

**CCC Report, May 10, 2004**

# **Solidification Stress Model in Abaqus**

**Seid Koric**

**Engineering Applications Analyst**

**National Center for Supercomputing Applications -NCSA**

**PhD Candidate at Mechanical and Industrial Engineering**

**University of Illinois at Urbana-Champaign**

**skoric@ncsa.uiuc.edu**

# Objectives

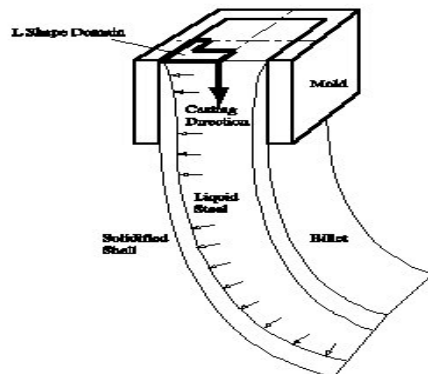
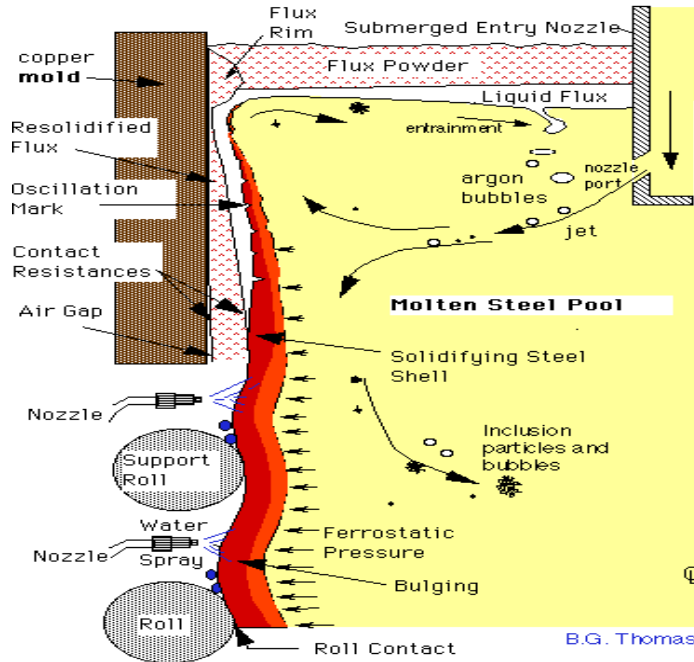
- To predict the evolution of **temperature, shape, stress and strain** distribution in the solidifying shell in continuous casting mold by **using world's leading nonlinear commercial multipurpose finite element package** with an accurate approach.
- **Validate the model with available analytical solution and benchmarks** with in-house code **CON2D**.
- **To apply new Abaqus model** to our real problems with even more complex phenomena.

# Why ABAQUS ?

- If its convergence problems can be overcome, ABAQUS offers a **wide range of capabilities**.
- It is **relatively simple to use**, other modelers in this field can largely benefit from this work, including our final customers – **the steel industry**.
- Abaqus has imbedded **pre and post processing tools** supporting import of the major CAD formats. All major general purpose pre-processing packages like Patran and I-DEAS support Abaqus.
- Abaqus is using **full Newton-Raphson scheme** for solution of global nonlinear equilibrium equations and has a powerful contact algorithm.
- Abaqus has a **rich library of 2D and 3D elements**.
- Abaqus has **parallel implementation** on High Performance Computing Platforms which can scale wall clock time significantly for large 2D and 3D problems.
- Abaqus can link with **external user subroutines** (in Fortran and C) linked with the main code than can be coded to increase the functionality and the efficiency of the main Abaqus code.

# Basic Phenomena

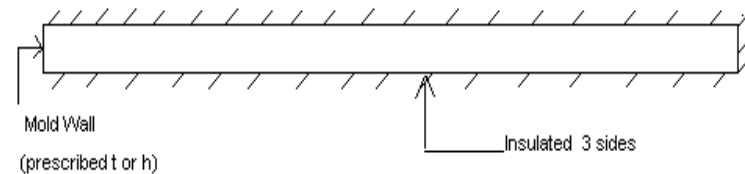
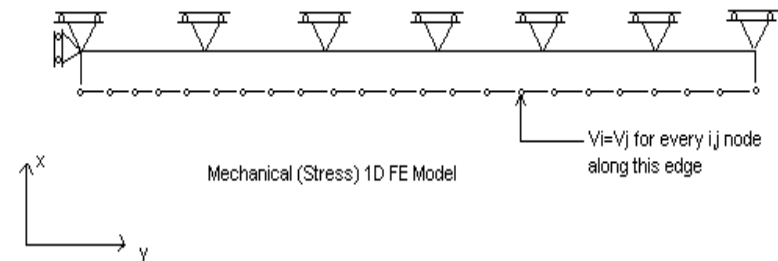
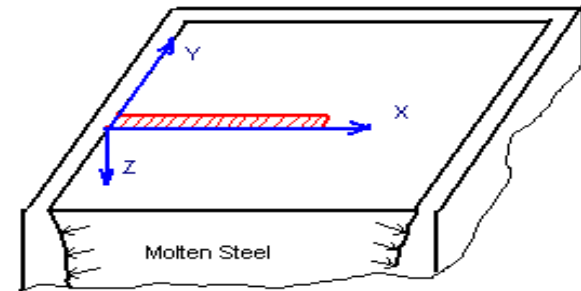
## Slab Casting Phenomena (Longitudinal section: not to scale)



- **Initial solidification** occurs at the meniscus and is responsible for the surface quality of the final product.
- **Thermal strains** arise due to volume changes caused by temp changes and phase transformations.  
**Inelastic Strains** develop due to both strain-rate independent plasticity and time dependant creep.
- At inner side of the strand shell the **ferrostatic pressure** linearly increasing with the height is present.
- The **mold taper** has the task to compensate the shell shrinkage yielding good contact between strand shell and mold wall.
- Many other phenomena are present due to **complex interactions between thermal and mechanical stresses** and micro structural effects. Some of them are still not fully understood.

