Future Computing Needs for Innovative Confinement Concepts

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Outline

- Introduction of Plasma Science and Innovation Center
- Current Computing Utilization and Resources
  - Simulation Highlights
- Near Term Needs
- Concluding Comments

The Disclaimer

- presentation reflects the PSI Center only
- PSI Center is not alone in ICC simulations
- e.g. E. Belova (PPPL), stellarator community, Tech-X and other SBIR/private companies

PSI-Center Mission

- provide practical and accurate tools to model physics needed for achieving high-confidence predictive simulations of innovative confinement concepts (ICC) in user-friendly codes
- facilitate and assist with simulations of collaborating experiments
- facilitate **V&V** of codes experimentally accessible parameter regimes
- **long term goal** - develop design tools for rapid and cost effective development of ICCs experiments

Personnel

Directors

Thomas R. Jarboe (Director)
Richard D. Milroy (Dep-Dir)

Two-Fluid and Transport

Carl R. Sovinec (U-Wisc)
Eric D. Held (USU)
Jeong-Young Ji (USU)

Interfacing

Brian A. Nelson
Charlson C. Kim

Boundary Conditions

Uri Shumlak
George J. Marklin
Alan H. Glasser
Eric T. Meier
Wes Lowrie
V. S. “Slava” Lukin (NRL)

Kinetic Effects

Richard D. Milroy
Charlson C. Kim

Collaborating Experiments

- Bellan Plasma Group, Caltech, PI: Paul Bellan
- CTH, Auburn U., PI: Steve Knowlton - planned collaboration
- CU-FRC, CU-Boulder, PI: Tobin Munsat; (A. D. Light and M. T. Schmidt)
- ELF Thruster, MSNW, PI: John Slough
- FRX–L, LANL, PI: Thomas P. Intrator
- HIT–II/HIT–SI, Univ. of Washington, PI: Thomas R. Jarboe
- LDX, M.I.T., PI(s): Jay Kesner and Mike Mauel; (D. Garnier)
- MST, Univ. of Wisconsin–Madison, PI: John Sarff
- PHD, Univ. of Washington, PI: John Slough
- SSPX, LLNL, PI: Harry McLean; (B. Cohen and E. B. Hooper)
- SSX, Swarthmore College, PI: Michael Brown
- TCS–U, Univ. of Washington, PI: Alan Hoffman
- ZaP, Univ. of Washington, PI: Uri Shumlak

PSI-Center Codes

- NIMROD and HiFi - two complementary 3D X-MHD codes
  - initial value codes using implicit time stepping
  - high order finite element spatial discretization
  - MPI parallelism
  - NIMROD uses nodal FE in 2D and Fourier in periodic direction - computationally efficient
  - HiFi uses 3D modal - geometric flexibility
  - NIMROD has PIC and continuum options
- PSI-Tet - 3D zero β plasma equilibrium solver
  - tetrahedral elements usign mimetic operators
  - hybrid OpenMP/MPI parallelism
- all rely on scalable sparse solver
- ‘piggyback’ on development related to tokamak simulations
  - particularly CEMM
  - in future with others, particularly through PIC/continuum

- ICC experiments typically smaller and cooler than tokamaks (notable exception is MST-U.Wisc)
- dimensionless parameters (e.g. S) within fidelity regime of available codes
- **BUT** simulations should not be considered easy
    - strongly driven
    - large flows
    - large gradients
    - density voids
    - field nulls
    - no strong background equilibrium field
    - numerous and varied geometries
- X-MHD effects are often primary effects (e.g. Hall physics)
- good testbed for developing extended models
- good opportunity for V&V
- exercises codes and algorithms over broad parameter range and configurations

Status of ICC Simulations

Experiment	**Simulation Topic**	**NIMROD**	**HiFi**
Bellan Group	Spheromak formation	✓✓	
ELF	FRC RMF/translation in neutrals	✓✓✓	✓✓
FRX–L	FRC translation	✓	✓
HIT–II	Coaxial helicity injection	✓✓	
HIT–SI	Steady-inductive HI	✓✓✓	In progress
LDX	Dipole interchange studies	✓✓	
MST	Kinetic particle effects	✓✓	
Pegasus	Relaxation current drive	✓✓	
PHD	FRC translation/compression	✓✓✓	✓
SSPX	Spheromak relaxation/transport	✓✓✓	
SSX	Spheromak equilibria/relaxation	✓✓	✓✓✓
TCS–U	RMF formation/kinetic effects	✓✓✓	
ZaP	Sheared-flow stabilization	✓	

