Abaqus ME498 Talk

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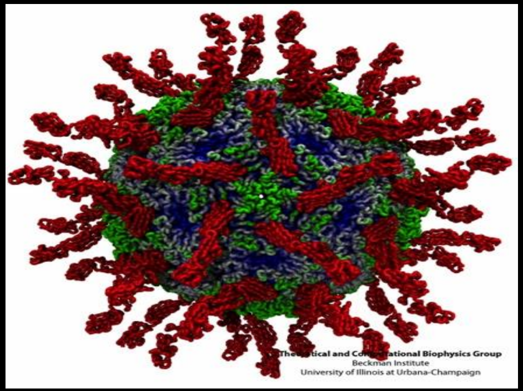
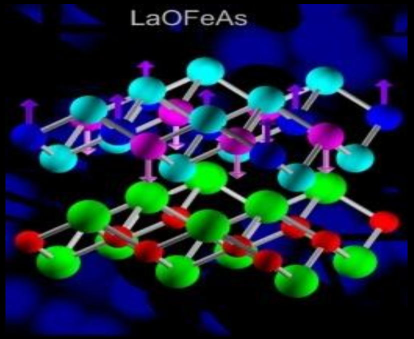
Who uses High Performance (Super) Computing ?

Answer: Anyone whose problem can not fit on a PC or workstation, and/or would take a very long time to run on a PC