# 1D Solidification Stress Problem for Program Validation

- **Analytical Solution** exists (Weiner & Boley 1963)
- **1D FE Domain** used for validation
- **Generalized plane strain** both in y and z direction to give 3D stress/strain state
- **Yield stress linearly drops** with temp. from 20Mpa @ 1000C to 0.07Mpa @ Solidus Temp 1494.35C
- Tested both internal PLASTIC Abaqus procedure and a **special high-creep function** to emulate Elastic-Perfect Plastic material behavior



Heat Transfer 1D FE Domain

# Governing Equations

## Heat Transfer Equation:

$$\rho \left( \frac{\partial H(T)}{\partial T} \right) \left( \frac{\partial T}{\partial t} \right) = \frac{\partial}{\partial x} \left( k(T) \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k(T) \frac{\partial T}{\partial y} \right)$$

## Equilibrium Equations 2D:

$$\frac{\partial \Delta \sigma_x}{\partial x} + \frac{\partial \Delta \tau_{xy}}{\partial y} = \Delta F_x$$

$$\frac{\partial \Delta \sigma_y}{\partial y} + \frac{\partial \Delta \tau_{xy}}{\partial x} = \Delta F_y$$

$$\int \Delta \sigma_z dA = \Delta F_z$$

$$\int x \Delta \sigma_z dA = \Delta M_x$$

$$\int y \Delta \sigma_z dA = \Delta M_y$$

# More Equations:

## Constitutive Equations:

$$\{\Delta\sigma\} = [D]\{\Delta\varepsilon_e\} + [\Delta D]\{\varepsilon_e\}$$

where,

$$\{\sigma\} = \{\sigma_x \quad \sigma_y \quad \sigma_z \quad \tau_{xy}\}^T$$

$$\{\varepsilon\} = \{\varepsilon_x \quad \varepsilon_y \quad \varepsilon_z \quad \varepsilon_{xy}\}^T$$

$$[D] = \frac{E(T)}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & 0 & \nu \\ \nu & 1-\nu & 0 & \nu \\ 0 & 0 & \frac{1-2\nu}{2} & 0 \\ \nu & \nu & 0 & 1-\nu \end{bmatrix}$$

## Generalized Plane Strain

$$\Delta\varepsilon_x = \frac{\partial\Delta u_x}{\partial x}$$

$$\Delta\varepsilon_y = \frac{\partial\Delta u_y}{\partial y}$$

$$\Delta\varepsilon_{xy} = \frac{1}{2} \left( \frac{\partial\Delta u_y}{\partial x} + \frac{\partial\Delta u_x}{\partial y} \right)$$

$$\Delta\varepsilon_z = a + bx + cy$$

## Finite Elements Implementations

$$[K] \{T\} + [C] \{\dot{T}\} = \{Q\}$$

$$[K] \{\Delta u\} = \{\Delta F_{\varepsilon_{th}}\} + \{\Delta F_{\varepsilon_{pl}}\} + \{F_{fp}\} + \{F_{el}\}$$

## Incremental Total Strain

$$\{\Delta\varepsilon\} = \{\Delta\varepsilon_e\} + \{\Delta\varepsilon_{th}\} + \{\Delta\varepsilon_{pl}\}$$

# Constants Used in Abaqus Numerical Solution of B&W Analytical Test Problem

Conductivity	[W/mK]	33.
Specific Heat	[J/kg/K]	661.
Elastic Modulus in Solid	[Gpa]	40.
Elastic Modulus in Liq.	[Gpa]	14.
Thermal Linear Exp.	[1/k]	2.E-4
Density	[kg/m <sup>3</sup> ]	7500.
Poisson's Ratio		0.3
Liquidus Temp	[° C]	1494.48
Solidus Temp	[° C]	1494.38
Initial Temp	[° C]	1495.
Latent Heat	[J/kgK]	272000.
Number of Elements		300.
Uniform Element Length [mm]		0.1

Artificial and **non-physical thermal BC** from B&W (slab surface quenched to 1000C), replaced by a **convective BC** with **h=220000 [W/m<sup>2</sup>K]**

