Scientific Discovery through Advanced Computing in Plasma Science

PICASso
(Program in Integrative Information, Computer and Application Sciences)

Successes of Computational Science Seminar

September 27, 2004

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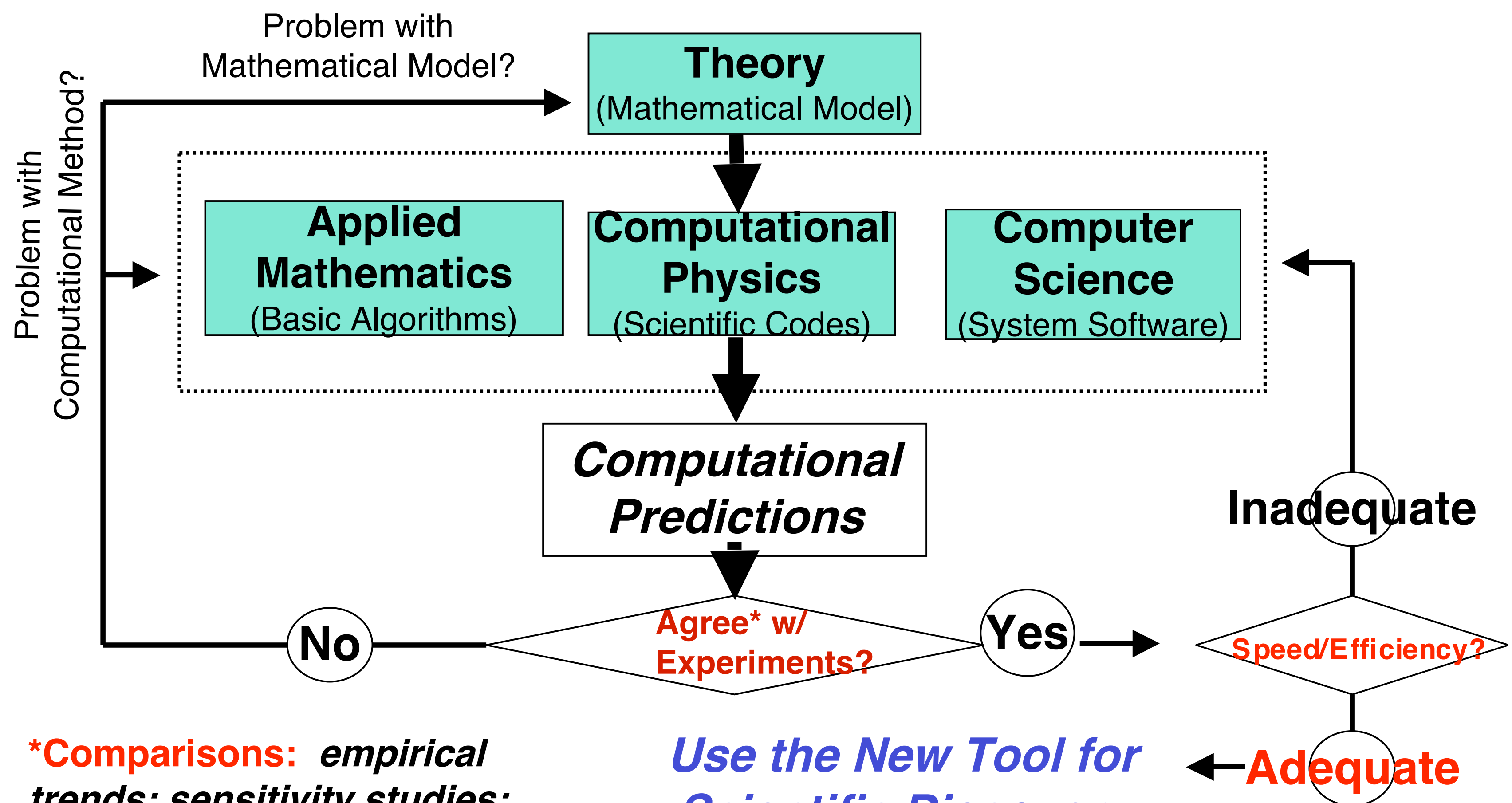
Princeton University

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 reliable predictions of complex properties of high temperature plasmas**
  - **Acquisition of *scientific understanding* needed for predictive models *superior to empirical scaling***

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



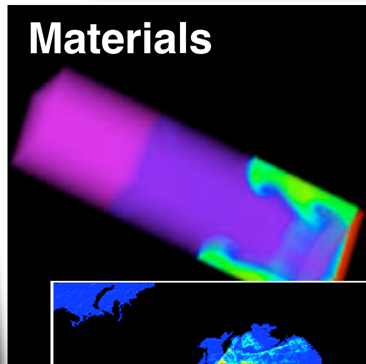
Use the New Tool for Scientific Discovery

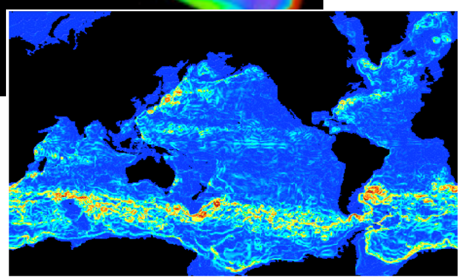
(<u>Repeat cycle as new phenomena encountered</u>)

Comparisons:** *empirical trends; sensitivity studies; detailed structure (spectra, correlation functions, …)

Advanced Computing

is Critical to Discovery in Many Scientific Disciplines

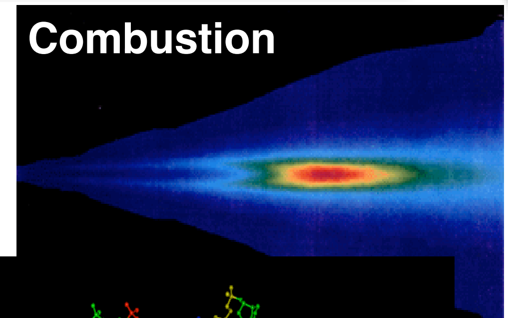


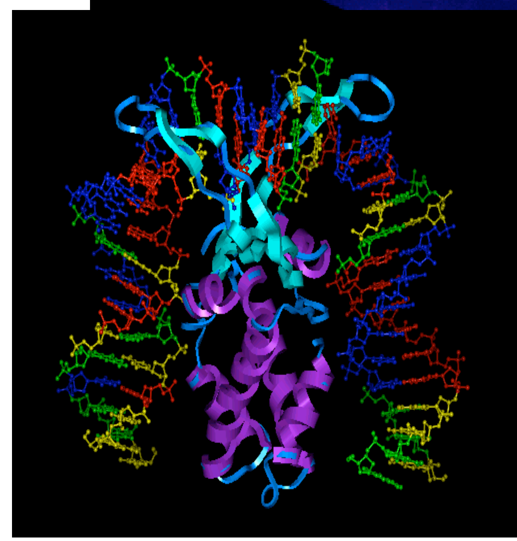


Global Systems

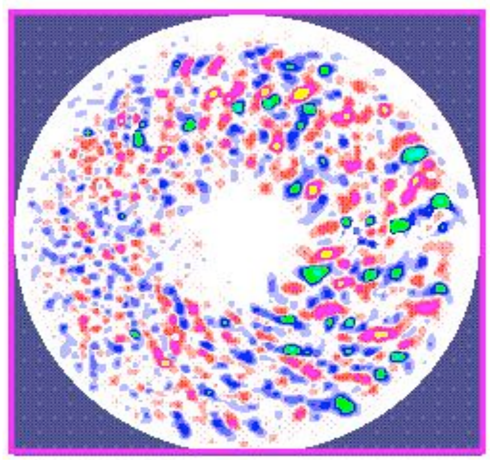
Dramatic Advances in Simulation Capabilities

