Lawrence Livermore National Laboratory

The Business Case for a Public-Private Sector Partnership in High Performance Computing (HPC)

Roger W. Werne, Ph.D.
Deputy Director, Industrial Partnerships
October 15, 2009

Lawrence Livermore National Laboratory, P. O. Box 808, Livermore, CA 94551
This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

LLNL-PRES-41224

The Business Case for a Public-Private Sector Partnership in High Performance Computing (HPC)

My talk will focus on three questions:

1. Why is HPC really important to business and government?
2. What are some “market” examples in business and government?
3. What kind of partnership makes sense?

Richard W. Hamming – circa 1957

"The purpose of computing is insight not numbers"

"Machines should work. People should think."

And insight is about creativity, options and ultimately decision making

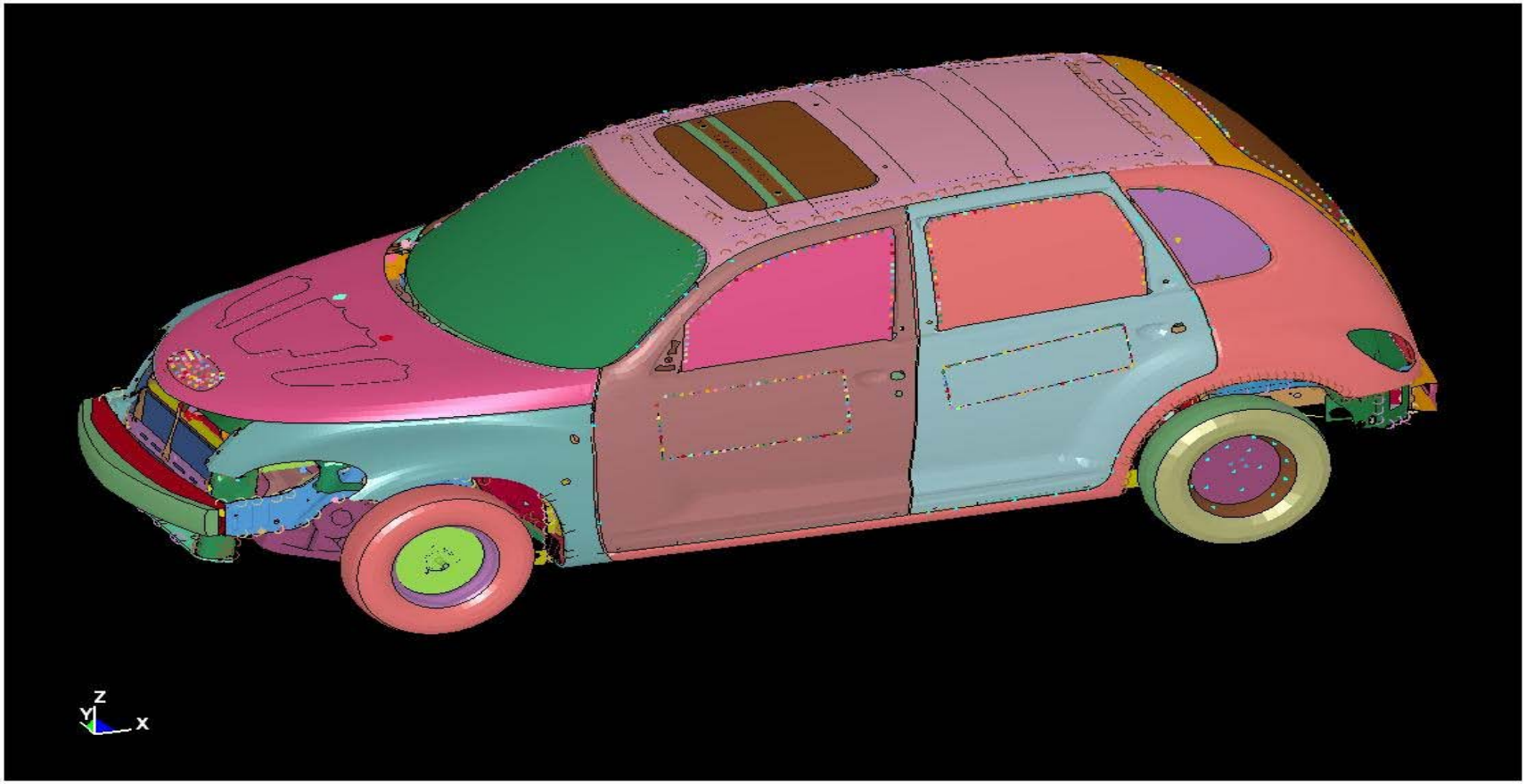
- Creativity is inventiveness, originality, thinking of things in new and different ways – exploring the unknown through numerical experiments, data mining, etc.
- Options are choices, pathways forward, alternatives – analyzing more design options within a given period of time
- Decisions are options, choices, pathways, or alternatives selected as a path forward – decisions that make your business “better, faster, cheaper”

Many industries/sectors have recognized the value of computing and are investing significant resources in predictive simulation

- Automobile and aircraft – performance optimization
- Oil and gas – seismic mapping, resource recovery
- Infrastructure management – emergency response
- Pharmaceutical – drug discovery
- Finance – financial market analysis and “prediction”
- Environment – weather prediction, environmental prediction, global climate change

