AMR Update and Future Plans in APDEC & CEMM

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SciDAC
Scientific Discovery
through
Advanced Computing

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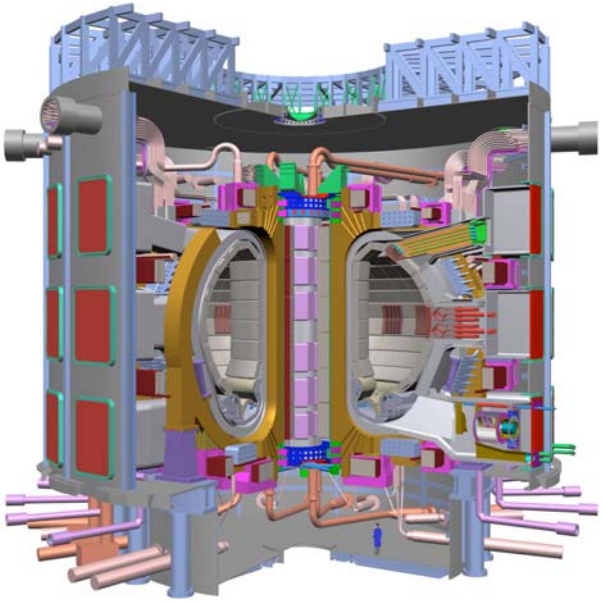
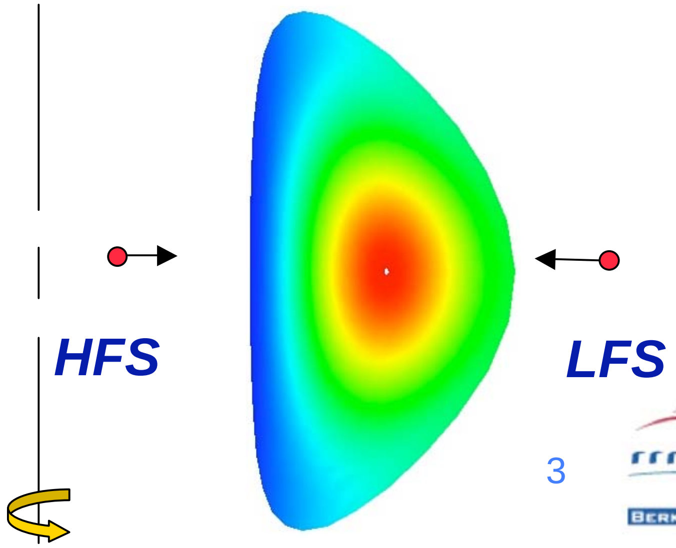
APDEC - SciDAC-2

- Applied Partial Differential Equation Center for Enabling Technology (APDEC) funded under SciDAC-2
  - *Goal: develop algorithms and software for simulating multiscale problems on structured grids.*
  - *Applications-driven approach: end-to-end development of software tools to meet specific DOE science requirements.*
- Lead Principal Investigator: P. Colella (LBNL, .3 FTE). Site project leads: D. Trebotich (LLNL), R. Samtaney (PPPL).
- Algorithm / software development team:
  - LBNL: B. van Straalen (team lead), D. Graves, T. Ligocki, P. Schwartz (.5 FTE), P. McCorquodale (.5 FTE).
  - LLNL: D. Trebotich, C. Bono, G. Miller (UCD summer faculty).
- Combustion application team (LBNL, all .5 FTE): J. Bell (team lead), M. Day, J. Grcar, M. Lijewski.
- MHD Application Team:
  - PPPL: R. Samtaney (team lead, PPPL).
  - LBNL: D. Martin (.5 FTE), T. Sternberg (.5 FTE).
- Other applications collaborators: Astrophysics (S. Woosley); FACETS magnetic fusion framework (J. Carey).
- Other CET / Institute collaborators: VACET (E. Bethel); others pending.

