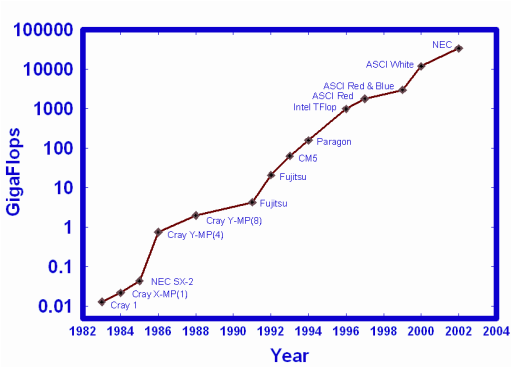
COMPUTATIONAL ENGINEERING SCIENCES IN THE 21ST CENTURY

Thomas C. Bickel

Engineering Sciences Center
Sandia National Laboratories
Albuquerque, New Mexico 87185-0841
tbickel@sandia.gov

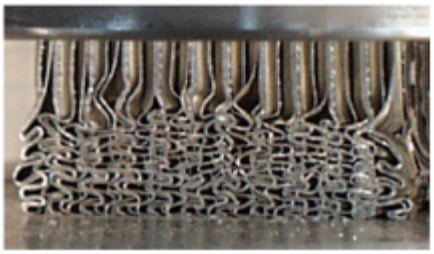
The field of Computational Engineering Sciences has made phenomenal advancements over the past century. To quote Michael Overton[1], *"The traditional two branches of science are theoretical science and experimental science. Computational science is now mentioned as a third branch, having a status that is essentially equal to, or perhaps eclipsing, that of its two older siblings."* Yet, we still struggle with peers who minimize the value of computational results. Examples abound, such as the statement attributed to the aero community by Pat Roache,[2] *"No one believes the computational fluid dynamics results except the one who performed the calculation, and everyone believes the experimental results except the one who performed the experiment."* Or as an NASA engineer said, referring to the investigation of the Columbia accident[3], *"All the analysis and investigating and theorizing in the world just goes right down the tubes as soon as you have experimental information."*

In 1994, The US Department of Energy/National Nuclear Security Agency (NNSA) established a ten year Accelerated Strategic Computing Initiative (ASCI) vision for the use of computational models to achieve its National Security mission goals**.** In ten years, there have been remarkable achievements within the ASCI program, including breaking the 10^{12} floating point operations/sec boundary with the goal of a petaflop, achieving a $>10^3$ increase in the fidelity of the computational models, realizing tremendous increases in our ability to manipulate and visualize data, introducing new computational software architectures, and utilizing new numerical approaches to nonlinear computational mechanics. Extrapolating these accomplishments into the next decade, while risky, highlights the need to integrate the three branches of science: theoretical, experimental, and computational. Our ability to verify the mathematical basis of our software, to explore new validation technologies for the comparison of experiment and simulation, and to develop new methods to quantify the uncertainty not only of computational results but also of experimental results, limits us today and will only become worse in the future unless we accelerate our development of these areas. In addition, we are realizing that the complexity of problem setup inhibits the ability to shorten the engineering design cycle.



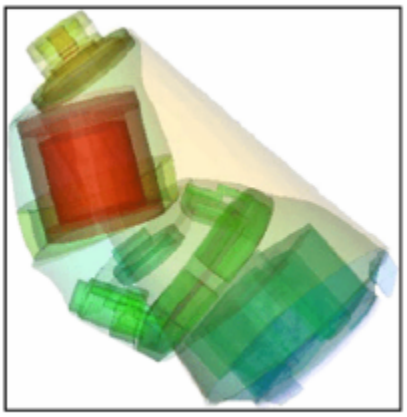
I will discuss the accomplishments made over the past decade at Sandia National Laboratories in the disciplines of continuum, computational engineering sciences important to our work:

- High-deformation, nonlinear, transient dynamics,
- Structural dynamics,
- Fire physics,
- Heat transfer, and,
- Compressible and incompressible fluid mechanics.

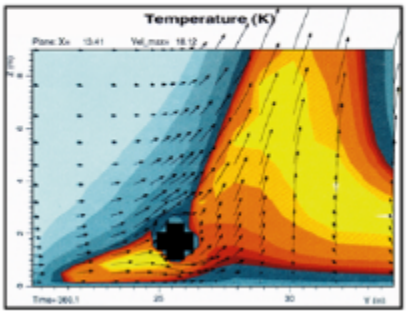


Transient Dynamics

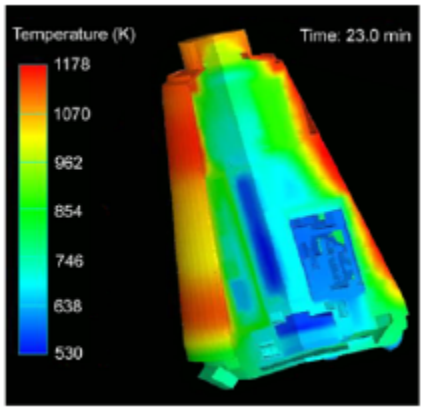
[1] Michael L. Overton, *Numerical Computing with IEEE Floating Point Arithmetic*, SIAM, 2001.
[2] Patrick J. Roache, *Verification and Validation in Computational Science and Engineering*, Hermosa Publishers, 1998.
[3] Anonymous, New York Times, May 30, 2003, byline: John Schwartz and Matthew L. Wald.



Structural Dynamics



Fire Physics



Heat Transfer

A review of the past decade will explore how we are merging experiment and computation at Sandia. A look to the future will examine our goals for the next decade. Finally, I will discuss our collaborations with industry and universities to illustrate the extension of this branch of science to future engineering practices.

To continue the achievements made within the field of computational sciences we must marry this branch with experimental and theoretical sciences at a time of explosive growth in evolving disciplines such as non-continuum mechanics, computational chemistry, and computational biology, to name a few. This will indeed be an even greater challenge than those we have faced over the past century.