U.S. Department of Energy's

Office of Science

Fusion Simulation Project

Status and Plans

Fusion Energy Sciences Advisory Committee Meeting

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OFES

March 2, 2007

www.ofes.fusion.doe.gov

Outline

- Introduction & Motivation
  - What is the FSP?
  - Why do we need it?
  - Why now?
- FSP Workshop Plans
- FES SciDAC Projects—Overview

Introduction & Motivation

What is the FSP?

- The **Fusion Simulation Project** (FSP)**—**led by OFES in collaboration with OASCR—is a computational initiative aimed at the development of a whole-device predictive simulation capability focusing on ITER, but also relevant to major current and planned toroidal fusion experiments

Why do we need it?

- Each pulse in ITER is expected to cost about $1M, so a reliable predictive simulation capability is needed to optimize discharge scenario and control
- It will make the U.S. the world leader in fusion plasma simulations

Why start it now?

- It is a challenging undertaking. It takes time to develop, verify, and validate such a comprehensive simulation code
- The U.S. fusion community—under the auspices of the Office of Science's *Scientific Discovery through Advanced Computing* (**SciDAC**) program—has taken advantage of today's leadership class terascale computing facilities to develop high-performance computational tools that have given us new and significant insights into questions of fundamental importance in fusion plasma science
- The success and strength of these ongoing efforts as well as the emerging availability of petascale computing resources support the timeliness of the FSP initiative

FSP Workshop Plans

- An FSP workshop is planned for May 2007 to develop a detailed roadmap with major scientific and computational milestones
- The FSP Workshop Panel is co-chaired by Prof. Arnold Kritz of Lehigh University and Prof. David Keyes of Columbia University
- The main product of this workshop will be an FSP Report by the end of June 2007. There will be a FESAC charge to evaluate this report and recommend a course of action

Status of FES SciDAC Projects

- The FSP will build on the success of our existing SciDAC projects
- Multi-institutional teams of plasma physicists, applied mathematicians and computer scientists have been working together using high performance computing resources to solve complex problems in fusion plasma science
- Currently, there are six projects in the OFES SciDAC portfolio: three original SciDAC projects focused on topical science areas, and three Fusion Simulation Prototype Centers focused on code integration

OFES SciDAC Projects

Gyrokinetic Particle Simulation Center (GPSC)

- **Turbulent transport in burning plasmas using PIC codes**
- **PI: W.W. Lee (PPPL)**
- **PPPL, UC Irvine, ORNL, U Colorado, UCLA, U Tennessee, UC Davis, Columbia**

Center for Extended Magnetohydrodynamic Modeling (CEMM)

- **Macroscopic stability and nonlinear dynamics using 3D extended MHD codes (M3D & NIMROD)**
- **PI: S. Jardin (PPPL)**
- **PPPL, U Wisconsin, Tech-X, MIT, NYU, U Colorado, U Utah, Utah State U**

Center for Simulation of Wave-Plasma Interactions (CSWPI)

- **Launching, propagation and absorption of high power EM waves and RF-driven modifications to the background plasma distribution function (TORIC, AORSA, CQL3D)**
- **PI: P. Bonoli (MIT)**
- **MIT, ORNL, CompX, Lodestar, General Atomics, Tech-X, PPPL**

Fusion Simulation Prototype Centers

Center for Simulation of Wave Interactions with MHD (SWIM)

- Brings together state of the art extended MHD and RF codes to investigate the interactions of waves with MHD and the mitigation of instabilities
- Develop Integrated Plasma Simulator (IPS) – framework to allow coupling of virtually any fusion code, not just RF and MHD
- PI: D. Batchelor, ORNL
- ORNL. Indiana U, Columbia U, General Atomics, COMPX, U Wisconsin, MIT, NYU, LBNL, Lehigh U, Tech-X

Center for Plasma Edge Simulation (CPES)

- Develop integrated predictive plasma edge simulation package applicable to burning plasma experiments; integrates edge gyrokinetics with extended MHD codes
- PI: C-S Chang (NYU)
- Caltech, Columbia U, LBNL, Lehigh U, MIT, ORNL, PPPL, Rutgers, UC Irvine, U Colorado, U Tennessee, U Utah

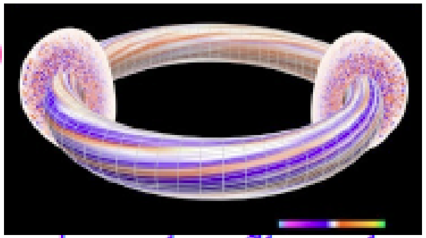
Framework Application for Core-Edge Transport Simulations (FACETS)

