

Computation across the curriculum

Ivan Babic, Earlham College - OU 2012

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

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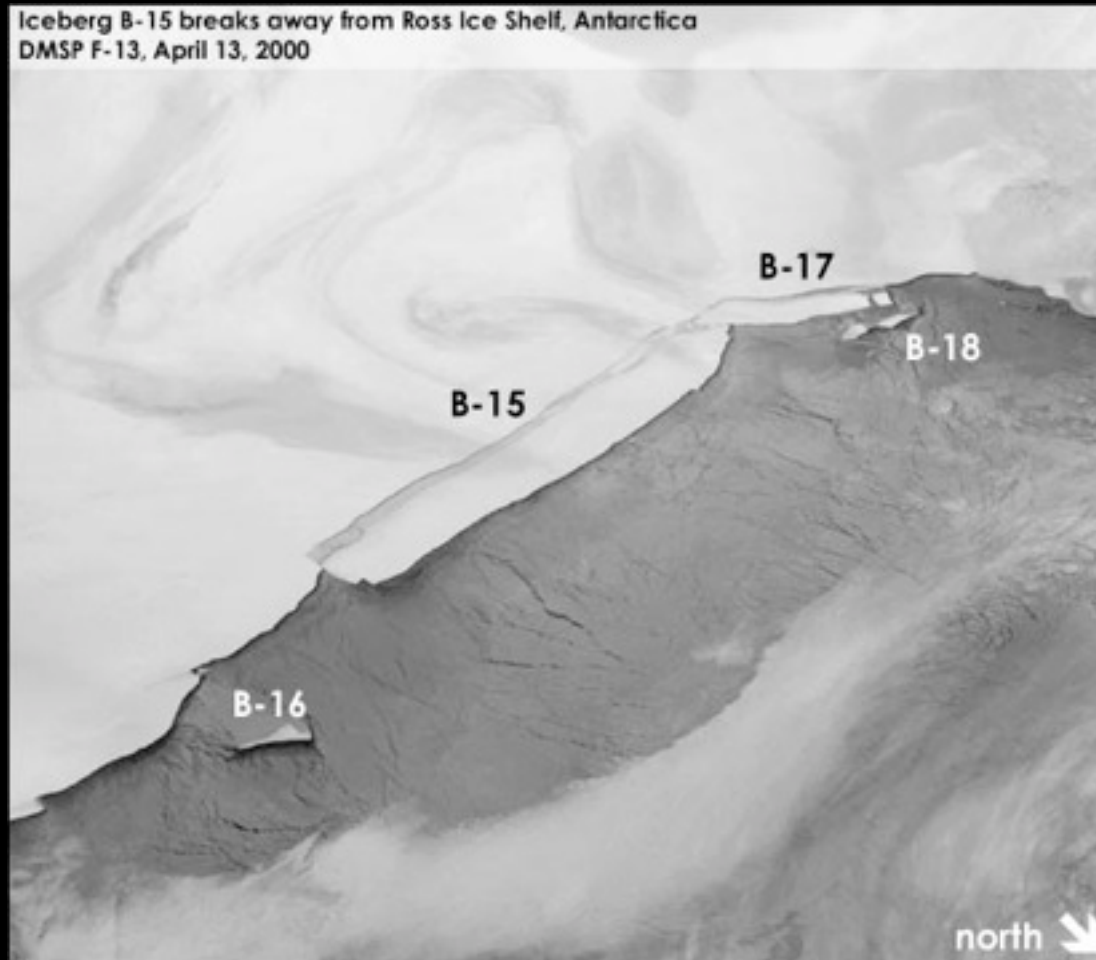
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✕	✕	me			Ticket - MEAL EQUIPMENT BOEING 777-300/300 - Babić Ivan Drawer 390, Earham College 801 National Road West Richmond, IN 47374	12/11/11
✕	✕	me - Marko, Zeljka (27)	Inbox	Facebook	Yarna Ivan, nova karta - EQUIPMENT BOEING 777-300/300 >>> BRITISH AIRWAYS - BA 296 > MON 07MAY CHICAGO IL LONDON GB 0005 0945 >	11/15/11
✕	✕	Miles & More Newsletter	Inbox		Your current mileage balance in October - A Boeing 777 will take off every Wednesday from Vienna to this island paradise. During the	10/18/11
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Wednesday, August 1, 12

All Science is
Interdisciplinary

B-15



Who were those people?

