

Outline

- Noteworthy news items:
 - 50 refereed and IAEA papers in 04-07 grant period
 - Close connections with SWIM and CPES
 - Well attended APS and Sherwood CEMM Meetings
 - SIAM news article
 - OFES Joule milestones for both FY05 and FY06
 - Parallel scaling studies extended to over 4000 p for both NIMROD and M3D
 - Graduate Education
- Recent Activities and Accomplishments
 - Model Development
 - Code and Algorithm Development
 - Applications
- New Planned research we would like the PAC's guidance on
 - Physics Model Development
 - Algorithm and other Code Development
 - Applications
 - Verification and Validation plans
- New partnerships with CS/Applied Math

CEMM Software Roadmap developed with D. Keyes/TOPS

"Brute force" extrapolation from CDX-U to ITER gives a factor of 10¹² in space-time points required (explicit, linear elements, uniform mesh)

This should be achievable as follows:

- 1.5 orders: increased parallelism
- 1.5 orders: processor speed and efficiency
- 4 orders: adaptive gridding
- 1 order: higher order elements
- 1 order: field-line following coordinates
- 3 orders: implicit algorithms

Should be possible. Requires manpower to implement and customize mostly known algorithms in leading codes Note: Hardware (3) : Software (9) !!

SIAM News: Volume 39, Number 7, Sept 2006

Interview with David Keyes

"The current issue of SIAM News features an article by Michelle Sipics The article deserves not only interest but also praise. It is timely, absorbing, trenchant."

Paul Saylor (U. Illinois) in NA-Digest

Taking on the ITER Challenge, Scientists Look to Innovative Algorithms, Petascale Computers

By Michelle Sipics

The promise of fusion as a clean, selfsustaining and essentially limitless energy source has become a mantra for the age, held out by many scientists as a possible solution to the world's energy crisis and a way to reduce the amounts of greenhouse gases released into the atmosphere by more conventional sources of energy. If self-sustaining fusion reactions can be realized and maintained long enough to produce electricity, the technology could potentially revolutionize energy generation and use.

ITER, initially short for International Thermonuclear Experimental Reactor, is now the official, non-acronymic name (meaning "the way" in Latin) of what is undoubtedly the largest undertaking of its kind. Started as a collaboration between four major parties in 1985, ITER has evolved into a seven-party project that finally found a physical home last year, when it was announced that the ITER fusion reactor would be built in Cadarache, in southern France. (The participants are the European Union, Russia, Japan, China, India, South Problems remain, however—notably the years, and perhaps decades, of progress needed to attain such a goal. In fact, even *simulating* the proposed ITER tokamak is currently out of reach. But according to David Keyes, a computational mathematician at Columbia University and acting director of the Institute for Scientific Computing Research (ISCR) at Lawrence Livermore National Laboratory, the ability to perform such simulations may be drawing closer.

Hardware 3, Software 9

"Fusion scientists have been making useful characterizations about plasma fusion devices, physics, operating regimes and the like for over 50 years," Keyes says. "However, to simulate the dynamics of ITER for a typical experimental 'shot' over scales of interest with today's most commonly used algorithmic technologies would require approximately 10^{24} floating-point operations." That sounds bleak, given the 280.6 Tflop/s (10^{12} flops/s) benchmark performance of the IBM BlueGene/L at Lawrence Livermore National Laboratory—as of June

CEMM Successfully completed the only OFES Theory Annual Program Performance Target¹ for both FY05 and FY06 (Joule Milestone)

FY 2006 Science Accomplishments

High-Resolution Nonlinear Simulations of Edge Localized Modes

Predicting the behavior and optimizing the confinement in a tokamak burning plasma device such as ITER requires improved simulations of the entire plasma region, particularly the plasma edge. The steep gradients present at the edge give rise to a class of quasi-periodic nonlinear oscillations known as Edge Localized Modes or ELMs. The simulation of the nonlinear physics of these events is very challenging due to the fine-scale structures that develop and influence the ELM frequency and magnitude. This year, the large nonlinear extended MHD codes being developed in the U.S.— NIMROD and M3D—have been able to substantially increase the realism of their simulations by increasing the resolution of their models, allowing the inclusion and study of physical processes previously neglected—most notably sheared plasma rotation. These high resolution simulations, including sheared plasma flow, help to illuminate the important plasma properties that determine different ELM behavior. This knowledge is key to begin developing control techniques to modify ELM behavior, leading to higher performance in ITER.