- Multi-physics, parallel framework application for full-scale fusion reactor modeling; initial focus is core to wall transport modeling
- PI: J.R. Cary (Tech-X Corp)
- Tech-X, LLNL, PPPL, ANL, UCSD, CSU, ORNL, ParaTools, GA, Columbia U, LBNL, Indiana U, MIT, NYU, Lodestar

Additional Slides

Viewgraphs provided by the SciDAC PIs

SciDAC Center for Gyrokinetic Particle Simulation of Turbulent Transport in Burning Plasmas (GPSC)



(Oct. 2004 - Oct. 2007)

W. W. Lee, S. E. Parker, Z. Lin, D. E. Keyes et al.

Achievements:

• Developing general geometry GTC-s and GTC-neo codes interfaced with experimental profiles and conducting nonlocal turbulent and neoclassical transport studies for D3D and NSTX. [Wang et al., PoP **13**, 082501 (2006); PoP **13**, 092505 (2006); Wang et al. IAEA-CN-149-TH-2-6Ra (2006)]

• Porting and optimizing GTC on various massively parallel platforms (MPP) and achieving 8.5 TeraFlop/sec performance on Jaguar (ORNL), BlueGeneL (Watson) and the Earth Simulator (Japan) [Ethier, Fall Creek Falls Conference (2006)]

• Carrying out discrete particle noise convergence studies for ITG modes [Lee et al, IAEA-CN-149-TH/2-6Rb (2006)], and applying the Fluctuation-Dissipation Theorem to the nonlinearly saturated system with the finding that discrete particle noise has no effect on steady state transport [Jenkins and Lee, PoP to appear].

• Studying ETG convergence and the short-wavelength TEM modes [Lin et al, IAEA-CN-149-TH/P2-8(2006)] with the discovery that wave-particle decorrelation is responsible for ETG transport [Holod and Lin, PoP, to appear].

• Developing global electromagnetic capability in GTC for both MHD and kinetic shear-Alfven waves [Nishimura et al., submitted to PoP].

UCDAVIS UCIrvine UCLA Colorado ornl PPPL

Achievements (cont.)

• GEM now includes radially-global electromagnetic physics based on general equilibrium and profiles with multiple ion species interface with experimental data [Chen and Parker, JCP **220,** 839 (2007)].

• GEM code has also been extended to interface with TRANSP and NCLASS, and studies of ITG-TEM modes, microtearing modes, and KBMs in NSTX are underway. [Rewoldt et al. APS (2006)].

• Particle-Continuum method to limit weight-growth in long-time simulations [Chen and Parker, APS (2006)].

Future Plans

• Implement electron dynamics capability in GTC-s and carry out systematic studies on turbulent and neoclassical transport in D3D and NSTX with multi-species ions using GTC-s, of which plasma rotation and momentum transport are of particular interest - PPPL.

• Participate in the OMB's Joule applications for software effectiveness using GTC-s as recommended by ASCR as well as engage in the petascale campaign at ORNL in preparation for ITER simulations - PPPL.

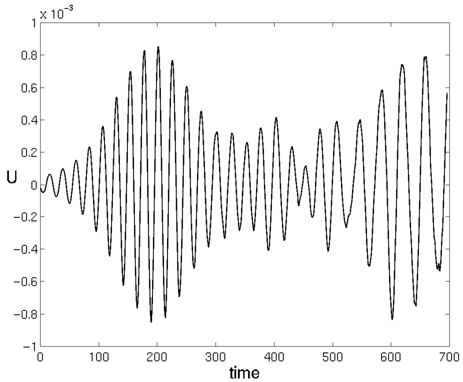
• Carry out electromagnetic microturbulence simulations using GTC with kinetic electrons - UCI

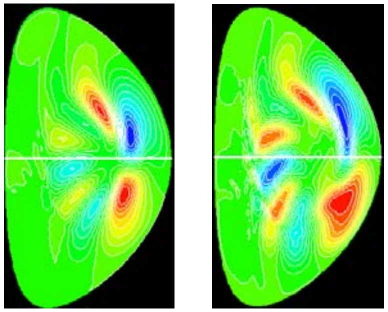
• Perform kinetic simulations of energetic particle driven modes using GTC and compare the results with experimental measurements - UCI.

