PLASMA SCIENCE ADVANCED COMPUTING INSTITUTE REPORT FROM JUNE 3-4 PAC MEETING

PRESENTATION TO FUSION ENERGY SCIENCES ADVISORY COMMITTEE MEETING

W. M. TANG

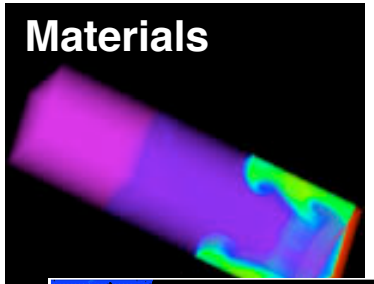
26-27 July 2004

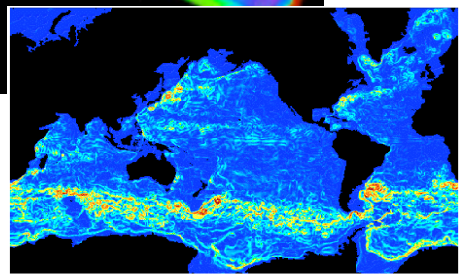
Advanced Computing

is Critical to Discovery in Many Scientific Disciplines

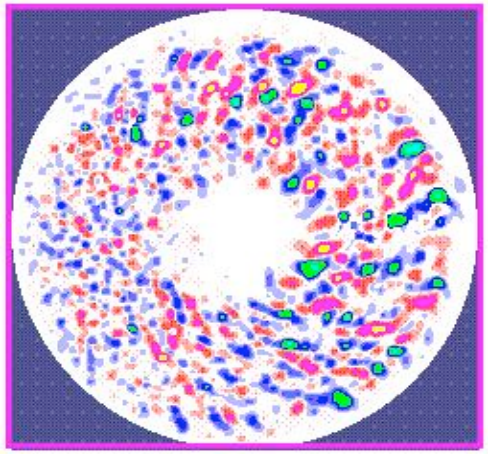
U.S. DOE SciDAC (Scientific Discovery through Advanced Computing) Program

Need Dramatic Advances in Simulation Capabilities To Meet Mission Goals

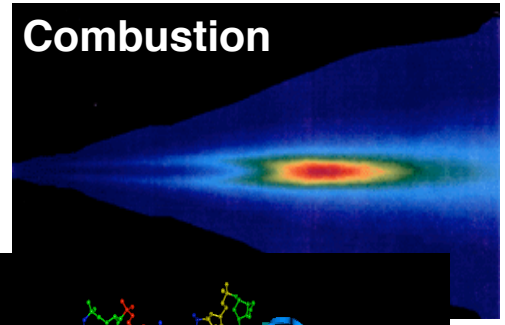


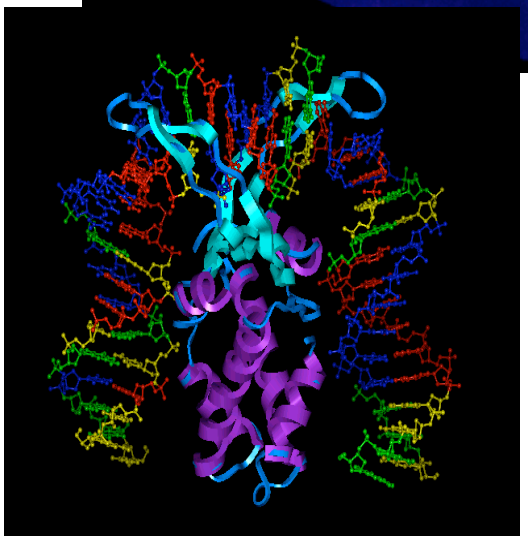


Global Systems



Fusion Energy





Health Effects, Bioremediation

PSACI Program Advisory Committee

William Kruer, *PAC Chairman*, Chief Scientist for Inertial Fusion Plasma Physics, LLNL
James Callen, Professor of Engineering Physics, U. of Wisconsin
Ronald Cohen, Head, MFE Theory Program, LLNL
Ronald Davidson, Professor of Astrophysical Sciences, Princeton U.
Patrick Diamond, Professor of Physics, UCSD
James Drake, Professor of Physics & Astronomy, U. of Maryland
*Brian Gross, Deputy Director and Head of Computing, Geophysical Fluid Dynamics Laboratory
*Robert Harrison, Chief Scientist for Computational Chemistry, ORNL
Russell Hulse, Nobel Laureatte and Distinguished Laboratory Fellow, PPPL
*Kai Li, Professor of Computer Sciences, Princeton U.
*William McCurdy, Senior Faculty Scientist, LBNL
*Steven Orszag, Professor of Mathematics and Chairman, Applied Math Department, Yale U.
*Malcolm Stocks, Corporate Fellow & Co-Director of Computational Science
& Materials Research Institute, ORNL

