I Want To Be a Computational Mathematician

(with apologies to Paul Halmos)

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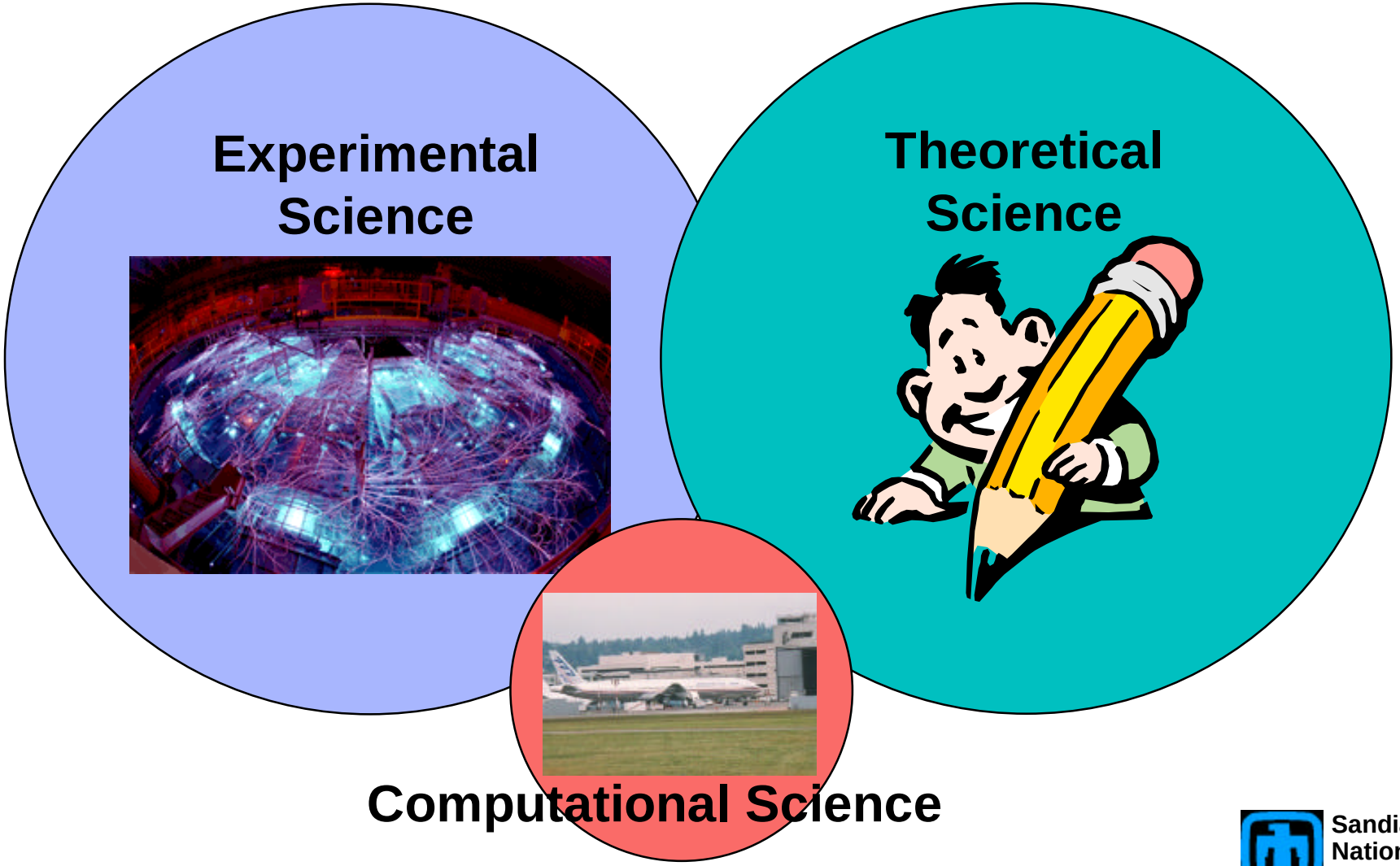
Science in the 1890's