• Include equilibrium ion parallel flows in input to radially-global version of GEM and use input data from TRANSP and NCLASS, as well as investigate ETG modes using a separate flux-tube (radially-local) version of the GEM code, including fine scale zonal flows - Colorado

• Rigorously quantify the amount of dissipation introduced by the particle-continuum method - Colorado

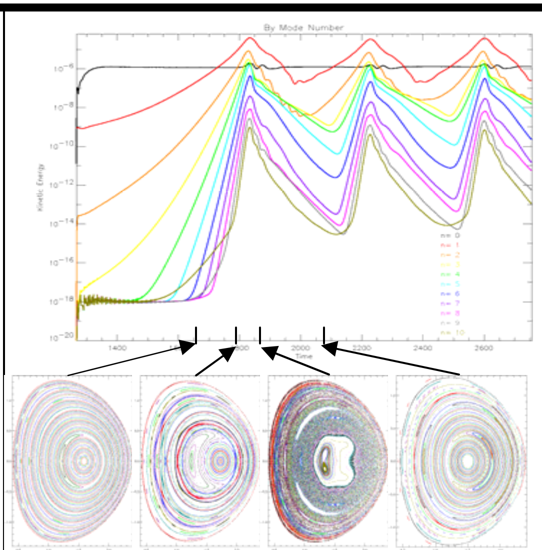
The Center for Extended Magnetohydrodynamic Modeling (current activities)



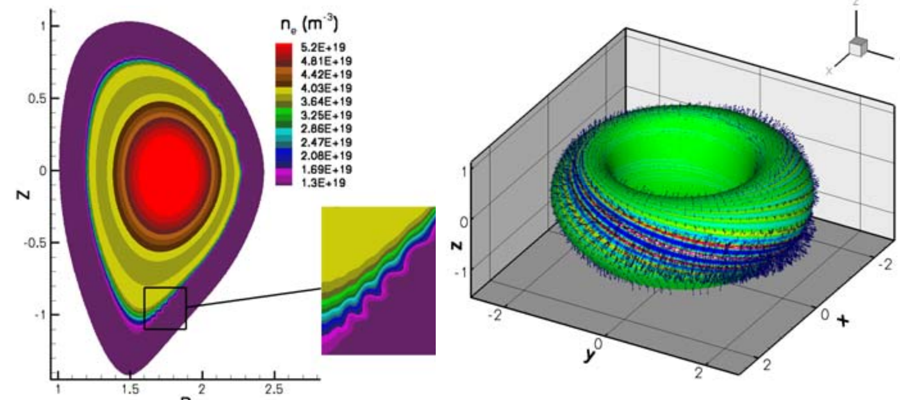


t=0.0 t=336

Beam-driven modes in NSTX show nonlinear frequency chirping

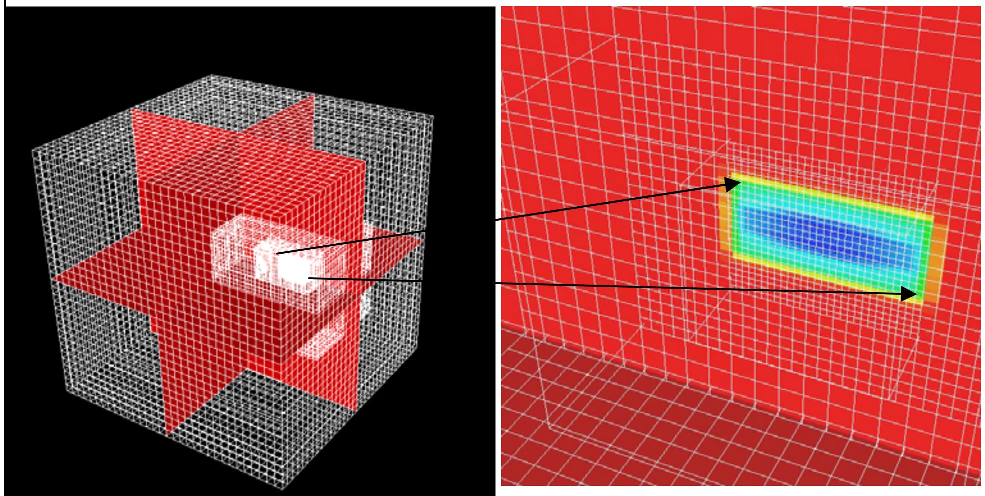


- Repetitive sawtooth cycles in CDX-U show periods of stochastic field lines
- M3D and NIMROD predict similar but different behavior. Now trying to under-stand differences in non-linear results



ELM Theory Milestone: with n>40modes:

- shows helically localized ripple structures
- T_e perturbations less than n_e perturbations



