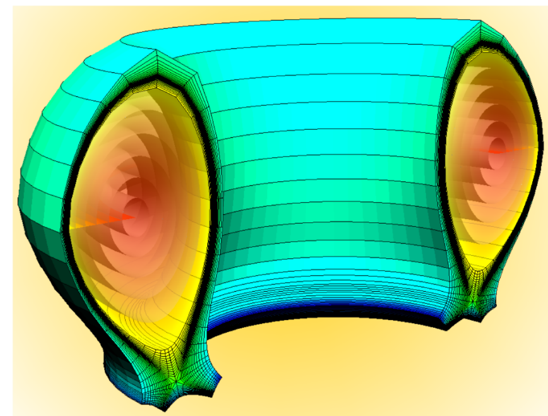
Applied Math Algorithms in FACETS

Proto-FSP Review, Sept 1, 2010, PPPL



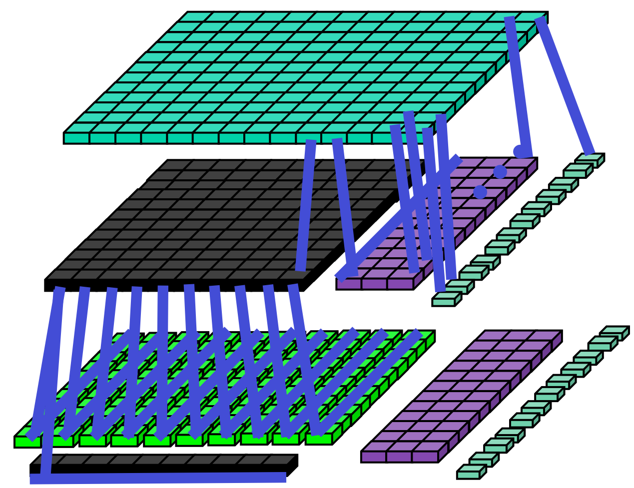
Speaker: Lois Curfman McInnes, ANL

Core: Alexander Pletzer, Tech-X

- **John Cary, Johan Carlsson, Tech-X:** Core solver
- **Srinath Vadlamani, Tech-X:** Turbulent flux computation via FMCFM
- **Ammar Hakim, Mahmood Miah, Tech-X:** FACETS infrastructure
- **Greg Hammett, PPPL:** Time stepping schemes
- **Alexei Pankin, Lehigh University**: Core transport benchmark against ASTRA

Edge: Tom Rognlien, LLNL

- **Satish Balay, ANL:** Portability and systems issues via TOPS
- **John Cary et al., Tech-X:** FACETS integration
- **Ron Cohen, LLNL:** Edge physics, scripting
- **Ben Dudson, Univ of York:** BOUT++ physics and design, no FACETS funding
- **Sean Farley, IIT:** Math grad student: BOUT++ solvers and componentization
- **Mike McCourt, Cornell:** Applied math grad student: UEDGE solvers
- **Maxim Umansky, LLNL:** BOUT++ physics, no FACETS funding
- **Hong Zhang, ANL:** Nonlinear solvers



Coupling: Don Estep, CSU

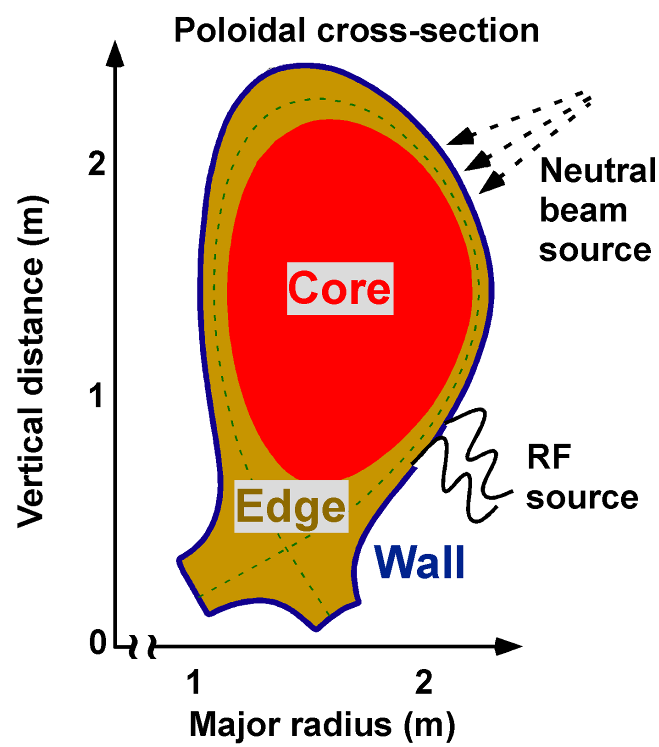
- **Brendan Sheehan, Simon Tavener, CSU:** Stability and accuracy issues in coupling
- **Ammar Hakim, Tech-X:** Explicit coupling in FACETS
- **Johan Carlsson, Tech-X**: Implicit coupling in FACETS
- **Ron Cohen, Tom Rognlien, LLNL:** Physics issues in coupling

SciDAC Scientific Discovery through Advanced Computing
Office of Science
Tech-X · Argonne National Laboratory · Colorado State University · General Atomics · LLNL · ORNL Oak Ridge National Laboratory · ParaTools · PPPL Princeton Plasma Physics Laboratory · UCSD · Lehigh

FACETS simulations rely on time-dependent, nonlinear PDEs

- **Current focus**
  - **Core** (new core solver, Tech-X)
  - **Edge** (UEDGE and BOUT++, LLNL)
  - **Core-edge coupling**

- **Discussion emphasizes**
  - **Collaboration with SciDAC TOPS Center**
  - **Implicit algorithms**
  - **Scalability**
  - **Stability and accuracy issues**

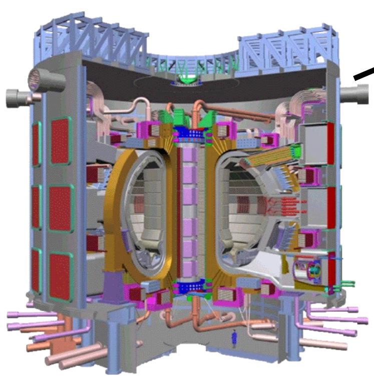


TOPS provides enabling technology to FACETS; FACETS motivates enhancements to TOPS