- Forensic analysis
- Archeology
- Genome sequencing
- Anthropology



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

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

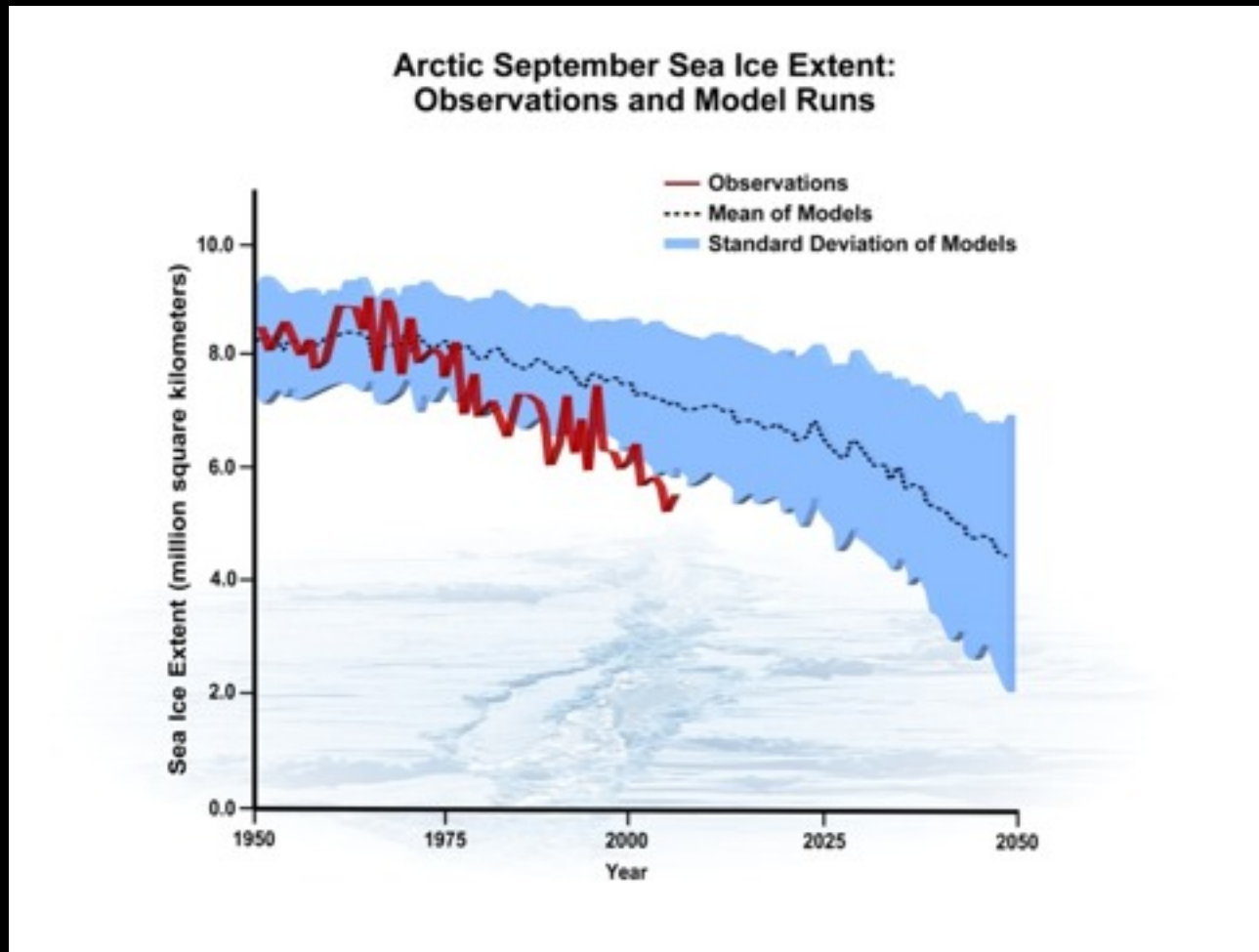
- Modeling and Simulation
 - Protein folding
 - Earthquakes
 - Phylogenetic reconstruction
 - Genome construction
- Data Sets
 - Sloan Digital Sky Survey
 - Protein Data Bank
 - Arctic aerial photographs
 - Geographical information systems (GIS)

