Introduction

CSC 7443:
Scientific Information Visualization

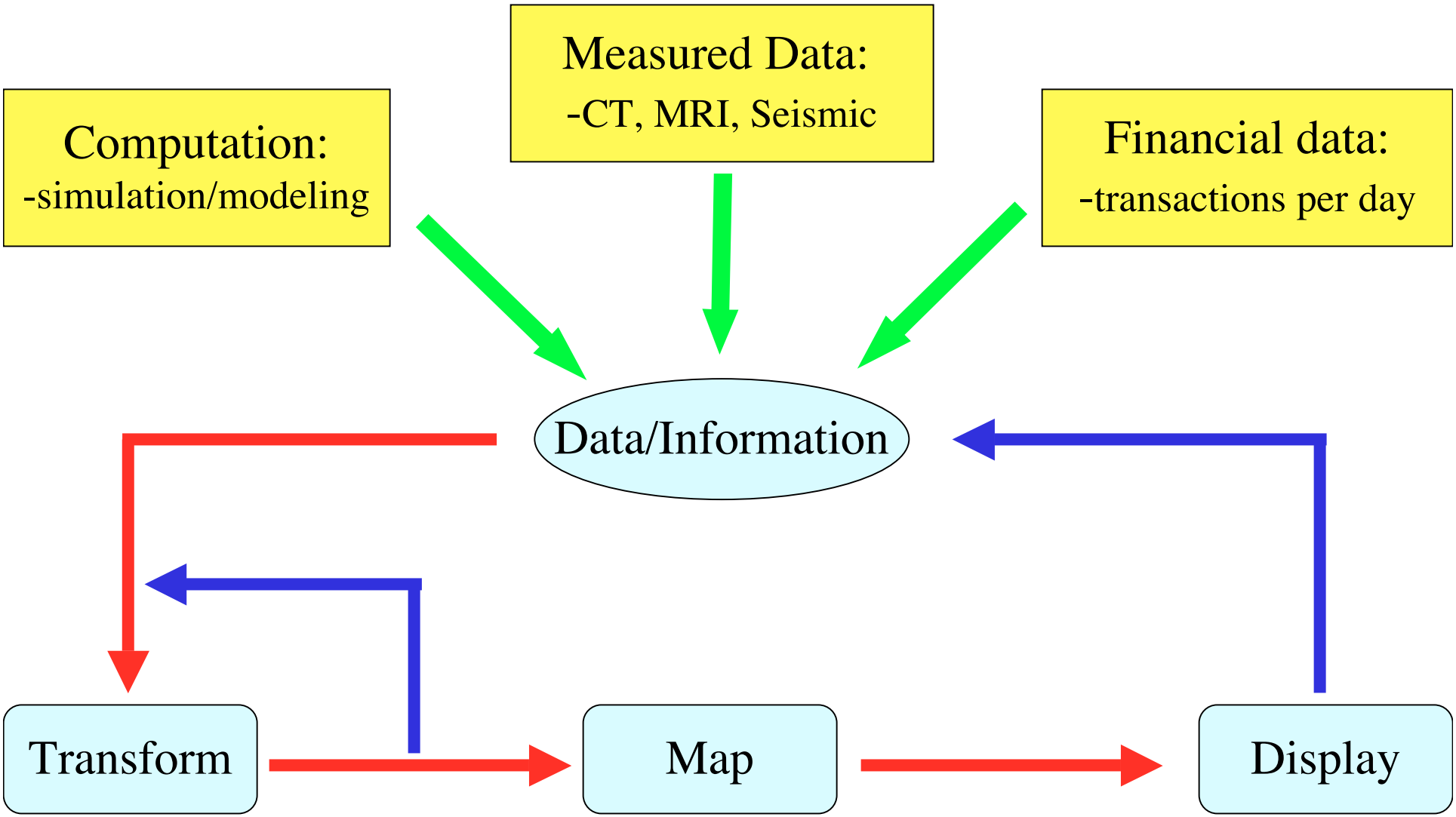
Definition and Concept

What Is Visualization?

- Process of making a computer image or graph for gaining an insight into data/information
  - Transforming abstract, physical data/information to a form that can be seen
  - Interpreting in visual terms or putting into visual forms (i.e., into pictures)

- Cognitive process
  - Form a mental image of something
  - Internalize an understanding

Visualization Process



Example: Visual Representation of Data

- Look at the data table for a biomolecule
  - Table shows atomic types, positions etc.
  - Can you get any information? How does its structure look like?

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HEADER    DEOXYRIBONUCLEIC ACID                   04-JAN-93   111D     111D   2
COMPND    DNA (5'-D(*CP*GP*CP*AP*AP*AP*TP*TP*GP*GP*CP*G)-3') 111D  3
CRYST1   25.230   41.160   65.010  90.00  90.00  90.00 P 21 21 21    8  111D  43
ATOM      1  O5*   C A   1      19.185  35.253  25.139  1.00  0.00      111D  50
ATOM      2  C5*   C A   1      19.533  35.044  23.748  1.00  0.00      111D  51
ATOM      3  C4*   C A   1      20.280  33.726  23.644  1.00  0.00      111D  52
ATOM      4  O4*   C A   1      19.606  32.677  24.281  1.00  0.00      111D  53
ATOM      5  C3*   C A   1      20.487  33.261  22.214  1.00  0.00      111D  54
ATOM      6  O3*   C A   1      21.753  32.648  21.999  1.00  0.00      111D  55
.....................
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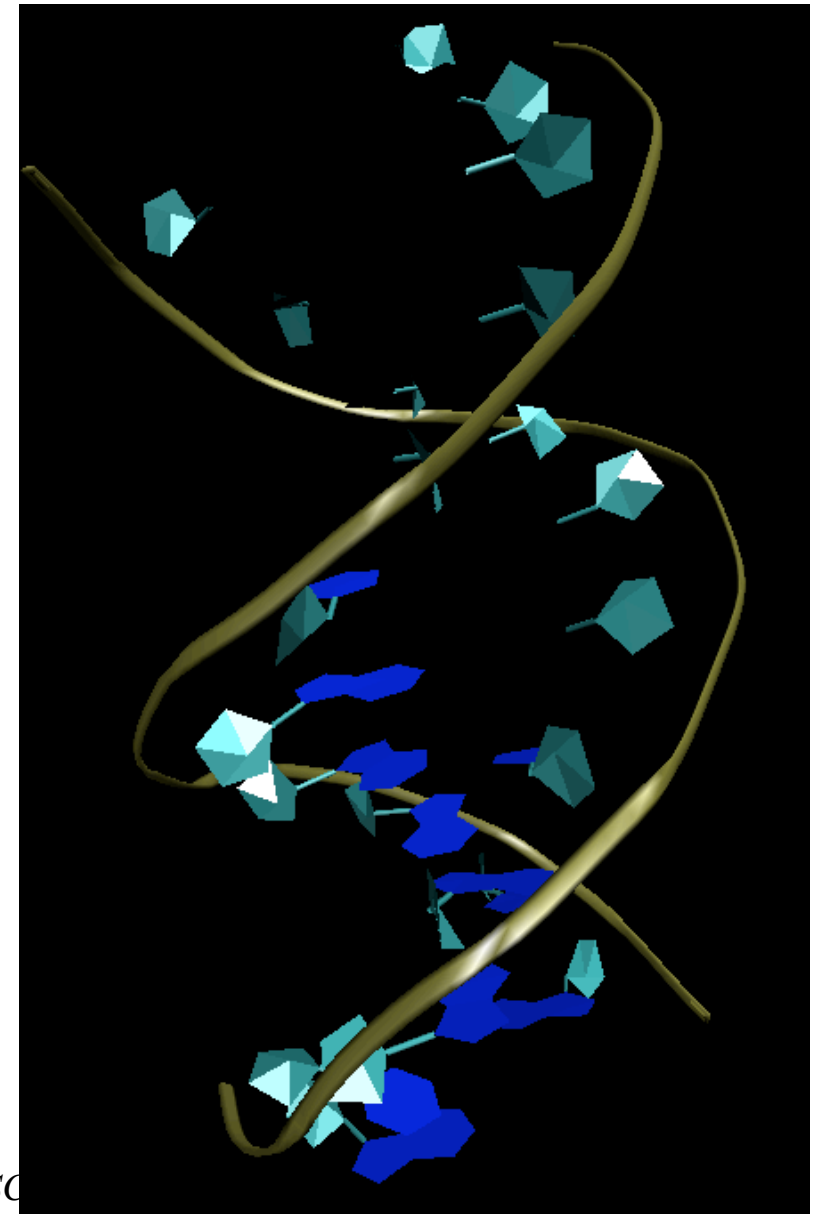
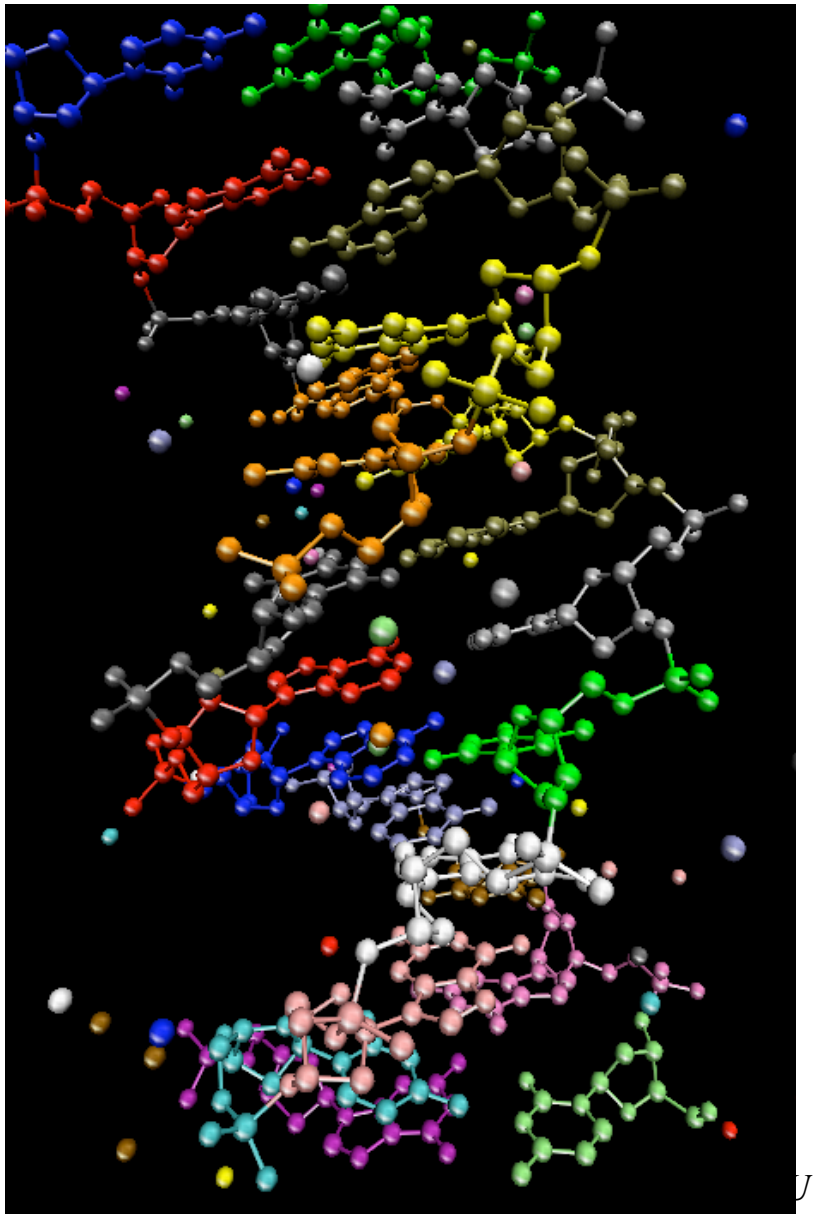
VMD Outputs





