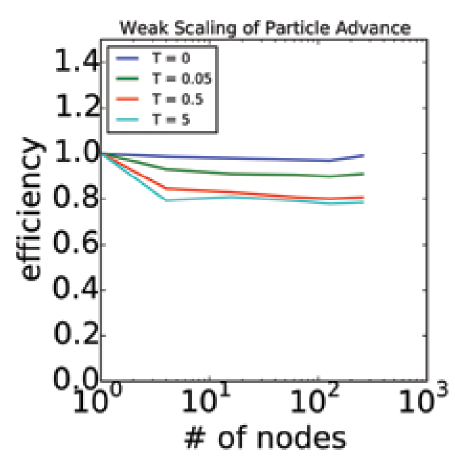

FIGURE 2: Weak scaling test of hPIC on Blue Waters with 32 million particles per node, mesh of 55,000x55,000 on each Blue Waters node (1 million particles per MPI process, 100 particles per cell, 100x100 mesh on each MPI process). The weak scaling holds well with efficiency close to 100% for T=0 (cold plasma), ~91% for T=0.05 (typical ions) and ~80% for T=5 (typical electron plasma).

NEXT GENERATION WORK

The HPC resources available with the next-generation of Track-1 systems will allow us to perform large-scale 2D-3V plasma simulation of the plasma-material interface, potentially simulating a large portion of the divertor private region of a tokamak (a device that uses a magnetic field to confine plasma in a torus), a large portion of the scrape-off layer facing the first wall, or a full-scale industrial plasma device. The code is also ready to explore the first small 3D simulations of the plasma material boundary. Three-dimensional effects are expected to play a vital role at the boundary of stellarator fusion devices, like the Hybrid Illinois Device for Research and Applications (HIDRA) recently acquired by the University of Illinois at Urbana-Champaign.