The Center for Extended Magnetohydrodynamic Modeling

(Global Stability of Magnetic Fusion Devices)

S. Jardin—lead PI

a SciDAC activity…
Partners with:
TOPS
TSTT
APDEC

General Atomics: D. Brennan*
MIT: L. Sugiyama, J. Ramos*
NYU: H. Strauss
PPPL: J. Breslau, J. Chen, G. Fu, S. Klasky, W. Park, R. Samtaney
SAIC: D. Schnack, A. Pankin*
TechX*: S. Kruger
U. Colorado: S. Parker , D. Barnes*
U.Wisconsin: J. Callen, C. Hegna, C. Sovinec, C. Kim*
Utah State: E. Held

*new

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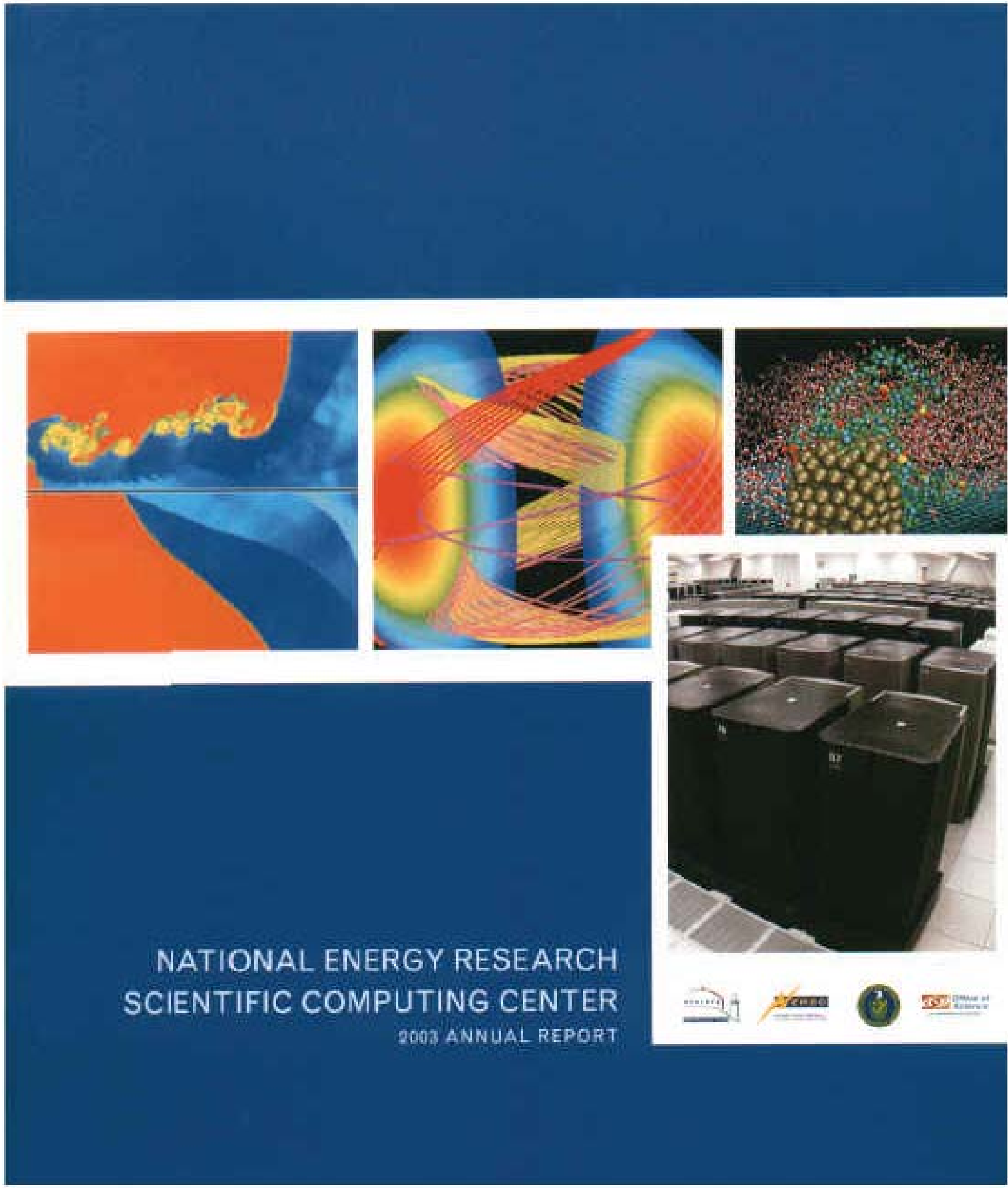
We have had (and are having) a very productive period

- 2 of the 3 cover pictures, and "Advances in Computational Science" in the fusion area in the NERSC 2003 annual report came from the CEMM project
- During the last 2 ½ years we have had Invited APS/ Sherwood talks from: Breslau, Brennan, Held, Park, Sovinec, Strauss, Sugiyama
- SIAM Session Talks by: Jardin, Schnack, Sovinec
- ICNSP'03 talks by Kruger, Strauss, Samtaney, Breslau
- Many others (IAEA, EPS, etc.), and many journal papers



NATIONAL ENERGY RESEARCH
SCIENTIFIC COMPUTING CENTER
2003 ANNUAL REPORT

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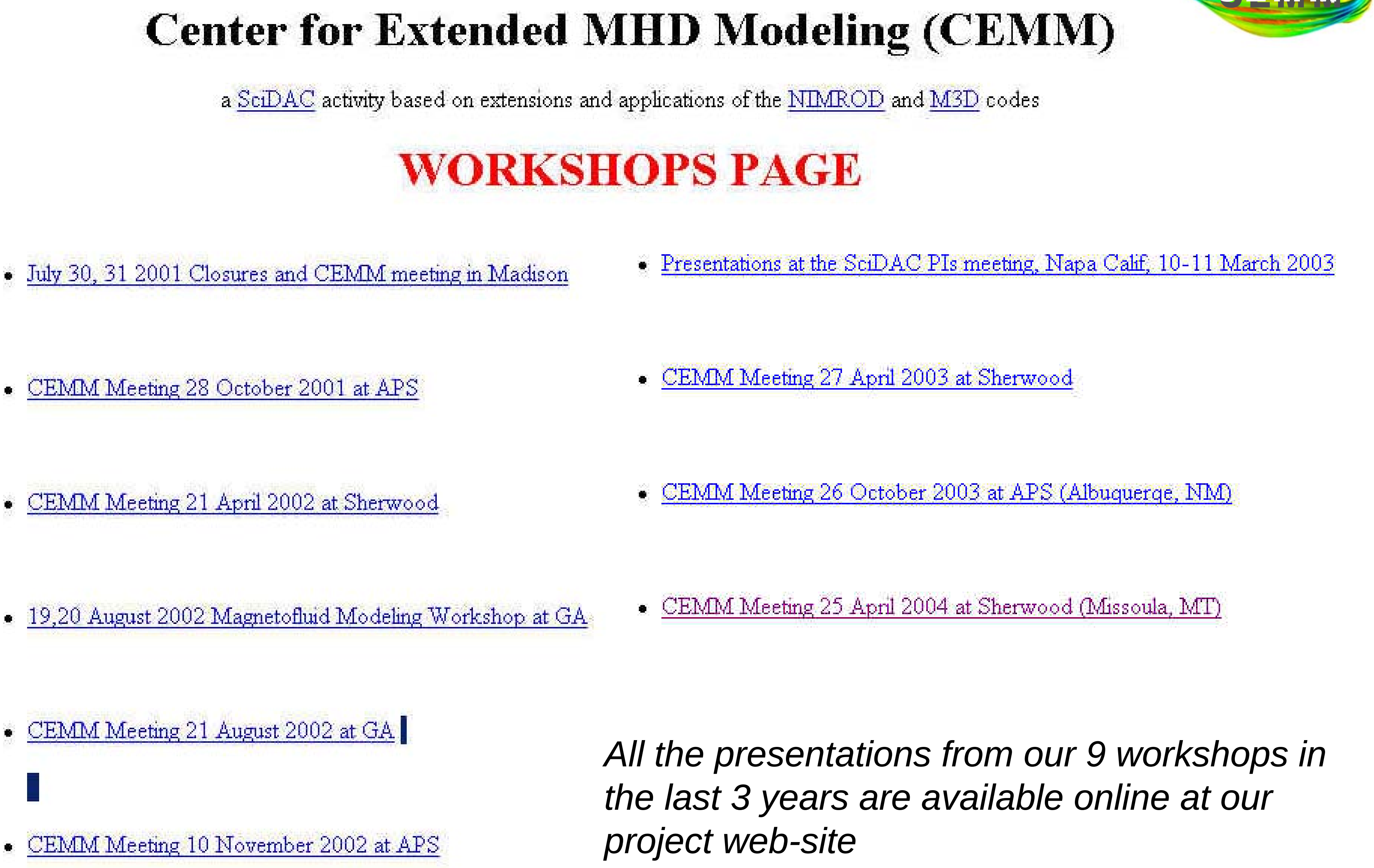

Center for Extended MHD Modeling (CEMM)

a SciDAC activity based on extensions and applications of the NIMROD and M3D codes

WORKSHOPS PAGE

- July 30, 31 2001 Closures and CEMM meeting in Madison
- CEMM Meeting 28 October 2001 at APS
- CEMM Meeting 21 April 2002 at Sherwood
- 19,20 August 2002 Magnetofluid Modeling Workshop at GA
- CEMM Meeting 21 August 2002 at GA
- CEMM Meeting 10 November 2002 at APS
- Presentations at the SciDAC PIs meeting, Napa Calif, 10-11 March 2003
- CEMM Meeting 27 April 2003 at Sherwood
- CEMM Meeting 26 October 2003 at APS (Albuquerqe, NM)
- CEMM Meeting 25 April 2004 at Sherwood (Missoula, MT)

All the presentations from our 9 workshops in the last 3 years are available online at our project web-site

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CEMM project has met most milestones while only 50% funded.