NEEDED TO ACCELERATE PROGRESS IN PLASMA SCIENCE

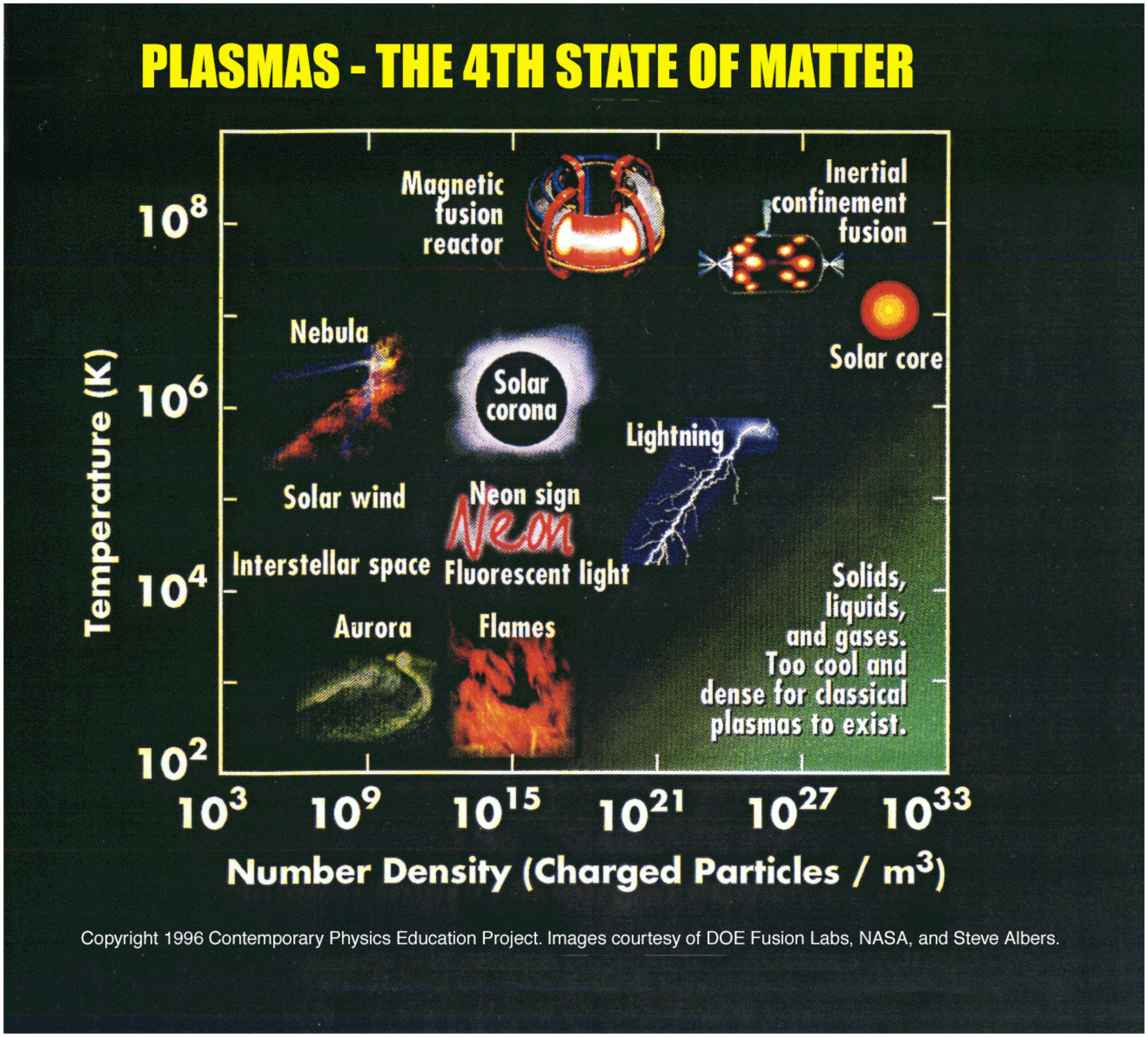




Health Effects, Bioremediation



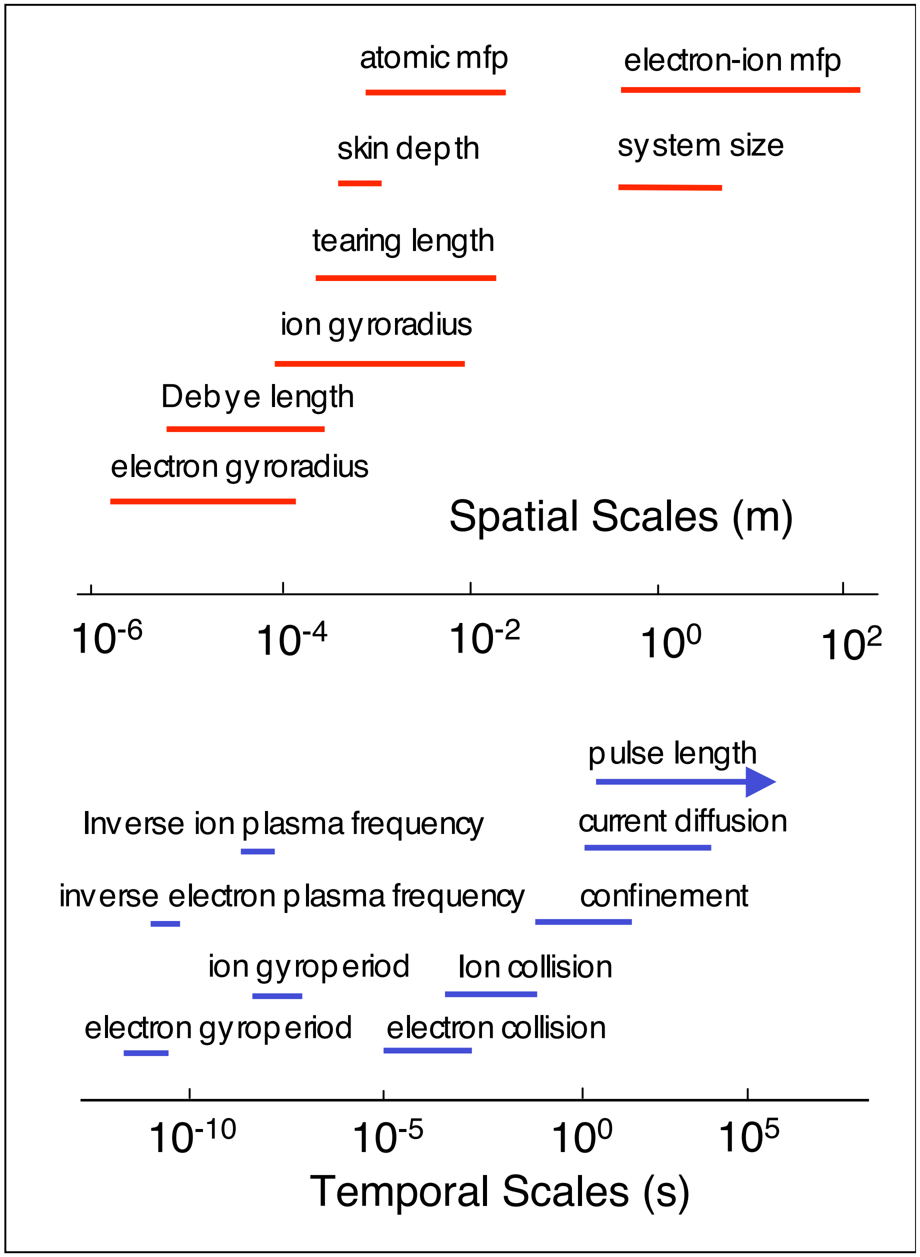
Fusion Energy


PLASMAS - THE 4TH STATE OF MATTER
Magnetic fusion reactor
Inertial confinement fusion
Nebula
Solar corona
Solar core
Lightning
Solar wind
Neon sign
Neon
Interstellar space
Fluorescent light
Solids, liquids, and gases. Too cool and dense for classical plasmas to exist.
Aurora
Flames
Temperature (K)
10^8
10^6
10^4
10^2
10^3
10^9
10^15
10^21
10^27
10^33
Number Density (Charged Particles / m^3)
Copyright 1996 Contemporary Physics Education Project. Images courtesy of DOE Fusion Labs, NASA, and Steve Albers.

