Computational Methods Across the Curriculum

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Introduction to Parallel Programming and Cluster Computing @ UW 2011

Computational Methods

- Simulations based on models
- Analysis of large data sets
- Visualization of large data sets
- In general techniques that depend on high performance computing gear to be practical
- Third method of scientific inquiry
- 20th vs 21st century science; atoms and icebergs

Computational Methods

- Why use simulations?

  too small (atoms, molecules)

  too large (galaxies, the universe)

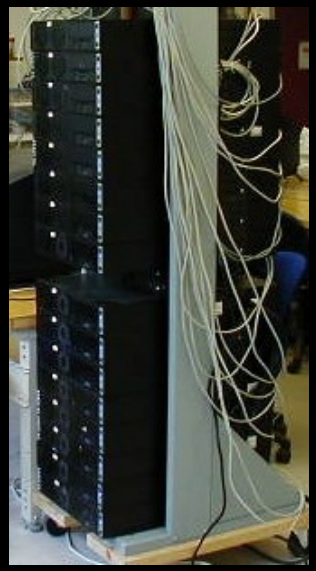
  too fast (photosynthesis, protein folding)

  too slow (geological processes, climate change)

  too complex (blood circulation, weather)

  too dangerous (toxic materials, nuclear stockpile stability)

High Performance Computing Gear




	Bazaar	Cairo	BobSCEd	Al-salam
Year	2000	2003	2006	2010
GFLOPS	18	128	666	~3000
Size	32U	16U	8U	13U

Moore’s law, every 18 months the density of transistors in integrated circuits roughly doubles

Flops indicates how many mathematical operations involving decimal fractions the computer can handle in one second.

For PCs it is measured in millions of flops (megaflops),

For mainframe computers in billions of flops (gigaflops),

For super computers in trillions of flops (teraflops)

(floating point operations per second (Flops))

(800 000 000 / (10^6) =
800 mega FLOPS)

yotta FLOPS	10^24
zetta FLOPS	10^21
exa FLOPS	10^18
peta FLOPS	10^15
tera FLOPS	10^12
giga FLOPS	10^9
mega FLOPS	10^6
kilo FLOPS	10^3

Moore’s Law in Action

1950	32 Bytes	10^0	phone booth
1975	640 KB	10^3	shoe box
2000	256 MB	10^6	pack of gum
2008	2 GB	10^9	credit card
2030	1 TB	10^12	?

Typical amount of RAM in a “desktop” computer

Data > Information > Knowledge

- Complete works of Shakespeare - ~ 5 MB
- Human genome - ~ 1 GB
- Complete works of Beethoven - ~ 20 GB
- Medical imaging - ~ 30 GB per scan
- Library of Congress - ~ 10 TB
- All US academic libraries - ~ 2 PB
- Large Hadron Collider - ~1.5 GB/second

Increasingly Readings > Data ...

Parallel and Distributed Computing

- Decomposing large problems into smaller ones, solving the smaller problems, and then reducing those answers to find “the answer”
- Domain decomposition
- Functional decomposition
- Shared memory systems
- Message passing systems

Natural Sciences

- Modeling and Simulation
  Protein folding
  Earthquakes
  Phylogenetic reconstruction
  Genome construction
- Data Sets
  Sloan Digital Sky Survey
  Protein Data Bank
  Arctic aerial photographs
  Geographical information systems (GIS)