task	status
Expand M3D MPP version to stellarators	**Done.** Several talks and papers based on this
Incorporate 2-fluid version in M3D MPP version	**Done.** Several talks and papers based on this
Develop energetic particle module in M3D & NIMROD	**Done**. M3D version being used for production runs. NIMROD version in benchmark phase
Implement parallel non-Hermitian matrix solves in NIMROD	**Done**. SuperLU or GMRES option
Devlelop CEL-gased stress tensor for electrons	Post-doc not funded. Will proceed in renewal.
M3D mesh module for vacuum region with separatrix	**Done**. (halo-current and RWM calculations)
Apply energetic particle hybrid level to stellarators	Capability in place. Applications starting.
Implement majority ion δf computation and closure based on simulation particles in M3D	**Done**. Being used for collisionless RWM studies
Implement majority electron closures based on CEL	Heat flux done. Post-doc not funded
Improve the Hall and gyroviscous advances in NIMROD	In progress. Several presentations have been made on this. Still being optimized
Implement AMR methods in global simulations	**Done**. Applied to reconnection, pellets, Richtmyer-Meshkov instability
Further development of multi-fluid closures including parallel dynamics and parallel dynamics	Being worked on—present emphasis
Implement collisional effects in simulation-particle δf to address filamentation	Being worked on.
Analyze semi-implicit approaches with CEL closure	Post-Doc not funded
Incorporate implicit advection in NIMROD	**Done.**

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CEMM Simulation Codes:

	NIMROD	M3D	AMRMHD*	M3D-C^{1*}
Poloidal discretization	High order quad C^0 finite elements	Triangular linear finite elements	Structured adaptive grid	High order triangular C^1 finite elements
Toroidal discretization	Pseudo-spectral	Finite difference	Structured adaptive grid	spectral
Time integration	Semi-implicit	Partially implicit	Upwind, Partially implicit and time adaptive	Fully implicit linear terms
Enforcement of $\nabla\cdot\mathbf{B} = 0$	Error Diffusion	Vector Potential	Projection Method	Vector Potential
Libraries	SuperLU(LBL)	PETSc (ANL)	CHOMBO (LBL)	SuperLU
Sparse Matrix Solver	Direct and CG	GMRES, ICCG, and HYPRE	Conjugate Gradient	Direct
Preconditioner	Direct solve of approximate matrices	Incomplete LU	Multigrid	Analytic reduction

*Exploratory projects

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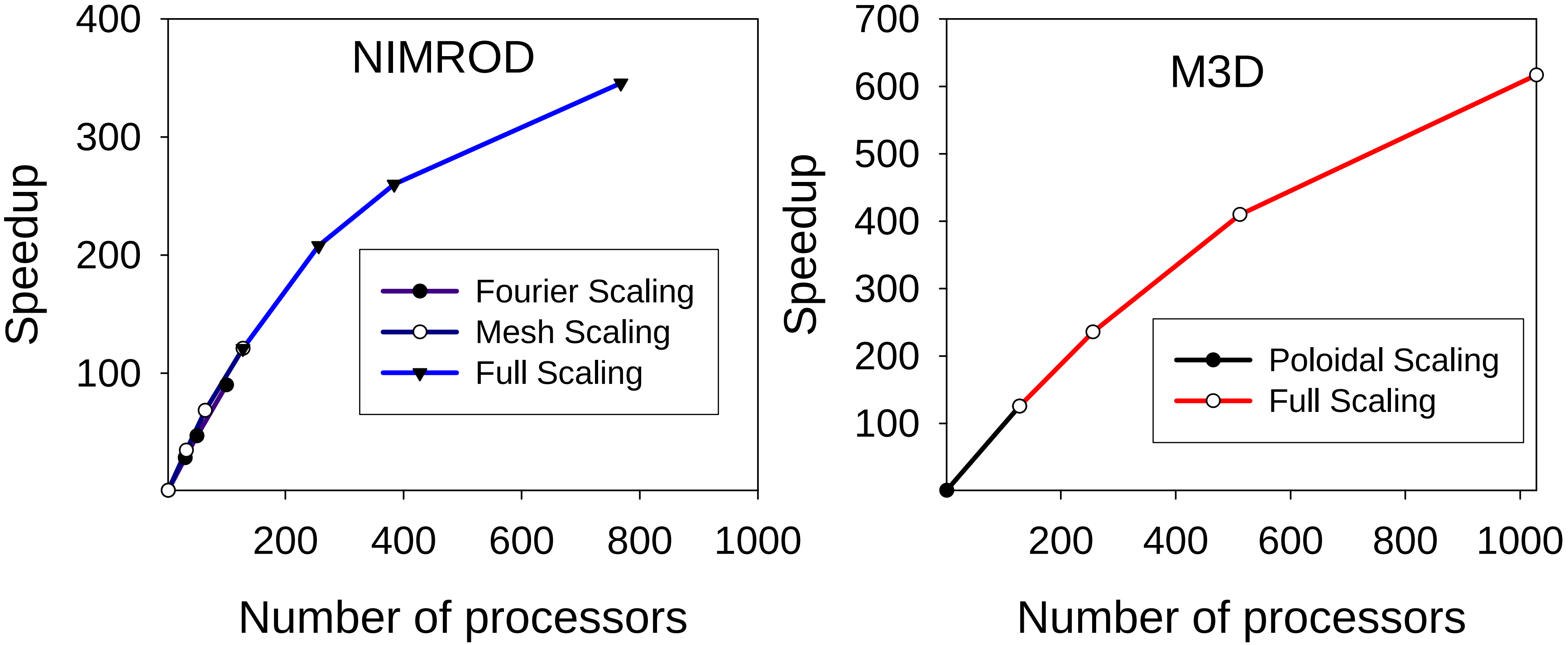
Parallel Scaling of NIMROD and M3D



Note: This is for strong scaling (problem size held fixed) for realistic problem sizes. Scaling would appear more ideal for weak scaling (problem size increases with processor number).

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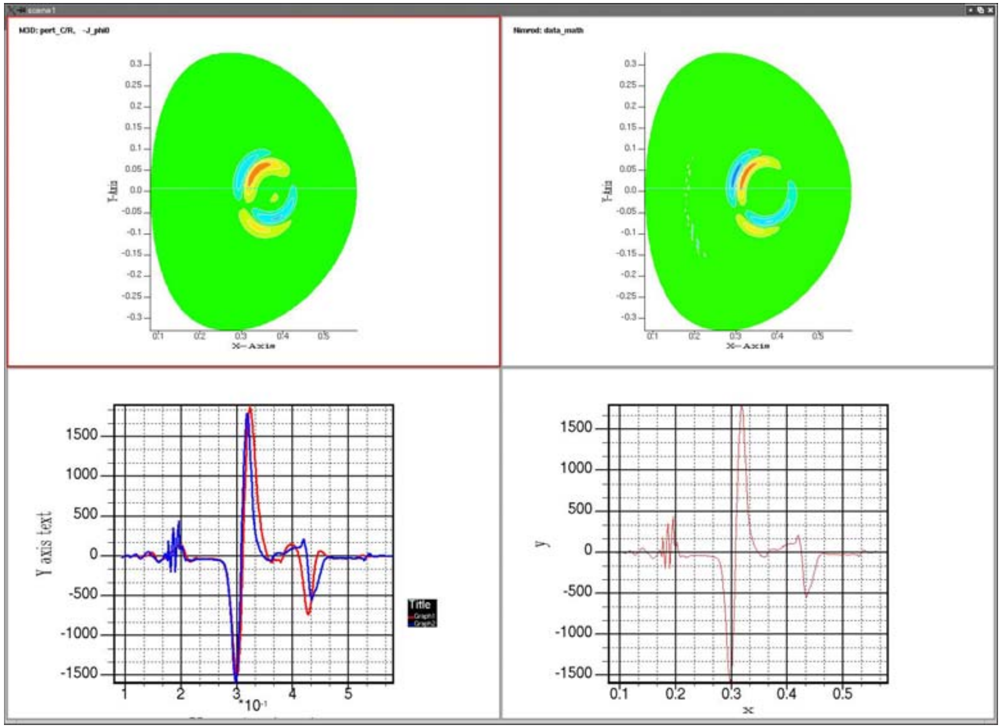
Common Visualization

- joint AVS package available for comparing NIMROD and M3D output
- custom packages available for both NIMROD and M3D as stand-alone
- abandoned (for now) the use of MDS-plus
    - not suitable for exploring the large volumes of data simulations generate
    - awkward for unstructured and AMR data types



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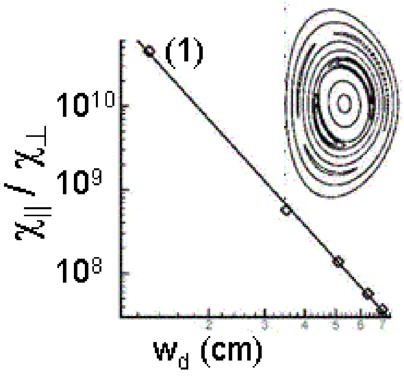
Applications Highlights Years 1-2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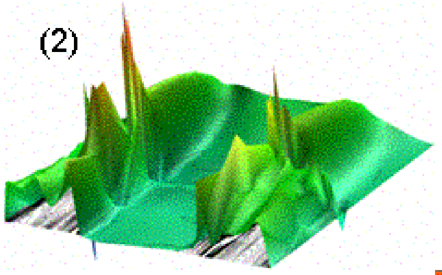
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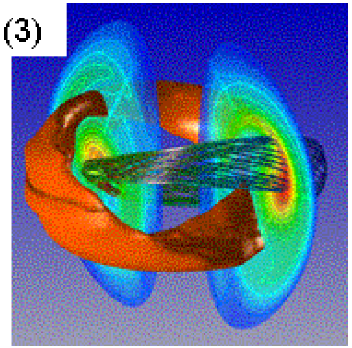
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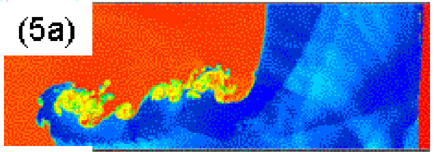
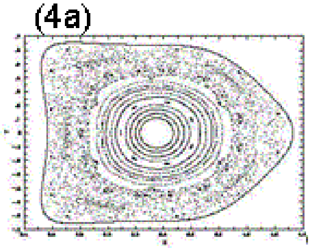
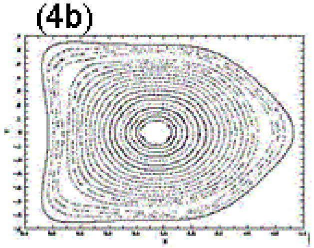
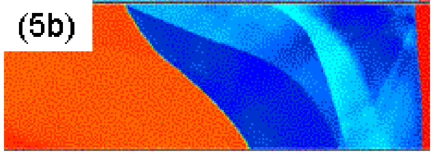