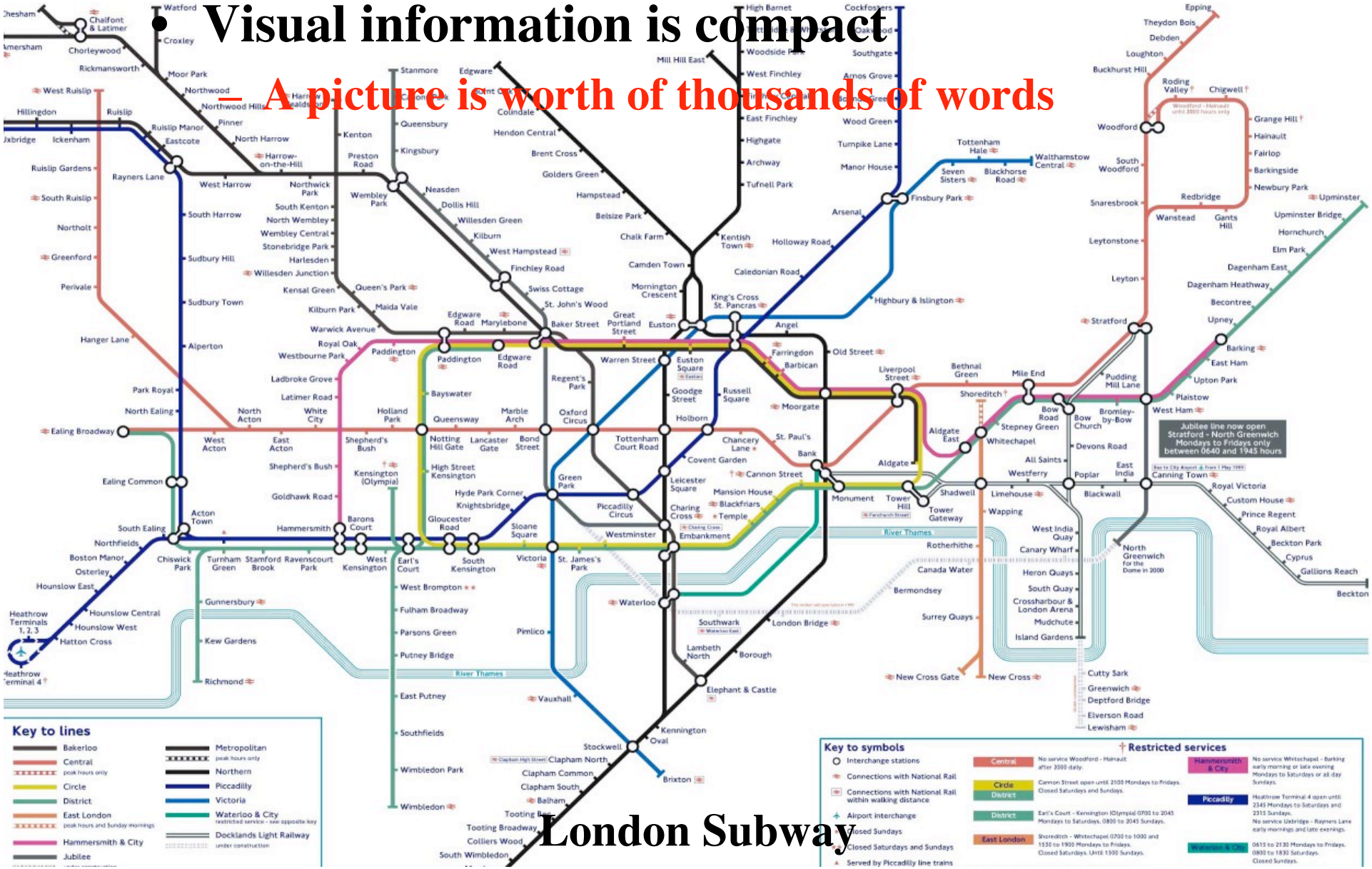
Why Visualization?

- Vision is most important human perception
  - Seeing is believing
- Is there any state in US which is connected to 8 states?

Why?

- Visual information is compact

A picture is worth of thousands of words



London Subway

Why?

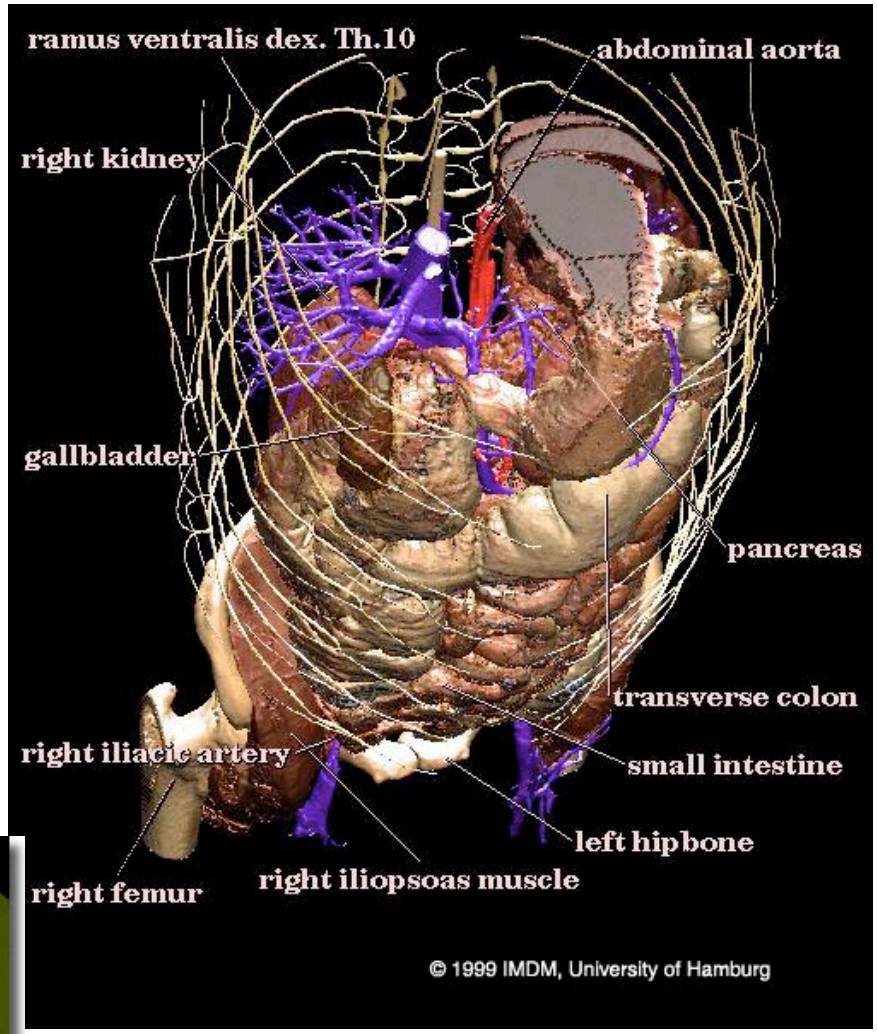
- Extends our vision
  - Removes limits of human vision in space, time, frequency and complexity
  - Creates images or pictures of things that otherwise can not be seen

