

Computational Science and Engineering

Ecom-Icomp Experts Address Series

Feb 27, 2008

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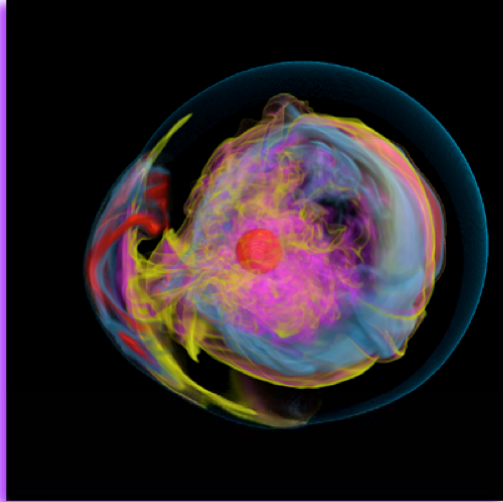
"The first great scientific breakthrough of the 21st century – the decoding of the human genome announced in February 2001 – was a triumph of large-scale computational science. When the Department of Energy (DOE) and the National Institutes of Health (NIH) launched the Human Genome Project in 1990, the most powerful computers were 100,000 times slower than today's high-end machines; private citizens using networks could send data at only 9600 baud; and many geneticists performed their calculations by hand....it was expected to take decades."

---Report to the President, June 2005, "Computational Science:
Ensuring America's Competitiveness"

This validates an additional way of "doing science"

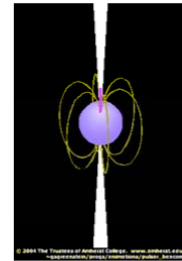
A New Way of Discovery

Discovery of the SASI (Standing Accretion Shock Instability)



Blondin & Mezzacappa Nature 445, 58-60 (4 January 2007)

- Wholly computational discovery
- Instability serves to move the shock outward
→ explosion?
- Provides 'natural' explanation for neutron star spin up



NATIONAL CENTER
FOR COMPUTATIONAL SCIENCES
Oak Ridge National Laboratory

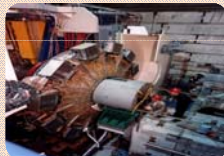
U.S. Department of Energy

How To "Do Science"

The four methods of "doing modern science"



Observational
Science



Experimental
Science

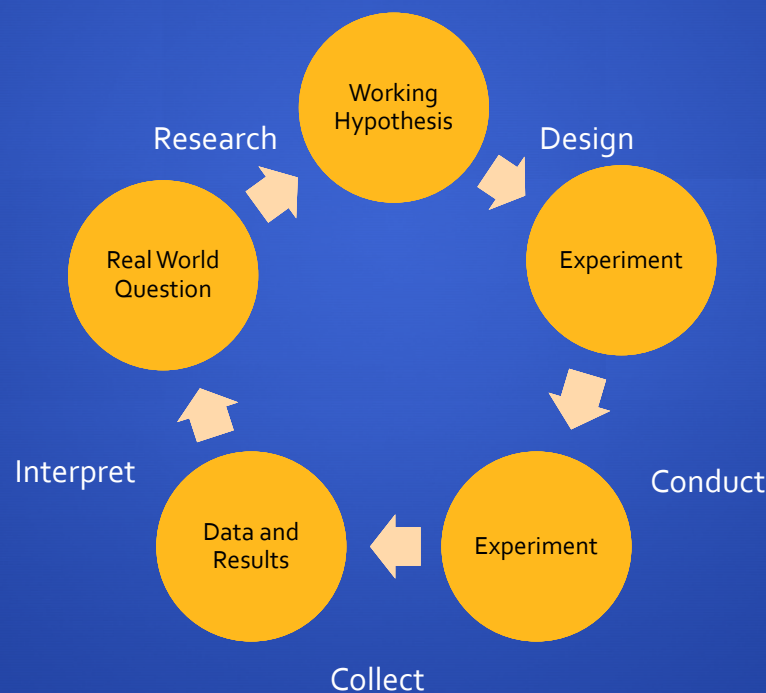


Theoretical
Science



Computational
Science

Scientific Method Process (1/2)



Scientific Method Process (2/2)

- First described ~400 years ago
- Is not constant – evolves as a result of technology
 - Peer review is a result of print
 - Repeatability of experiments is a result of peer review and collaboration (societies, not just letters)
 - Statistical sampling is due to advancements in mathematics
 - Etc.
- The impact of computing is only now being realized

“The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be solvable.”

--Paul Dirac, Royal Academy, London, 1929

“It is nice to know the computer understands the problem, but I would like to understand it too.”

--Eugene Wigner (when confronted with the computer generated results of a quantum mechanics calculation)

What is Computational Science? (1/5)

- Computational science is the integration of computing technology into scientific research
- It is the application of computer simulation and other computational methods to the solution of scientific problems and the understanding of scientific phenomenon
- Computing becomes a “full partner” in scientific discovery
- It is not to be confused with computer science which is the study of topics related to computers and information processing

Visualization of Computational Science Definition

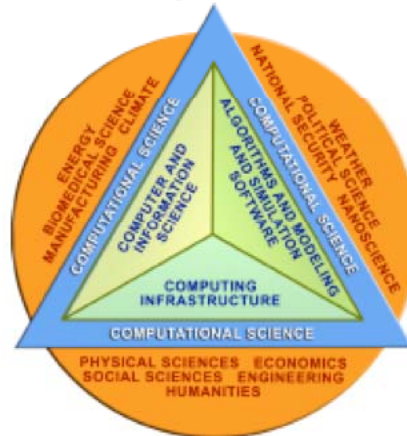


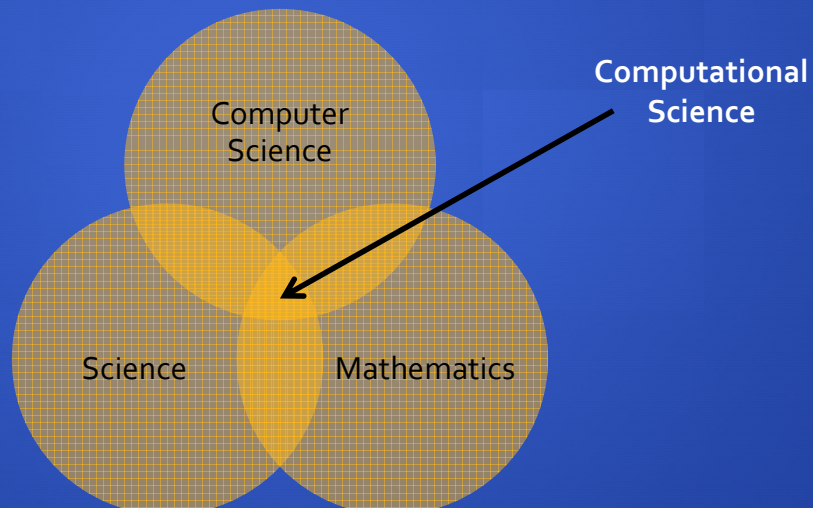
Figure 1

It takes scientific contributions across many disciplines to successfully fit software, systems, networks, and other IT components together to perform computational tasks. And it takes teams of skilled personnel representing those disciplines to manage computing system capabilities and apply them to complicated real-world challenges, much as it takes a medical team with many skills – not just a surgeon with a scalpel – to perform a complex surgical procedure. Indeed, the PITAC believes that the multidisciplinary teams required to address computational science challenges represent what will be the most common mode of science and engineering discovery throughout the 21st century.

The multidisciplinary teams required to address computational science challenges represent what will be the most common mode of 21st century science and engineering R&D.

What is Computational Science? (3/5)

Computational science seeks to gain an understanding of scientific processes through the use of mathematical methods on computers



What is Computational Science? (4/5)

- Used to:
 - Perform experiments that might be too dangerous to perform in a lab
 - Perform experiments that happen too quickly or too slowly
 - Perform experiments that might be too expensive
 - Perform experiments that are only solvable using computational approaches
 - Visualize phenomenon in the past, present, or future
 - Perform “what-if” experiments
 - Data mine through huge datasets
 - Etc., etc.