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**



Plasma Physics Challenges

NRC Plasma Science Committee

Macroscopic Stability

Fusion: What limits the pressure in plasmas?

Space Physics: Geomagnetic substorms

Wave-particle Interactions

Fusion: How do hot particles and plasma waves interact in the nonlinear regime?

Solar Physics: Solar coronal heating

Microturbulence & Transport

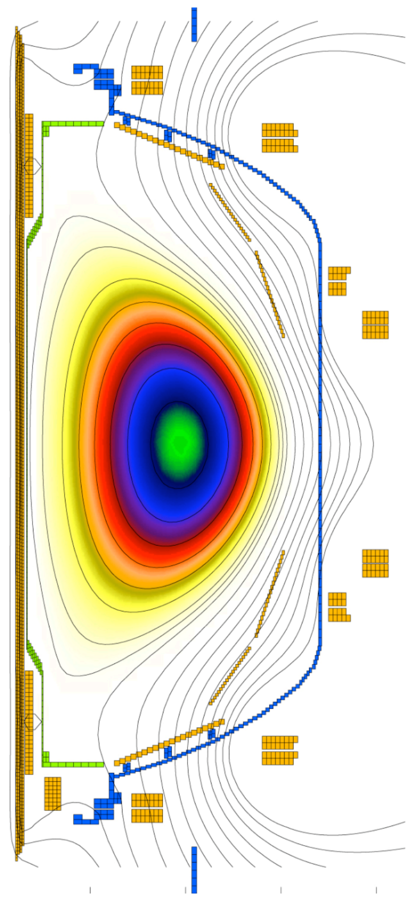
Fusion: What causes plasma transport?

Astrophysics: Accretion disks (black holes)

Plasma-material Interactions

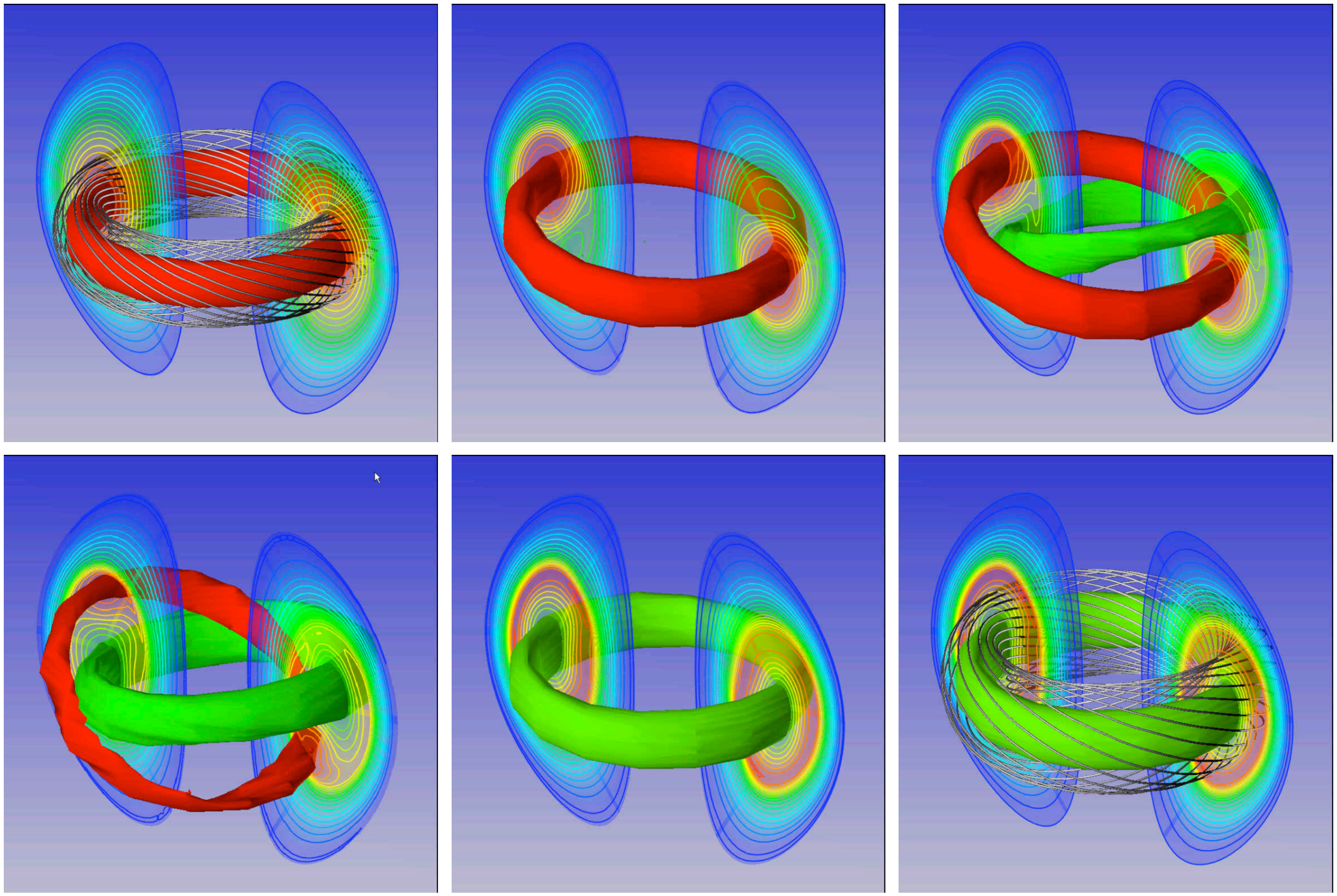
Fusion: How can high-temperature plasma and material surfaces co-exist?