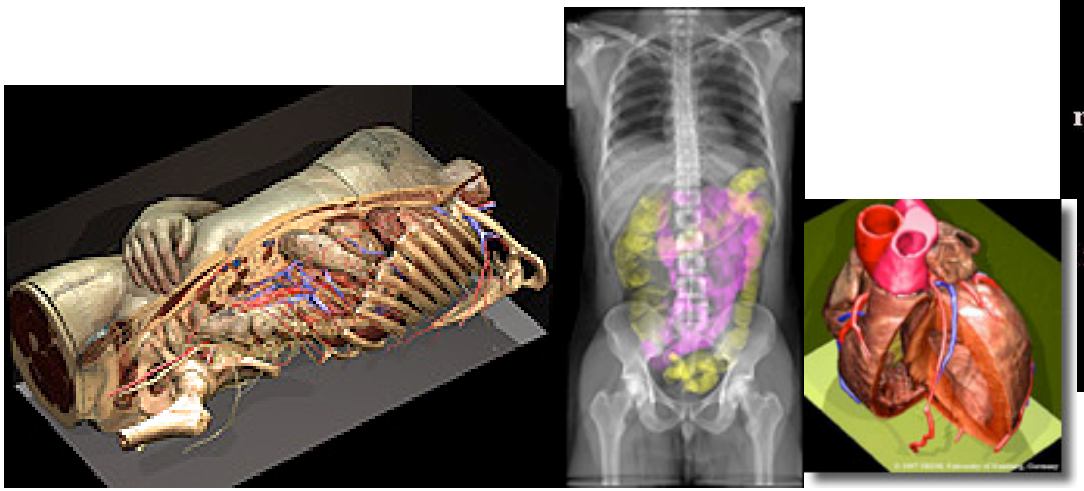
    - See an object's internal structure (visible man)
    - See things that are far away (stars and nebulas)
    - See microscopic world (crystal structure)
    - See things that move very fast (molecular dynamics)

Human Inner Organs

- Visible (voxel) man
  - Reconstruction of human body from tomographic datasets of dissected real body

www.uke.uni-hamburg.de



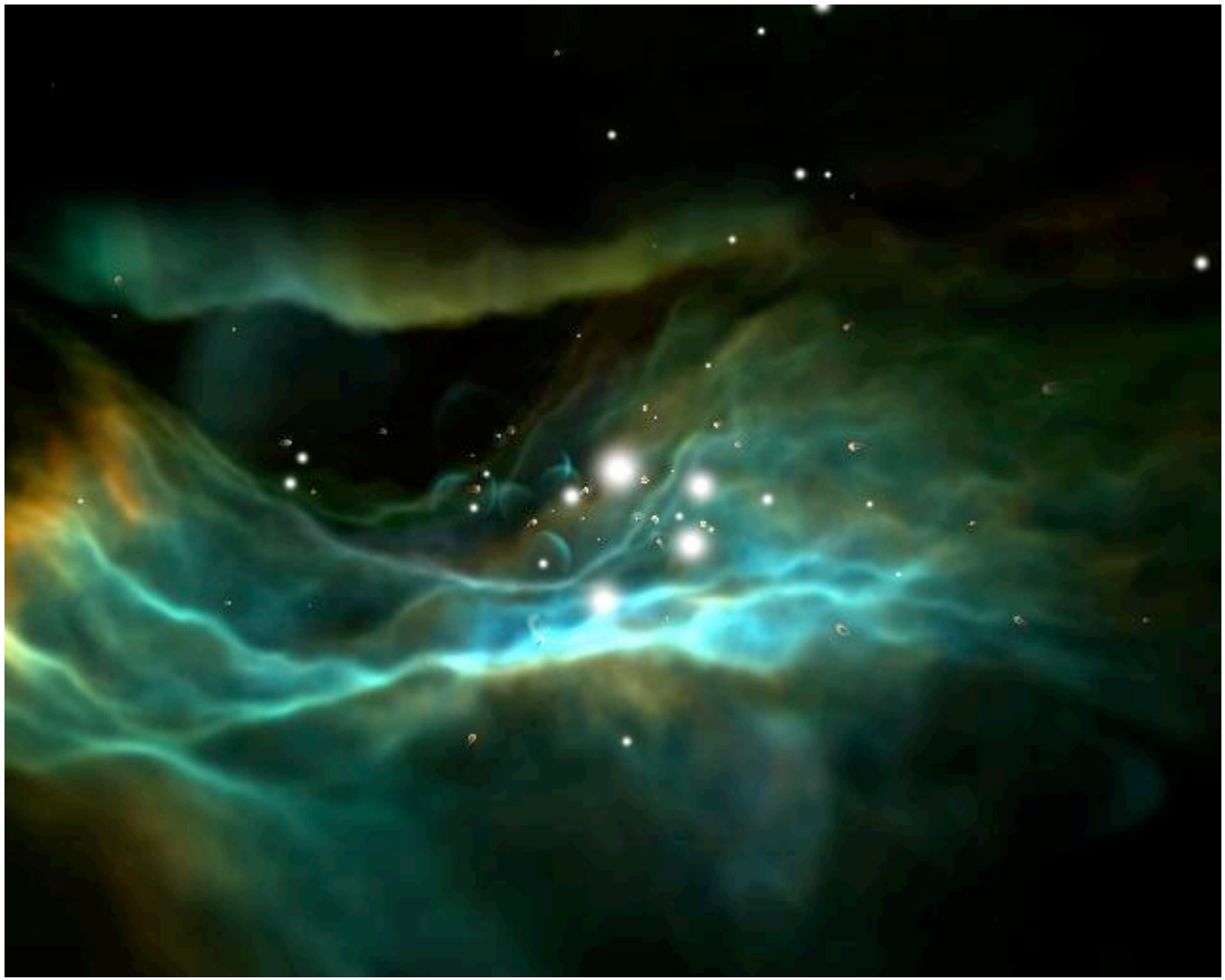


B. B. Karki, LSU

Stars and Emission Nebulas

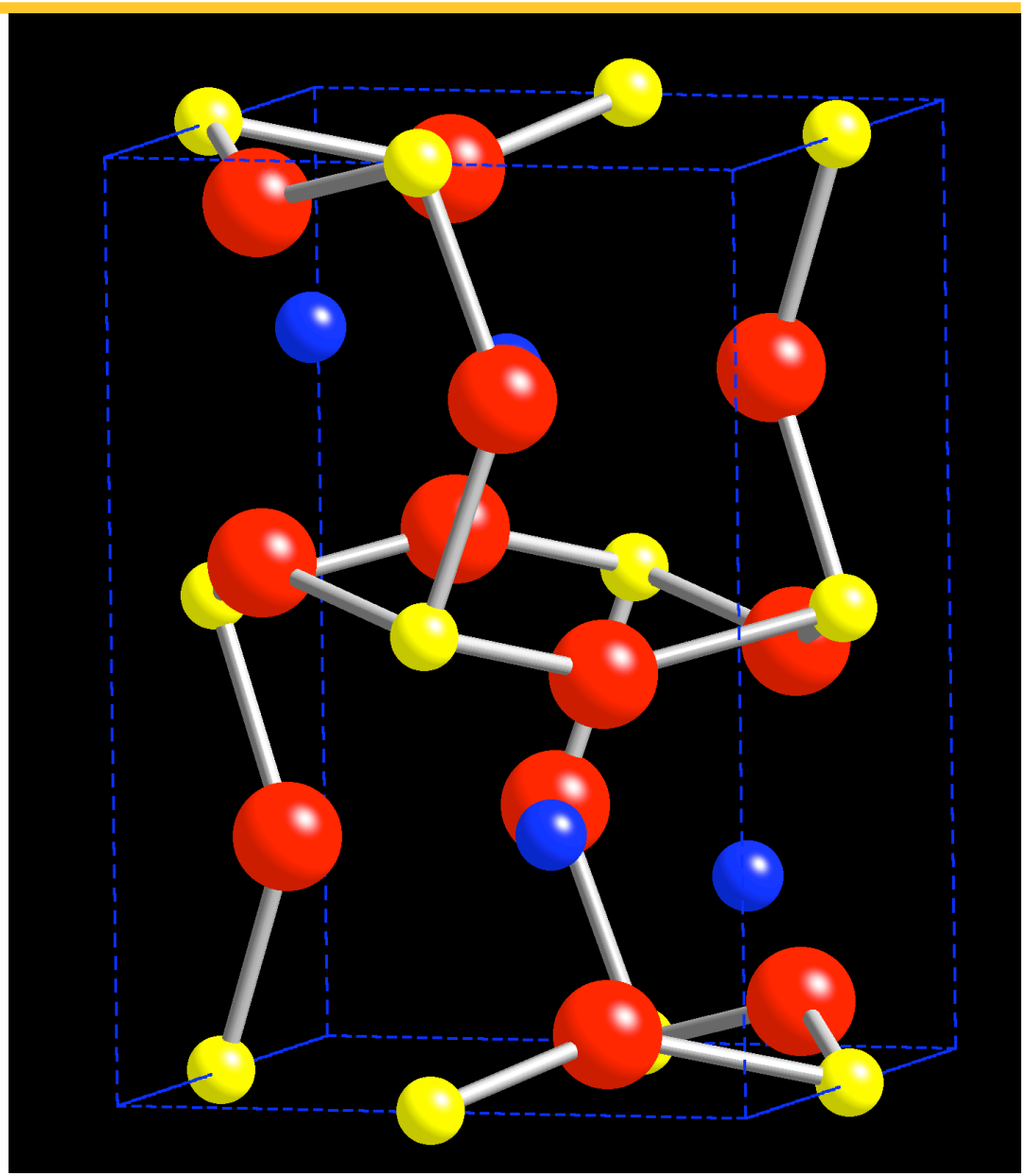
- Visualizing Orion Nebula:
  - Ionization and emissive gas layers, proplyds and shock fronts, and stars