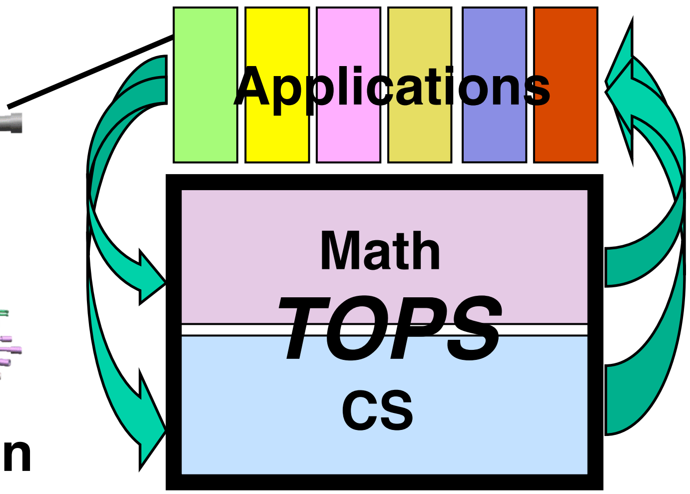
TOPS Overview

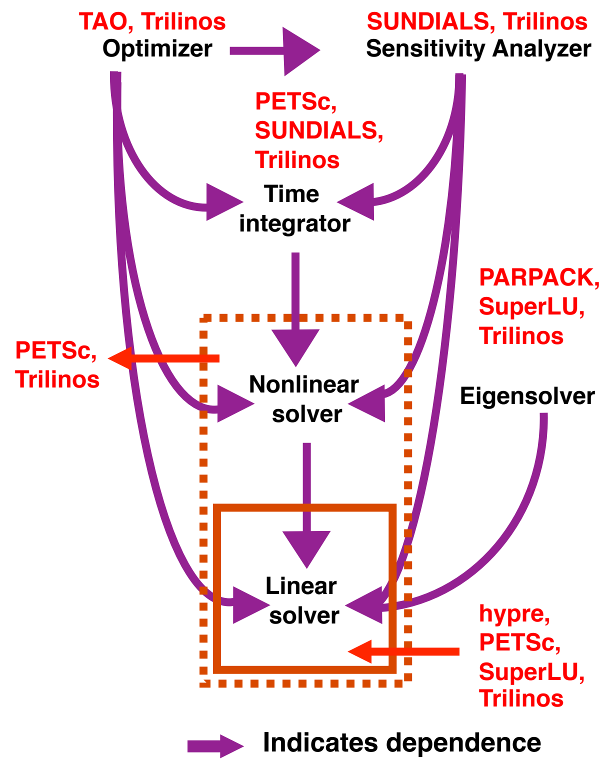
- **TOPS develops, demonstrates, and disseminates robust, quality engineered, solver software for high-performance computers**
- **TOPS institutions:** ANL, LBNL, LLNL, SNL, Columbia U, Southern Methodist U, U of California, Berkeley, U of Colorado, Boulder, U of Texas, Austin

TOPS
Towards Optimal Petascale Simulations
PI: D. Keyes, Columbia Univ.
www.scalablesolvers.org



FACETS fusion





Primary emphasis of TOPS numerical software

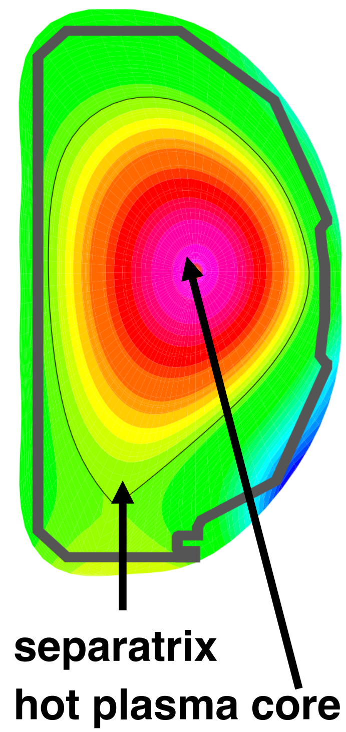
Tech-X, Argonne National Laboratory, Colorado State University, General Atomics, LLNL, ORNL Oak Ridge National Laboratory, ParaTools, PPPL Princeton Plasma Physics Laboratory, UCSD

FACETS' infrastructure allows high-order integration schemes for core

- Plasma core is the region well inside the separatrix
- Transport along field lines >> perpendicular transport, leading to homogenization in poloidal direction
- Core satisfies 1D conservation laws: $$\frac{\partial q}{\partial t} + \nabla \bullet F = s$$

  q = {plasma density, electron energy density, ion energy density}
  F = highly nonlinear fluxes including neoclassical diffusion, electron/ion temperature gradient induced turbulence, etc.
  s = particle and heating sources and sinks

- New core capabilities (A. Pletzer, Tech-X):
  - Get *s* from NUBEAM (PPPL)
    - has its own time advance algorithms
  - Arbitrarily high-order time steppers can be assembled for core at runtime
  - Employ nested iterations for improved convergence



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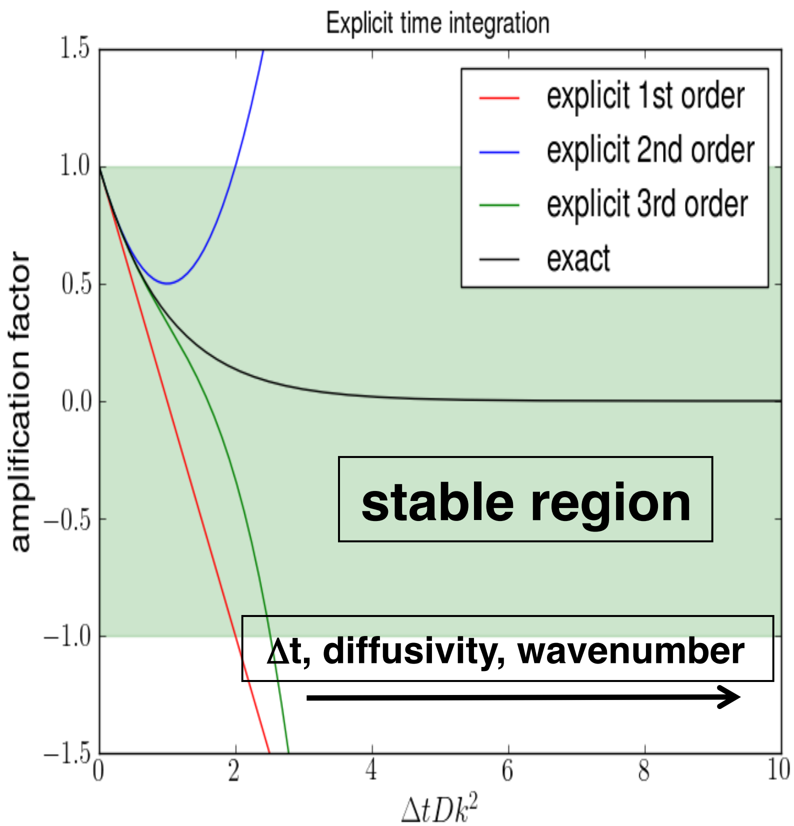
Turbulence makes core transport equations extremely stiff (nonlinear)

