CTTS Overview

Stephen C. Jardin

Theory and Simulation of Disruptions Workshop

PPPL, August 5-7, 2019
CTTS Participants

PHYSICS TEAM

- **PPPL**: C. Clauser, N. Ferraro, I. Krebs, S. Jardin, C. Liu, C. Zhao
- **GA**: V. Izzo, C. Kim, L. Lao, B. Lyons, J. McClenaghan, P. Parks
- **Utah State U**: E. Held
- **Tech X**: E. Howell, J. King, S. Kruger
- **SBU**: R. Samulyak
- **HRS Fusion**: H. Strauss

HPC TEAM

- **RPI**: M. Shephard, S. Seol, W. Tobin
- **LBL**: N. Ding, X. Li, Y. Liu, S. Williams
- **PPPL**: J. Chen
- **SBU**: R. Samulyak

30 participants (part time)
9 institutions
1. Code Descriptions

2. Forces due to Vertical Displacement Events

3. Disruption Mitigation via Impurity Injections
   3.1 Stand Alone
   3.2 via code coupling

4. Runaway Electrons interacting with MHD

5. High-Performance Computing
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**M3D-C¹ and NIMROD solve 3D MHD Equations in Toroidal Geometry including Impurity Radiation and Runaway Electrons**

\[
\begin{align*}
\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{V}) &= \nabla \cdot D \nabla n_i + S_n \\
\frac{\partial n_Z^{(j)}}{\partial t} + \nabla \cdot (n_Z^{(j)} \mathbf{V}) &= \nabla \cdot D \nabla n_Z^{(j)} + I_Z^{(j-1)} n_Z^{(j-1)} - \left( I_Z^{(j)} + R_Z^{(j)} \right) n_Z^{(j)} + R_Z^{(j+1)} n_Z^{(j+1)} + S_Z^{(j)} \\
\frac{\partial A}{\partial t} &= -\mathbf{E} - \nabla \Phi \\
\nabla \cdot \left( \frac{1}{R^2} \nabla \Phi \right) &= -\nabla \cdot \left( \frac{1}{R^2} \mathbf{E} \right) \\
\mathbf{B} &= \nabla \times \mathbf{A} \\
\frac{\partial \mathbf{B}}{\partial t} &= -\nabla \times \mathbf{E} \\
\nabla \cdot \mathbf{B} &= 0
\end{align*}
\]

{:#equation M3D-C1 NIMROD}

\[
\begin{align*}
\rho \left( \frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} \right) + \nabla p &= \mathbf{J} \times \mathbf{B} - \nabla \cdot \mathbf{\Pi} - \mathbf{\omega} \times \mathbf{V} + S_m, \\
E + \mathbf{V} \times \mathbf{B} &= \eta (\mathbf{J} - \mathbf{J}_{RA}) + S_{CD} \\
\frac{3}{2} \left[ \frac{\partial p_e}{\partial t} + \nabla \cdot (p_e \mathbf{V}) \right] &= -p_e \nabla \cdot \mathbf{V} + \mathbf{J} \cdot \mathbf{E} - \nabla \cdot \mathbf{q}_e + Q_\Delta + S_{eE} \\
\frac{3}{2} \left[ \frac{\partial p_i}{\partial t} + \nabla \cdot (p_i \mathbf{V}) \right] &= -p_i \nabla \cdot \mathbf{V} - \mathbf{\Pi}_i : \nabla \mathbf{V} - \nabla \cdot \mathbf{q}_i - Q_\Delta + \frac{1}{2} \mathbf{\omega} \mathbf{V}^2 + S_{iE}
\end{align*}
\]

- Also, separate equations for resistive wall and vacuum regions
- Different options for Runaway Electron current \( \mathbf{J}_{RA} \)
- Option for energetic ion species (not used here)
M₃D-C¹ and NIMROD have very different numerical implementations

### M₃D-C¹

<table>
<thead>
<tr>
<th>Direction</th>
<th>Field Type</th>
<th>Implementation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poloidal Direction</td>
<td>Tri. C² Reduced Quintic FE</td>
<td>High. Order quad C⁰ FE</td>
</tr>
<tr>
<td>Toroidal Direction</td>
<td>Hermite Cubic C¹ FE</td>
<td>Spectral</td>
</tr>
</tbody>
</table>

### NIMROD

<table>
<thead>
<tr>
<th>Field Type</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Magnetic Field</td>
<td>[ B = \nabla \psi \times \nabla \phi - \nabla_{\perp} f' + F \nabla \phi ]</td>
</tr>
<tr>
<td>Velocity Field</td>
<td>[ \mathbf{V} = R^2 \nabla U \times \nabla \phi + \omega R^2 \nabla \phi + R^{-2} \nabla_{\perp} \chi ]</td>
</tr>
</tbody>
</table>