GENERAL VIEW

(1) Fusion SciDAC Program is effectively utilizing advanced computing to produce significant *new scientific insights/conceptual breakthroughs* that could not otherwise be achieved and which are well appreciated by the FES Program as well as the general scientific community

(2) Partnerships with Computer Science/Applied Math components of SciDAC Program have delivered *new* capabilities -- *collaboratively building the necessary software, visualization, networking, etc. to enable effective use of hardware to accelerate scientific progress*

(3) Fusion SciDAC Program can play a key role in helping development/planning of future experimental facilities such as ITER -- *cost-effective assessment of new ideas and operating scenarios*

CHARGE FOR PSACI PAC MEETING

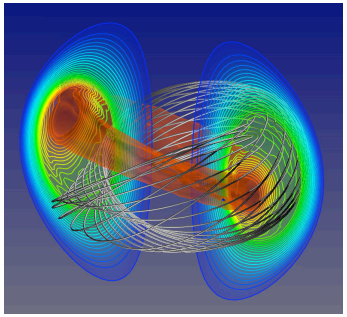
- **Assessment of the accomplishments of the previous Fusion SciDAC Projects (over 3 years, ending in June '04)**
  - ***Accountability*: How has each project made tangible progress toward achieving scientific targets originally proposed by Fusion SciDAC projects?**
  - ***Supercomputing Relevance*: How have high-end computing resources been effectively utilized to accelerate progress toward achieving these goals?**
  - ***Effectiveness of Collaborations*: Are productive collaborative activities evident within each project and with other SciDAC activities (including relation between projects and enabling technology resource centers)?**

PSACI PAC REPORT

- **Assessment of the accomplishments of the previous Fusion SciDAC Projects [PRESENTATIONS by PI's POSTED @ http://w3.pppl.gov/theory/PSACI04.html]**
  - **Impressive technical and computational advances achieved and reported in *journal publications and invited papers at major meetings*.**
  - **FES advances in computational modeling of complex multi-scale physics are *highly visible in presentations to other scientific communities and funding agencies*.**
  - **FES SciDAC projects have brought together physicists, applied mathematicians and computer scientists *"in close and productive working relationships which are a model for future research."***

Previous Fusion SciDAC Projects

Extended MHD Modeling

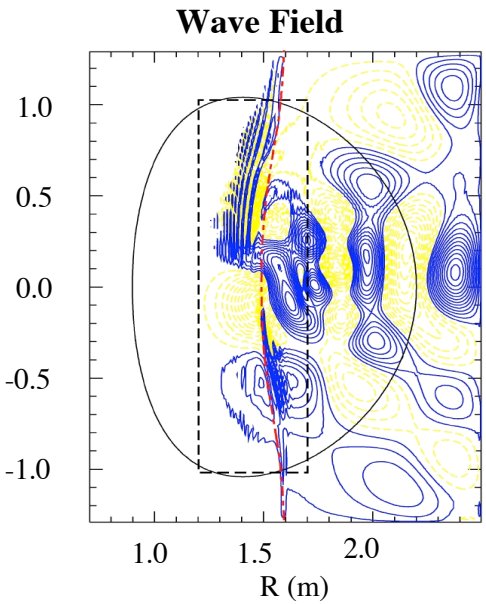


N=1 Plasma Instability

PPPL, SAIC, U. Wisconsin, NYU, U. Colorado, MIT, Utah State U., GA, LANL, U. Texas

