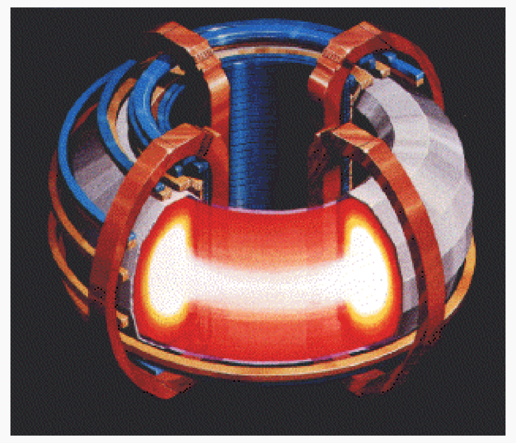
Scalable Preconditioners for Coupled Plasma/Neutral Boundary Transport Simulations

Michael McCourt[1,2], Tom Rognlien[3], Lois Curfman McInnes[2], Hong Zhang[2]

[1]Cornell University, [2]Argonne National Laboratory, [3]Lawrence Livermore National Laboratory

Office of Science
U.S. Department of Energy

Introduction



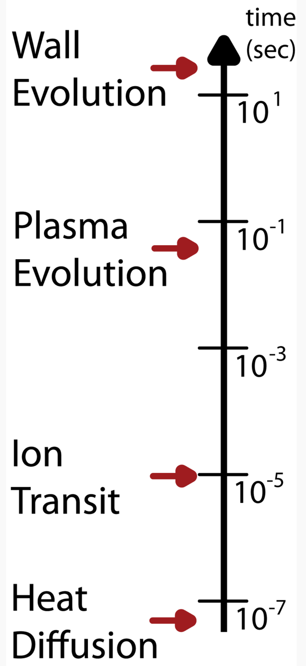
- We study simulations of the edge region of a Tokamak magnetic confinement fusion reactor using UEDGE.
  - UEDGE is a 2D parallel edge plasma application developed by T. Rognlien et al. (LLNL)
- UEDGE is one of the edge plasma transport components in FACETS.
  - FACETS: Framework Application for Core-Edge Transport Simulations based at Tech-X Corporation
  - PI: John Cary, `https://www.facetsproject.org`
  - FACETS goal: Strong coupling between core, edge and wall Tokamak regions during simulation

Governing Physics

UEDGE uses a fluid transport model, conserving particles, momentum and energy.

- Simulations use $\Delta t \in [10^{-4}, 10^{-3}]$ sec, appropriate for coupling to time-dependant core models.
  - Coupled plasma/neutral simulations involve a large range of spatial and temporal scales.
- Several coupled variables interact in the basic simulation:
  - Deuterium ion D^+ temperature
  - Deuterium ion D^+ density
  - Deuterium ion D^+ parallel velocity
  - Electron e temperature
  - Neutral Deuterium D density
- Strong nonlinearities can yield ill-conditioned simulations

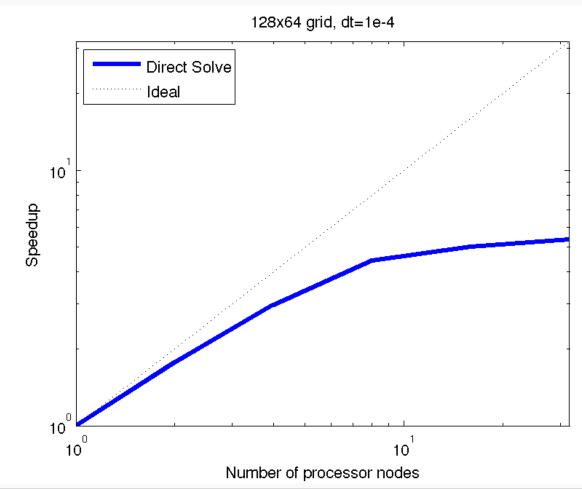
Competing Time Scales

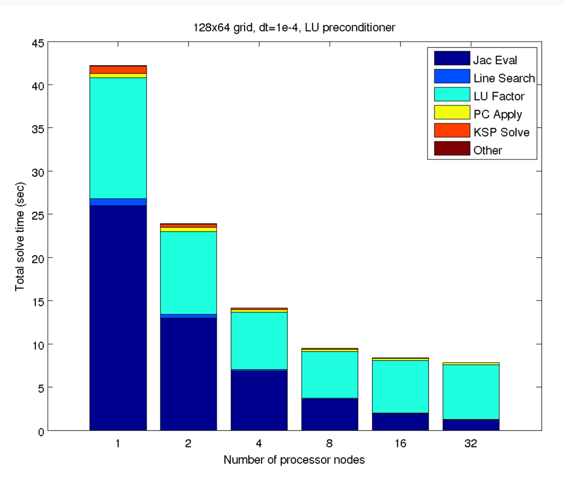


- Impurities in the plasma arise from:
  - Plasma sputtering of material walls, and
  - Edge transport competing with ionization/recombination.
  - Solving each charge state (or bundle) creates large systems.

