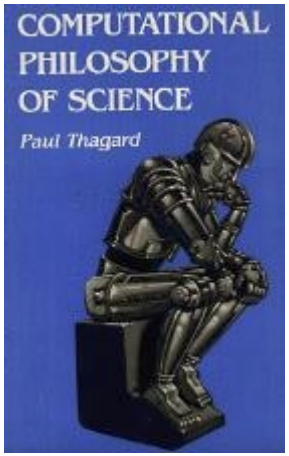
PETAFLOPS



Applications for PetaFLOPs

Rick Stevens

Argonne National Laboratory

University of Chicago

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PetaFLOPS Applications Discussions

- PetaFLOPS I
- Bodega Summer Study
- Frontiers Workshops
- NSF Point Designs
- DOE ASCI
- HTMT Project
- DOE SSI
- NSF PACI and Apex

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Bodega Bay Applications Workshop

Artificial Intelligence

Astrophysics

Climate

Computational Biology

Computational Chemistry

Computational Physics

Cryptography

Digital Libraries and Multimedia

Dynamical Systems

Economics

Computational Electromagnetics

Electronic Device Simulation

Fluid Dynamics

Geophysics

Graph Theory

Mathematics and Logic

Medicine

Multidisciplinary Problems

Optimization

Particle-in-cell models

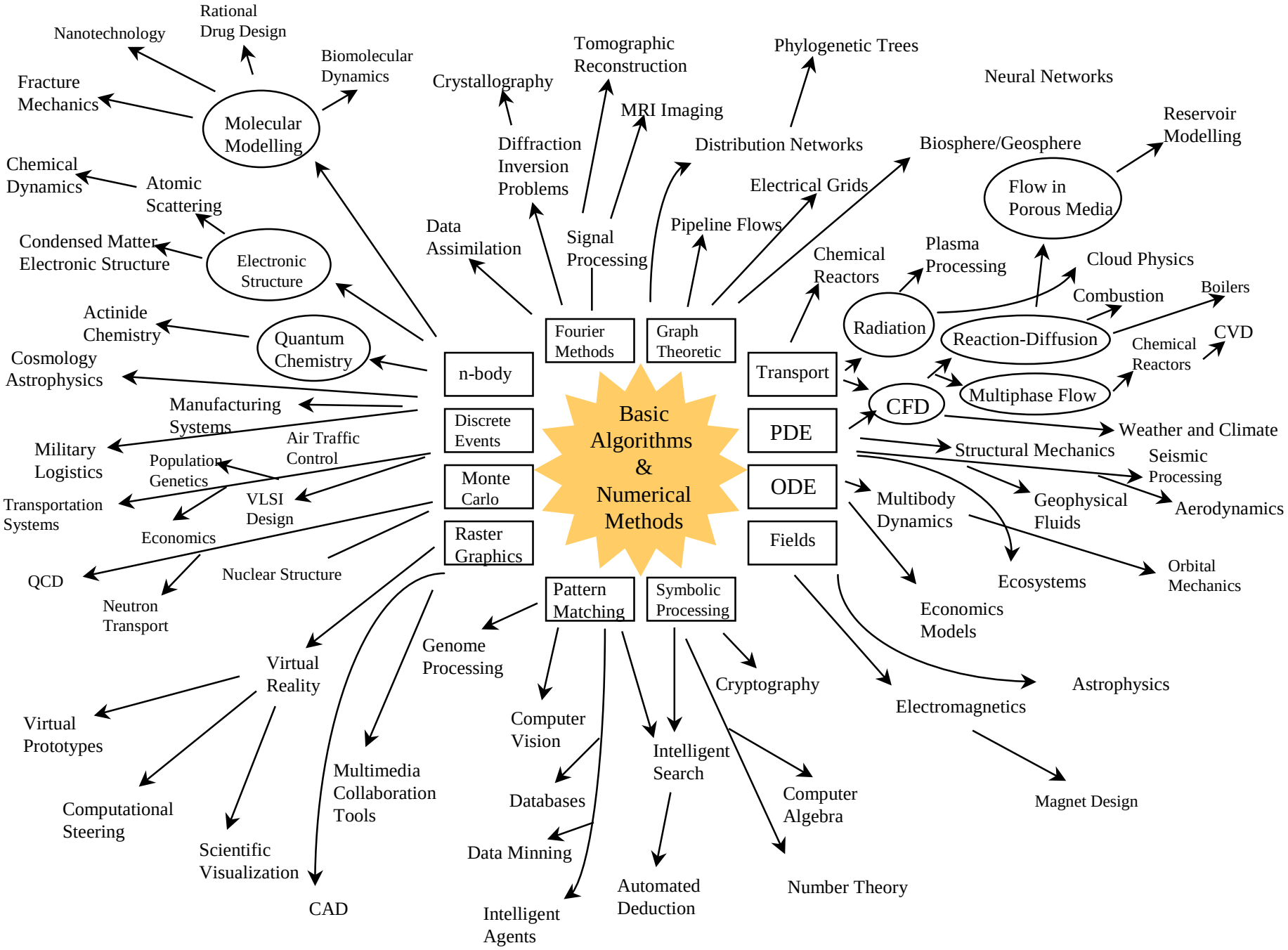
Real-time/Time critical

Signal Processing

Shock physics

Structural mechanics

Vision and Geometric Computing


Basic Algorithms & Numerical Methods
n-body
Discrete Events
Monte Carlo
Raster Graphics
Fourier Methods
Graph Theoretic
Transport
PDE
ODE
Fields
Pattern Matching
Symbolic Processing
Molecular Modelling
Nanotechnology
Rational Drug Design
Biomolecular Dynamics
Fracture Mechanics
Electronic Structure
Chemical Dynamics
Atomic Scattering
Condensed Matter Electronic Structure
Quantum Chemistry
Actinide Chemistry
Cosmology Astrophysics
Manufacturing Systems
Military Logistics
Air Traffic Control
Population Genetics
Transportation Systems
VLSI Design
Economics
QCD
Nuclear Structure
Neutron Transport
Crystallography
Tomographic Reconstruction
Phylogenetic Trees
Neural Networks
Diffraction Inversion Problems
MRI Imaging
Distribution Networks
Biosphere/Geosphere
Reservoir Modelling
Data Assimilation
Signal Processing
Pipeline Flows
Electrical Grids
Flow in Porous Media
Chemical Reactors
Plasma Processing
Cloud Physics
Radiation
Combustion
Boilers
Reaction-Diffusion
CVD
Chemical Reactors
CFD
Multiphase Flow
Weather and Climate
Structural Mechanics
Seismic Processing
Multibody Dynamics
Geophysical Fluids
Aerodynamics
Ecosystems
Orbital Mechanics
Economics Models
Astrophysics