Nadeau et al., Computer Graphs Forum, 20: 27 (2001)



Crystal Structure

- $MgSiO_3$ perovskite
- An orthorhombic unit cell
- Atomic coordination



Molecular Dynamics

Alkanethiol molecular chains on gold substrate: Collective behavior as time elapses in picoseconds (10^{-12} seconds)

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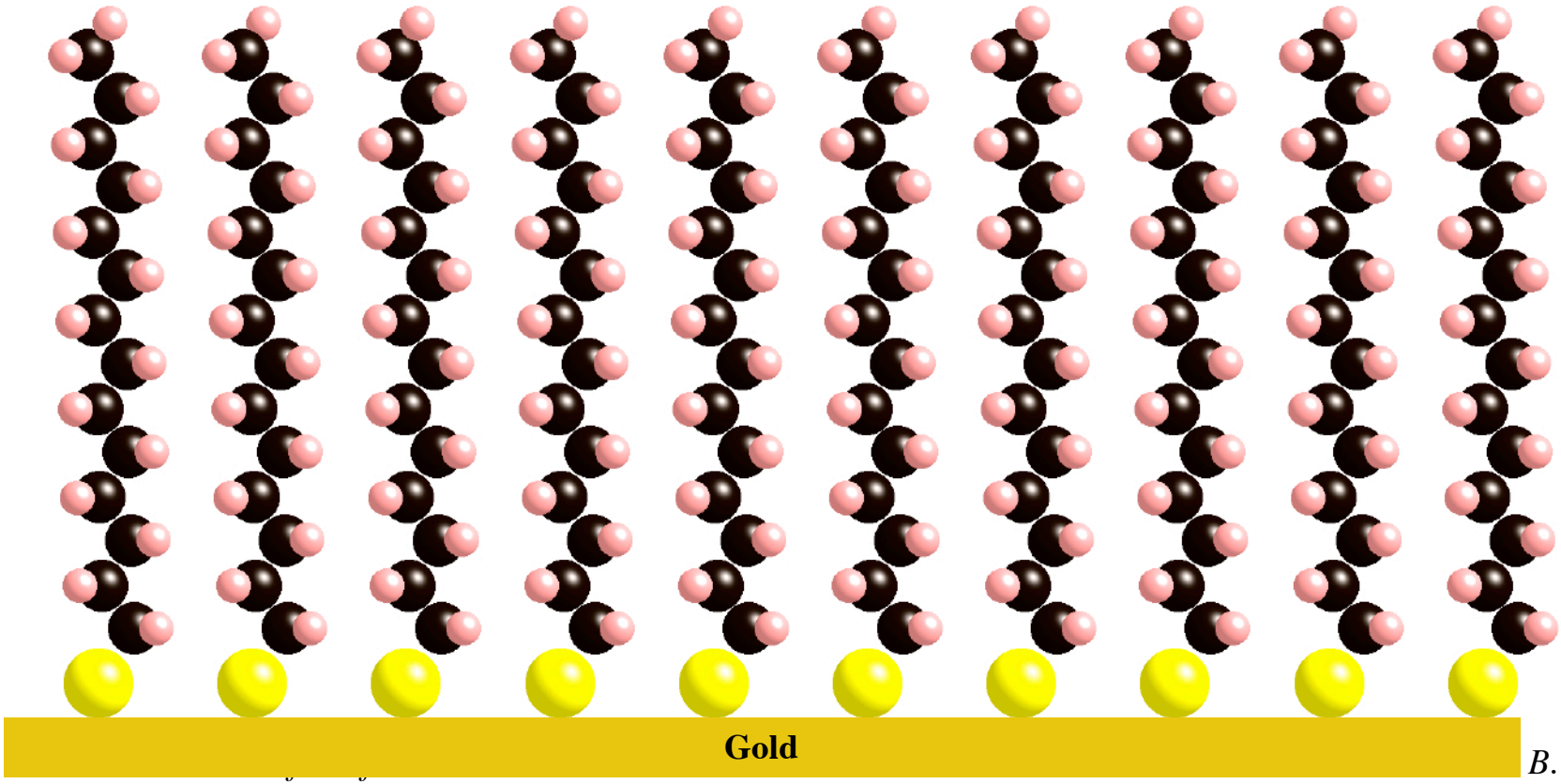

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Why?

- Improves activities
  - Demonstrate, analyze, understand, explore, enlighten
  - Provides a frame of reference (a temporary storage) to help us think

Visualization as a Formal Discipline

- A part of our everyday life
  - Research/education
  - Business/finance
  - Entertainment industry
- Being developed as an important discipline or field
  - 1987 NSF report on visualization in scientific computing
  - IEEE visualization, ACM SIGGRAPH conferences
  - Several more international conferences

Types and Applications

Types of Visualization

- Scientific Visualization
  - Scientific data
- Information Visualization
  - Hypertext, abstract data structures
- Data Visualization
  - A more general term
  - data sources beyond science such as financial, marketing, or business data
  - Broad enough to encompass both scientific and information visualization

Scientific Visualization

- Relates to and represents something physical or geometric
  - Images of human brain
  - Air flow over a wing

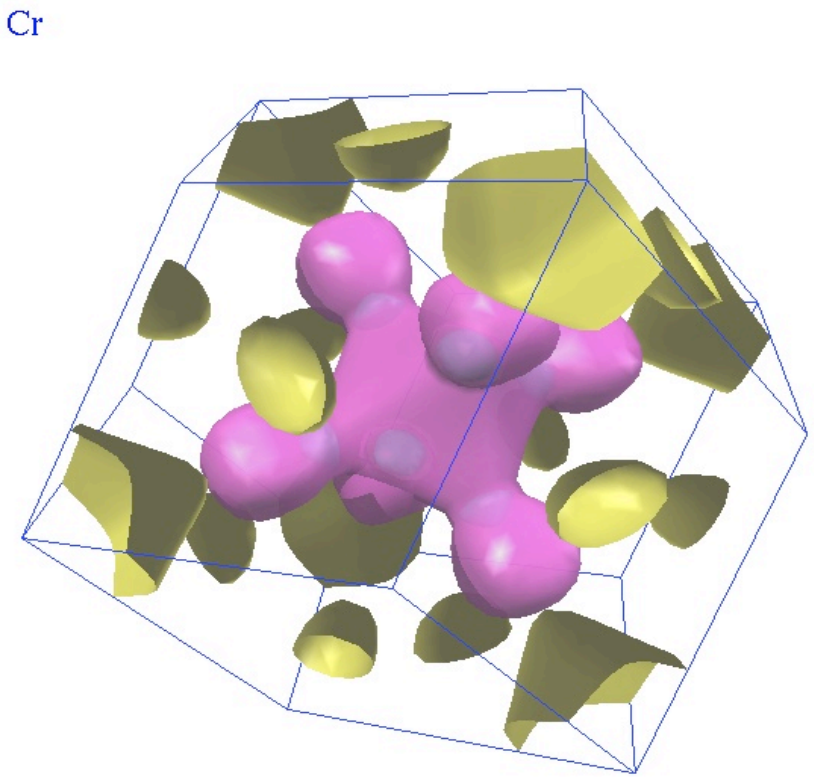
- Data come from scientific computing and measurements

Scientific Computing

- Real materials simulation/modeling
  - Electronic calculations
  - Atomistic MD (molecular dynamics) modeling
  - Finite element (continuum) modeling