Science/Fusion Energy Sciences/Science Page 396 FY 2008 Congressional Budget

This was the only OFES Theory/Computation accomplishment included in the FY 2008 President's budget request.

¹(see http://www.science.doe.gov/ofes)

Parallel Scaling Studies



- M3D 3D weak scaling: 71% efficiency to 4960 p on Jaguar
- M3D 3D strong scaling: 87% efficiency up to 3072 p on Jaguar
- NIMROD strong scaling: 70% efficiency up to 4096 p on Seaborg

See http://w3.pppl.gov/m3d/scale.html

And http://w3.pppl.gov/CEMM/Sherwood2007/Held.pdf

Graduate Education

- Presently have 10 Graduate Students with CEMM-related research for their PhD thesis
 - Princeton (3)
 - University of Wisconsin (6)
 - Utah State University (1)
- One student was selected by Princeton University for an "Honorific Fellowship" for his final year
- One UW student was awarded a DOE Computational Science Graduate Fellowship
- Students are encouraged to attend CEMM meetings and make presentations as appropriate.

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Model Development-1

 NIMROD and M3D-C¹ now have full (Braginskii) gyroviscous tensor and 2-fluid terms incorporated and have verified these on test problems

$$\begin{split} & \frac{\partial n}{\partial t} + \nabla \bullet (n\vec{V}) = 0 & \text{Present since Day 1} \\ & \text{Recently been added and tested} \\ & \frac{\partial \vec{B}}{\partial t} = -\nabla \times \vec{E} & \mu_0 \vec{J} = \nabla \times \vec{B} & \text{Known, but not yet tested} \\ & \text{Still being developed (|| closures)} \\ & nM_i (\frac{\partial \vec{V}}{\partial t} + \vec{V} \bullet \nabla \vec{V}) + \nabla p = \vec{J} \times \vec{B} - \nabla \bullet \Pi_{GV} - \nabla \bullet \Pi_{||} - \nabla \bullet \Pi_{\perp} \\ & \vec{E} + \vec{V} \times \vec{B} = \frac{1}{ne} (\vec{R} + \vec{J} \times \vec{B} - \nabla p_e - \nabla \bullet \Pi_{||}^e) \\ & \frac{3}{2} \frac{\partial p_e}{\partial t} + \nabla \bullet (\frac{3}{2} p_e \vec{V}) = -p_e \nabla \bullet \vec{V} + \frac{\vec{J}}{ne} \bullet [\frac{3}{2} \nabla p_e - \frac{5}{2} \frac{p_e}{n} \nabla n + \vec{R}] - \Pi_e : \nabla (V - \frac{\vec{J}}{ne}) \\ & -\nabla \bullet \vec{q}_{e\perp}^c - \nabla \bullet \vec{q}_{e\parallel}^c - \nabla \bullet \vec{q}_{e\parallel} + Q_{\Delta} \\ & \frac{3}{2} \frac{\partial p_i}{\partial t} + \nabla \bullet (\frac{3}{2} p_i \vec{V}) = -p_i \nabla \bullet \vec{V} - \Pi_i : \nabla V - \nabla \bullet \vec{q}_{i\perp}^c - \nabla \bullet \vec{q}_{i\parallel} - Q_{\Delta} \end{split}$$

• We are pursuing several approaches to develop the parallel (||) closures in a computationally tractable form

Model Development-2

Several approaches are being pursued within CEMM to develop the *low collisionality* parallel (||) closures in a computationally tractable form

• D. Barnes and S. Parker (NIMROD) and W. Park and G. Fu (M3D) are pursuing PIC-type δf closures for the stress tensor: new techniques to evolve Maxwellian and bound RMS particle weights.