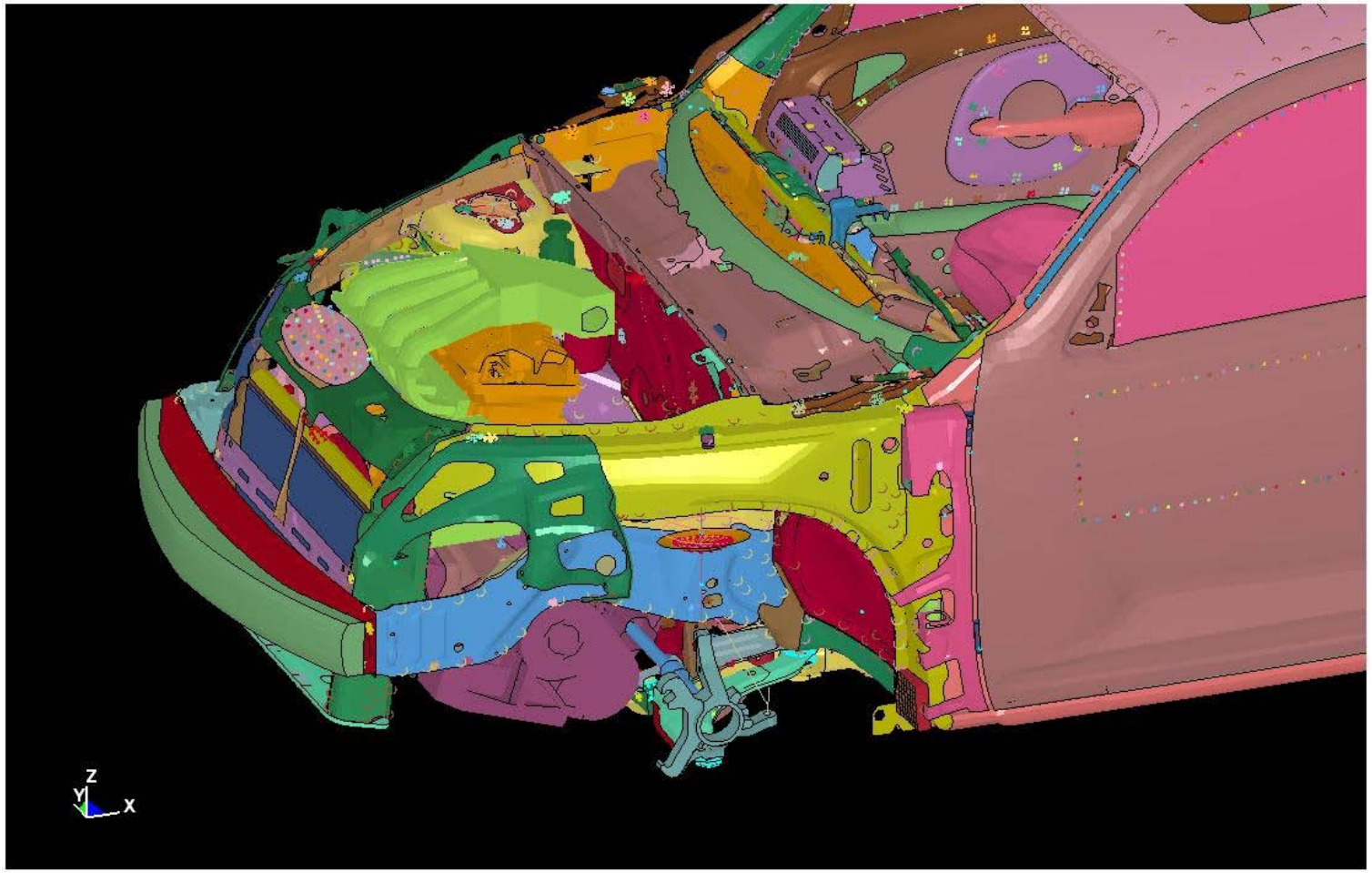
A few examples ----

Automotive Market: In the late ‘80s the DYNA3D code, commercialized as LSDYNA by Livermore Software Technology Corporation, revolutionized crash simulation in automotive design*

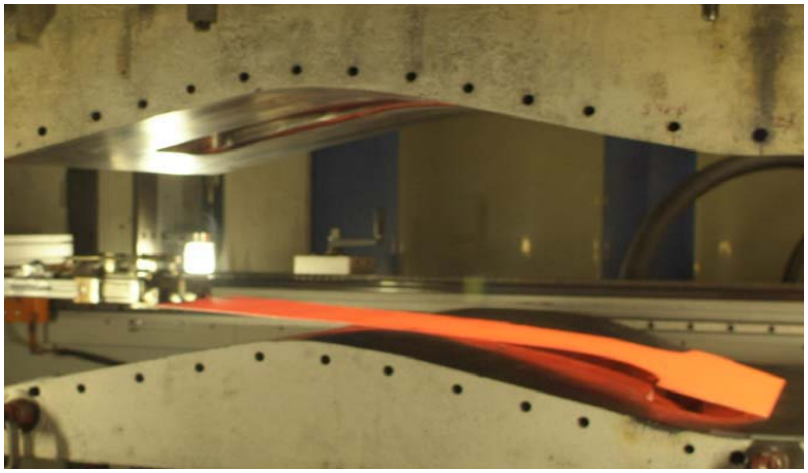


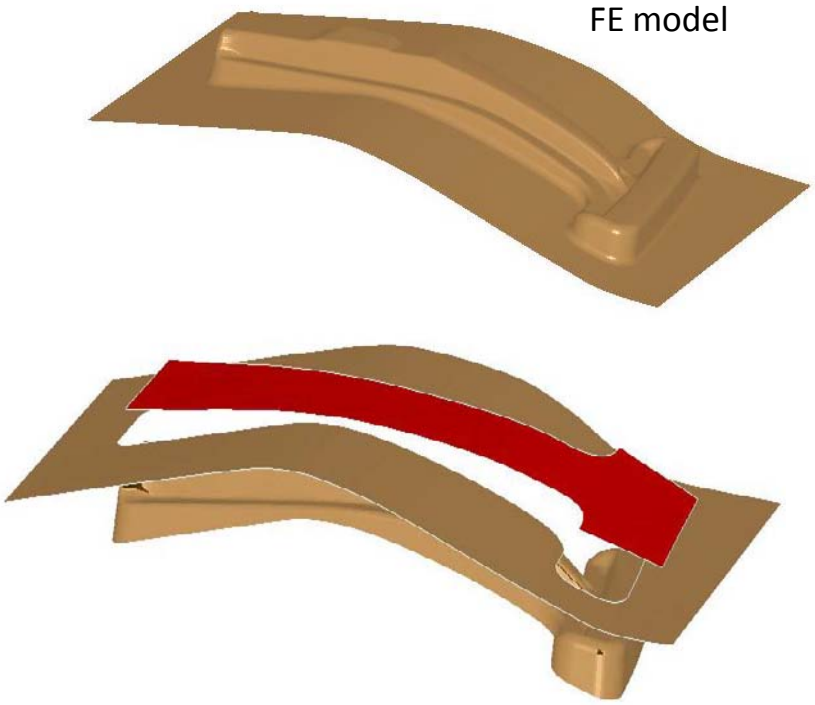
*compilments of Art Shapiro, PhD, LSTC

Detailed structural models, which include body structure, and spot welds, suspension, and tires allow crash safety to be analyzed without expensive full scale testing



Manufacturing: Thermo-mechanical Models of the manufacturing process also save time and money - a goal is to model the manufacturing of the part and insert it, residual stresses and all, into the assembled automobile model*

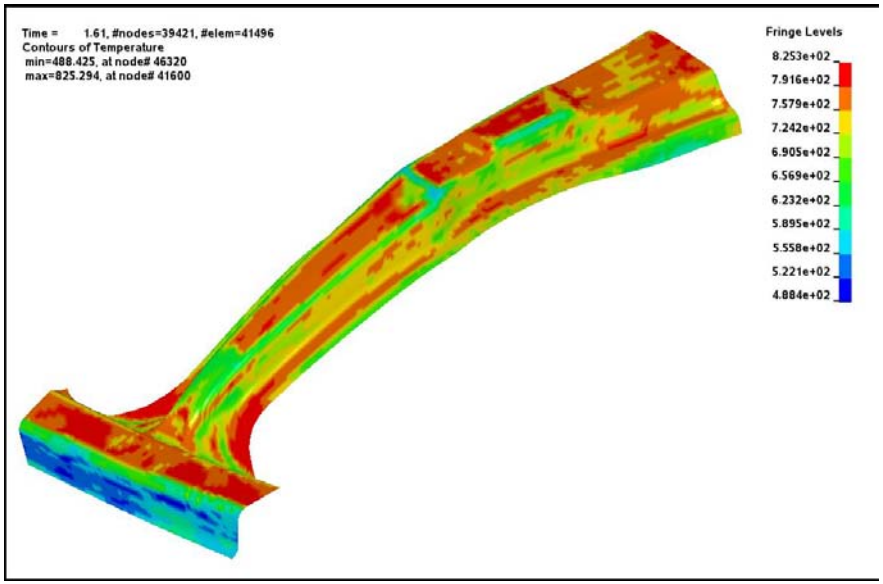




* Compliments of Art Shapiro, PhD, LSTC

Successfully “hot forming” a part requires accurate estimates of cooling rates which affect grain size and therefore material properties – therefore “time” is an important element in the manufacturing process

