Theory and Advanced Scientific Computing

Presentation to
Dr. Walt Polansky
Acting Director, MICS Division
Office of Science, Department of Energy

Dr. William Tang
Chief Scientist, Princeton Plasma Physics Laboratory
August 29, 2002

PPPL THEORY PROGRAM
Has Well-Defined Target & Approach

- ***TARGET* --- RELIABLE PREDICTIONS OF PROPERTIES OF FUSION PLASMAS**
  - **Scientific Challenge*:* *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 improvements of energy confinement systems *(longer-term impact)***

PPPL THEORY/ADVANCED SCIENTIFIC COMPUTING PROGRAM
Emphasizes Accountability & Partnerships in Advancing Plasma Science

- ***ACCOUNTABILITY***
  - **Strong track record for producing seminal theories & reliable codes**
  - **Well-motivated goals with deliverables & associated time-lines (*Theory Department 5-Year Plan document*)**
  - **Steering Committee to facilitate productivity & communication**
    - **IFE & Non-MFE Plasma Science (Davidson); MHD (Jardin); Transport (Hahm); Waves/Energetic Particles (Cheng); Non-Axisym. Systems (Reiman); Laser-Plasma Interactions (Valeo)**
- ***PARTNERSHIPS***
  - **With theorists and theory groups, nationally & internationally**
  - **With experimentalists and experimental groups, nationally & internationally**
  - **With advanced scientific computing community**
  - **With technology development**

ADVANCED COMPUTING IS AN INCREASINGLY POWERFUL TOOL FOR SCIENTIFIC DISCOVERY

- **Advanced computation in tandem with theory and experiment is powerful *new tool for scientific understanding and innovation* in research**

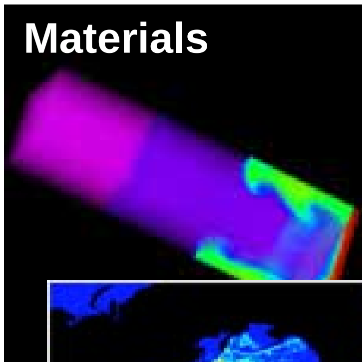
- **Plasma Science is *effectively utilizing* the exciting advances in Information Technology and Scientific Computing**
  - ***Reference*: *Advanced Computations in Plasma Physics* Physics of Plasmas 9 (May, 2002)**

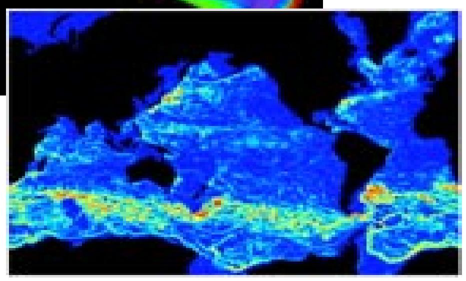
- **Accelerates progress toward Theory Goal for reliable predictions of complex properties of high temperature plasmas**
  - **Acquire the *scientific understanding* needed for predictive models *superior to empirical scaling***

Advanced Computing

is Critical to Discovery in Many Scientific Disciplines

Materials

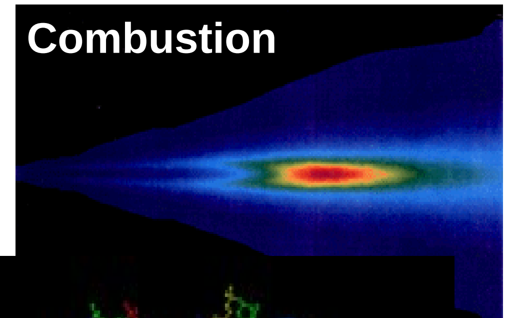


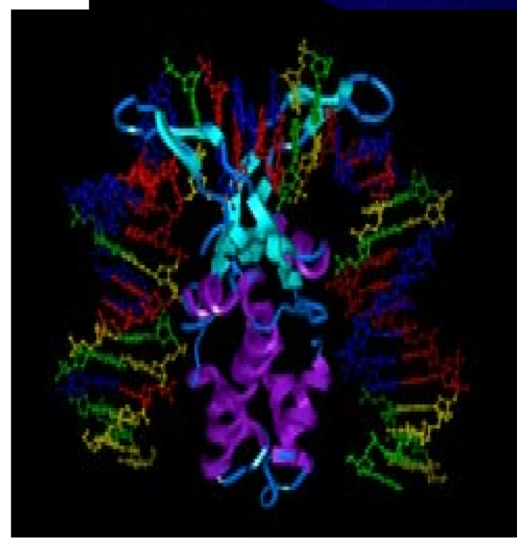


Global Systems

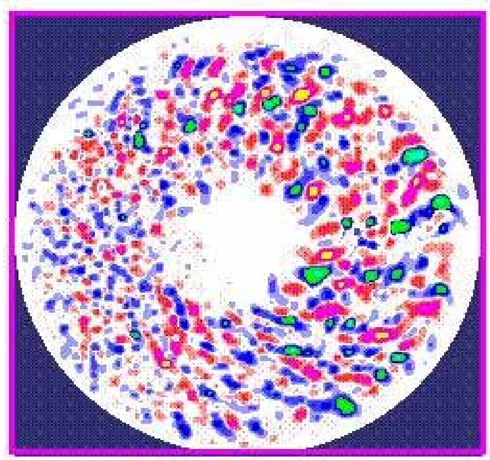
Dramatic Advances in Simulation Capabilities are Needed to Meet the Mission Goals of DOE

