PPPL Theory Department Review:

Advanced Scientific Computing & Concluding Comments

W. M. Tang

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PPPL THEORY PROGRAM
Addresses a Wide Range of Scientific Areas

- **Scientific Objectives have been identified together with expected deliverables over next two to five years**
  - **Consistent with Scientific Challenges highlighted by FESAC Priorities Panel, ITPA/ITER, and project needs**

- **Advanced Scientific Computing (e.g. SciDAC Projects) plays key role in all areas of research: (*synergistic cross-cuts*)**
  - **CENTER FOR EXTENDED MAGNETOHYDRODYNAMIC MODELING (S. Jardin, 26% to PPPL)**
  - **CENTER FOR GYROKINETIC PARTICLE SIMULATION OF TURBULENT TRANSPORT IN BURNING PLASMAS (W. Lee, 32% to PPPL)**
  - **CENTER FOR SIMULATION OF WAVE-PARTICLE INTERACTIONS (P. Bonoli, 28% to PPPL)**
  - **PROTO-FSP INTEGRATION CENTER FOR PLASMA EDGE SIMULATIONS (C. S. Chang, 12% to PPPL)**
  - **PROTO-FSP INTEGRATION CENTER FOR SIMULATION OF WAVE INTERACTIONS WITH MHD (D. Batchelor, 30% to PPPL)**

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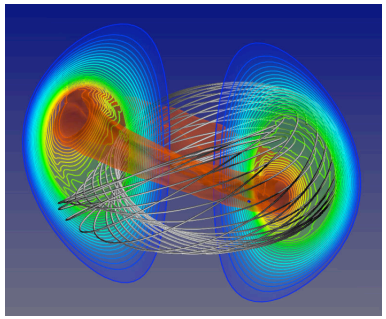
Key Science Problems Collaboratively Addressed via Fusion SciDAC Projects

Extended MHD Modeling (CEMM)



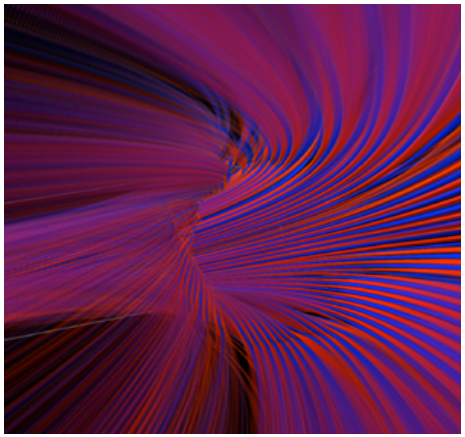
n=1 Plasma Instability

PPPL, NYU
U. Wisconsin, SAIC,
U. Colorado, MIT,
General Atomics,
LANL, ISICs, SAPP

Plasma Microturbulence

(CGPS)

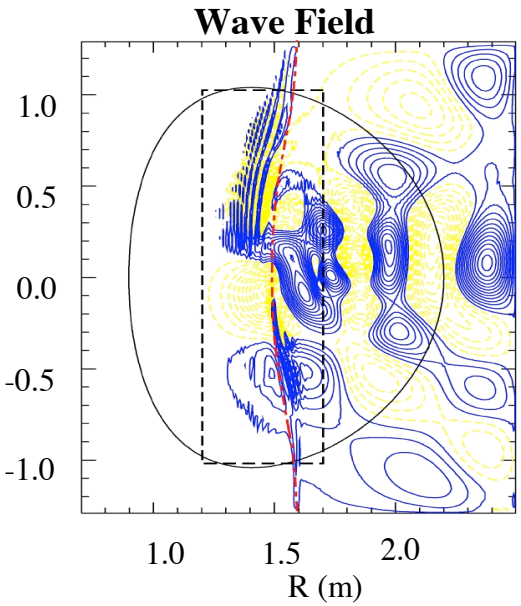
PPPL, UC Irvine,
U. Colorado, UCLA,
ISICs, SAPP