Algorithms

- Implicit time discretization with nonlinear solves via preconditioned Jacobian-free Newton-Krylov
  - The choice of preconditioner is vital to achieving scalability
- PETSc is used to conduct the simulation in parallel
- Early experiments showed limited scalability
  - The direct solver becomes overwhelmed by the cost of LU factorization and associated communication.

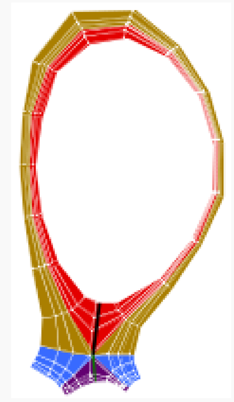




Motivating a Physics Preconditioner

Physics issues to consider for computational stability/accuracy/efficiency:

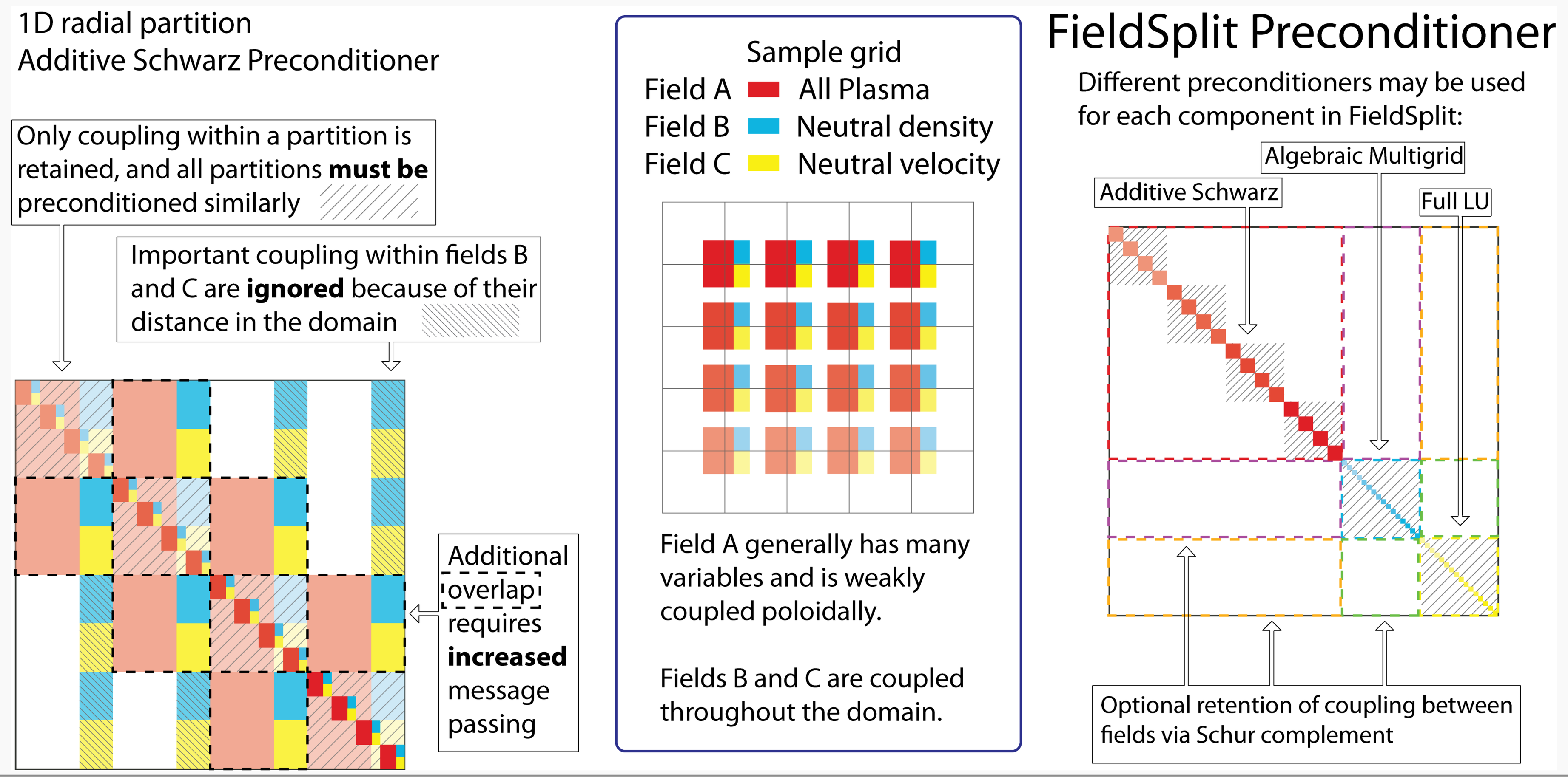
- Solving plasma and neutral equations on the same mesh simplifies their strong coupling; this is helpful to ensure an accurate simulation.
  - Wall particle recycling and ionization can result in long physical times to reach equilibrium; this competes with the fast edge plasma transport.
- To accommodate the dominant plasma transport, the discretization is highly anisotropic.
  - For standard Δt the plasma terms are well-conditioned enough to use an easily scalable preconditioner such as Additive Schwarz.
- However, neutral collisional diffusive transport is isotropic, and very ill-conditioned on an anisotropic mesh.