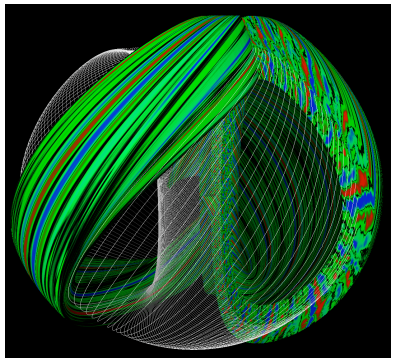
RF/Wave Plasma Interactions

ORNL, PPPL, MIT, Lodestar, CompX



Plasma Microturbulence

LLNL, GA, PPPL, U. Maryland, U. Texas, U. Colorado, UCLA

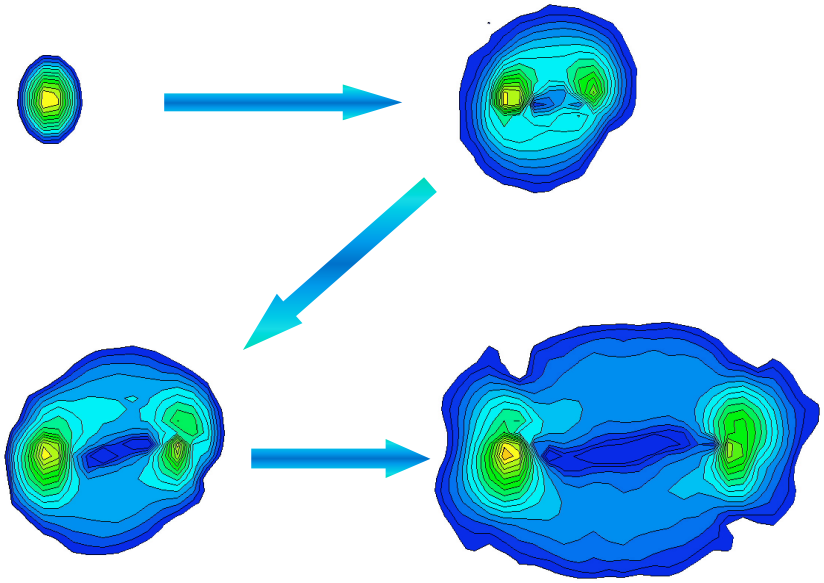


Turbulent Eddies in Plasmas

Previous Fusion SciDAC Projects

Terascale Atomic Physics

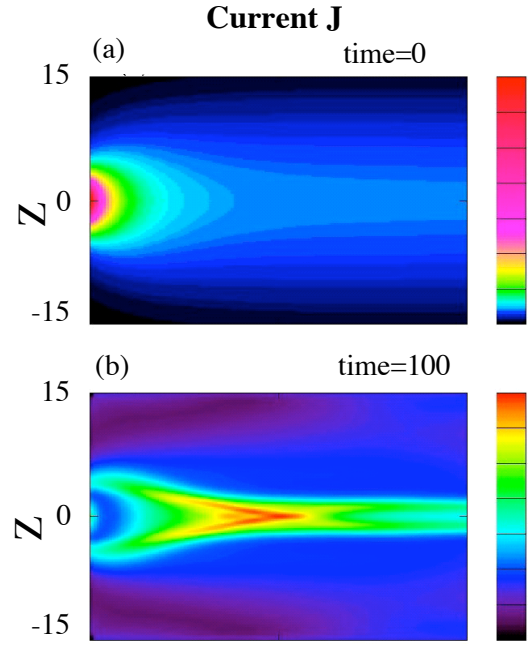
Auburn University
Rollins College
Oak Ridge National Laboratory



Magnetic Reconnection Physics

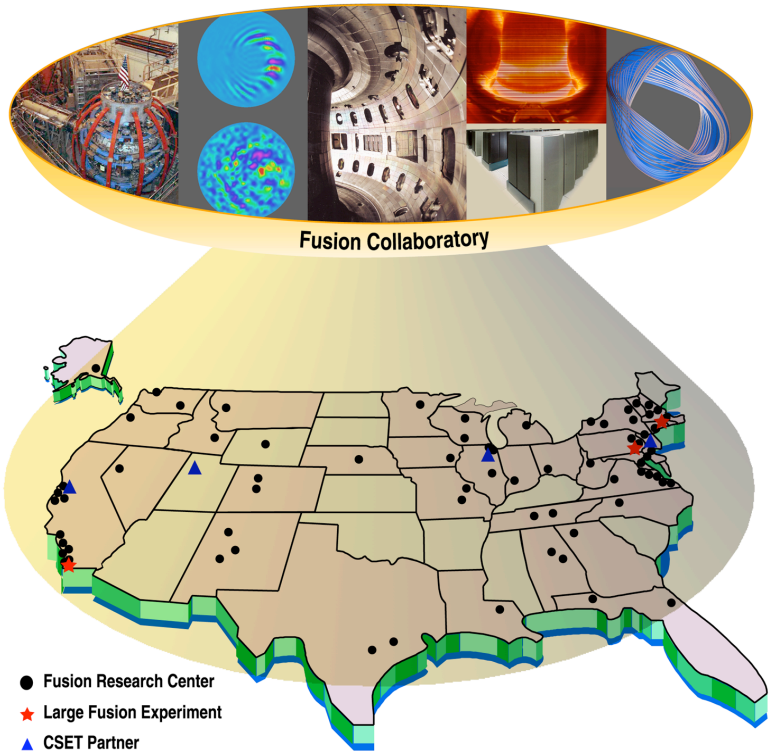
University of Iowa
University of Chicago
University of Texas