Electromagnetics
Magnet Design
Genome Processing
Cryptography
Virtual Reality
Virtual Prototypes
Computational Steering
Scientific Visualization
Multimedia Collaboration Tools
CAD
Computer Vision
Databases
Data Minning
Intelligent Agents
Intelligent Search
Automated Deduction
Computer Algebra
Number Theory

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Can PetaFLOPS Transition us from Computing as a means for Explanation to Computing as a mode for Discovery?

- Modes of Discovery
  - getting to a new place first!!
  - staying in the new place with the time to look around
- Needs
  - reliable infrastructure (discovery happens at the edges)
  - predictable and abundant availability of resource (time)
  - freedom from pressure to avoid failure (dumb ideas)
- To make this transition we need to make scientific computing resources more abundant, more available and more usable

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Getting to a New Place First

- Moving Fast
  - small teams
  - well equipped, but self contained
- Traveling Light
  - minimum of infrastructure and gear
  - living by wit and courage
- Not Staying Long
  - taking pictures and sending them home
  - moving on

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Staying a Long Time and Looking Around

- Building Homes
  - bring our history, tools and infrastructure with us
  - making our selves comfortable
- Planting Gardens
  - figuring out what will grow here and what's good to eat
  - learning the climate and growing season
- Building Schools
  - settling in for the long haul
  - building community

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Best Prepared Applications Communities

- Astrophysics
  - stars, supernovae, neutron stars, cosmology
- Weapons Simulations
  - burn codes, 3D hydrodynamics, 3D structures
- Climate and Weather Modeling
- Computational Chemistry
- Molecular Modeling
- Cryptography

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Less Prepared Applications Communities

- Computational Linguistics
- Computational Economics
- Operations Research
- Bioinformatics
- Computational Logic
- Complex Systems Simulation
- Engineering/Design Simulations