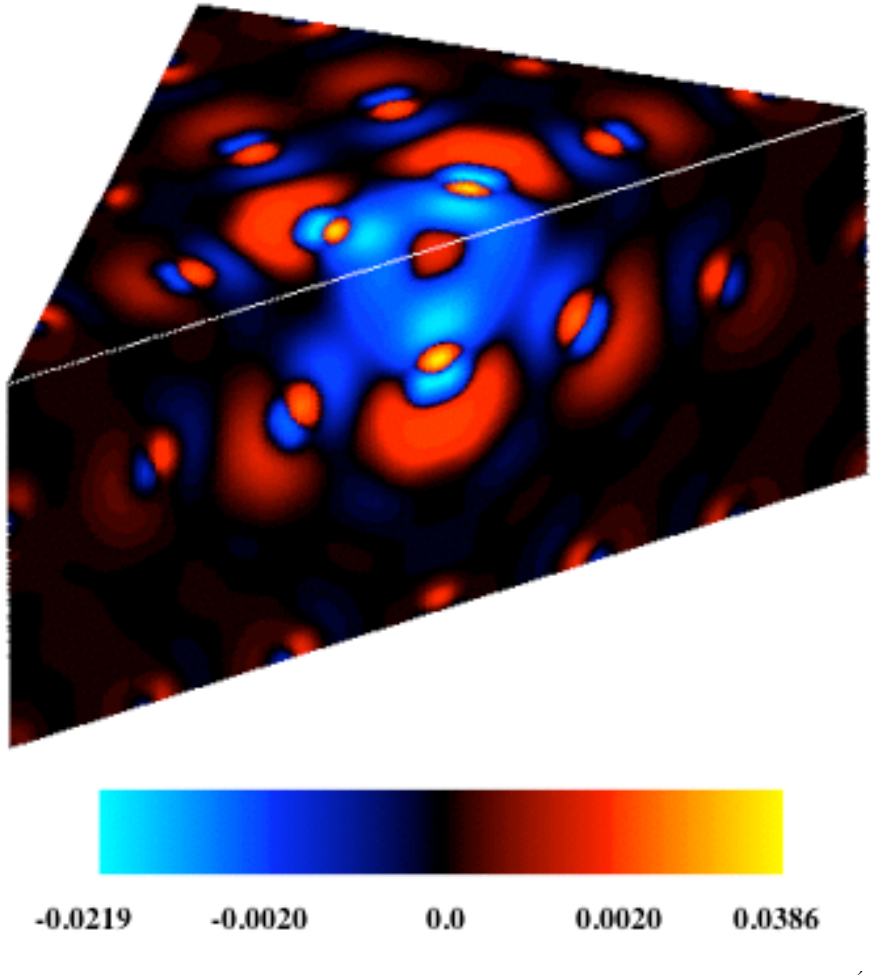
- Solving differential equations
  - Computational fluid dynamics
  - Temperature distribution
  - Electromagnetic field

Example: Electronic structures

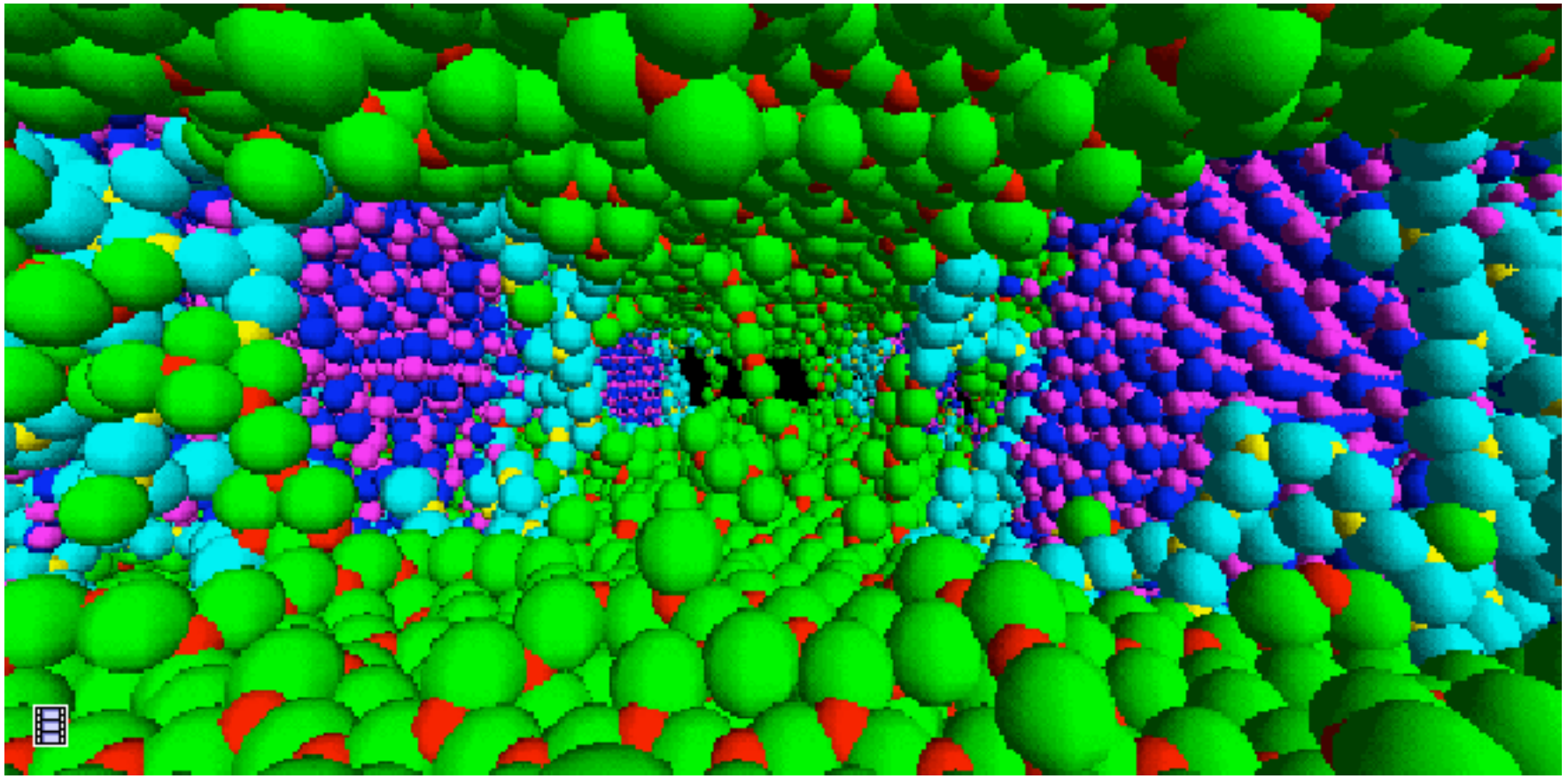


Fermi Surface of Chromium
(3 bands are shown)
http://www.phys.ufl.edu/fermisurface/

Electronic charge density in MgO around a vacancy defect (Red: deposition, Blue: depletion)