Combustion





Health Effects, Bioremediation

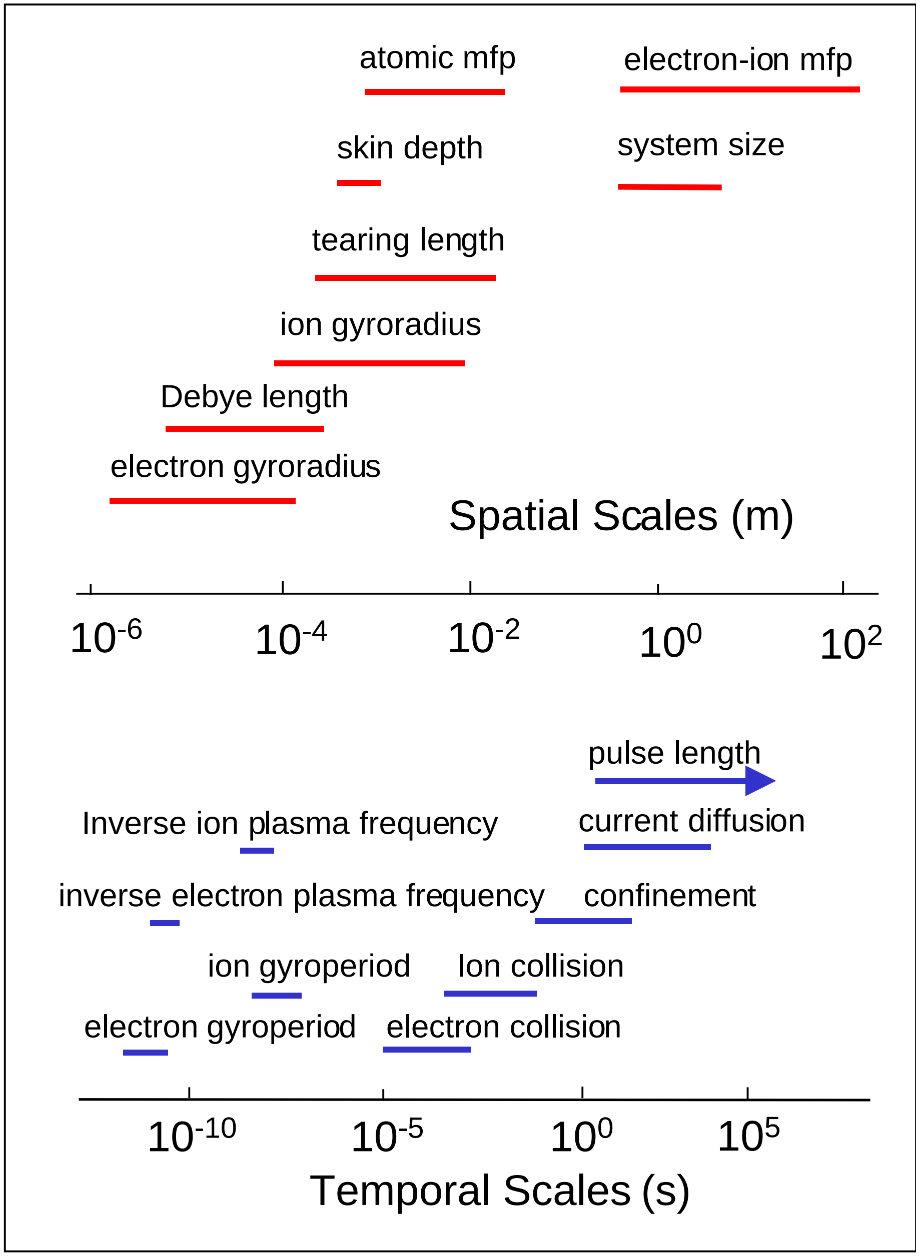


Fusion Energy

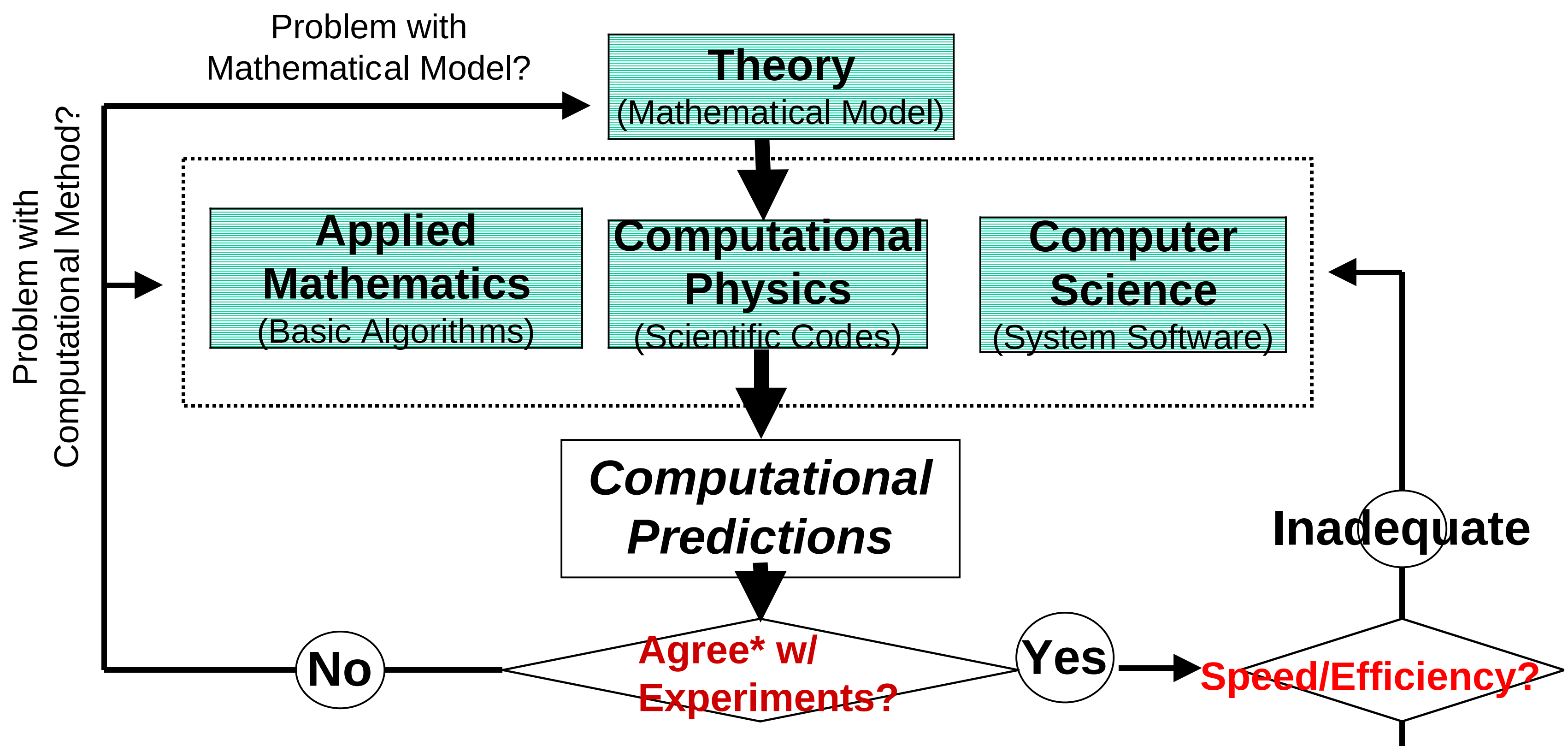
Spatial & Temporal Scales Present Major Challenge to Theory & Simulations