Turbulent Eddies in Plasmas

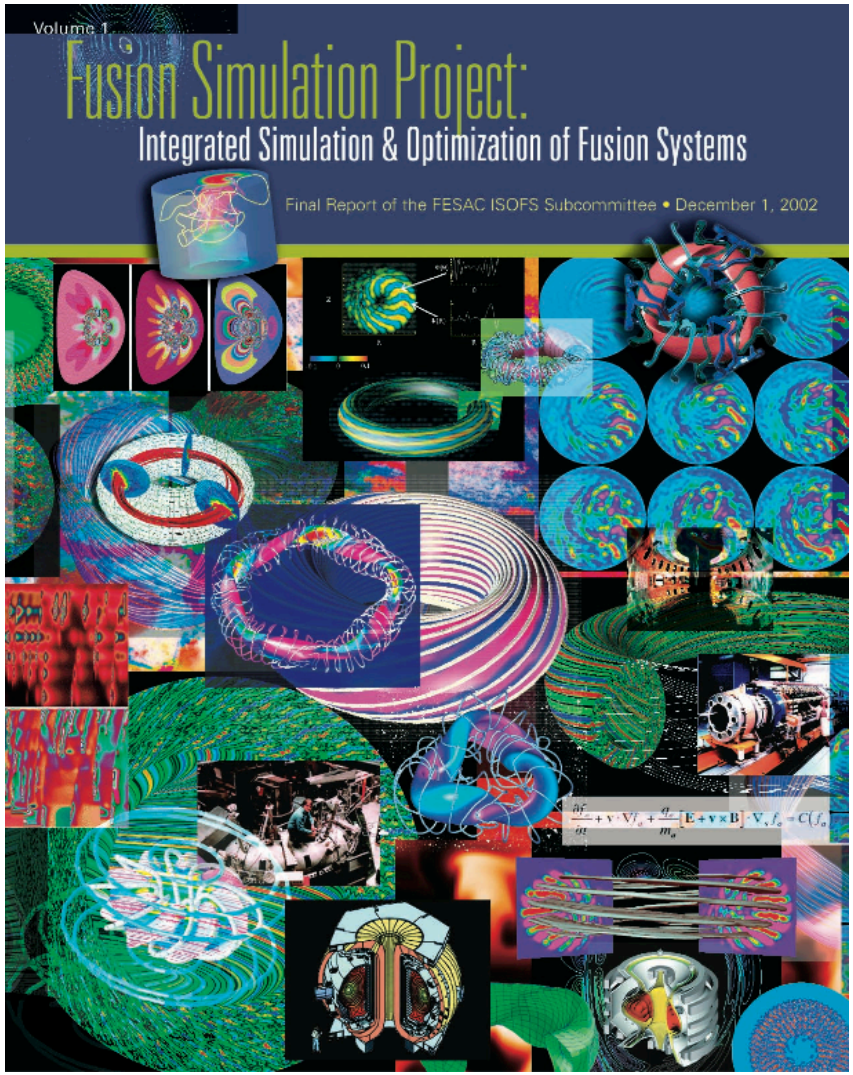
Wave Plasma Interactions (CWPI)

ORNL, PPPL, MIT,
Lodestar, CompX, SAPP



SciDAC INTEGRATED MODELING:
"Proto-Fusion Simulation Project"

- **Two new $2M/yr (for 3 yrs.) "Proto-FSP" projects just launched jointly from OFES & OASCR within SciDAC Program]**
- **Center for Plasma Edge Integration (C. S. Chang, NYU) will address integration challenges associated with transport, MHD, and boundary physics issues**
- **Center for Simulation of Wave Interactions with Magnetohydrodynamics (D. Batchelor, ORNL) will address integration challenges associated with RF and MHD physics issues**
- **Plan to leverage results from *SciDAC Program* for fundamental physics foundations and from Applied Math/CS communities for needed algorithms**



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ADVANCED SCIENTIFIC COMPUTING ACCOMPLISHMENTS

- **Advanced computation in tandem with theory and experiment has proven to be a powerful *new tool for scientific understanding and innovation* in FES research**