• E. Held, et al, have developed continuum techniques to calculate parallel heat flow and the parallel stress tensor from the solution of the integral parallel kinetic equation: Extension of Chapman Enskog technique to low collisionality (CEL)

• J. Ramos has extended the formal fluid theory of magnetized plasma dynamics at low collisionality up to the stress and stress-flux tensors. The higher order terms still need to be closed kinetically. Simplified equations in some asymptotic regions.

Model Development-3

There are two generic types of extended MHD problems:

(J. Callen, Closures Workshop 2006, SWIM proposal, 2005):

- > **Fast MHD** ($\omega > v_1 \sim 10^3 \text{ s}^{-1}$) phenomena occur on *Alfven* timescale
 - Sawtooth, Disruption, ELMs: Only need 2-fluid + Gyroviscosity
- > Slow MHD ($\omega < v_1 \sim 10^3 \text{ s}^{-1}$) phenomena occur on *dissipative* timescale
 - NTM, RWM: All transport effects important, need parallel closures

Our strategy is to primarily pursue applications in the Fast MHD area as we work to better refine models and algorithms in the Slow MHD area.

Code Development - NIMROD

• A new implicit leapfrog algorithm including *implicit advection*, in addition to an *implicit Hall electric field*, was implemented.

- A matrix-free quasi-GMRES algorithm has been implemented.
- The SuperLU_dist parallel solver library is used to provide preconditioning.
- This was used for the FY07 Joule milestone, nonlinear two-fluid ELM computation.

• The fluid (ion) stress now has *additive options* for kinematic, isotropic, parallel, and Braginskii *gyro-viscous* components.

• The implementation is implicit for each of the terms, and the anisotropic options include the full three-dimensional and time-dependent variations of the magnetic field.

- The simulation-particle model for *minority hot ions* has been improved.
 - It uses the high-order representation of field quantities.
 - Full-orbit trajectories and kinetics is a new option.

• A new scheme has been implemented to separate the parallel decomposition of *non-local kinetic closure* computations from the decomposition of the fluid advance.

- In this scheme, a separate group of processors performs the computationally demanding closures and exchanges data with the fluid processors.
- Scaling to 4000 processors achieves 70% efficiency.



Code Development M3D

- *Parallel scaling:* We have extended our studies of the parallel scaling of the newly configured M3D code on the ORNL Cray XT3 (Jaguar)
 - include both 3D weak and 3D strong scaling.
 - Involved new grid partitioning, HYPRE Algebraic Multigrid (TOPS)
- *Finite Element Representation:* New classes of 2nd and 3rd order elements and mass-lumped elements have been implemented in M3D as an option.
 - Another class of higher order spectral elements has also been developed and tested in a model code. These will be fully implemented in M3D during the next proposal period.
- *Implicit Algorithm Improvement:* An improved partially implicit algorithm has been implemented in M3D resulting in a time-step increase of a factor of 5 over the older method.
 - This was achieved by solving an additional 3D elliptic equation each time step that isolates the component of the fluid vorticity in the poloidal plane.
 - The large time-step increase more than compensates the 50% increase in computational cost per step for the new 3D solve.
- Add Collision effects to fast ions: We have implemented a pitch angle scattering operator in the M3D code
 - demonstrated existence of bootstrap current

Code Development – M3D- C^{1}

• Reformulation of the M3D code using high-order triangular elements with *continuous first-derivatives*

• makes possible efficient implicit solution algorithm

• Physics model has been extended to *full 2D implicit* 8-field 2-fluid MHD model including Hall terms and full gyroviscous tensor

- JCP Paper submitted
- Triangular element based code has been modified to be *fully unstructured*
 - has been interfaced with ITAPS mesh adaptivity tools
 - collaboration with SCOREC team at RPI



- Has been extended from slab to toroidal geometry
 - is being used to calculate accurate 2-fluid toroidal equilibrium with flow that are stationary on all time scales
- Implicit formulation and algorithms have been developed for 3D
 - Linear 3D option being formulated (MARS++)
 - Nonlinear solution algorithm being tested
 - Preliminary tests show excellent parallel scaling efficiency

Code Development - AMRMHD

- Pellet Injection using Adaptive Mesh Refinement:
 - The AMRMHD code has now been converted to *magnetic coordinates*
 - for increased efficiency when applied to tokamak pellet fueling calculations.
 - We have implemented a detailed *local physics model* in neighborhood of pellet
 - includes ablation and long mean-free-path electron heating



- Begun steps to make this AMR code fully implicit,
 - we have worked with TOPS to demonstrate the feasibility by making a uniform mesh code with the same form of the finite difference equations fully implicit
 - uses the Newton-Kyrlov technique
 - present emphasis is on improved pre-conditioners

Code Verification – Gravitational Mode¹





• We extended the analytic dispersion relation of 2F stabilization of the gravitational mode (due to Roberts and Taylor) to the high- β regime.