AMR simulation of Pellets predicts difference between inboard & outboard launch

The Center for Extended Magnetohydrodynamic Modeling (Future plans)

Improved Closure Models

- Kinetic closure
- Improved fluid closures

More Efficient, More Scalable codes

- Fully 3D implicit solves
- scaling to 10,000's of processors on routine basis

Continue most applications into more relevant physics regimes:

- Sawtooth in a burning plasma – track down differences between codes
- Neoclassical tearing modes and techniques for stabilization
- ELM behavior and control
- Causes of disruptions
- Forces and heat loads due to disruptions\
- Plasma fueling
- Energetic Particle modes
- Resistive Wall modes

The SciDAC Center for Simulation of Wave – Plasma Interactions

L.A. Berry, D.B. Batchelor, E.F. Jaeger,
E. D`Azevedo, M. Carter

P.T. Bonoli, J.C. Wright

C.K. Phillips, E. Valeo
N. Gorelenkov, H. Qin

D. Smithe

R.W. Harvey, A.P. Smirnov
N.M. Ershov

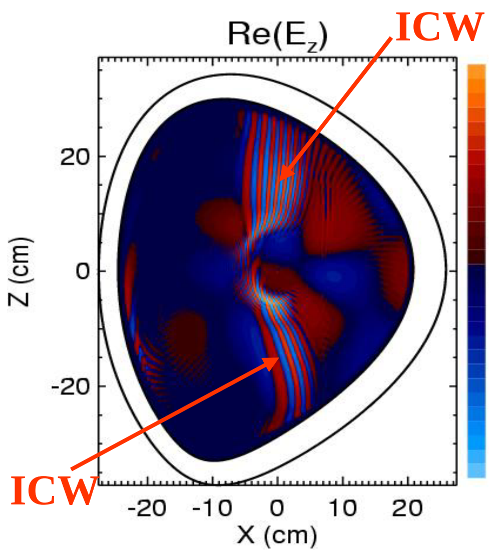
M. Brambilla
R. Bilato

M. Choi

C.S. Chang
J.M.-Kwon

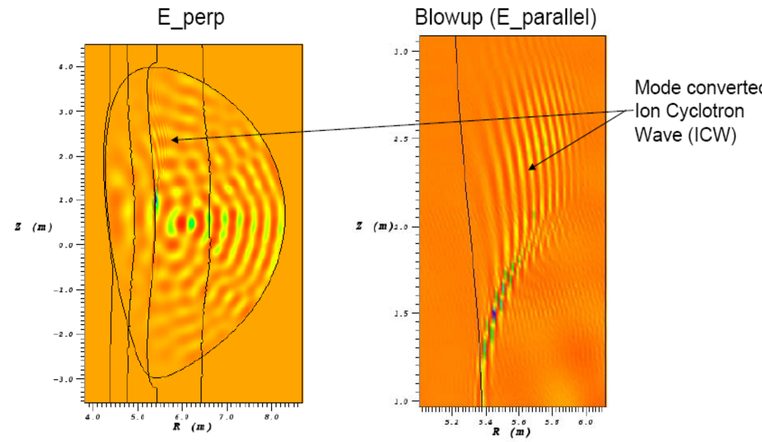
D. D'Ippolito, J. Myra - Lodestar Research

RF SciDAC Center – Scientific Accomplishments

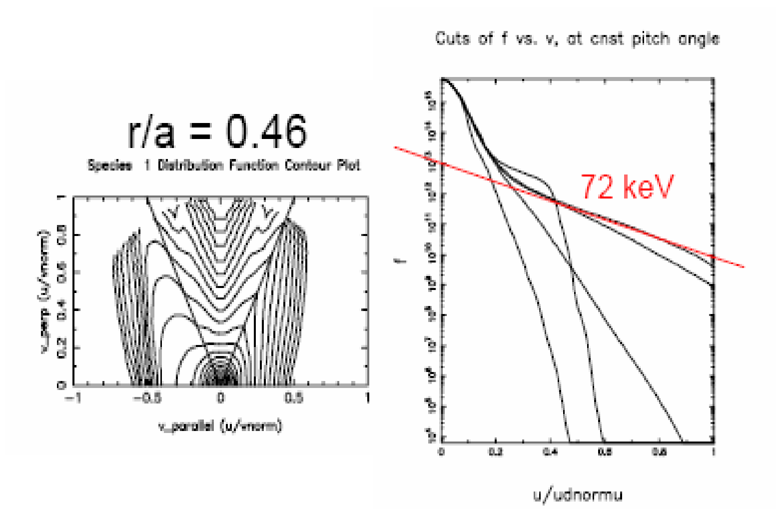


TORIC simulation of ICW in Alcator C-Mod

First ever simulations of multiple spatial scale fast wave to ion cyclotron wave (ICW) mode conversion in present day tokamaks and in ITER using the TORIC & AORSA solvers.