Pellet Injection & Edge Localized Modes

- Motivation
  - *Injection of frozen hydrogen pellets is a viable method of fueling a tokamak*
  - *Presently there is no satisfactory simulation or comprehensive predictive model for pellet injection (esp. for ITER)*
  - *H-mode operation of ITER will be accompanied by edge localized modes (ELMS) (ITER Physics Experts Group,Nucl. Fusion 1999)*
    - *H-mode (high-confinement mode) is a narrow transport barrier which forms at the plasma edge as the heating power is increased. A high pressure region forms which when steepened sufficiently will lead to an instability*
  - *Pellet injection related to ELMs (Gohill et al. PRL, 2001; Lang et al. Nucl. Fusion 2000)*
- Objectives
  - *Develop a comprehensive simulation capability for pellet injection and ELMs in tokamaks (esp. ITER) with adaptive mesh refinement for spatial resolution and fully implicit Newton-Krylov approach for temporal stiffness*





Scales and Resolution Requirements

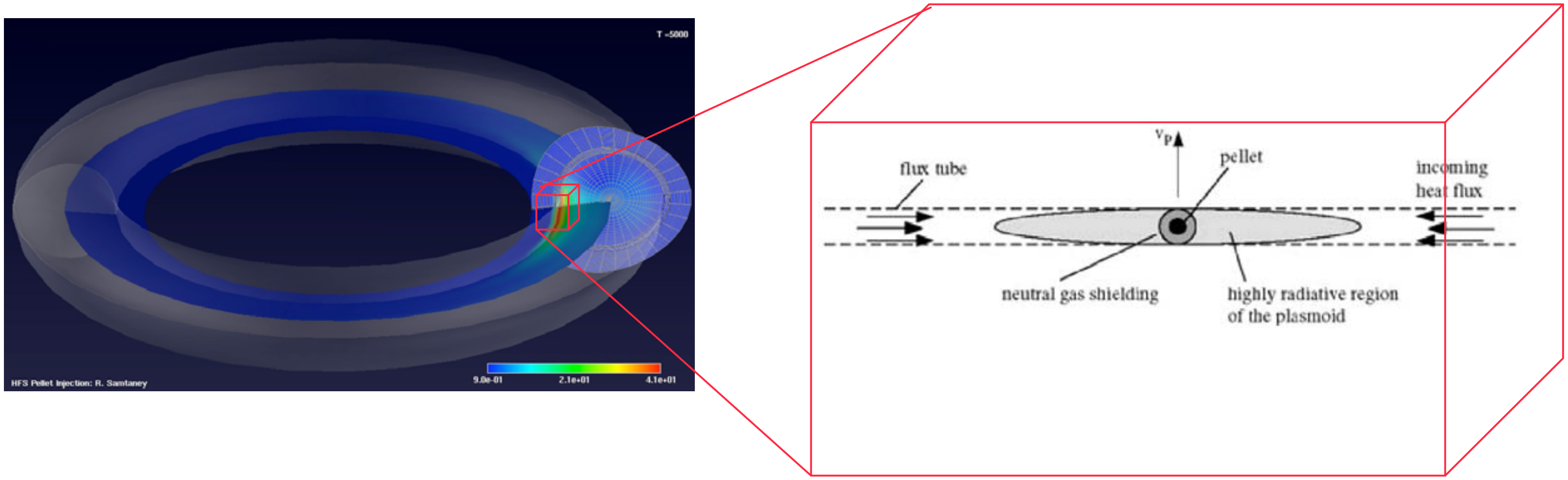
- Large separation of time scales ($\tau_e < \tau_f < \tau_a < \tau_c < \tau_p$)
- Spatial scales: Pellet radius r_p << Device size L ~$O(10^{-3})$
- Pellet cloud density ~ $O(10^4)$ times ambient plasma density
- Electron heat flux is non-local
- Large pressure and density gradients in the vicinity of cloud
- Pellet lifetime ~ $O(10^{-3})$ s →long time integrations

Resolution estimates

Tokamak	Major Radius	N	N_{steps}	Spacetime Points
CDXU (Small)	0.3	2×10^7	2×10^5	4×10^{12}
DIIID (Medium)	1.75	3.3×10^9	7×10^6	2.3×10^{17}
ITER (Large)	6.2	1.5×10^{11}	9×10^7	1.4×10^{19}