- Both NIMROD and M3D- C^1 agree with analytic result.
- Compressibility, gyroviscosity, Hall-term, finite β are all important

¹Suggested by D. Schnack (Roberts and Taylor 1963)

Code Verification – Hot particle modes



- NIMROD and M3D agree on the linear frequency and growth rates
- NIMROD now has option of Boris particle push (not guiding center)



• Anisotropic hot particle pressure induces real frequency



 nonlinear calculation shows flattening of distribution function and frequency chirping 17

Code Verification: tearing and interchange



- 2-fluid linear tearing growth rates have been computed in all regimes.
- reproduces analytic results from Mirnov, Hegna, Prager Phys. Plasmas 11, 4481 (2004)
- extending comparison to include parallel electron stress



- careful study of the nonlinear development of a localized interchange instability
- screw pinch geometry
- current sheets are found to form in the nonlinear development
- interchange-tearing coupling through current sheet formation and ensuing magnetic reconnection

Code Verification: Linear ELMs



- M3D linear growth rates comparable to ELITE and GATO for η_{inner} =10⁻⁶, η_{outer} =10⁻²
- However, results sensitive to values and profile of resistivity not in ELITE model
- 2-fluid, flow effects absent in this comparison



eigenfunctions for n=5

Nonlinear 2F ELM Computation with NIMROD

- Project's first large-scale 3D computation with Hall effect and Braginskii gyroviscosity.
- Nonlinear evolution from DIII-D 113317 equilibrium includes toroidal modes $0 \le n \le 42$.
- Linear two-fluid stabilization is obtained for large-n.
- Nonlinear coupling is producing poloidal localization, unlike our previous MHD results.





Number density in the $\phi=0$ plane at simulation time $t=82.3 \ \mu$ s has poloidally localized ripples.





Temperature perturbations reach 100 eV at this time (T_{ped} =400 eV) and show a nonlinear helical structure. Perturbed plasma flow vectors are superposed.

Nonlinear 2F ELM Calculations with M3D





- density and temperature profiles at same times as contour plots (right). Density is seen to change more than temperature.
- large parallel thermal conductivity equilibrates the temperature on open lines to the wall temperature
- when 3D magnetic perturbations are present, magnetic separatrix is ill-defined, stochastically connecting regions of closed and open field lines.
- plasma in original separatrix region is poorly confined
- toroidal current density at edge (not shown) also broadens and decreases in amplitude.



Close-up of pressure contours at $\phi=0$ at 3 times



CMOD – n=20 eigenfunction. Pressure (I) and stream function (r) 21

m=1 mode in CDX-U Tokamak



- Low aspect ratio ($R_0/a = 1.4 1.5$)
- Small ($R_0 = 33.5 \text{ cm}$)
- Elongation $\kappa \sim 1.6$
- $B_T \sim 2300$ gauss
- $I_p \sim 70 \text{ kA}$
- $n_e \sim 4 \times 10^{13} \text{ cm}^{-3}$
- $T_e \sim 100 \text{ eV} \rightarrow \text{S} \sim 10^4$
- Discharge time ~ 12 ms
- Goal is to reproduce repetitive sawtooth behavior using actual parameters of experiment
- Phase-I is to compare nonlinear results from NIMROD and M3D using exactly the same initial conditions, boundary conditions, and sources now successfully completed!
- Phase-II extensions will be discussed later



- Initial (unexpected) results showed that linearly unstable modes existed for *all values of toroidal mode number n*
- These have been identified as *resistive ballooning modes* and are found to be stabilized by sufficiently large thermal conductivity
- Physics of the stabilization of these modes with increasingly complete physics description still area of active research (physics spin-off)