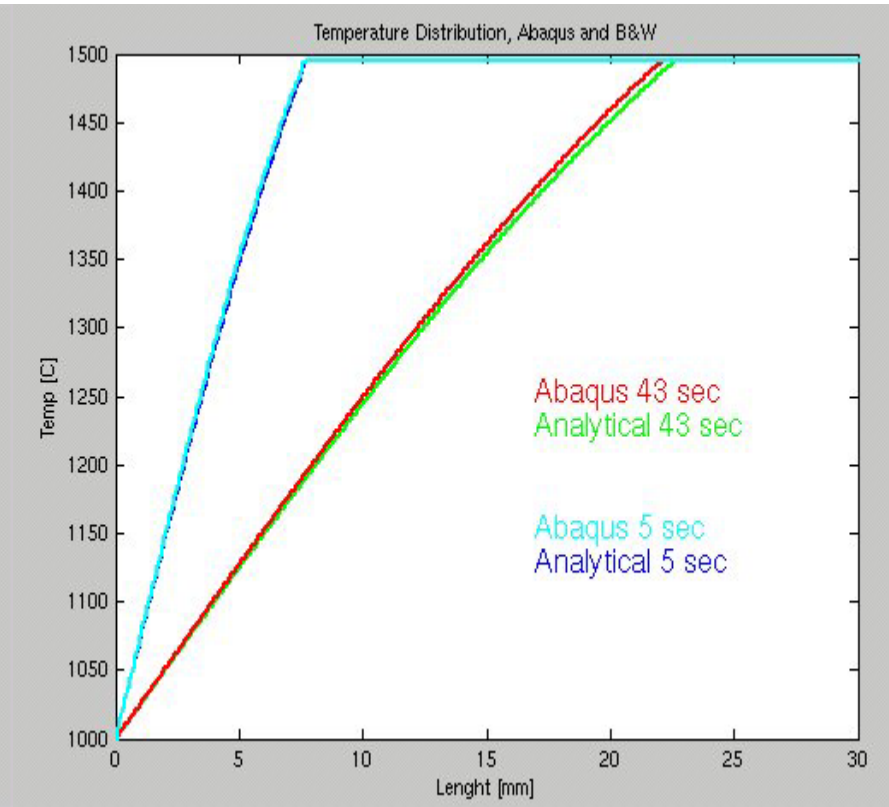
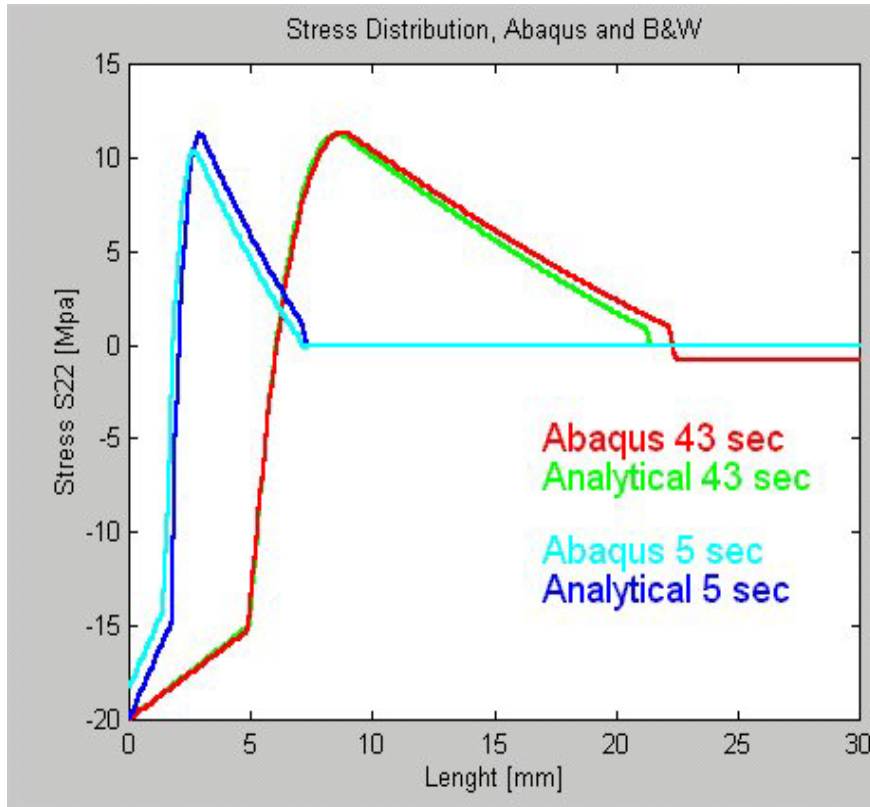
**Simple calculation to get h**, from surface energy balance at initial instant of time:

$$-k \frac{\partial T}{\partial x} = h(T - T_{\infty}) \quad \text{and for finite values } 33 \frac{495}{0.0001} = h \cdot 495$$



# Temperature and Stress Distributions for 1D Solidification

## Abaqus and Analytical (Weiner-Boley) Solutions



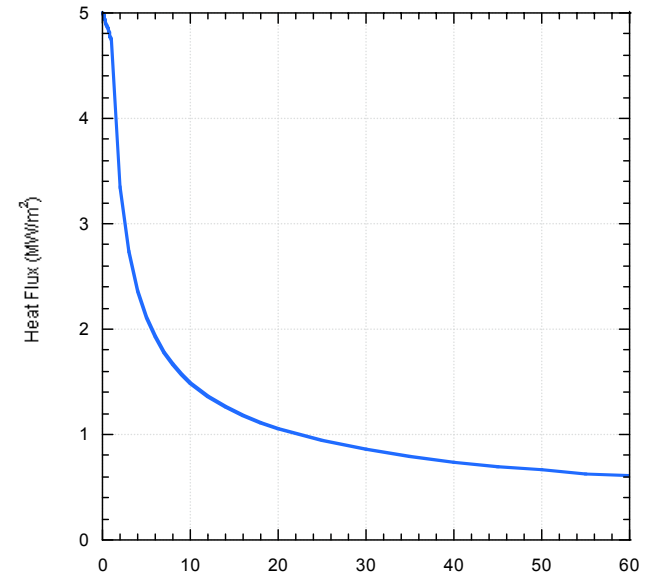
- The numerical representations from MATLAB and Abaqus produces almost **identical results**

- Model is **numerically consistent** and has **acceptable mesh**

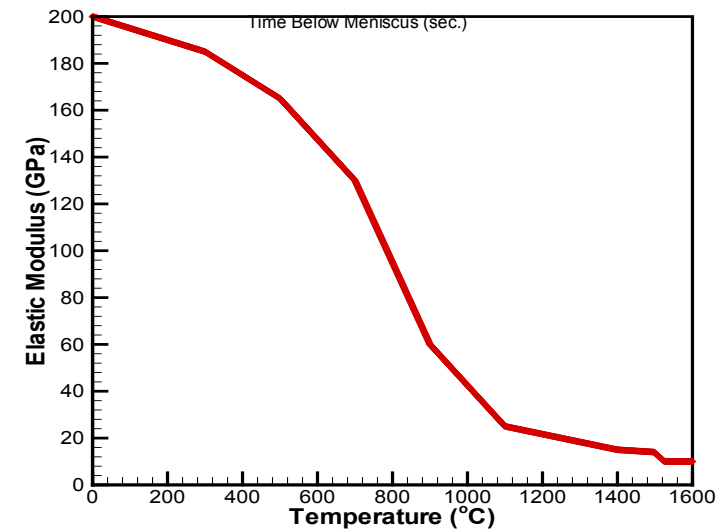
# Add more complexity (physics) to the Abaqus model by means of user subroutines