Substorm in the Magnetotail



FUSION ENERGY SCIENCES COLLABORATORY (OASCR-funded)

(***involves 40 US sites in 37 states***)



• Collaboratory Goals:

-- enable more efficient use of experimental facilities by developing more powerful *between pulse data analysis*

-- enable *better access by researchers* to analysis & simulation codes, data, and visualization tools

-- create *standard tool set* for remote data access, security, and visualization

• Collaboratory Partners:

-- ***3 large fusion experiments****

* C-MOD, DIII-D, NSTX

-- ***4 computer science centers*** **

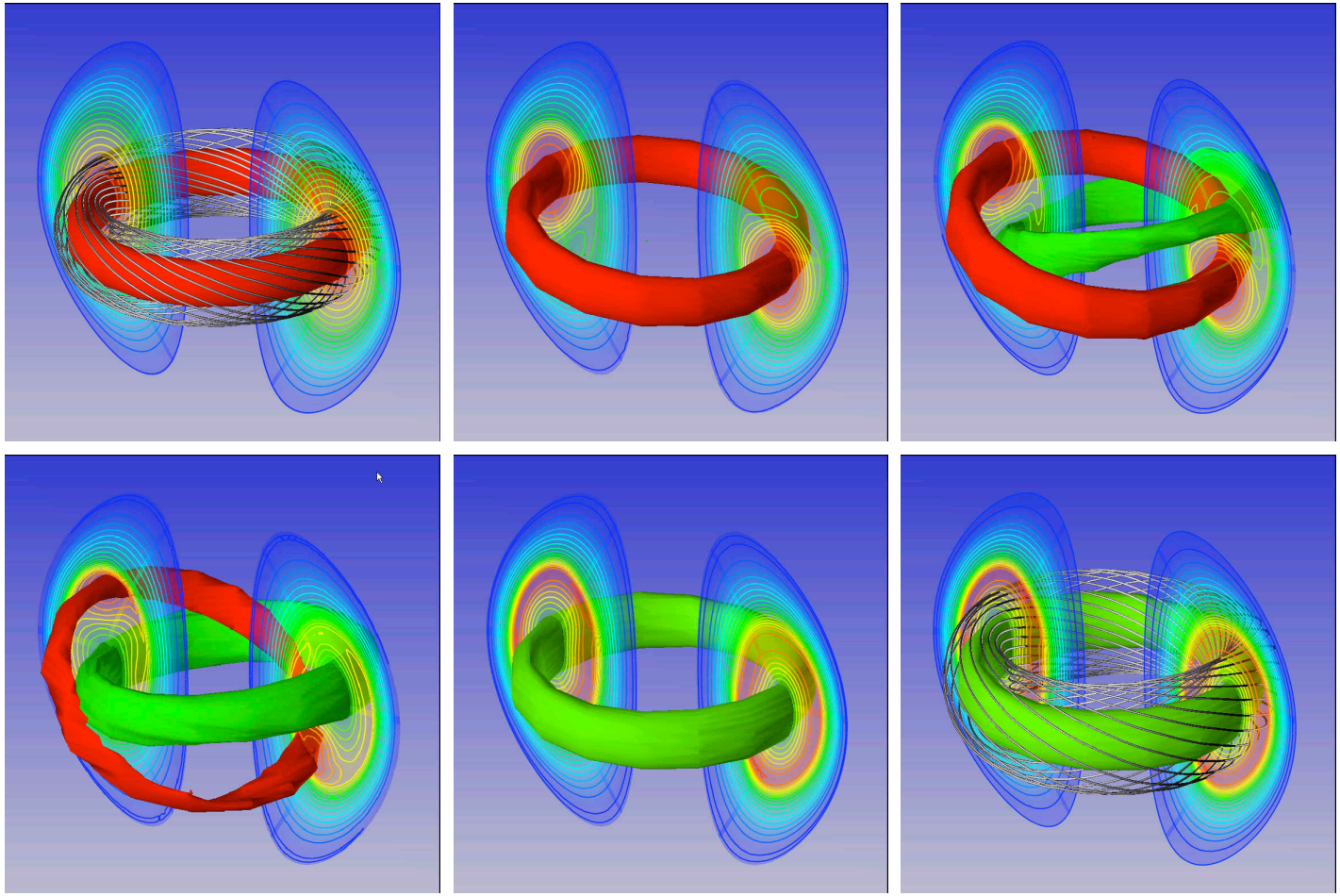
** ANL, LBNL, Princeton U., U. of Utah

Highlighted Advances: *(All dependent on significant SciDAC CS/Applied Math alliances)*