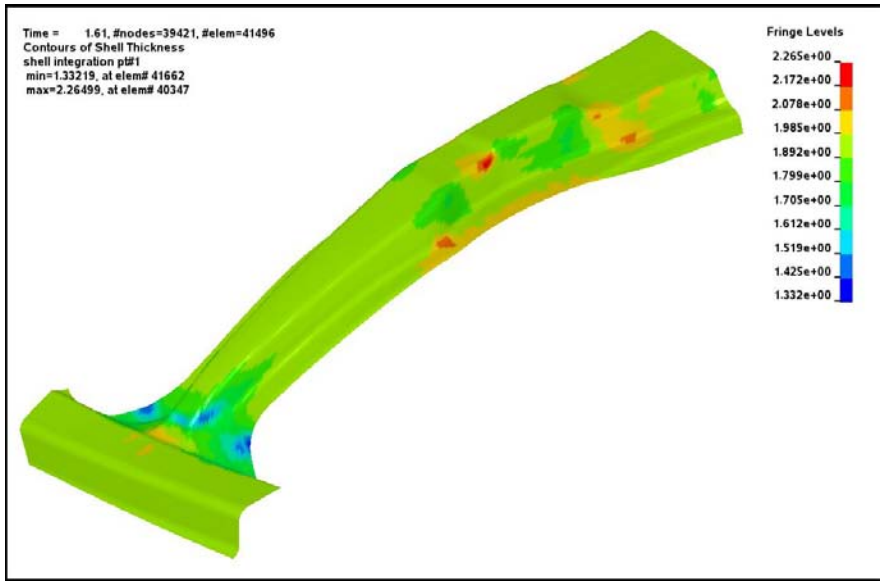
Results after forming



Temperature

min = 488C

max = 825C



Thickness

min = 1.33mm

max = 2.26mm

Studies show that scaling a given code to many processors is not straight forward*

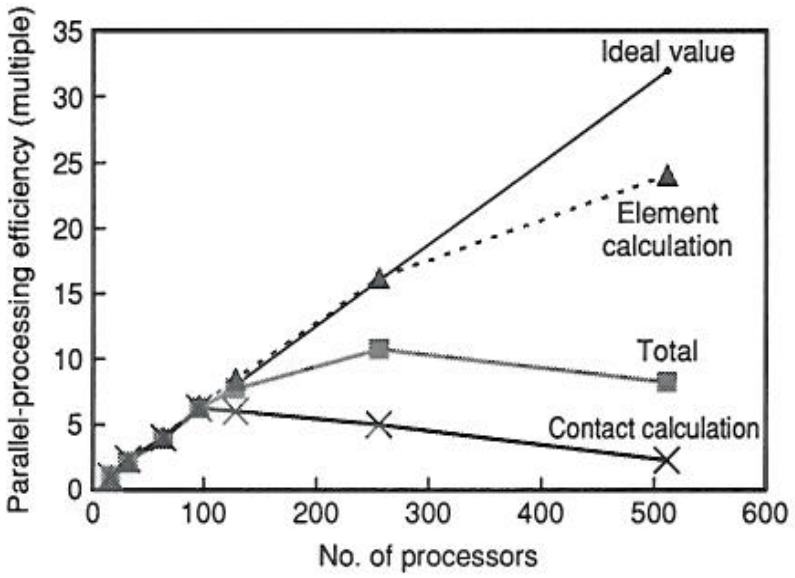


Figure 1
Parallel-processing efficiency for a 10-million-element model (before performance improvements).

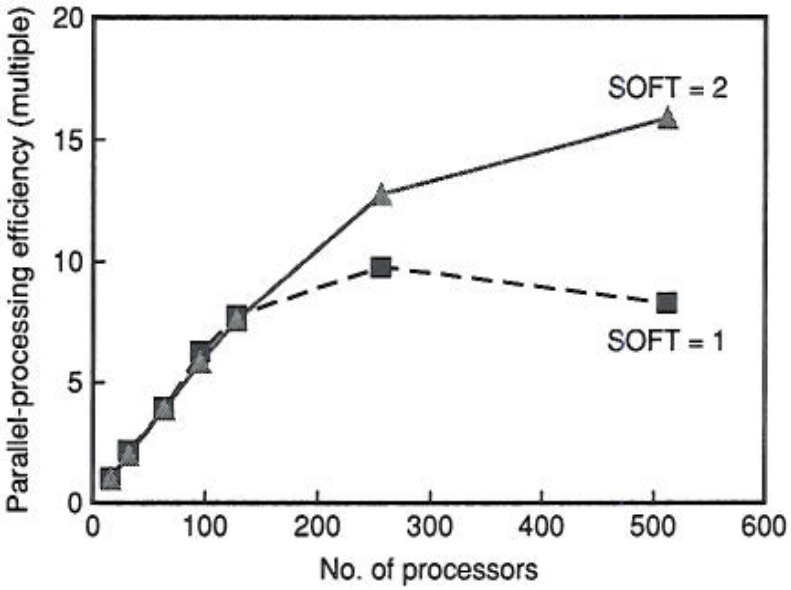
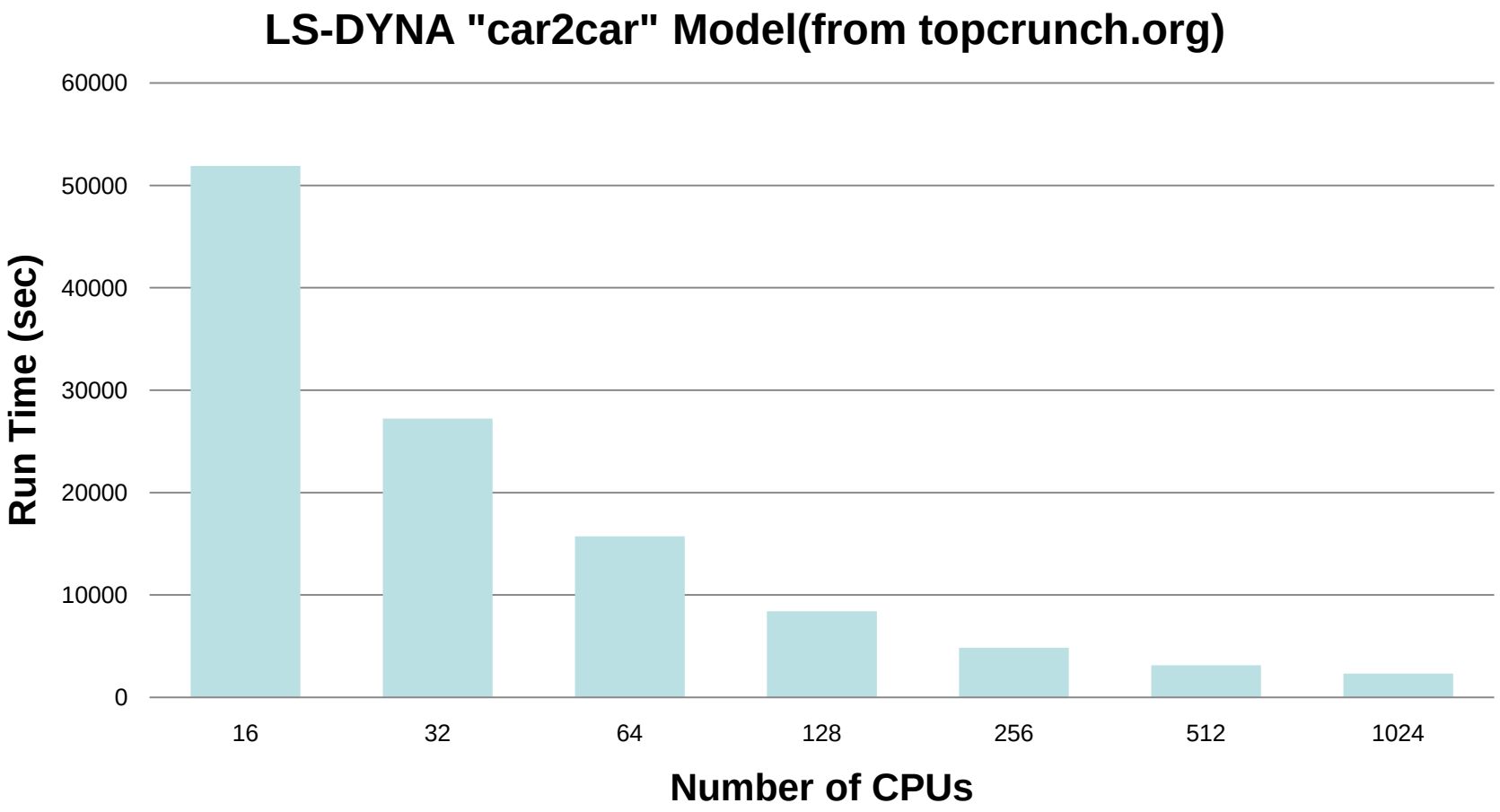