Applied instantaneous Heat Flux from a real plant  
measurements:

$$q \left( MW / m^3 \right) = \begin{cases} 5 - 0.2444t \text{ (sec.)} & t \leq 1.0 \text{ sec.} \\ 4.7556t \text{ (sec.)}^{-0.504} & t > 1.0 \text{ sec.} \end{cases}$$



Elastic modulus decreases as temperature increase:



The only difference between solid and liquid is a large creep rate in the liquid

$$\dot{\varepsilon} = \begin{cases} 10^{10} (|\sigma| - \sigma_{yield}) & \text{if } |\sigma| > \sigma_{yield} \\ 0 & \text{if } |\sigma| \leq \sigma_{yield} \end{cases}$$

(this is still a “milder” version of the liquid creep function used in CON2D)

Elastic visco-plastic model of Kozlowski for solidifying plain-carbon steel as our constitutive model:

$$\dot{\varepsilon} (1/\text{sec.}) = f(\%C) \left[ \sigma (MPa) - f_1(T(^{\circ}K)) \right] \varepsilon |\varepsilon|^{f_2(T(^{\circ}K)) - 1} \exp \left( - \frac{4.465 \times 10^4 (T(^{\circ}K))}{T(^{\circ}K)} \right)^{f_3(T(^{\circ}K))}$$

where

$$f_1(T(^{\circ}K)) = 130.5 - 5.128 \times 10^{-3} T(^{\circ}K)$$

$$f_2(T(^{\circ}K)) = -0.6289 + 1.114 \times 10^{-3} T(^{\circ}K)$$

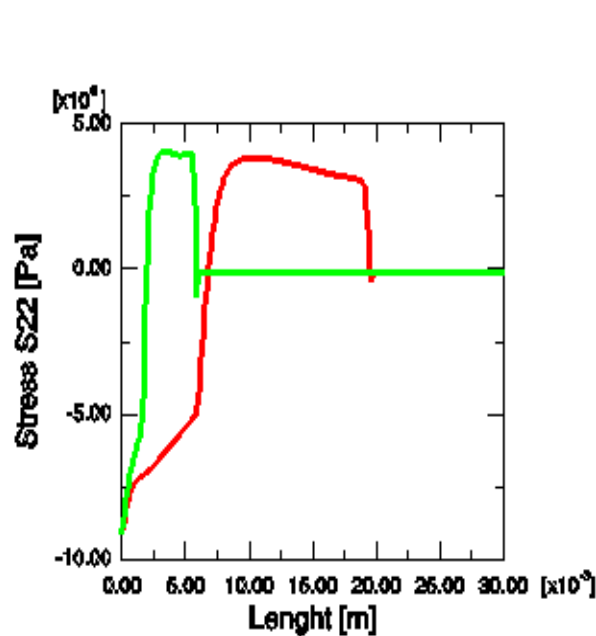
$$f_3(T(^{\circ}K)) = 8.132 - 1.54 \times 10^{-3} T(^{\circ}K)$$