What is Computational Science? (5/5)

“Computational Science was built on the vision that computers would represent a virtual laboratory where one could explore new concepts from simulations and comparison of these with experimental data.”

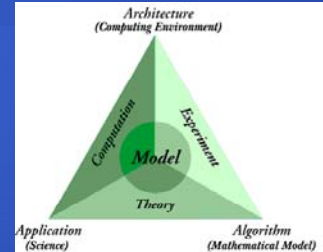
---Geoffrey Fox, Indiana University

Analyze - Predict

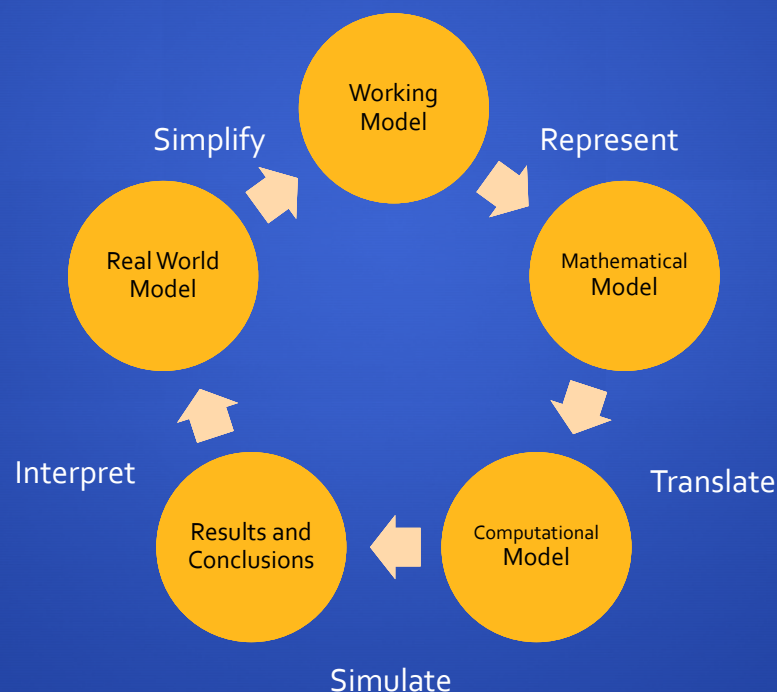
Computational Science Investigations

A Computational science investigation should include

- An application - a scientific problem of interest and the components of that problem that we wish to study and/or include.
- Algorithm - the numerical/mathematical representation of that problem, including any numerical methods or recipes used to solve the algorithm.
- Architecture – a computing platform and software tool(s) used to compute a solution set for the algorithm.



Computational Science Process



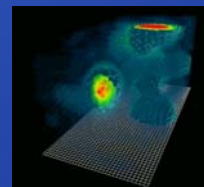
The Modeling Process

- Modeling is the application of methods to analyze complex real-world problems in order to make predictions about what might happen with various actions
- A system exhibits probabilistic or stochastic behavior if an element of chance exists. Otherwise, it exhibits deterministic behavior. A probabilistic or stochastic model exhibits random effects, while a deterministic model does not.
- A static model does not consider time, while a dynamic model changes with time.
- In a continuous model, time changes continuously, while in a discrete model time changes in incremental steps.

(Ref: Shiflet & Shiflet)

Major Approaches to Computational Science Problems

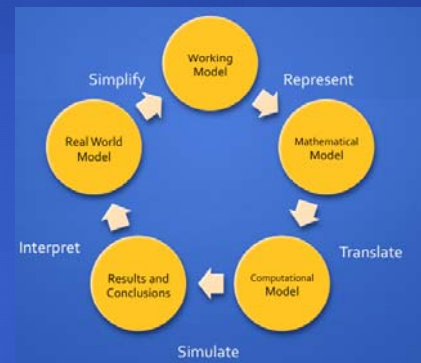
- System dynamics models provide global views of major systems that change with time (e.g., equation-based physics problems)
- Cellular automaton simulations (finite element) provide local views of individuals affecting individuals. The world under consideration consists of a rectangular grid of cells, and each cell has a state that can change with time according to rules (e.g., visualization of lattice gauge QCD)



Real World Problem

Identify *Real-World Problem*:

- Perform background research, workable problem
- Conduct investigations (Labs)
- Select computational tool
- *Understand current activity and predict future behavior*

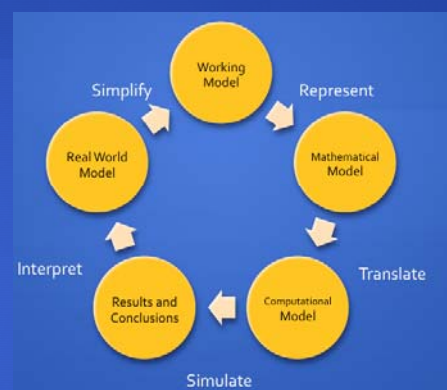


Working Model

Simplify → *Working Model*:

Identify and select factors to describe important aspects of *Real World Problem*; determine those factors that can be neglected.

- State simplifying assumptions
- Determine governing principles, physical laws
- Identify model variables and inter-relationships



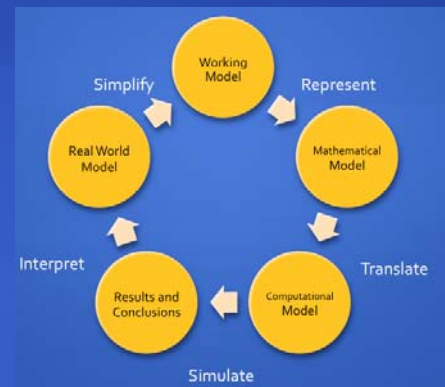
Mathematical Model

Represent → Mathematical Model:
Express the *Working Model* in

mathematical terms; write down

mathematical equations or an algorithm

whose solution describes the *Working Model*.

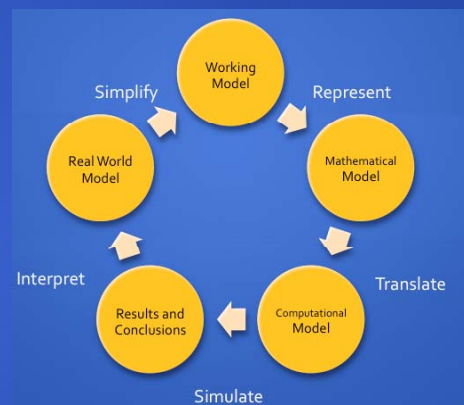


In general, the success of a mathematical model depends on how easy it is to use and how accurately it predicts.

Computational Model

Translate → Computational Model:

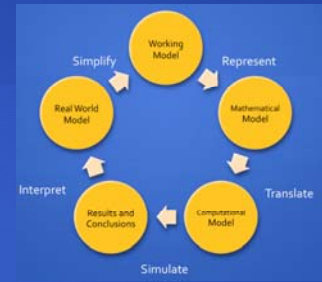
- Change *Mathematical Model* into a for computational solution.
- Computational models include tool-specifics.



Results/Conclusions

Simulate → *Results/Conclusions*:
Run “Computational Model” to obtain
Results; draw *Conclusions*.

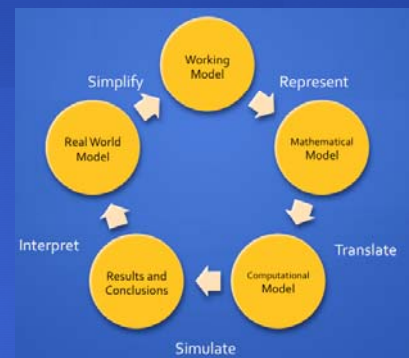
- Verify your computer program;
use check cases; explore ranges of validity.
- Graphs, charts, and other visualization
tools are useful in summarizing results
and drawing conclusions.