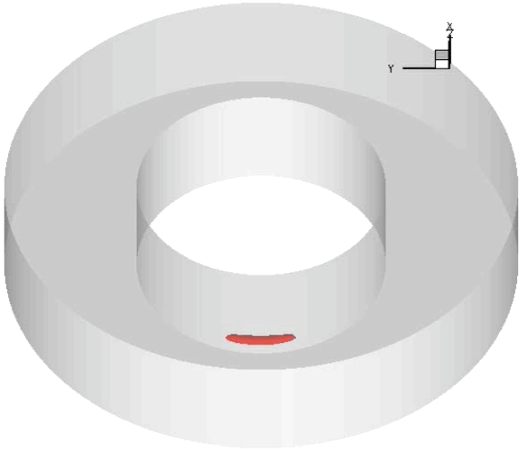
- **MHD:**
  - **new insights into high beta disruptions on DIII-D**
  - **visualization of internal reconnection in NSTX featured in R. Orbach's presentation at Supercomputing '03 Meeting**
  - **major algorithm improvements such as AMR implemented to aid new studies (e.g., pellet injection dynamics)**
  - **over 20 journal articles & many invited presentations at major conferences**
- **PMP:**
  - **new insights into scaling of heat transport with machine size**
  - **new EM drift-wave algorithms implemented**
  - **impressive NL cross-benchmarking between lead codes**
  - **porting of major codes to *"Leadership Class" supercomputers* -- ESC and ORNL Cray X1**
  - **over 20 journal articles & many invited presentations at major conferences**

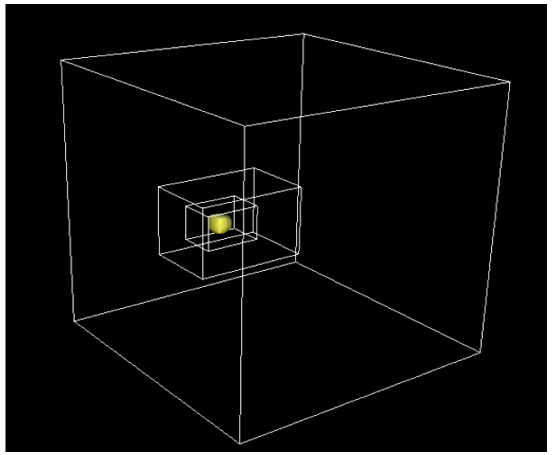
MHD Simulation of Internal Reconnection Event

Hot Inner Region Interchanges with Colder Outer Region via Magnetic Reconnection



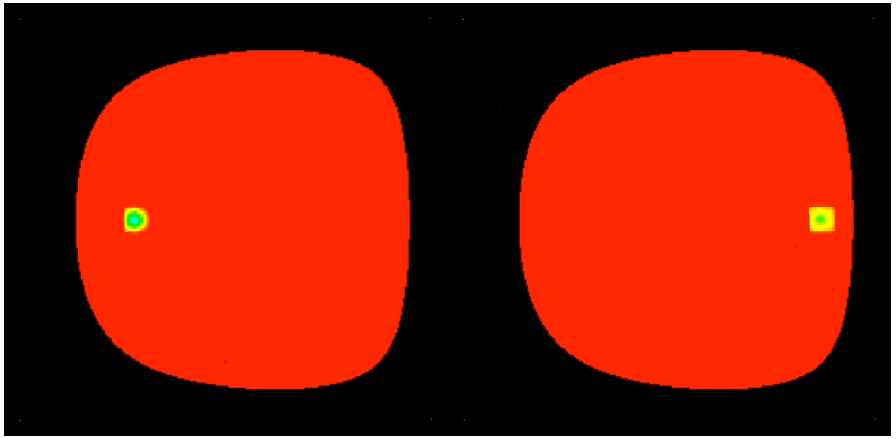
Fusion Codes Take Advantage of Latest Computational Advances for ITER-Relevant Calculations