$$f(\%C) = 4.655 \times 10^4 + 7.14 \times 10^4 \%C + 1.2 \times 10^5 (\%C)^2$$

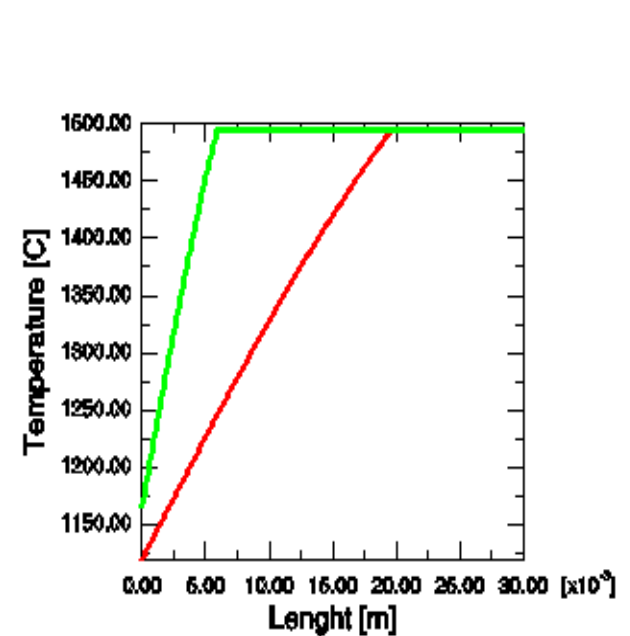
# Temperature and Stress Distribution

## Elastic-visco-plastic model by Kozlowski

Viewport: 1 Graph: XYPlot-1



Viewport: 1 Graph: XYPlot-1

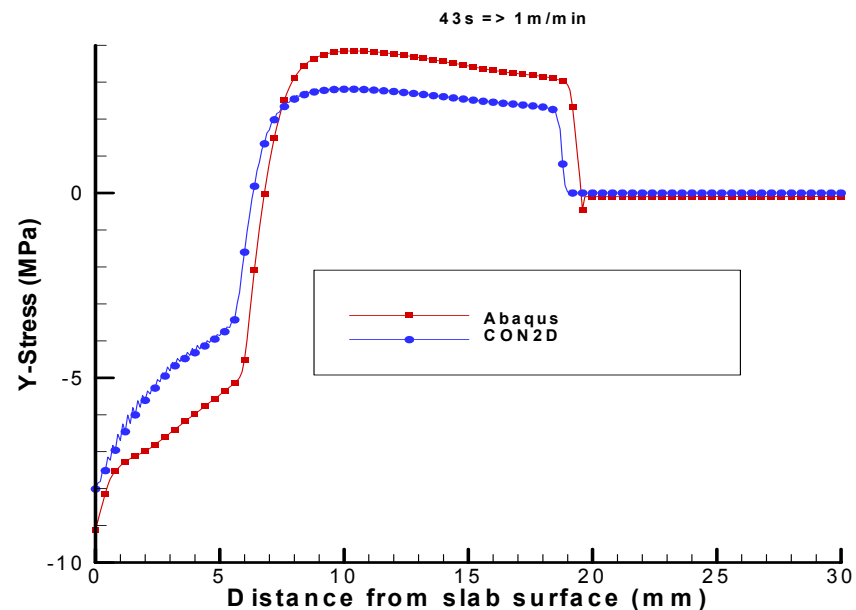
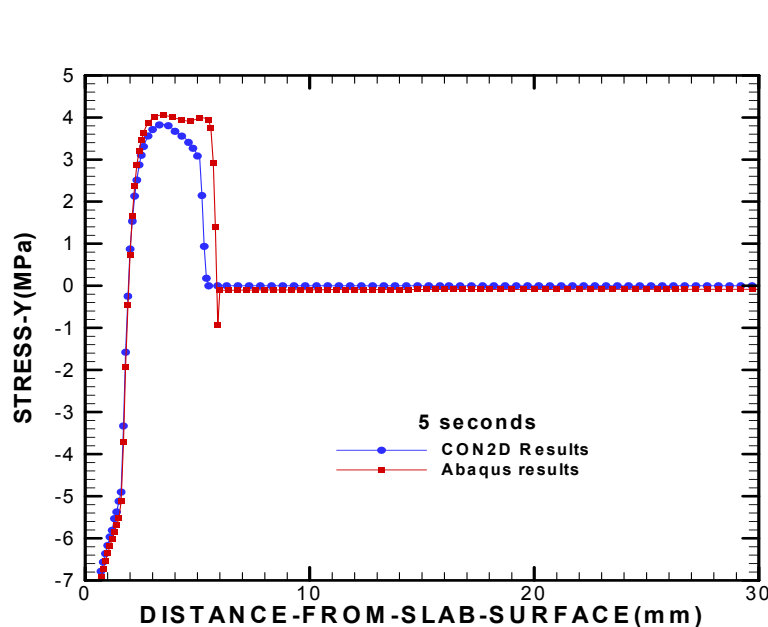


- Different residual stress values due to different creep rate function

- Lower temperatures due to real flux data

# Comparison of Abaqus and CON2D for previous complex model

	CON2D	ABAQUS/Native Explicit
Element type	6 node triangular	4 node rectangular
Number of elements	400	300
Number of nodes	1803	603
Initial time step	1.E-4	1.E-11
RAM used	350Mb	450Mb
Wall clock on IBMp690	5 minutes	5760 minutes (96 hours)



## Conclusions (Past Work):

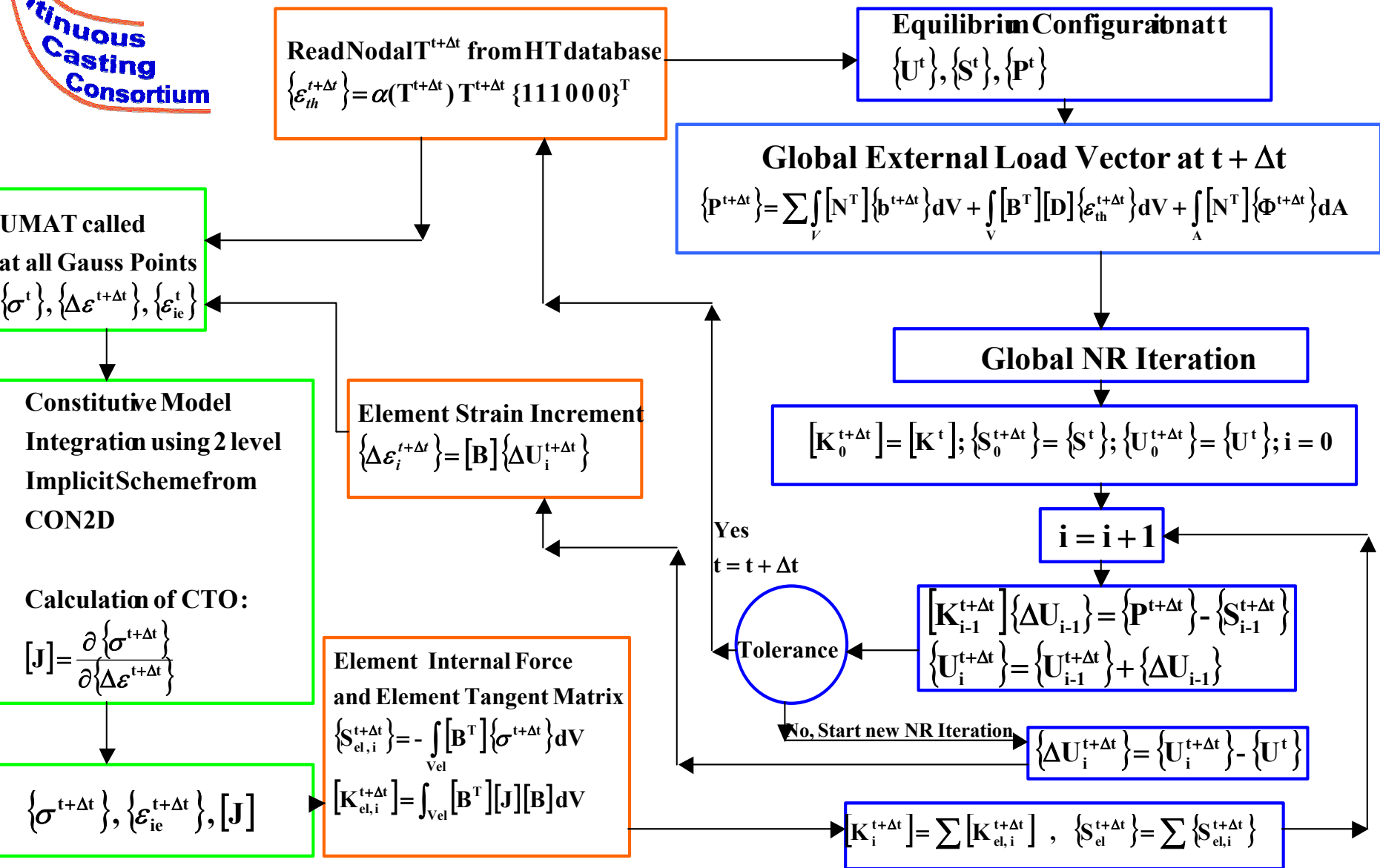
- Nowadays, **It is possible** to perform numerical simulations of steel solidification process in the Continuous Casting Mold with multipurpose commercial finite element code-Abaqus.
- **~1000 x more CPU** resources are needed with Abaqus explicit creep integration compared to in-house code CON2D for identical problem due to **superior CON2D robust integration scheme**
- **Main culprit** for Abaqus slow performance is the **integration** of the in creep functions.
- **Abaqus native implicit creep integration has failed completely** for this class of problems.
- **Quantitatively results are matching well, qualitative differences are under investigation.**