- Small changes in profiles can trigger large fluxes
- Explicit time stepping won't work, as explicit schemes have polynomial amplification factors A (bad!)
- Minimum stability requirement is A-stable ($|A| < 1$ for all Δt)
  - oscillations are damped after multiple iterations
- Also want L-stability ($|A| \to 0$ as $\Delta t \to \infty$)
  - oscillations are damped more rapidly for large Δt

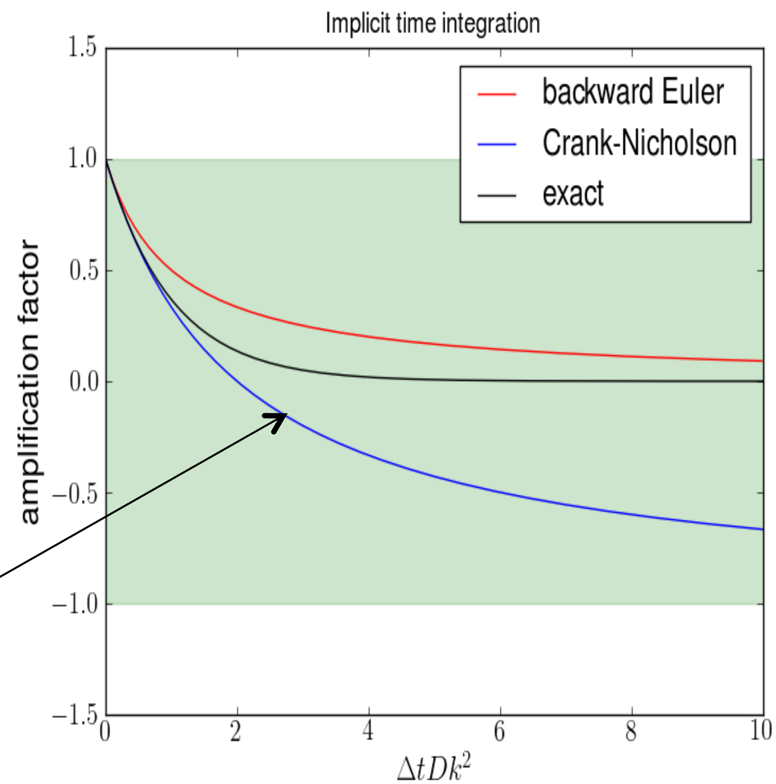
Amplification factor for the constant diffusion problem



Why flexibility in time integration is important

- **Backward Euler**
  - stable (yes)
  - 2nd order accurate (no)
- **Crank-Nicholson:**
  - stable (marginally)
  - 2nd order accurate (yes)
- **Can we have the best of both worlds? Accuracy and stability for large Δt**

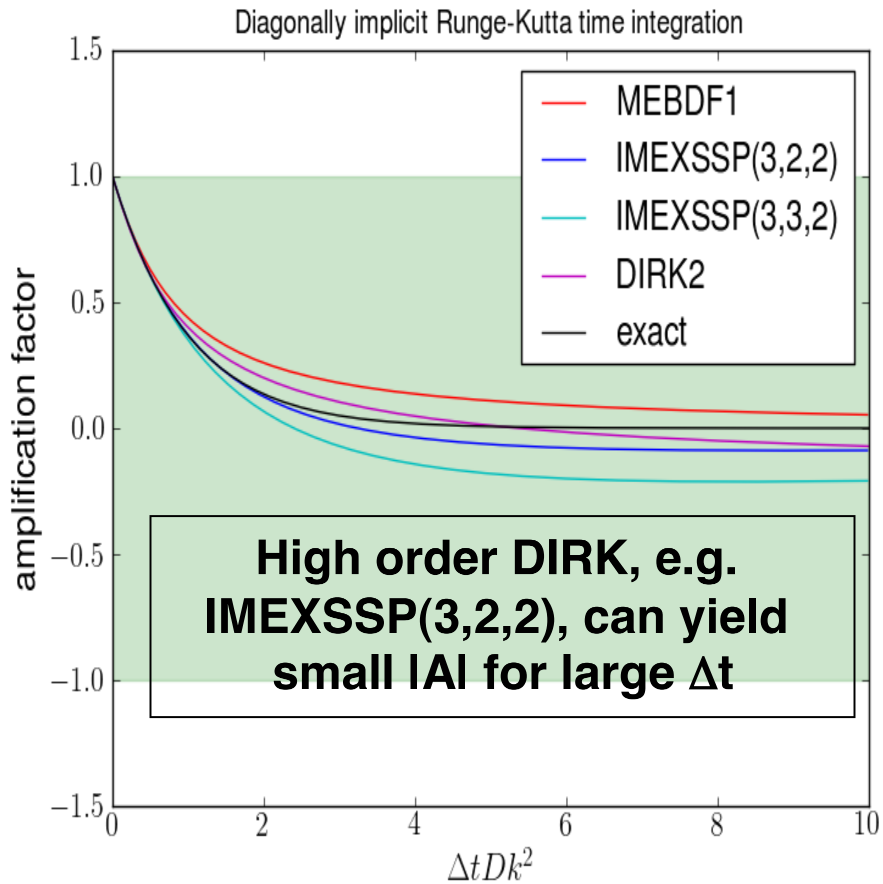
Tradeoff between accuracy and stability for some implicit schemes