- **Huge range of spatial and temporal scales**

- **Overlap in scales often means strong (simplified) ordering not possible**



Advanced Scientific Codes --- *a measure of the state of understanding of natural and engineered systems*



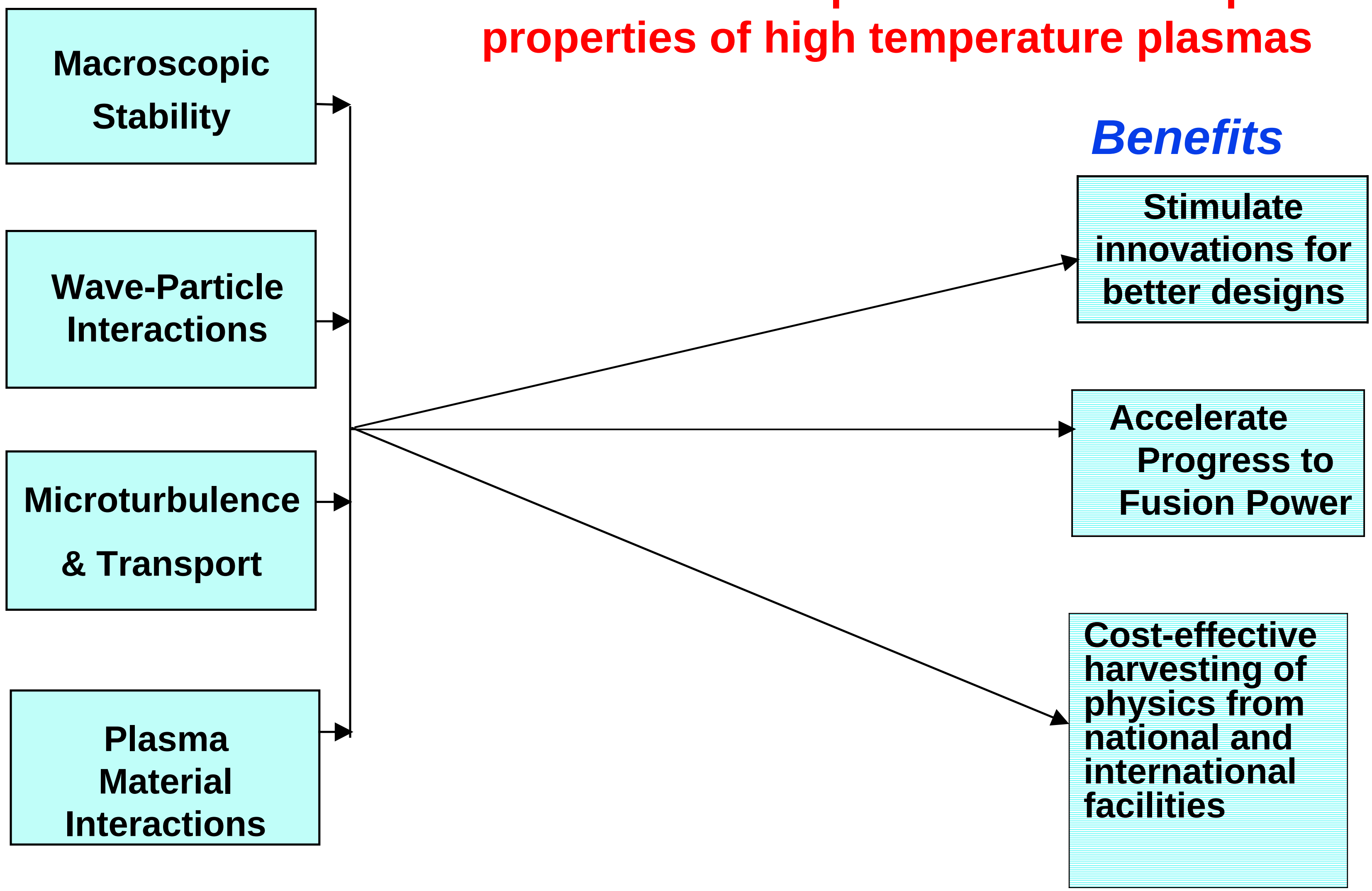
Comparisons:** *global trends; local dependences; detailed structure (spectra, correlation functions, …)

Use the New Tool for Scientific Discovery

(<u>Repeat cycle as new phenomena encountered</u>)

Science Areas *

GOAL: Reliable predictions of complex properties of high temperature plasmas



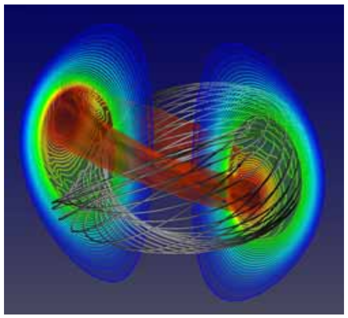
******All with strong coupling to experiments***

PPPL has helped establish stature/visibility of Plasma Science in Advanced Scientific Computing community

- **In response to OFES, PPPL has played a lead role in successfully establishing the *Plasma Science Advanced Computing Institute (PSACI)***
  - **Coordinates the Plasma Science component of DOE's SciDAC Program**
  - **Peer-reviewed projects include FES Collaboratory, Magnetic Reconnection, Wave Heating, Atomic Physics, Turbulent Transport, and MHD Simulations**
    - **Strong collaborative connections with CSET community**
    - **FES portfolio in excellent position for growth**
  - **Program Advisory Committee (with distinguished members from outside & within FES) provides excellent advice/guidance**