# Solutions to Abaqus Slow Performance

- **Solution 1:** Apply Kozlowski III model everywhere (liquid and solid) through the CREEP subroutine with its explicit integration, and **apply Abaqus native perfect plasticity for liquid**. Currently Abaqus Plasticity works only coupled with implicit creep integration. This issue has been addressed to HKS developers.
- **Solution 2:** Replace Abaqus native local integration model with fully **implicit local integration from CON2D followed by its robust two level bounded NR integration scheme** coded in another user defined subroutine UMAT. This work is currently under way. HKS has showed interest in our UMAT work.
- **Solution 2 is the focus of our current work !**

# Materially Non-Linear FEM Solution Strategy in Abaqus with UMAT

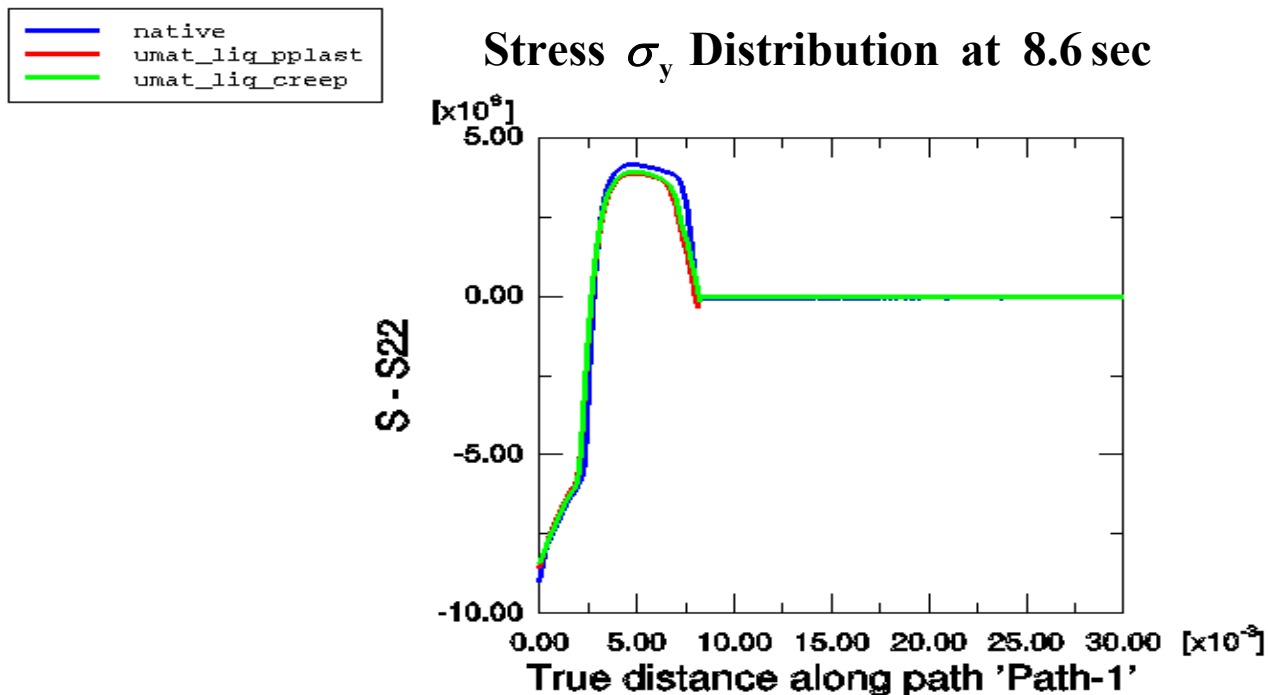
Continuous Casting Consortium





# Early Results with UMAT

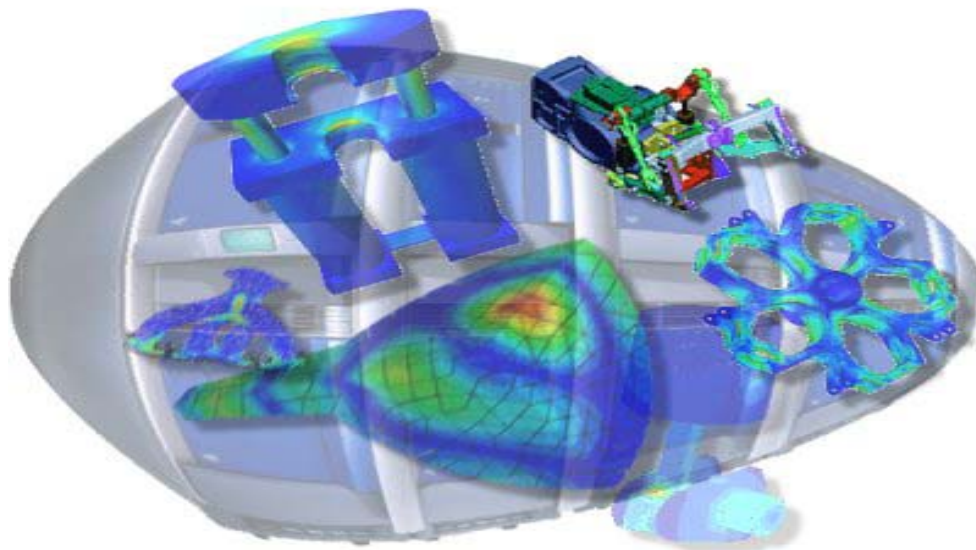
- Wall clock while keeping liquid creep function is ~25min, **230x Improvement** compared with Abaqus Native Explicit Integration, but still 5x slower then CON2D.
- Elastic-Perfectly Plastic constitutive law with very low Yield Stress coded for liquid phase replacing aggressive creep function and avoiding its integration. This implementation is actually **faster then CON2D, 4min** for this problem size and more then **1000x faster then Abaqus native explicit creep integration**.
- **Almost identical results for Stress Distribution** for both cases with UMAT and Native Explicit Creep Integration