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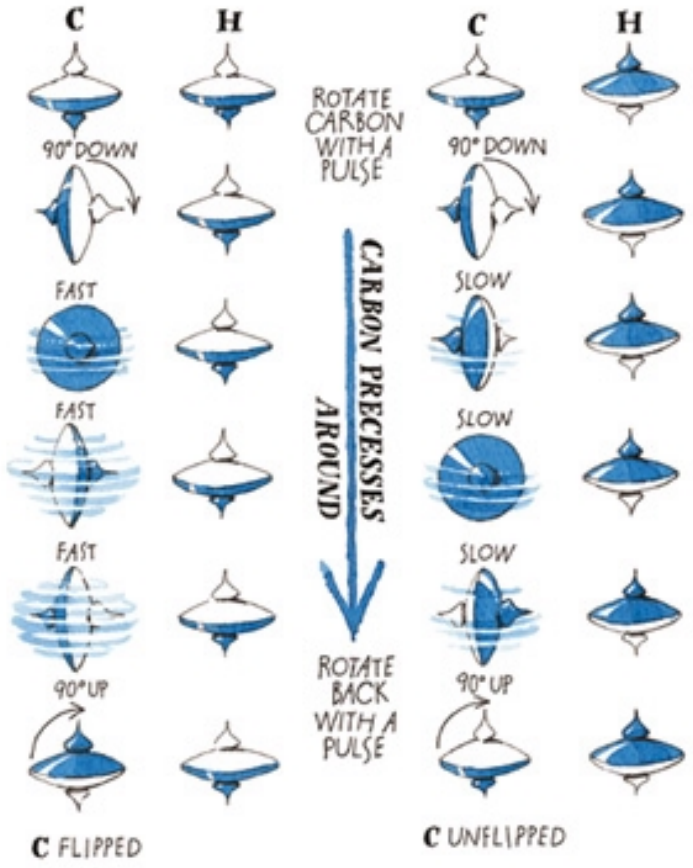
Quantum Computing

- Possible QC devices
- Exploration of Q Programming languages
- QC Algorithms
- Simulations



CONTROLLED-NOT LOGIC GATE

inverts one of two inputs conditionally on the state of the second.

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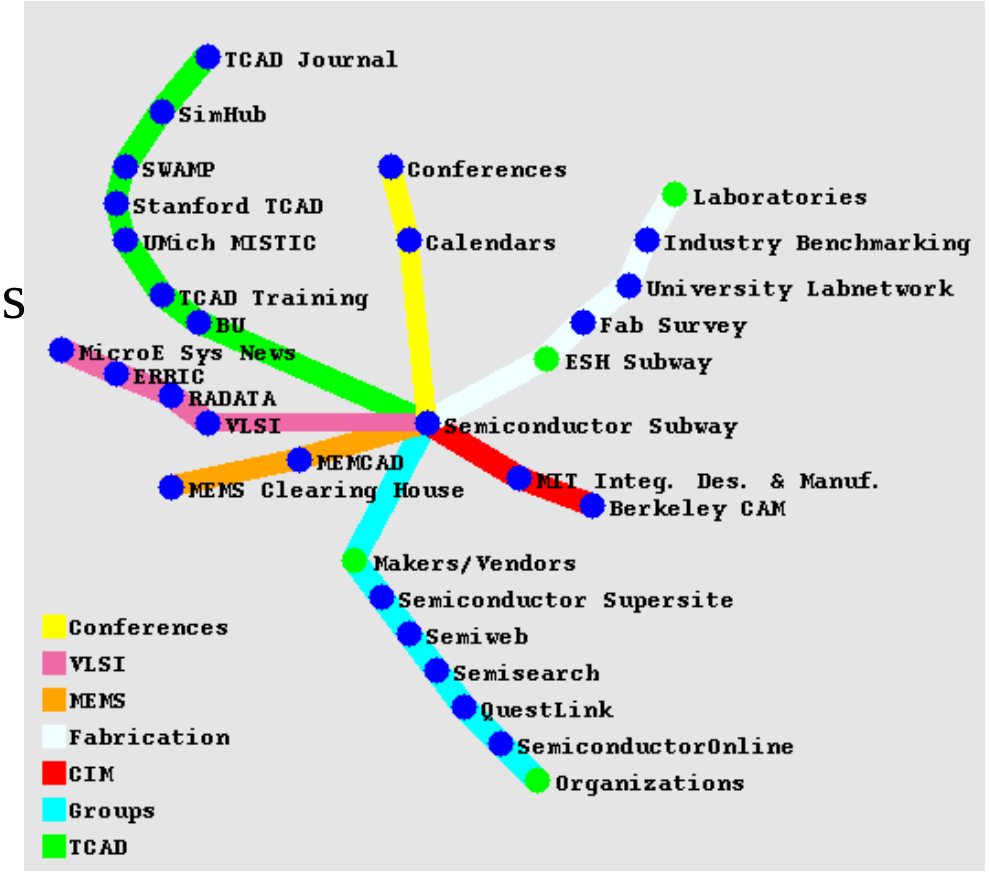
Computational Electronics

