BOUT++: Performance Characterization and Recent Advances in Design

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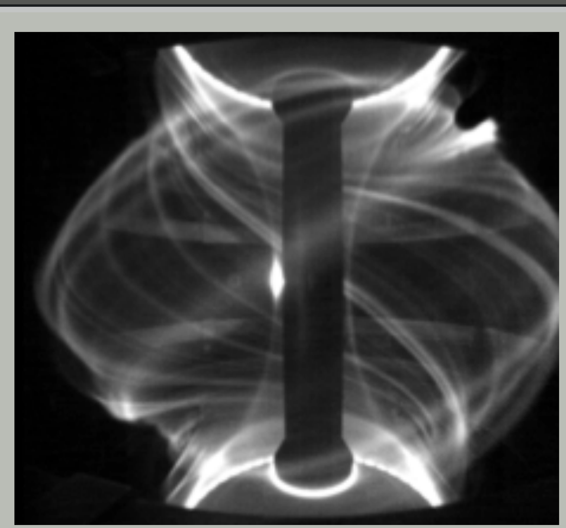
Edge Localized Modes

- Fast ($\sim 100\mu s$) eruption from the edge of tokamak plasmas
- If uncontrolled in ITER, these would release ~ 20 MJ
- World-wide effort to understand and control these events

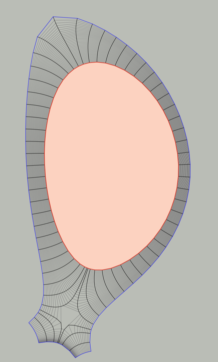


The BOUT++ Simulation Code

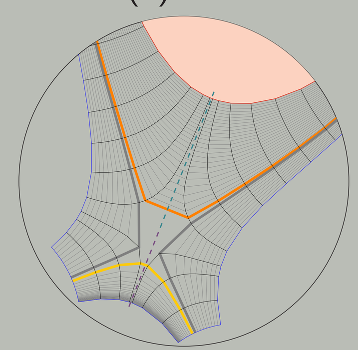
- Based on BOUT written by X. Xu, et. al. from LLNL [1]
- New 3D simulation code developed at York with LLNL and ANL
- Simulates plasma fluid equations in curvilinear coordinate systems
- Runs on workstations, clusters, large-scale machines, e.g., Cray XE6

ELM Equations

$$
\begin{aligned}
\rho_0\frac{d\omega}{dt} &= B_0^2 b\cdot\nabla\left(\frac{J_{||}}{B_0}\right) + 2b_0\times\kappa_0\cdot\nabla p\\
\frac{\partial A_{||}}{\partial t} &= -\nabla_{||}\phi\\
\frac{dp}{dt} &= -\frac{1}{B_0}b_0\times\nabla\phi\cdot\nabla p_0\\
\omega &= \frac{1}{B_0}\nabla_\perp^2\phi\\
J_{||} &= J_{||0} - \frac{1}{\mu_0}\nabla_\perp^2 A_{||}\\
\frac{d}{dt} &= \frac{\partial}{\partial t} + \frac{1}{B_0}b_0\times\nabla\phi\cdot\nabla
\end{aligned}
$$
[3]



(a) Mesh



(b) X-Point

References

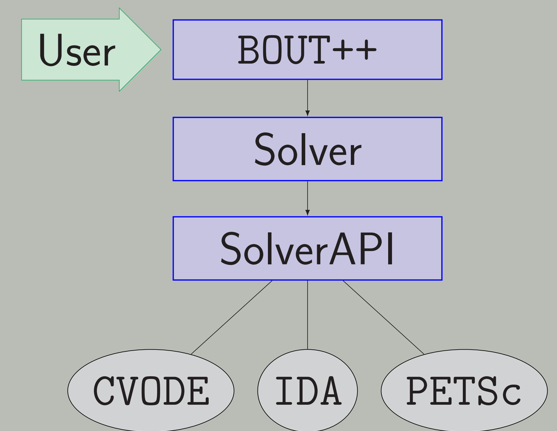
[1] BD Dudson et al. "BOUT++: A framework for parallel plasma fluid simulations". In: *Computer Physics Communications* 180.9 (2009), pp. 1467–1480.