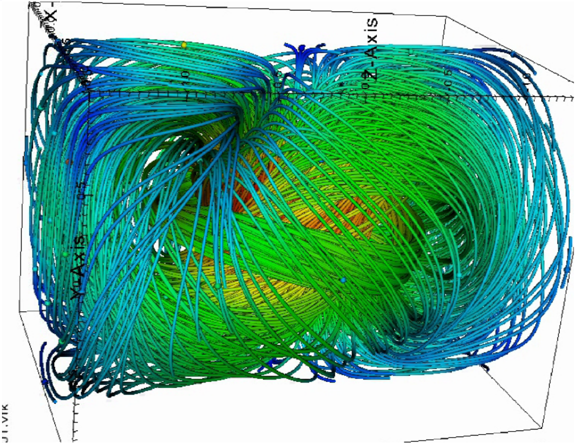
✓✓✓	Compared to experiment, continued study
✓✓	Codes running for specific experimental geometry
✓	General code runs of experimental interest performed

Current State of PSI Center Computing

- main computing resouce is local cluster - SGI Altix “ICE”
  - 192 × 2.8 GHz Xeon processors
  - 2 GB/processor 1600 MHz FSB RAM, Infiniband interconnects
  - $\sim$ 50% utilization
- $\sim .5M$cpuhrs at NERSC (PSI-Center and HIT-SI)
- most simulations are in their early stages
- typical production runs use $\sim$ 100 cores, $\sim$ 1GB/core
- ICC computations benefit from high throughput of modest sized jobs
- does not preclude need for large computations (e.g. LDX simulations)

PSI-Tet Calculates Taylor SSX Eigenmodes

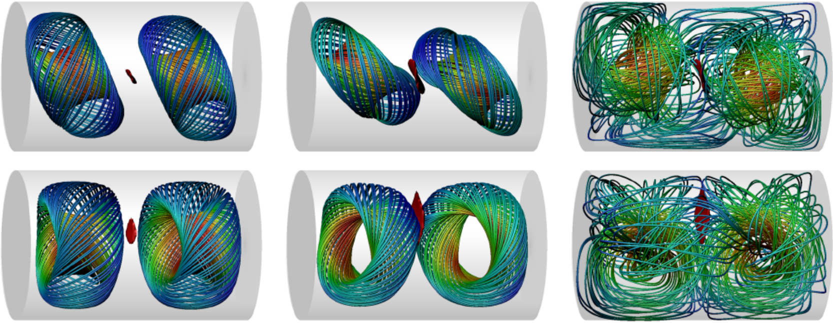
C. D. Cothran, M. R. Brown, T. Gray, M. J. Schaffer, and G. Marklin, *Phys Rev Lett* **103**(21), 215002, 2009.



Eigenstates compare well to data. ($\sim 10^6$ cells, 1hr×8procs)

Merging Spheromak simulations in HiFi

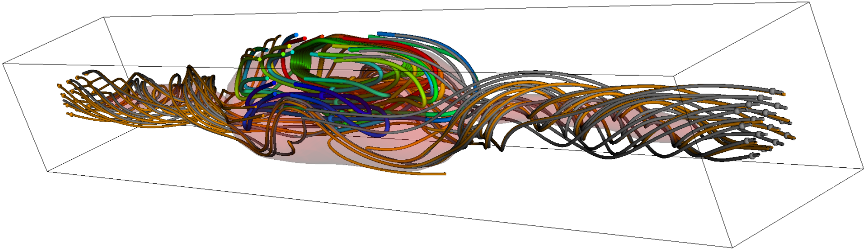
Gray et al., "Three-dimensional reconnection and relaxation of merging spheromak plasmas", to appear in PoP (2010)



Two orthogonal views of fieldlines and region of largest current density illustrates dynamic nature of evolution.
$\sim .25M$grid points, 512procs, $\sim$ 24hrs

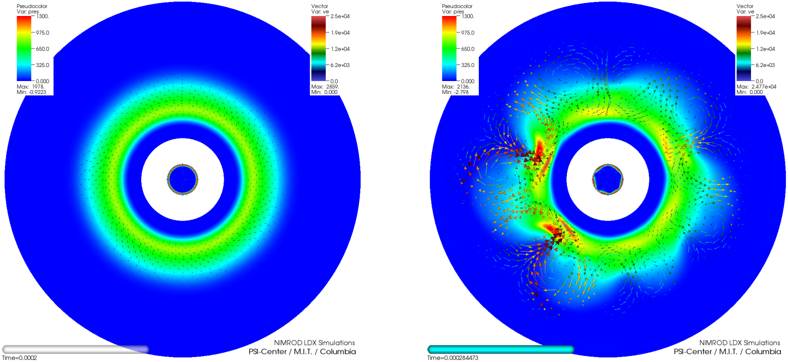
NIMROD FRC Simulations

R. D. Milroy, C. C. Kim, and C. R. Sovinec, *PoP* **17** 062502, 2010.



Field line traces during FRC formation - relies on Hall physics and algorithm advances of NIMROD (implicit advection and Fourier coupled preconditioner developed under **CEMM**)