- **Plasma Science is *effectively utilizing* the exciting advances in Information Technology and Scientific Computing**
  - ***References*: *Advanced Computations in Plasma Physics* Physics of Plasmas 9 (May, 2002) and *Advances and Challenges in Computational Plasma Science* Plasma Physics & Controlled Fusion 47 (February, 2005)**

- **Tangible progress toward more reliable predictions of complex properties of high temperature plasmas**
  - **Acquisition of *scientific understanding* needed for predictive models *superior to empirical scaling***
  - **Such models essential for future FES development for and beyond ITER**

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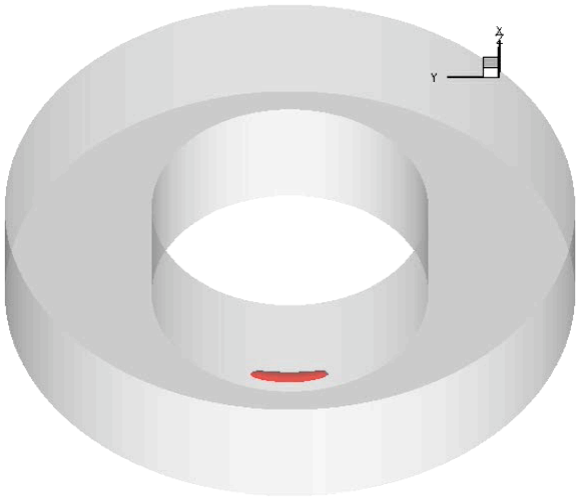
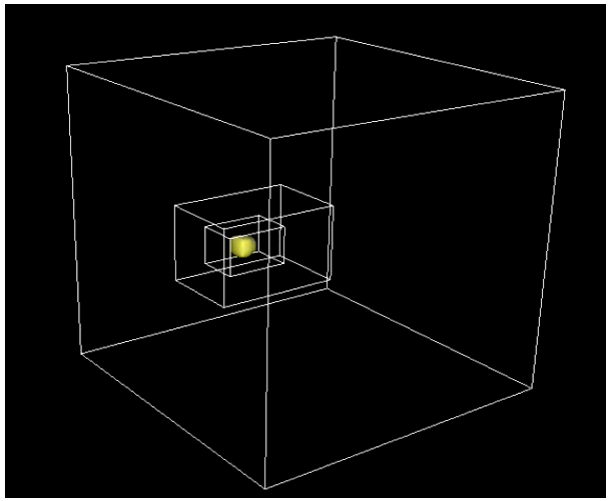
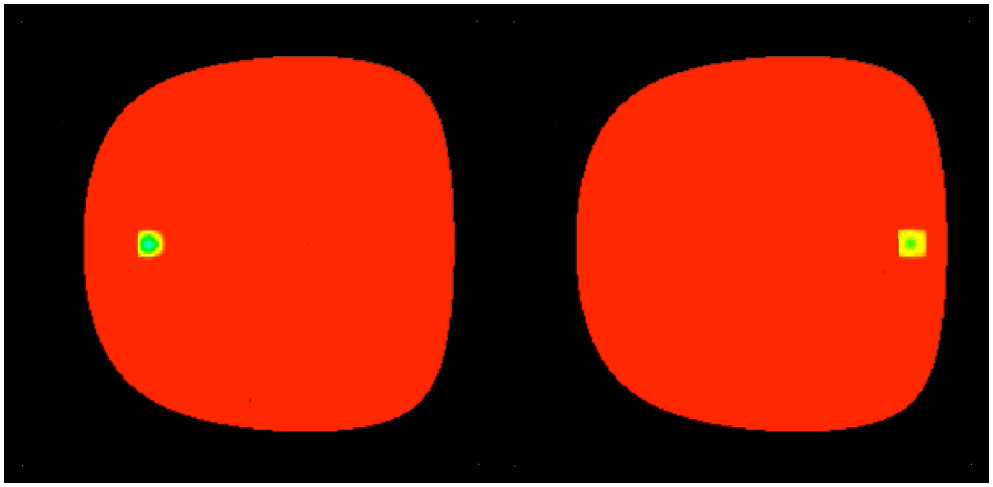
Fusion Codes at PPPL Take Advantage of Latest Computational Advances