Radial width is much greater than poloidal

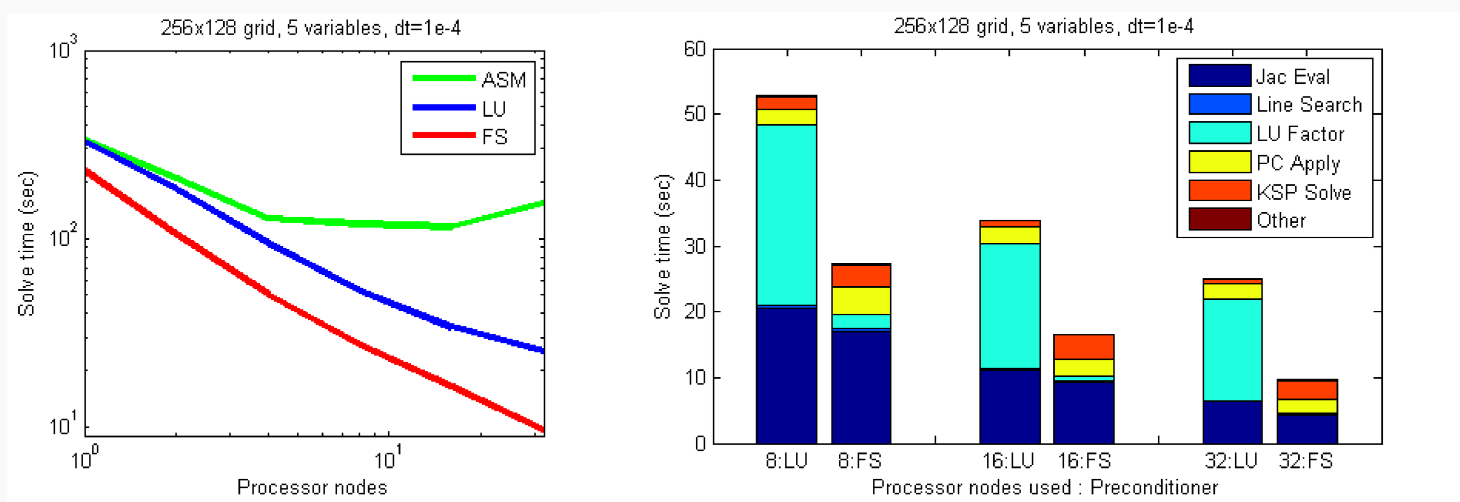
This physical knowledge implies that *separate* methods should be used to precondition the plasma and neutral terms within the nonlinear solver.

Designing a Physics Preconditioner: FieldSplit



Results: FieldSplit Preconditioning

- Initial FieldSplit structure - 2 separate fields preconditioned individually:
  - Field 1: 4 plasma terms solved with Additive Schwarz
  - Field 2: 1 neutral term solved with Algebraic Multigrid
- Component preconditioners are added together
- Coupling terms between fields are disregarded during preconditioning.