Molecular Science and Materials

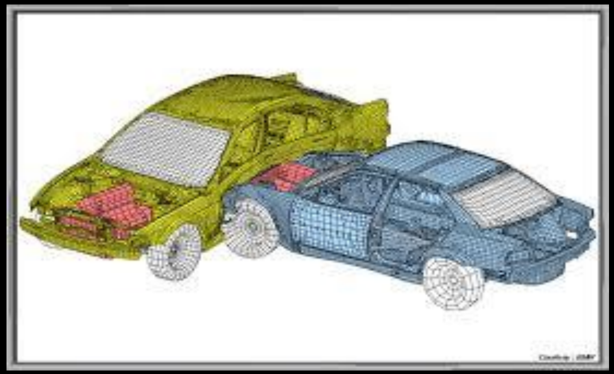




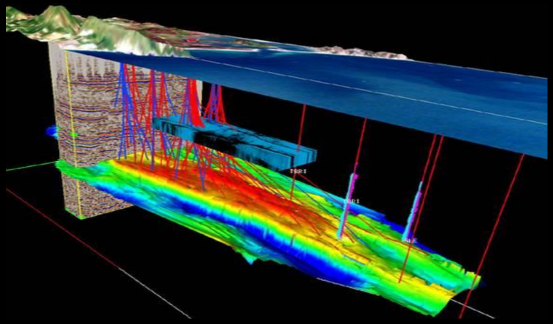
Weather & Climate

Astronomy

Engineering



Geoscience

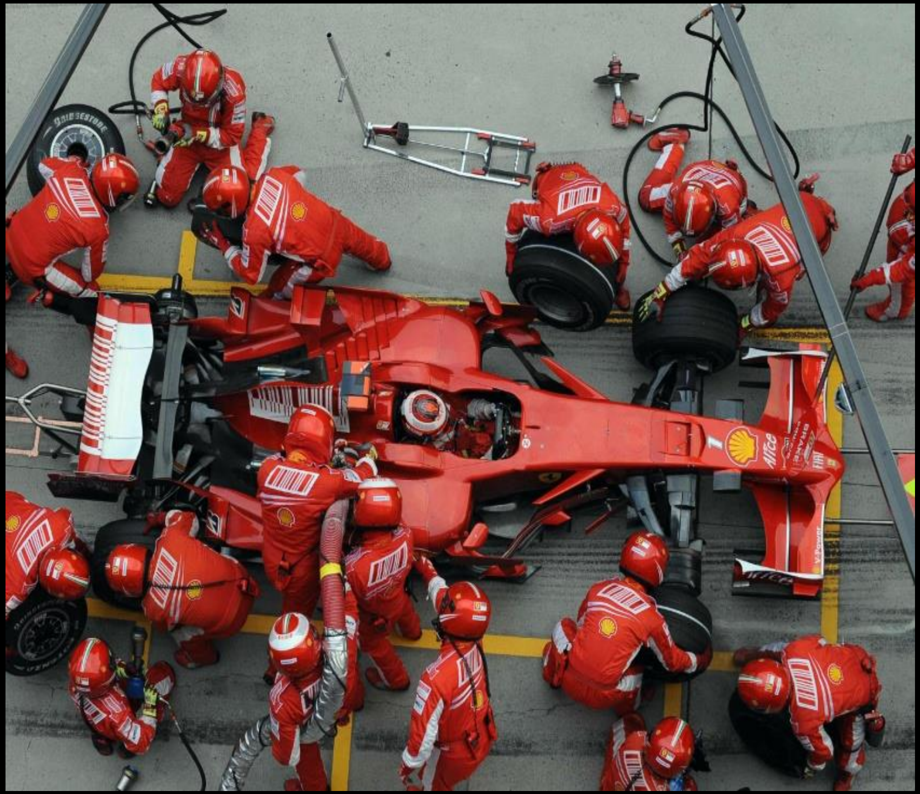


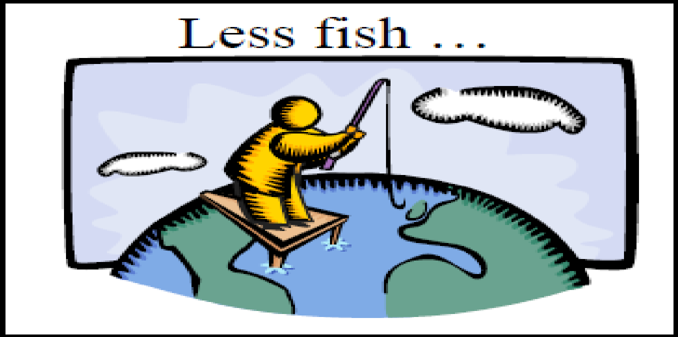
Health/Life Science

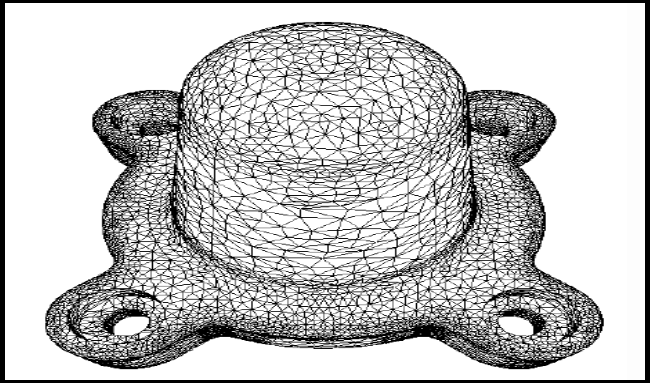
Finance Modeling

What makes HPC so "High Performance" ?

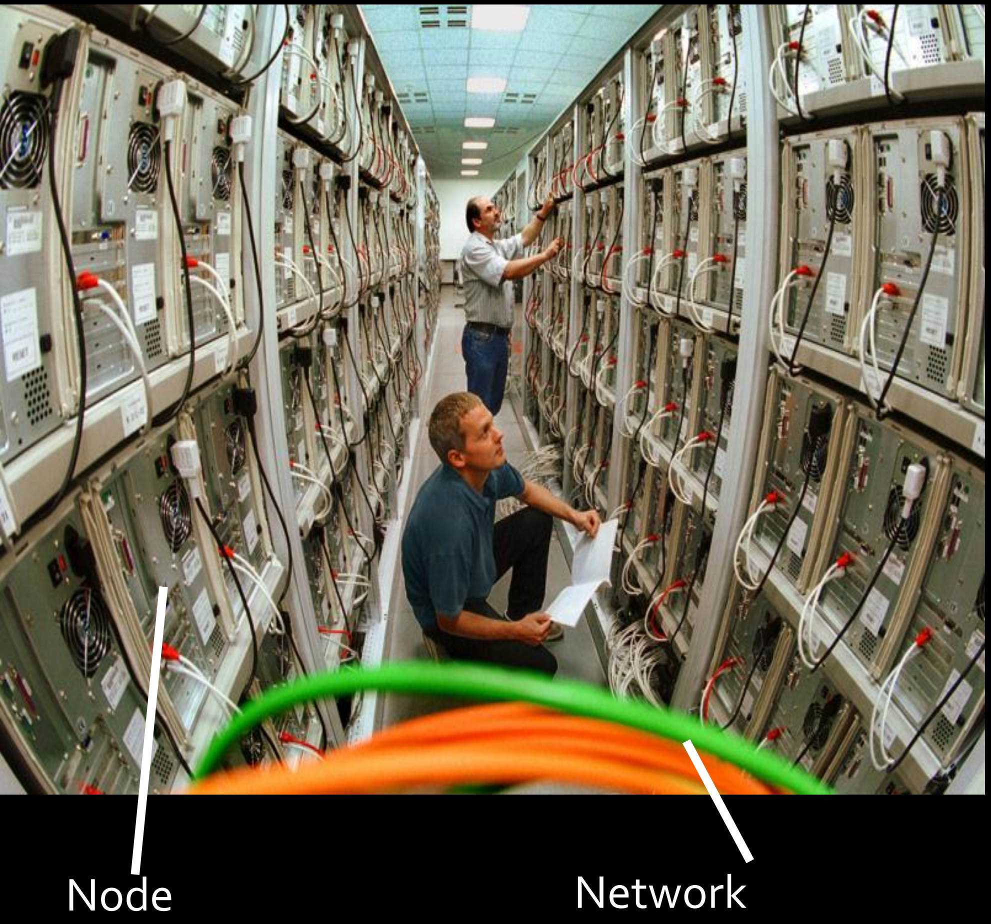
Answer: **Parallelism**, doing many things (computing) at the same time, or a set of independent processors work cooperatively to solve a single problem







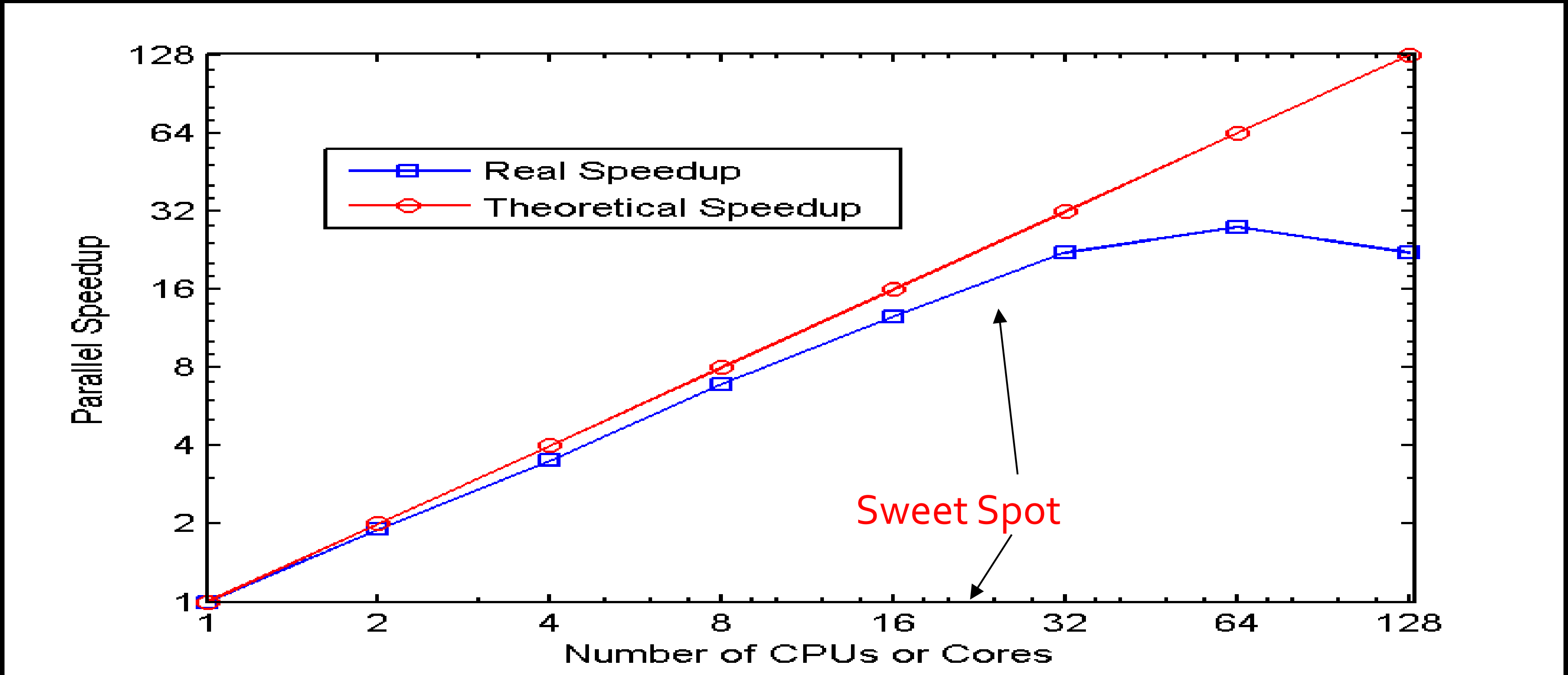
How a Supercomputer looks like ?