Plasma Physics Projects within DOE's (SciDAC) Program

Extended Magnetohydrodynamics

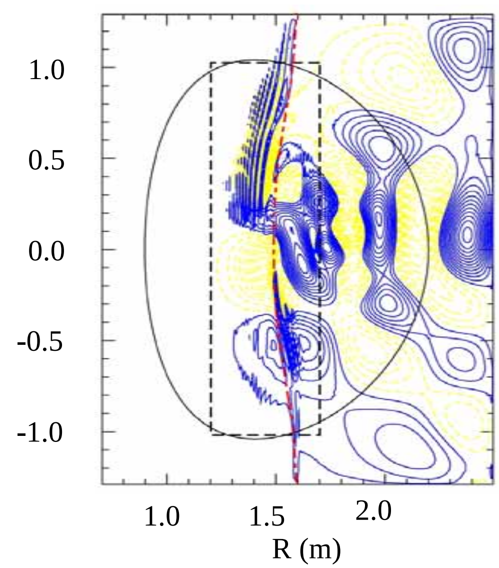


N=1 Plasma Instability

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

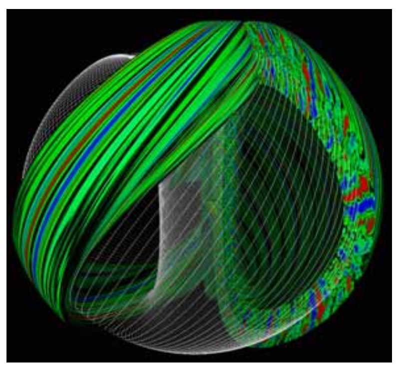
Wave-Plasma Interactions

ORNL, PPPL, MIT,
Lodestar, CompX



Plasma Microturbulence

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

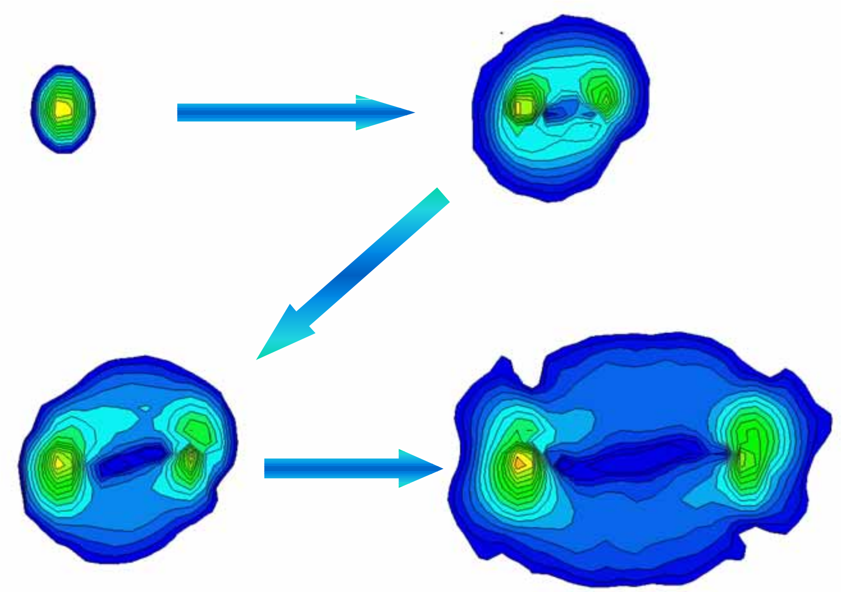


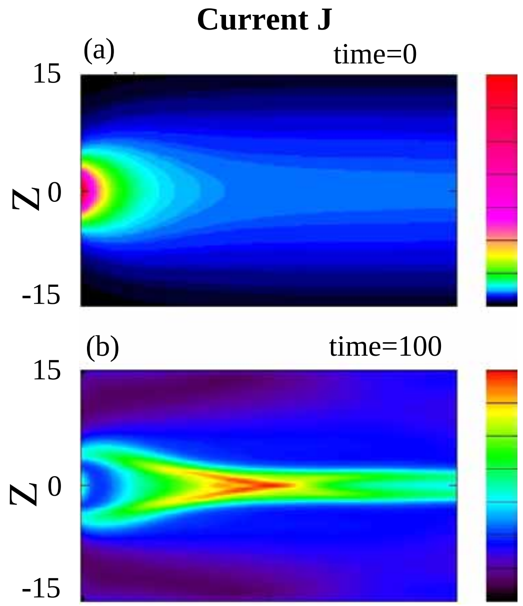
Turbulent Eddies in Plasmas

Plasma Physics Projects within DOE's (SciDAC) Program

Terascale Atomic Physics

Auburn University
Rollins College
Oak Ridge National Laboratory



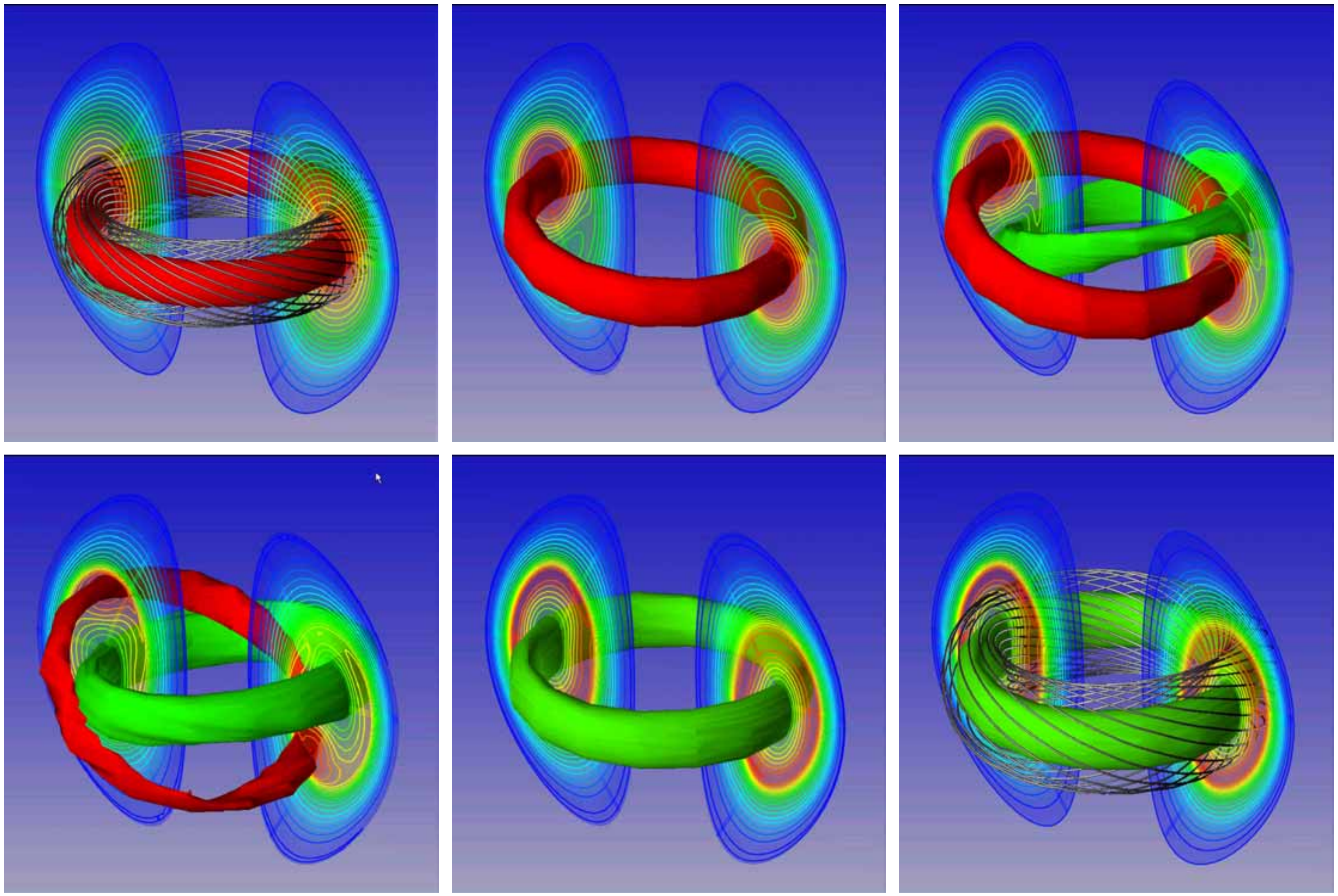


Magnetic Reconnection

University of Iowa
University of Chicago
University of Texas

MHD Simulation of Internal Reconnection Event

Hot Inner Region Interchanges with Colder Outer Region via Magnetic Reconnection



M3D simulation of NSTX

W. Park et al.

Visualization

S. Klasky et al.

PPPL
PRINCETON PLASMA
PHYSICS LABORATORY

UNDERSTANDING TURBULENT PLASMA TRANSPORT

An important problem:

⇐ **-- Size of plasma ignition experiment determined by fusion self-heating versus turbulent transport losses**

⇐ **-- Dynamics also of interest to other fields (e.g., astrophysical accretion disks)**

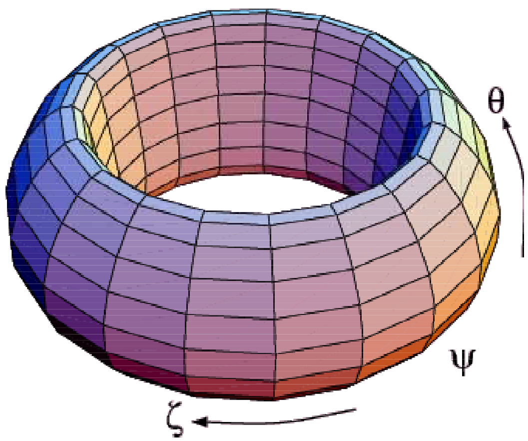
⇐ **A scientific *Grand Challenge* problem**

⇐

⇐ **A true terascale computational problem**

PROBLEM DESCRIPTION: Particle-in-cell Simulation of Plasma Turbulence

- **Key Issue**: confinement of high temperature plasmas by magnetic fields in 3D geometry



- Pressure gradients drives instabilities producing loss of confinement due to **turbulent transport**