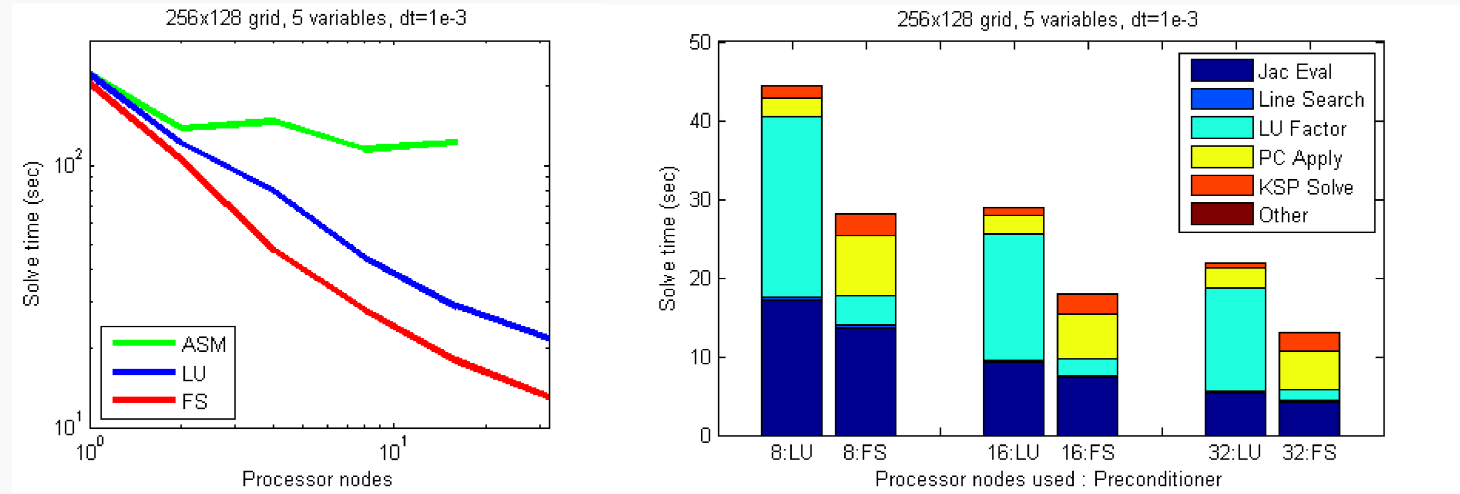


Solver	NP=32 results KSP its	Time (sec)
ASM	1585	154
LU	7	25
FS	44	10

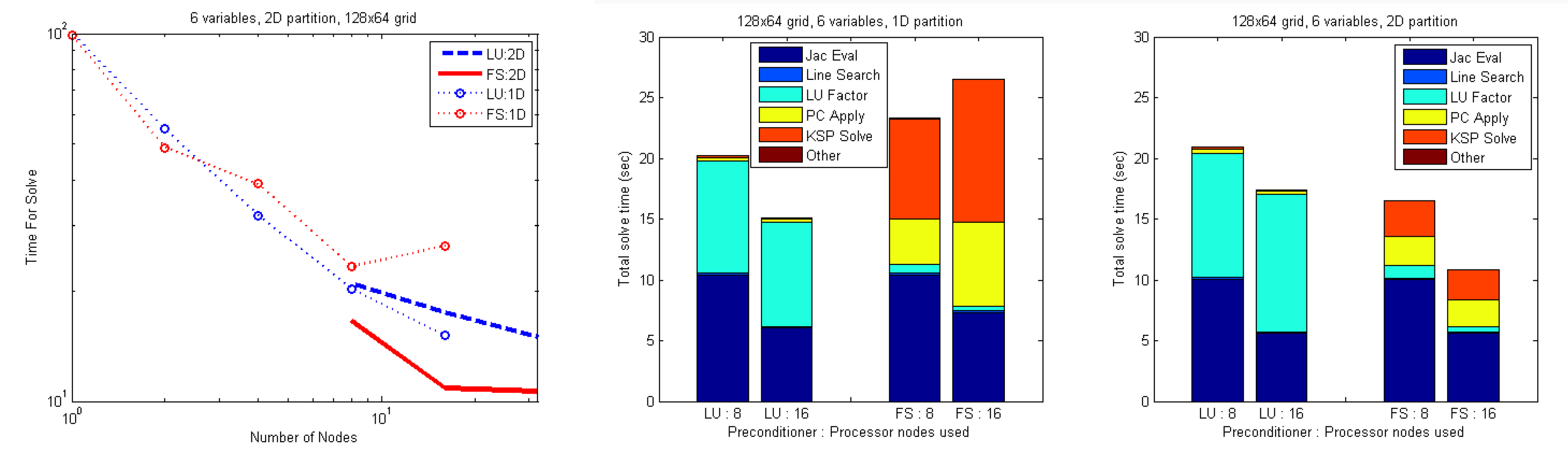
- By handling the troublesome fields (neutral gases) separately we can use a more scalable solver on the easier fields (plasma).
- 1D partitioning allows for the majority of fields (plasma) to be on their more optimal domain.