- Many computers, nodes, often in special cases for easy mounting in a rack
- One or more networks (interconnects) to connect the nodes together
- (Shared) File System for I/O
- Software that allows the nodes to communicate with each other (e.g. MPI)
and work in parallel
- Software that reserves resources to individual users

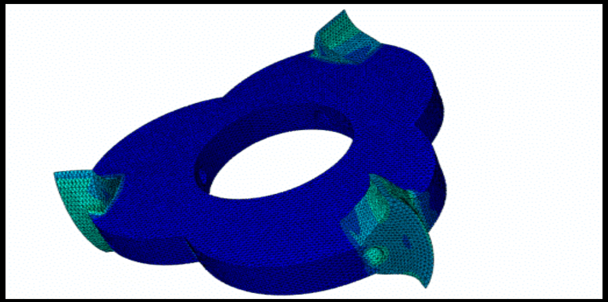
Scalable Speedup (Supercomputing 101)

- Speed-up (Sp) = wallclock for 1 core / wallclock # of Cores
- Speed-up reveals the benefit of solving problems in parallel
- Every problem has a “sweet spot”; depends on parallel implementation and problem size
- Real Sp is smaller then theoretical Sp due to: serial portions of the code, load imbalance between CPUs, network latency and bandwith, specifics in parallel implementation in the code, I/O, etc.

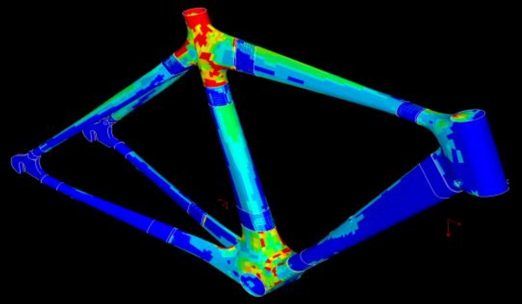


Think Big !

“It is amazing what one can do these days on a dual-core laptop computer. Nevertheless, the appetite for more speed and memory, if anything is increasing. There always seems to be some calculations that ones wants to do that exceeds available resources. It makes one think that computers have and will always come in one size and one speed: “**Too small and too slow”. This will be the case despite supercomputers becoming the size of football fields !”**



Tom Hughes, 2001, President of International Association for Computing Mechanics-IACM