Adaptive Mesh Refinement

Inside Pellet Launch →

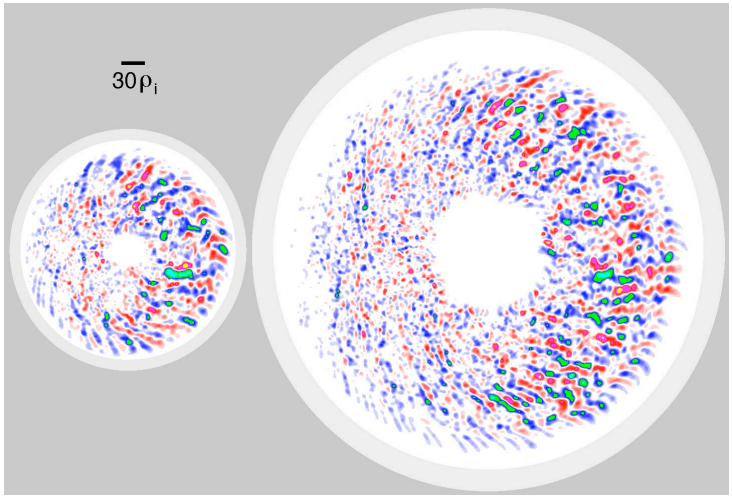


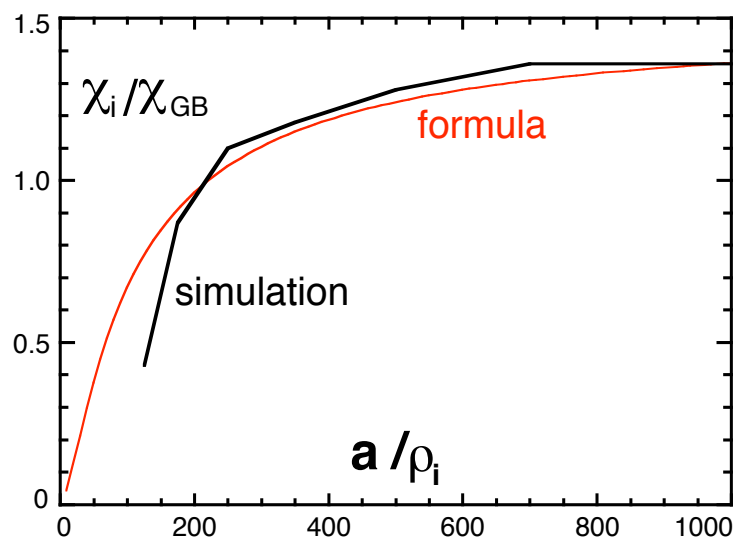
← **Outside Pellet Launch**

Simulation of Turbulence in future Ignition-Scale Experiments

Require State-of-the-Art 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**



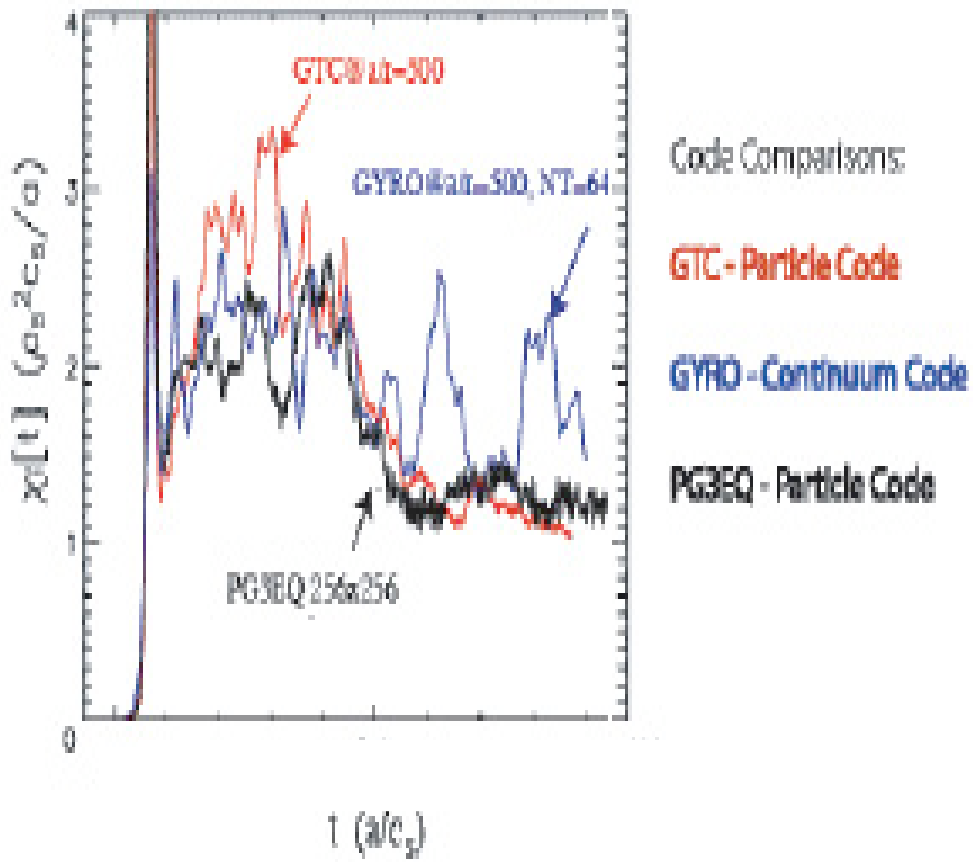


Comparisons of Nonlinear Results from Plasma Microturbulence Codes (*W. Nevins & SciDAC PMP Team*)

-- Nonlinear transport comparisons from very different major codes:

- ***PIC vs. Continuum***
- ***Local (Flux Tube) & Global Geometry***

-- Results indicate impressive level of agreement on measurements of χ_I



Highlighted Advances: *(All dependent on significant SciDAC CS/Applied Math alliances)*

- **RF:**
  - **new ability to model wave conversion processes in 2D for large-scale fusion devices enabled by increasing speed, resolution, and physics content of wave solvers**
  - **better understanding of ICRF mode conversion on C-MOD**
  - **over dozen journal articles published**

- **ATOMIC PHYSICS:**
  - **first accurate electron-impact excitation for fusion species enabled by new code applications**
  - **collisional radiative coefficients obtained to support transport studies in fusion systems**
  - **over ten PRLs published**

Highlighted Advances: *(All dependent on significant SciDAC CS/Applied Math alliances)*

- **RECONNECTION:**
  - **first 2-fluid Hall MHD code with AMR developed leading to new insights into "bursty" reconnection and sawtooth oscillations in tokamaks and magnetotail substorms**
  - **valuable interface with ASCI community**

- **FUSION COLLABORATORY:**