# Future Work

- More work on validation of results and comparison with CON2D.
- Add constitutive model for steels with delta-ferrite and temp dependant thermal linear expansion.
- Move to **2D and perhaps 3D** FE domains with Abaqus to **increase process understanding**.
- Derive and add **Consistent Tangent Operator for temperature** to UMAT and fully couple HT and Stress analysis.
- **Add more Complexity** (Physics) to the model: Internal BC with Ferrostatic Pressure, contact and friction between mold and shell, input mold distortion data, effects of superheat...
- If there are enough dofs (3D), **parallel Abaqus features** can be applied (each time increment solved in parallel).

# New Engineering Computational Resources at the National Center For Supercomputing Applications at the University Of Illinois



**Seid Koric**

**Engineering Applications Analyst**

<http://www.ncsa.uiuc.edu>

[skoric@ncsa.uiuc.edu](mailto:skoric@ncsa.uiuc.edu)

# NCSA Terascale Linux Clusters

- **Intel Xeon Linux Cluster of Parallel PC-s**

(currently #4 with 6.12 Tflops on the top 500 list of supercomputers)

- 1280 3.06 GHz dual processor nodes
- Myrinet 2000 interconnect between PC-s
- 3GB /node of RAM



- **Intel Itanium2 Linux Cluster of Parallel Itanium PC-s**

- 256 1.3Ghz dual processor nodes
- Myrinet 2000 interconnect between PC-s
- 4 and 12 GB/node of RAM

• Can solve a million equations with million unknowns in less than a minute by performing  $350 \times 10^9$  floating point operation per second



## NCSA machine room expansion

- capacity to 20 TF and expandable
- dedicated September 5, 2001

• **Great Potential to solve large scale problems in computational fluid dynamics and computational solid mechanics**

# Shared Memory NCSA Capabilities:

- Shared memory systems IBM Regatta, Power 4

- 2+ TF of clustered SMP
- 32 SMP CPUS, 1.3 Ghz
- large, 256 GB memory
- AIX IBM Unix OS

Perfect for engineering commercial software like:

**Abaqus, Ansys, Fluent, LS-Dyna, Marc, PRO/E..**

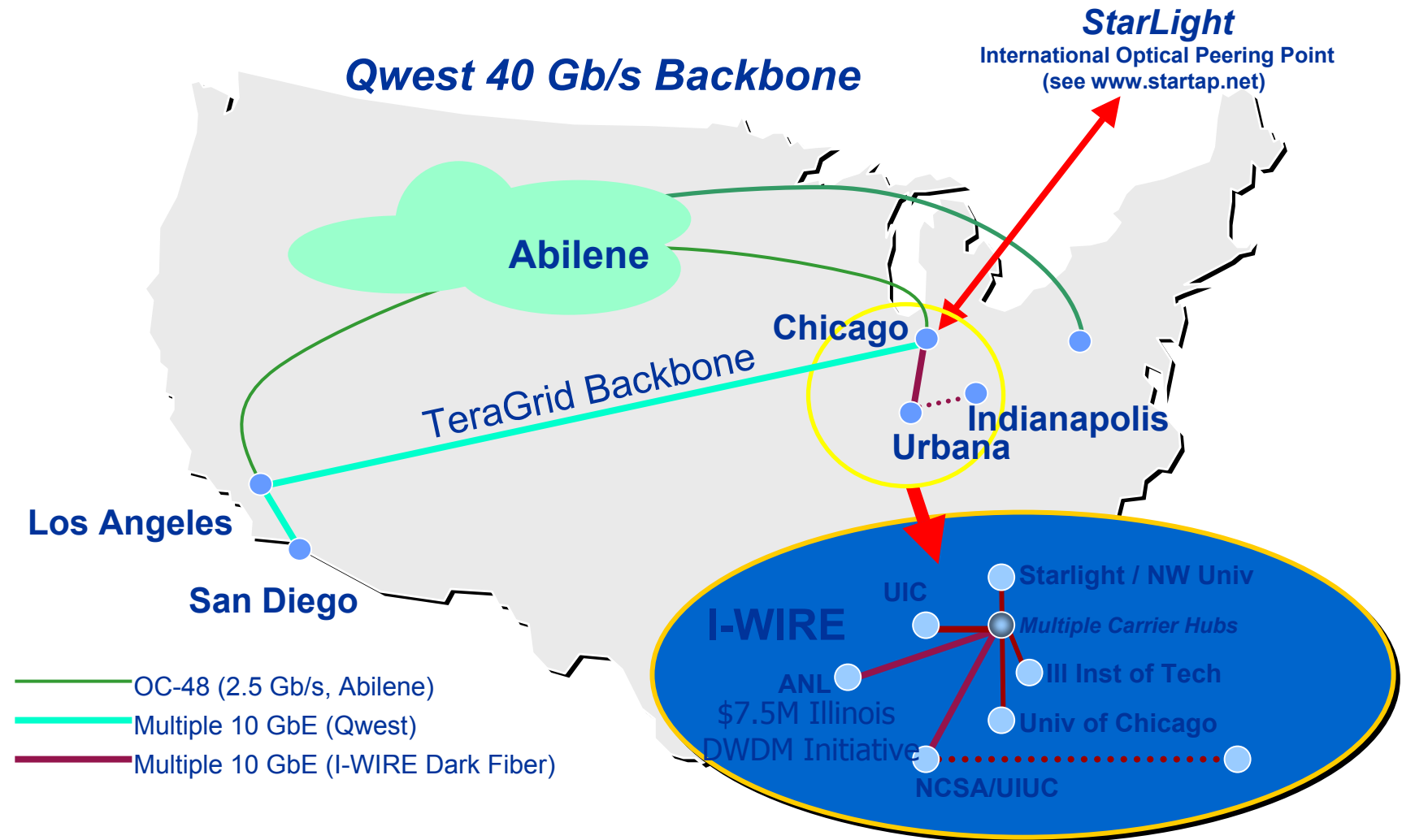


- Further SMP Expansions coming this year with newest SMP platform(s)
- Secondary and tertiary storage
  - 500 TB secondary storage SAN
  - 3.4 PB tertiary storage