(5a)

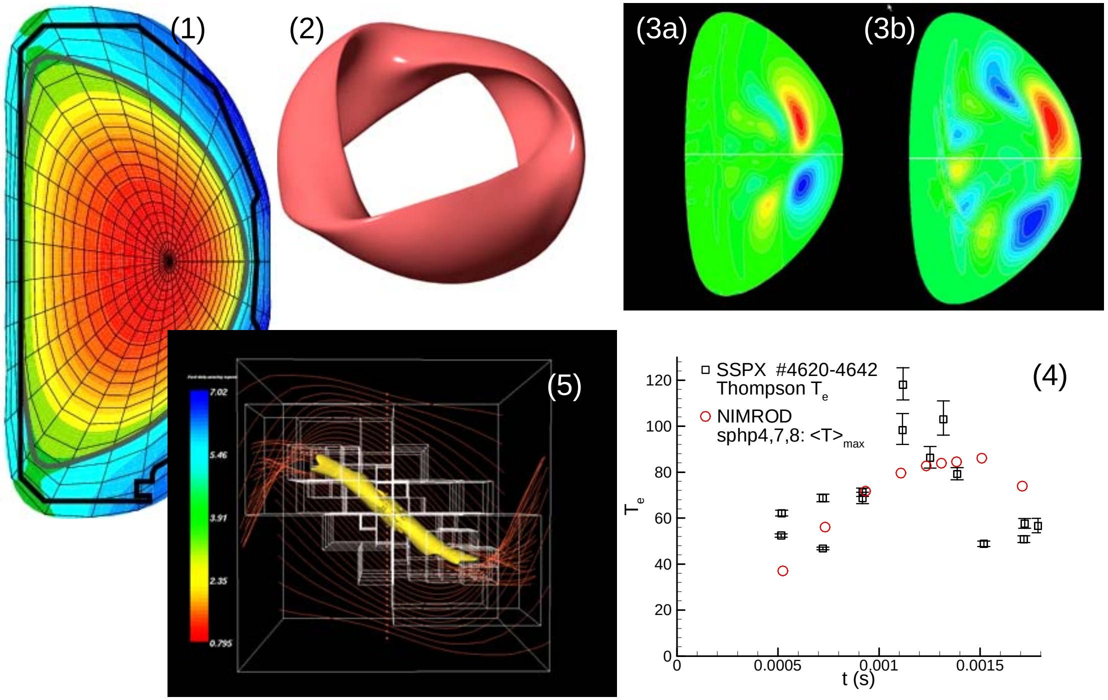

(4a)


(4b)


(5b)

1. Magnetic Island Thermalization at Realistic Parameters
2. Physics of the Current Hole
3. Effects of Strong Toroidal Shear on MHD Modes
4. Diamagnetic Stabilization of Instabilities in Stellarators
5. Suppression of the Richtmyer-Meshkov Instability by a Magnetic Field

Applications Highlights Years 2-3



1. The Dynamics of high-beta disruptions
2. Realistic limits on Stellarator performance
3. Energetic particle driven modes in spherical tokamaks
4. MHD behavior in small laboratory experiments
5. Pellet fueling of a tokamak

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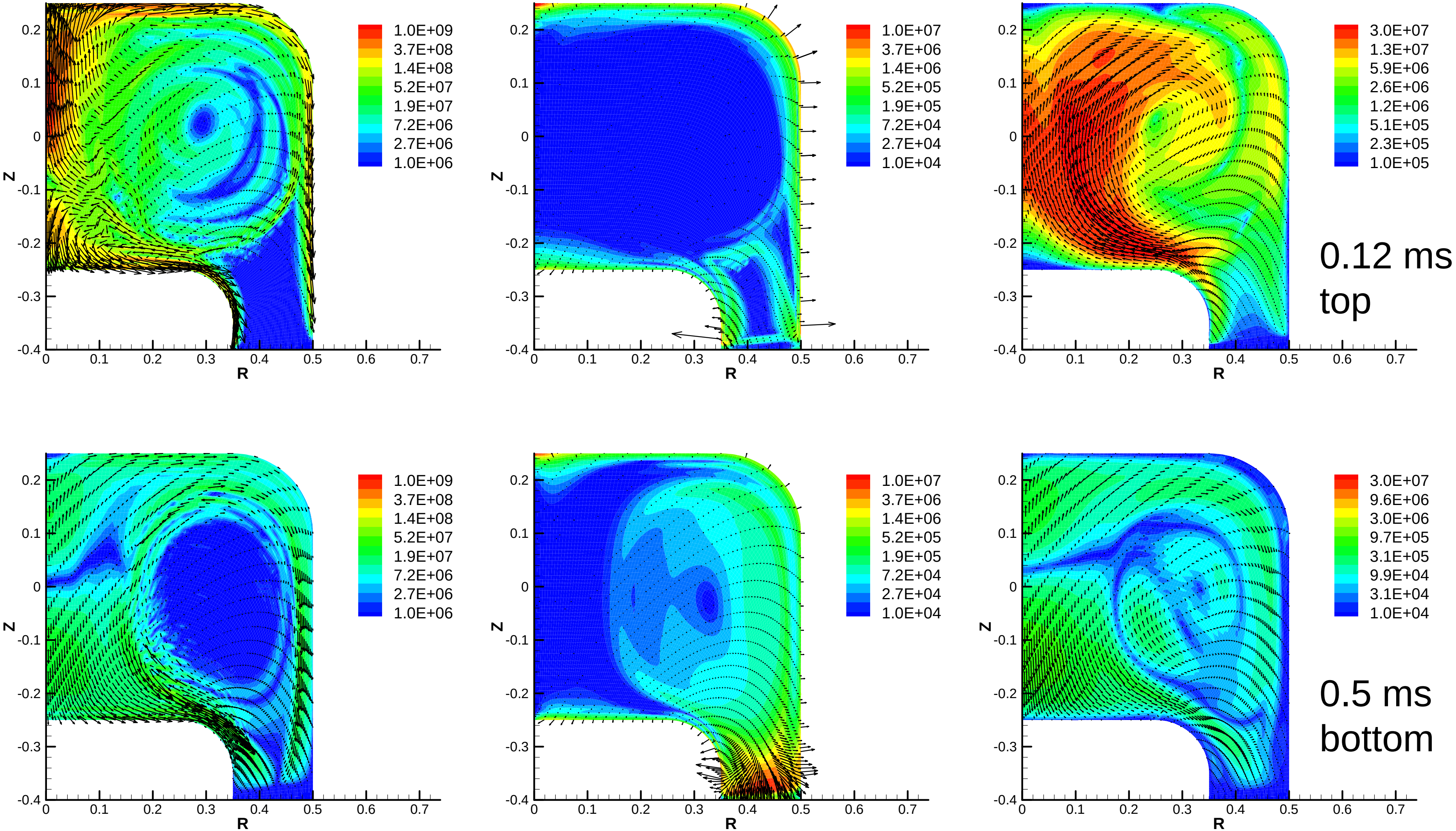
Sovinec presentation at recent ICC meeting showed that NIMROD simulation was able to reproduce many details of LLNL Spheromak experiment, providing validation of MHD model in this regime



0.12 ms top

0.5 ms bottom

conductive $\langle q_{\|} \mathbf{B}_{pol} \rangle$ conductive $\langle \mathbf{q}_{\perp pol} \rangle$ convective $\langle 2nT\mathbf{V}_{pol} \rangle$

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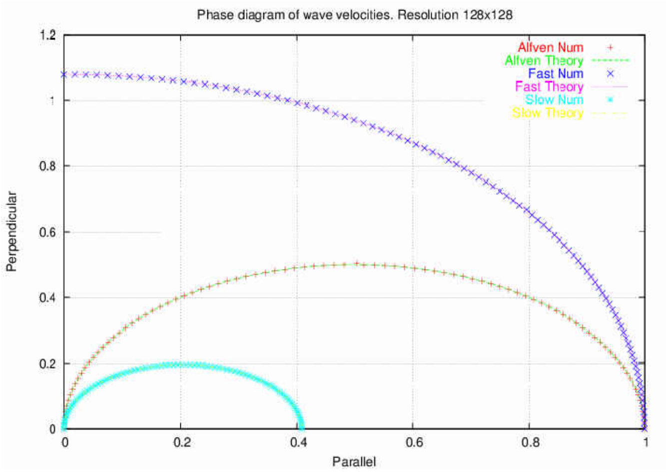
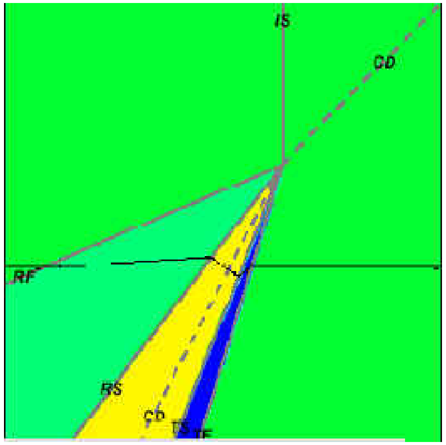
APDEC

- Implemented and fully verified resistive MHD equations in Chombo framework
    - uses unsplit generalized upwinding method
    - Godunov symmetrizable 8-wave formulation
    - $\nabla . B = 0$ enforced by projection technique

- Production version used for several applications
    - Richtmyer-Meshkov stabilization by B
    - magnetic reconnection at high S
    - pellet injection into tokamaks

- Future directions
    - nonlinear implicit Newton-Krylov version
    - flux coordinates
    - higher order to better handle anisotropy





“ We greatly underestimated how difficult it was to solve the extended MHD equations for fusion applications ”…*P.Colella, 2004*