Pellet Injection

- Combine global MHD simulations in a tokamak geometry with detailed local physics including ablation, ionization and electron heating in the neighborhood of the pellet



- AMR techniques to mitigate the complexity of the multiple scales in the problem
- Implicit time-stepping (Jacobian-free Newton-Krylov approach) for wide range of temporal scales

AMR - Current Status & Future Work

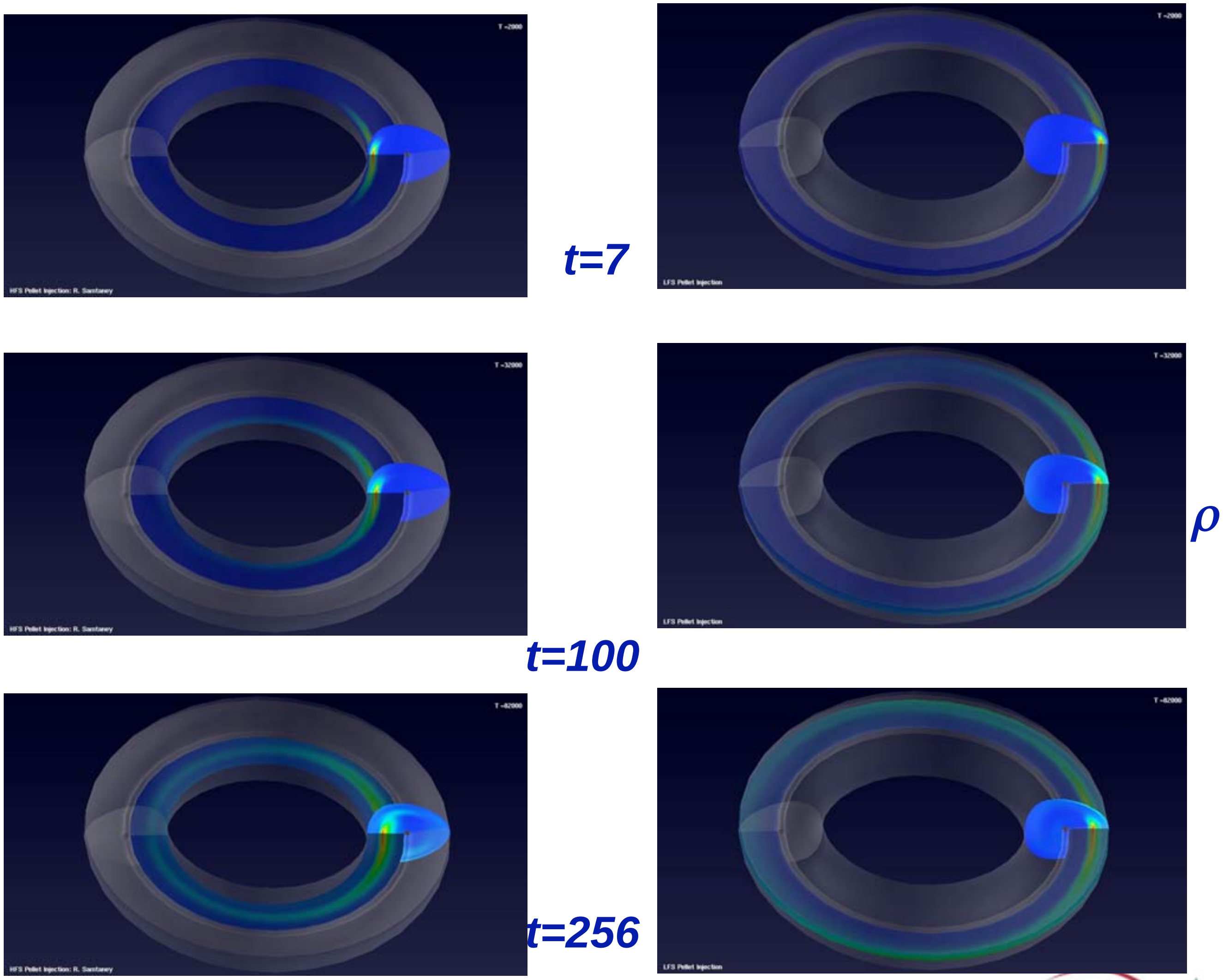
- AMRMHD code in flux coordinates for pellet injection
  - *Hyperbolic fluxes are evaluated using upwind methods*
  - *Includes models for pellet ablation & electron heat flux*
  - *Alternative approach: MHD = Hydro + EM*
    - *Godunov methods for hydrodynamics*
      - *J x B source in momentum equations, and J.E source in total energy/vol equation*
    - *Dissipation-free method for Faraday (auto preservation of solenoidal condition)*