Experimental Science

Theoretical Science

Science in the 1990's



Modeling and simulation are being used in safety critical situations

http://www.boeing.com/commercial/777family

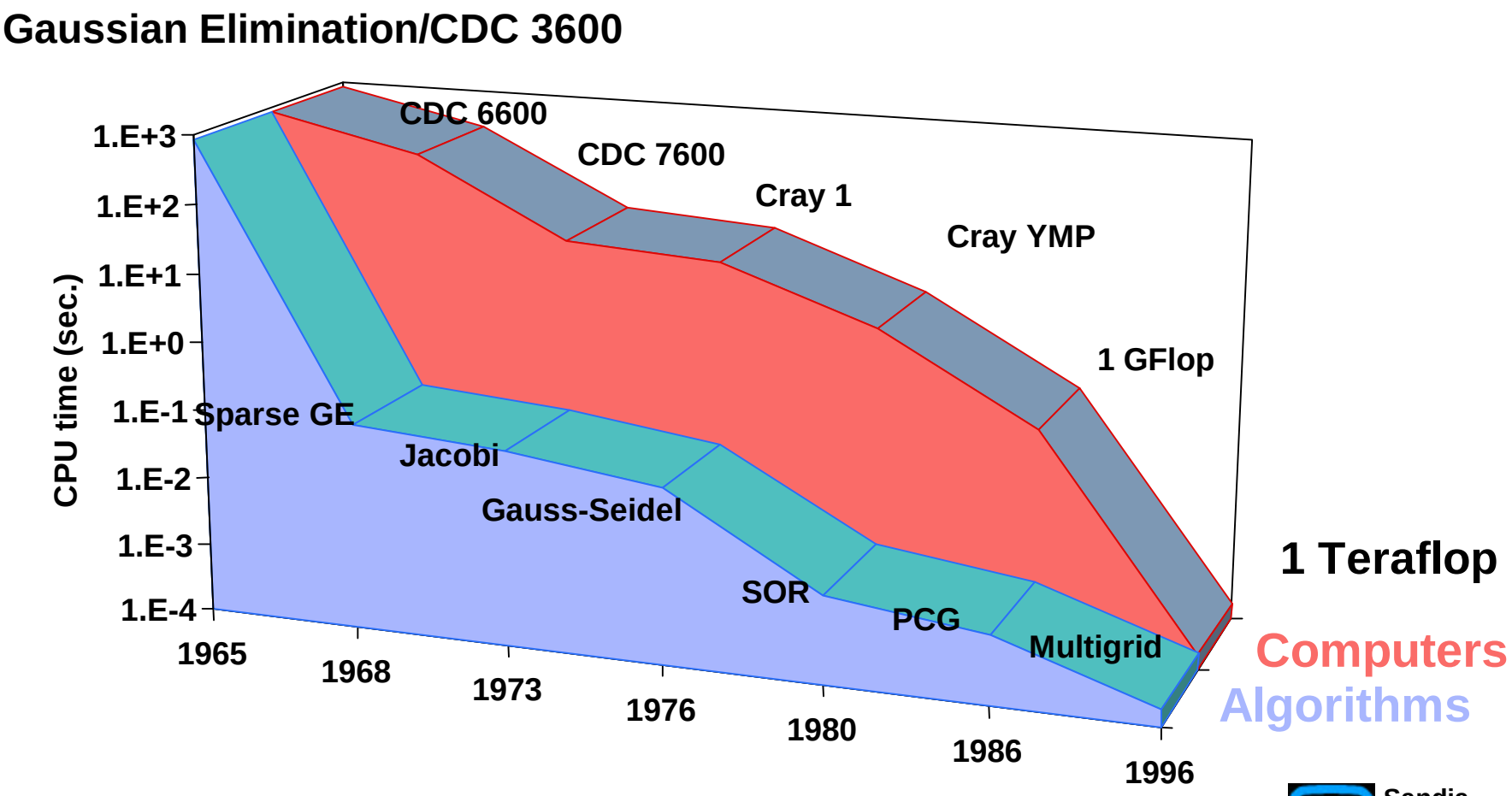
- The Boeing 777 is the first jetliner to be 100 percent digitally designed using three-dimensional solids technology.
- Throughout the design process, the airplane was preassembled on the computer, eliminating the need for a costly, full-scale mock-up.

Boeing expects 20% less manufacturing errors.

What's different today from yesterday?

- Experimental science has become increasingly difficult and expensive to do
- Computing power has increased tremendously
- Computational sciences and mathematics has taken on a new role
- Improvements in algorithm development have outpaced computing improvements !!!