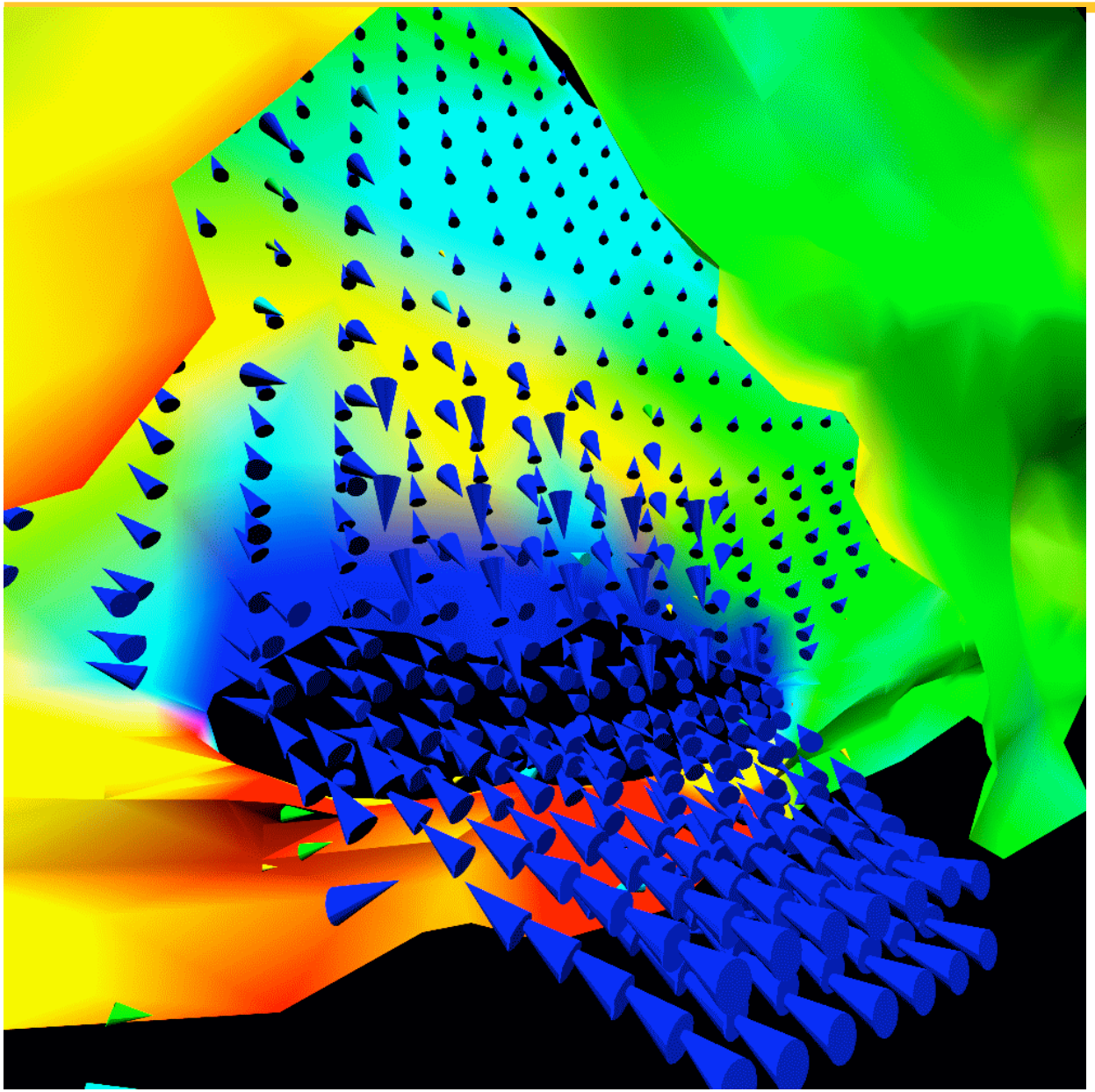
Example: Fracture in Fiber Composite



A billion-atom MD simulation of fracture in SiN-matrix SiC-fiber composite

Nakano et al., 2000

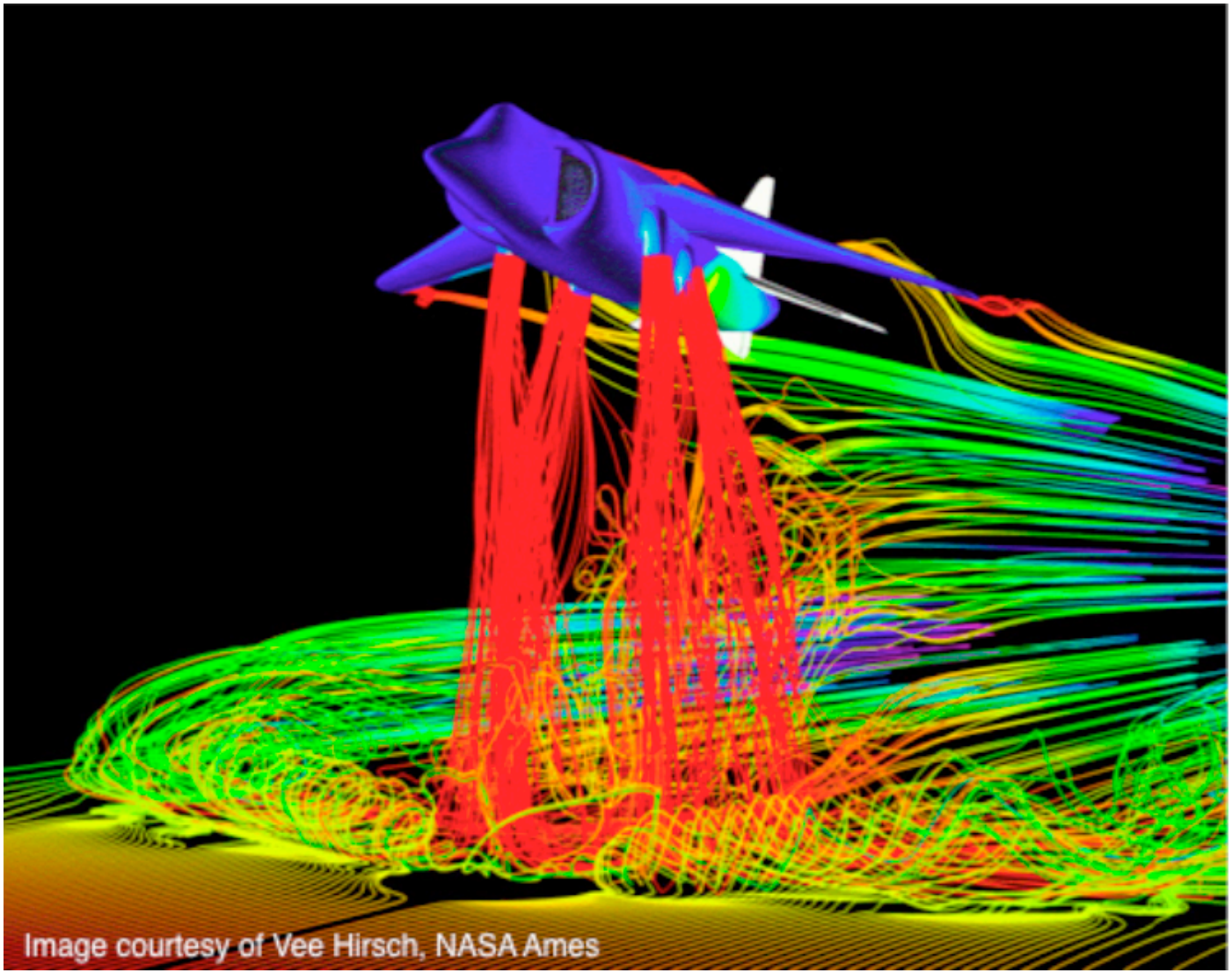
Example: Air Flow over Windshield



Air flow coming from a dashboard vent and striking the windshield of an automobile

http://www-fp.mcs.anl.gov/fl

Example: Air Flow Around Plane



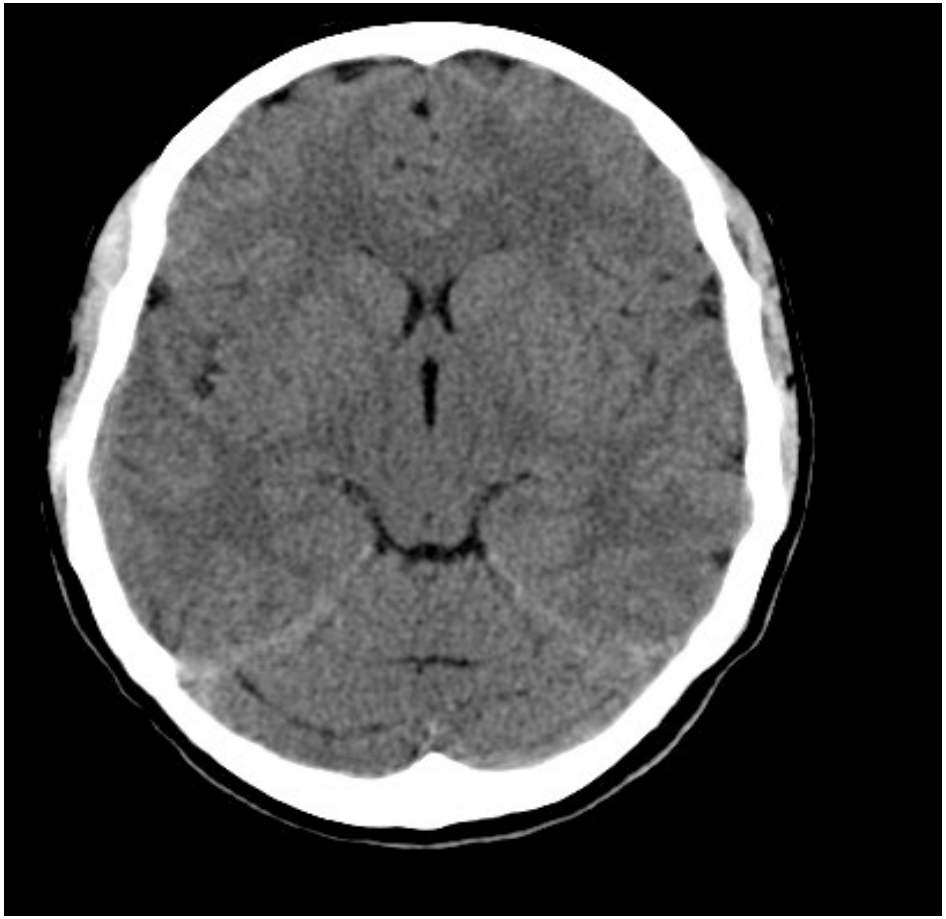
Streamline representation of air flow (vector field)