Adaptive Mesh Refinement

Inside Pellet Launch →



← **Outside Pellet Launch**

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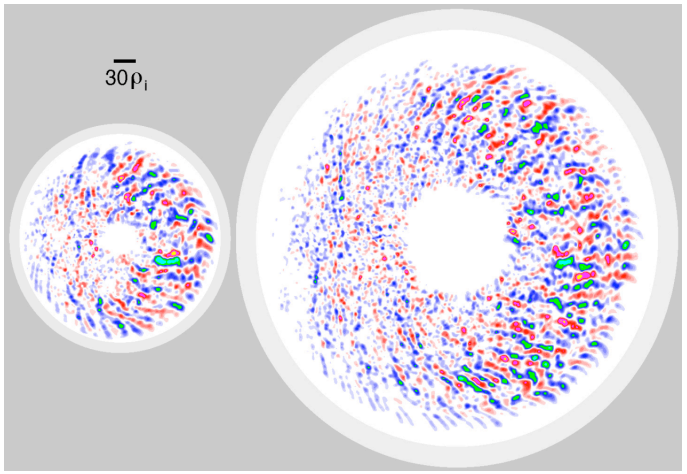
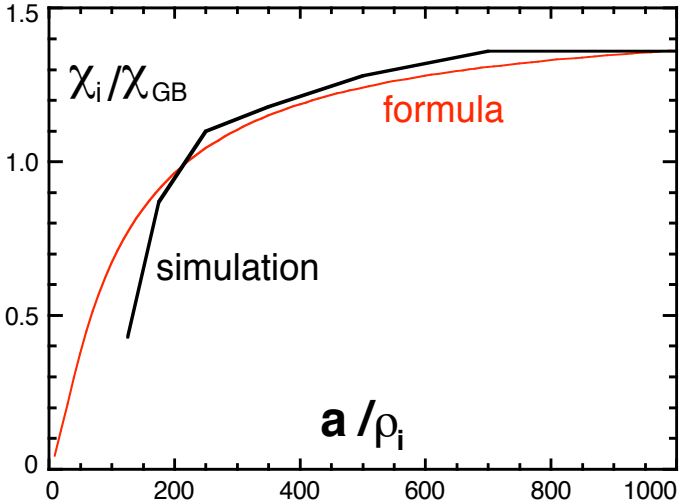
Simulation of Turbulence in Future Ignition-Scale Experiments
Requires Leadership-Class Computers

- **Recent Microturbulence Simulations for range including:**
  - **a/ρ_i = 400 (largest present lab experiment) through**
  - **a/ρ_i = 1000 (ignition experiment)**
- **Enabled by access to powerful supercomputers (e.g., 5TF IBM-SP @ NERSC)**
- ***PIC simulations: 1 billion particles, 125M spatial grid points; 7000 time steps***
- **Large-scale simulations indicate transition to more favorable scaling of plasma confinement**