- Diffusion terms - implicit treatment requires solving elliptic equations
  - *Presently the method of choice is geometric multi-grid with BiCGSTAB*
  - *Future: Robust and scalable solvers required for*
    - *Nonlinear properties* ($\eta \equiv \eta(T)$)
    - *Mapped grids*
    - *Anisotropies due to mapped grids and plasma properties*

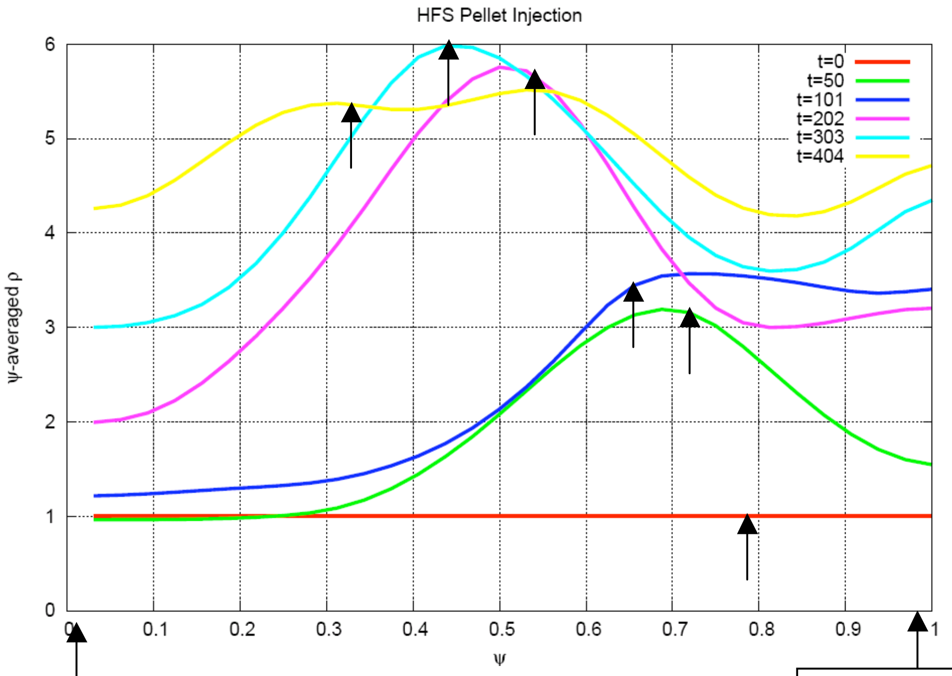
- **Initial Equilibrium:** Express $B=1/R(\phi \times \nabla \psi + g(\psi)\, \phi) \neq \mathrm{fnc}(\phi)$.
  - *A Chombo implementation of a robust Grad-Shafranov solver is desirable*