National Petascale Computing Facility

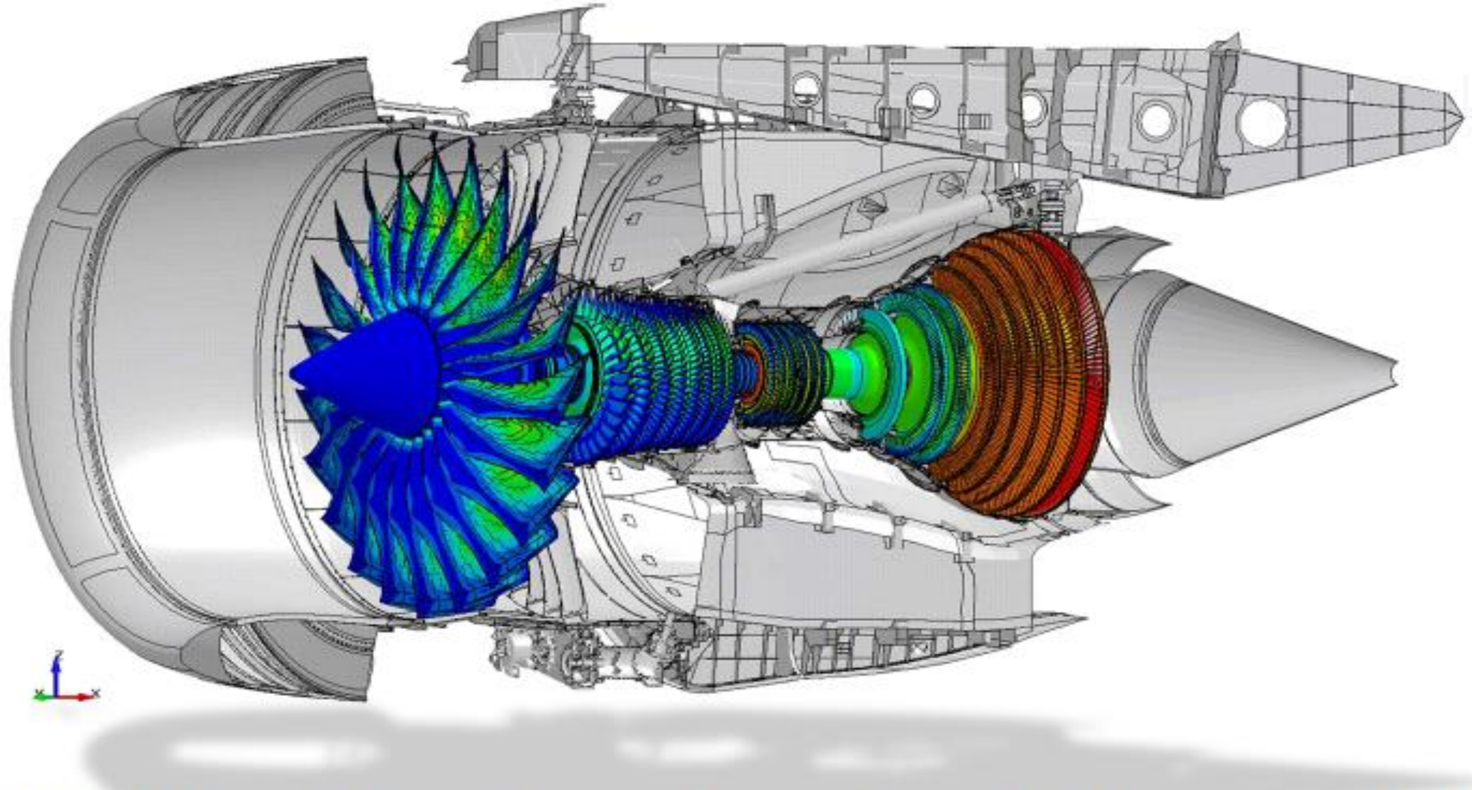
iFORGE

BLUE WATERS

SUSTAINED PETASCALE COMPUTING

A vision from our Industrial Partner

Dr. Yoon Ho, Rolls Royce, ISC14

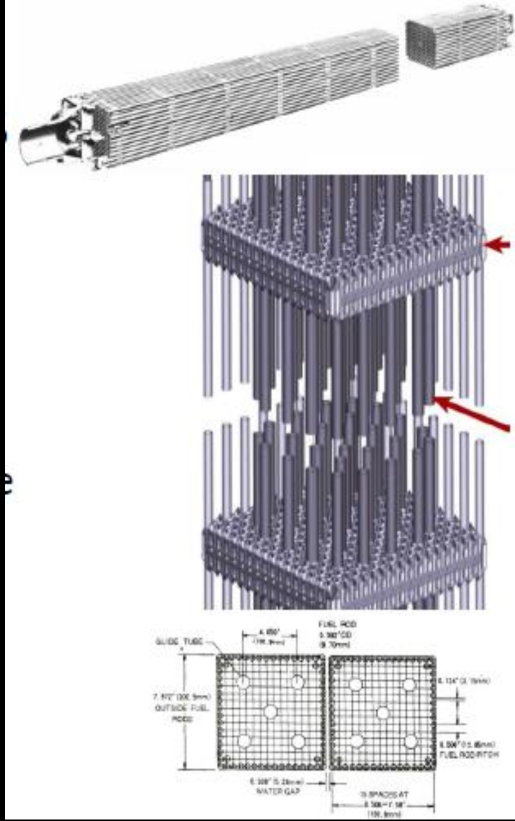


High fidelity virtual engine simulation and design

- > 1 trillion degrees of freedom (DOF)
- > 1 billion core hours per calculation

Direct Numerical Simulation of the Multiphase Flow in Nuclear Reactor Core (Year 2060 ?)

- About 160 fuel Assemblies (17x17 each, 4m long)
- Reynolds Number of 5,000 (typical reactor condition)
- Mesh Size 40,000T elements
- Should run up to 320B cores at 128K elements/core
- Would resolve 13.6B bubbles at average 1% void fraction
- **Number of Grid Points ~ $Re^{9/4}$ Overall cost ~Re^3**



Prof. Igor Bolotnov, NCSU, HPC-User Forum (2014)

Alya - Multiphysics on Extreme-Scale HPC

Designed by the Barcelona Supercomputer Center as a multiphysics parallel FEA code

Unstructured high order spatial discretization, explicit and implicit high order integration in time

Staggered schemes (with iterations) for coupled physics on a single mesh

Mesh partitioning and hybrid parallel implementation

Uses built-in iterative CG solver with various preconditioning techniques

Highly modular, with each module representing a different physics; easy to combine them at job launch

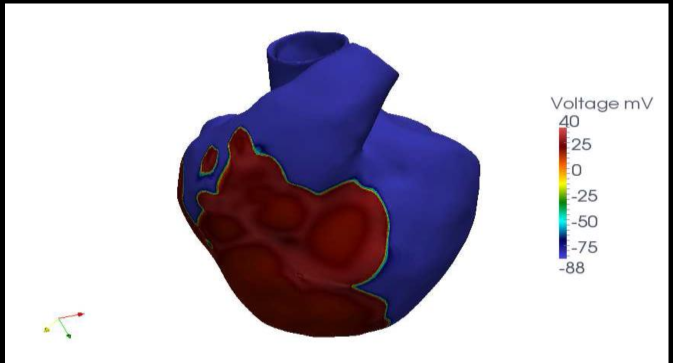
Ported to Blue Waters in 2014

Top Supercomputing Achievement – HPCwire Readers Choice at SC 2014 !