Scientific Experiments

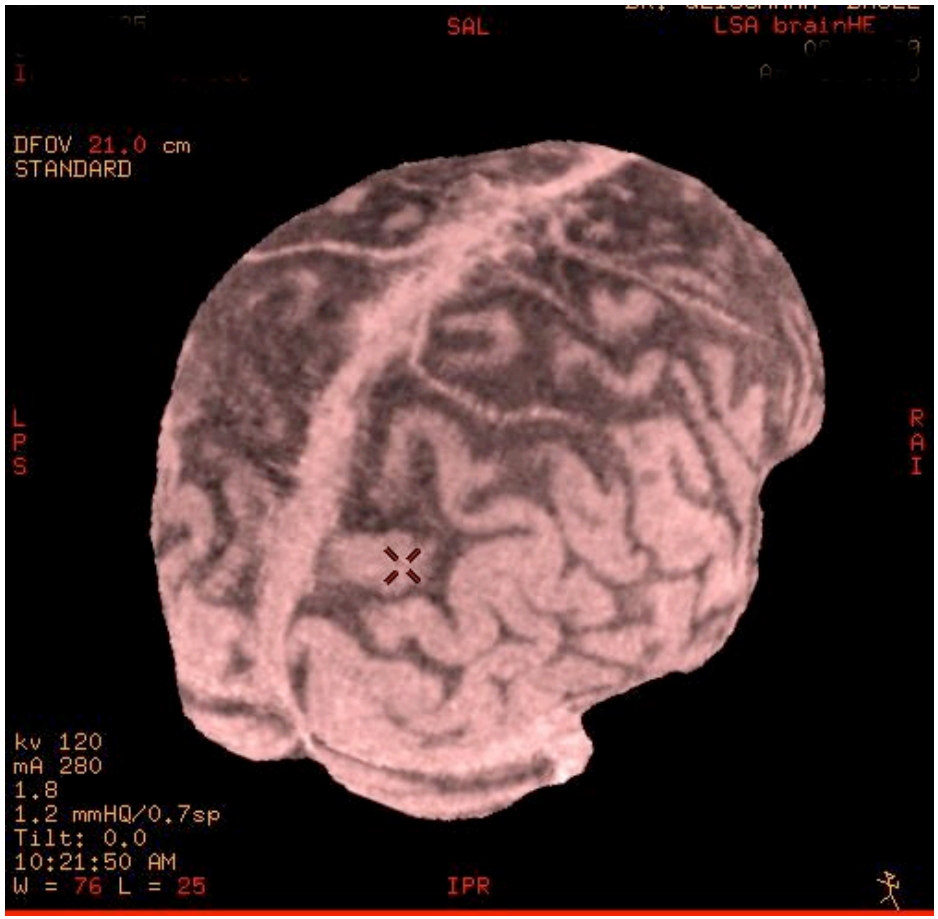
- Medical
  - Magnetic resonance imaging (MRI)
  - Computed tomography (CT)
  - Ultrasound
- Biological
  - Confocal microscope
  - Electron microscope
- Physical
  - Scanning tunnel microscope (STM)
  - Atomic force microscope (AFM)
- Earth science
  - Space station
  - Seismic tomography
- Object shape capture
  - 3D laser scanner

Example: Medical Imaging

Standard brain CT image

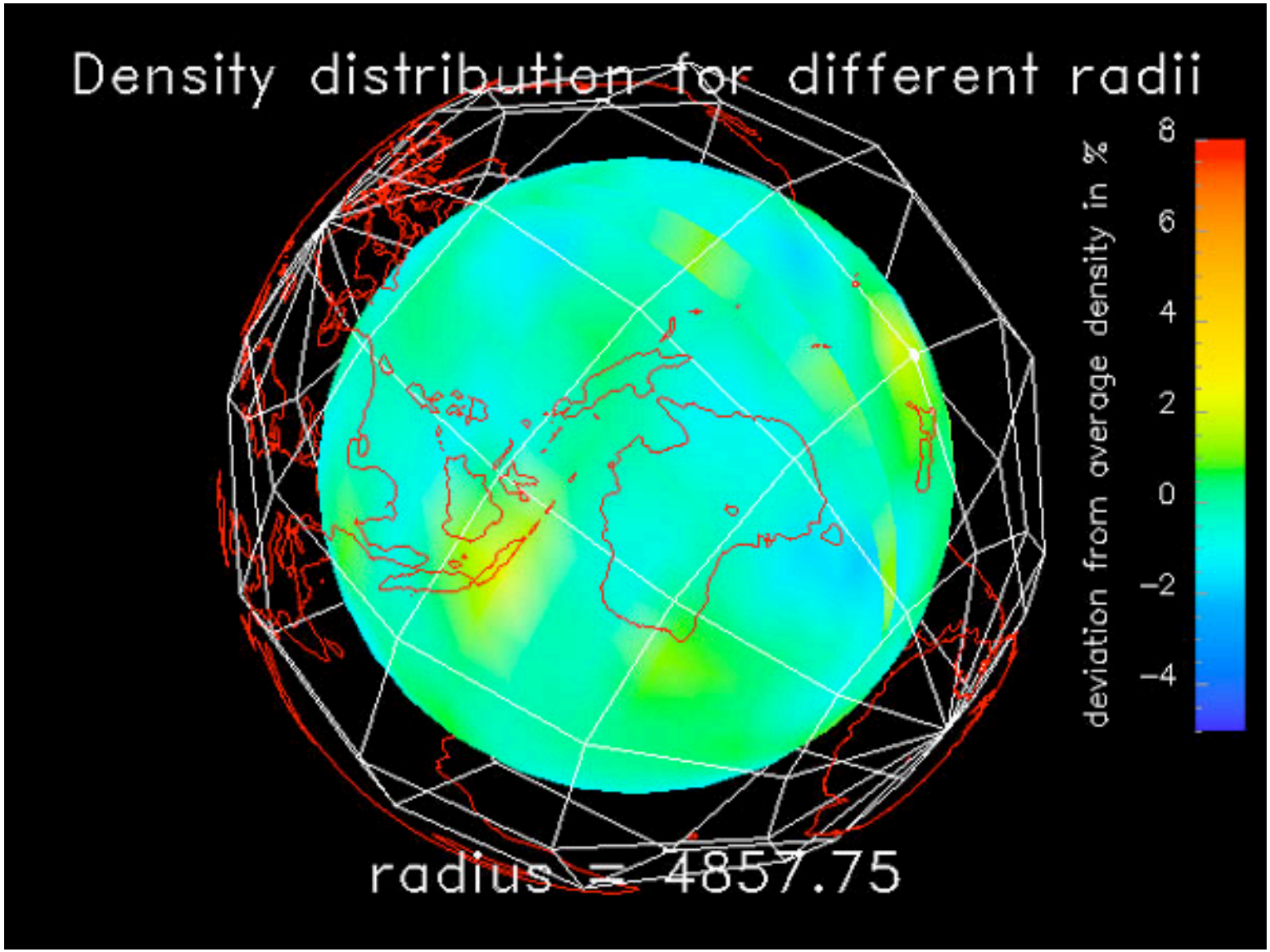


Volume rendered brain image



http://www.gemedicalsystems.com

Example: Convection in Earth's Mantle



www.vislab.usyd.edu.au/education/sv3/2001

Information Visualization

- What is information?
  - Items, entities, things which do not have a direct physical relevance, e.g, stock trends, baseball statistics, car attributes
  - Text, statistics, financial/business data, internet information

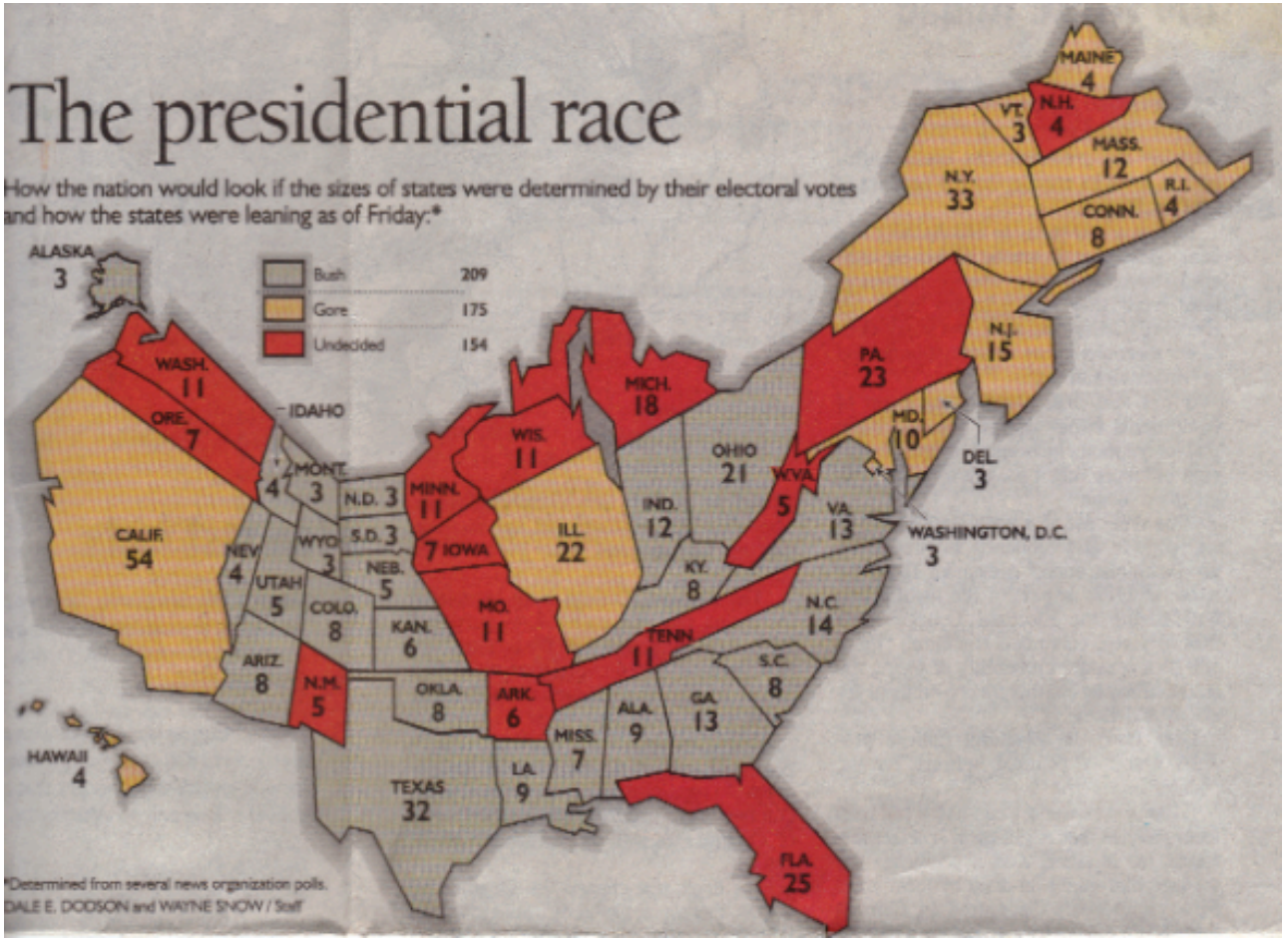
- Visual representation of abstract entities
  - To amplify cognition
  - Useful for analysis, explanation and decision making