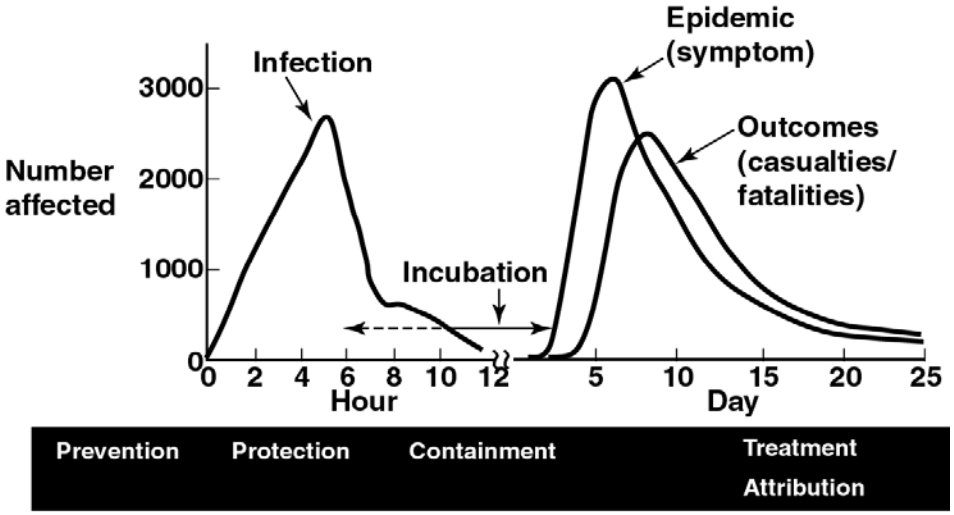
Figure 2
Parallel-processing efficiency for two types of contact definitions.

* Kondo & Makino, FUJITSU Sci.Tech. J. Oct. 2008

LS-DYNA scales very well with the number of processors



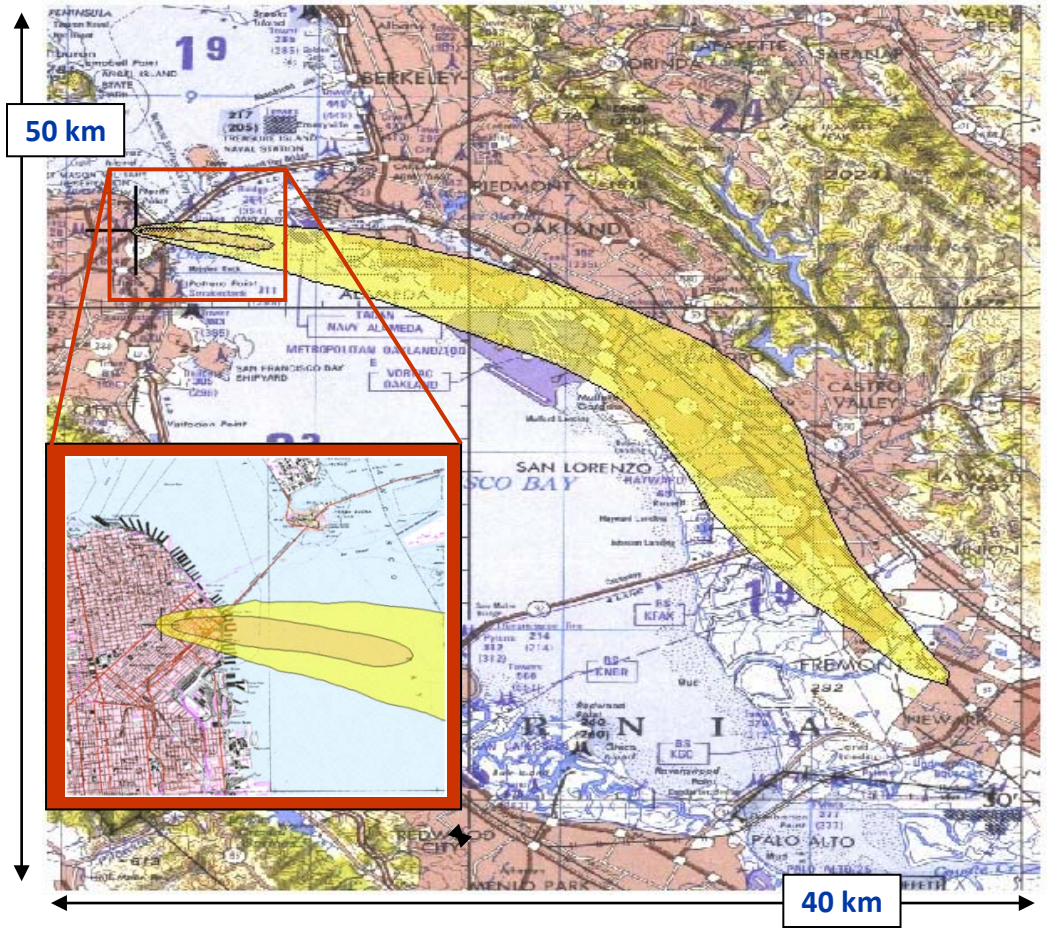
Homeland Security: Biological weapons represent significant threat because they are difficult to detect until symptoms appear



- Infections can usually be cured if vaccinations are given before symptoms manifest (within days)
- Detect to treat is the strategy ----

The threat is real --Aum Shinrikyo Headquarters — 1993

What appears to be a local WMD event can quickly become a regional problem*



Hypothetical release at the Embarcadero in San Francisco

Bio-agent Dose

Color	Area (km^2)	Description
	3.3	15% of the exposed population could receive a lethal dose Population: 1600
	148	2% of the exposed population could receive a lethal dose Population: 308,192

Release location:

In the San Francisco Financial District

At 3rd and Market Streets

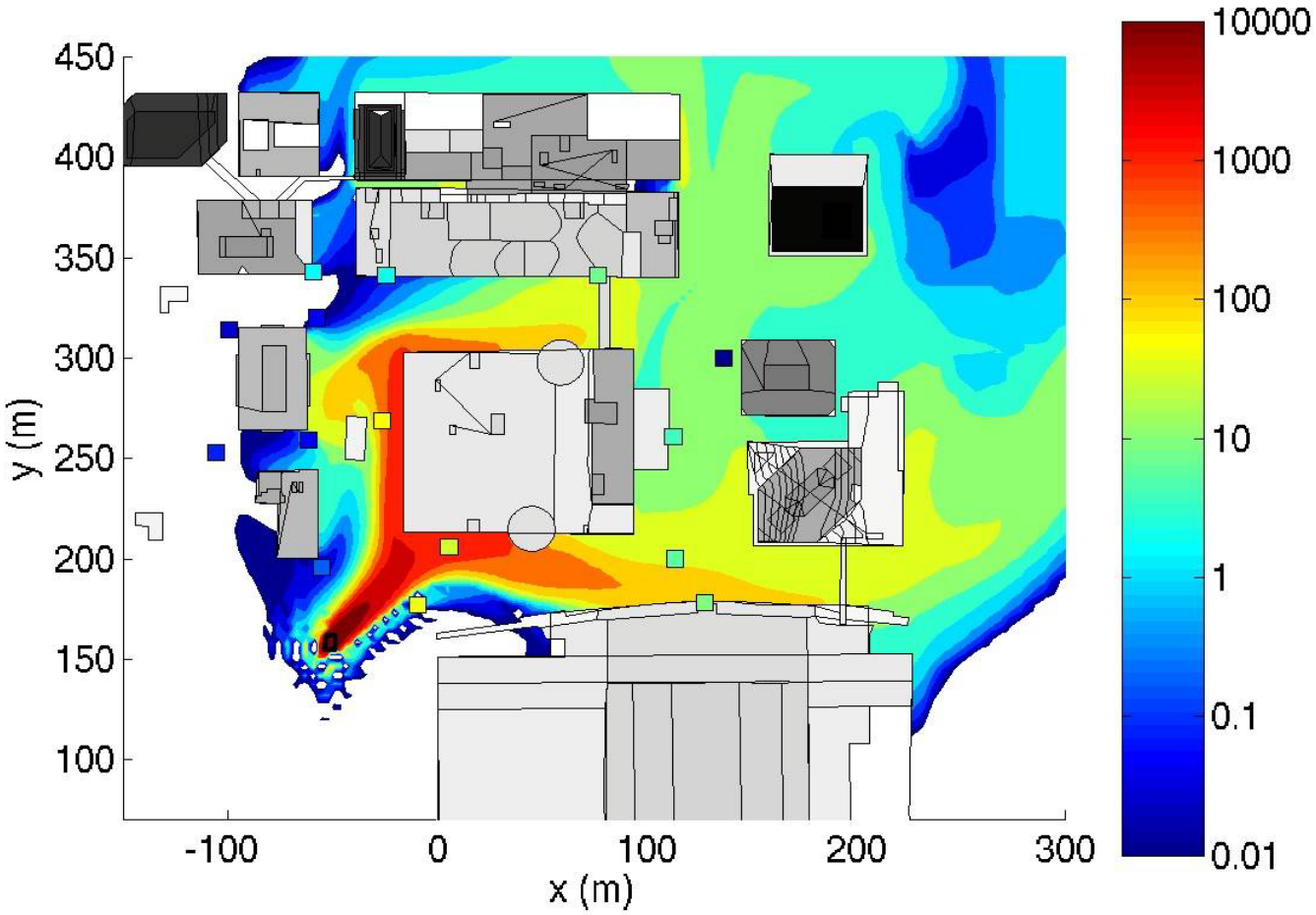
Lat/Long: 37° 47’ 14” N

122° 24’ 07” W

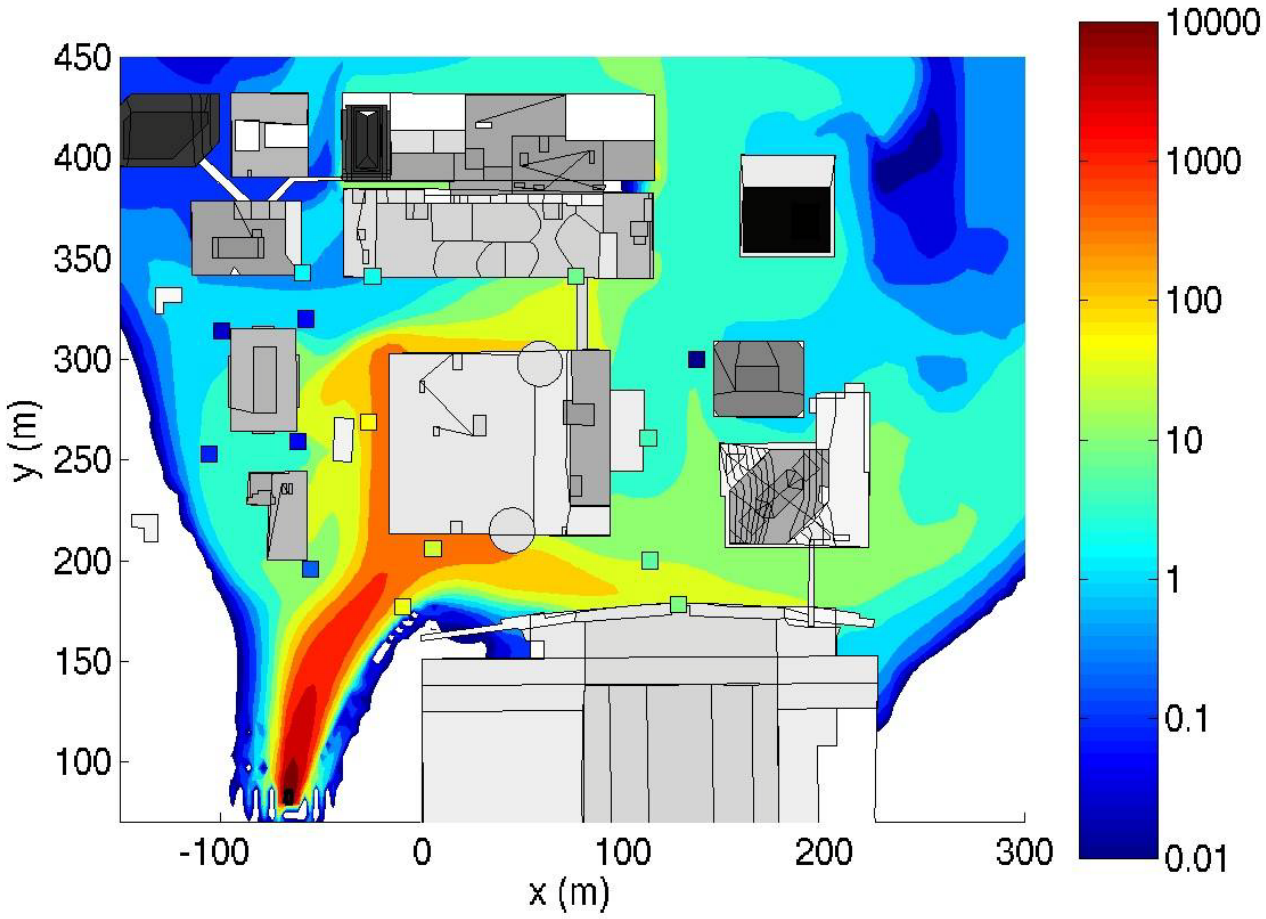
Meteorology: Observed winds at 5 PM PDT, 28 May 2003

*National Atmospheric Release and Advisory Capability

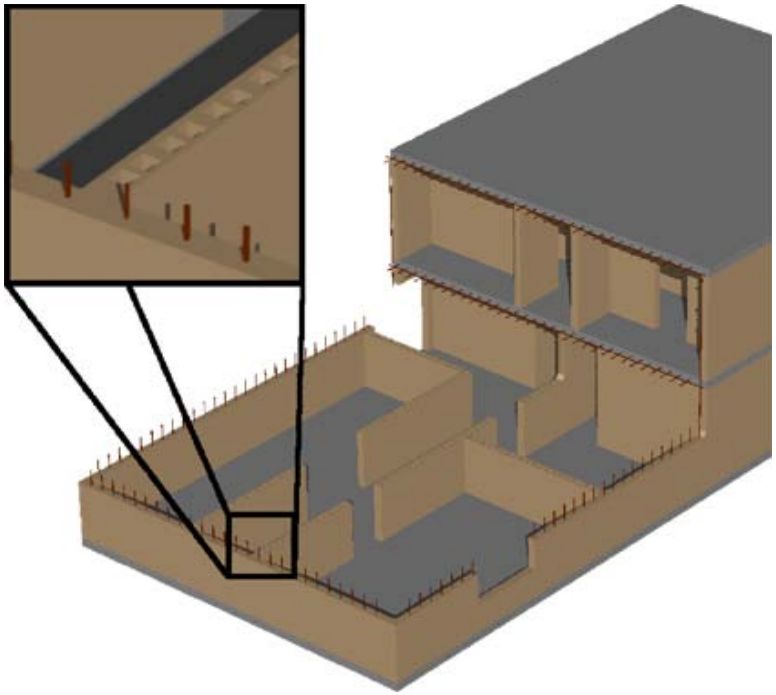
Locally, predicting source location in a complex flow environment is key – calculated flow from known source

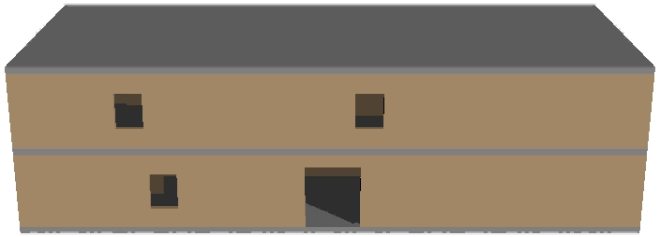


Given “field measurements”, predict the source location, i.e., solve the inversion problem – much more difficult!