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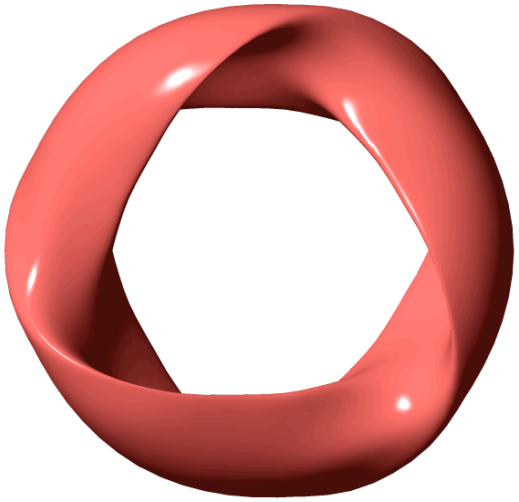
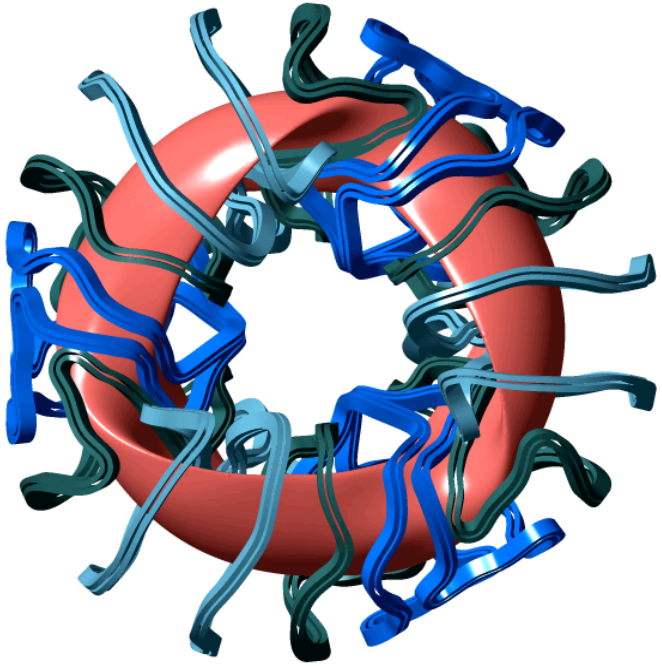
NCSX DESIGN STUDIES





- Optimization of Stability, Transport, and Constructability for Designing Future Experiments such as NCSX and QPS
- Utilization of MPP Computations Essential for Optimizations involving assesssments of over a half-million configurations

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PSACI Helps FES Community to Respond to Exciting Computational Science Funding Opportunities

(1) *Challenge* is for Fusion SciDAC projects to effectively utilize tera/peta-scale computing to produce significant *new scientific insights/conceptual breakthroughs* with impact on FES mission as well as the general scientific community -- "SciDAC-II" promises to offer enhanced funding opportunities for the next 5-year phase of the program.

(2) Need to clearly demonstrate how the partnerships with OASCR are helping to deliver *new* capabilities -- *collaboratively building the necessary software, visualization, networking, etc. to enable effective use of modern hardware to accelerate scientific progress*

(3) Fusion SciDAC Program should demonstrate how it can enable for the US -- *via a meaningful scientific leadership role and cost-effective participation on new facilities located abroad such as ITER*

-- impact real decision-making in the large "scientific options space"

-- harvest knowledge from major US investment in ITER and from collaborations on other facilities abroad