Real World Problem

Interpret *Conclusions*:
Compare with *Real World Problem* behavior.

- If model results do not “agree” with
physical reality or experimental
data, reexamine the Working Model
(relax assumptions) and repeat modeling steps.
- Often, the modeling process proceeds
through several “cycles” until model is “acceptable”



Example: Projectile Motion

Determine the motion of a projectile starting from a height H , above the ground with initial velocity V .

Working Model (1/2)

- Governing principles: $d = v \cdot t$ and $v = a \cdot t$
- Simplifying assumptions:
 - Gravity is the only force acting on the body
 - Flat earth
 - No drag (air resistance)
 - Model variables are $H, V, g; t, s,$ and v

Working Model (2/2)

Form a discrete-in-time model to determine the position and velocity of the projectile above the ground at equally spaced times, $t_0, t_1, t_2, \dots, t_n$; e.g. $t_0 = 0$ sec, $t_1 = 1$ sec; $t_2 = 2$ sec, etc.

v_0	v_1	v_2	...	v_n
s_0	s_1	s_2	...	s_n
t_0	t_1	t_2	...	t_n

Mathematical Model

Given an initial time, t_0 , an initial height, H , and an initial velocity, V , generate the time history of heights, s_n , and velocities, v , by the formulas

$$s_0 = H, v_0 = V$$

$$\Delta s_n = v_{n-1} \Delta t, s_n = s_{n-1} + \Delta s_n$$

$$\Delta v_n = -g \Delta t, v_n = v_{n-1} + \Delta v_n$$

$$n = 1, 2, \dots$$

Computational Model

Pseudo-Code

Input

t_o , initial time; V , initial velocity; H , initial height
 g , acceleration due to gravity; Δt , time step;
 i_{\max} , maximum number of steps

Output

t_i , t-value at time step i
 s_i , height at time t_i
 v_i , velocity at time t_i

Example: Projectile Motion

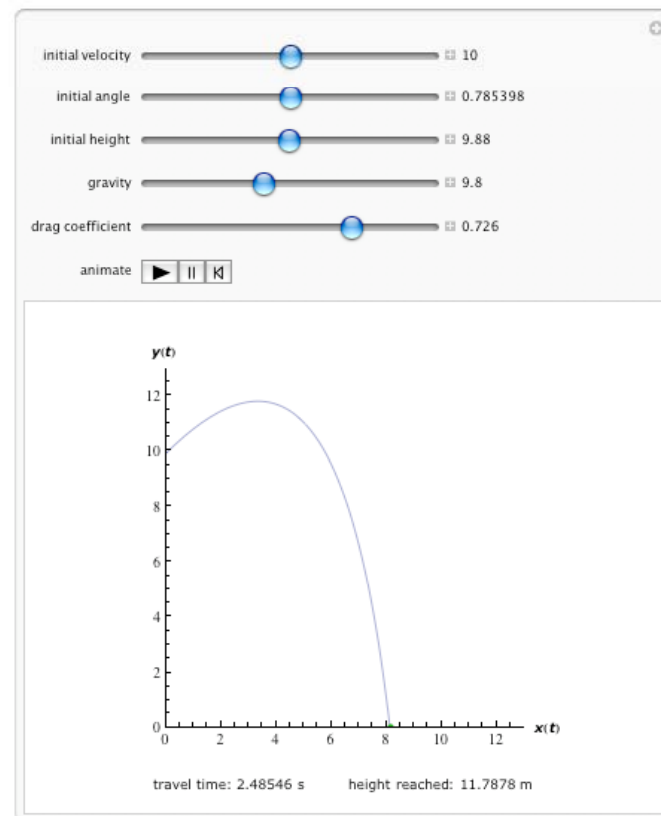
Initialize

set $t_i = t_o = 0$; $v_i = v_o = V$; $s_i = s_o = H$
print t_i , s_i , v_i

Time stepping: $i = 1, i_{\max}$

set $t_i = t_i + \Delta t$
set $s_i = s_i + v_i * \Delta t$
set $v_i = v_i - g * \Delta t$
print t_i , s_i , v_i
if ($s_i \leq 0$), quit

Animated Projectile Motion



Interpretation

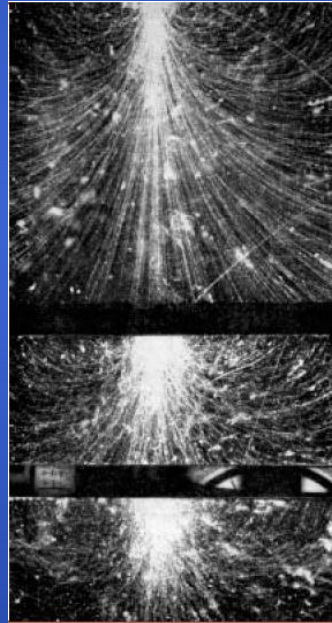
- To create a more realistic model of a moving projectile, some of the simplifying assumptions could be dropped; e.g., incorporate drag - depends on shape of the projectile, is proportional to velocity
- Improve discrete model:
 - Approximate velocities in the midpoint of time intervals instead of the beginning.
 - Reduce the size of Δt .

**Most Scientific Computing
Problems are More Complex Than
Moving Projectiles**

Scientific Simulation

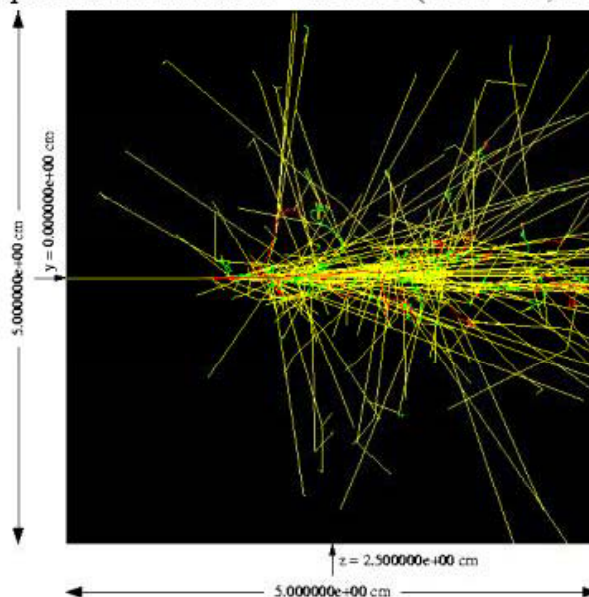
Example – Electron-Gamma Showers (EGS)

- To simulate the interaction of particle beams of varying energies on fixed targets of various materials and geometries
- To study the resulting particle showers
- Simulations based upon known laws of physics and observed interactions (cross sections) between particles
- Allows “what-ifs” not possible or feasible in the laboratory



1 GeV Photon Shower

1 GeV photon shower in 10 r.l. of Pb ($E_{\text{cut}}=0.1$, $P_{\text{cut}}=0.01$ Mev)



EGS Applications

- Materials physics
- Radiation/health physics
- Radiation medicine
- Education
- Etc.