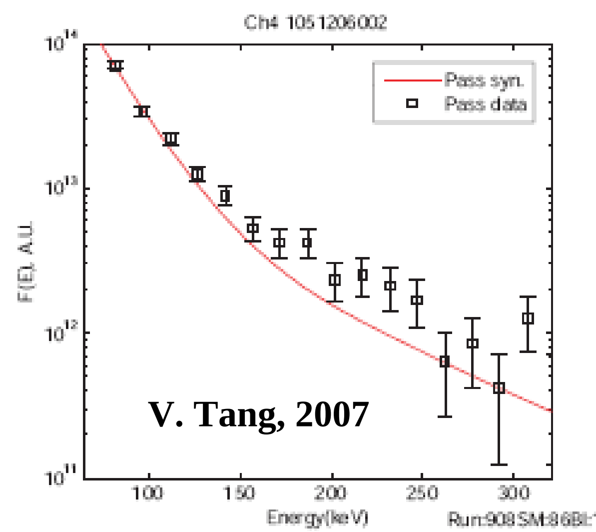


AORSA simulation of ICW in ITER



Predicted ion tail dist. in C-Mod from AORSA-CQL3D

First-principle simulation of ICRF generated ion tails using AORSA – CQL3D and synthetic diagnostic code comparison with experiment.



Synthetic Code Comparison with measured ion dist. In C-Mod

RF SciDAC Center – Future Plans

- **Evaluate the compatibility of ICRF and LHRF antennas with edge plasma and develop a predictive capability to launch desired wave spectra in present day devices and in ITER:**
  - TOPICA antenna code coupled to the linear 3D wave fields from TORIC and AORSA.
  - Implementation of nonlinear RF sheath boundary conditions in full-wave solvers.
  - Employ PIC approach (VORPAL) to simulate nonlinear RF edge interaction.

- **Predictive description of how externally launched ICRF and LH waves interact with energetic particles in a burning plasma - (fast fusion alphas, fast NB ions, ICRF tails, and LHRF electron tails):**
  - Closed loop computation of ICRF interaction with fast ions including finite ion orbit width and spatial diffusion effects:
    - Numerical distributions from orbit following Monte Carlo or from gyrokinetic codes coupled to full-wave solvers (AORSA and TORIC).
    - RF operators from direct particle orbit integration.
  - Closed loop computation of LHRF electron tail generation in LH current drive, including interaction with fusion alphas.
    - Full-wave LH fields coupled to bounce averaged Fokker Planck treatment for complete wave field description (diffraction and focusing).

- **Predictive description of self-generated waves in plasmas (Alfven eigenmodes and cascades, parametric decay waves):**
  - Application of full-wave solvers to modes at Ω_{ci} (Compressional Alfven Eigenmodes) and modes at << Ω_{ci} (TAE's).
  - Evaluate onset of parametric decay instability in ICRF and LHRF regimes using realistic tokamak geometry and RF wave fields.

Center for Simulation of Wave Interactions with MHD (SWIM)