  - **worldwide data access on the FusionGrid achieved; used for collaborations on JET experiment**
  - **overall significant impact on more efficient use of experimental facilities and integration of experiment, theory, & modeling**
  - **OASCR will continue to fund this project which has been a "*remarkable success*."**

CHARGE FOR PSACI PAC MEETING

- **Consider and provide guidance on the key areas targeted in the *next 3-year phase of the FES SciDAC Program* (beginning in June of '04)**
  - ***Scientific Potential*: What is the likelihood of timely delivery of significant new scientific insights/conceptual breakthroughs enabled by the FES SciDAC Program?**
  - ***New Tools for Assessing Burning Plasmas*: What is the likelihood of timely delivery of reliable computational modeling capabilities addressing burning plasma physics issues relevant to ITER?**
  - ***Major Integrated Modeling Effort*: How can the FSP (Fusion Simulation Project) component of the FES SciDAC Program best be organized to successfully achieve the targeted goals of this new effort.**

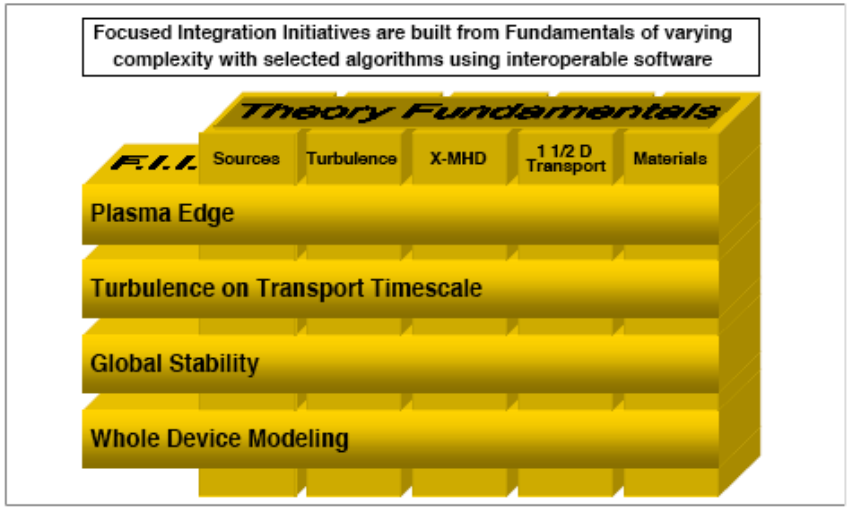
PSACI PAC REPORT

- **On New Fusion SciDAC Projects:**
  - **Selection Process:** ***"The PAC applauds the DOE for its timely execution of an excellent review process for the new projects in the FES portfolio."***
  - **Two Projects Selected:** ***"The new centers for Extended MHD Modeling and for Gyrokinetic Particle Simulations of Plasma Turbulence are very high quality projects with focused and well-defined deliverables in the vital areas of MHD and plasma microturbulence."***
    - ***Specific technical feedback provided by PAC to PIs***