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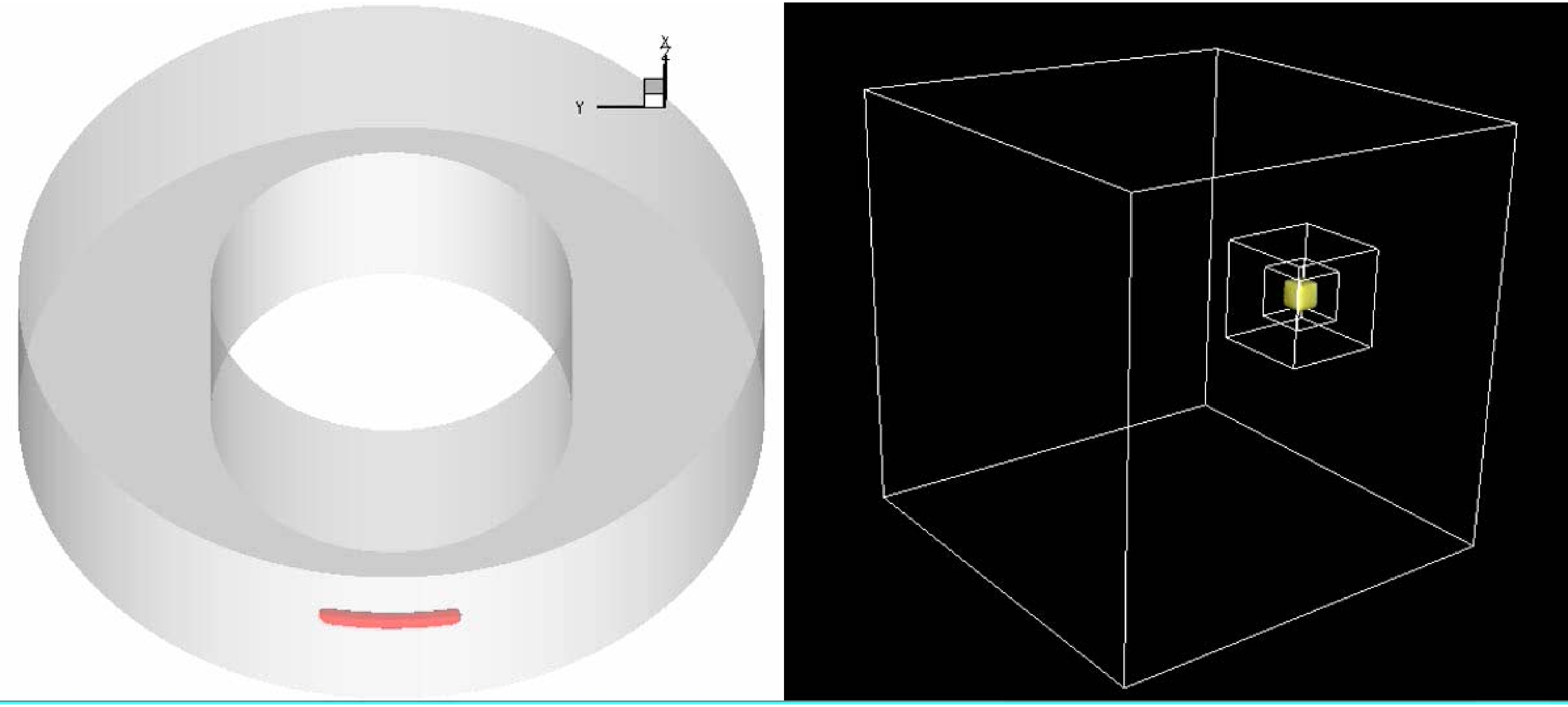
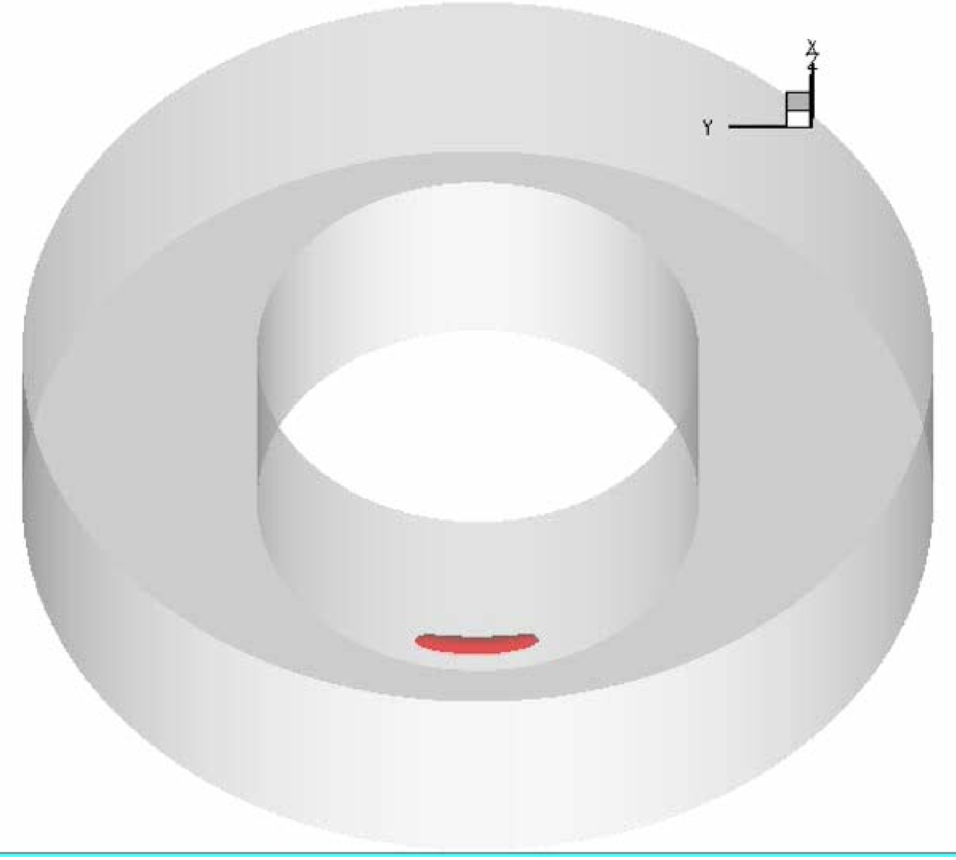
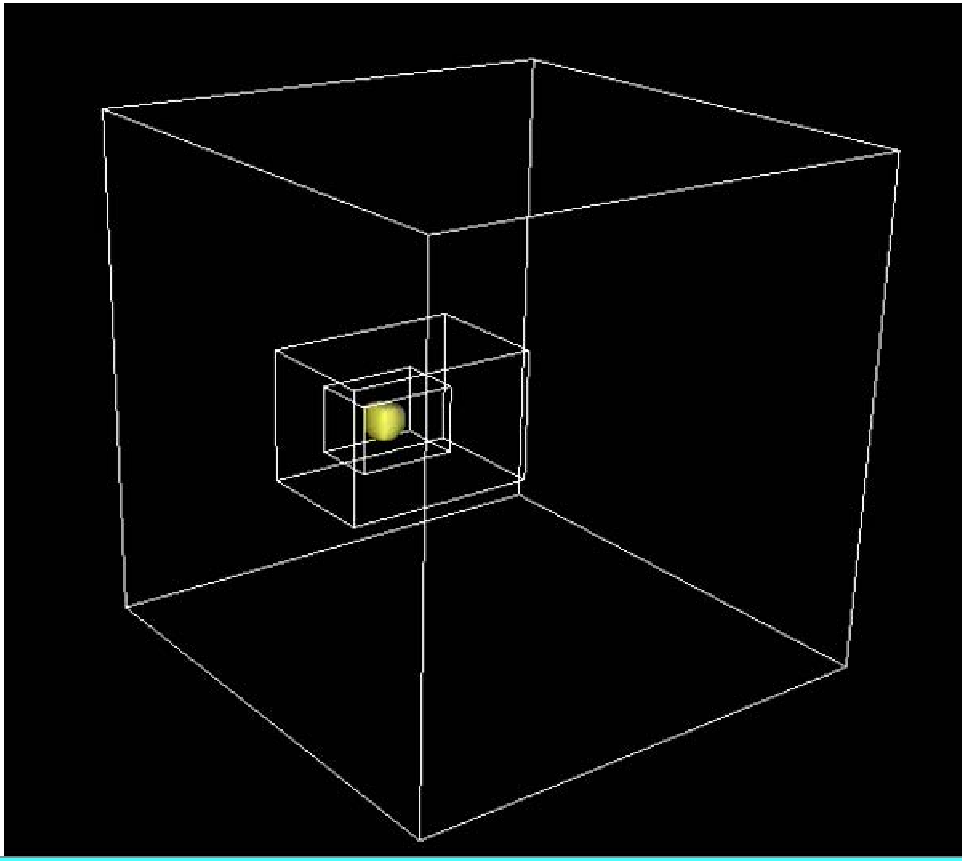
Low-field side pellet injection