Material Science: Materials processing



MHD Simulation of Internal Reconnection Event

Hot Inner Region Interchanges with Colder Outer Region via Magnetic Reconnection



M3D Simulation by:

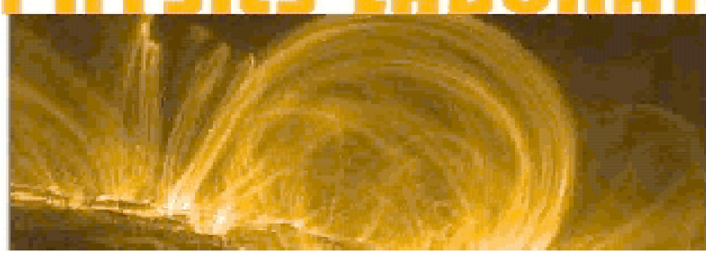
W. Park et. al

Visualization by:

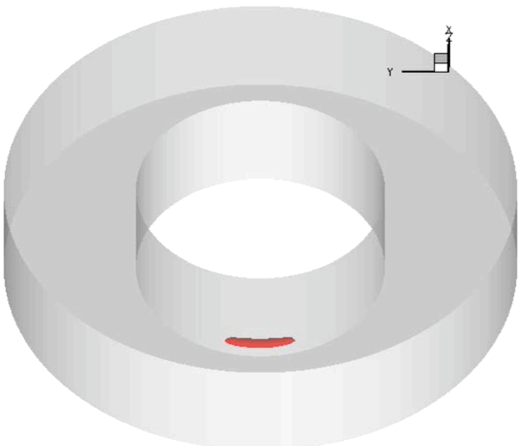
S. Klasky & W. Park

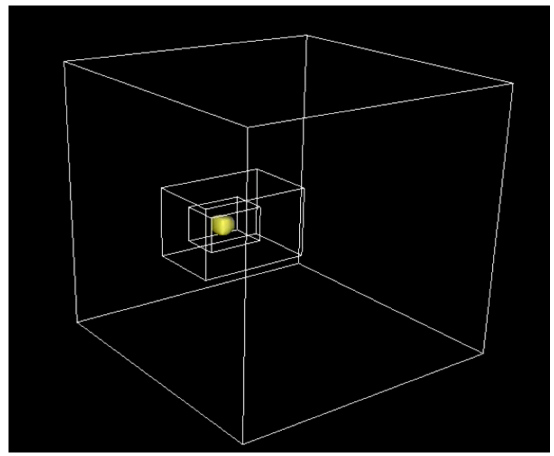
PPPL

PRINCETON PLASMA PHYSICS LABORATORY



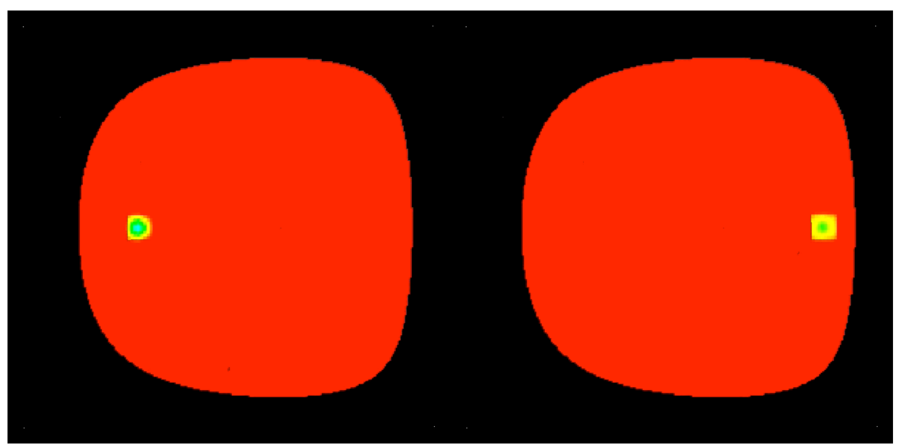
Fusion Codes Take Advantage of Latest Computational Advances





Adaptive Mesh Refinement

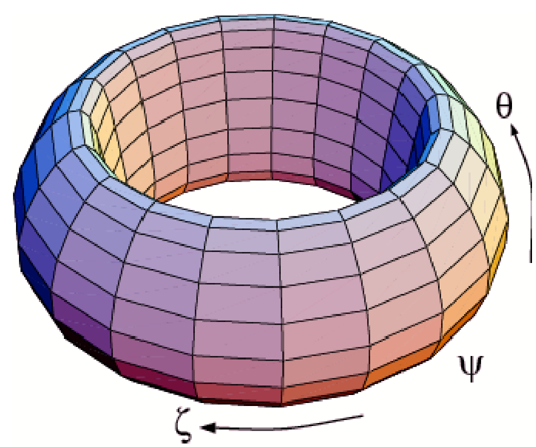
Inside Pellet Launch →



← **Outside Pellet Launch**

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

Particle Simulation of the Boltzmann-Maxwell System

- The Boltzmann equation (Nonlinear PDE in Lagrangian coordinates):

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \mathbf{v} \cdot \frac{\partial F}{\partial \mathbf{x}} + \left(\mathbf{E} + \frac{1}{c} \mathbf{v} \times \mathbf{B} \right) \cdot \frac{\partial F}{\partial \mathbf{v}} = C(F).$$

- "Particle Pushing" (Linear ODE's)

$$\frac{d\mathbf{x}_j}{dt} = \mathbf{v}_j, \qquad \frac{d\mathbf{v}_j}{dt} = \frac{q}{m} \left(\mathbf{E} + \frac{1}{c} \mathbf{v}_j \times \mathbf{B} \right)_{\mathbf{x}_j}.$$

- Klimontovich-Dupree representation,

$$F = \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_j)\delta(\mathbf{v} - \mathbf{v}_j),$$