- Plasma turbulence is ***nonlinear, chaotic, 5-D problem***

- **Particle-in-cell simulation**

→distribution function - integrate along characteristics with particles advanced in parallel

→interaction - self-consistent EM fields

The Physics Model

Magnetic Coordinates:

$\boldsymbol{B=\nabla\alpha\times\nabla\psi}$

Perturbed 5-D Distribution Function:

$\boldsymbol{h_s=h_s(\psi,\alpha,\theta,\varepsilon,\mu)}$

Gyrokinetic equation:

$$\left(\frac{d}{dt}+v_{\|}\hat{\mathbf{b}}\cdot\nabla+i\omega_d\right)h=i\omega_*^T\Phi-q\frac{\partial F_0}{\partial\varepsilon}\frac{\partial\Phi}{\partial t}$$

where:

$$\Phi=J_0\left(\tfrac{k_\perp v_\perp}{\Omega}\right)\left(\phi-\frac{v_{\|}}{c}A_{\|}\right)+\frac{J_1\left(\frac{k_\perp v_\perp}{\Omega}\right)}{\frac{k_\perp v_\perp}{\Omega}}\frac{mv_\perp^2}{q}\frac{\delta B_{\|}}{B}$$

Reduced Maxwell's Equations:

Electrostatic potential:

$$\nabla_\perp^2\phi=4\pi\sum_s q\int d^2v\left[q\phi\frac{\partial F_0}{\partial\varepsilon}+J_0\left(\tfrac{k_\perp v_\perp}{\Omega}\right)h\right]$$

$\boldsymbol{\delta B_\perp}$:

$$\nabla_\perp^2 A_{\|}=-\frac{4\pi}{c}\sum_s\int d^2v\ \ qv_{\|}J_0\left(\tfrac{k_\perp v_\perp}{\Omega}\right)h$$

$\boldsymbol{\delta B_{\|}}$:

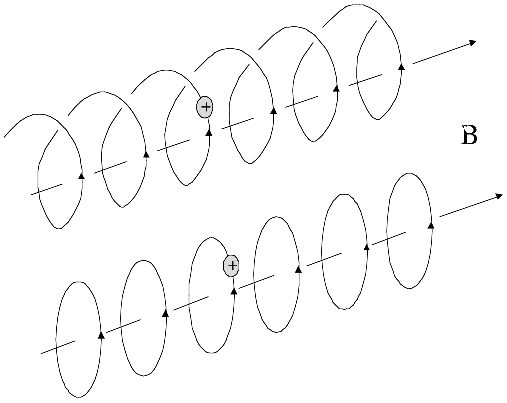
$$\frac{\delta B_{\|}}{B}=-\frac{4\pi}{B^2}\sum_s\int d^2v\ \ mv_\perp^2\frac{J_1\left(\frac{k_\perp v_\perp}{\Omega}\right)}{\frac{k_\perp v_\perp}{\Omega}}h$$

Gyrokinetic Particle Simulation

- **[*W. Lee, PF ('83); JCP ('87*)]**

- **Gyrophase-averaged Vlasov-Maxwell equations for low frequency microinstabilities**.