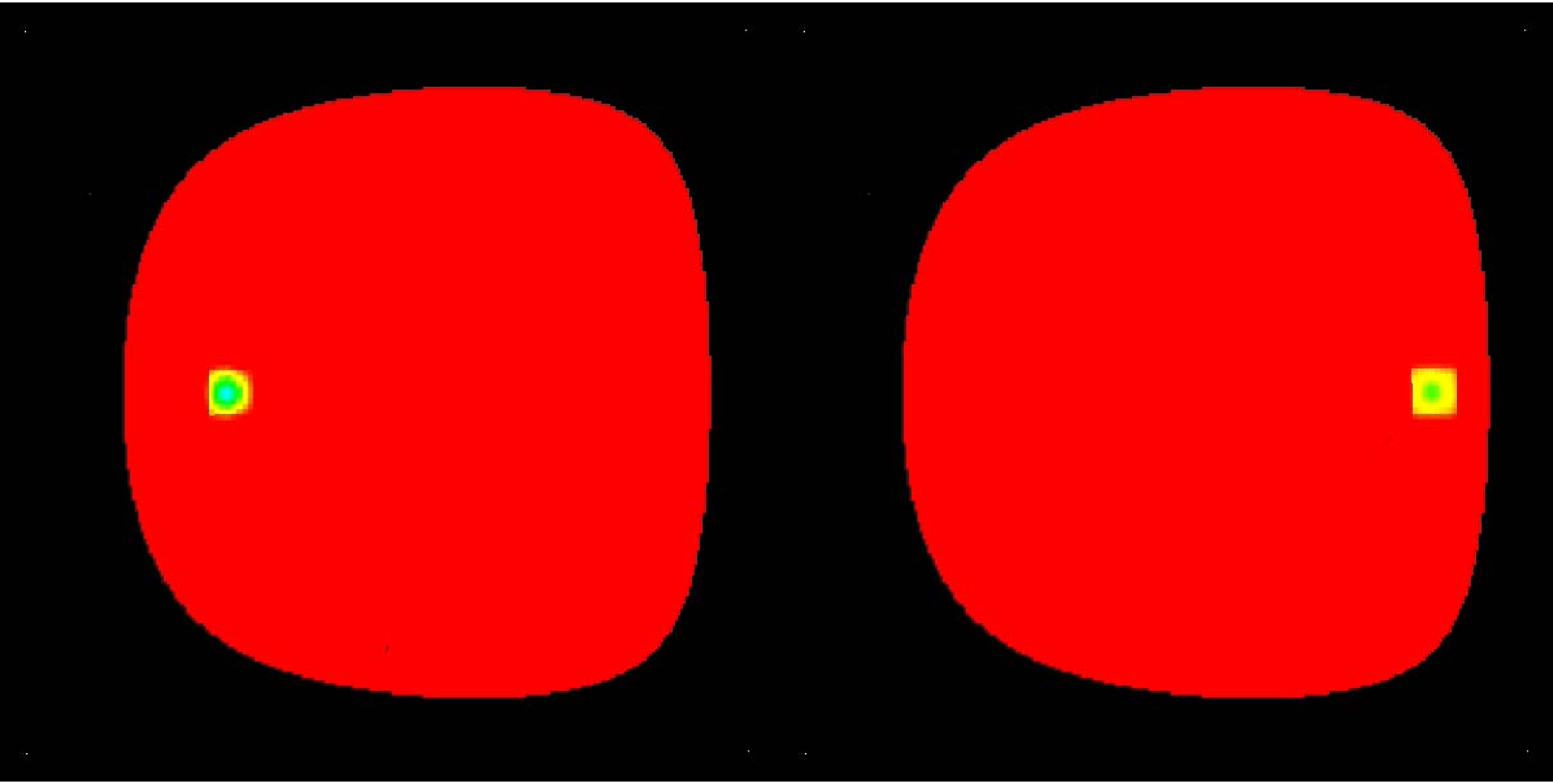


High-field side pellet injection





Comparison of LFS and HFS



Poloidal projection of density

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TOPS

Focus has been on improving the linear solvers in M3D and in NIMROD

- NIMROD switched from a CG solver to the optimized direct sparse matrix solver SuperLU
  - Factor 4-5 improvement in computational time for real applications
  - Improvement due to the ill-conditioned nature of the matrices
- M3D was able to reformulate it's elliptic equations in a symmetric form and switch from GMRES to ICCG to gain a factor of 2 in running time
- Hypre multi-grid package is also now implemented. This is the fastest solver for the largest problems.

TSTT

- Focus has been on implementing high-order finite elements in M3D, and in interfacing with custom mesh generator for NIMROD (CUBIT)
- Developed a set of “Challenge Problems” to introduce applied mathematicians to multi-scale fusion problems
  - Paul Fisher (ANL) wrote a paper on the anisotropic heat conduction problem quantifying the value of high-order elements
  - M.Shephard, J.Flaherty, and a post-doc (RPI) wrote a paper on the ability of h/p-refinement to deal with current singularities
  - Carol Woodward and postdoc (LLNL) are attempting resistive reconnection challenge problem
  - Through these papers, and many discussions, we have chosen a particular C^1 triangular finite element and a direct implicit finite difference method for the M3D-C^1 project

What have we learned from the ISICs?

- It has been confirmed that high order (3-5th) finite elements are a big win for fusion MHD:
  - a must for highly anisotropic heat conduction
  - leads to smaller matrices for same accuracy, making an implicit time advance feasible
  - jury is still out concerning C^0 vs C^1 elements
- Adaptive Mesh Refinement is a powerful tool for some transient problems with a range of space scales,
  - but it's usefulness for slow-growing MHD modes has not been demonstrated.
- It is valuable to have multiple, interoperable linear solvers available.
  - this is especially true now that the Cray X-1 is in the mix of architectures available to us

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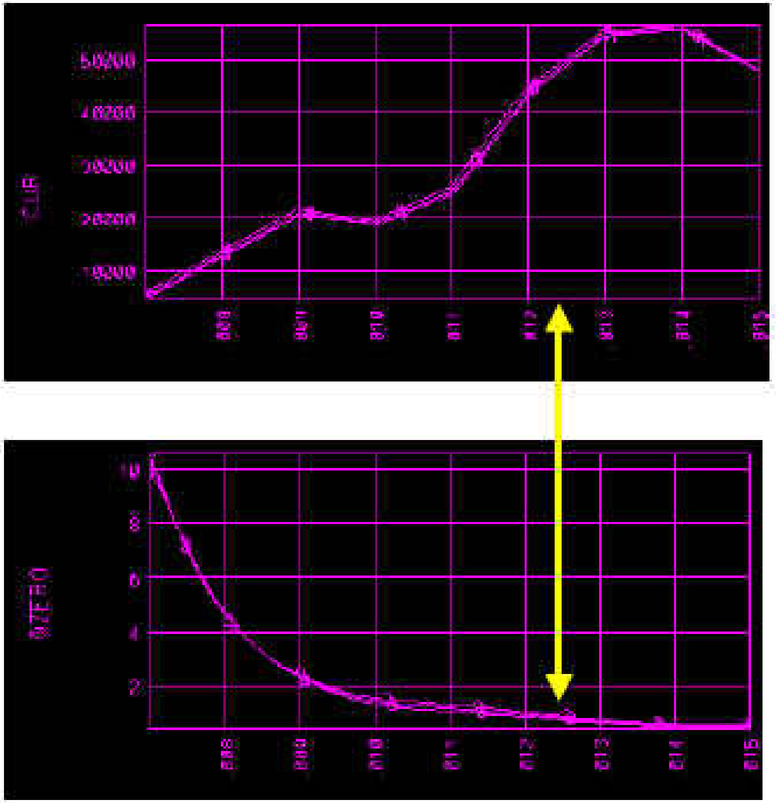
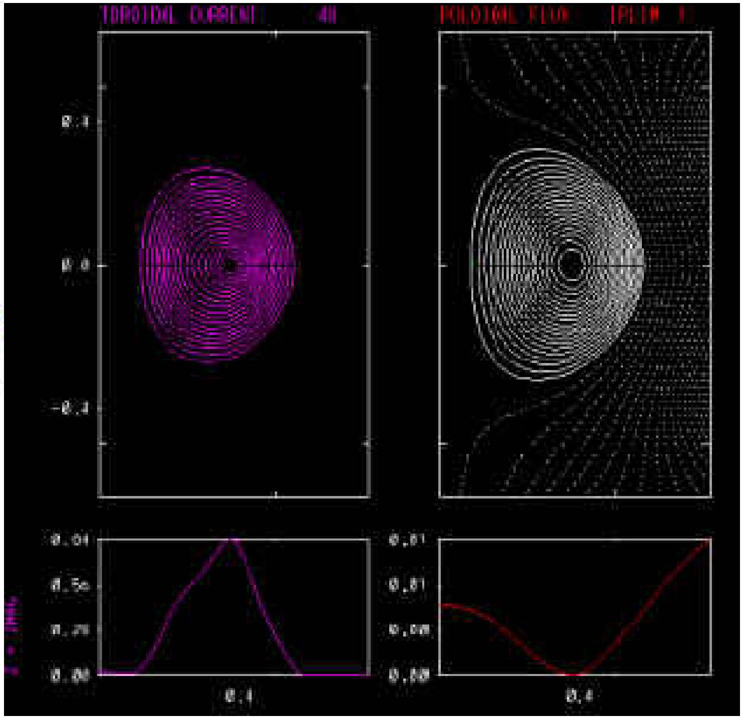
Status of The CDX-U validation/verification exercise