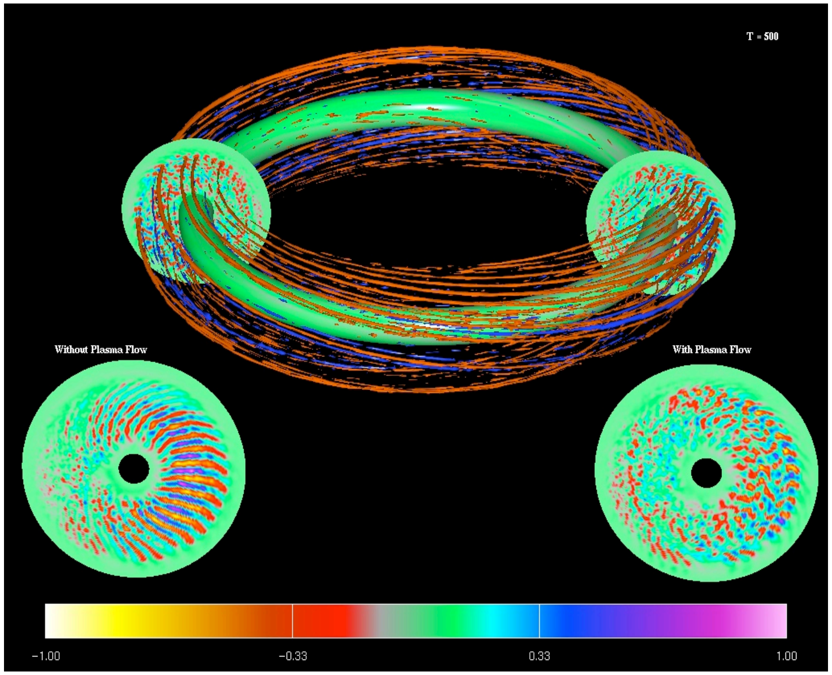
- Poisson's Equation: (Linear PDE in Eulerian coordinates (lab frame)

$$\nabla^2 \phi = -4\pi \sum_{\alpha} q_\alpha \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_{\alpha j})$$

- Ampere's Law and Faraday's Law [Linear PDE's in Eulerian coordinates (lab frame)]

3-D TURBULENCE SIMULATIONS ON POWERFUL NEW MPP COMPUTERS

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

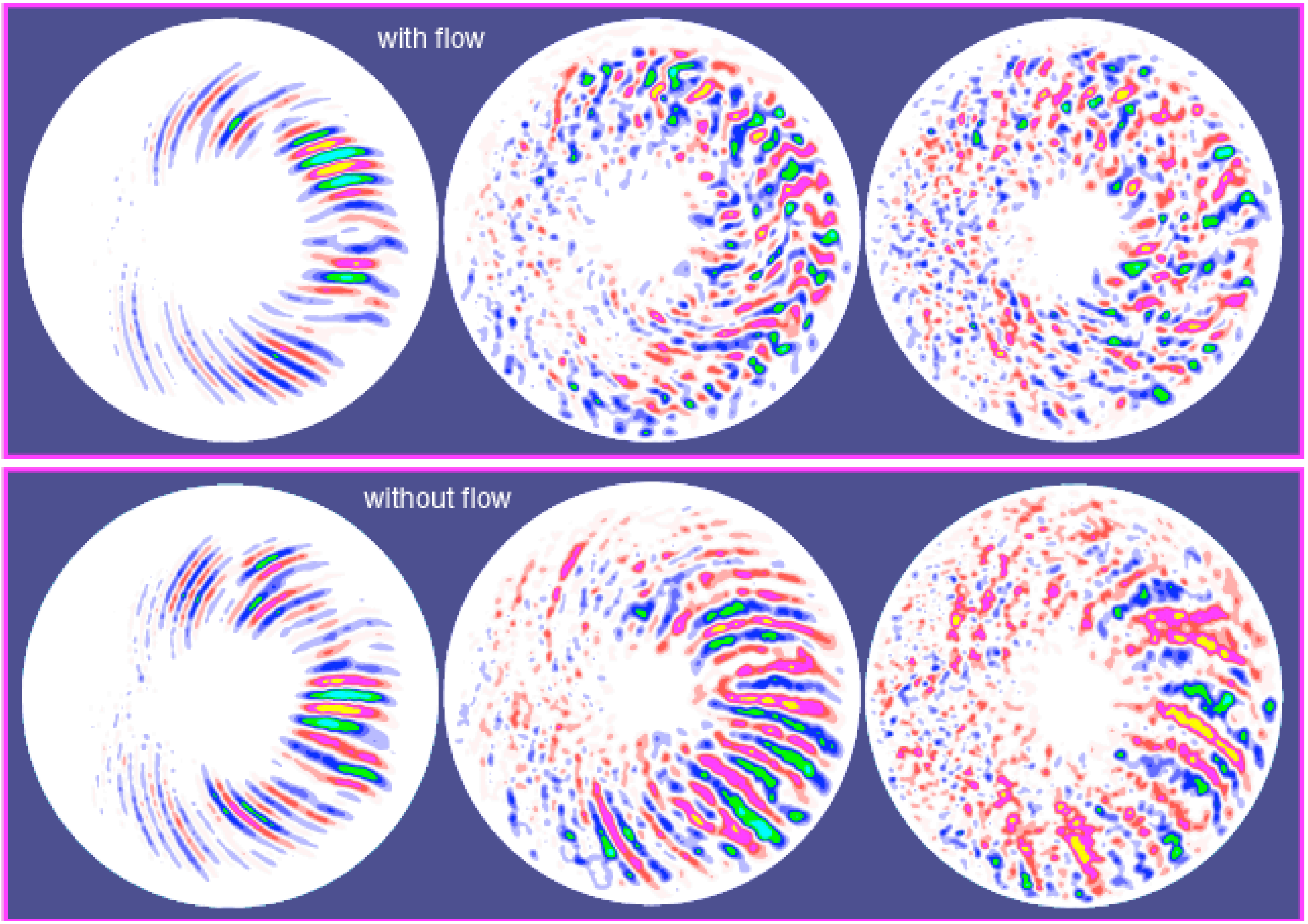


- **Advanced simulations utilize full power of modern MPP's**

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

- **Highly-dimensional data requires advanced visualization: PU/PPPL Display Wall collaboration**

Turbulence Decorrelation by Self-generated E x B Flow in Gyrokinetic Simulation



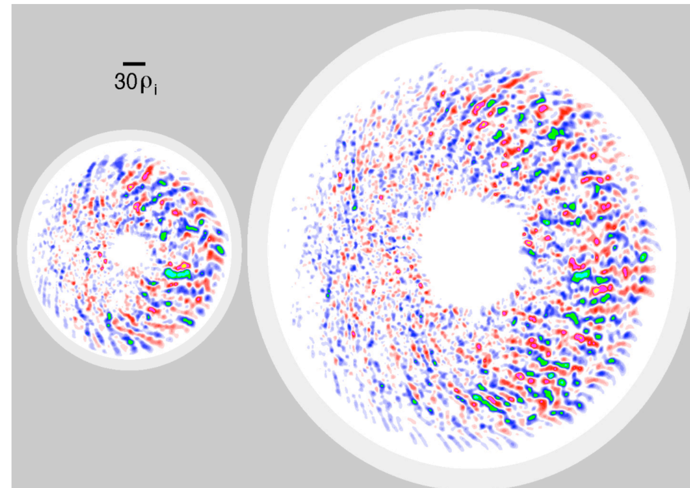
3D Particle Simulation of Plasma Turbulence: Massively Parallel Computation