Finite Element and Lattice Methods

Finite Element Method (FEM)

- Many problems in engineering and applied science are governed by differential or integral equations
- The solutions to these equations would provide an exact, closed-form solution to the particular problem being studied
- However, complexities in the geometry, properties and in the boundary conditions that are seen in most real-world problems *usually* means that an exact solution cannot be obtained or obtained in a reasonable amount of time

Finite Element Method (2/2)

- In the FEM, a complex region defining a continuum is discretized into simple geometric shapes called *elements*
- The properties and the governing relationships are assumed over these elements and expressed mathematically in terms of unknown values at specific points in the elements called *nodes*
- An assembly process is used to link the individual elements to the given system. When the effects of loads and boundary conditions are considered, a set of linear or nonlinear algebraic equations is usually obtained
- Solution of these equations gives the *approximate* behavior of the continuum or system

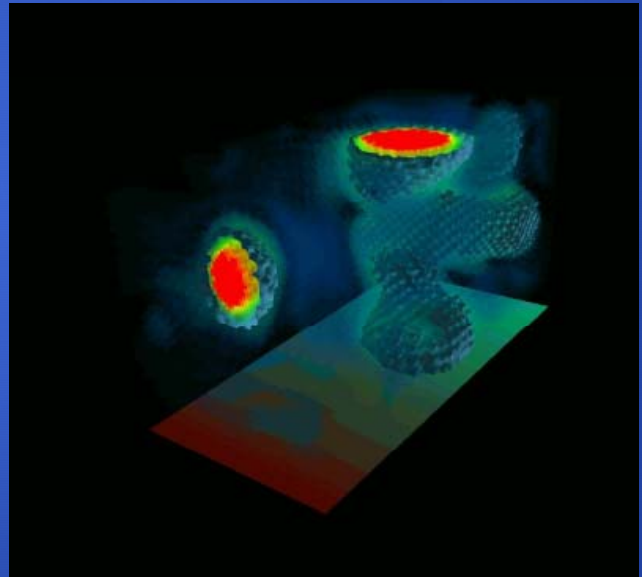
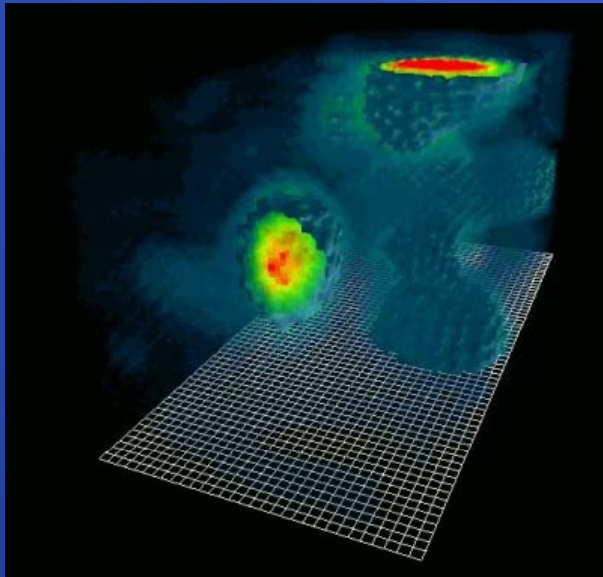
Example – Lattice QCD Simulation (1/3)

- In quantum theories such as QCD, particles are represented by fields
- To simulate the quark and gluon activities inside matter on a computer, physicists calculate the evolution of the fields on a four-dimensional lattice representing space and time
- A typical lattice simulation that approximates a volume containing a proton might use a grid of $24 \times 24 \times 24$ points in space evaluated over a sequence of 48 points in time
- The values at the intersections of the lattice approximate the local strength of quark fields
- The links between the points simulate the rubber bands—the strength of the gluon fields that carry energy and other properties of the strong force through space and time, manipulating the quark fields.

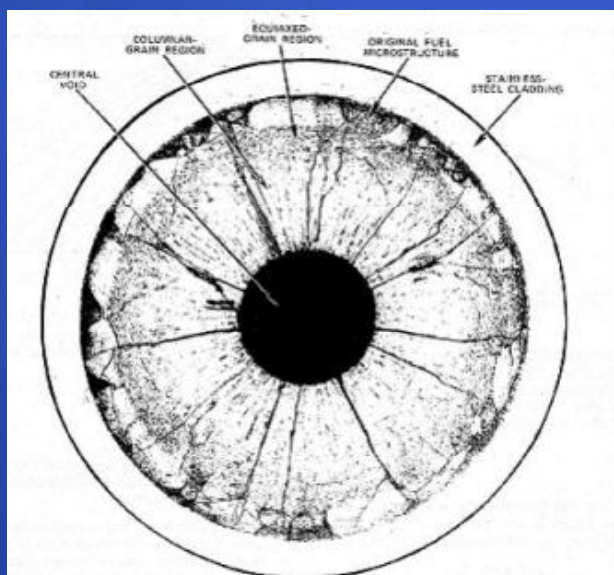
Example – Lattice QCD Simulation (2/3)

- At each step in time, the computer recalculates the field strengths at each point and link in space
- The algorithm for a single point takes into account the changing fields at the eight nearest-neighbor points, representing the exchange of gluons in three directions of space—up and down; left and right; front and back—and the change of the fields over time—past and future.

Example – Lattice QCD Simulation (3/3)



Nuclear Fuel Rod Degradation



Advanced Test Reactor Simulation at INL (Idaho National Laboratory)



Simulation vs. CGI?

- <http://www.youtube.com/watch?v= FIKonHQF8Y>

Topics in Computational Science and Engineering

- High Performance Computing
- Data Mining
- Simulation
- Scientific Visualization
- Programming (Traditional and Symbolic Manipulation Tools)
- Collaboration systems/E-Science
- Analysis Packages
- Display and text processing systems

Data Mining

Data Mining

- Modern science is driven by data analysis like never before. We have an ability to collect and process data that is increasing exponentially!
- "...the analysis of (often large) observational data sets to find unsuspected relationships and to summarize the data in novel ways that are both understandable and useful to the data owner."
- The extraction of useful patterns from data sources, e.g., databases, texts, web, image.

- Sequential pattern mining:

A sequential rule: $A \rightarrow B$, says that event A will be immediately followed by event B with a certain confidence

- Deviation/anomaly/exception detection:
discovering the most significant changes in data
- Data visualization: using graphical methods to show patterns in data
- High performance computing
- Bioinformatics

Why Data Mining

- Rapid computerization produces huge amounts of data
- How to make best use of data?
- A growing realization: knowledge discovered from data can be used for competitive advantage and to increase intelligence

Purposes of Data Mining

- Locating phenomenon from spatially, temporally, or logically related factors, each of which is defined at different levels of abstraction
- Content based searching and browsing
- Feature extraction
- Reduction in data volume
- Scientific analysis
- Searching for anomalies

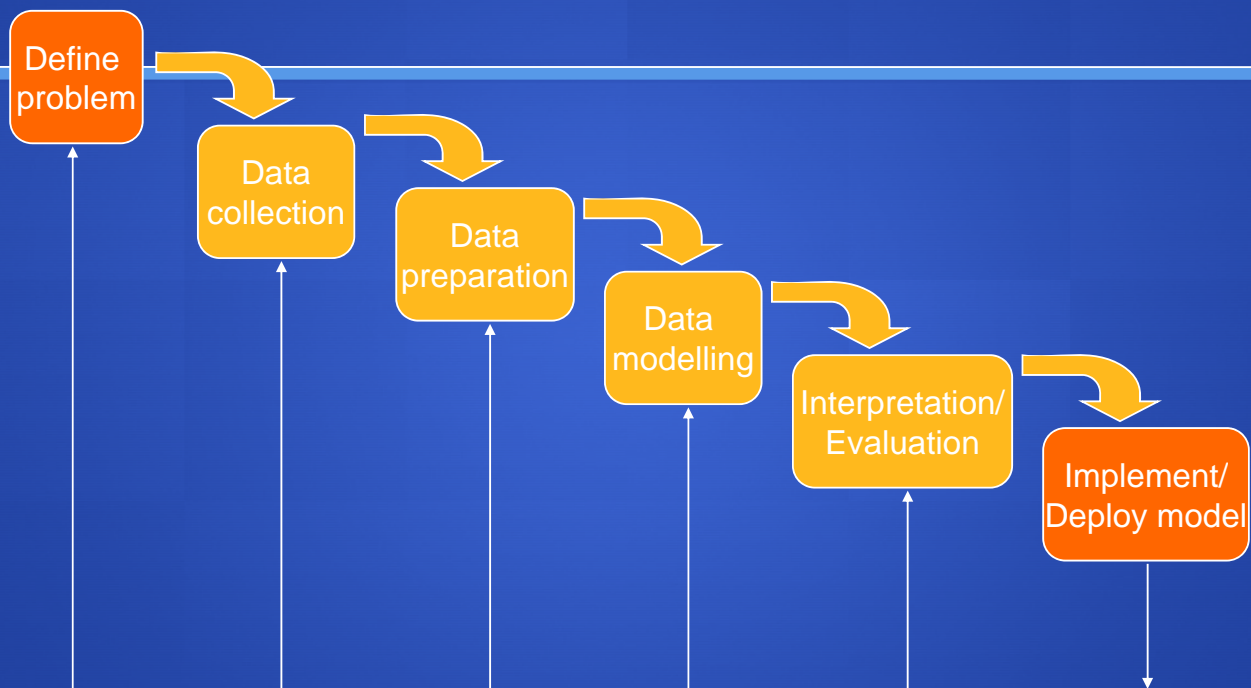
Data Mining Fields

- Data mining is an emerging multi-disciplinary field:
 - Statistics
 - Machine learning
 - Databases
 - Visualization
 - Data warehousing
 - High-performance computing
 - ...