Earthquakes

Combined view with Camera Match

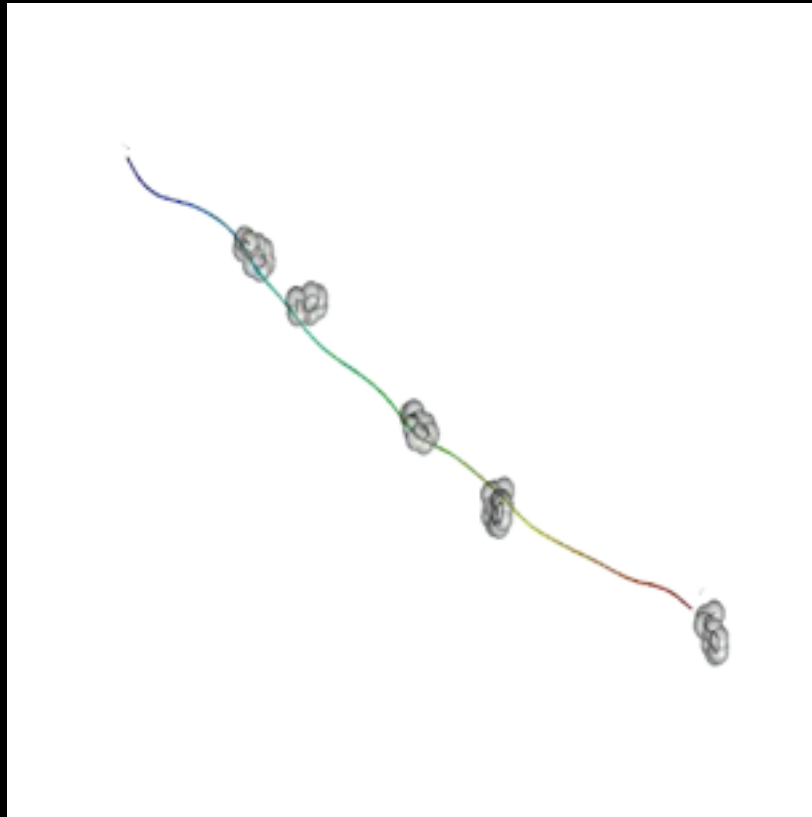
Source: San Diego Supercomputer Center

Climate Change



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

Protein Folding



Source: Pande Lab, Stanford University

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

Is that really a Van Gogh?



Source: Christian Science Monitor

Vase with 15 Sunflowers

Humanities

- Modeling and Simulation

Game theory

Topic modeling

Text analysis

- Data Sets

Library of Congress

Project Gutenberg

Newspaper morgues

Rome Reborn



Source: University of California Irvine

Looking out from the Roman Forum in a complete interactive 3D model of Rome

Arts

- **Modeling and Simulation**

Animation and rendering

Painting provenance

Digital music

- **Data Sets**

Photograph archives

Scanned paintings, sculptures, buildings

Digital recordings

Social Sciences

- Modeling and Simulation

 - Teacher matching

 - Social systems

 - Derivatives analysis

- Data Sets

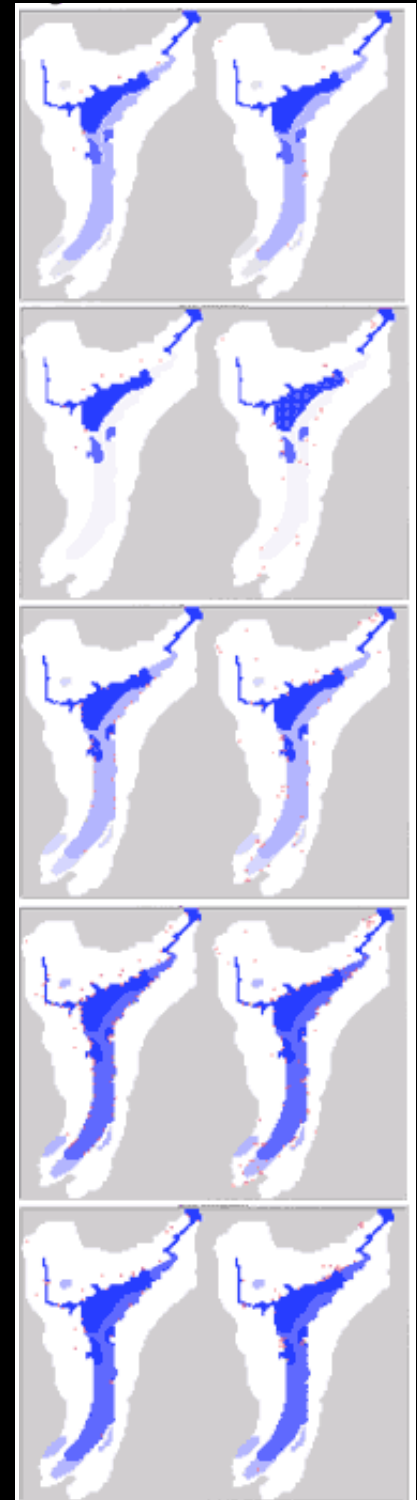
 - Census

 - Geographical information systems (GIS)

 - Voting records

 - Transaction records (commercial and civil)

What happened to the Anasazi?



Source: Jonathan Rauch, The Atlantic

Technology in the Wild



Education, Outreach, and Training

- National Computational Science Institute/SC Education Program/Blue Waters UPEP
- Workshops for undergraduate faculty and students
- 1800 participants at 80 workshops over the past 7 years
- Specialize in first-touch to handoff to a regional provider
- 3D Internet - metaverse and web-based interactive applications
- Curriculum development
- Outreach to high schools



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