Example: Power Costs

Average cost per month

Wall Street Journal, August 16, 2001

Example: Electoral College



Atlanta Journal, November 5, 2000

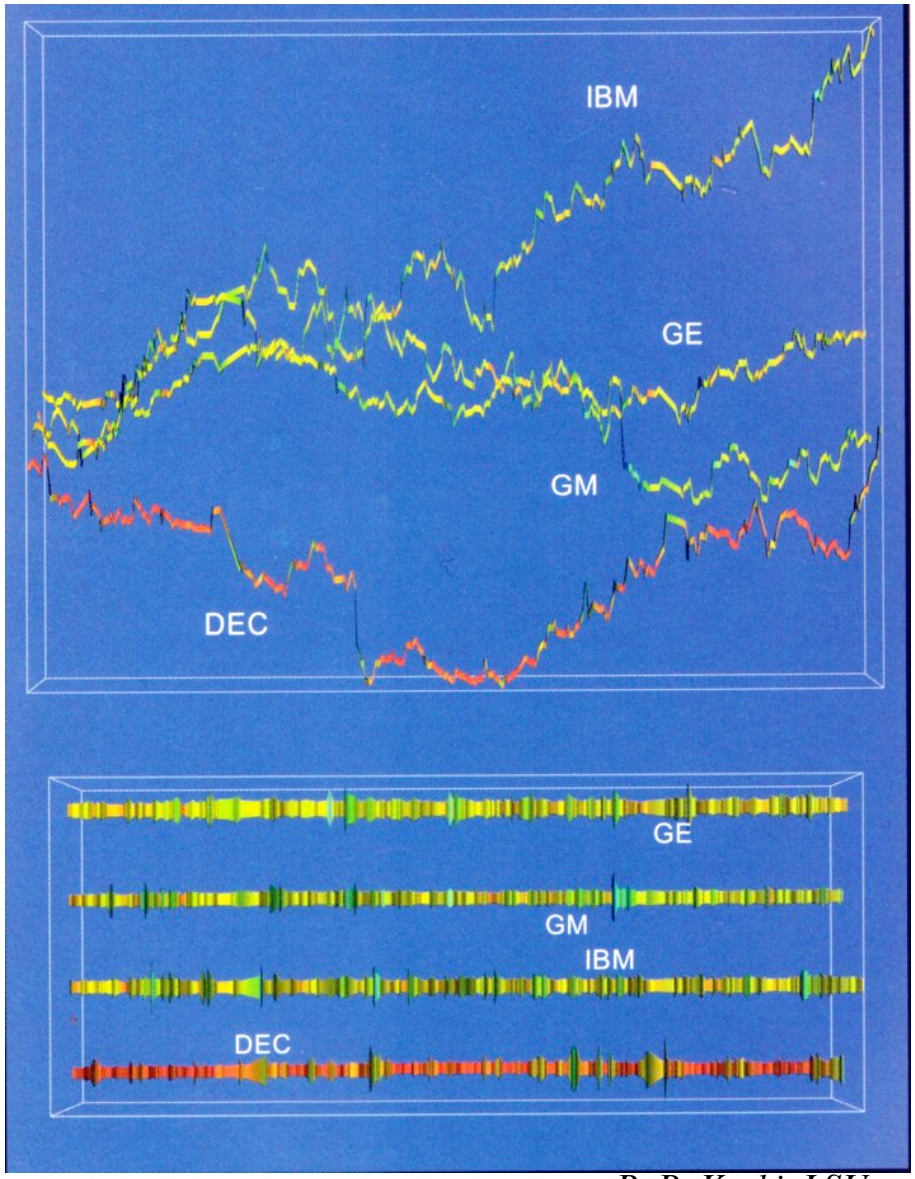
Example: London Subway

www.londontransport.co.uk/tube

Example: Stock Market Data

- Financial visualization of stock market
  - Four stocks over time
- Lines are wrapped with variable radius tubes
  - Side view: History of stock closing prices
  - Top view: Changes in stock volume with time

Visualization Toolkit, Schroeder et al., 1997



Application Areas

- Medical
- Biology
- Physics
- Astronomy
- Chemistry
- Earth sciences
- Engineering
- Metrology
- Business
- Finance
- Computer science

Issues

What make Visualization Challenging?

- Scale
- Dimensionality
- Data types
- Visual mapping
- Interactivity

Data Explosion

- How to make sense out of the datasets when they become very large
- Scientific data
  - A million-atom simulation: 7 GB/step
  - Satellite or space station: TB/day
  - MRI dataset: 256^3 = 16 MB/slice
  - Laser scanning: 2 million points/minute
  - Geographically distributed data
- Complex society
  - There simply is more stuff
  - Access to an incredible amount of data (news, sports, purchases) by computers, internet and web
  - New York stock market: billion transactions/day

Dimensionality

- Three dimensional (trivariate) data
  - We are in 3D world
  - Volume visualization (mapping 3D data to 2D screen)
- Time-varying data
  - Dynamic nature
- Multi-dimensional (hypervariate) data
  - Car attributes: Make, model, year, miles per gallon, cost, no. of cylinders, size, weight
  - Financial data: Investment as a function of interest rate, initial investment, time, income, and so on
  - How to display relationships between many variables

Data Types

- Structured versus unstructured data
  - Unstructured (irregular) data are less compact and efficient
  - Preprocessing of data
- Scalar, vector and tensor data
  - Data from flow dynamics
  - Stress-strain data
- Multiple data sets
- Non-numerical data
  - Ordinal: days of the week
  - Categorical data: names of animals

Visual Mapping

- Display without ambiguity
  - Colors, lighting, translucent, animation, texture mapping
- Too much data for too little display area (screen)
  - Too many cases
  - Too many variables
- Need to highlight particular cases or variables

Interactivity

- Visualization is naturally interactive
- Show multiple different perspectives on the data
- Real-time interactions
  - Immersive interactive (virtual reality) environments

Available Programs and APIs

OpenGL

- Industry standard for a graphics API (Unix, PCs, Macs)
- Assembler language of computer graphics
  - One can have ultimate control in developing application
  - Faster execution
  - Most software is based on OpenGL
- Access from C/C++, Fortran, JAVA
- Window-system and operating system independent
- Source: *www.opengl.org*

Visual Molecular Dynamics (VMD)

- Designed for biological macromolecules
- Immersive and interactivity
- Freely available for Unix, Mac and PCs
- Source: *http://www.ks.uiuc.edu/Research/vmd/*

Visualization Toolkit (VTK)

- An open source, freely available software system
- Visualize any data in 3D -- medical, scientific or financial
- Build applications with C++, Java or Tcl
- Implemented on Unix-based platforms and PCs
- Source: *http://public.kitware.com/VTK*

Advanced Visual Systems (AVS)

- AVS/Express, OpenViz
- Object-Oriented (C++, Java, Visual Basics)
- 3D stereo immersion and interactivity
- OpenViz for displaying business data
- Source: *www.avs.com*

OpenDX (Data Explorer)

- Open source software version of IBM visualization DX
- Unix, Linux, Macs and Pcs
- Work in client/server environment, and distributed processing
- Source: *www.opendx.org*

Open Inventor

- Object-oriented toolkit (C and C++)
- Window system and platform independent
- Supports SGI graphics
- Serves as the basis for virtual reality modeling language
- Source: *www.sgi.com/software/inventor*

Amira

- Based on OpenGL and open inventor
- Window, Unix, Linux
- Automatic and interactive segmentation of data
- Various file formats such as tiff, jpeg, binary data
- Source: *www.amiravis.com*