Results: Scalability for More Complex Problems

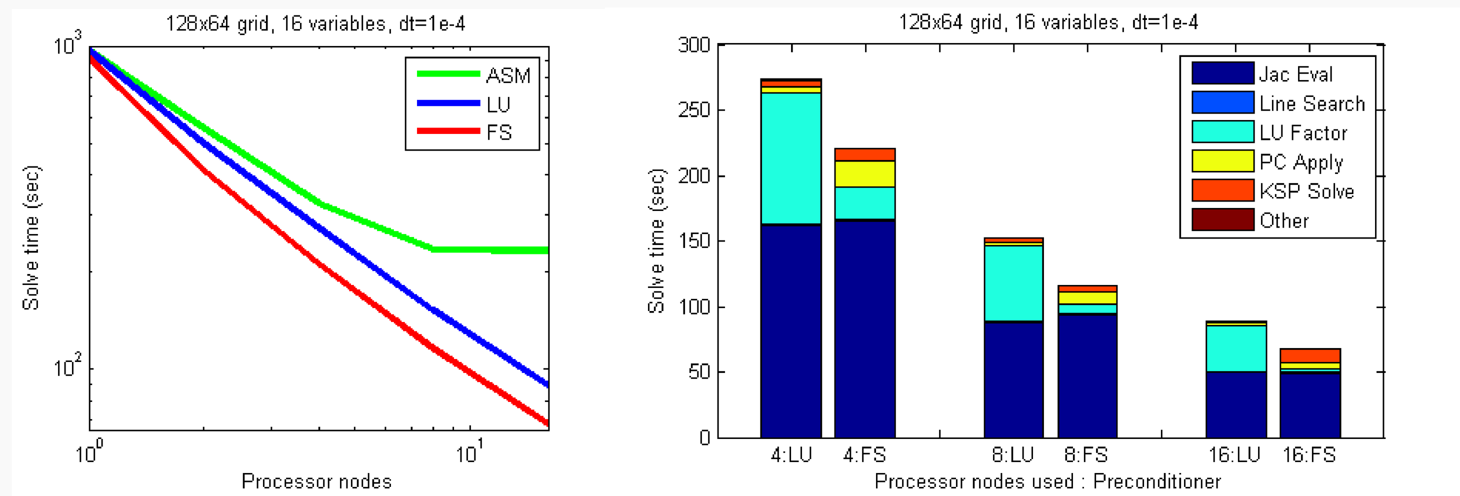
- FieldSplit performs well for larger time steps, so long as the plasma terms can still be solved scalably.



- Initially the neutral D velocity was computed with a simpler algebraic model. Below are results with its inclusion in the nonlinear solve.
  - A 2D partitioning is preferred for this problem, which is first available at NP=8.



- We also enjoy improved performance in the presence of a Neon impurity and the 11 new individual fields added as a result.



Conclusions

- FieldSplit overcomes a major obstacle to parallel scalability for an implicit coupled neutral/plasma edge model.
  - This allows greatly reduced runtimes when using multiple processors.
  - Little code manipulation is required.
- Jacobian-free Newton-Krylov within PETSc using FieldSplit preconditioning provides flexibility for optimizations such as
  - Redundant preconditioning on comparatively small fields,
  - Variable Additive Schwarz overlap, and
  - Jacobian lagging both within and across time steps.

Future Work

- As different species (e.g., He and C) are added and larger Δt used, how can FieldSplit be optimized?
- The goal of the FACETS project is Core-Edge-Wall coupling
  - How can this physics preconditioning be applied in a multiphysics setting?
  - What techniques developed here can be used in 3D edge codes, e.g., BOUT++?
- Coupling terms can be retained via the Schur complement.
  - Cost is greater than Additive FieldSplit.
  - While not needed so far, will this coupling be useful in multiphysics preconditioning?

Acknowledgements

Special thanks to Charles Van Loan, Satish Balay, and Barry Smith.