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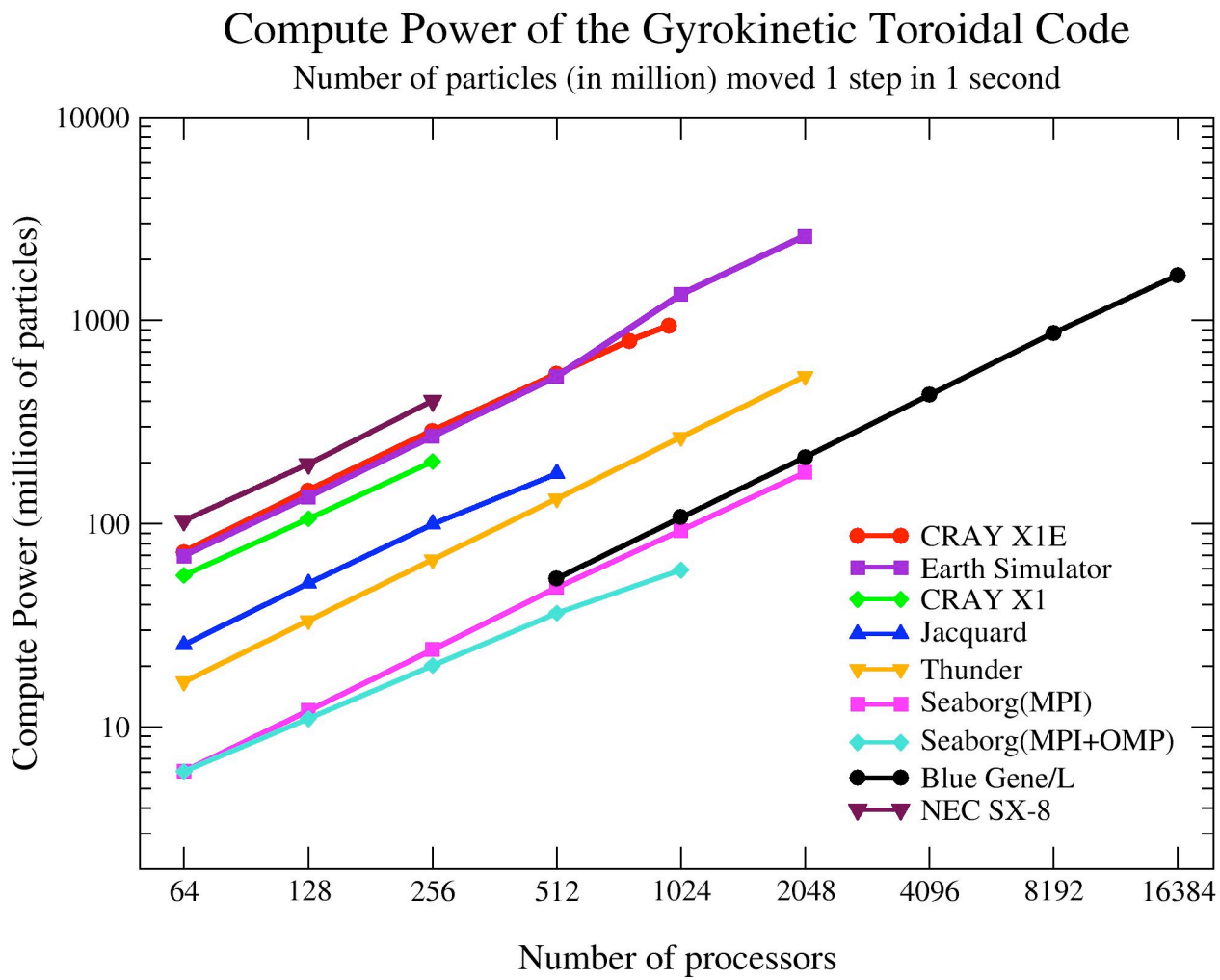
OUTSTANDING LEADERSHIP CLASS COMPUTING ACCOMPLISHMENT ENABLED BY ALLIANCES WITH OFES, OASCR, AND PRINCETON UNIVERSITY