Typical Data Mining Tasks

- Classification:
 - mining patterns that can classify future data into *known* classes
- Association rule mining:
 - mining any rule of the form $X \rightarrow Y$, where X and Y are sets of data items
- Clustering:
 - identifying a set of *similar* groups in the data

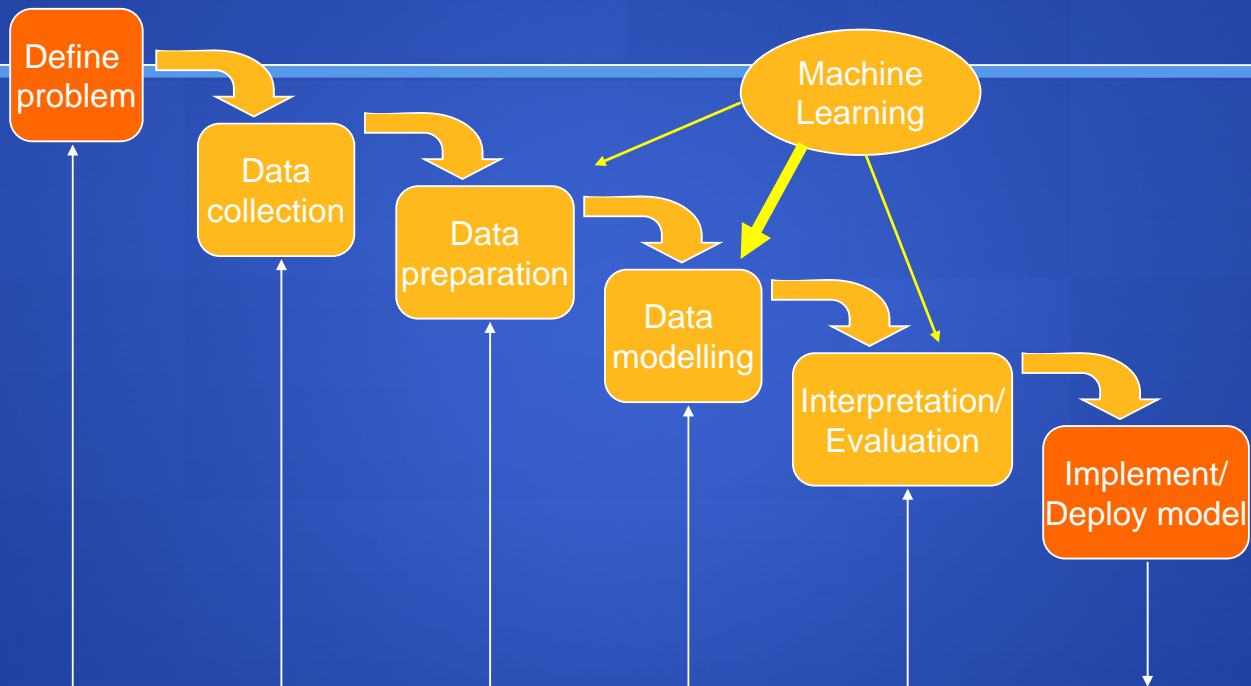
Data Mining



Machine Learning

- "...the study of computer algorithms capable of learning to improve their performance on a task on the basis of their own experience."
 - Often this is "learning from data".
- A sub-discipline of artificial intelligence, with large overlaps into statistics, pattern recognition, visualization, robotics, control, ...

Data Mining



Patterns (1/2)

- Patterns are the relationships and summaries derived through a data mining exercise
- Patterns must be:
 - valid
 - novel
 - potentially useful
 - understandable

Patterns (2/2)

- Patterns are used for
 - prediction or classification
 - describing the existing data
 - segmenting the data (e.g., the market)
 - profiling the data (e.g., your customers)
 - Detection (e.g., intrusion, fault, anomaly)

Data(1/2)

- Data mining typically deals with data that have already been collected for some purpose other than data mining
- Data miners usually have no influence on data collection strategies
- Large bodies of data cause new problems: representation, storage, retrieval, analysis, ...

Data (2/2)

- Even with a very large data set, we are usually faced with just a sample from the population.
- Data exist in many types (continuous, nominal) and forms (credit card usage records, supermarket transactions, government statistics, text, images, medical records, human genome databases, molecular databases).

Data Modelling and the Scientific Method

- Data modelling plays an important role at several stages in the scientific process:
 1. Observe and explore interesting phenomena
 2. Generate hypotheses
 3. Formulate model to explain phenomena
 4. Test predictions made by the theory
 5. Modify theory and repeat (at 2 or 3)
- The explosion of data suggests that we need to (partially) automate numerous aspects of the scientific method

Pattern Recognition

Pattern Recognition

- Pattern recognition is a research area in which pattern in data are *found, measured*, and used to *recognize, classify* and *discover* objects
- This is a catchall phrase that includes:
 - Classification
 - Clustering
 - Data mining
 - etc

Pattern Recognition Approaches

- **Statistical Pattern Recognition**
 - The data is reduced to vectors of real numbers that measure objects features. Statistical modeling is then used for recognition, classification, etc
- **Structural Pattern Recognition**
 - The data is converted to a discrete and structured form such as trees, graphs, grammars, etc. Techniques related to computer science subjects such as graph matching and parsing are used

Scientific Visualization

The Challenge

- Transform the *data* into *information* (understanding, insight) thus making it useful to people.
- Support specific tasks
- Improve performance as compared to existing mechanisms

Information Visualization

- Provide tools that present data in a way to help people understand and gain insight from it
- Cliches
 - “Seeing is believing”
 - “A picture is worth a thousand words”

“The use of computer-supported, interactive, visual representations of abstract data to amplify cognition.”