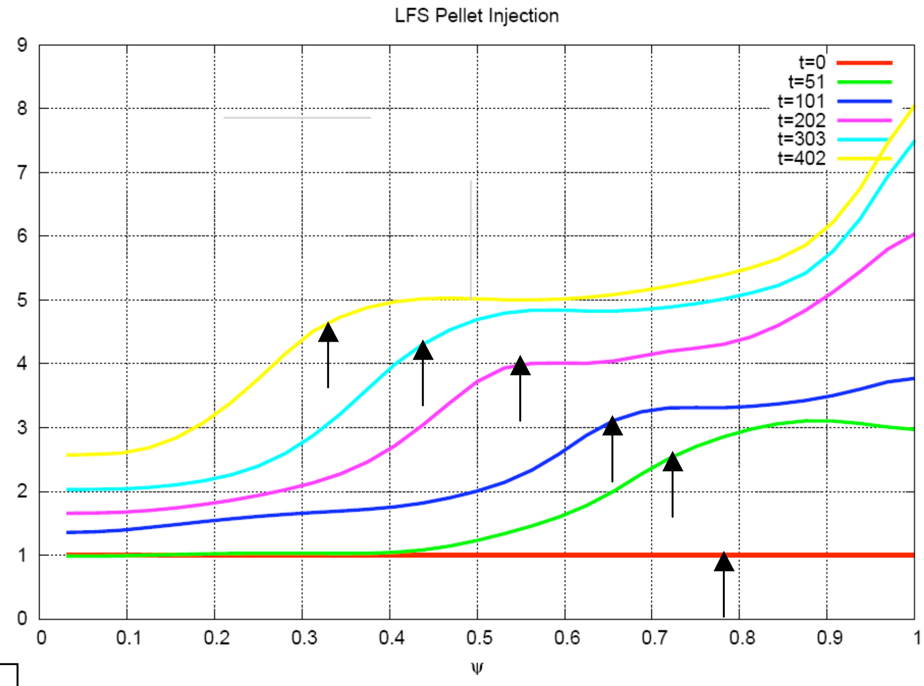
Results - HFS vs. LFS

B_T = 0.375T
n_0=1.5× 10^{19}/m^3
$T_{e\infty}$=1.3Kev
β=0.05
R_0=1m, a=0.3 m
Pellet: r_p=1mm,
v_p=1000m/s
HFS shows better core fueling than LFS
Transport of ablated pellet material in direction of major radius is due to an interchange instability
(Oral presentation VO1.00009 Thursday afternoon)



HFS vs. LFS - Average Density Profiles





Core

Edge

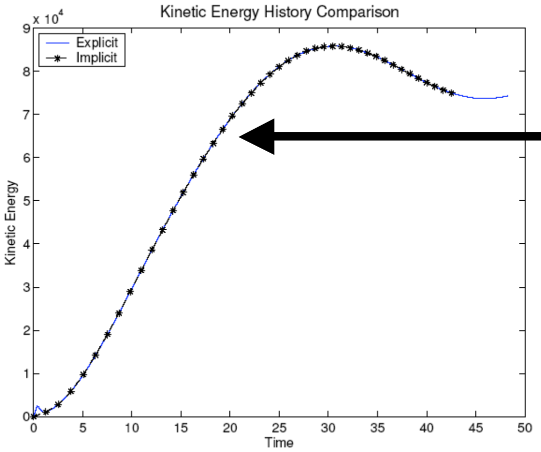
HFS Pellet injection shows better core fueling than LFS

New Interpretation: Nonlinear manifestation of the interchange instability is responsible for fast motion across flux surfaces in direction of increasing R (APS -DPP 2006)