Crank-Nicholson's A → -1 for large Δt

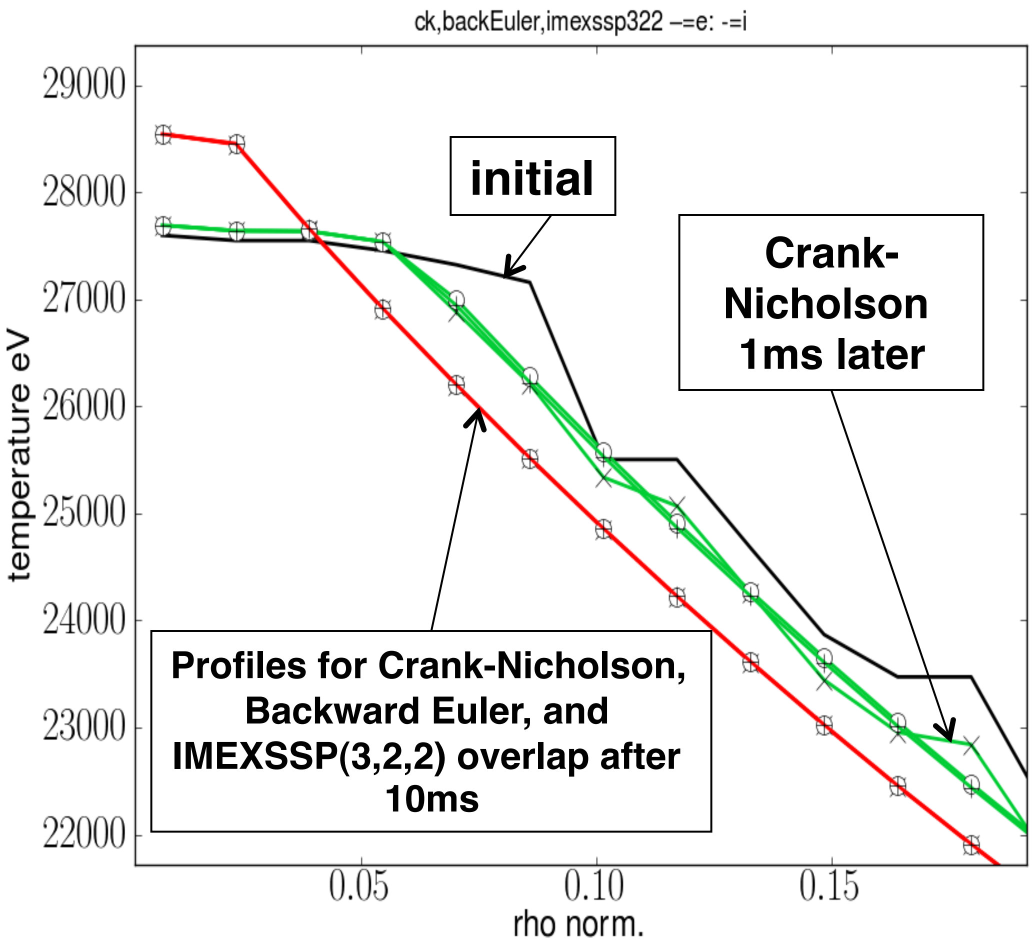
DIRK time stepping schemes can be stable *and* accurate

- **DIRK = Diagonally Implicit Runge-Kutta**
- **Multi-stage method, each stage involves an implicit solve (PETSc/SNES)**
- **Example of 3-stage DIRK:**
  - Solve dQ1 = Δt*F(qOld + a11*dQ1)
  - Set q1 = qOld + a21*dQ1
  - Solve dQ2 = Δt*F(q1 + a22*dQ2)
  - Set q2 = qOld + a31*dQ1 + a32*dQ2
  - Solve dQ3 = Δt*F(q2 + a33*dQ3)
  - Set qNew = qOld + b1*dQ1 + b2*dQ2 + b3*dQ3
  - Repeat…



[Collaboration with G. Hammett, PPPL]

Order of integration scheme affects transients in FACETS



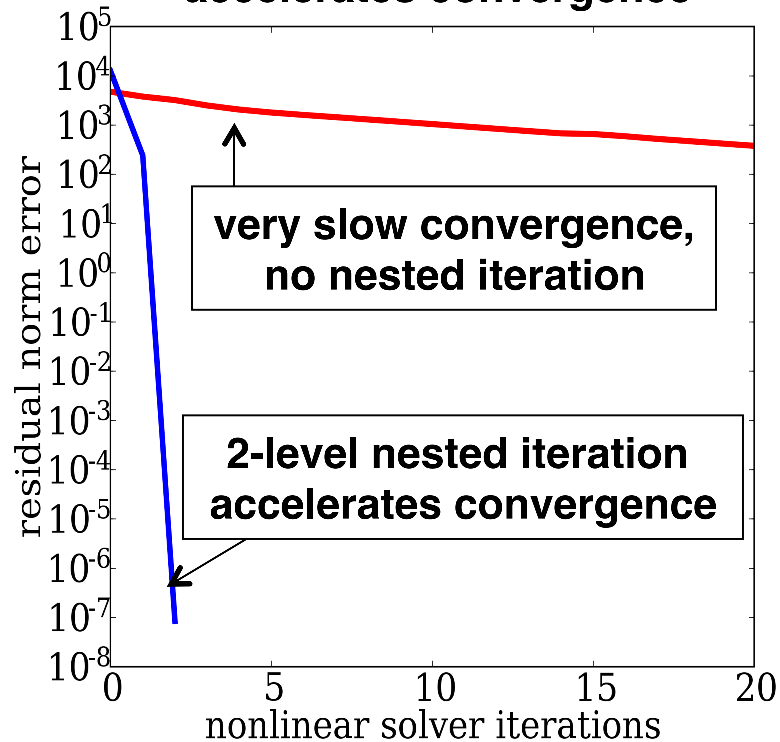
Green: 1ms
Red: 10ms

Detail of ion temperature (Ti) as time evolves using different integration schemes (ITER geometry). Initially, Ti has oscillations, which are damped over time. Damping is most effective for backward Euler and IMEXSSP(3,2,2).

FACETS applies nested iteration to improve convergence of time integrators

- Nonlinear solvers often have difficulty converging
- Convergence is faster on coarse grid
- Recursively solving from coarser to finer mesh was found to improve convergence (nested iterations)
- FACETS does not rely on profile smoothing
- Small time steps ~1ms are taken initially; larger Δt ~100ms can be taken later

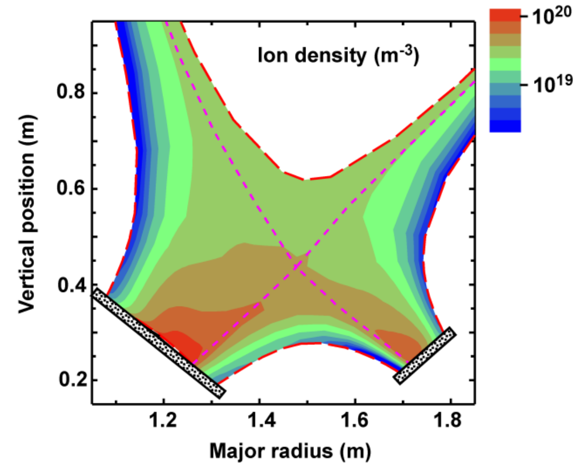
nested iteration accelerates convergence