TSC follows 2D (axisymmetric) evolution of typical CDX-U discharge





R_0 = 33.5 cm

R/a = 1.5

κ = 1.6

B_T = 2300 g

T_e = 100ev

I_p = 70 kA

$n_e = 4 \times 10^{13}$ cm^{-3}

Equilibrium at t=12.40ms (as q_0 drops to 0.92) is used to initialize 3D runs

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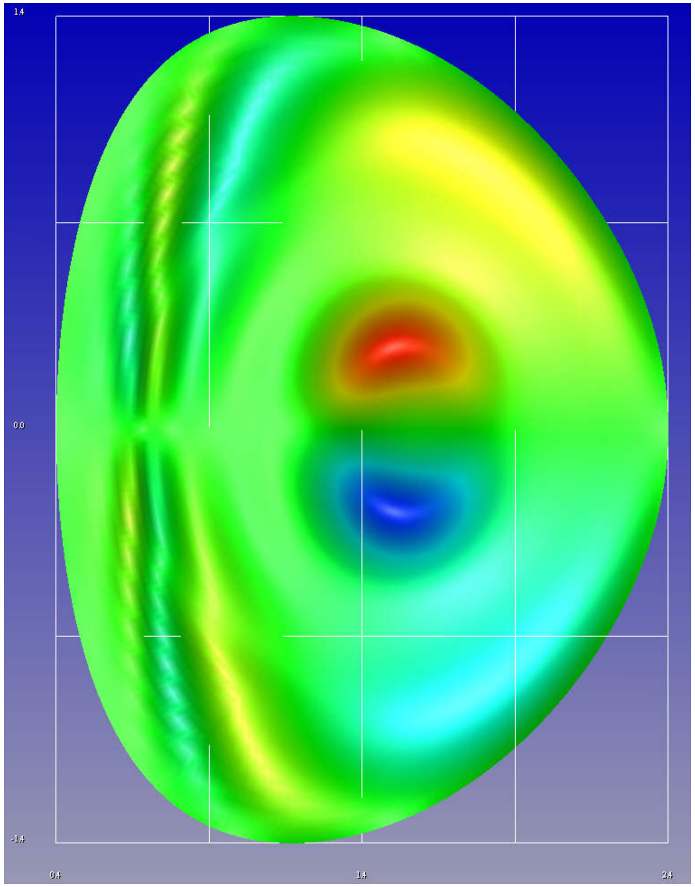
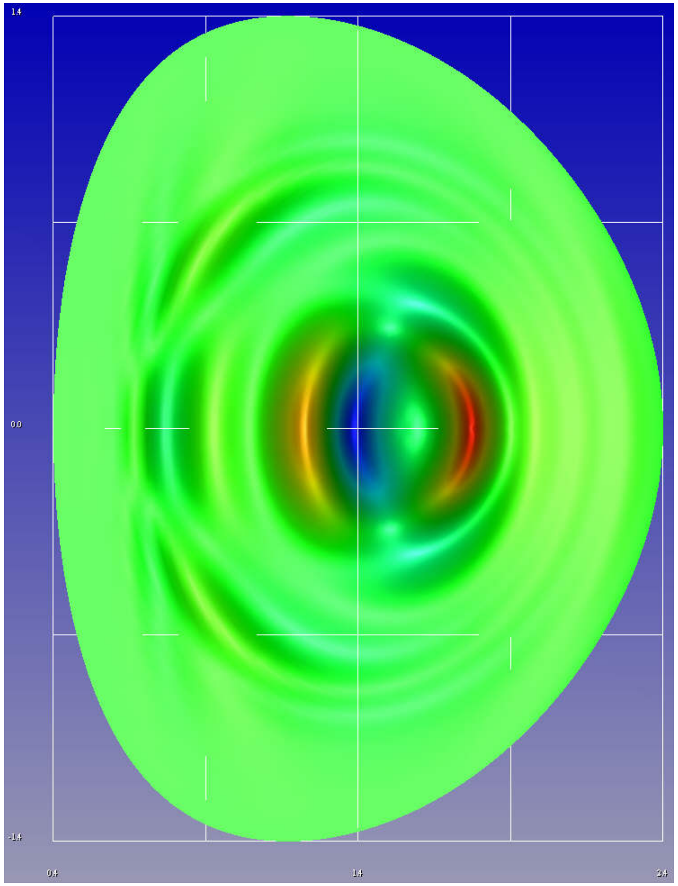
CDX-U: *n*=1 Eigenmode

Incompressible velocity
stream function U



Toroidal current density
J_ϕ



$\gamma \tau_A = 8.61 \times 10^{-3} \rightarrow$ growth time = 116 τ_A

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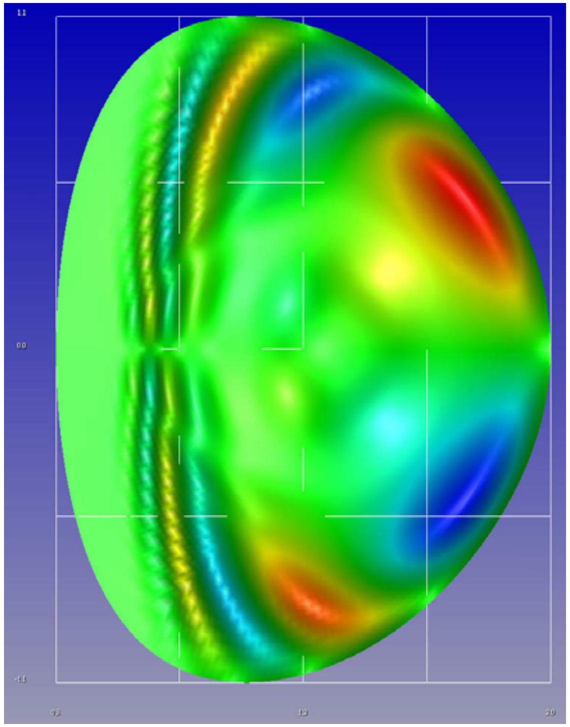
CDX-U: Higher *n* Eigenmodes

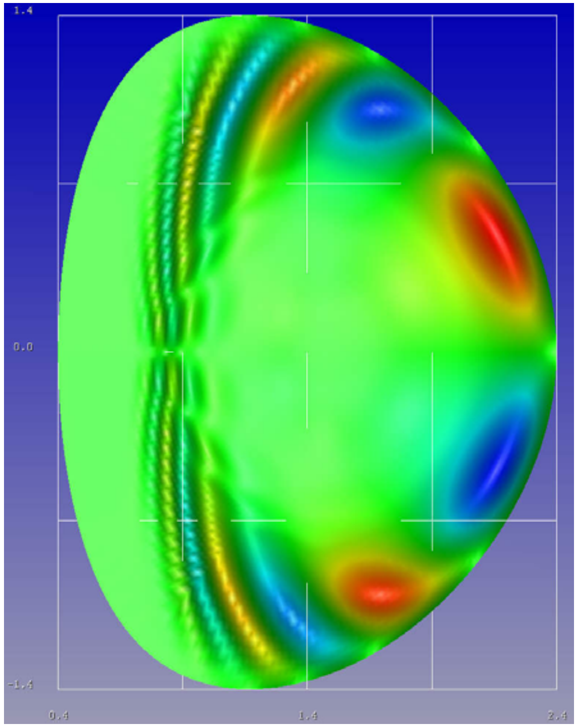
Incompressible velocity
stream function U

$n = 2$



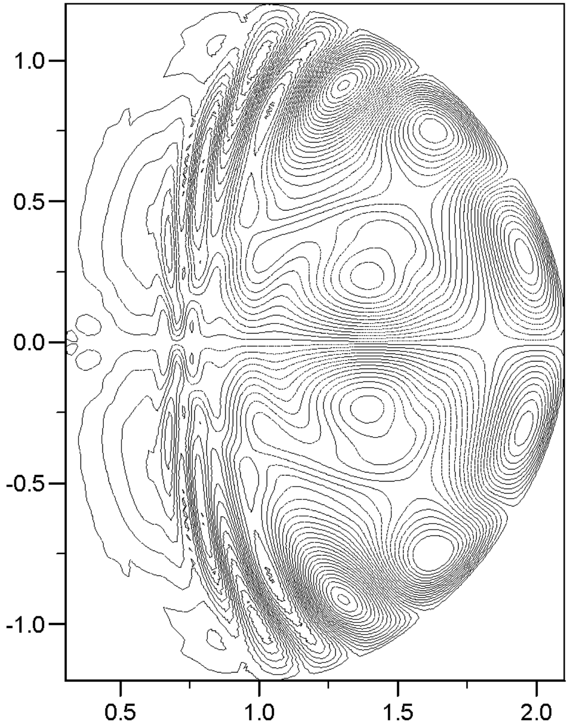
m ≥ 5
$\gamma \tau_A = 1.28 \times 10^{-2}$

$n = 3$



m ≥ 7
$\gamma \tau_A = 1.71 \times 10^{-2}$

$n = 4$ (projected)