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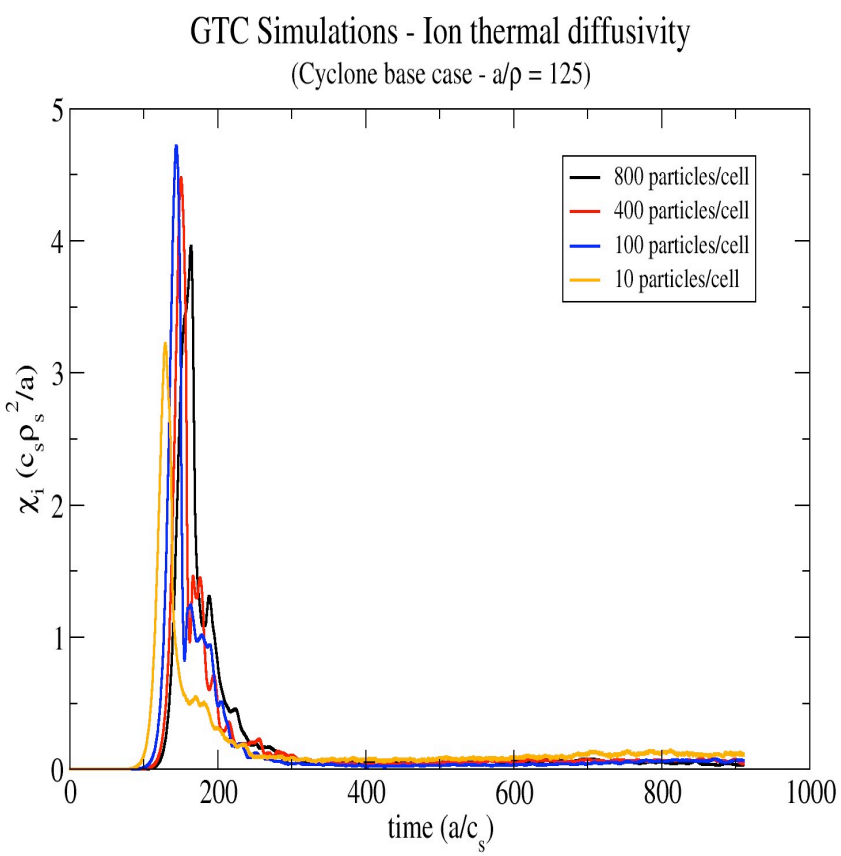
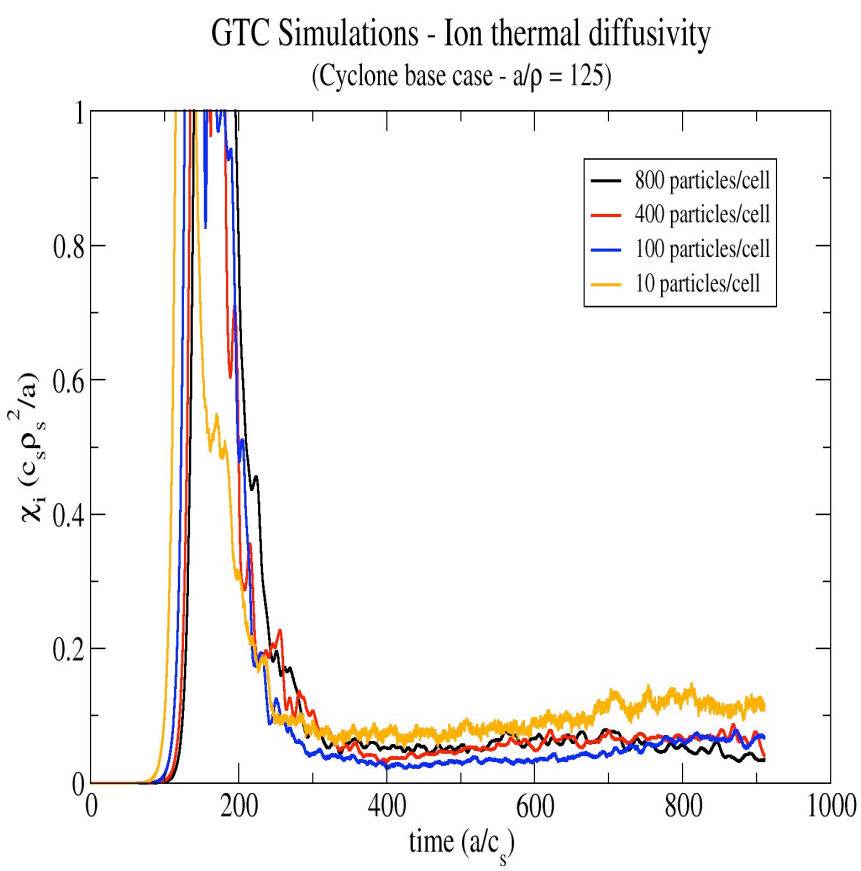
UTILIZATION OF LEADERSHIP CLASS COMPUTER (CRAY X1E) TO ADDRESS SCIENTIFIC UNDERSTANDING: *NOISE RESOLUTION IN PIC CODES VIA DRAMATIC INCREASE IN NUMBER OF PARTICLES USED*