D. B. Batchelor, L. A. Berry, S. P. Hirshman, W. A. Houlberg, E. F. Jaeger, R. Sanchez – *ORNL Fusion Energy*

D. E. Bernholdt, E. D'Azevedo, W. Elwasif, S. Klasky– *ORNL Computer Science and Mathematics*

S. C. Jardin, G-Y Fu, D. McCune, J. Chen, L- P Ku, M. Chance, J. Breslau – *PPPL*

R. Bramley – *Indiana University*, D. Keyes – *Columbia University*, D. P. Schissel, D. Aswath – *General Atomics*,

R. W. Harvey – *CompX*, **D. Schnack** – *U. Wisconsin*, **J. Ramos, P. T. Bonoli, J.Wright** – *MIT*

S. Kruger – *TechX*, **G. Bateman** – *Lehigh University*,

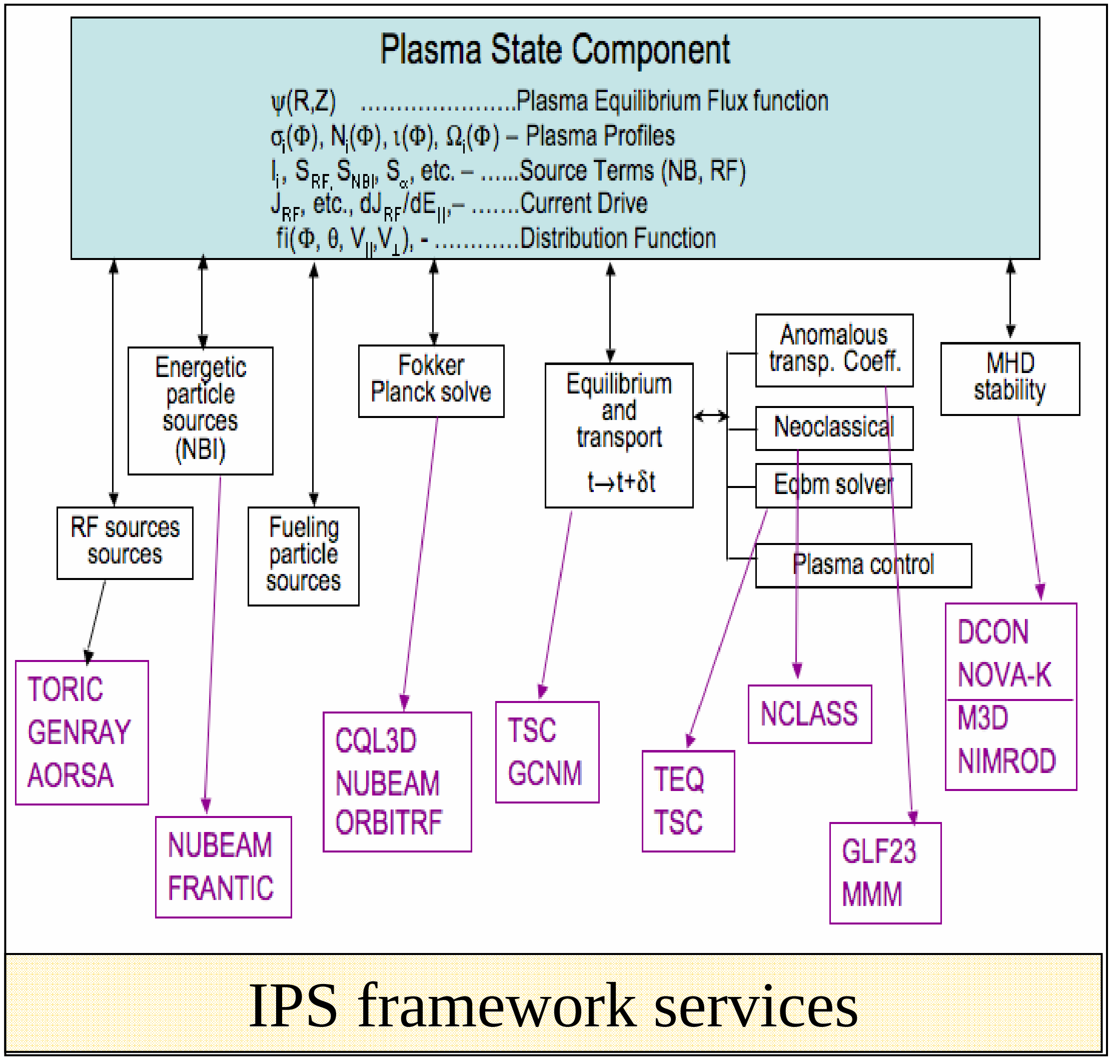
Unfunded participants:

L. Sugiyama – *MIT*, **C. C. Hegna** – *University of Wisconsin*, **H. Strauss** – *New York University*, **P. Collela** – *LBNL*

H. St. John – *General Atomics*

SWIM – design of Integrated Plasma Simulator (IPS) is complete, initial implementation undergoing testing

- **Plasma State component provides an extensible facility to exchange simulation data between physics components**
  - **Allows coupling of any physics code**
  - **Has already been adopted by other simulation projects → pTRANSP**
- **IPS incorporates multiple, well tested, state-of-the-art codes to implement each functional component**
- **IPS framework is derived from already developed computer science products**
  - Portal
  - Event logging
  - Data management
  - Workflow management



SWIM Project Plans – development of physics-based models of RF control of sawtooth oscillations and neoclassical tearing modes

Development of the Integrated Plasma Simulator (IPS)