New algorithms have yielded greater reductions in solution time than hardware improvements



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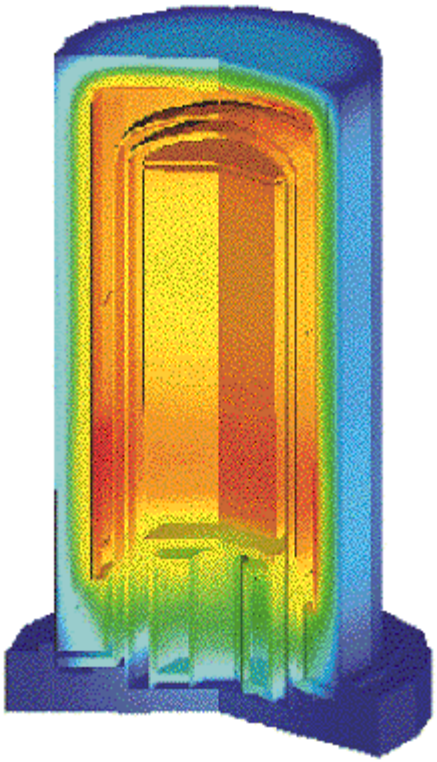
Quick tour of projects at Sandia

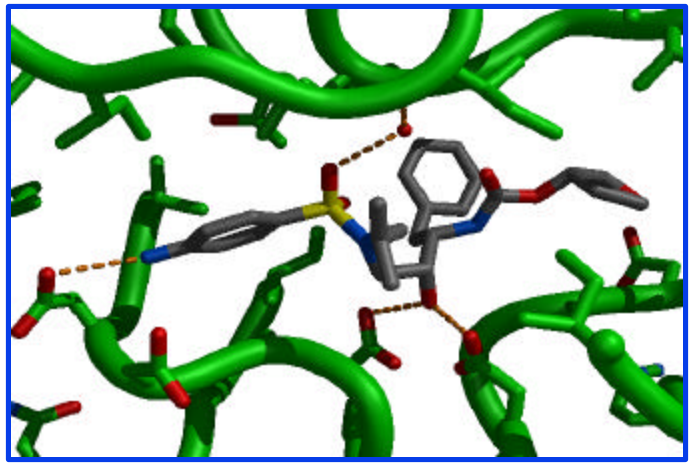
- Computational mathematics at Sandia is applications driven
- I'll only touch on 2 major areas
  - optimization
  - iterative methods for linear systems
- (Many) More details can be found at
  - http://csmr.ca.sandia.gov
  - http://www.cs.sandia.gov

Optimization methods are used in a variety of applications



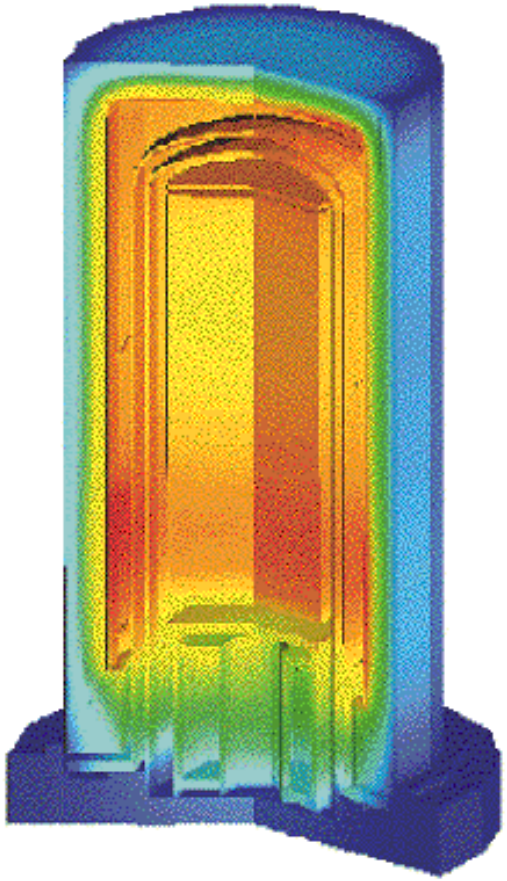
Temperature fields in a vertical, stacked-wafer, low-pressure, chemical-vapor-deposition furnace