Infrastructure: A 10B zone 3D EM problem was calculated to study radar reflections from the interior surfaces of buildings.*



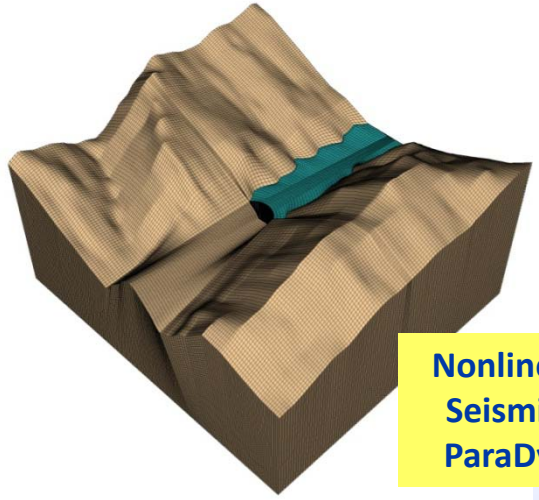


*compliments of Mark Stowell, PhD, LLNL

Infrastructure Management: Nonlinear seismic analysis of concrete dams*

- “In the design of practically all dams the difficulties of analysis are so great the consequences of failure so serious, and the cost of appreciably changing the probabilities of failure are of such high magnitude that refined model and analytical studies are almost always in order.” – Newmark & Rosenblueth

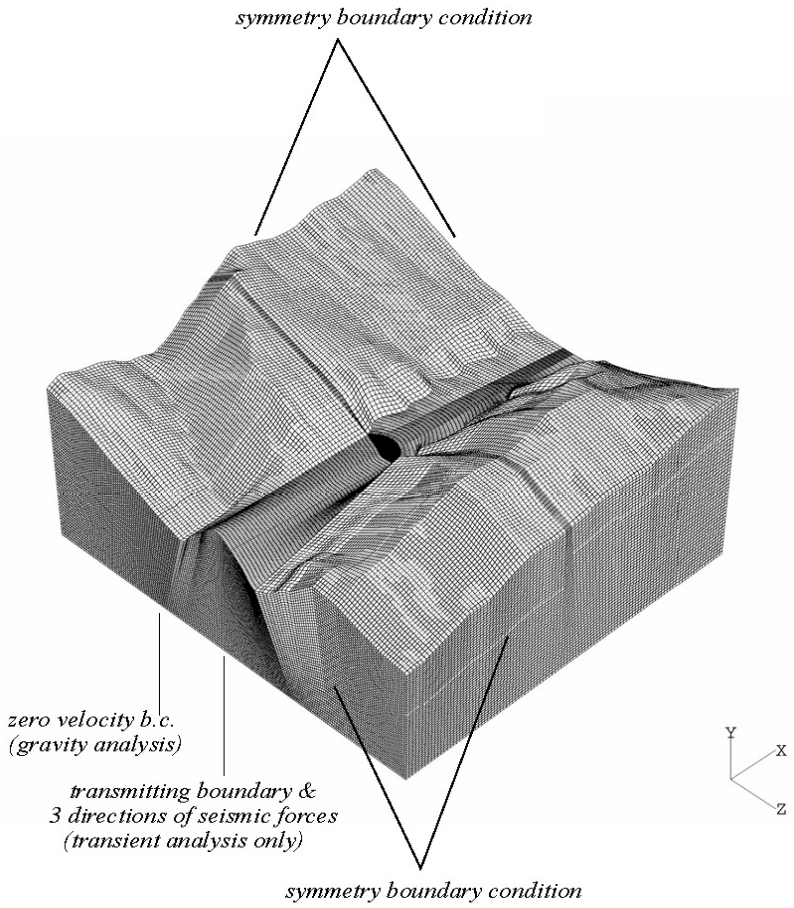
So, if one wishes to assess, through computational simulation, the integrity of a large concrete arch dam under realistic seismic excitation, then what aspects of this enormously complex problem must one truly get right?