Main Idea

- Visuals help us think
 - Provide a frame of reference, a temporary storage area
- External cognition
 - Role of external world in thinking and reason
 - Multiplication exercise

Information Visualization

- What is “information”?
 - Items, entities, things which do not have a direct physical correspondence
 - Examples: baseball statistics, stock trends, connections between criminals, car attributes...
- Scientific Visualization
 - Primarily relates to and represents something physical or geometric
 - Examples
 - Air flow over a wing
 - Stresses on a girder
 - Weather over Pennsylvania

Key Attributes

- Scale
 - Challenge often arises when data sets become very large
- Interactivity
 - Want to show multiple different perspectives on the data
- Tasks
 - Want to support specific tasks – not just to create a cool demo
 - Support discovery, decision making, explanation

Visualization Success Stories

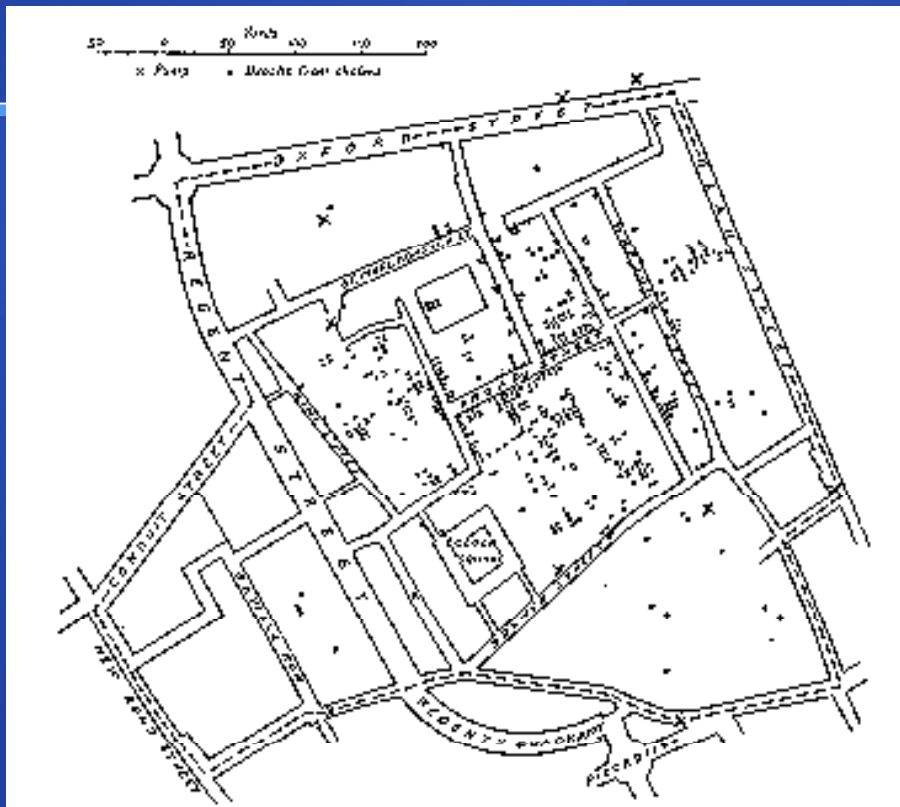
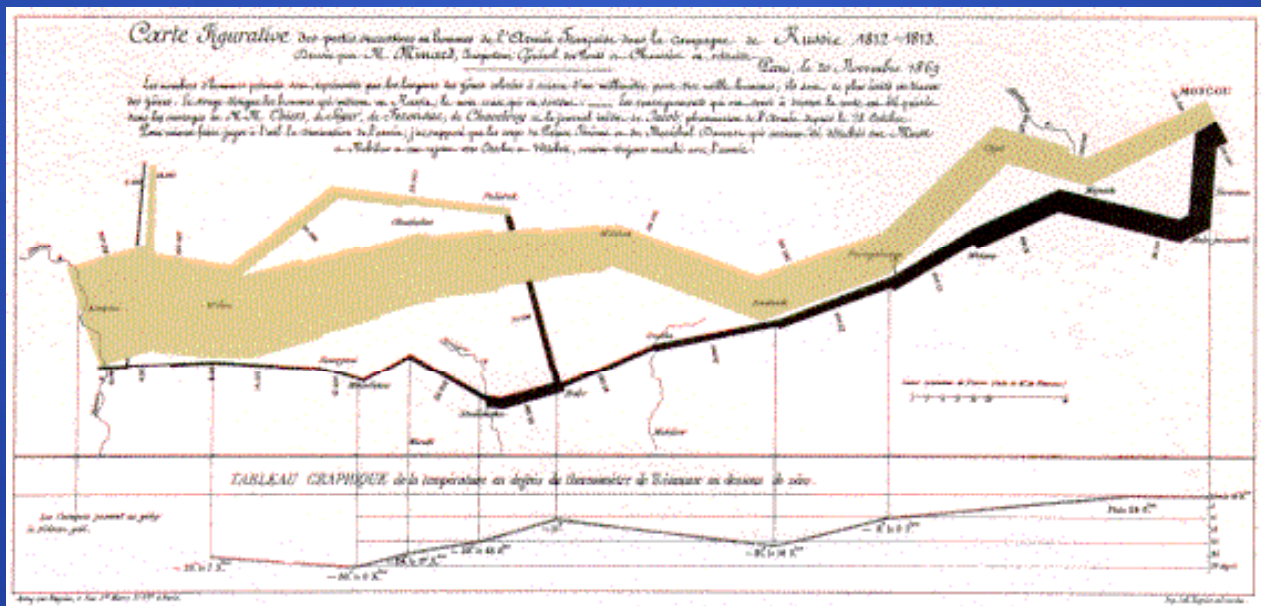


Illustration of John Snow's deduction that a cholera epidemic was caused by a bad water pump, circa 1854.

Dots indicate location of deaths.

From Visual Explanations by Edward Tufte, Graphics Press, 1997

Napoleon's March



Minard graphic

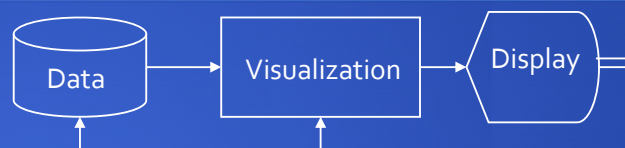
```
size of army
direction
```

latitude
longitude

```
temperature
date
```

What is Scientific Visualization?

- It is a transformation of abstract data into readily-comprehensible images
- It relies on human cognitive processes



Geometric and Visual Computing Areas

- Computer Aided Geometric Design (CAGD): Curves/surfaces
- Solid Modeling: Representations and Algorithms for solids
- Computational Geometry: Provably efficient algorithms
- Computer-Aided Design (CAD): Automation of Shape Design
- Computer-Aided Manufacturing (CAM): NC Machining
- Finite Element Meshing (FEM): Construction and simulation

New Topics in Computational Science and Engineering

- “Collaboratories” and scientific workspaces of the future
- Scientific research in virtual worlds
- Exascale Science
- Web Science

Programming and Mathematical Solvers

Popular Symbolic/Mathematical Software Packages (1/2)

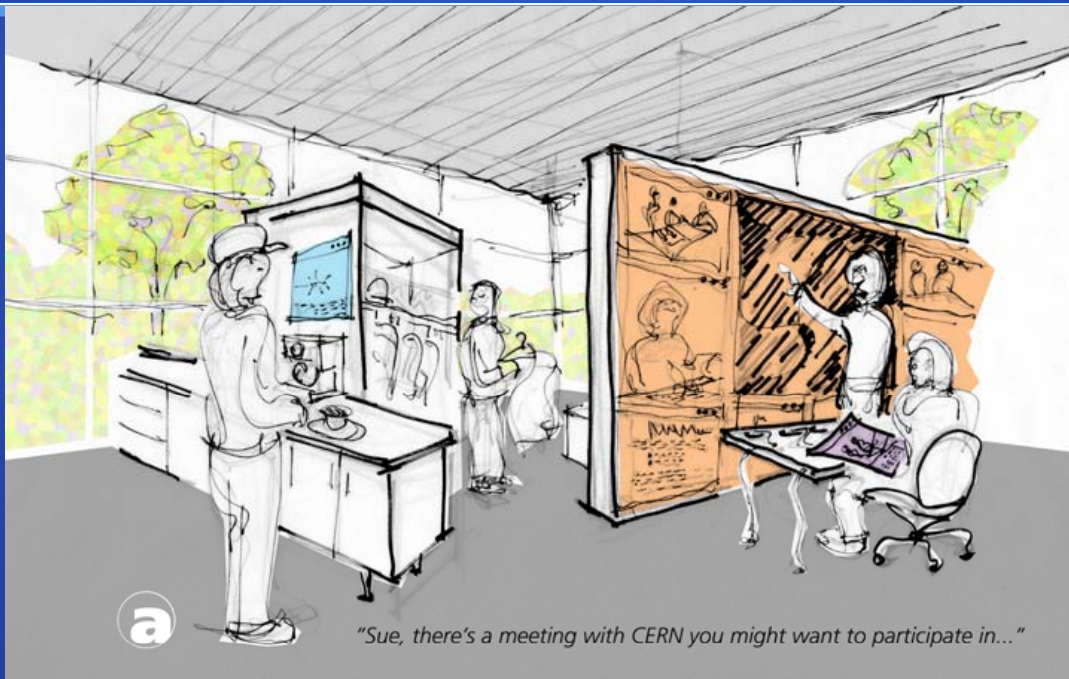
- **Mathematica**
 - Advantages - premier all-purpose mathematical software package; It integrates swift and accurate symbolic and numerical calculation, all-purpose graphics, and a powerful programming language
 - Disadvantages – Steep learning curve, expensive; premier all-purpose mathematical software package. It integrates swift and accurate symbolic and numerical calculation, all-purpose graphics, and a powerful programming language
- **Matlab**
 - Advantages - combines efficient computation, visualization and programming for linear-algebraic technical work and other mathematical areas
 - Disadvantages - Not for analytical/symbolic math

