Characterizing Large-Scale Computational Physics

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Biases

- **Intentional**
  - Large-scale

- **Inevitable**
  - Department of Energy
    - NERSC
    - Advanced Computing Laboratory (LANL)
    - Argonne Leadership Computing Facility
  - Plasma physics
  - USA
Questions

- **Is it physics?**
  - Lattice QCD
  - Plasma simulation
  - Molecular dynamics
  - Electronic Structure
  - Protein folding

- **Is it large-scale?**
  - 20% of leadership-class machine
  - Distributed-memory parallelism
  - Too large/slow for O(100) processor cluster
Sources

- **Journals**
  - Physical Review
  - Journal of Computational Physics
  - IEEE Computer

- **Proceedings**
  - SC, IPDPS
  - Extreme Scale workshops

- **Computer center annual reports**
  - NERSC, ALCF, OLCF, PSC, TACC

- **Reviews/reports**
  - SciDAC Review
  - Computation as a Tool for Discovery in Physics (NSF report, 2002)

- **Books**
  - Petascale Computing: Algorithms and Applications (Bader, 2008)
  - Various “Computational Physics” texts
## Physics Areas

<table>
<thead>
<tr>
<th>Condensed Matter</th>
<th>High Energy</th>
<th>Astrophysics/Relativity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plasma</td>
<td>Atomic/Molecular</td>
<td>Nuclear</td>
</tr>
<tr>
<td>Climate/weather</td>
<td>Turbulence</td>
<td>Geophysics</td>
</tr>
<tr>
<td>...</td>
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<td></td>
</tr>
</tbody>
</table>
Application Types

- Lattice QCD
- Electronic Structure
- Electromagnetics
- Accelerator Beam
- Monte Carlo Transport
- Climate
- Nuclear Structure
- Combustion
- Nuclear Burn
- DDT

- Plasma
  - PIC
  - Kinetic
  - Fluid(s)

- CFD
  - DNS
  - Lattice Gas/Boltzmann
  - LES/RANS
  - SPH

- Cosmology Structure Evolution
- Structural Mechanics
- Earthquake
- Seismic Wave Propagation
- Dynamic Rupture
- Atomistic Molecular Dynamics

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Wide Range of Scales of Interest
Turbulence

Turbulent Fluid Flow.

- **Range of length scales in 3D turbulence** ~ $R_e^{9/4}$
- **State-of-the-art DNS (direct numerical simulation):** $R_e = O(10^4)$
  - Range of length scales = $O(10^9)$

- **Need for more**
  - Physical $R_e$ for commercial jet aircraft = $O(10^7 – 10^8)$
  - Physical $R_e$ for atmospheric flow = $O(10^7 – 10^8)$
Cosmology: Simulate evolution of large-scale structure of the universe

- **State-of-the-art simulation:** resolve galaxy-halo-sized structures
- **Range of length scales is** $> 10^5$  
  - Simulation domain 1 Gpc on a side  
  - Force resolution $O(10)$ kpc
- **Range of mass scales is** $10^4$-$10^5$  
  - 1 ptcl is 1-10 billion $M_{\text{sun}}$  
  - Milky Way dark matter halo is 60 billion - 3 trillion solar masses  
  - 10 billion ptcles
- **Need for more**  
  - Resolve galaxies (“baryonic” matter)...stars
Plasma Physics

Fusion energy applications.

(http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=5644908&isnumber=5644843)
Plasma Physics

Electrostatic ion microturbulence in a tokamak

- Need for more
  - Electron kinetics, full-\(f\)
  - Magnetic fluctuations
Geophysics

Seismic Wave Propagation.

- **State-of-the-art simulation**
  - M8: magnitude-8 on San Andreas Fault
    - 800 x 400 km area in Southern California (85 km deep)
    - Frequencies 0-2 Hz
    - 6 minutes simulated time
    - Grid resolution 40 m => 436 billion grid cells
    - CFL => 160,000 timesteps

- **Need for more**
  - Sub-skyscraper building relevance: 3-10 Hz
Brute Force Computational Approach
Turbulence

Turbulent Fluid Flow.

- **Direct Numerical Simulation: Discrete solution of Navier-Stokes equations**
  - Finite volume
  - Spectral
  - Pseudospectral
  - Spectral element

- **Less brutish, but less general**
  - Reynolds-averaged Navier-Stokes (RANS)
  - Large-eddy simulation (LES)
Simulate evolution of large-scale structure of the universe.

- **Dark matter: Particle-mesh**
  - Poisson solve for long-range interactions
  - Short-range interactions
  - \texttt{MC^3} code: local particle-particle interaction
  - \texttt{Enzo} code: AMR
Plasma Physics

Fusion energy applications: tokamak ion microturbulence

- **Ions:** Vlasov equation for phase-space distribution $f(x,p)$
  - Reduce to *gyrokinetic* form representing sufficient
  - **GTC** code: particle-in-cell (PIC) ions
  - **GYRO** code: discretize $(x,p)$ phase space

- **Electromagnetic fields:** Maxwell's equations
  - Reduce to Poisson equation in electrostatic limit

Figure: Tang, ALCF Early Science Kick-Off Workshop (http://workshops.alcf.anl.gov/esp10/agenda/)
Seismic Wave Propagation.

- **Discrete solution of equations for anelastic solids**
  - Finite difference (FD)
  - Finite volume
  - Spectral element
  - Finite element

- **AWP-ODC code: staggered FD scheme**
  - $4^{th}$ order in space, $2^{nd}$ order in time
  - Split-node algorithm for dynamic fault rupture modeling
  - M8 problem: uniform mesh
Persistent Players
Live Long
END