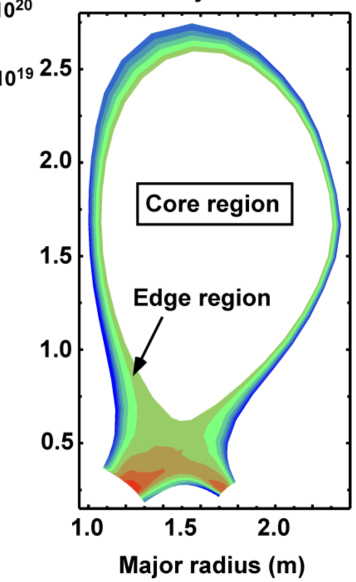
UEDGE demands robust parallel solvers to handle strong nonlinearities

Challenges in edge modeling

- Extremely anisotropic transport
- Extremely strong nonlinearities
- Large range of spatial and temporal scales



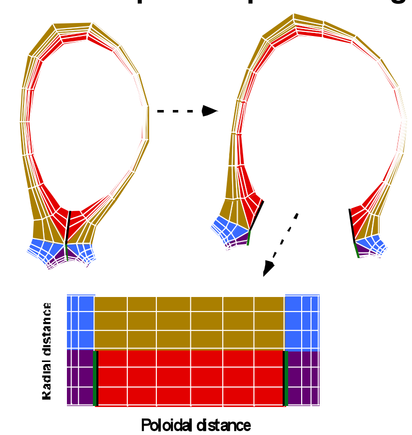
Poloidal cross-section of ion density for DIII-D



UEDGE (T. Rognlien, LLNL)

- Test case: Magnetic equilibrium for DIII-D single-null tokamak
- 2D fluid equations for plasma/neutrals
  - variables: n_i, u_{pi}, n_g, T_e, and T_i (ion density, ion parallel velocity, neutral gas density, electron and ion temperatures)
- Finite volumes, non-orthogonal mesh
- Volumetric ionization, recombination & radiation loss
- Boundary conditions:
  - core – Dirichlet or Neumann
  - wall/divertor – particle recycling & sheath heat loss
- Problem size 40,960: 128x64 mesh (poloidal x radial), 5 unknowns per mesh point

UEDGE parallel partitioning



UEDGE approach: Fully implicit, parallel Newton solvers via PETSc

Solve F(u) = 0: Matrix-free Newton-Krylov:

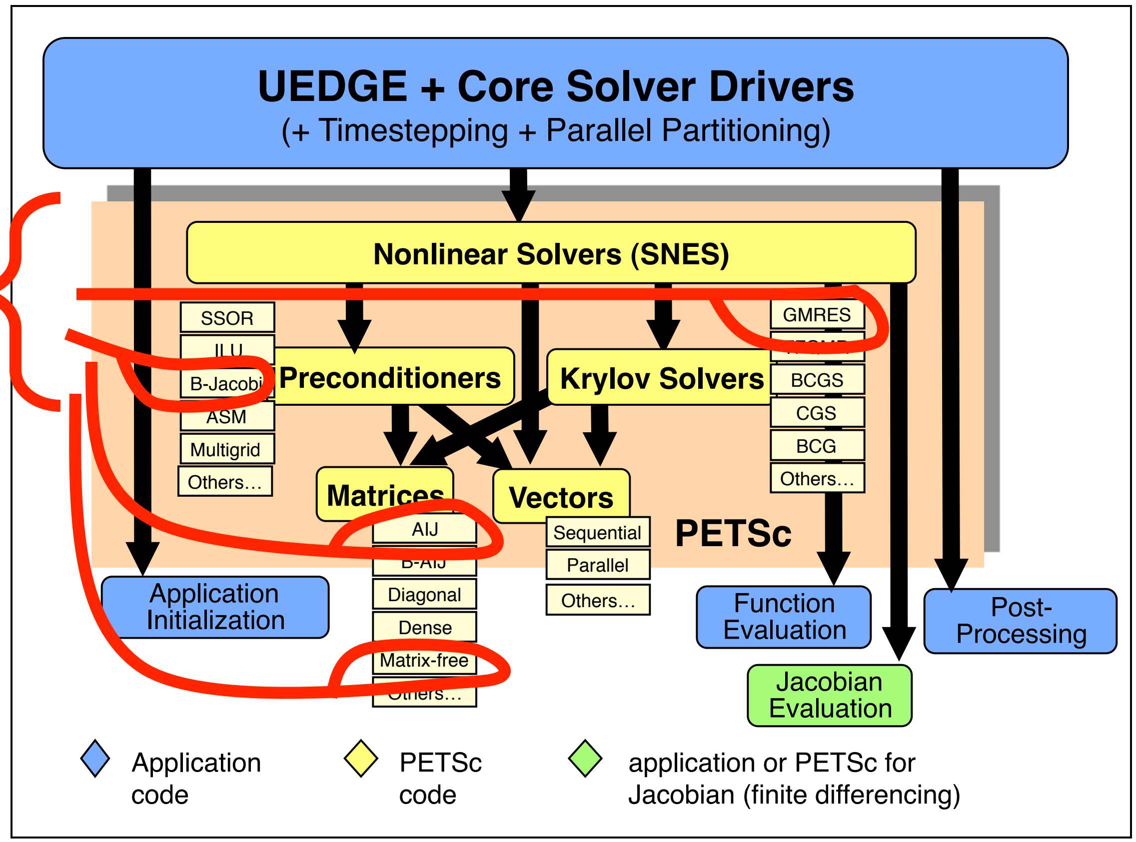
$$F'(u^{l+1})\,\partial u^{l} = -F(u^{l-1})$$

$$u^{l} = u^{l+1} + \lambda\,\partial u^{l}$$

- **Solve Newton system with preconditioned Krylov method**

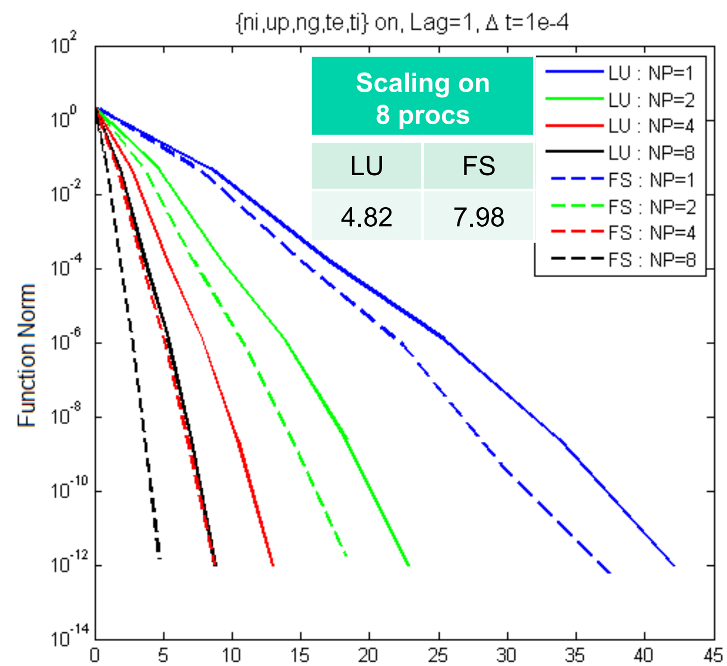
Options originally used by UEDGE

- **Matrix-free: Compute Jacobian-vector products via finite difference approx; use cheaper Jacobian approx for preconditioner**