Popular Symbolic/Mathematical Software Packages (2/2)

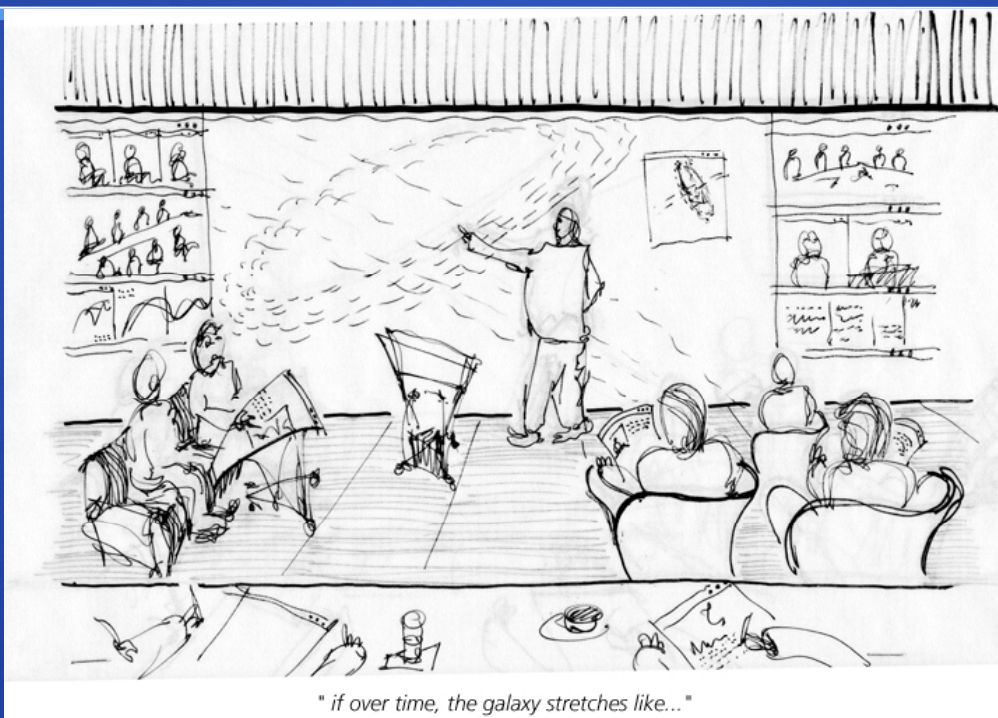
- **Maple**
 - Advantages - powerful analytical and mathematical software which does the same sorts of things that Mathematica does, with similar high quality; programming language is procedural -- like C or Fortran or Basic -- although it has a few functional programming constructs.
 - Disadvantages - Worksheet interface/typesetting not as developed as Mathematica's, but it is less expensive
- **IDL (Interactive Data Language)**
 - Advantages - excels at processing real-world data, especially graphics, and has a reasonably simple syntax, especially for those familiar with Fortran or C; makes it as easy as possible to read in data from files of numerous scientific data formats
 - Disadvantages - Does not do symbolic math

Scientific Workspace of the Future (SWOF)