- **Spiral motion of a charged particle is modified as a rotating charged ring subject to guiding center electric and magnetic drift motion as well as parallel acceleration -- *speeds up computations* by 3 to 6 orders of magnitude in time steps and 2 to 3 orders in spatial resolution**



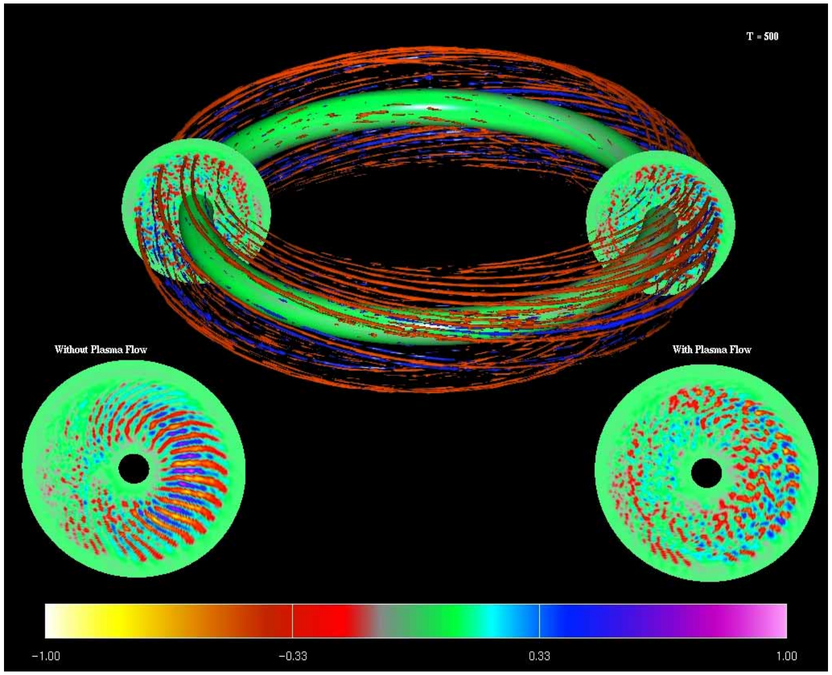
3-D TURBULENCE SIMULATIONS ON POWERFUL NEW MPP COMPUTERS

- **Advanced simulations utilize full power of modern MPP's**

- **Reduction of turbulence needed to keep fusion plasmas well confined**

- **<u>SCIENCE</u> Vol. 281, 1835 (1998)** {***Presidential Early Career Award to*** **Z. Lin (Nov. 2000)**}

- **Large volume and high-dimensionality of data requires data management and advanced visualization**



3D Particle Simulation of Plasma Turbulence: Massively Parallel Computation

Turbulent Transport Reduction by Zonal Flows

Princeton Plasma Physics Laboratory
Princeton University

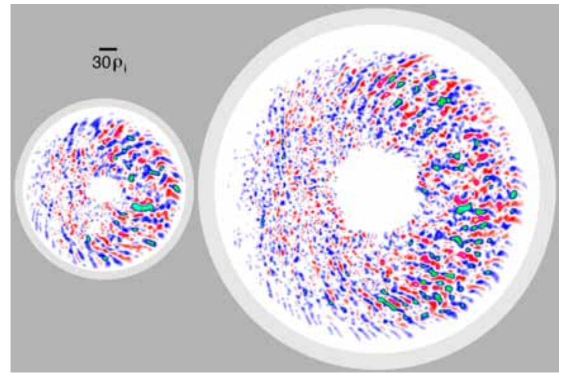
PPPL
PRINCETON PLASMA PHYSICS LABORATORY

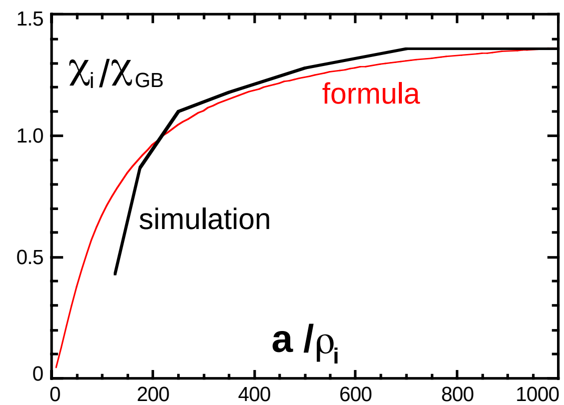
Simulation of Turbulence in an Ignition-Scale Tokamak

- **Recent Microturbulence (ITG) Simulations for**
  - **a/ρ_i = 125 (small lab tokamak) through**
  - **a/ρ_i = 1000 (ignition tokamak)**
- **Size-scaling of transport**
  - **Bohm-like at small a/ρ_i**
  - **Transitions to gyroBohm at large a/ρ_I**
- **Enabled by access to 5TF IBM-SP @ NERSC**
- **1 billion particles, 125M spatial grid points; 7000 time steps**
- **Large-scale simulations indicate transition scaling as:**

$$\chi_i \approx \chi_{gyroBohm}/(1+50\ \rho_i/a)^2$$

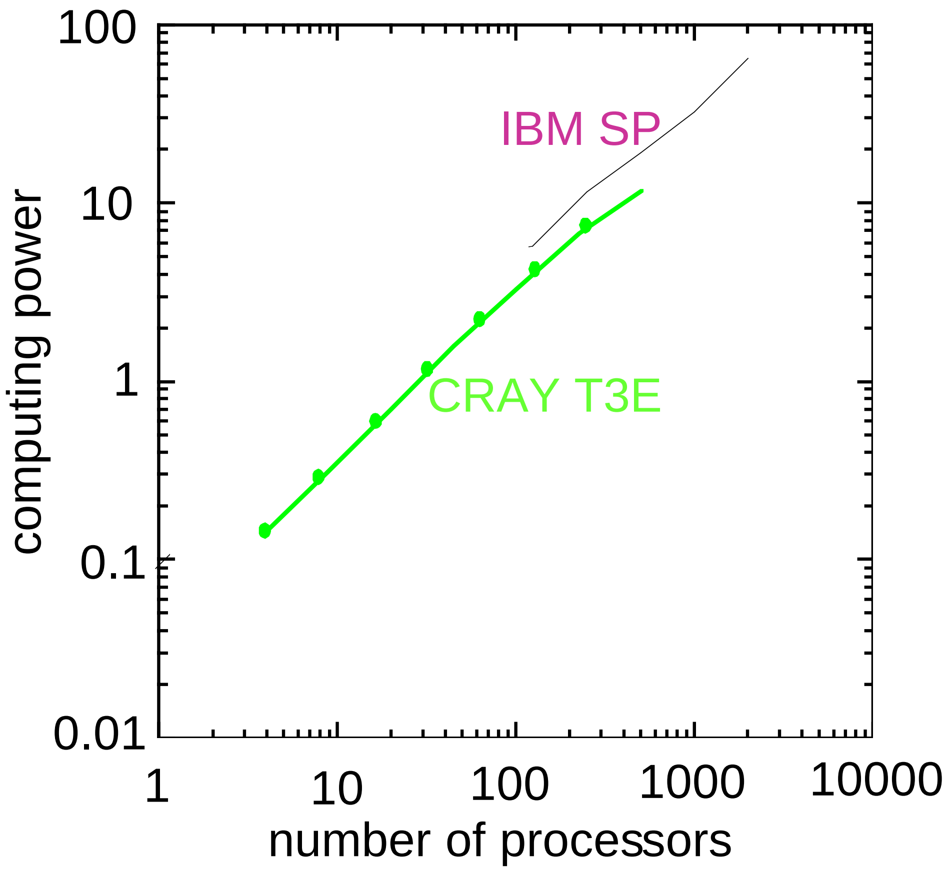
motivates new theoretical studies





3D Gyrokinetic Toroidal Code (GTC)