Predictive fire codes can help fight aircraft fires

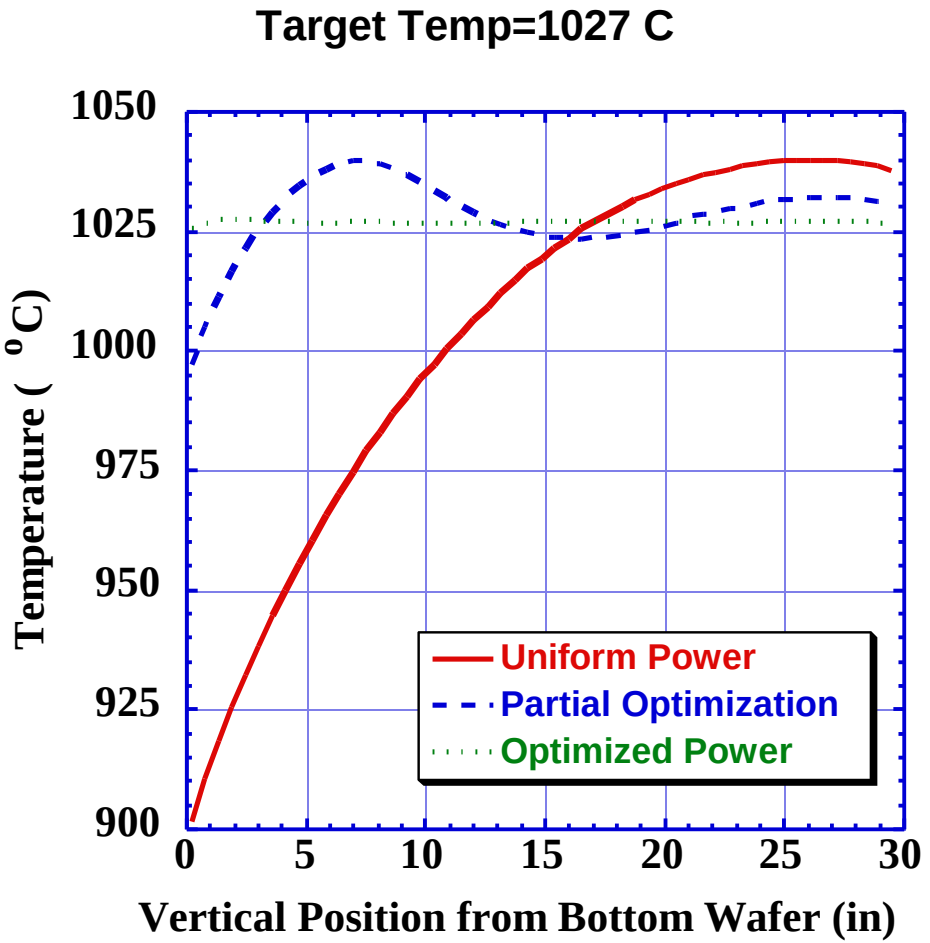


HIV-1 Protease complexed with Vertex drug VX-478

Optimized power distribution enhances wafer temperature uniformity for steady-state open-loop operation



Temperature fields in a vertical, stacked-wafer, low-pressure, chemical-vapor-deposition furnace



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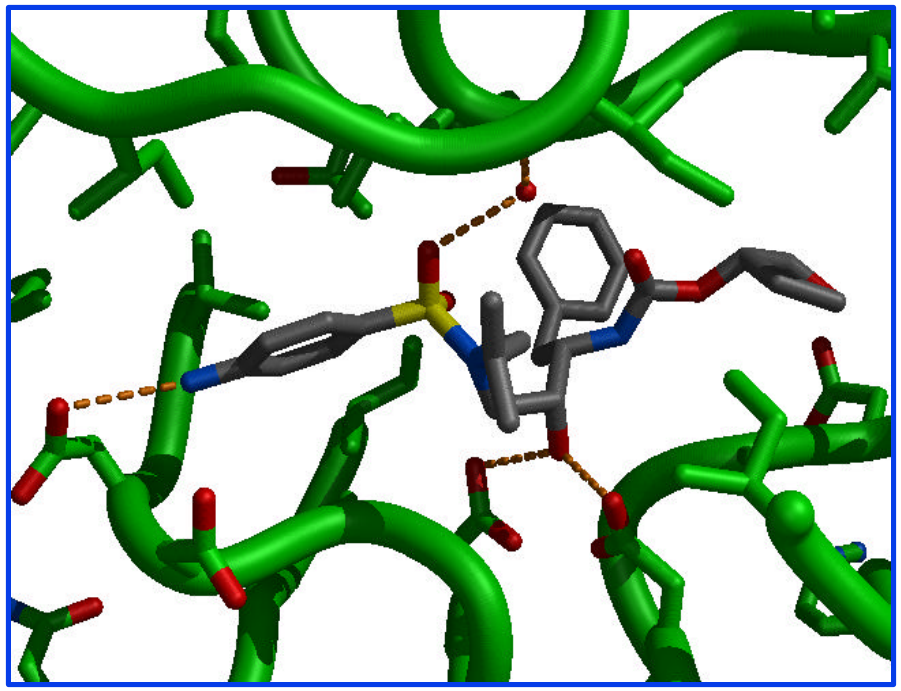
Model-based safety assessments can be used to simulate accident scenarios