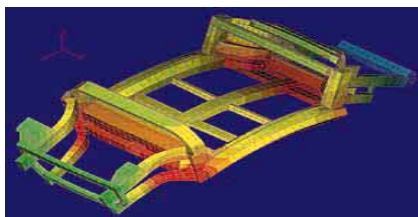
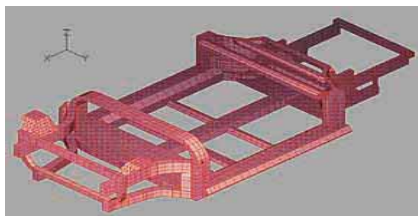


# Computing in 21<sup>st</sup> Century, a story of TeraGrid

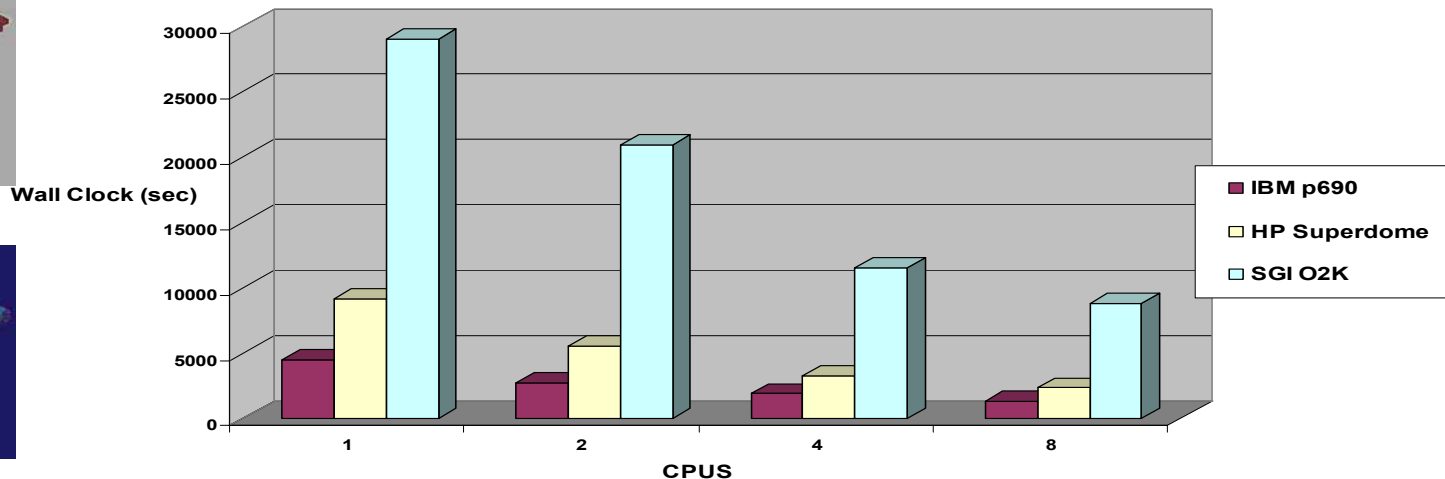
*Computing Resources: Anytime, Anywhere*



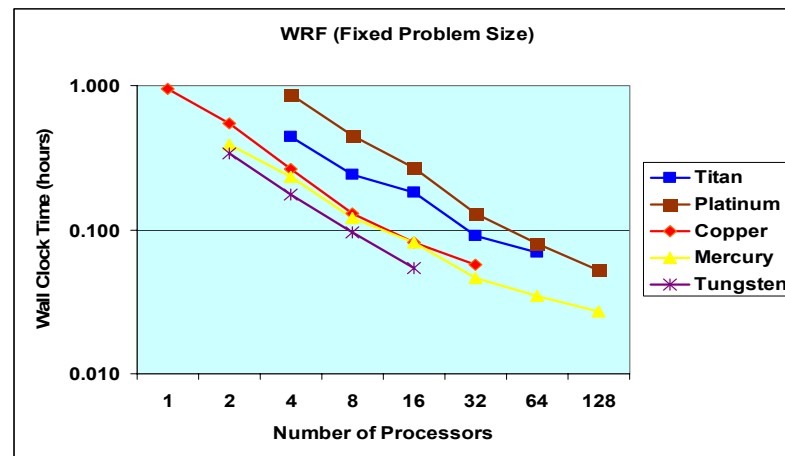
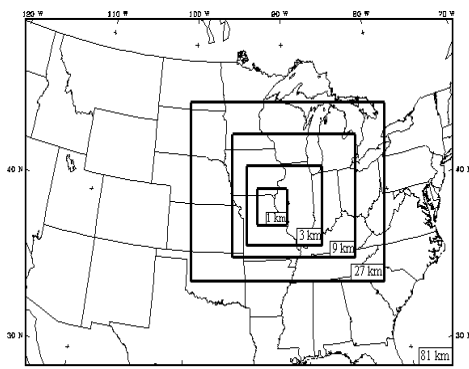
# Some CSM and CFD Applications on NCSA machines



Abaqus/Standard, SMP Solver, 1m dofs



Reference: Bob  
Wilhelmson (NCSA)  
Severe Weather  
Forecast



# Acknowledgments:

- **Prof. Brian G. Thomas**
- **Chungsheng Li, PhD, Former UIUC student**
- **Caludio Ojeda, Former Visiting Scholar**
- **National Center for Supercomputing Applications**