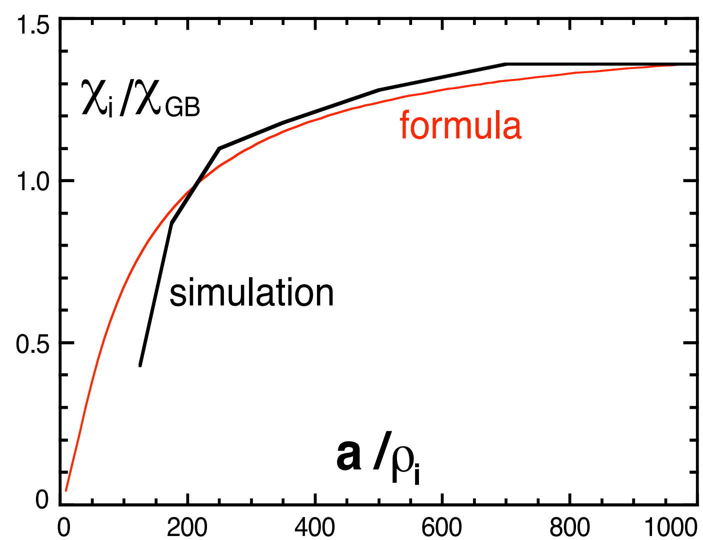
Turbulent Transport Reduction by Zonal Flows

Princeton Plasma Physics Laboratory
Princeton University

Simulation of Turbulence in future Ignition-Scale Experiments
Require State-of-the-Art Computers

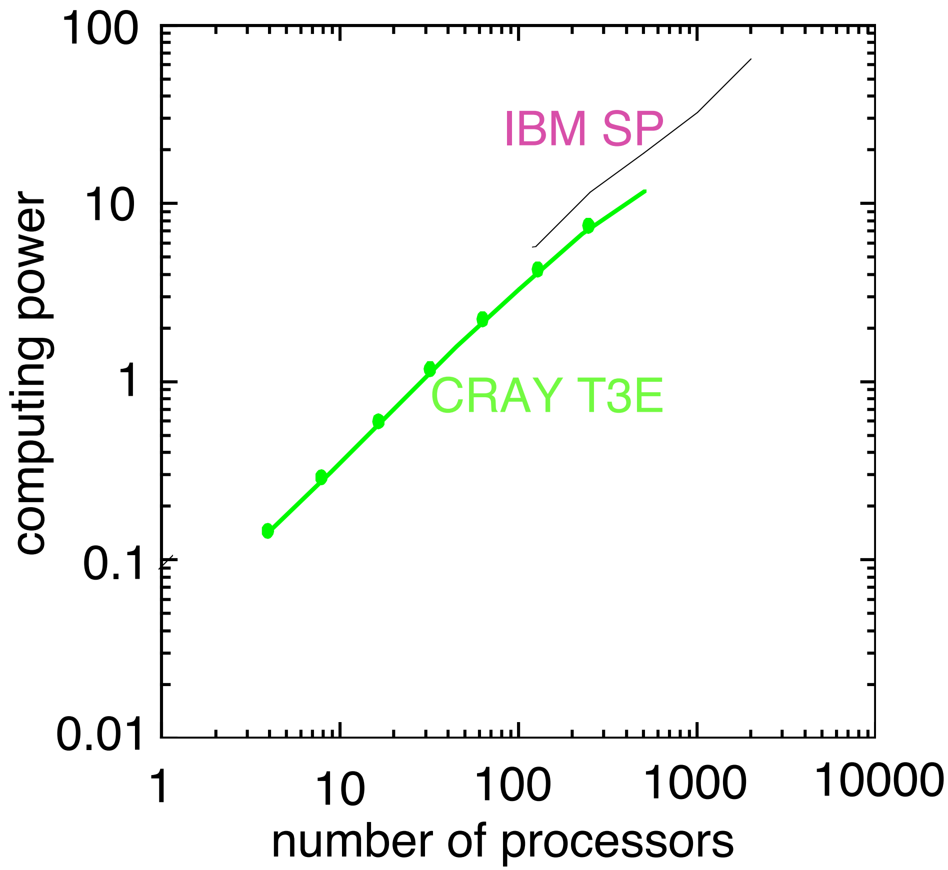
- **Recent Microturbulence Simulations for range including:**
  - **a/ρ_i = 400 (largest present lab experiment) through**
  - **a/ρ_i = 1000 (ignition experiment)**
- **Enabled by access to powerful supercomputers (e.g., 5TF IBM-SP @ NERSC)**
- ***PIC simulations: 1 billion particles, 125M spatial grid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