New preconditioners have improved robustness and scalability of parallel UEDGE

- **Original parallel UEDGE**
  - **Supported only block Jacobi preconditioner**
    - **No convergence in parallel for difficult nonlinearities (e.g., neutral gas)**
- **New capabilities**
  - **Scalable parallel Jacobian computation using matrix coloring for FD**
    - **Complete parallel Jacobian data enables more robust parallel preconditioners**
    - **Impact: Enables inclusion of neutral gas equation (difficult for highly anisotropic mesh)**
  - **PCFieldSplit solves the neutral terms with LU and other terms with Additive Schwarz**
    - **Exploit understanding of the physics**
    - **Impact: Improves scalability for neutral gas cases**
  - **More investigations**
    - **1D vs. 2D partitioning:** without neutrals, 1D is preferred
    - **Choice of timestep:** ASM converges scalably for Δt≈10-4



Time for nonlinear solve: LU and PCFieldSplit on 1,2,4,8 procs

Exploiting physics knowledge in custom preconditioners … with no changes to UEDGE

New PCFieldSplit simplifies multi-model algebraic system specification and solution.

UEDGE runtime option:

```
prec['7']=['-pc_type fieldsplit','-pc_fieldsplit_block_size 5',
'-pc_fieldsplit_type additive','-pc_fieldsplit_0_fields 0,1,2,3
','-pc_fieldsplit_1_fields 4','-fieldsplit_0_pc_type asm','-fie
ldsplit_0_sub_pc_type lu','-fieldsplit_0_sub_pc_factor_mat_solv
er_package mumps','-fieldsplit_1_pc_type lu','-fieldsplit_1_pc_
factor_mat_solver_package mumps']
```

$$\begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{pmatrix}$$

base ordering (all variables per mesh point)

physics-based reordering (for PC only)

$$\begin{pmatrix} A_1 & A_2 \\ A_3 & A_4 \end{pmatrix}$$

components are separated

A_1 Non-neutral terms only

A_2 Neutral to Non-neutral

A_3 Non-neutral to neutral

A_4 Neutral terms only

Leveraging knowledge of the different component physics in the system produces a better preconditioner.

$$\begin{pmatrix} A_1^{-1} & \\ & A_4^{-1} \end{pmatrix}$$

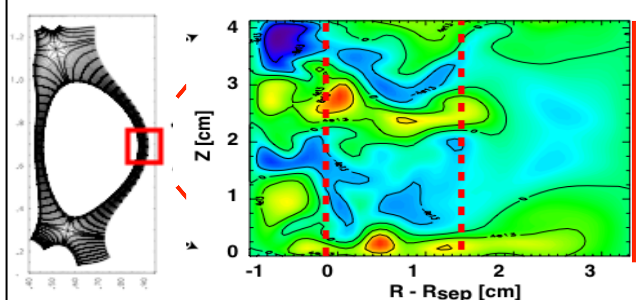
additive componentwise preconditioner

A_1^{-1} Additive Schwarz, LU on blocks → Additive Schwarz provides scalability

A_4^{-1} Full LU solve via MUMPS → LU handles the neutrals only

New BOUT++ capabilities exploit both SUNDIALS (implicit integrators) and PETSc (preconditioners)

- BOUT++ (BOUndary Turbulence), LLNL and University of York (B. Dudson)
  - Radial transport driven by plasma turbulence; BOUT++ provides fundamental edge model
    - 2D UEDGE approx turbulent diffusion
    - 3D BOUT++ models turbulence in detail
  - Ion and electron fluids; electromagnetic
  - Full tokamak cross section
  - Finite differences, 2D parallel partitioning
  - Implicit time advance via SUNDIALS



BOUT edge density turbulence, $\delta n_i/n_i$

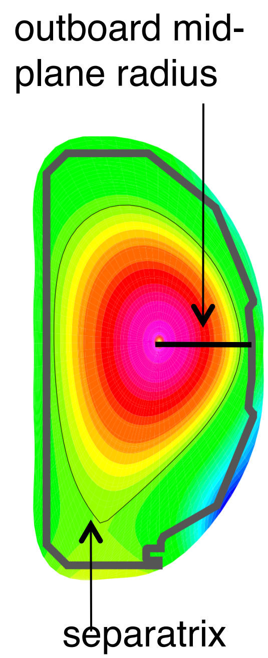
- Recent progress
  - Parallel BOUT++/PETSc/SUNDIALS verified against original BOUT
  - Extended design for flexibility and robustness
    - Enables runtime experimentation with algorithms
    - Facilitates incorporation as a FACETS component
  - Currently adding new physics, exploring various options for preconditioners, time integration, Newton-Krylov, etc.

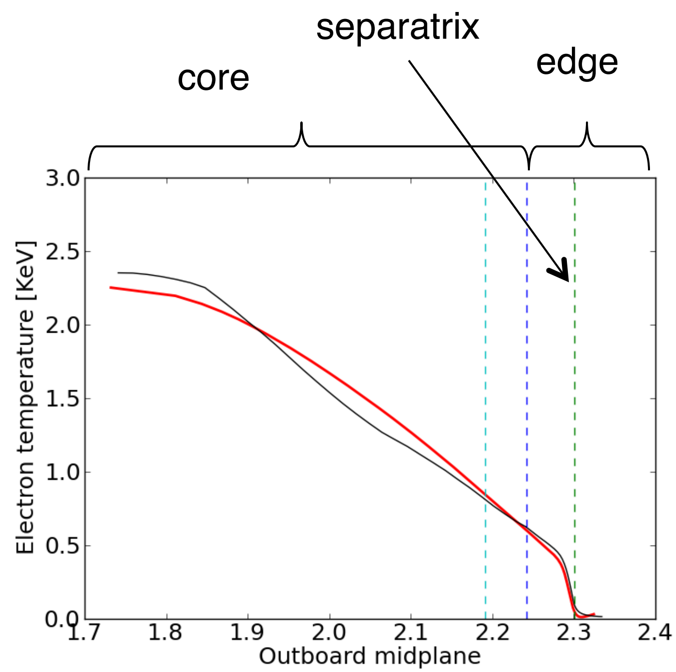
Several issues need to be resolved in a proper core-edge coupling scheme