2 Real-World Cases

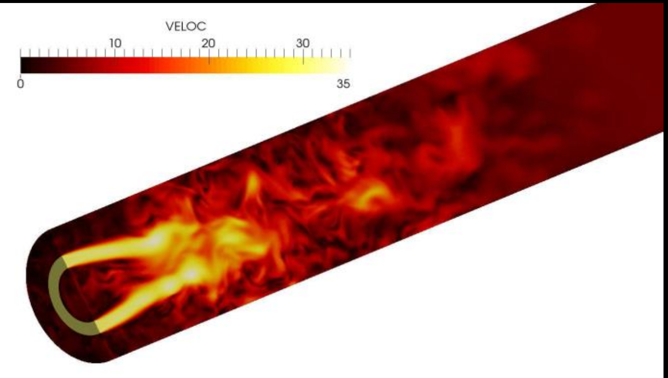
Human Heart

Non-linear solid mechanics
Coupled with electrical propagation
3.4 billion elements, scaled to 100,000 cores

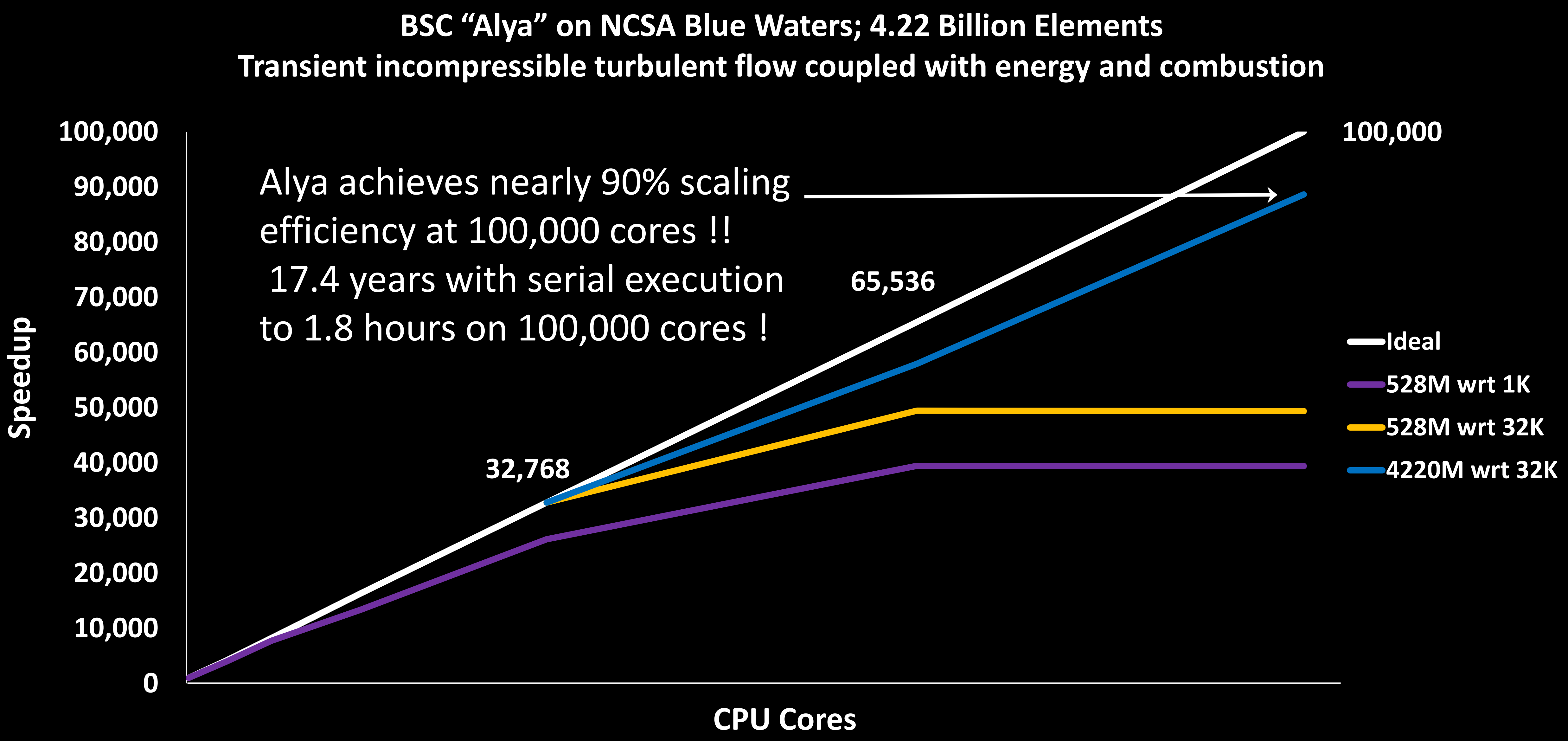


Kiln Furnace

Transient incompressible turbulent flow
Coupled with energy and combustion
4.22 billion elements, scaled to 100,000 cores



Alya – Kiln Furnace



Why Abaqus ?