- Figure shows *kinetic energy vs time* for each of first 10 toroidal modes for nonlinear NIMROD and M3D calculations with same initial conditions, sources, and boundary conditions
- Codes now are in very good agreement in most all aspects (difference in n=0 energy due to different treatment of equilibrium in the 2 codes)
- Times t₁ and t₂ displayed in next vg

Flux surfaces (Poincaré plots)



Obtaining agreement between the 2-codes was a long process, and a number of lessons were learned that we documented in a 3/30/2007 memo to DOE. These were in the following areas:

- Defining the Physical Parameters
 - need precise specification of everything
 - in a regime where n=1 robustly unstable, n>1 stable
- Communication between code teams
 - need much more frequent communication than ~6 months
- Necessary modifications to the M3D code
 - \bullet form of $\kappa_{||}\, \text{and}\, \kappa_{\perp}\, \text{and}\, \text{viscosities}$
 - switched to conservative form of field evolution equation
- Necessary modifications to the NIMROD code
 - more accurate form for equilibrium interpolation



Helical current density during crash

- Show movie
- Sequence of Poincaré plots showing breakup and formation of flux surfaces
- Color coded according to q-value
- Illustrates many physics issues related to magnetic field topology



Energetic Particle Effects in ITER

- Linear stability of n=1 mode in ITER including *thermal ion kinetic effects*
 - Alpha particle stabilization is reduced by elongation
 - Thermal ion kinetic effects are strongly stabilizing
 - Fishbone mode is stable at nominal ITER parameters
- Initial linear runs of α -particle driven TAE with mode number up to n=5
 - No TAE instability was found





The stability of fishbone mode in ITER



GEM 2-Fluid Reconnection



- Codes now give good agreement for GEM 2F nonlinear magnetic reconnection test problem
- Now being extended to large guide-field regime (more tokamak relevant)



Current density at t=32



Pellet Injection

- AMR now done in equilibrium flux surface geometry
- Improved ablation, ionization and electron heating model for pellet
- Implicit treatment of resistive diffusion
- Demonstrated improved fuelling efficiency for inside launch



Logical space showing AMR levels

- Scaling to ITER parameters requires implicit treatment
- JFNK method developed for uni-mesh resistive MHD using SUNDIALS package
- Being extended to AMR



Density contours in outside (u) and inside (l) launch

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Physics Model Development

- Nonlocal Parallel Closures
 - CEL-DKE nonlocal closures for parallel electron and ion heat flows and stresses have been implemented in NIMROD and calculation scales to 1000s of p
 - Now limited to slowly-evolving instabilities such as NTMs
 - These will be generalized to include time-dependence into the CEL-DKE solution
- Study of Heat Transport in Stochastic Magnetic Fields
 - Developing new techniques based on cantori, chaotic-coordinates, and Devil's staircase analysis
 - Proposing tests of this vs nonlocal parallel closures approach
- Implicit Electron Stress
 - Implementing improved form of electron stress in Ohm's law equation.
- Kinetic-Ion MHD
 - Implicit ion-kinetic closure using an evolving Maxwellian δf method with bounded weights
 - Extend to non-linear model, arbitrary polarization, and evaluate on test problems.



Algorithm Development - M3D

- Incremental improvements in M3D
 - Extend present FEM method (now up to 3rd order) to high-order spectral elements
 - Further improve the partially implicit algorithm to allow larger time steps
- M3D-C¹ development
 - 5th order triangular elements with C¹ continuity
 - Fully (linearly) implicit time integration
 - Fully tested in 2D slab geometry (3 papers) with full 2F model
 - Detailed study of 2F toroidal equilibrium with flow
 - Free boundary
 - Extensions to 3D underway
 - Linear 3D will provide rapid screening of 2F equilibrium for stability properties
 - Nonlinear 3D projects multi-teraflop performance

Algorithm Development - NIMROD

- Improved Preconditioning
 - Present preconditioning is for each toroidal harmonic separately
 - Propose to add a toroidal preconditioning step