- Goal is to determine the worst-case response
- Simulation of coupled sub-systems requires new methods
- Complex physics and 3D geometries make this a difficult problem

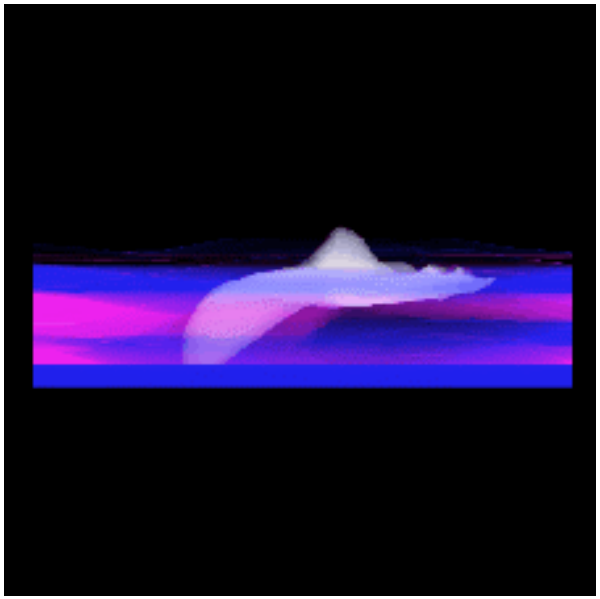
Drug design can be viewed as an energy minimization problem in computational chemistry



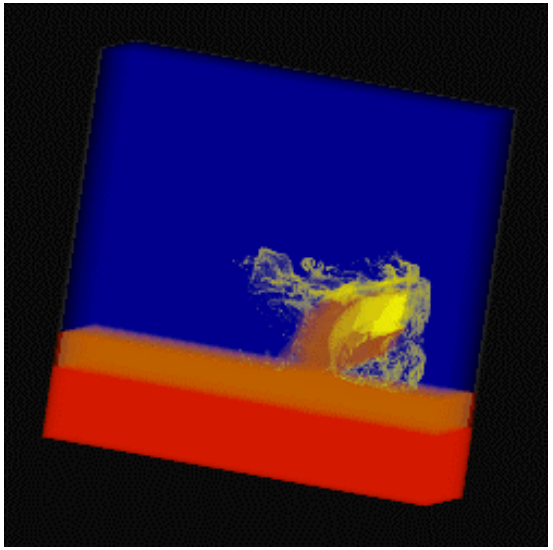
HIV-1 Protease Complexed with Vertex drug VX-478

- A single new drug may cost over $200 million to develop and the design process is typically takes about 13 years
- Typically there are thousands of parameters and constraints
- There are thousands of local minima

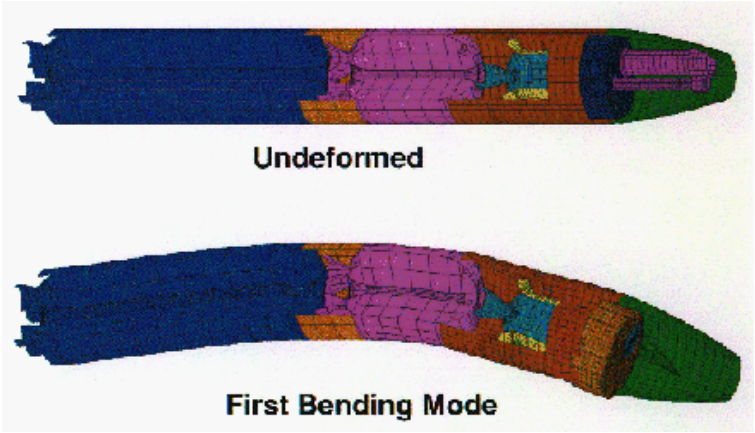
Other interesting mathematical problems arise in the solution of large linear systems of equations



Simulation of 1 km comet splashing into the Atlantic ocean using 50 M cell calculation



Visualization of a large oil and gas data set (about 100 million cells).