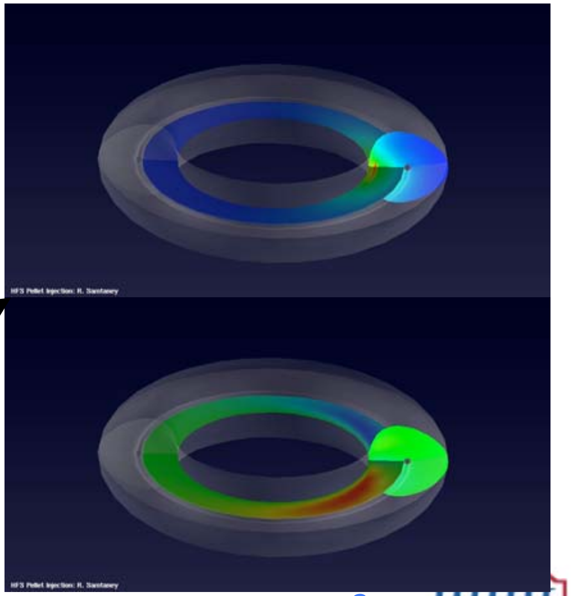
Arrows indicate average pellet location

JFNK Fully Implicit Approach for Resistive MHD

- Time step set using explicit CFL condition of fastest wave
- Pellet Injection: Explicit codes require $O(10^{6\text{-}7})$ time steps.
- For d-dimensions, time interval T, CFL type stability restrictions imply that total execution time $E \propto T\, S^{1+\alpha/d}\, P^{\alpha/d}$ where P is the total number of processors, S is the total storage on each processor, and α is the degree to which Δt depends upon mesh spacing (Keyes et al., SciDAC 2006)
- In SciDAC-1, a JFNK code for for Resistive MHD was developed using the SUNDIALS package (Collaboration with TOPS; D. R. Reynolds and C. S. Woodward)



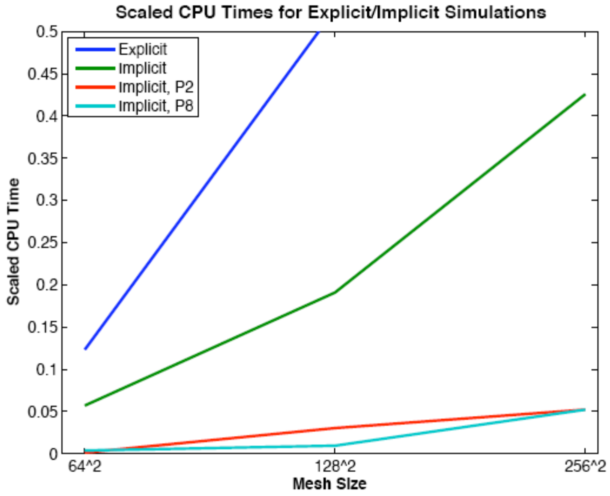
Good agreement between explicit and implicit methods for model pellet problem

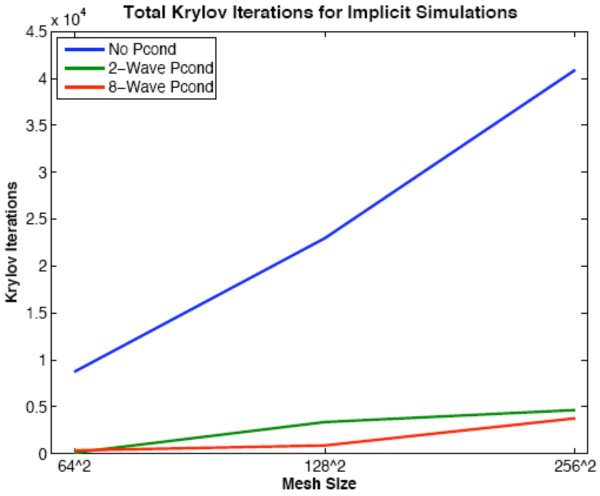


Implicit simulations in a toroidal geometry. $\Delta t = 100\, \Delta t_{explicit}$

Preconditioning - Preliminary Results

- Test problem: linear wave propagation (t_{end}=50)
- Preconditioner: Instead of J δ U = R we solve (J P^{-1}) P δ U = R
- Operator split into hyperbolic and diffusive parts $P^{-1} = P_h^{-1} P_d^{-1}$
- Hyperbolic: decompose into local wave structure; employ ADI to get block tridiagonal matrices which are easily inverted
- Diffusive: investigating multi-grid methods for preconditioning





Scaled CPU : Total CPU / Total number of spatial cells.
Horizontal line ==> perfect scaling.
Poster JP1.00110 Tuesday Afternoon

ELMs: Challenges

- Most descriptions are empirical and models tend to be phenomenological
  - *Experiments indicate a precursor mode initially localized toroidally which grows to span the entire plasma circumference*
  - *ELM time scale is O(ms) & frequency is O(20-100 Hz). ELMs appear as short separated bursts*