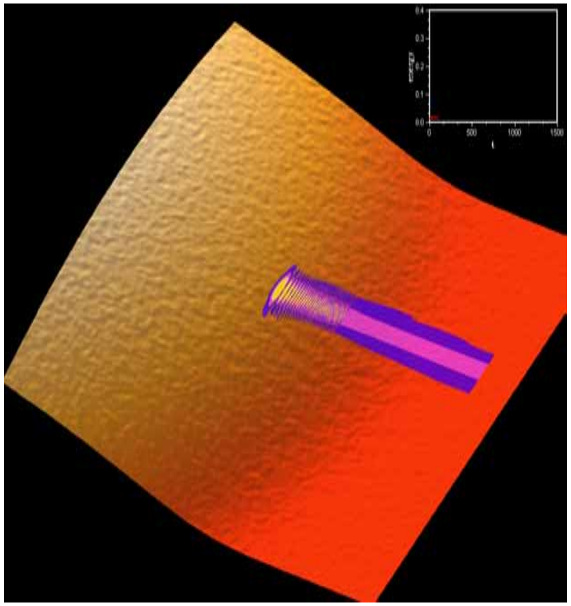
Scalable on Massively Parallel Computers



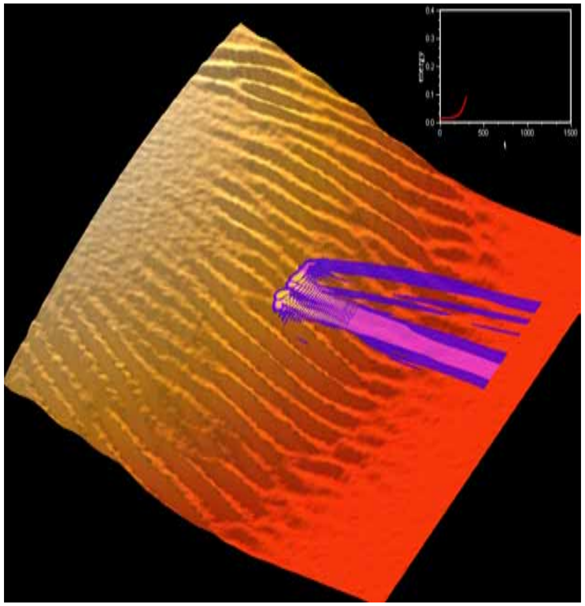
Y-axis: number of particles (in millions) which move one step in one second

New Cross-Disciplinary Opportunities for Diagnosing and Understanding Turbulence

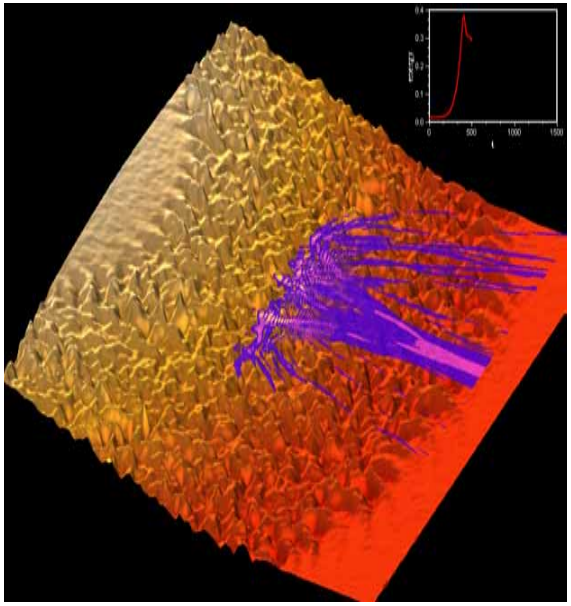
Break-up and scattering of microwaves from plasma turbulence



Target plasma



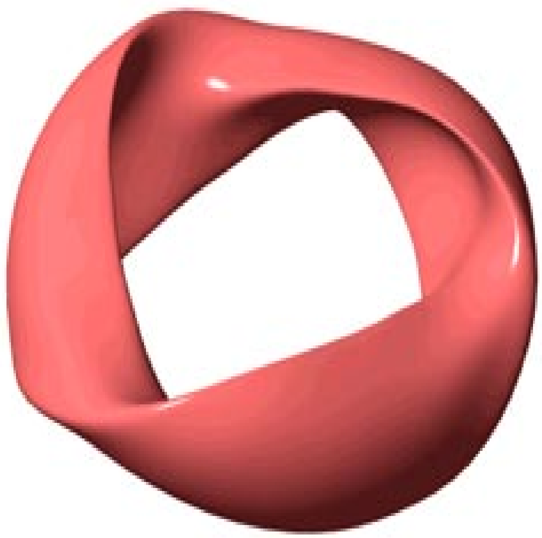
Growth of Radial structures

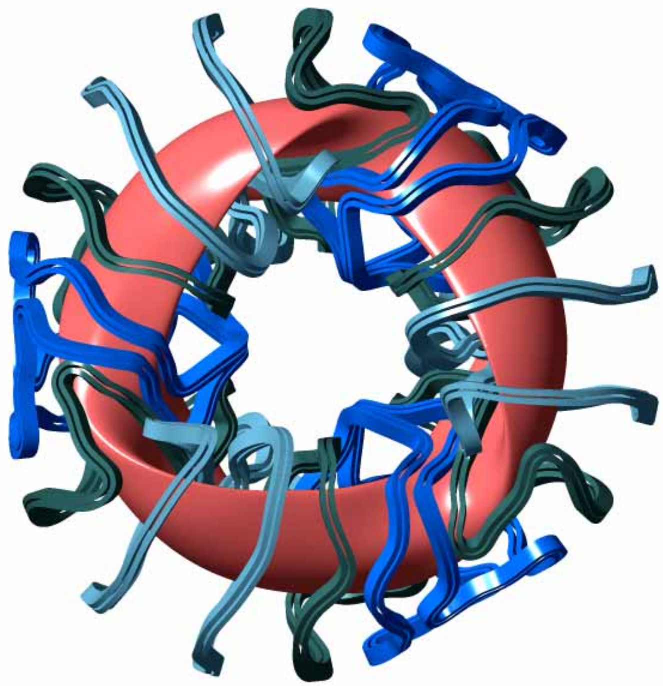


Zonal flows and decorrelation

Z. Lin, GTC Simulation
G.J. Kramer, E. Valeo, R. Nazikian, Full Wave Simulation of μ-wave Reflection
S. Klasky, I. Zatz, Visualization