Linear structural dynamics analysis requires MP eigensolvers

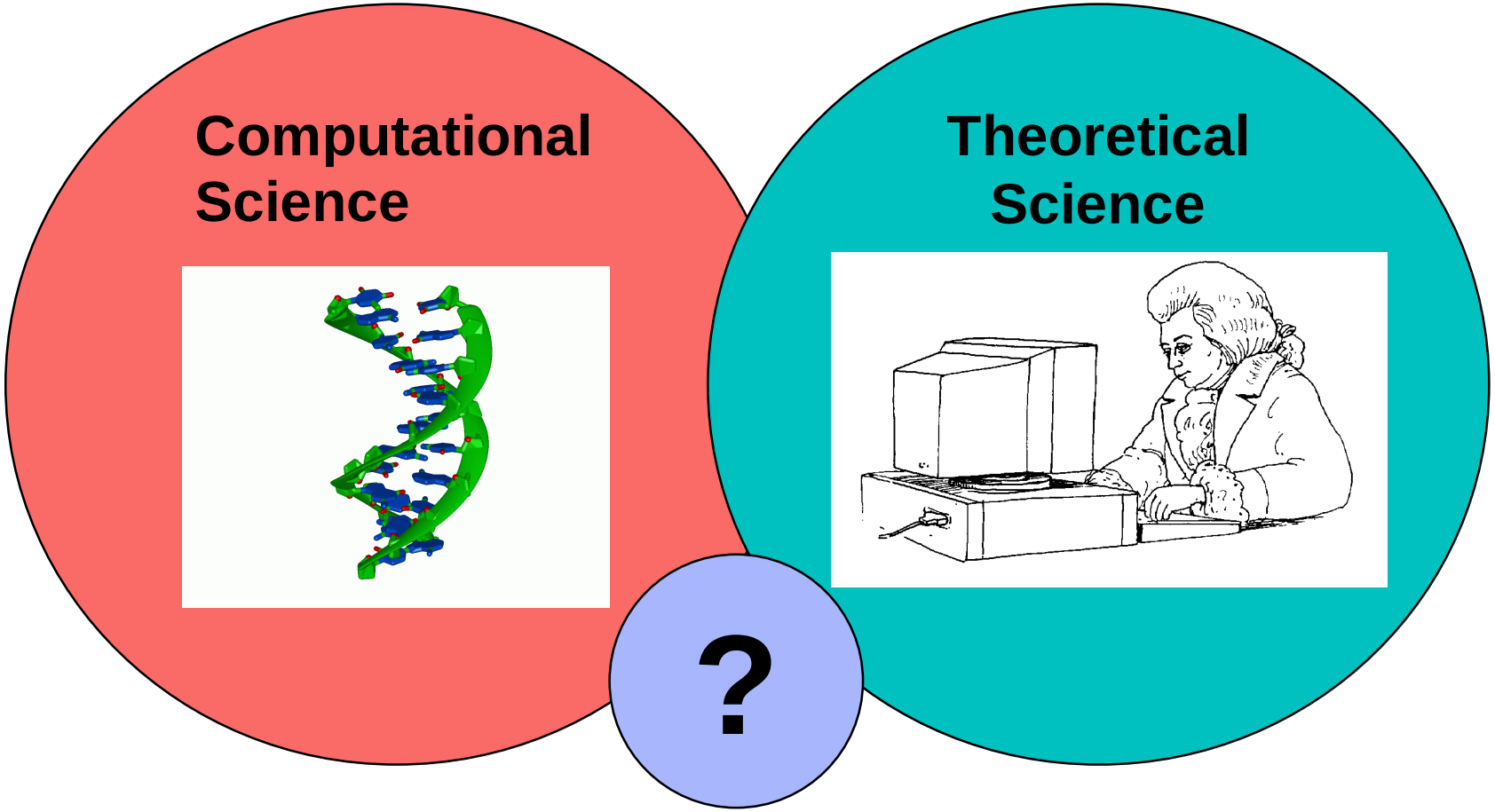
Recap

- Modeling and simulation have taken on a new role in scientific discovery
  - Many projects are in relatively new fields
  - Almost all projects are interdisciplinary
  - Solutions to these problems require intensive computational resources
- Computational mathematics is at the heart of most simulations
- New computing paradigms force us to constantly change our way of thinking

A few areas of research include:

- Basic algorithm development, especially in the area of scaleable parallel algorithms
- Parallel optimization methods for large-scale nonlinear constrained problems
- Parallel linear solvers for problems with > 10 billion unknowns

Science in 2050 ?



Where do we go from here

- We desperately need to have more people in computational mathematics
- Must have a fundamental understanding of the mathematics
- Must have a strong computing background
- Need to have new ways of thinking about problems

Why do I want to be a computational mathematician?

- Challenging problems of national importance
- Wide range and diversity of problems
- FUN !!!!