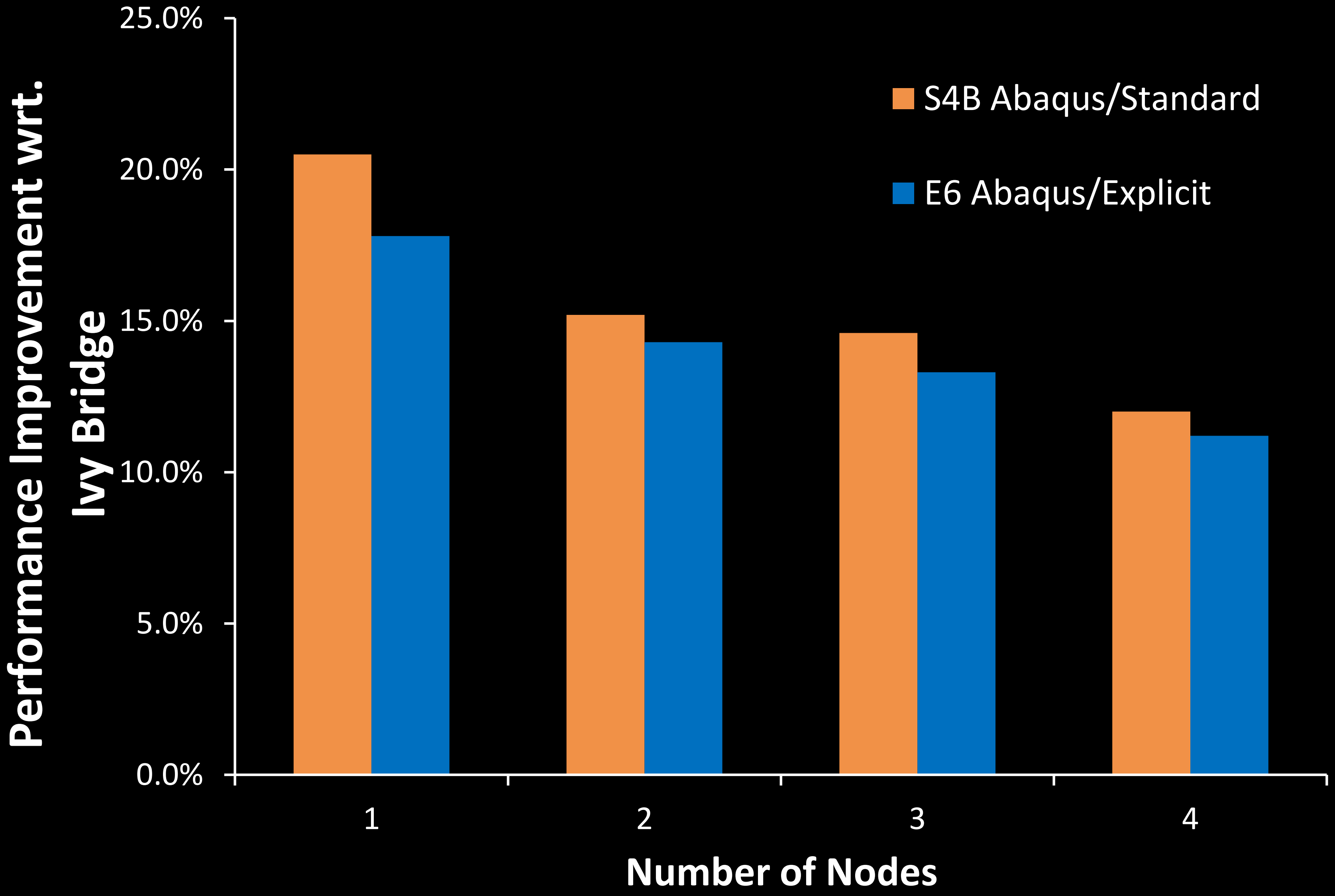
- Abaqus is the most popular FEA ISV Software, heavily used by both academia and industry

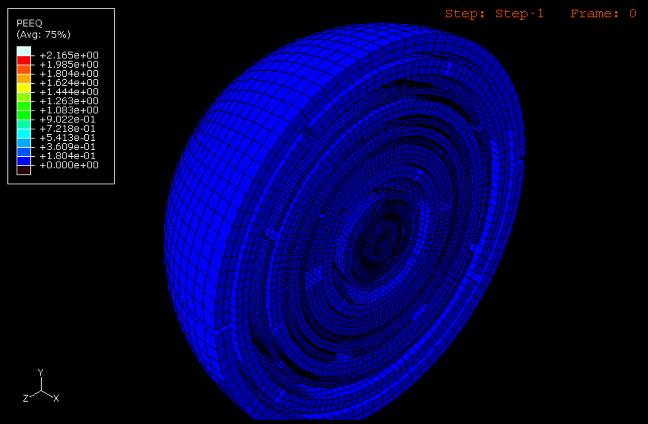
- Academic and open source FEA codes are hand-tailored to the numerical problem to be solved and often feature only basic numerical algorithm and are difficult to use. They are often missing imbedded pre and post processing capabilities, contact, nonlinear material constitutive models, mesh adaptivity, and flexible coupling of different elements and physics –all the crucial features in industry and research

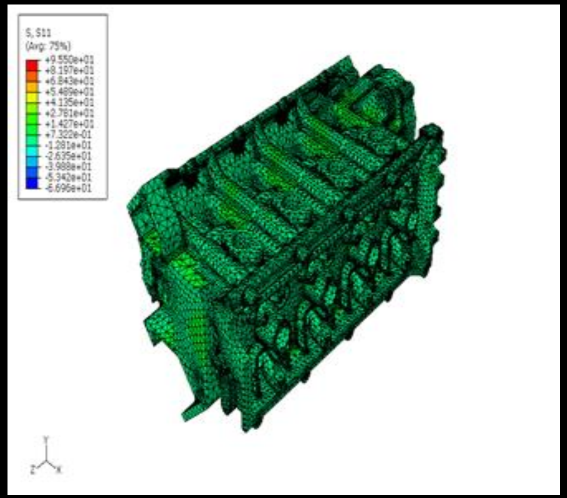
- Abaqus has a modern and friendly GUI CAE for pre and post processing coupled with the robust implicit and explicit parallel solvers and even CFD solvers.

- Its direct implicit solver scales on modern HPC better than any other ISV direct solver we have tested. It accelerates on GPUs better than any other ISV code.