    [PRESENTATIONS of goals and associated scientific roadmaps posted @http://w3.pppl.gov/theory/PSACI04.html]
- **Additional Observations/Recommendations:**
  - ***Desirable that funding be found to encourage work in the RF and Atomic Physics areas.***
  - ***Access to computer time and computer science resources should be maintained for previous SciDAC-funded scientists***
  - ***Concern that there is no SciDAC project on the vital topic of plasma edge modeling***

INTEGRATED MODELING: *U.S. Fusion Program has proposed "Fusion Simulation Project" (FSP)*

- **Proposed $20M/yr with start-up planning activity in FY '05 at about $2M - *potentially valuable US contribution to ITER***



- **Need to *effectively leverage ongoing SciDAC Program* for fundamental physics foundations and for needed algorithms, etc. from Applied Math/Computer Science communities**

PSACI PAC REPORT

- **On proposed Fusion Simulation Project (FSP):**
  - **Presentation from Doug Post (Chair of FSP Planning Committee)**
  - **SciDAC Director Michael Strayer noted that the FSP is expected to be a component of FES SciDAC portfolio**
  - **$2M set aside in FY'05 for FSP start-up planning ($1M from FES SciDAC and $1M from OASCR)**

"The PAC strongly supports the goal of integrated modeling and the proposed FSP (previously endorsed by FESAC and by DOE leadership). … The PAC stresses the importance of a more detailed technical plan for the use of these significant start-up resources."

PSACI PAC REPORT

- **Recommendations:** ***"We strongly recommend that the FSP Planning Activity:"***

  (1) "Plan how to *leverage the past and ongoing FES SciDAC projects into the FSP* and identify key *missing scientific areas for the integrated modeling* of a fusion burning plasma."

  (2) "Propose an appropriate *balance between the needed physics R & D and computational science* developments during the early, middle, and mature stages of the FSP Project."

  (3) "Make progress on some multi-scale (in both space & time) integrated modeling challenges by identifying and facilitating "*prototype modeling*" *of a few key multi-scale scientific issues for burning plasmas*."

  -- e.g. sawtooth crash dynamics; ELMs; ITB formation & growth while maintaining MHD stability; RF effects on plasma flows & in forming transport barriers

PSACI PAC REPORT

- **Recommendations for FSP Planning Activity (continued):**

  (4) "Plan how to integrate relevant SciDAC ISICs (*Integrated Software Infrastructure Centers*) into the FSP as part of broader plan to have the computer science & physics elements developed in parallel from the beginning and throughout the evolution of the FSP."

  (5) "Identify key *burning plasma focal points* for the early, middle, and mature stages of the FSP."

CONCLUSIONS

- **PSACI PAC review of the accomplishments of the FES SciDAC Program over the past 3 years concludes that it is**

  "clear that FES is at the very forefront in using high-end computing to successfully model complex multi-scale physics, and have brought together physicists, applied mathematicians, and computer scientists in close and productive working relationships, which are a model for future research."

- **Selection Process:** ***"The PAC applauds the DOE for its timely execution of an excellent review process for the new projects in the FES portfolio."***

- **Projects Selected:** ***"The new centers for Extended MHD Modeling and for Gyrokinetic Particle Simulations of Plasma Turbulence are very high quality projects with focused and well-defined deliverables in the vital areas of MHD and plasma microturbulence."***

CONCLUSIONS (continued)

- **On the FSP:** ***"The PAC strongly supports the goal of integrated modeling and the proposed FSP" and "stresses the importance of a more detailed technical plan for the use of these significant start-up resources."***

- **FSP Plan needs to:**
  - **"*leverage* past and ongoing FES SciDAC projects into FSP" and "*identify key missing scientific areas* for the integrated modeling of a fusion burning plasma"**
  - **establish "*balance between needed physics R & D and computational science developments*"**
  - **identify and facilitate *"prototype modeling" of a few key multi-scale scientific issues* for burning plasmas**

CONCLUSIONS (continued)

- **SUMMARILY:**

  Fusion SciDAC Program is effectively utilizing advanced computing to accelerate progress toward new scientific insights & conceptual breakthroughs that could not otherwise be achieved.