- **Initial conditions need to be consistent across the core edge boundary**
  - How to ensure two different models use the same initial conditions?
- **Flux models need to be consistent in both the core and the edge at the core-edge interface**
  - How to ensure fluxes transition smoothly at the coupling interface?
- **Grids need to be carefully aligned to get second-order coupling scheme**
  - How to ensure that spatial order is not reduced while exchanging data across different grids?
- **Temporal and spatial discretization need to be of the same order for both models to maintain overall order**

Current core-edge simulations have been done using explicit coupling

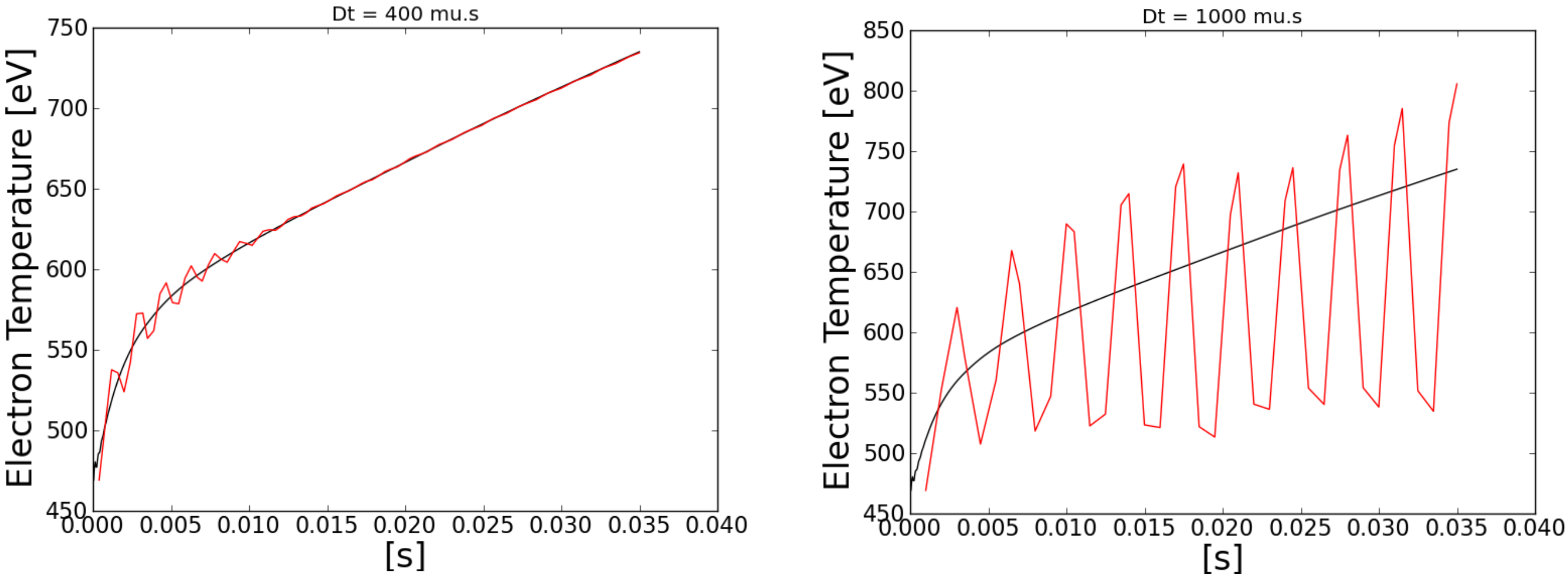
- **Pass the *contravariant* particle and energy fluxes from core to edge**
- **Pass the flux-surface averaged values from edge to core**
- **Core and edge run concurrently on each coupling time-step**
- **Core and edge component can sub-step if needed**
- **Data is exchanged at the end of the step and process repeated**





Electron temperature (black) compared to experiment (red)

Limitations of explicit coupling scheme: consistency and stability



- **Small initial discontinuity in flux makes scheme unstable with increasing timestep (1 ms).**
- **For full discharge simulation we will need order of 10 ms timesteps.**
- **Implicit methods are needed to "relax" the system and allow larger coupled timesteps.**

Implicitly coupled components are in self-consistent state

- **For large time steps, explicitly coupled components can end up in inconsistent state**
  - **For example, core and edge transport components can disagree on electron temperature at coupling interface**
- **Implicit coupling keeps components in self-consistent state even for large time steps**
- **Implicit coupling described by nonlinear system:**

$$\begin{cases} x = h(y) \\ y = g(x) \end{cases}$$

  - **Code G (e.g., core) takes input x and generates output y**
  - **Code H (e.g, edge) takes input y and generates output x**

FACETS supports both Picard and Newton iterative implicit coupling

- **FACETS supports 2 implicit coupling schemes:**
  - **Picard iteration:**
    $$\begin{cases} x^{n+1} = h(y^n) \\ y^{n+1} = g(x^n) \end{cases}$$
  - **Quasi-Newton iteration on equation**
    $$f(x,y) = [x - h(y), y - g(x)] = 0$$

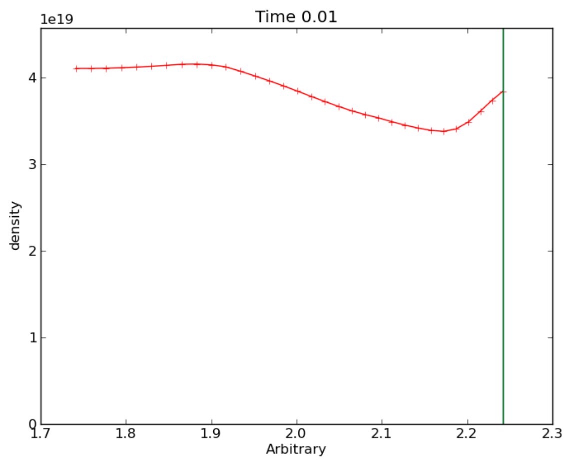
  by iteratively solving Jacobian system: $J^n[\delta x^n, \delta y^n] = -f^n$

  and adding the increments
  $$[x^{n+1}, y^{n+1}] = [x^n + \delta x^n, y^n + \delta y^n]$$