- **Populate the IPS with additional physics components – RF solver (AORSA and TORIC), Fokker Planck (CQL3D), Equilibrium and Transport, MHD (DCON), NUBEAM**
- **Carry out initial tests and simulations**
  – CQL3D + Equilibrium and Transport, runaway electron production in ITER startup
  – AORSA + CQL3D, energetic minority tail formation in C-Mod rate of increase of tail
- **Public release of IPS**

Control of Sawtooth oscillations by RF modification of profiles and energetic particle populations

- **Improvement of reduced sawtooth models to include RF effects**
- **ITER scenario analysis to mitigate deleterious sawtooth effects**

RF control of Neoclassical Tearing Modes

- **Complete closures analysis for MHD fluid closures including effects of RF heating and current drive**
- **Direct coupling of 3D nonlinear MHD with RF codes**
- **Investigation of power requirements for RF stabilization of NTM in ITER**

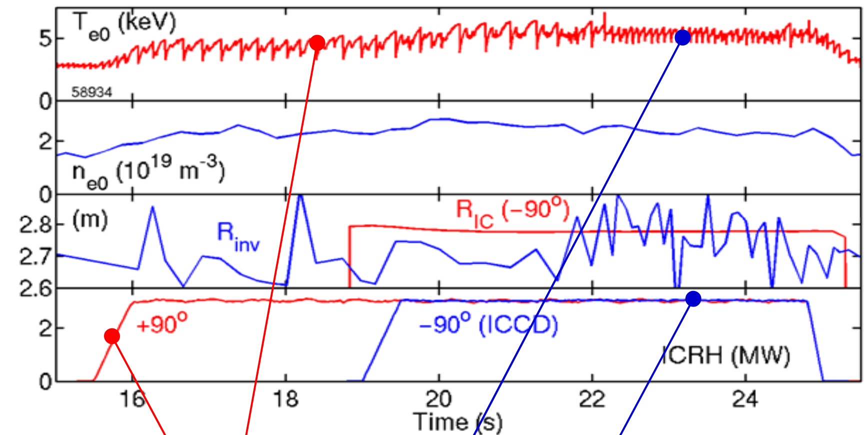
***See our fun website at:* www.cswim.org**

SWIM brings together state of the art extended MHD and RF codes to investigate the interactions of waves with MHD and the mitigation of instabilities

Applied to:

- **Effect of RF waves on sawtooth stability and other fast MHD events**
- **RF control of neoclassical tearing modes and other slow macroscopic instabilities**
- **Effect of RF and other sources on profile evolution and scenario optimization**
- **Developing Integrated Plasma Simulator (IPS) – framework to allow coupling of virtually any fusion fusion code, not just RF and MHD.**

Sawtooth control on JET with Minority Current Drive on JET



co current drive **counter current drive**

ICRF minority current drive can either increase or decrease sawtooth period and amplitude depending on phasing of antenna

SciDAC FSP Prototype Center for Plasma Edge Simulation (CPES)

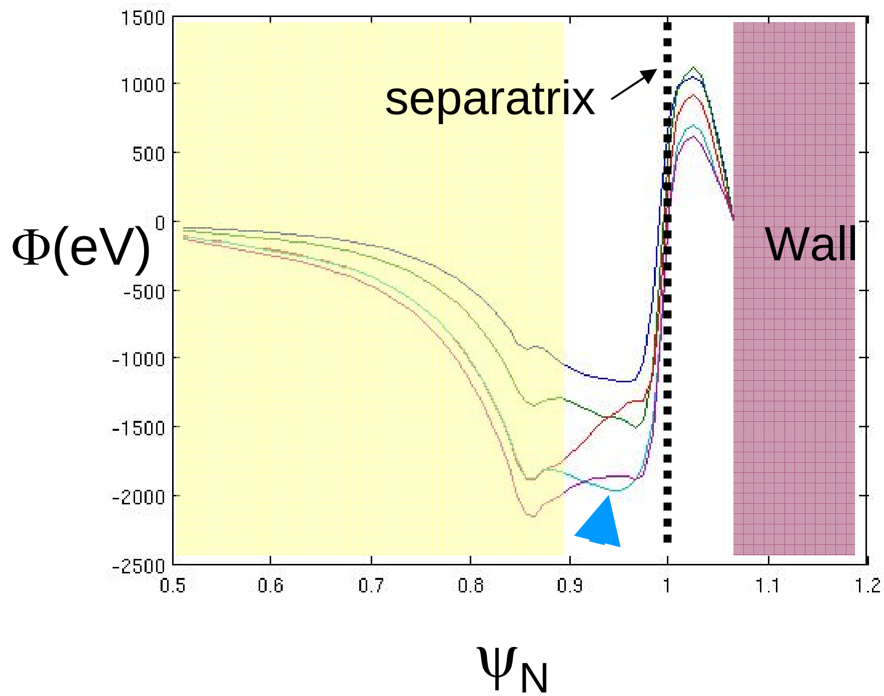
Lead PI: C-S Chang, NYU

CPES Center for Plasma Edge Simulation

1st year highlights

- XGC obtained first axisymmetric gyrokinetic edge solution by averaging over 5D turbulence in realistic edge geometry
- Shows strong enough neoclassical sheared ExB flow for turbulence suppression in the entire edge (scrape-off & pedestal).
- ITG solution is verified using cyclone plasma.