- Device modeling
  - Electronics
  - mechanical properties
- Circuit modeling
- Materials modeling
- Process modeling



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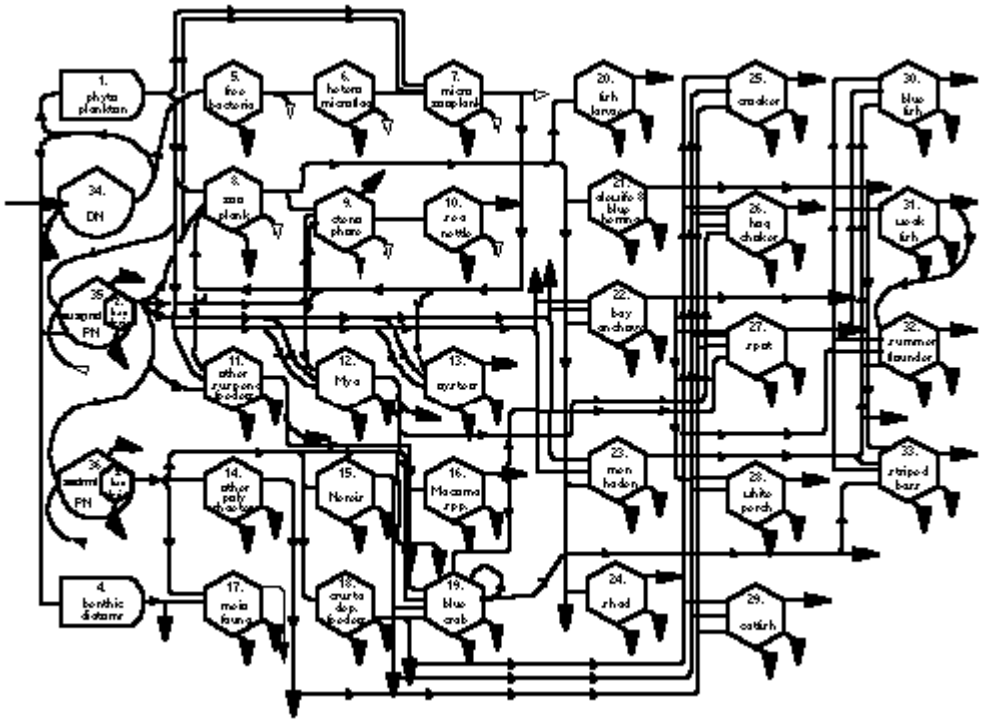
Computational Ecology

- Large-scale ecosystems models
- Individual-base models
  - age specific
  - behaviors
- Integration with Geochemical process cycles
- Ecosystem Network Analysis



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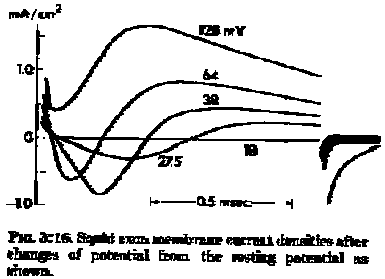
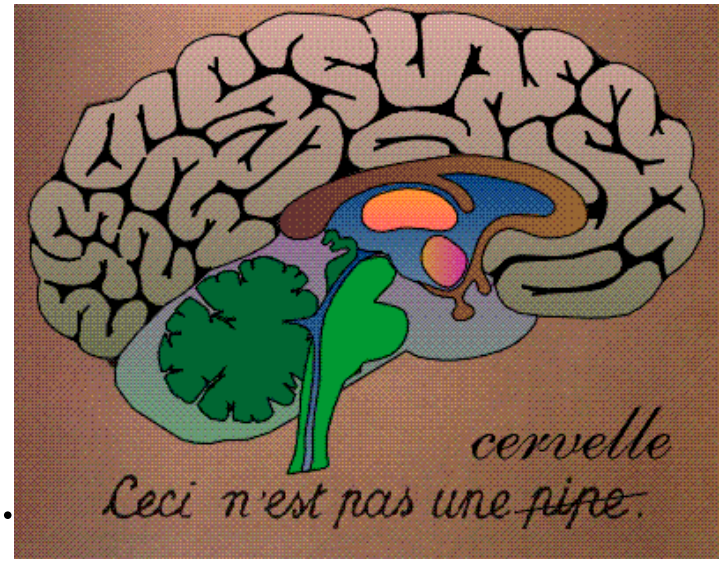
Computational Neuroscience



- Simulations of real neurons and neuronal systems
  - growth and development
  - signal transmission (membrane action potentials)
  - emergent behaviors
- Connectionist models
- Near term feasibility
  - Largest scale NEURON 3.0 simulation on MPP
  - Scalability of ANNs on MPP

SEAC 1/2 hour for 5 ms axon time, 1959.