PPPL COMPUTING INFRASTRUCTURE

- PPPL has made cost-effective investment in ***capacity computing*** by combining dedicated funding from OFES Theory, PPPL Projects, and Princeton U. partnerships
- 450 CPUs, including
  - 32 and 64 bit dual-processor clusters (all with Gbit interconnects and also 24 with Infiniband)
  - 16 processor SGI Altix SMP (20% contribution from PU) with primary focus on SciDAC CEMM applications needs
  - Partnership with PU providing access to at least 25% of new 64 processor SGI Altix System (located & maintained on Campus) with primary focus on Burning Plasma/ITER modeling needs
  - Visualization display wall (6 processor SGI Altix SMP)

- Aggregate capacity (4,000,000 CPU hrs/yr) is helping to address the increasingly critical capacity computing needs at PPPL
  - ***Requires dedicated funding to maintain and provide necessary upgrades (every 3 years)***

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PPPL THEORY PROGRAM
Has Well-Defined Target & Approach

- ***TARGET* --- RELIABLE PREDICTIONS OF PROPERTIES OF FUSION PLASMAS**
  - **<u>Scientific Challenge</u>*: Understanding* of complex physics phenomena impacting plasma performance & *Integration* of such knowledge into predictive models that prove superior to empirical scaling**

- ***APPROACH*:**
  - **Planning and interpretation of experiments on existing facilities; design of new facilities; cross-cuts to other areas of science *(shorter-term impact)***
  - **Develop innovative new tools for analyzing wider range of phenomena with greater accuracy *(medium-term impact)***
  - **Generate seminal concepts advancing basic physics as well as new ideas for confinement systems improvements *(longer-term impact)***

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PPPL THEORY PROGRAM Emphasizes Accomplishments & Synergistic Partnerships

- *ACCOMPLISHMENTS*
  - Strong track record for producing seminal theories (TAE, Turbulence Spreading, …) & reliable codes (M3D, GTC, ….)
  - Well-motivated goals with deliverables & associated time-lines (Roadmaps)
  - Steering Committee and strong linkages with projects (NSTX, NCSX, Off-Site) to facilitate productivity & responsiveness

- *SYNERGISTIC COLLABORATIONS*
  - With other theorists (e.g., UCSD, UCI, Frascati, NIFS on turbulence spreading studies)
  - With experimentalists (e.g, JET on current hole studies)
  - With advanced scientific computing community (e.g, SciDAC Projects and PSACI)

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Summary

- PPPL's strong presence in DOE's SciDAC Program provides *natural bridge for fruitful collaborations* between FES, Computer Science, & Applied Math with demonstrable impact on key science problems in FES.
  -- stronger alliances within SciDAC-2 to produce critically needed innovations in CS/Applied Math and also with National Computing Facilities (ORNL, NERSC, ….)

- The PPPL Theory Program via strong synergistic alliances across the FES community is helping to *accelerate progress* toward gaining the knowledge needed to strategically impact plans for the future (e.g, participation in ITER and beyond) by producing modeling capabilities to enable the most effective harvesting of physics from domestic and international experimental facilities.

- PPPL Theory has uniquely and very effectively *leveraged investments* made in facilities (NSTX, NCSX, Off-Site Collaborations, & ITER) as well as other programs (DOE's SciDAC and OASCR programs, PU Graduate Education Program)

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Summary

- **Timely achievement of the targeted goals will require additional investment:**
  (1) $350K for maintaining and upgrading capacity computing capabilities at PPPL
  (2) $200K for PPPL theory post-doctoral program
  (3) $100K for new incoming collaborators at PPPL

- **Guided by a Strategic Plan formulated under the strong leadership of J. Manickam including**
  - **Well-motivated goals with deliverables & associated time-lines (Roadmaps),**
  - **Pro-active Steering Committee with strong linkages to projects (NSTX, NCSX, Off-Site) for facilitating productivity & responsiveness,**

The PPPL Theory Program is well-positioned to achieve its targeted goals

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