Scientific Discovery through Advanced Computing in Plasma Science

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

*Successes of Computational Science Seminar*

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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

- 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*

- **Theory** (Mathematical Model)
- **Applied Mathematics** (Basic Algorithms)
- **Computational Physics** (Scientific Codes)
- **Computer Science** (System Software)

**Problem with Mathematical Model?**

- **Problem with Computational Method?**

**Computational Predictions**

- **Agree* w/ Experiments?**

**Inadequate**

- **Use the New Tool for Scientific Discovery**
  
  (Repeat cycle as new phenomena encountered)

**Yes**

- **Speed/Efficiency?**

**Adequate**

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*Comparisons: empirical trends; sensitivity studies; detailed structure (spectra, correlation functions, …)
Advanced Computing
is Critical to Discovery in Many Scientific Disciplines

Dramatic Advances in Simulation Capabilities

NEEDED TO ACCELERATE PROGRESS IN PLASMA SCIENCE

- Materials
- Global Systems
- Fusion Energy
- Combustion
- Health Effects, Bioremediation
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*
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)
  \[
  \frac{dx_j}{dt} = v_j, \quad \frac{dv_j}{dt} = \frac{q}{m} \left( \mathbf{E} + \frac{1}{c} \mathbf{v}_j \times \mathbf{B} \right)_{x_j}.
  \]

- 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


• 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:
  - \( a/\rho_i = 400 \) (largest present lab experiment) through
  - \( a/\rho_i = 1000 \) (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
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.

particle array scatter operation

grid array
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

121 Million grid points

Heat Potential

Temperature

Time
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
  - 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
Princeton University’s
PICASso Program

Program in Integrative Computer and Application Sciences

The Computational Pipeline

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.