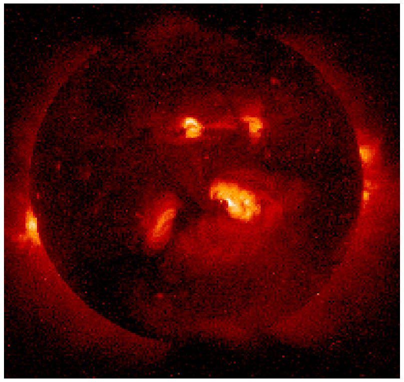
STELLARATOR DESIGN





- **Optimization of Stability, Transport, and Constructability for Designing National Compact Stellarator Experiment (NCSX)**
- **Utilization of MPP Computations Essential for Optimizations**

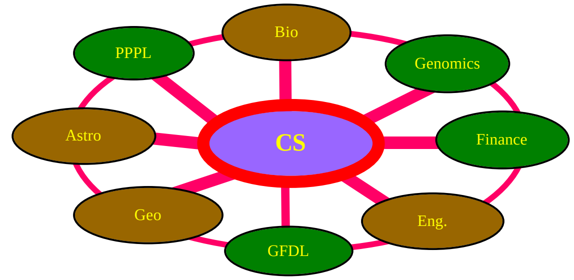
Relation to other scientific disciplines



- ***Space Physics***
  – reconnection in Earth's magnetosphere, solar corona, astrophysical plasmas
  – dynamos, collective phenomena, …….
- ***High Energy Physics***
  – Collective dynamics impacting advanced accelerator design
- ***Industrial Applications***
  – Plasma Processing, Xerography, Flat Panel Display, ….
- ***Computational Physics -- issues common to many areas***
  – advances in solving partial differential equations in complex geometry,
  – adaptive mesh refinement in 3D,
  – parallel methods for inverting sparse matrices
  – etc.

Driving Applications

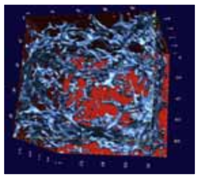
Princeton University's PICASso Program



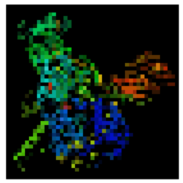
Program in Integrative Computer and Application Sciences

Science/Engineering

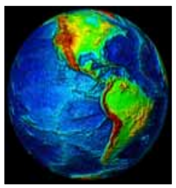
Astrophysics



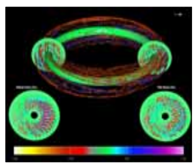
Biology, Genomics



Geosciences



Plasma Physics



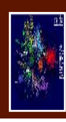
The Computational Pipeline

Models	Methods	Software	Scalable Systems	Networks and Distributed Systems	Data Management	Visualization

Integrative Research and Training in Entire Computational Pipeline

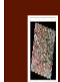
Scalable Services

Internet Services



Mobile Services

Information Archives



PPPL is developing important new Plasma Science Advanced Computing Projects

- **PPPL has recently been awarded the *<u>Pilot Topical Computing Facility for Fusion Energy Sciences</u>***
  - **Will explore *optimal architecture for FES computational applications***
    - **includes dedicated clusters, grid computing, benchmarking on ESC node (SX-6 @ Chippewa Falls via NERSC collaboration and @ Alaska via ORNL collaboration), and benchmarking on IBM Blue Gene L and C via collaboration with IBM and CalTech**
  - **Strong *partnership with community* (FES SciDAC PI's) and with *Princeton University* (matching funds and active participation of Princeton Institute for Computational Science and Engineering (PICSciE)**

- **PPPL is actively exploring a *Joint Computing Partnership* with NOAA's Geophysical Fluid Dynamics Laboratory and Princeton University**

CONCLUSIONS

- **PPPL Theory/Advanced Scientific Program combines:**
  - long-standing ***commitment to academic and educational*** excellence
  - ***accountable progress*** on many of most important, scientifically challenging problems facing FES research
  - ***strong partnerships*** with universities, laboratories, & industry

- **PPPL Theory/Advanced Scientific Computing Program is key National/International Resource:**
  - highly desired for many ***external collaborations***
  - critical to ***cost-effective innovation*** in fusion research
  - enables ***optimal leveraging*** of major national/international investments in experimental facilities
  - attracts ***bright young people essential for the future***

Pilot FES Topical Computer Facility

(S. Davis and E. Valeo)

Location	PPPL Project	Pilot FES TCF DOE/LPDA	Pilot FES TCF PU/GFDL
FCC	76 Dual AMD 2000+	64 Dual AMD 2000+/Myrinet??	
PPLCC	35 Dual Mainly Intel		**18 Dual AMD 2100+ w/Gigabit**
VisLab			**1 graphics node**
PU		**Grid Computing Experiments**	**10 Dual AMD 2100+ w/Gigabit**
GFDL			**10 Dual AMD 2100+ w/Gigabit**

Pilot FES TCF Attributes

- **Integration** (into PPPL UNIX Cluster)
  - Firewall protected
  - Common Authentication
  - AFS shared application software
  - NFS shared home, project, scratch disks
  - Backup to automated tape library
  - 2TByte dedicated project/scratch file server (RAIDZONE)
- **Administration** (quite efficient)
  - Manpower required is insensitive to number of nodes
  - "Golden" system image is replicated to new systems
  - System specific configuration files are automatically generated and distributed from an administrative directory tree (under CVS management)
- **Networking**
  - Gbit for PU/GFDL Pilot TCF
  - 100 Mb (+ Myrinet?) for DOE Pilot TCF nodes, Gbit uplink
  - Private network (172.16.1.X) with mapping to public address at PPPL router

Pilot FES TCF Status (08/29/02)

- 18 AMD rack-mounted dual-CPU units up and running for 1 month
- TCF room refurbishing essentially complete
  - Removal of CICADA remnants, including under floor cables
  - New floor, cable trays
  - Reconditioning of AC
- Much has already arrived: console concentrators, network switches, racks, …
- 120 AMD units due to arrive by 09/01
- Systems should be operational/available for use by Sept. 15 (pending PDU hardware arrival)