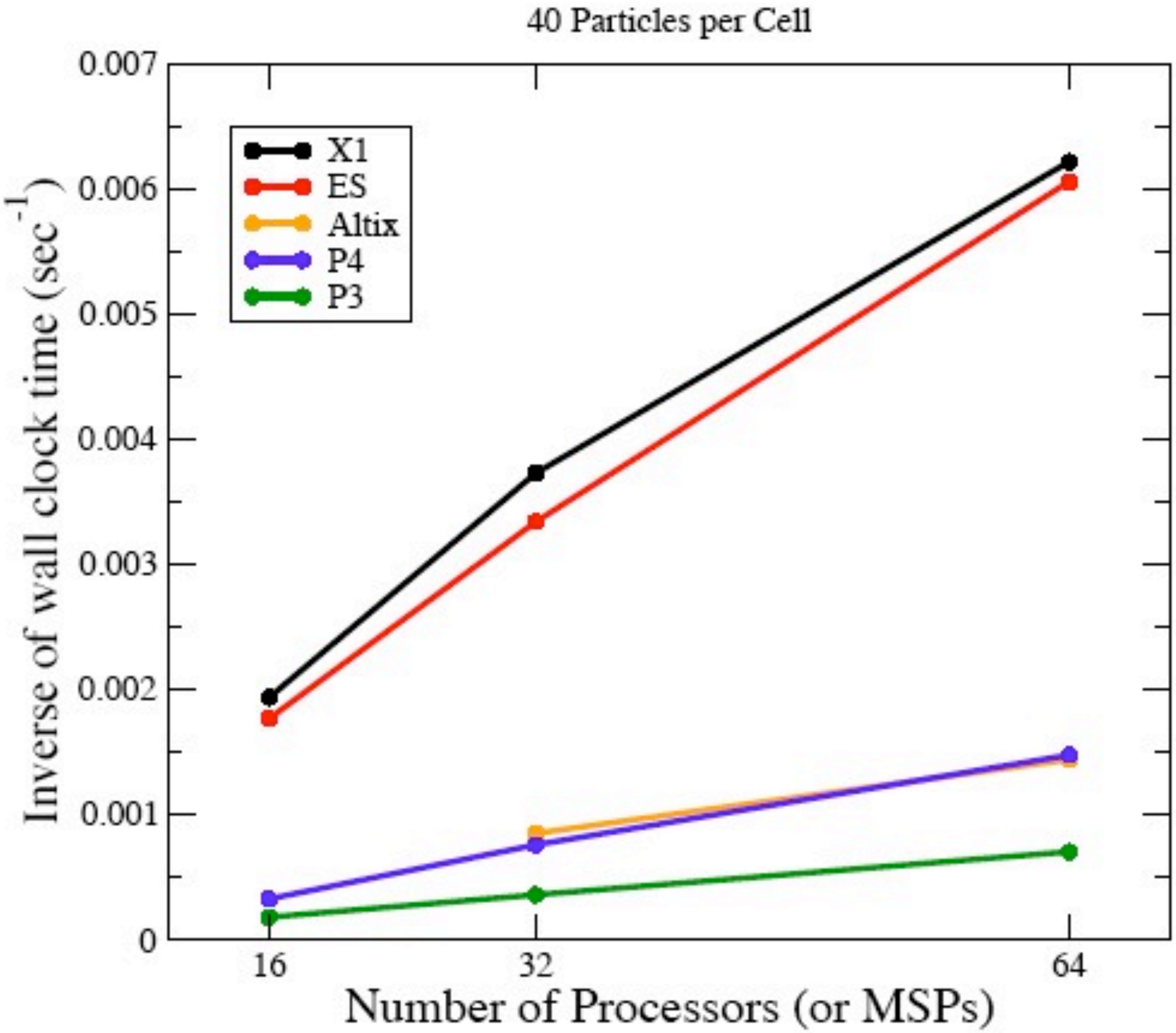


3D Particle-in-Cell Simulations

Scalable on Massively Parallel Computers



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

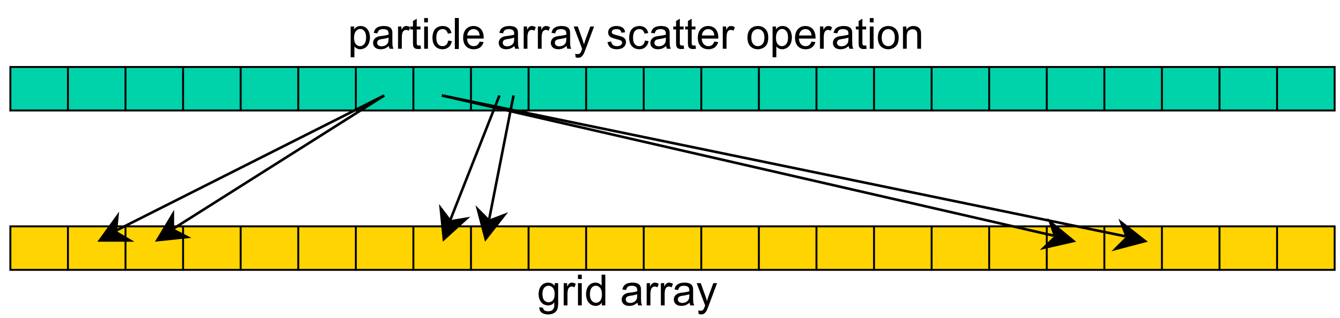

40 Particles per Cell
Inverse of wall clock time (sec^{-1})
Number of Processors (or MSPs)
X1
ES
Altix
P4
P3
0
0.001
0.002
0.003
0.004
0.005
0.006
0.007
16
32
64

Computational Challenges

- ***Fast and Efficient Elliptic (Poisson) Solvers:***
  - Required for both Particle-in-Cell (PIC) kinetic codes and Magneto-hydrodynamics (MHD) fluid codes.
    - PIC applications involve extremely large sparse matrix system (10^8 X 10^8 grid points)
  - Deal with non-Cartesian irregular grid in toroidal geometry.
  - Need efficient pre-conditioner to speed-up the solve (e.g., pre-arranging matrix)
  - Portable parallel solver
- ***Optimization of Parallel Algorithms:***
  - Improve scalability and efficient utilization of increasing numbers of processors
  - Properly distribute particles over simulation domain.
  - Improve load balancing

Computational Challenges

- ***“Gather-Scatter” operation in PIC codes***
  - The particles are randomly distributed in the simulation volume (grid).
  - Particle charge deposition on the grid leads to indirect addressing in memory (see below).
    - need to arrange data to enable “direct-addressing” (at least for some time period)
    - also a problem in computer games
  - Not cache friendly.
  - Need to be tuned differently depending on the architecture.