### Coupling to Conductors

- M₃D-C¹: same matrix
- NIMROD: Separate matrices w interface

### Both codes use:
- Split Implicit Time advance
- Block-Jacobi preconditioner based on SuperLU_DIST
- GMRES based iterative solvers
- Impurity ionization and recombination rates from KPRAD
Center for Tokamak Transient Simulations Outline

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Vertical Displacement Events: (VDEs)

K. Bunkers: The influence of boundary conditions on NIMROD Axisymmetric VDE computations

C. Sovinec: Update on axisymmetric VDE benchmarking

Strauss: Thermal quench and asymmetric wall force in ITER disruptions

Clauser: Vertical Force during VDEs in ITER and the role of halo currents

Jardin: Coupling of M3D-C¹ to Carridi

5.3 T 15MA ITER
M3D-C$^1$ is being interfaced with the CARRIDI engineering code to produce realistic forces for ITER

- CARRIDI is presently interfaced with the 2D equilibrium evolution code CARMAoNL
- Above benchmark between M3D-C$^1$ & CARMAoNL was presented at 2019 EPS

- CARRIDI detailed electro-magnetic model of ITER structure.
- Now interfacing M3D-C$^1$ VDE simulation with CARRIDI to extend analysis to 3D plasma

C. Clauser, F. Villone
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Disruption Mitigation via Impurity Injections -- Stand Alone

B. Lyons ... Recent progress in 3D modeling of disruption mitigation

V. Izzo ... Modeling of shell pellet injection for disruption mitigation on DIII-D

S. Jardin ... Modeling of Electromagnetic pellet injector in NSTX-U

Ferraro, NF, 2019
Electromagnetic pellet injector offers advantages for ITER; proposal to test on NSTX-U

- Very fast response time (2-3 ms)
- Speeds up to 1 km/s
- High resolution modeling of 1 mm Carbon pellet as 2.5 cm (poloidal) x 25 cm (toroidal) Gaussian source

Electron Temperature

- $T_e(0) = 2$ keV
- $n(0) = 2 \times 10^{19}$ m$^{-3}$
- $I_p = 600$ kA
- $\beta_p = 0.73$
- $l_i(3) = 0.6$

R. Raman
4 time slices in a M3D-C¹ simulation of a 1 mm Carbon pellet injected into NSTX-U via EPI

Injection Plane Contours at different times

Change in Electron Temp.
(a) - 0.6 keV
(b) - 1.7 keV
(c) - 1.7 keV
(d) - 1.7 keV

Carbon Density:
(a) $6.8 \times 10^{19} \text{ m}^{-3}$
(b) $5.2 \times 10^{19} \text{ m}^{-3}$
(c) $5.2 \times 10^{19} \text{ m}^{-3}$
(d) $3.1 \times 10^{19} \text{ m}^{-3}$

Radiation source:
(a) - 3.2 GW/m³
(b) - 1.0 GW/m³
(c) - 1.1 GW/m³
(d) - 0.4 GW/m³
Contours at $t=0.13$ ms at 4 toroidal locations for M3D-C$^1$ simulation of 1 mm Carbon EPI in NSTX-U

Same time ($t=0.130$ ms), different toroidal locations

**Change in Electron Temp.**
- (a) – 969. eV
- (b) - 1062 eV
- (c) – 1034 eV
- (d) - 1067eV

**Carbon Density:**
- (a) $8.20 \times 10^{19}$ m$^{-3}$
- (b) $1.86 \times 10^{19}$ m$^{-3}$
- (c) $0.07 \times 10^{19}$ m$^{-3}$
- (d) $1.86 \times 10^{19}$ m$^{-3}$

**Radiation source:**
- (a) - 4400 MW/m$^3$
- (b) - 40. MW/m$^3$
- (c) - 0.5 MW/m$^3$
- (d) -40. MW/m$^3$
Convergence study of toroidal resolution and toroidal pellet extent

Plasma properties and pellet source distributed over the Gaussian Distribution:

\[ S = \frac{1}{(2\pi)^{3/2} V_p^2 V_t} \exp \left[ - \frac{(R - R_p)^2 + (Z - Z_p)^2}{2 V_p^2} - \frac{R R_p \left(1 - \cos(\phi - \phi_p)\right)}{V_t^2} \right] \]