LDX Interchange simulations with NIMROD

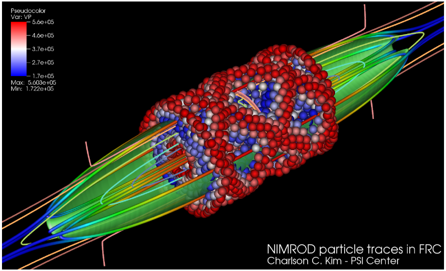


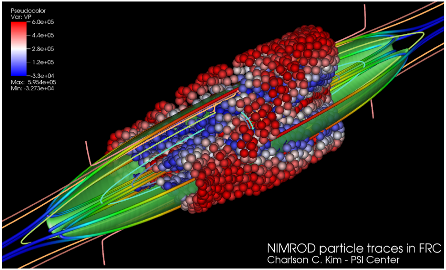
Pressure (colors) and velocity (arrows)

Interchange spectra mostly in $n = 5, 6, 7$

- an exception to the modest computation, $> 10^6$ gridpoints
- typically run on local (MIT) cluster (J. Kesner)

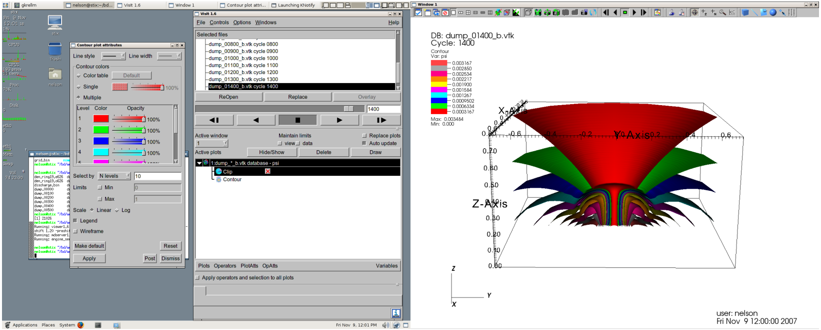
PIC in NIMROD





Single Lorentz particle traces in an FRC. PIC module (and continuum module) best candidates for parallel gains. PIC performance is constrained by particle sorting on nonuniform mesh. Uses same domain decomposition as fluid - load balance issues.

VisIt Provides Powerful Interactive 3D Plotting



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2	🟩	100%
3	🟦	100%
4	■	100%

Select by N levels 10
Limits ☐ Min 0
☐ Max 1

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dump_00900_b.vtk cycle 0900
dump_01000_b.vtk cycle 1000
dump_01100_b.vtk cycle 1100
dump_01200_b.vtk cycle 1200
dump_01300_b.vtk cycle 1300
dump_01400_b.vtk cycle 1400

1400

Active window 1

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Clip
Contour

DB: dump_01400_b.vtk
Cycle: 1400
Contour
Var: psi

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- 0.002850
- 0.002534
- 0.002217
- 0.001900
- 0.001584
- 0.001267
- 0.0009502
- 0.0006334
- 0.0003167

Max: 0.003484
Min: 0.000

user: nelson
Fri Nov 9 12:00:00 2007

- NIMROD dump files converted with NimPy Python module
- SEL/HiFi and PSI-TET can write HDF5 or VTK files for VisIt
- plans to implement synthetic diagnostics

Formula for Extrapolating

- heuristic/ad hoc formula for computational work (CW)

$$\mathrm{CW} = \frac{L}{\delta x} \times \frac{T}{\delta \tau} \times \mathrm{H} \tag{1}$$

  L system size, T simulation time, $(\delta x, \delta \tau)$ minimum required resolution, H is the Hartman number

$$\mathrm{H} = \frac{LB}{\sqrt{\eta \rho \nu}} \tag{2}$$

  B magnetic field, η diffusivity, ν viscosity, ρ mass density

- use computer work to extrapolate from a known computation to future needs

e.g. extrapolating needs for FRC simulations

- baseline FRC formation simulation $\sim 100 cpuhrs$
- projected needs for full device FRC simulation $\times 10^4$

L	δx	T	$\delta\tau$	B	η	ν	ρ
$\times 5$	$\times 4^{-1}$	$\times 10$	1^*	$\times 3$	1	$\times 10^{-1}$	1

* $\delta\tau$ is constrained by CFL

- actual need requires scaling information
- example demonstrates large scale computing can be utilized by ICC simulations
- more typical of ICC sim's $\sim \times 10^{2-3}$ (L is usually fixed)

Concluding Comments

- ICC simulations test algorithms in a broad range of parameters and geometries
- typical ICC simulations use < 100procs
  - could increase $\sim \times 10$
  - need longer run time
- projections show ICC simulations would benefit most from high throughput of modest size jobs (100's-1000 proc) over longer run times
- PIC and continuum method are best candidates to benefit from new architecture
- significant coordinated effort needed for sparse scalable solvers to take advantage of new architecture/paradigm

NERSC can help facilitate user end experience

- queue policy for modest jobs over longer walltimes
- queue policy for ensemble runs
- support codes through modules (reduce redundant compiles and executables)
- provide workflow tools (some already exist)
- web-based archiving interface
- unified filesystem across all machines (already in place?)
- continued and expanded visualization (VisIt) support
- many of these exist already, e.g. NERSC Analytics Program