[2] P Narayanan et al. "Performance Characterization for Fusion Co-design Applications". In: *Proceedings of CUG* (2011).

[3] XQ Xu et al. "Nonlinear Simulations of Peeling-Ballooning Modes with Anomalous Electron Viscosity and their Role in Edge Localized Mode Crashes". In: *Physical review letters* (2010).

Software Design Issues

- Time integration and Newton-Krylov nonlinear solves using SUNDIALS (LLNL) or PETSc (ANL)
- Coordinate system and differential operators
- Parallel communications using MPI



SUNDIALS: `https://computation.llnl.gov/casc/sundials`
PETSc: `http://www.mcs.anl.gov/petsc`

Jacobian-free Newton-Krylov Method

At each timestep, we solve the nonlinear system

$$F(x) = 0,$$

where $F : \mathbb{R}^n \to \mathbb{R}^n$ by a Newton-Krylov method

$$x_{k+1} = x_k - [F'(x_k)]^{-1}F(x_k), \quad k = 0, 1, \ldots,$$

where x_0 is an initial approximation to the solution and $F'(x_k)$, the Jacobian, is nonsingular at each iteration. In practice, the Newton iteration is implemented by the following two steps:

1. (Approximately) solve $F'(x_k)\Delta x_k = -F(x_k)$.
2. Update $x_{k+1} = x_k + \alpha\Delta x_k$.

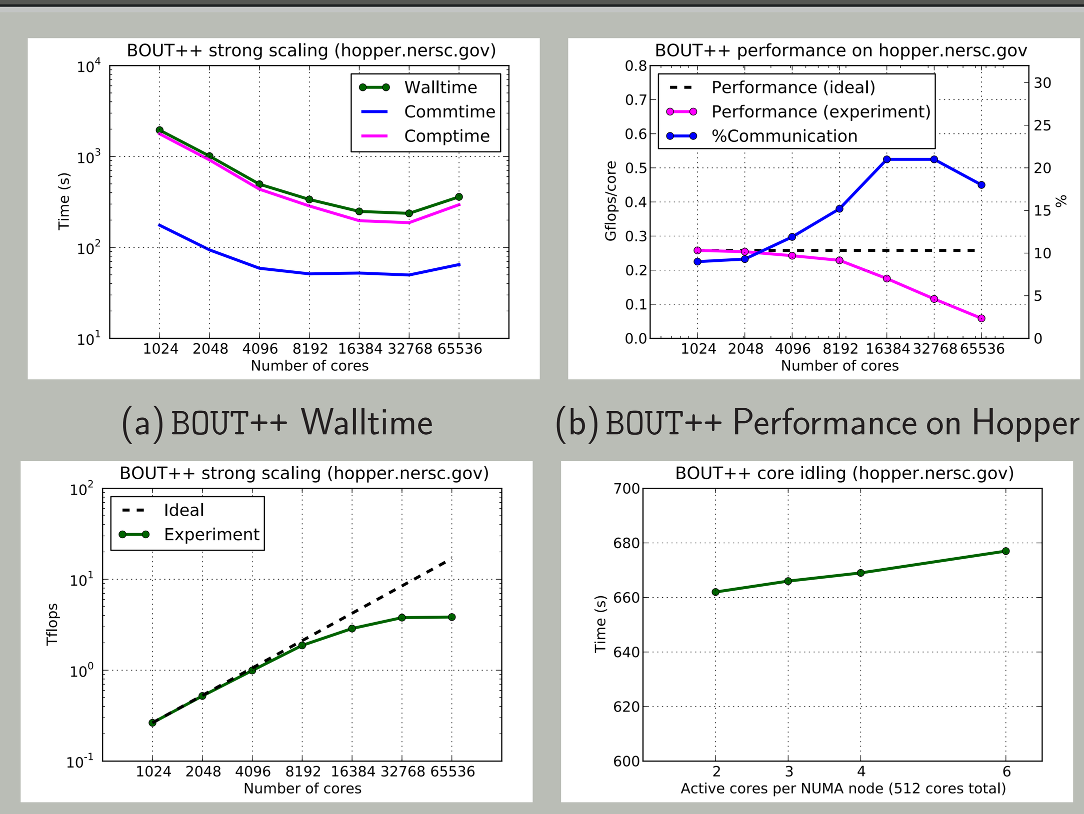
where $0 < \alpha \leq 1$ is a scalar. Jacobian-vector products in Krylov methods are computed matrix-free via