- Evaluation of Newton-Krylov Solves
 - Allows time-centering of nonlinear terms
 - Will compare accuracy and efficiency with existing leapfrog-based linearly implicit method

Common Algorithm Development

- Common vacuum treatment
 - Interfacing a *common vacuum fields module* for M3D, M3D-C¹, and NIMROD

- Evaluation of FETI-DP
 - Dual-Primal Finite Element Tearing and Interconnecting Domain Decomposition
 - Method of domain substructuring that should lead to a *perfectly scalable* iteration technique
 - Divides matrix into 3 parts:
 - Diagonal block matrix that requires only local solves
 - Moderate-sized coarse, global "primal" matrix that can be solved by SuperLU-Dist
 - Large, sparse "dual" matrix for Lagrange multipliers which is solved by preconditioned Krylov methods

New Physics Applications - 1

- Sawtooth validation studies
 - Building on the successful M3D/NIMROD benchmark
 - Switch to experimentally more relevant source terms and B.C. for validation
 - Extend to larger, hotter tokamak where 2F model is required
- Sawteeth with an energetic ion component
 - Simulate an entire sawtooth cycle with an energetic particle component
 - Study triggering, reconnection, stochastic fields, seed islands, redistribution
- NTMs: Excitation
 - Resume studies of NTMs including new closures with 2F and FLR effects
- NTMs: Control
 - Study the effect of externally supplied current drive on the nonlinear development of the resistive tearing mode --- tied to SWIM workscope

New Physics Applications - 2

- ELM modeling
 - Understand the small ELM regime
 - Understand Edge Harmonic Oscillations
 - Understand ELM suppression via RMP
 - Nonlinear Evolution of Type-I ELMs
 - Tied to CPES workscope
- RWM
 - Linear simulations including resistivity, 2F model, and rotation
 - ITER geometry
 - Nonlinear studies including disruption onset
- Error Field Studies
 - benchmarking with linear studies of island formation
 - Mode locking and rotation damping studies
- Disruption Mitigation Studies
 - Coupled NIMROD/KPRAD to study Massive Gas Injection (MGI)



Verification and Validation Plans

In addition to V&V activities mentioned elsewhere, we are deriving new analytic results specifically for verification exercises:

- Two-fluid axisymmetric equilibria with flow:
 - The effect of FLR, gyroviscosity, diamagnetic heat flux, parallel heat fluxes, and pressure anisotropy on equilibrium with flow
- Drift-Tearing Mode
 - Numerical simulations in analytically tractable geometries
- m=1 internal mode
 - Low collisionality regime, including toroidal effects.

Research Partners

- CPES, SWIM, and PSI-C are making use of NIMROD and M3D codes
- APDEC
 - Collaborating in the further development of the AMR MHD code for pellet injection and for ELMs
- ITAPS(1)
 - We are collaborating with R. Samulyak and J. Glimm in the development of a multi-scale simulation capability of tokamak refueling
- ITAPS(2)
 - We are collaborating with RPI on developing adaptive unstructured grids for the M3D-C¹ code
- TOPS
 - NIMROD, M3D, and M3D-C¹ use the TOPS solvers. We are collaborating with them to make solver improvements.
- VACETs
 - We are moving away from AVS and towards VISIT with their help
- SDM
 - We are exploring ways to facilitate rapid and seamless data transfer and storage

Summary

- 2F plasma models now in routine use
- Active research on 3 approaches to low collisionality parallel closures:
 - PIC, continuum, higher-order moments
- Parallel scaling now to 4000+ processors with good efficiency
- Improved implicit algorithms in NIMROD and M3D
- Several successful linear V&V activities
- Nonlinear ELM calculations with NIMROD and M3D fulfill OFES Joule Milestone
- Major success in nonlinear sawtooth M3D/NIMROD benchmark calculation
- Energetic Particle effects evaluated for ITER
- New research planned:
 - Model development: parallel closures and stochastic heat transport
 - Algorithm improvement: M3D, M3D-C¹, NIMROD, and FETI-DP
 - Applications: Sawtooth, NTM, ELM, RWM, Error Field, Disruption Mitigation
 - V&V: New analytic tests in 2F equilibrium with flow, drift-tearing, m=1