BOUT++: Performance Characterization and Recent Advances in Design*

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Simulating turbulence and transport in edge plasma is one of the most critical areas of tokamak fusion modeling because the edge region sets key engineering constraints for the plasma-facing material components and plays a crucial role in plasma confinement for maximum fusion gain. The edge is also one of the most challenging regions to simulate due to complex physics and the magnetic geometry. Analyzing the performance and parallel communication patterns of numerical methods is essential to achieve efficient, robust, and scalable simulations. Moreover, attention to software design to facilitate multiphysics coupling is becoming increasingly important.

This work characterizes the performance and describes recent advances in the design of BOUT++, a parallel framework for three-dimensional plasma fluid simulations in the divertor tokamak boundary region. BOUT++ inherited some key concepts from the original fluid edge code BOUT but is much more general. The aim of BOUT++ is to automate common tasks and to separate implementation details from physics modules, so that users can easily work with a broad range of physics models for multiple fluid variables in general coordinate systems We explain the use of design patterns in BOUT++ to facilitate interfacing to time integration capabilities in two complementary libraries, SUNDIALS and PETSc. This approach provides flexibility in selecting different runtime options for the libraries, thereby facilitating experiments with a variety of numerical methods and enabling the incorporation of newly developed algorithms.

BOUT++ simulations have been profiled on a petascale Cray XE6 platform to identify critical performance characteristics, including scalability, memory/network bandwidth limitations, and communication overhead. We analyze the performance of implicit time integration algorithms that employ Jacobian-free Newton-Krylov methods to solve the nonlinear systems that arise at each timestep, and we determine opportunities for future algorithmic enhancements. We also discuss recent changes in the design to enable BOUT++ to function within the FACETS framework, which has the goal of providing integrated modeling of the core, edge, and wall regions of fusion devices.

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