<table>
<thead>
<tr>
<th>nplane</th>
<th>( V_t )</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>1.00</td>
</tr>
<tr>
<td>16</td>
<td>0.50</td>
</tr>
<tr>
<td>32</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Convergence study in # of toroidal planes indicates the highest toroidal resolution used so far may not be high enough.....Still in progress.
Te contours for different toroidal resolutions (injection plane)

8 planes
var_tor = 1.00 m

t = 0.065ms
T_{max} = 2000ev

t = 0.130ms
T_{max} = 1500ev

t = 0.650ms
T_{max} = 270ev

t = 0.1000ms
T_{max} = 270ev

16 planes
var_tor = 0.50 m

32 planes
var_tor = 0.25 m
Center for Tokamak Transient Simulations
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Disruption Mitigation via Impurity Injections – via code coupling

R. Samulyak...Simulation studies of the ablation of Neon pellets and SPI fragments for plasma disruption mitigation in tokamaks

NIMROD simulation domain showing ablated material obtained from LP code

LP simulation of pellet ablation cloud

\( \nabla B \)-drifted ablation material

Mass flow, thermodynamic data, and energy sinks from LP to TK

B, \( n_e \), \( T_e \) from TK to LP
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Runaway Electrons interacting with MHD

C. Zhao .. Simulation of MHD instabilities with runaway electron current using M3D-C¹

G. Wang ... Reduced models of runaway electrons in NIMROD ... (poster)

- A collaboration between PPPL, GA, and ORNL is initialized to couple both M3D-C¹ and NIMROD with KORC to model runaway electron diffusion and its back reaction to MHD instabilities

KORC: Highly scalable PIC RE code using GPUs (ORNL)
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5. High-Performance Computing
Must Address Communication to Improve Scaling Performance

- SuperLU Preconditioners are essential for the solvers in M3D-C¹ and NIMROD
- Solver performance is dominated by MPI communications in the triangular solve
- Performance improvements in SpTRSV improves application performance and scalability

- **COMPARED SIX MATRICES**
  - 1 from FES code M3D-C¹ A30
  - 5 from SuiteSparse Matrix Collection

- **COMMUNICATION ~70% - 90% FOR ALL LARGE SPARSE MATRIX SOLVES**

Solve time break down on NERSC’s Cori/KNL using 1024 processes

SpTRSV: SuperLU_dist triangular solve
Implementing One-Sided Communication:

- Remote direct memory access (RDMA) is a process to directly access memory on remote processes without involvement of the activities at the remote side.
- Light-weight asynchronous primitives provides a pathway to efficient DAG execution and accelerator-based exascale solvers
- Shown below: fompi one-sided communication greatly improves bandwidth over MPI two-sided

DAG: Directed Acyclic Graph
Performance model for Sparse Triangular Solvers

- LBL built a critical path analysis tool to determine the critical path with consideration of process decomposition
  - Circles can represent:
    - a DGEMV or TRSMV in SpTRSV
    - a kernel in the application
  - Edges can represent:
    - data dependencies
    - execution flow

- LBL modeled mat-vecs and communication in SpTRSV using the critical path analysis tool
  - Empirical observations of performance fit within the model’s performance bounds

DGEMV & TRSMV are matrix-vec operations
SpTRSV: SuperLU_dist triangular solve

Critical path visualization

Potential benefits from better task placement

N. Ding, S. Williams, S. Li, Y. Liu
One-Sided Communication implemented for Sparse Triangular Solvers

- LBL created a one-sided MPI version of SpTRSV on Cray system
- Attained a 2.2x speedup for M3D-C¹ matrix at 4096 processes on Cori(NERSC) over the existing two-sided in SuperLU_DIST
Communication-avoiding 3D sparse LU factorization in SuperLU_dist

- **Algorithm innovation:** 3D grid of MPI processes, Z-dimension has some data replication, but results in reduced communication and increased parallelism

- Shown in graph is improvement in M3D-C¹ velocity matrix for 32, 128, 512 MPI processes: (1.3x, 1.8x, 5x)
Velocity Matrix Restructuring for Improved Preconditioning

- M3D- C\(^1\) uses a physics-based Helmholtz-like decomposition of the velocity field:
  \[ \mathbf{V} = R^2 \nabla U \times \nabla \phi + \omega R^2 \nabla \phi + R^{-2} \nabla \chi \]

- The old ordering mixed these three physically different velocity variables in the same vector.

- New ordering allows us to separate these, facilitating a more efficient preconditioning strategy.

(R, \(\phi\), Z) coordinates
Adjacency – based reordering has potential to improve performance

- Colors correspond to mesh numbering: blue → red
- Re-ordering can improve cache misses and Particle-in-Cell performance
- Now being evaluated for M3D-C¹ and NIMROD

E. Seol, M. Shephard, W. Tobin
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