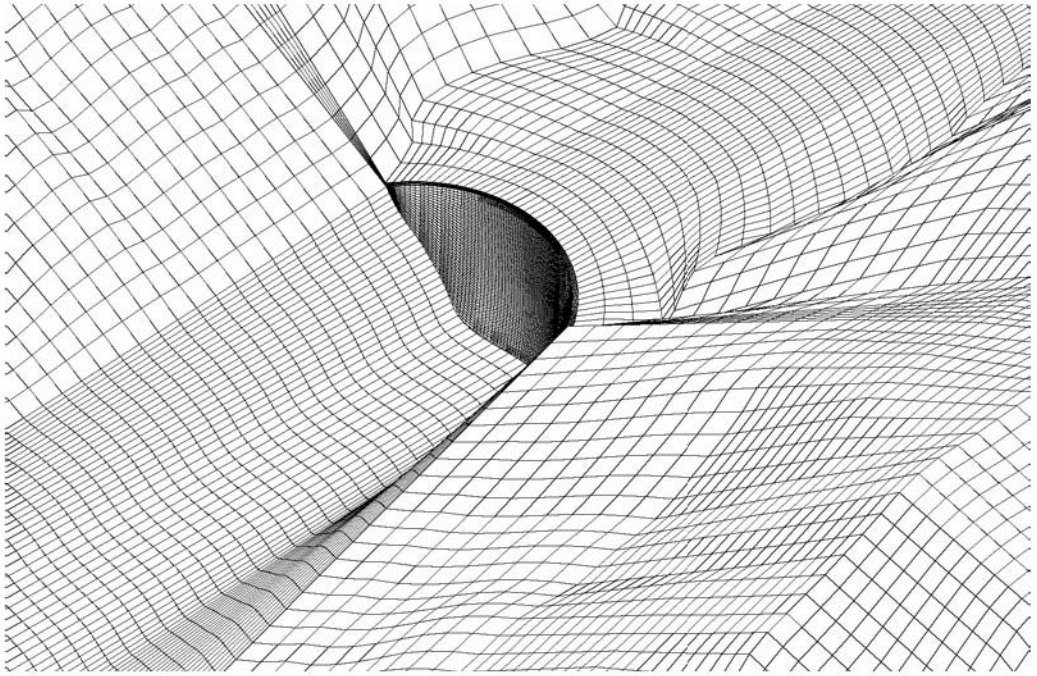


Nonlinear Seismic: ParaDyn

*compliments of Chad Noble, PhD, LLNL

3D dam/reservoir/foundation finite element model of Morrow Point Dam





ParaDyn Model

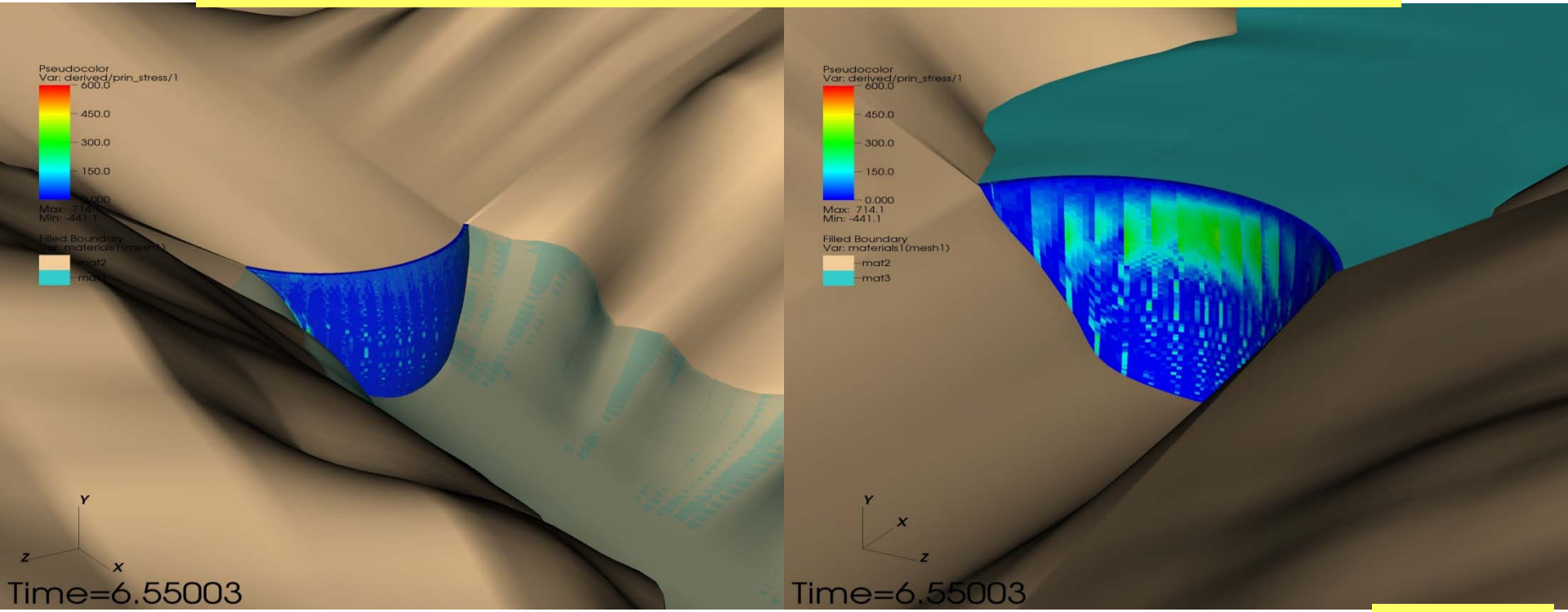
1,071,625 solid hexahedral elements

1,120,280 nodes

32 processors on MCR (LLNL)

Principal tensile stress at maximum displacement

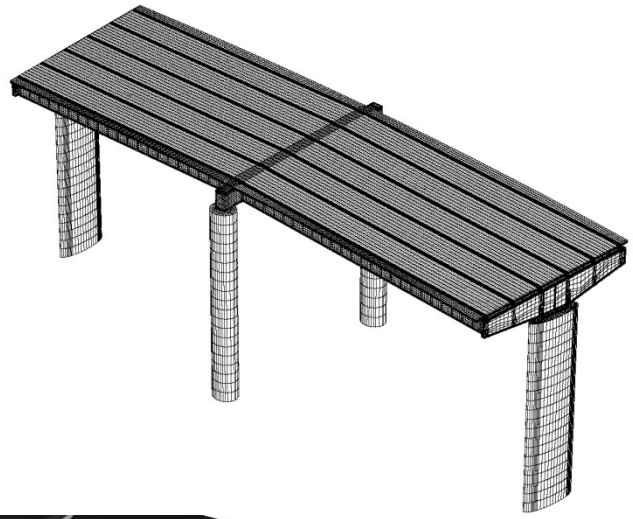
Maximum displacement at T = 6.55 seconds predicted to be 2.4 inches in the upstream direction



No significant damage predicted from M6.7 earthquake

Nonlinear Seismic: ParaDyn

Highway 580 Bridge Collapse due to a truck fire on *April 29, 2007 at 4:02 AM**



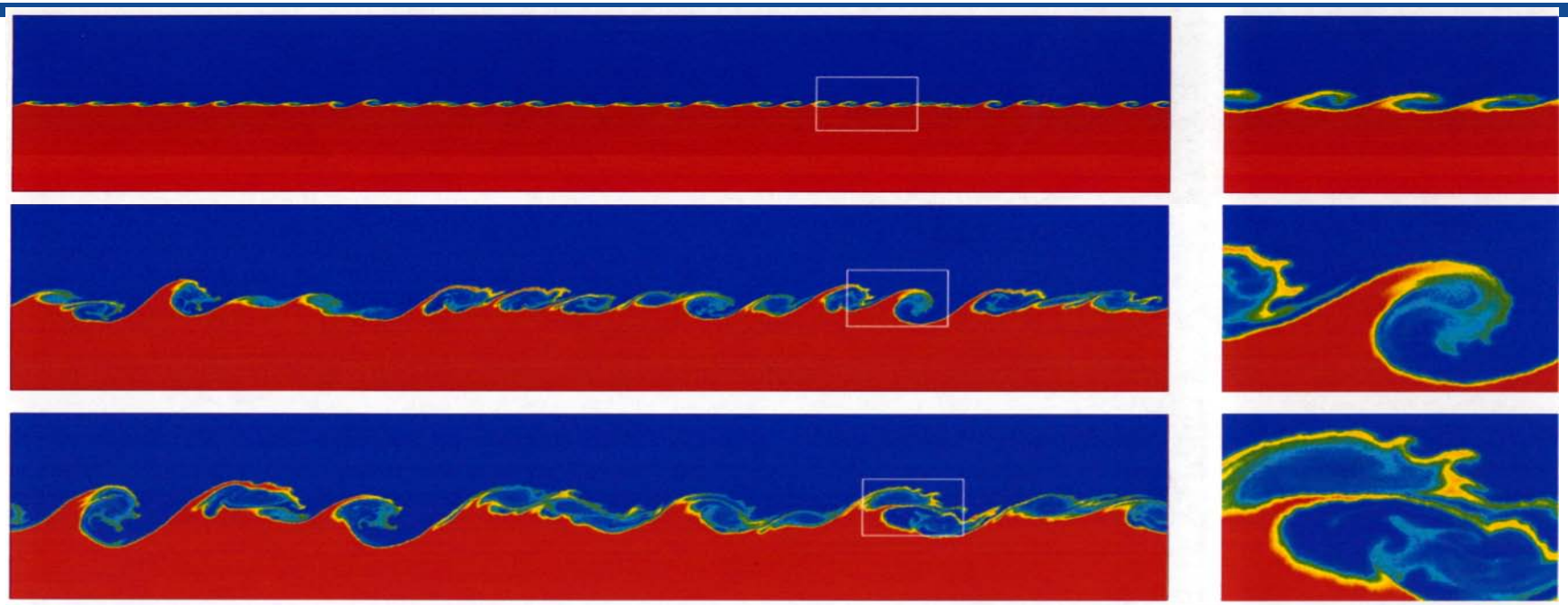
Objective: validate computer simulation so that effective fire and progressive collapse mitigation measures can be studied

Nonlinear thermal/structural:

TOPAZ3D/NIKE3D/DIABLO

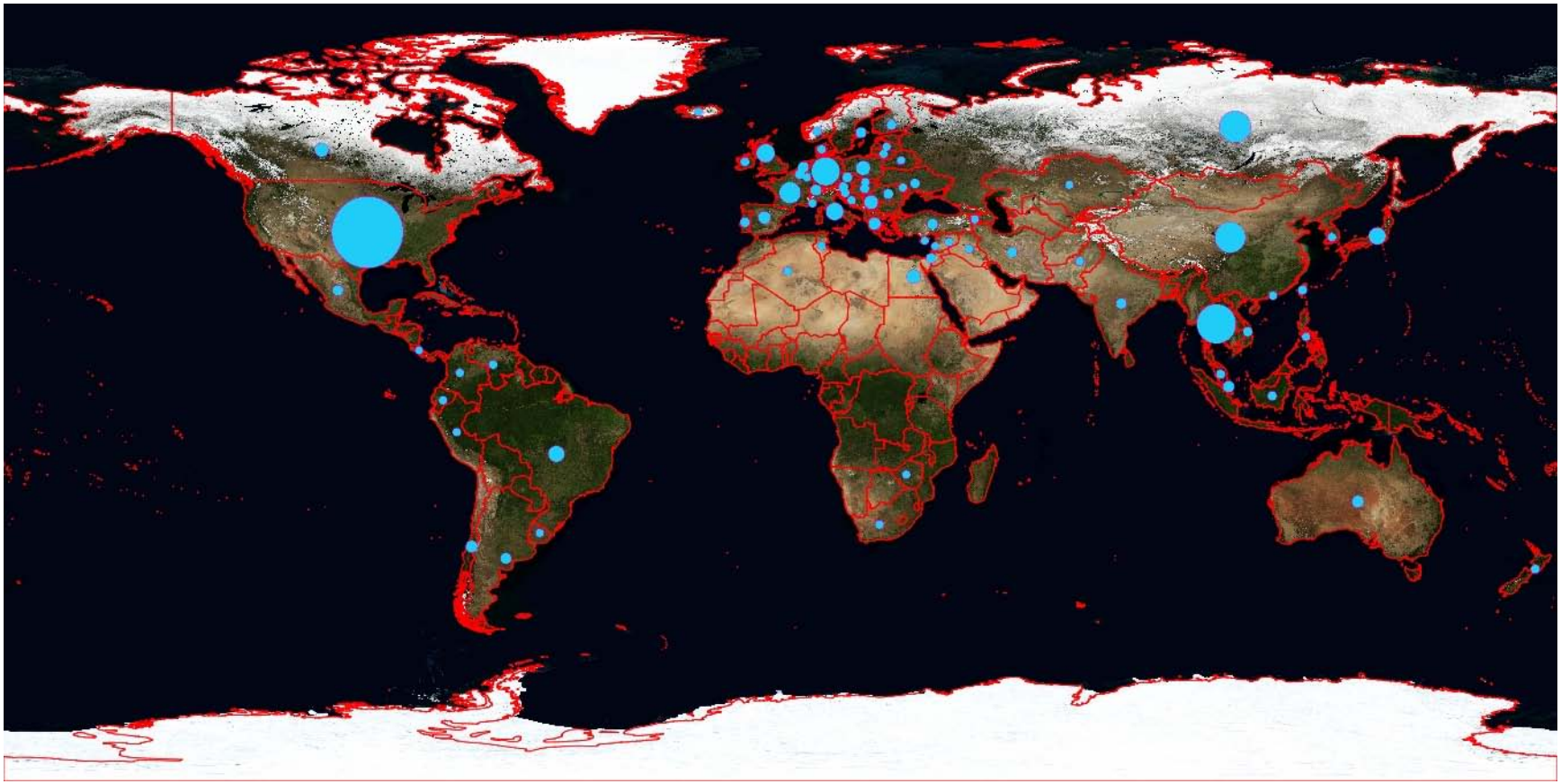
*compliments of Chad Noble, PhD. LLNL

Research: Computational Experiments - Initiation of Kelvin-Helmholtz Instability using Molecular Dynamics Simulation



- **Molten metals of differing densities undergoing a constant shear**
- **5.0 μm x 2.9 μm simulation of more than 2 billion atoms using ddcMD code for 8 days on all 131,072 processors of BGL - finalist for 2007 Gordon Bell Prize**
- **First atomistic simulation to develop Kelvin-Helmholtz instability at hydro scale**
- **This is the moral equivalent of Ab Initio 2D Hydro**

The HPC market is predicted to be > $15.5B in 2011. An example of interest: VISTA an LLNL open source HPC code: Over 88,000 downloads worldwide in 2007



The businesses in the HPC market fall into three categories

1. The **Users** who utilize HPC to better compete in their markets

2. The **Independent Software Vendors (ISVs)** who develop and sell the HPC tools to the **Users.**

3. The **Computer Vendors (CVs)** who sell hardware and operating systems to the **Users** and **ISVs**

The “Users” are the ones with the business problems to solve; they drive development of the ISV’s and CVs

- In terms of “Decision Making”, time is always of the essence for the “Users”. For example:
  - Financial markets – seconds to months
  - Oil and gas – days to months
  - Auto and Aircraft – hours to days
  - Emergency response – minutes to hours
  - Infrastructure management – days to months

Increasingly, the Users are requiring larger predictive simulation problems to be solved in shorter periods of time: better, faster, cheaper decisions

However, the barriers to entry for the Users are significant

- Cost of the tools – start-up costs for hardware, software and personnel training can be significant as can be maintenance costs.
- Cost of money – many businesses want a factor of ten in five years, i.e., 58.5% discount rate. Or at least three-year payback or 28% per year.
- Resistance to change – “We’ve always done it this way; there’s no need to change”.
- A new level of intellectual sophistication is required in the business

So how do we lower the barrier for businesses wanting to become more competitive through the use of HPC resources?

- At LLNL, we believe that one answer is a Public-Private Partnership between a National Laboratory and businesses in the HPC market, e.g.,

Hyperion

A state-of-the-art HPC facility located at Lawrence Livermore National Laboratory

Hyperion Collaborations Allow Partners to Build A Resource None Could Afford Alone

Founding Members:

- **Intel, Dell, and Supermicro**
  - Processors, Nodes, Racks and Integration
- **QLogic, Cisco and Mellanox**
  - IBA switches & HCAs
  - Ethernet switches & NICs
  - IBA Ethernet routers
- **DDN, Sun, LSI**
  - Storage Hardware
- **RedHat**
  - Linux Testing and System Admin
- **Sun and RedHat**
  - Parallel File Systems

Hyperion* is next generation Linux cluster and is the largest testbed of its kind in the world

- 1152 nodes – 9216 cores
- 100-teraFLOP/s peak
- > 9TB memory
- InfiniBand 4X DDR interconnect & access to > 47 GB/s Raid disk bandwidth
- Two storage area networks(Data Center Ethernet & InfiniBand)

*for further information contact Mark Seager, PhD, LLNL.

The benefit to Hyperion commercial partners is competitive advantage

- Access to a world-class HPC capability at a reasonable cost
- Access to LLNL's and partners' expertise in HPC
- Shared risk with other parties
- Test new hardware and software products in a demanding HPC environment – try before you buy!
- Low risk approach to explore new capabilities/possibilities

Benefits to LLNL are also significant

- Access to the latest hardware and software
- Access to many smart people in industry
- Ability of LLNL to help U.S. industry maintain leadership in the competitive HPC world market
- Help LLNL understand HPC commercial market directions

Contact Information:

- Roger W. Werne, PhD
- Deputy Director – Industrial Partnerships
- Lawrence Livermore National Laboratory
- PO Box 808, L-795
- Livermore, CA 94550
- Phone: 925-423-7302
- Email: werne1@llnl.gov