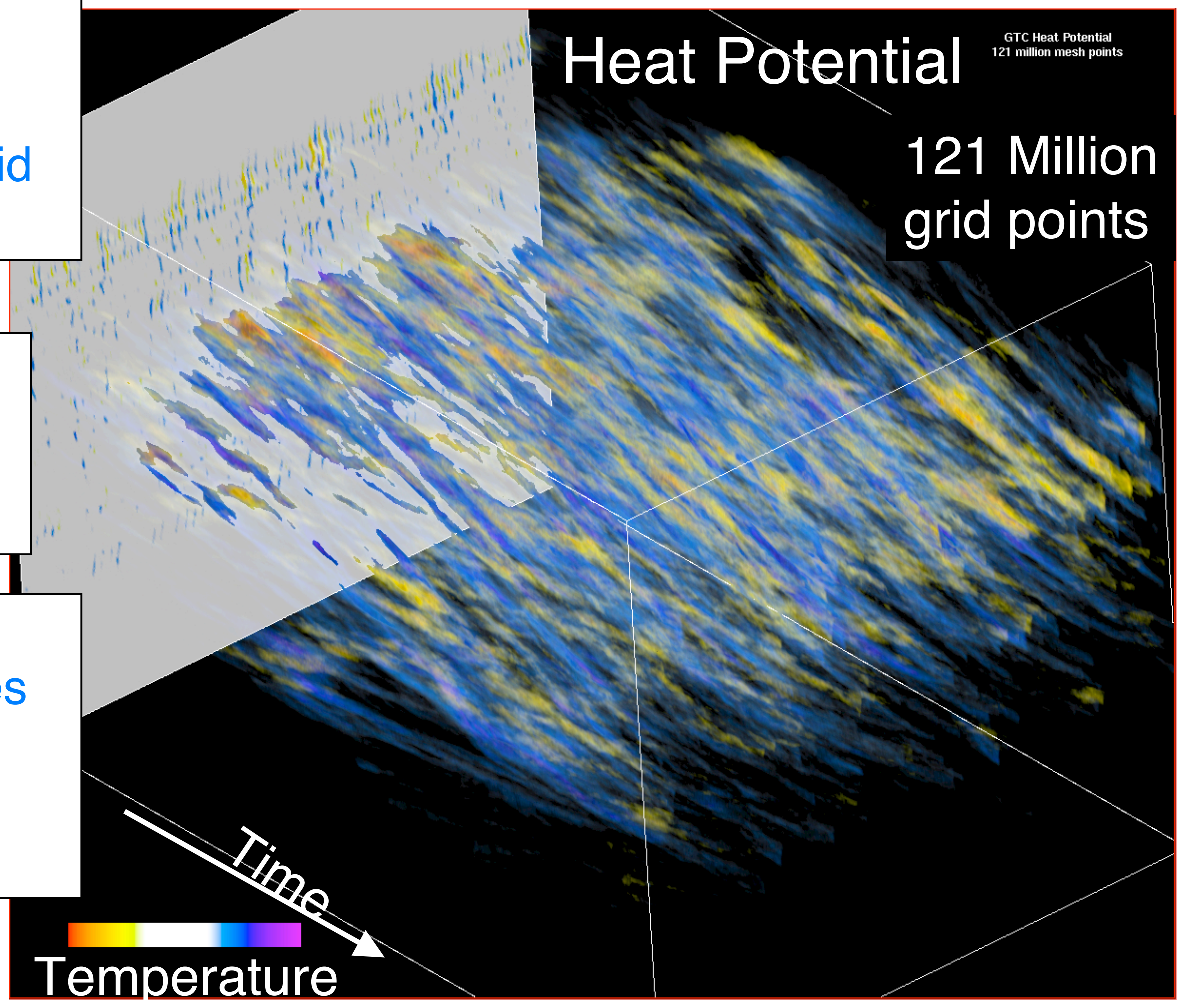
Data Management and Visualization Challenges

Terabytes of data are now generated at remote location (Data Management, Data Grid technologies)

Data must be efficiently analyzed to compute derived quantities

New advanced visualization techniques are needed to help identify key features in the data

Particle in Cell Turbulence Simulation



Data Management & Visualization Challenges

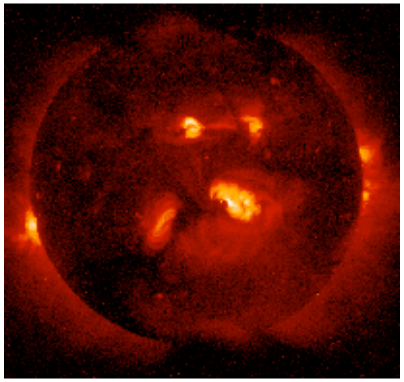
- Data-management challenge in some scientific areas already exceeding compute-power challenge in needed resources
- Automated Workflow Environment:
  - Tera- to Peta-bytes of data to be moved *automatically* from simulations to analysis codes
  - Feature Detection/Tracking to harvest scientific information -- impossible to understand without new data mining techniques
- Parallel I/O Development and Support - define portable, efficient standard with interoperability between parallel and non-parallel I/O
  - Massively parallel I/O systems needed since storage capacity growing faster than bandwidth and access times
- Real-time visualization to enable “steering” of long-running simulations

"Capability & Capacity" Computing in Plasma Science

- ***Pilot Topical Computing Facility for Fusion Energy Sciences*** **(involves PPPL/PU collaboration via PICSciE)**
  - **Explores** ***optimal architecture for FES computational applications***
    - **dedicated clusters & grid computing for "capacity" applications (includes new SGI Altix)**
    - **"capability" applications on "leadership class" computers:** ***Earth Simulator Supercomputer in Japan*** **and the new** ***Cray X1 Supercomputer at ORNL***

- **Positioning for participation in exciting new US interagency (DOE, NSF, DOD, …) initiative for developing interdisciplinary computational research program**
  - **HECRTF's** ***Federal Plan for High End Computing (May 10, '04)*** **("High End Computing Revitalization Task Force" Report to Congress)**
  - **Recognition of common hardware, software, data management & networking challenges**

Relation to other scientific disciplines

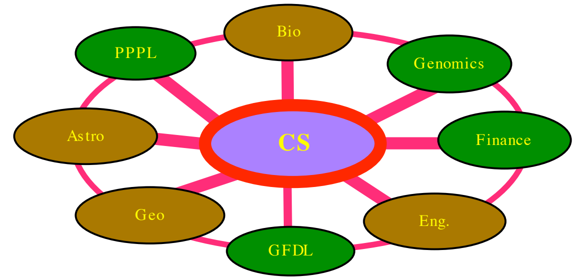


- ***Space Physics***
  - Astrophysics (e.g., Magnetorotational Instabilities as driver for momentum transport in accretion disks)
  - Solar physics (e.g., Sigmoids [from force-free magnetic fields] as precursors to solar eruptions)
  - Magnetospheric Physics (e.g., Kinetic Ballooning Instabilities as driver for substorms)
- ***High Energy Physics***
  - Collective dynamics impacting advanced accelerator design (e.g., electron-proton two-stream instability as driver for excess electron population in proton storage ring experiments)
- ***Computational Physics -- many issues common to many areas***
  - advances in solving partial differential equations in complex geometry,
  - adaptive mesh refinement in 3D
  - multiple other examples

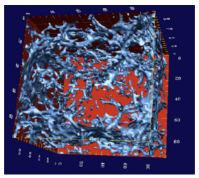
Science/Engineering

Driving Applications

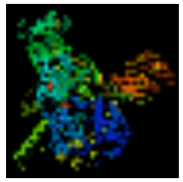
Princeton University's
PICASso Program



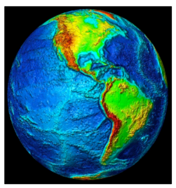
Astrophysics



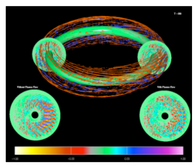
Biology, Genomics



Geosciences



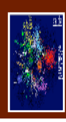
Plasma Physics



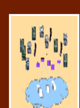
Program in Integrative Computer and Application Sciences

Scalable Services

Internet Services



Mobile Services



Information Archives

The Computational Pipeline

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

Integrative Research and Training in Entire Computational Pipeline

CONCLUSIONS

- **Advanced Computations is a *natural bridge* for fruitful collaborations between Plasma Science and other scientific disciplines (*Computer Science, Applied Math, other Physics Applications areas*).**

- **Advanced Computations is *accelerating progress* toward gaining the physics knowledge needed to harness fusion energy by enabling efficient interpretation of present experiments and planning future devices.**

- **Plasma Science *expects to participate in* the exciting advances in Information Technology and Scientific Computing to address *new scientific challenges.***

- **Computational Plasma Science is helping to attract, educate, & retain *young talent* essential for the future of this field.**