- MHD Models: ELMs are driven by high pressure gradients or toroidal density gradient or a combination of both
  - *Ideal MHD: ELMs are somewhere in between kink modes (low n)/peeling modes (high n) and ballooning modes (very high n).*
  - *Type I ELMs may be investigated with Ideal MHD.*
  - *Resistive MHD: Important for Type III ELMs.*

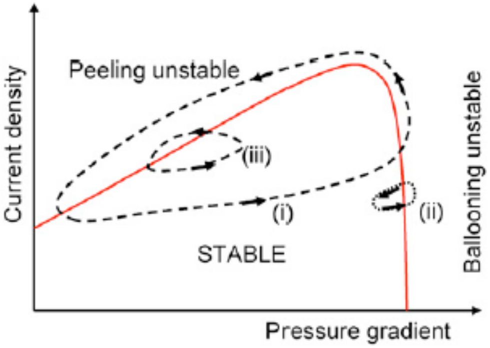


Figure from H. R. Wilson et al, Plasma Phys. Control. Fusion 2006

- Vacuum modeled as a high resistive cold plasma
  - *Large variation in properties at edge will stress the elliptic solvers*
- Upwind methods are suitable for large gradients of pressure and density encountered at the edge
- “Localized” character makes them amenable to AMR

Requirements for Fusion MHD

- Geometry
  - *Toroidal geometry*
    - *Mapped grid approach*
    - *Multi-block grids*
- Anisotropic transport
  - *Parallel conduction of heat is orders of magnitude larger than perpendicular heat conduction* $(\chi_{||}/\chi_{\perp} = O(10^8))$
    - *Higher order* $(O(h^4))$
    - *Second order finite volume approach (Gunter et al. JCP 2005; Sharma & Hammet - preprint)*
- Implicit time stepping
  - *Preliminary JFNK work shows promise*
  - *Implicit treatment of fast compressive and shear Alfven waves*
- Extended MHD Models
  - *Not within the scope of the current APDEC SciDAC*
- Other application specific requirements
  - *Inclusion of ionization, dissociation, sublimation models for pellet injection*
- Scalable software on petascale computing platforms is essential
- Visualization/data analysis for mapped multi-block AMR data

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Scientific, Technological & Algorithmic Impact

- Scientific questions
  - *What are the MHD mechanisms for “anomalous” transport across flux surfaces in pellet injection?*
  - *What causes the cloud striations observed in pellet injection experiments?*
  - *What are the underlying MHD mechanisms and precursors leading to ELMs?*
  - *What are the physical processes in pellet-injection induced ELMs?*
  - *What is the mechanism for suppressing ELMs by inducing ergodicity of magnetic fields at the edge?*

- Technological/Engineering questions
  - *What are the optimal pellet parameters (size, speed, launch trajectories) for ITER?*
  - *What are the heat loads on divertors in ELMs?*
  - *What is the frequency of occurrence of ELMs?*

- Algorithmic advances
  - *Combining JFNK with AMR will provide a powerful simulation tool for MHD fusion applications*

Leveraged Collaborations

- Brookhaven National Laboratory: Heterogeneous Multiscale Algorithms for Multiscale MHD (PI: R. Samulyak)
  - *Coupling of AMR MHD code with FronTier MHD code*
- University of Minnesota & Oak Ridge National Laboratory (PI: P. Woodward)
  - *Pushing AMR MHD to petascale on ORNL computing platforms*
- General Atomics (P. Parks and P. Perkins)
  - *Pellet injection MHD models and ablation physics*
- Towards Optimal Petascale Simulations (TOPS, PI: D. E. Keyes)
  - *JFNK and preconditioners for resistive MHD (?)*
- Center for Plasma Edge Simulations (CPES, PI: C. S. Chang)
  - *Coupling of kinetic codes with MHD at the plasma edge*

Summary

- Two Fusion MHD applications crucial to ITER have been identified
  - *Pellet injection & Edge Localized Modes*

- Proposed work under SciDAC-2: Combine adaptive and implicit methods to manage the wide range of spatial and temporal scales, and to provide a comprehensive simulation tool for pellet injection & ELMs in ITER