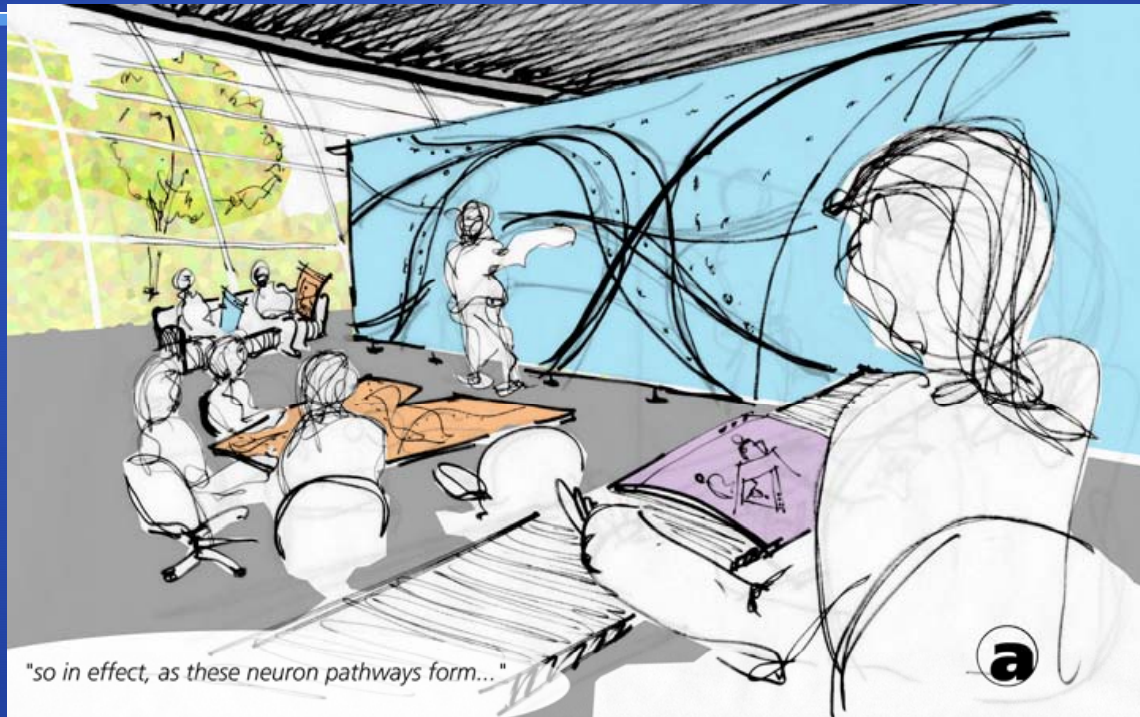
Ad Hoc Collaboration



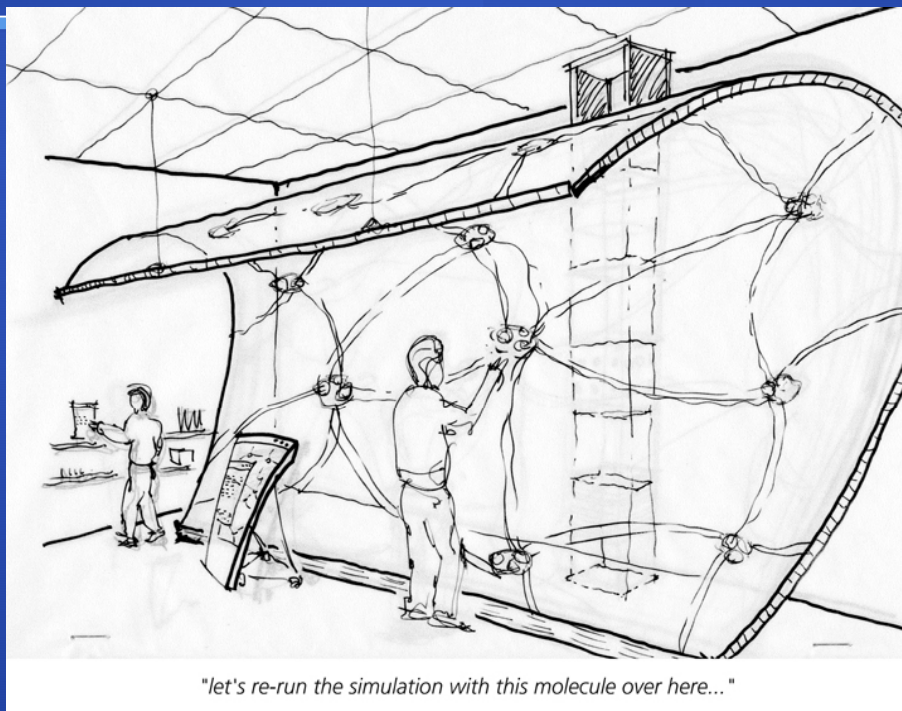
Distance Learning



Distributed Exploratory Analysis



Interactive Scientific Computing



The Scientific Research Potential of Virtual Worlds

William Sims Bainbridge

Online virtual worlds, electronic environments where people can work and interact in a somewhat realistic manner, have great potential as sites for research in the social, behavioral, and economic sciences, as well as in human-centered computer science. This article uses Second Life and World of Warcraft as two very different examples of current virtual worlds that foreshadow future developments, introducing a number of research methodologies that scientists are now exploring, including formal experimentation, observational ethnography, and quantitative analysis of economic markets or social networks.

Recent technological developments in building online worldlike environments have made possible new kinds of research in the social and behavioral sciences, new interesting challenges for computer and information science, and suggest new potential for education across all the sciences (1, 2). We can use the term "virtual world" to describe an electronic environment that visually mimics complex physical spaces, where people can interact with each other and with virtual objects, and where people are represented by animated characters. The diversity of current virtual worlds can be represented by the creativity-oriented environment Second Life (SL) and the massively multiplayer online role-playing game World of Warcraft (WoW). To date, about 6.5 million people have entered SL, and WoW reports that it has 8.5 million subscribers, so the impact of this technology is beginning to be felt by society.

The user enters each via a personal computer running special software that connects to one or more servers that pass information back and forth between users over the Internet. Both simulate very large three-dimensional environments filled with virtual objects through which the user may subjectively walk, swim, or fly, and in the case of WoW, with thousands of simple artificial intelligence (AI) characters to interact with. Each user is represented by an avatar and can talk with the others by typing in a chat channel or through optional voice communication (3). Both worlds sustain complex internal economies with their own currencies, both enable users to do world work for each other, and both offer software tools to facilitate social interaction, although some of their specific features are quite different (4-6) (Fig. 1).

In terms of scientific research methodologies, one can do interviews and ethnographic research in both environments, but other methods would work better in one than the other. SL is especially well designed to support formal experiments in social psychology or cognitive

science, because the researcher can construct a facility comparable to a real-world laboratory and recruit research subjects. WoW may be better for noninvasive statistical methodologies examining social networks and economic systems, because it naturally generates a vast trove of diverse but standardized data about social and economic interactions. Both allow users to create new software modules to extract data.

The present moment marks a major historical transition. Video games and computer games are as the process of evolving into something much richer, namely virtual worlds, at the same time that electronic games are surpassing the nation picture industry in dollar terms and beginning to cut into television. Already, many families forgo watching TV dramas to quest together in WoW. Previously separate forms of electronic commu-

nication are merging in what Americans call ubiquitous computing and Europeans call pervasive computing. The current generation of video game systems—Xbox 360, PlayStation 3, and both the Nintendo Wii and the Nintendo DS portable—all connect to the Internet, and games designed for cell phones or Internet-connected pocket computers are proliferating. Researchers are exploring the methods needed to create an entirely new generation of games, called pervasive LARPs (live-action role-playing games), that have players act in the real world while simultaneously interacting over the Internet via wireless mobile connections (7-9).

During this time of transition, when there is active speculation about the investment opportunities, it is exceedingly difficult to estimate the current economic impact of virtual worlds, let alone project the future. For example, a Web site called *Reckless* that was merely about WoW recently sold for 1 million dollars, and the game's \$15 monthly charge across many subscribers could generate hundreds of millions of dollars per year (10). Virtual worlds differ as to whether their internal currency can be exchanged for dollars (SL, WoW, etc.), so economists face the scientific dilemma of how to count wealth generation inside the games, in addition to the external dollar investments and returns. Exploratory studies by Nick Yee suggest that most players are in fact white, disproportionately male, but with a wide variety of occupations and demographic characteristics (11), so virtual worlds are not simply a childish fad. However



Fig. 1. The Stormwind Auction House in WoW. The three figures wearing vests and standing on platforms are the computer-generated auctioneers, whereas the dozen other figures are characters belonging to real human beings participating in auctions involving a thousand or more people. The one wearing in the center is the avatar of a scientist who is studying this virtual world and the computer-assisted systems it provides to facilitate social interaction and economic exchange.

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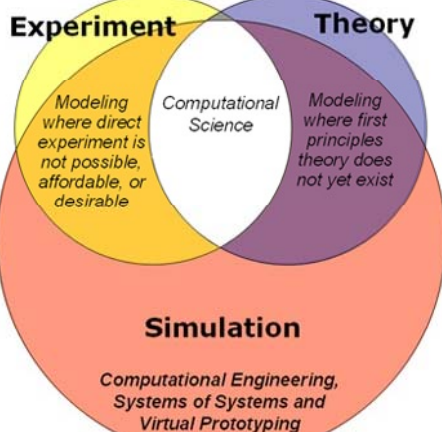
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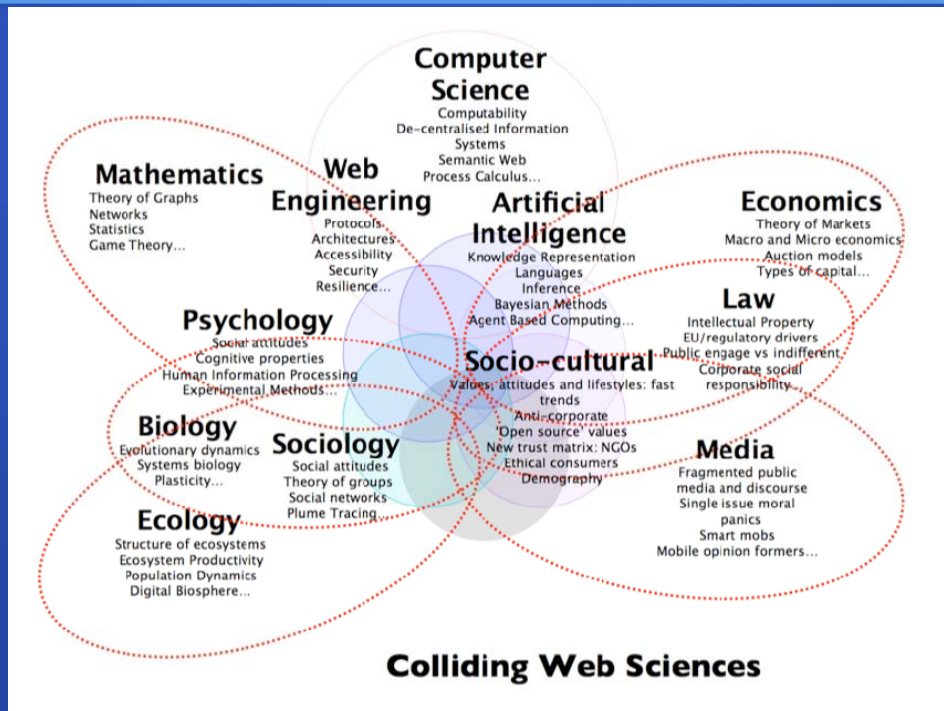


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July 21, 1995

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Thank You

Questions, Comments?

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