m ≥ 8
not converged

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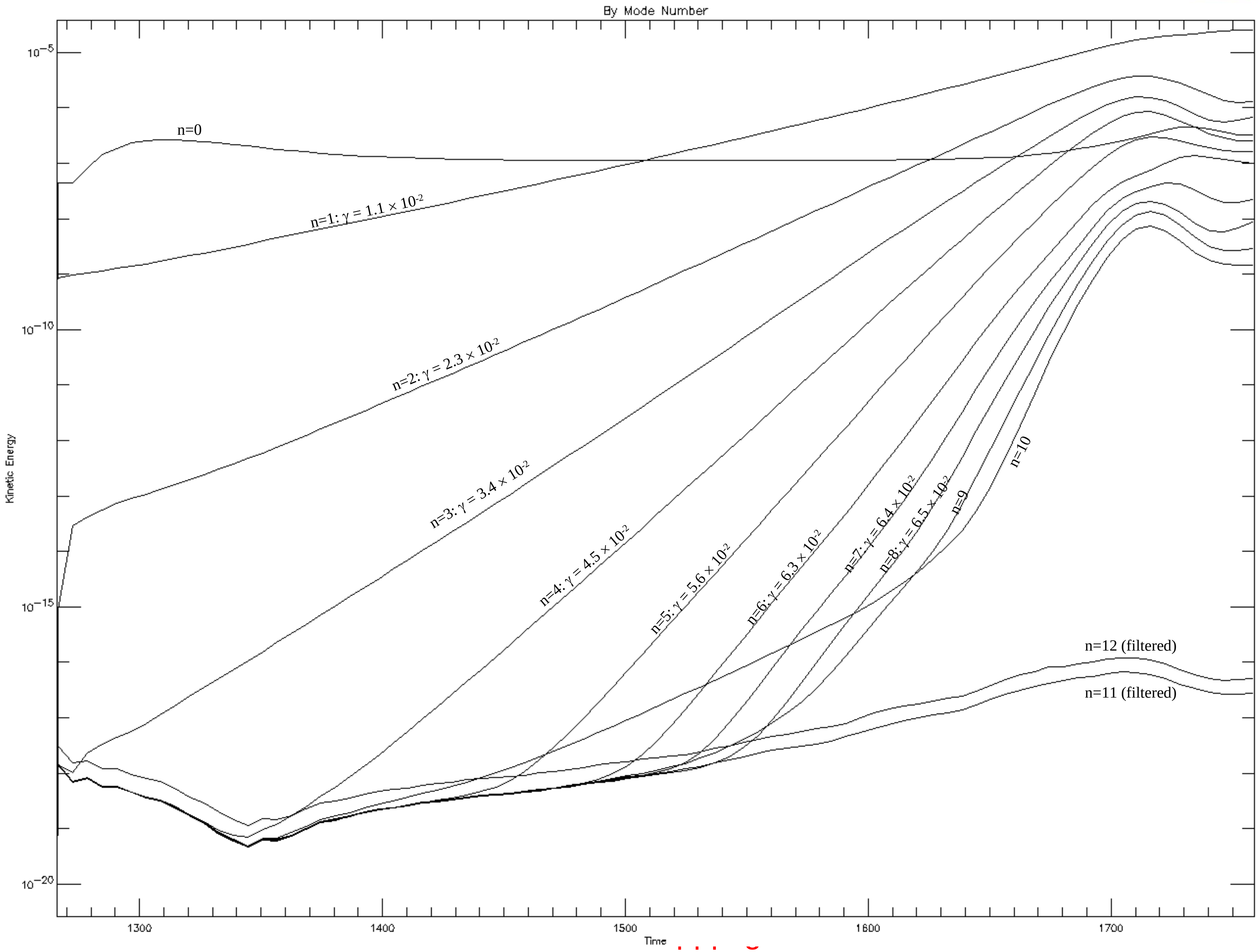
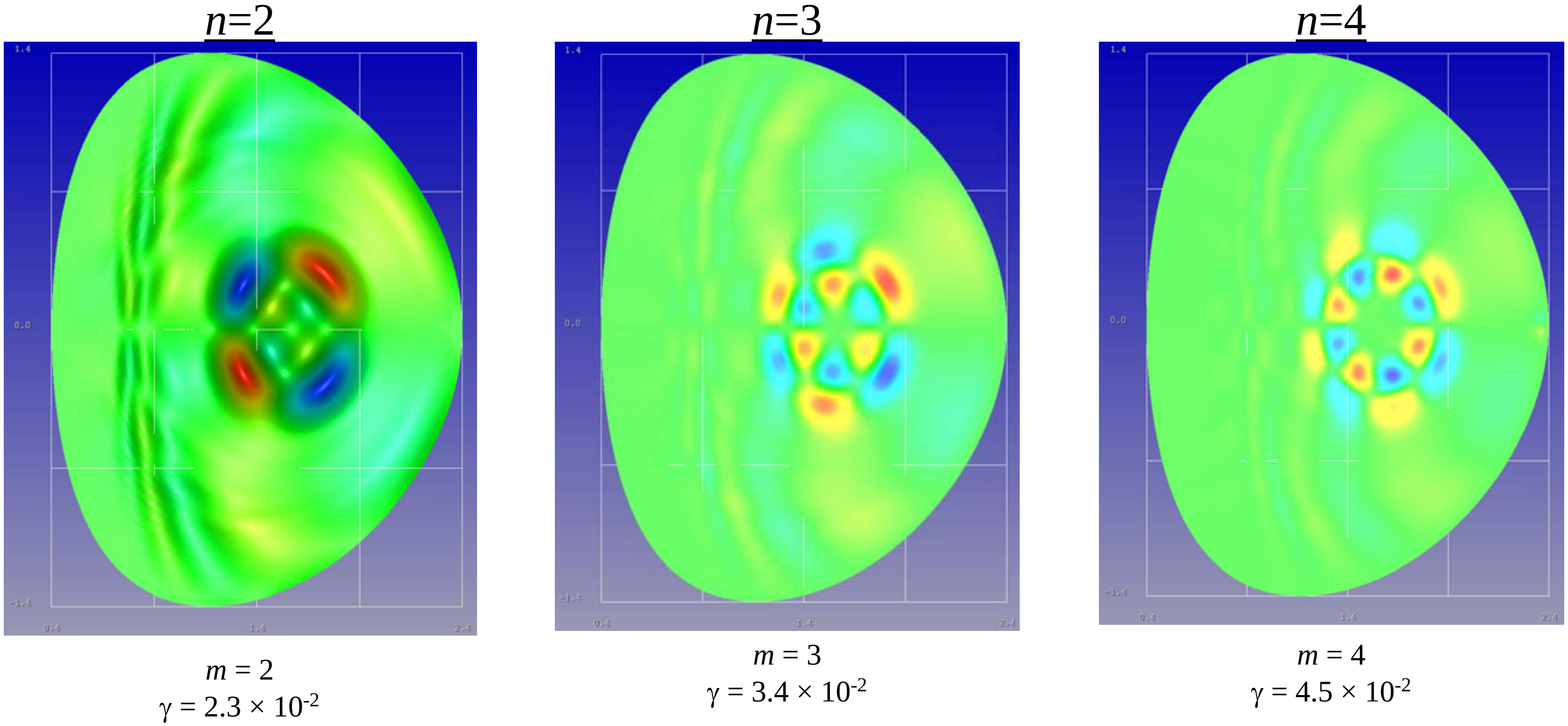
Nonlinear Kinetic Energy History



“Linear” high-*n* modes are driven, not eigenmodes

Incompressible velocity stream function *U*

Component of “linear” mode
in nonlinear run



n=2

$m = 2$
$\gamma = 2.3 \times 10^{-2}$

n=3

$m = 3$
$\gamma = 3.4 \times 10^{-2}$

n=4

$m = 4$
$\gamma = 4.5 \times 10^{-2}$

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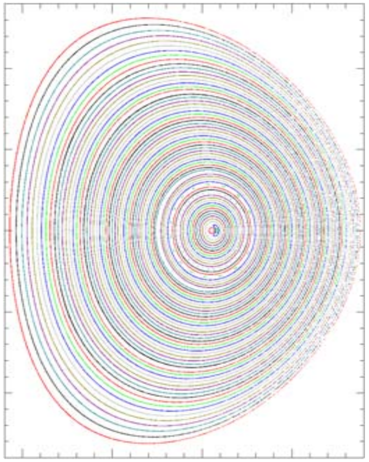
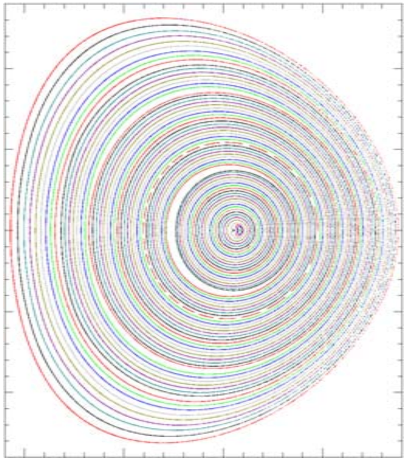
CDX-U: Nonlinear Time Series

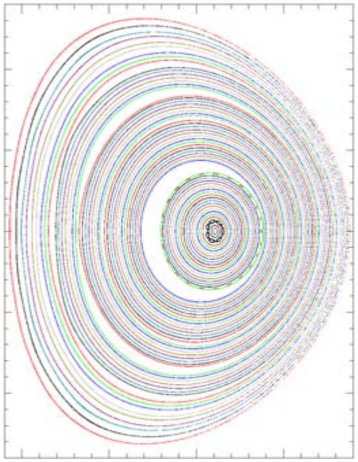
Poincaré Plots



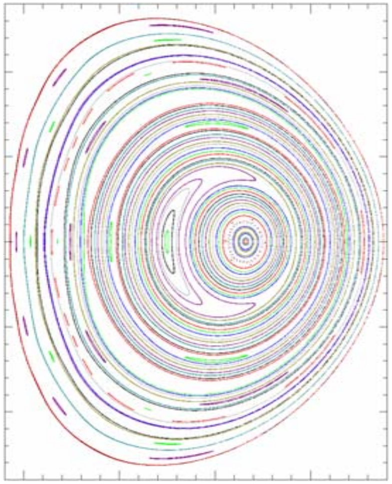
t = 1266.17



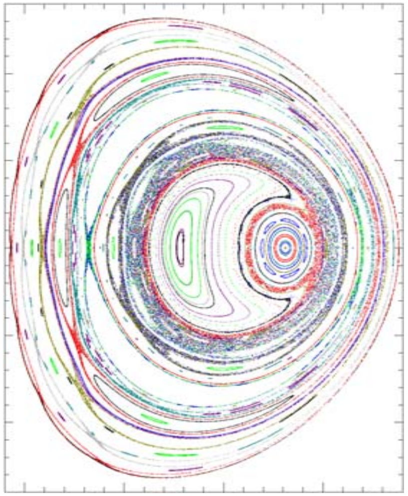
t = 1404.57



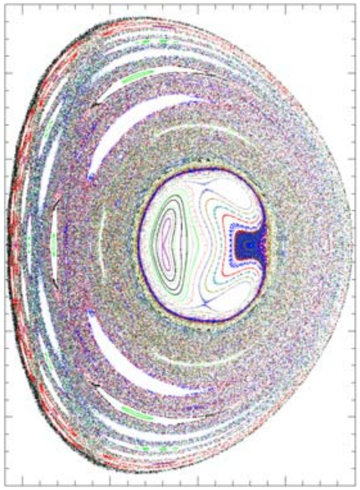
t = 1548.68



t = 1620.62



t = 1686.41



t = 1758.34

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Summary: CDX-U Simulation

- All toroidal modes of the q_0=0.92 CDX equilibrium are linearly unstable in resistive MHD model
  - n=1 is an internal kink mode
  - n>1 are resistive ballooning instabilities
  - Higher n modes have higher growth rates
- Nonlinear resistive MHD evolution beginning with just an n=1 perturbation disrupts within a sawtooth crash time
- Adding toroidal flow reduces the growth rate but does not stabilize
- Adding large parallel thermal conductivity reduces growth rate, but does not stabilize
- Adding the ω* term does not appreciably alter the growth rate

- **Realistic treatment of these modes requires a more complete extended MHD model—this is our present focus**

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Future Directions

- Get serious about extended-MHD
  - Evaluate several sets of equations with different orderings
  - Efficient algorithms for solving the extended MHD equations with dispersive waves
- Working towards burning plasma problems
  - 7 critical problems identified that are of interest to ITER
- Improved infrastructure
  - Further expand common visualization packages
  - Unified data management
- Integration Activities
  - Integrated calculation with RF
  - Hybrid calculation of neoclassical closures