Protein Folding

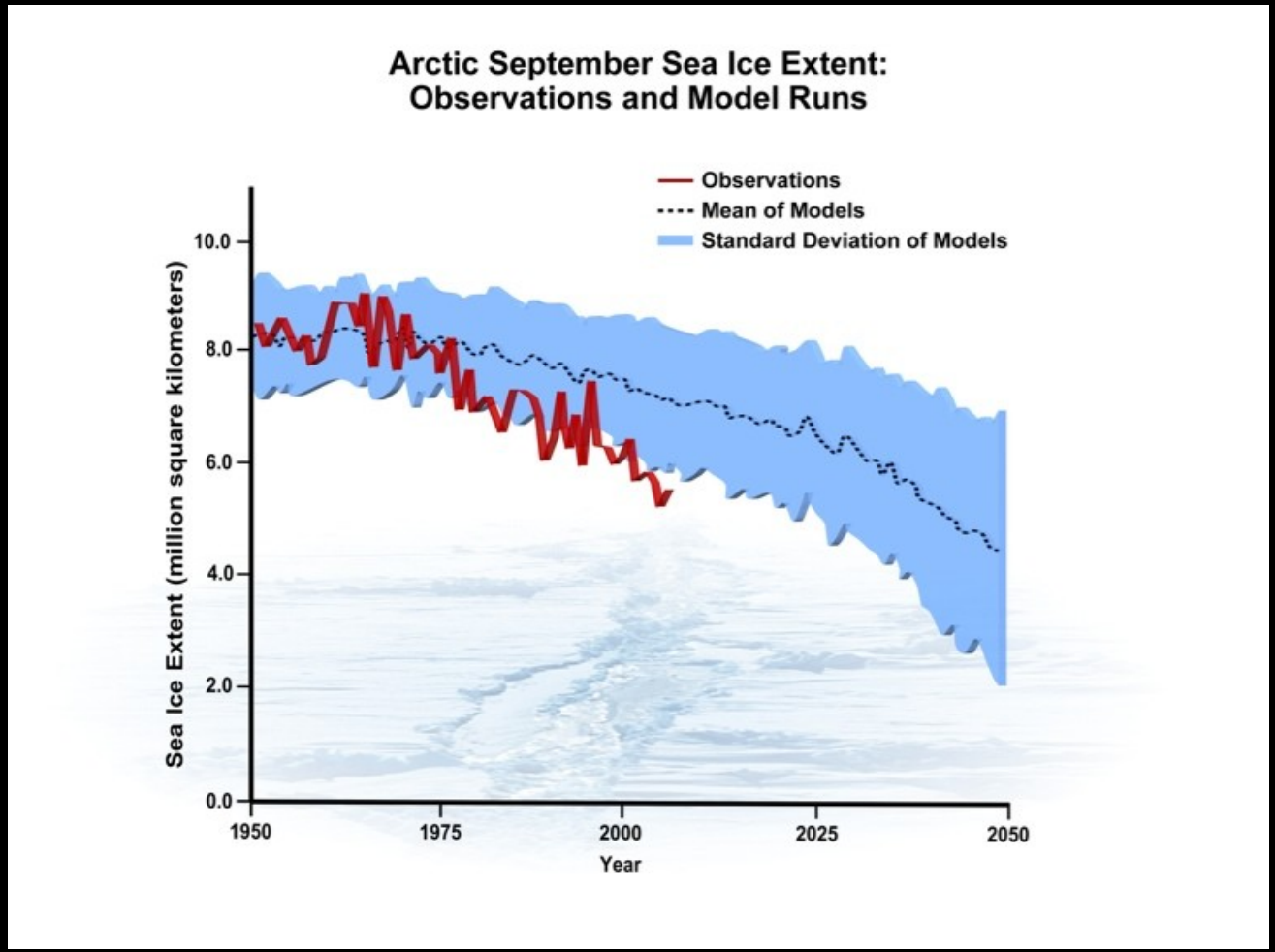
Source: Pande Lab, Stanford University

Result of an ensemble molecular dynamics simulation (Gromacs) of the villin headpiece

Earthquakes

Source: San Diego Supercomputer Center

Climate Change



Source: National Center for Atmospheric Research (NCAR) and the University of Colorado's National Snow and Ice Data Center (NSIDC)

Humanities

- Modeling and Simulation
  - Game theory
  - Topic modeling
  - Text analysis
- Data Sets
  - Library of Congress
  - Project Gutenberg
  - Newspaper morgues

Arts

- Modeling and Simulation
  - Animation and rendering
  - Painting provenance
  - Digital music
- Data Sets
  - Photograph archives
  - Scanned paintings, sculptures, buildings
  - Digital recordings

Is that really a Van Gogh?

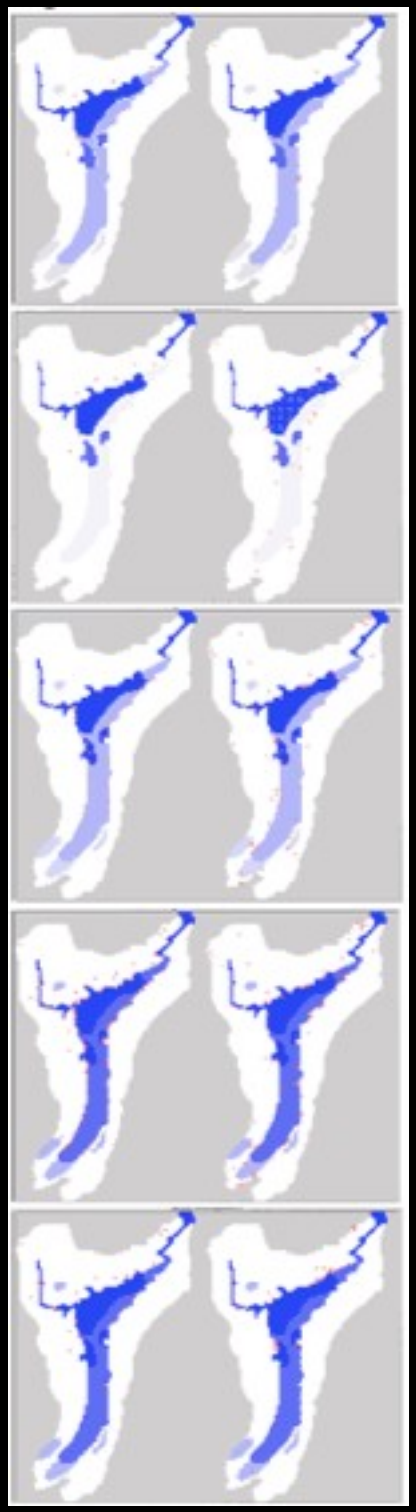
Source: Christian Science Monitor

Vase with 15 Sunflowers

Social Sciences

- Modeling and Simulation
  - Teacher matching
  - Social systems
  - Derivatives analysis
- Data Sets
  - Census
  - Geographical information systems (GIS)
  - Voting records
  - Transaction records (commercial and civil)

What happened to the Anasazi?



Source: Jonathan Rauch, The Atlantic

Why Do All This?

- President’s Information Technology Advisory Committee: “...computational science is one of the most important technical fields of the 21st century...”
- Rising Above The Gathering Storm: “...vastly improving K-12 and undergraduate science and mathematics education...”
- Bio2010: “...exposure during the early years of their undergraduate careers will help life science students use current computer methods and learn how to exploit emerging computer technologies as they arise...”

Future

- Software
  Making sense of all that stuff we are collecting
  [Readings] > Data > Information > Knowledge
  Visualization, interactive interfaces
- Grid
  Science portals, e.g. TeraGrid, Nanohub, Open Science Grid
  Humanities, Arts, and Social Science portals
- Hardware
  Specialized CPUs, e.g. FPGA and graphics chips
  Cores, cores, and more cores

References

*** This presentation is based on Charlie's presentation “Computation across curriculum”**