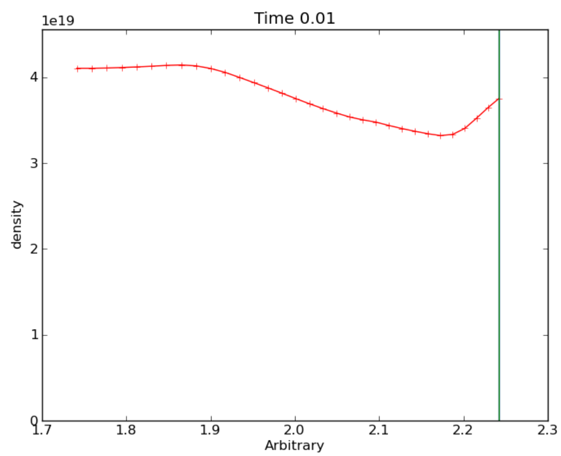
- **New generic implicit coupling component**
  - `FcImplicitContainerUpdater`
  - **Can couple any 2 (so far)** `FCComponents`

Implicit core-edge coupling enables larger timesteps

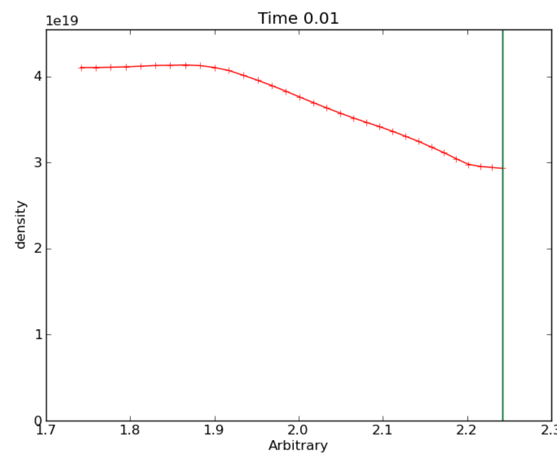
- **For verification, coupling was done between the real core component (`FcCoreComponent`) and a "toy" edge component (`FcExprComponent`)**
- **The implicit coupler (`FcImplicitContainerUpdater`) gives identical steady-state solution as explicit coupling (`FcNestedComponentUpdater` + `PcBcDataTransferUpdater` + `FcBcDataTransferUpdater`)**
- **For transients, explicit coupling with large Δt gives error:**



Implicit, Δt = 10 ms



Explicit, Δt = 1 ms



Explicit, Δt = 10 ms

Physics/math partnership in investigating stability for dynamic multiphysics coupling

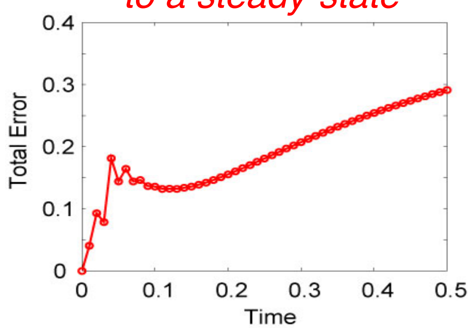
Coupled parabolic problems on neighboring intervals

$$
\begin{cases}
T_t^c = T_{xx}^c + S^c & \text{core} \\
T_t^m = \frac{1}{2} T_{xx}^m + S^m - 10^3 \left(T^m - T^d\right) & \text{edge midplane} \\
T_t^d = \frac{1}{2} T_{xx}^d + S^d + 10^3 \left(T^m - T^d - T^d \theta\left(x - x_s\right)\right) & \text{edge divertor} \\
T^c = \frac{1}{2}\left(T^m + T^d\right), \quad T_x^c = \frac{1}{2}\left(T_x^m + T_x^d\right) & \text{interface}
\end{cases}
$$

Implicit coupling:

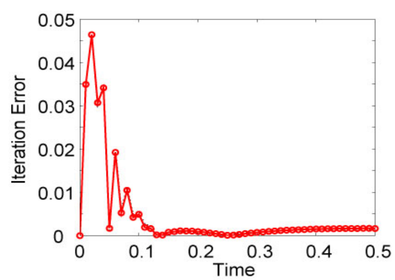
- **Implicit Euler for each component solve**
- **"Nonoverlapping" coupling**
- **$\Delta x = 10^{-2}$, $10^{-4} < \Delta t < 10^{-2}$**
- **1 iteration per step**

Solution should converge to a steady-state

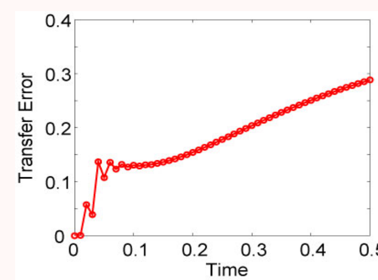


Total error grows with time

Detailed a posteriori error analysis:



Error due to incomplete iteration decays to zero



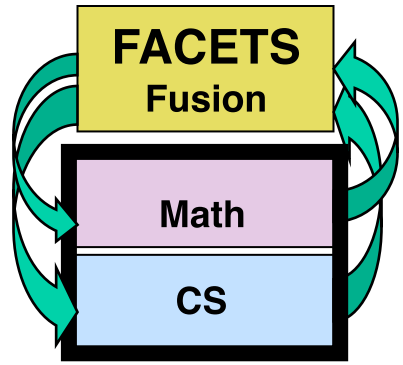
Error passed in gradients accumulates

Progress in analysis of accuracy and stability for multiphysics coupling

- **A posteriori error analysis:** Computational approach to error estimation that uses:
  - **Residuals** to describe introduction of error
  - **Adjoint (dual) problems** to describe the effect of stability
  - **Variational analysis** to produce **accurate** error estimates
  - The estimate provides a detailed description of causes of error
  - This is a computational approach that can deal with complex problems
- **Recent extensions multiscale, multiphysics models**
  - Treats general coupling strategies
  - Handles differences in discretization scale and solution representation
  - Handles complex stability of multiphysics problems
- **Results** (see http://www.math.colostate.edu/~estep)
  - Coupling of elliptic/parabolic problems through a boundary (3 papers, 1 preprint)
  - Coupling of elliptic problems through parameter passing (1 paper, 1 preprint)
  - Overview book chapter
  - Operator splitting and multirate integration methods (1 paper, 2 preprints)
  - Extension to finite volume schemes (1 paper, 1 preprint)
- **New CSU postdoc (B. Sheehan):** Analyzing stability and error of core-edge coupling via hands-on work with physicists & FACETS framework

Physics and math/algorithms synergy inspires new research and builds fundamental tools

- FACETS core-edge coupling has motivated
  - Multiphysics extensions to stability and error analysis (CSU)
  - Support for strong coupling between models in PETSc nonlinear solvers (ANL/TOPS)
  - Support for parallel interface to matrix coloring for sparse FD Jacobian computations (ANL/TOPS)



- These new applied math capabilities are feeding back into FACETS simulations
- Future work includes
  - Multiphysics issues in time integration algorithms and software
  - More multiphysics extensions to stability and error analysis
  - Algorithms for additional physics components
    - E.g., kinetic edge models, wall