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Extended MHD Models

Model	Momentum Equation	Ohm's law	Whist-lers[1]	KAW[2]	GV[3]	Slow dynamics[4]
General	$mn\frac{d\mathbf{V}}{dt} = -\nabla(p_e + p_i)$ $+\mathbf{J}\times\mathbf{B} - \nabla\cdot(\Pi_{\Vert e} + \Pi_{\Vert i}) - \nabla\cdot\Pi_i^{gv}$	$\mathbf{E} = -\mathbf{V}\times\mathbf{B} + \eta\mathbf{J}$ $+\frac{1}{ne}\left(\mathbf{J}\times\mathbf{B} - \nabla p_e - \nabla\cdot\Pi_{\Vert e}\right)$	Yes	Yes	Yes	Either
Generalized Hall MHD[5]	$mn\frac{d\mathbf{V}}{dt} = -\nabla(p_e + p_i)$ $+\mathbf{J}\times\mathbf{B} - \nabla\cdot(\Pi_{\Vert e} + \Pi_{\Vert i})$	$\mathbf{E} = -\mathbf{V}\times\mathbf{B} + \eta\mathbf{J}$ $+\frac{1}{ne}\left(\mathbf{J}\times\mathbf{B} - \nabla p_e - \nabla\cdot\Pi_{\Vert e}\right)$	Yes	Yes	No	No
Neoclassical-MHD	$mn\frac{d\mathbf{V}}{dt} = -\nabla(p_e + p_i)$ $+\mathbf{J}\times\mathbf{B} - \nabla\cdot(\Pi_{\Vert e} + \Pi_{\Vert i}) - \nabla\cdot\Pi_i^{gv}$	$\mathbf{E} = -\mathbf{V}\times\mathbf{B} + \eta\mathbf{J} - \frac{1}{ne}\nabla\cdot\Pi_{\Vert e}$	No	No	Yes	Yes
Generalized resistive MHD[5]	$mn\frac{d\mathbf{V}}{dt} = -\nabla p + \mathbf{J}\times\mathbf{B} - \nabla\cdot\Pi_{\Vert}$	$\mathbf{E} = -\mathbf{V}\times\mathbf{B} + \eta\mathbf{J}$	No	No	No	No
Generalized drift[6]	$mn\frac{d\mathbf{V}}{dt} = -mn\mathbf{V}_{di}\cdot\nabla\mathbf{V}_{\perp} + \upsilon_{gv}$ $+nm\mu\nabla_{\perp}^2\mathbf{V} - \nabla\cdot(\Pi_{\Vert e} + \Pi_{\Vert i})$ $-\nabla(p_e + p_i) + \mathbf{J}\times\mathbf{B}$	$\mathbf{E} = -\mathbf{V}\times\mathbf{B} + \eta\mathbf{J}^*$ $-\frac{1}{ne}\left[\nabla_{\Vert} p_e + \nabla\cdot\Pi_{\Vert e}\right]$	No	Yes	Yes	Yes

Higher order modes present in Extended MHD models present new numerical challenges

Mode	**Origin**	**Wave Equation**	**Dispersion**	**Comments**
Whistler	in Ohm $\mathbf{J}\times\mathbf{B}$	$\frac{\partial^2\mathbf{B}}{\partial t^2}=-\left(\frac{V_A^2}{\Omega}\right)^2(\mathbf{b}\cdot\nabla)^2\nabla^2\mathbf{B}$	$\omega^2=V_A^2k^2\left[1+\frac{1}{\beta}\left(\rho_i k_\parallel\right)^2\right]$	•electron response •finite $k_\parallel$
KAW	in Ohm $\nabla_\parallel p_e$	$\frac{\partial^2\mathbf{B}}{\partial t^2}=\left(\frac{V_A V_{th*}}{\Omega}\right)^2(\mathbf{b}\cdot\nabla)^2\,\nabla\times\left[\mathbf{bb}\cdot\nabla\times\mathbf{B}\right]$	$\omega^2=V_A^2k_\parallel^2\left[1+\left(\rho_s k_\perp\right)^2\right]$	•ion and e$^-$ response •finite $k_\parallel$ $k_\perp$
Parallel ion GV	η_4 term in $\nabla\cdot\Pi^{GV}$	$\rho\frac{\partial^2\mathbf{V}_\perp}{\partial t^2}=-\eta_4^2\nabla_\parallel^4\mathbf{V}_\perp$	$\omega_{\frac{L\pm}{R\pm}}=V_A k_\parallel\left[\pm1\pm\frac{1+\beta}{2\sqrt{\beta}}\left(\rho_i k_\parallel\right)\right]$	•ion response •finite $k_\parallel$
Perp. ion GV	η_3 term in $\nabla\cdot\Pi^{GV}$	$\rho\frac{\partial^2\mathbf{V}_\perp}{\partial t^2}=-\eta_3^2\nabla_\perp^4\mathbf{V}_\perp$	$\omega^2=V_A^2k_\perp^2\left[1+\frac{\gamma\beta}{2}+\frac{\beta}{16}\left(\rho_i k_\perp\right)^2\right]$	•ion response • finite $k_\perp$

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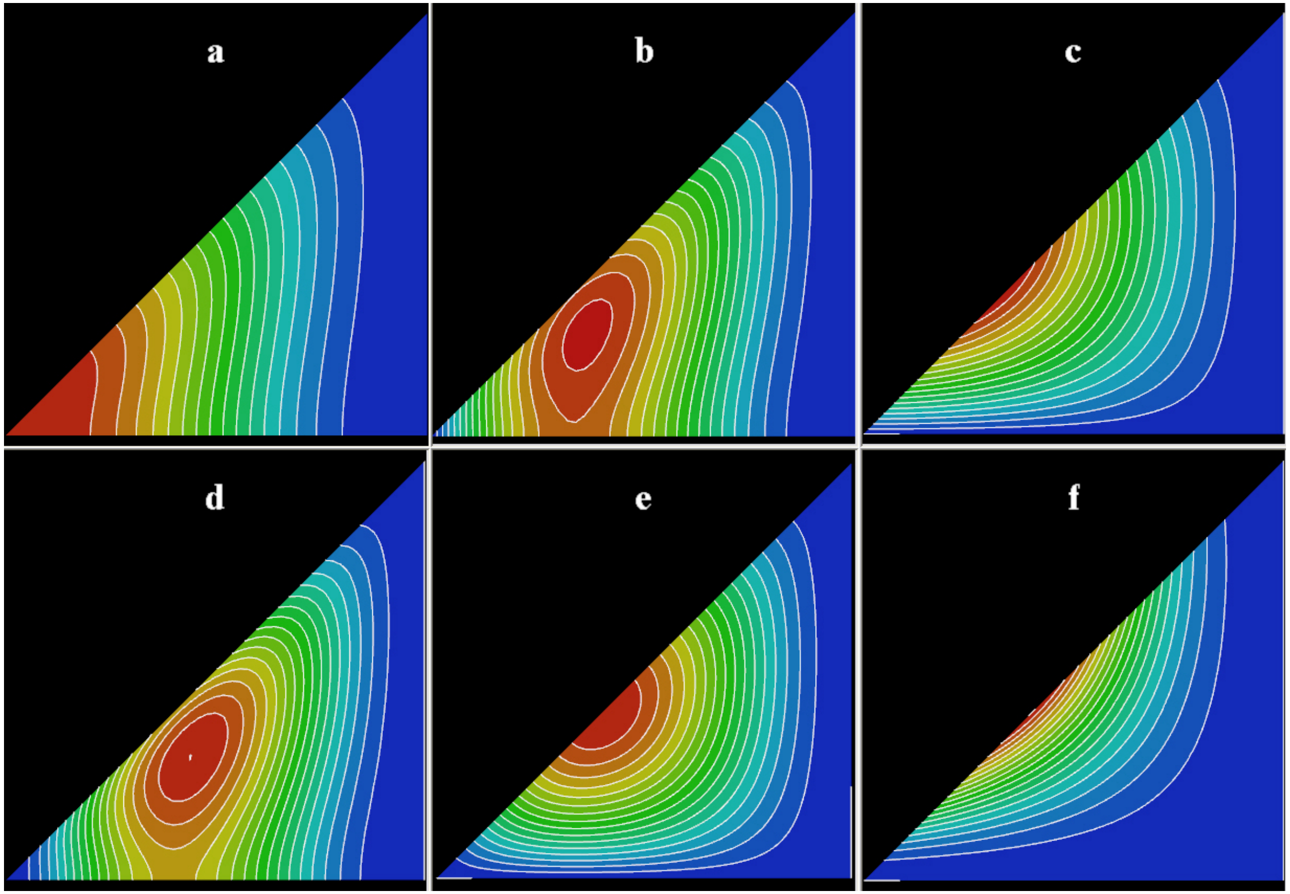
$a_i = g_{ij}\,\Phi_j$

The M3D C^1 Trial Functions:

$$\phi = \sum_{i=1}^{20} a_i\, \xi^{m_i}\eta^{n_i} = \sum_{i=1}^{20}\sum_{j=1}^{18} g_{ij}\Phi_j \xi^{m_i}\eta^{n_i} = \sum_{j=1}^{18} v_j\Phi_j$$

$$v_j = \sum_{i=1}^{20}\xi^{m_i}\eta^{n_i} g_{ij}$$



These are the trial functions. There are 18 for each triangle.

The 6 shown here correspond to one node, and vanish at the other nodes, along with their derivatives

Each of the six has value 1 for the function or one of it's derivatives at the node, zero for the others.

Note that the function and it's derivatives (through 2nd) play the role of the amplitudes

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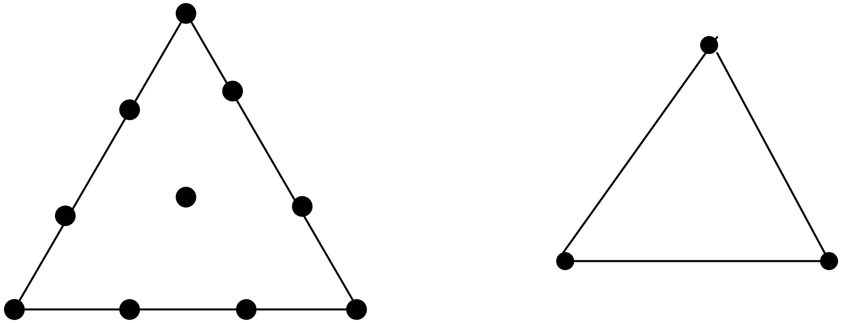
Comparison of reduced quintic to other popular triangular elements

	Vertex nodes	Line nodes	Interior nodes	accuracy order h^p	UK/T	continuity
linear element	3	0	0	2	½	C^0
Lagrange quadratic	3	3	0	3	2	C^0
Lagrange cubic	3	6	1	4	4½	C^0
Lagrange quartic	3	9	3	5	8	C^0
M3D C^1	18	0	0	5	3	C^1



UK/T is the number of unknowns per triangle

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Summary

- CEMM is functioning well
  - Productive in terms of results, lively meeting
  - Achieving milestones
  - M3D and NIMROD groups playing together nicely

- Interaction with ISICs going well
  - Very much a 2-way street…each learning from one another

- CDX-U Verification/Validation problem leading to interesting physics
  - Driver for developing better extended-MHD model
  - Common problem being addressed by both codes

- Emphasis in the near future is on Extended-MHD
  - Which set of equations to use
  - How to solve them
  - Understand the physics output
  - Implications for ITER-class burning plasmas

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