- Prototype coupling framework between XGC and MHD for pedestal-ELM cycle is established



Future plans in CPES

Center for Plasma Edge Simulation

<u>Edge gyrokinetic code XGC</u>

- Integrate new electrostatic turbulence capability with established neoclassical-neutral capability
- Simulate L-H transition and pedestal growth, together with scrape-off physics
- Add electromagnetic turbulence capability
- Add rf antenna effect on edge plasma
- Integrate with a core turbulence code

<u>Edge kinetic-MHD coupling</u>

- Couple XGC to nonlinear MHD/2-fluid codes (M3D and NIMROD) for ELM
- Simulate pedestal-ELM cycle with run-time monitoring

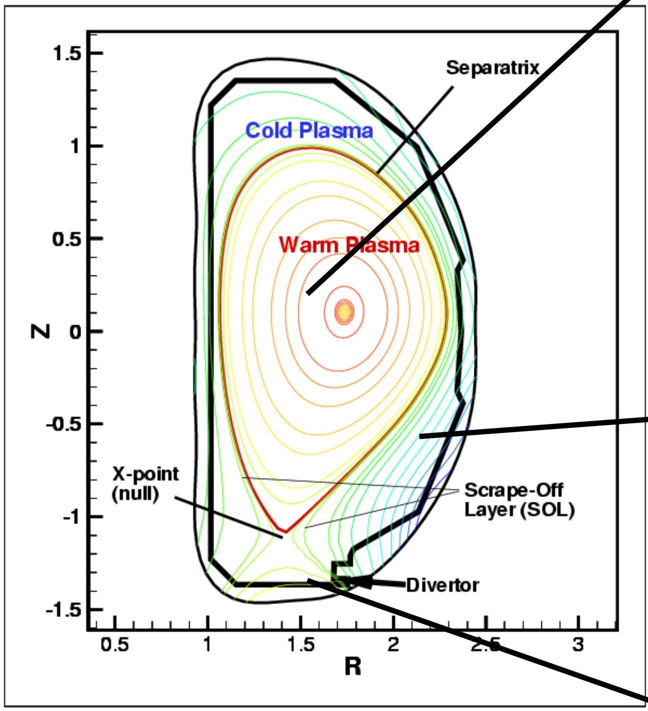
<u>Final goal</u>

- Predict ITER edge performance from complete package of first principles physics
- Integrate with core codes for whole device prediction

FACETS: Framework Application for Core-Edge Transport Simulations

- Multi-institutional, interdisciplinary project: Tech-X (Lead, Physics, CS/AM); LLNL (Physics, CS/AM); PPPL (Physics); ANL (CS/AM); UCSD (Physics); CSU (AM); ORNL (CS, perf); ParaTools (CS, perf); GA (Physics); Columbia (CS/AM); LBNL (CS/AM); Indiana (CS); MIT (Physics), NYU (Physics), Lodestar (Physics)
- Funded January 15, 2007
- Massively parallel to produce rapid, whole-device modeling capability
- Core to wall modeling of transport in 5 years. Rough timeline:
  - core/fluid-edge coupling with simplified transport models; dynamic wall model developed
  - core/fluid-edge/wall
  - equilibrium coupled
  - core transport coefficients from core gyrokinetic turbulence code (primary thrust of GA-ORNL SAP) &
  - edge transport and turbulence from edge gyrokinetic code

FACETS will integrate the core-edge-wall interaction



Closed field lines: slow perpendicular + fast parallel transport
⇒Quantities 1D, but embedded 3D turbulence
Hot plasma
⇒Collisionless, little significant atomic physics (except beams)

Open field lines: so parallel transport must balance perpendicular
⇒Quantities are 2D, but embedded 3D turbulence
Cool plasma
⇒Collisional, atomic physics is important

Wall: absorption and release of hydrogenic species
⇒Multiple 1D (into wall) equations
⇒Materials science important