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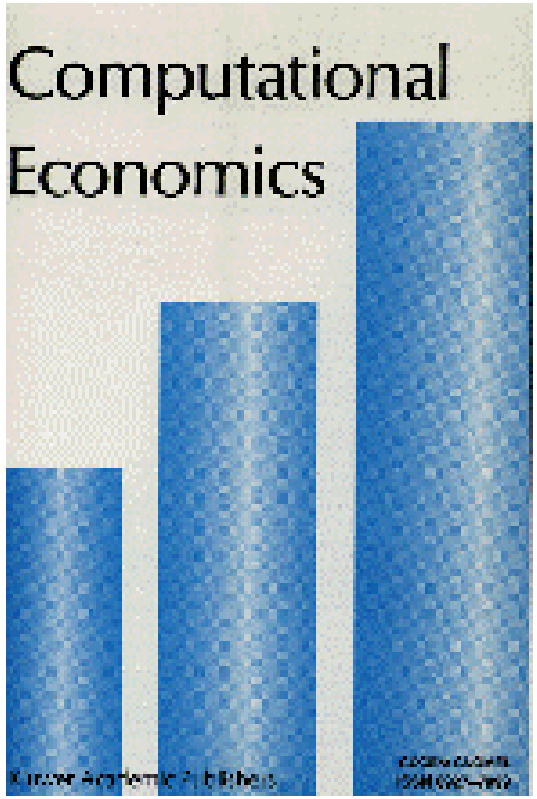
Computational Economics

- NSF Workshop in Computational Economics
  - Econometrics
  - Microeconomics
  - Sector Economics
  - Growth and Development
  - International Trade
  - Economic Theory
- Example…..



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Computational Economics Example

- Consider the following situation:
- Agents are seated in an auditorium listening to a brilliant economics lecture. At the end of the talk, after wiping away the tears, the applause begins, and perhaps a standing ovation ensues.
- Model, using whatever techniques you desire, the process of a standing ovation.
    - Explicitly state your model.
    - Summarize any results.
    - Suggest some potentially interesting future directions for the model.
- Suggest some economic scenarios that could be usefully modeled using such a process.

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Planetary and Geoscience

- Planetary formation
- Structure and dynamics of the Mantle
- Origin and dynamics of petroleum reservoirs
- Plate tectonics
- Earthquake prediction
- Paleoclimate predictions

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Web Mining

- Largest source of publicly available data
- Maybe an Important resource for social and humanities research
- More complex than data mining due to unstructured nature of the data
- Combines data mining and computational linguistics, image understanding and social theory

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Computational Epistemology

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Applications Areas for Petaflops

- Materials simulations that bridge the gap between microscale and macroscale (bulk materials)
- Coupled electro-mechanical simulations of nano-scale structures (dynamics and mechanics of micromachines)
- Full plant optimization for complex processes (chemical, manufacturing and assembly problems)
- High-resolution reacting flow problems (combustion, chemical mixing and multiphase flow)
- High-realism immersive virtual reality based on realtime radiosity modeling and complex scenes

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Applications Areas for Petaflops

- Time dependent simulations of complex biomolecules (membranes, synthesis machinary and dna)
- Multidisciplinary optimization problems combining structures, fluids and geometry
- Modeling of integrated earth systems (ocean, atmosphere, bio-geosphere)
- Improved 4d/6d data assimilation capability applied to remote sensing and environmental models
- Computational cosmology (integration of particle models, astrophysical fluids and radiation transport)

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Applications Areas for Petaflops

- Computational testing and simulation as a replacement for weapons testing (stockpile stewardship)
- Simulation of plasma fusion devices and basic physics for controlled fusion (to optimize design of future reactors)
- Design of new chemical compounds and synthesis pathways (environmental safety and cost improvements)
- Comprehensive modeling of groundwater and oil reservoirs (contamination and management)
- Modeling of complex transportation, communication and economic systems