$$F'(u)a \approx \frac{F(u + h\cdot a) - F(u)}{h}$$

FACETS

- Framework Application for Core-Edge Transport Simulations
- PI: John Cary, `http://www.facetsproject.org`
- FACETS goal: Modeling of a fusion device from the core to the wall
- Work in progress: Incorporating BOUT++ as a FACETS component

Performance Analysis



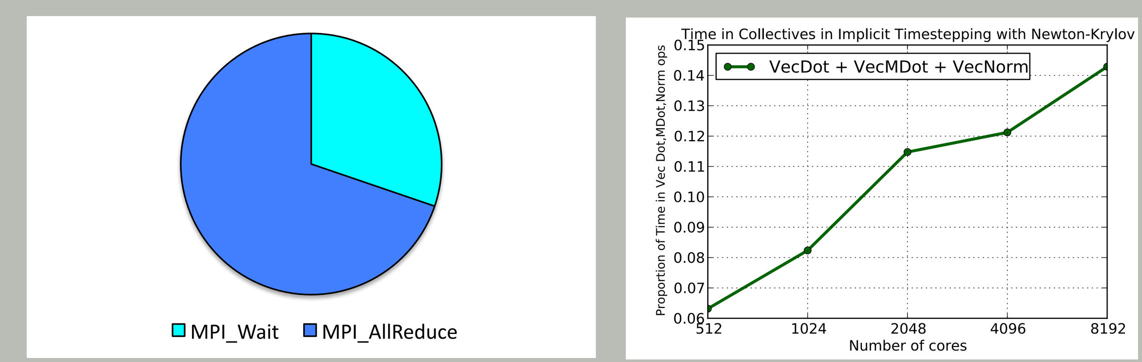
(a) BOUT++ Walltime (b) BOUT++ Performance on Hopper

(c) BOUT++ Strong Scaling (d) BOUT++ Core Idling

Figure 1: Strong scaling using CrayPAT on Hopper (NERSC) using ELM pb (nx=516, ny=512, nz=64) [2]

Figure 1(a) shows overall walltime, time spent in communication, and time spent in computation. Figure 1(b) presents the flops performance (Y-axis on left) and the communication as percentage of runtime (Y-axis on right). Figure 1(c) demonstrates strong scaling. Figure 1(d) illustrates that BOUT++ is relatively insensitive to bandwidth contention. [2]

MPI Collectives



(a) (b)

Figure 2: MPI Collectives on Hopper (NERSC)

Figure 2(a) shows the role of MPI collectives at high concurrency (65,536 processors) for test case 1. Figure 2(b) indicates that the cost of `MPI_Allreduce()` calls inside Newton-Krylov solver are a significant scalability barrier for ELM pb: nx=516, ny=64, nz=16, global vector dimension: 1,585,152. Data from 10 timesteps, Newton with restarted GMRES, no preconditioning

Ongoing and Future Work

- Research on robust and scalable preconditioners
  - Algebraic approaches that use sparse approximate Jacobian information
  - Leverage physics knowledge, including field splits for fast Alfven waves, fast magnetosonic waves, and thermal conductivity along the field lines
- Experiments with communication-reducing Krylov methods
- Exploration of IMEX techniques for flexible timestepping
- Incorporation into FACETS and exploration of multiphysics coupling issues
- Research on additional modeling capabilities

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