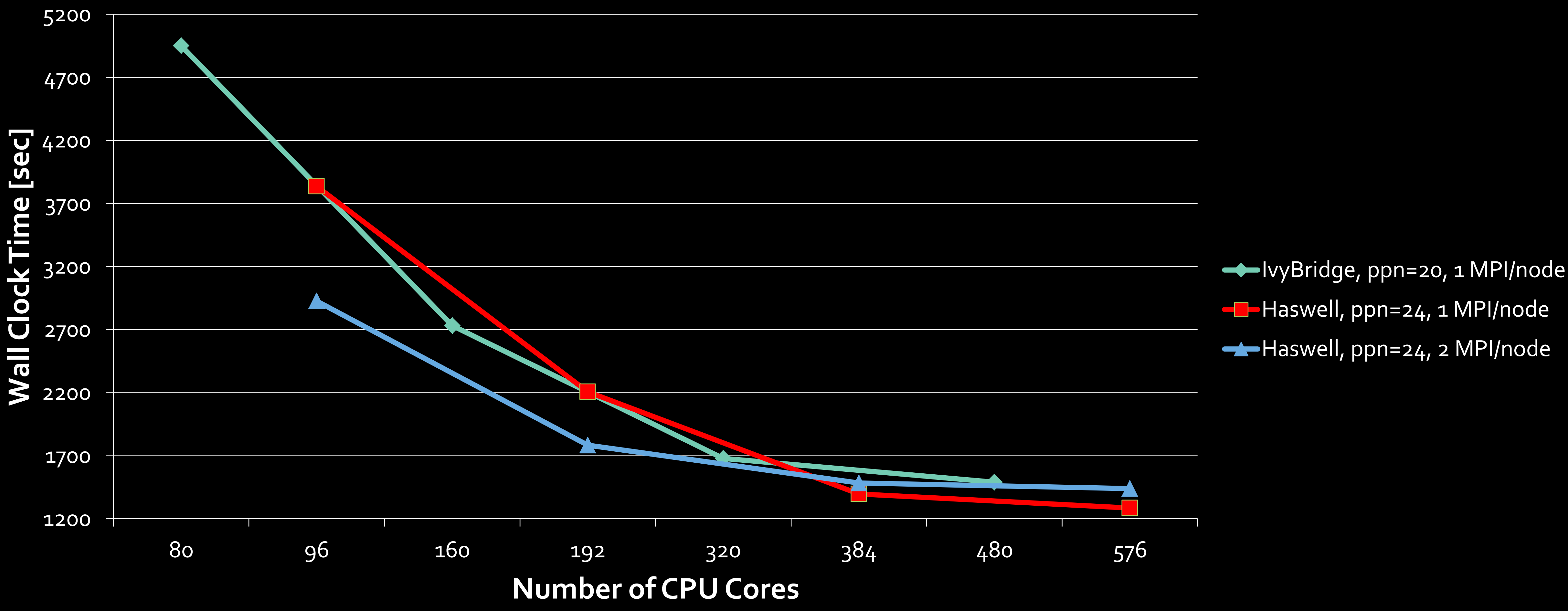
Abaqus on Intel Haswell Nodes of iForge



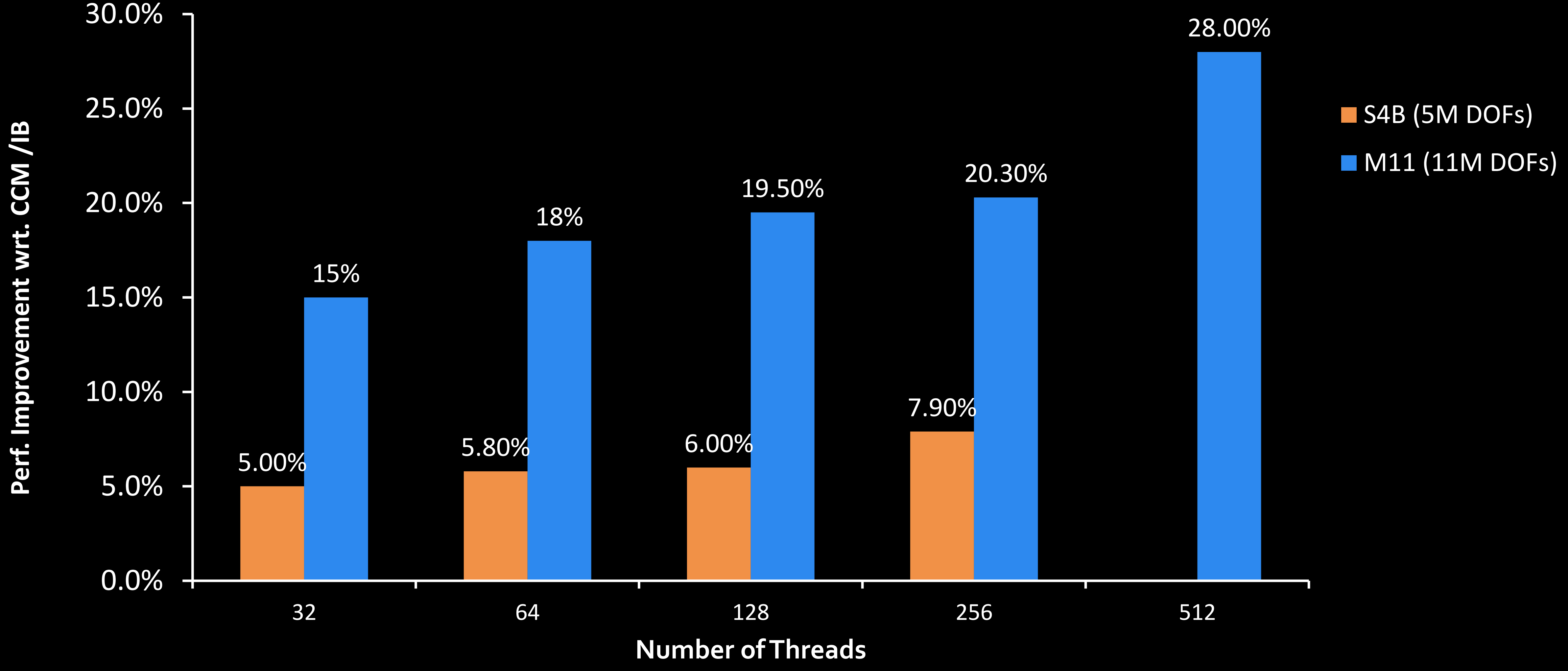




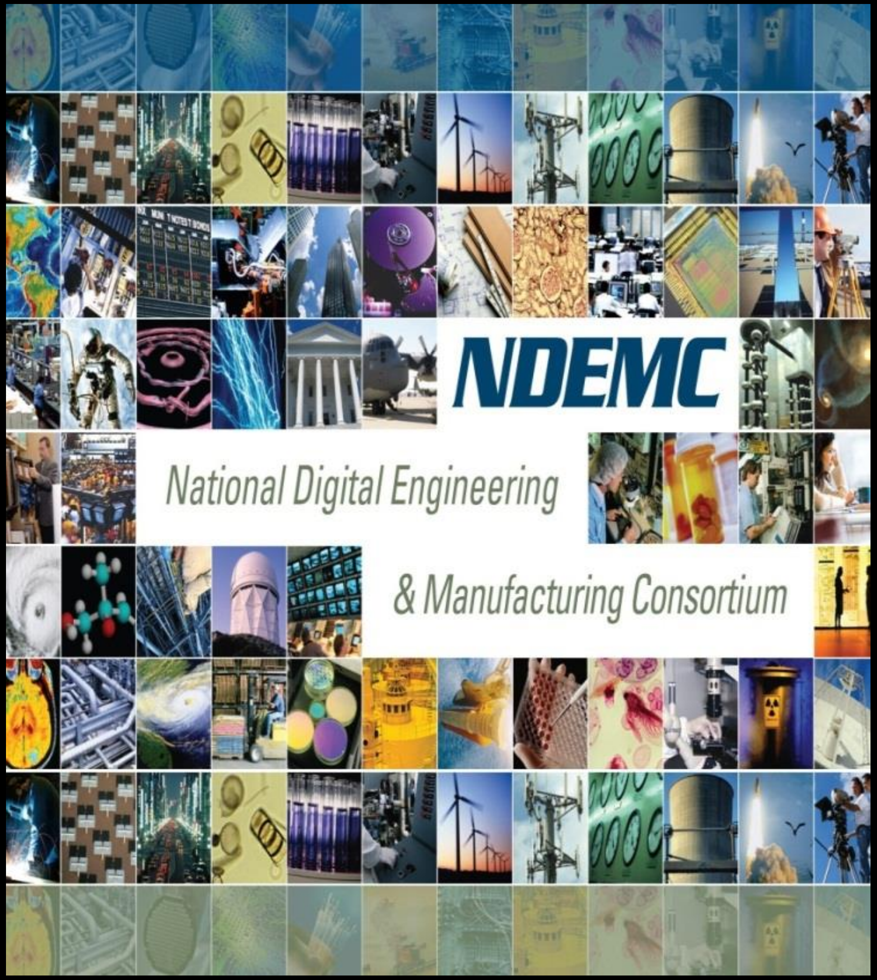
Abaqus on iForge
15M DOFs S4E(refined S4B)



Abaqus on Cray Linux Environment and Gemini



NDEMC Public-Private Partnership 2012-2014

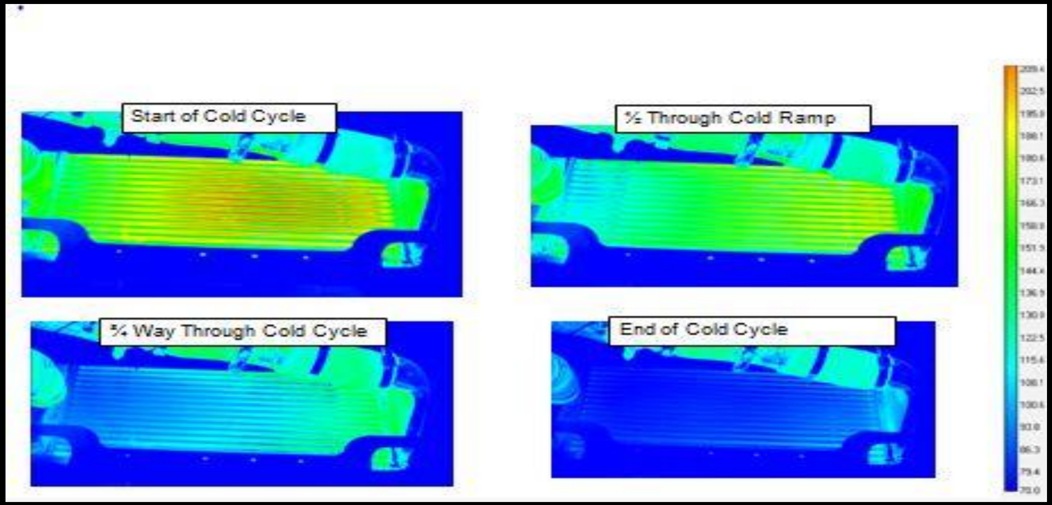


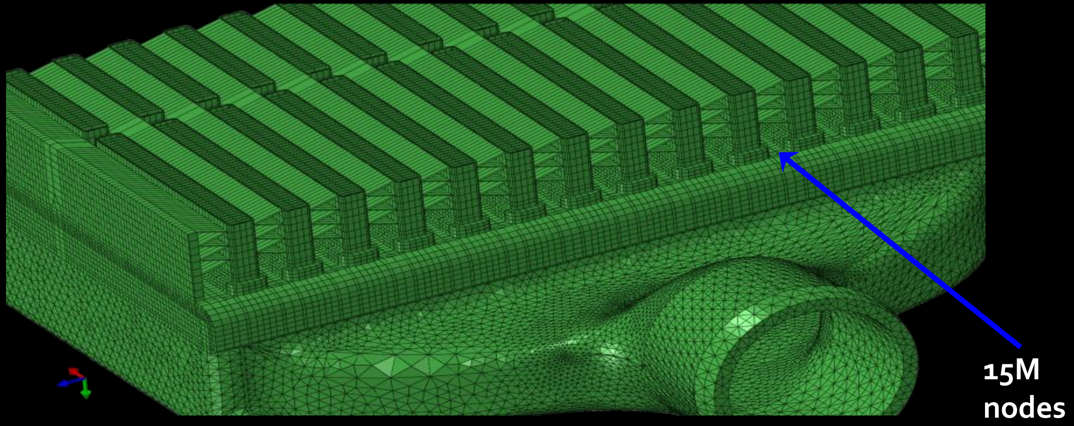
•US OEMs have gained a competitive edge through the use of high performance computing (HPC) with modeling simulation and analysis (MS&A).

• Council of competitiveness recognized that small and medium sized enterprises (SMEs) are not able to take advantage of HPC

• Starting in Spring of 2011 a regional pilot program was started in the Midwestern supply base.

Project: Multiphysics Simulation of Charge Air Cooler (CAC) during a thermal cycle



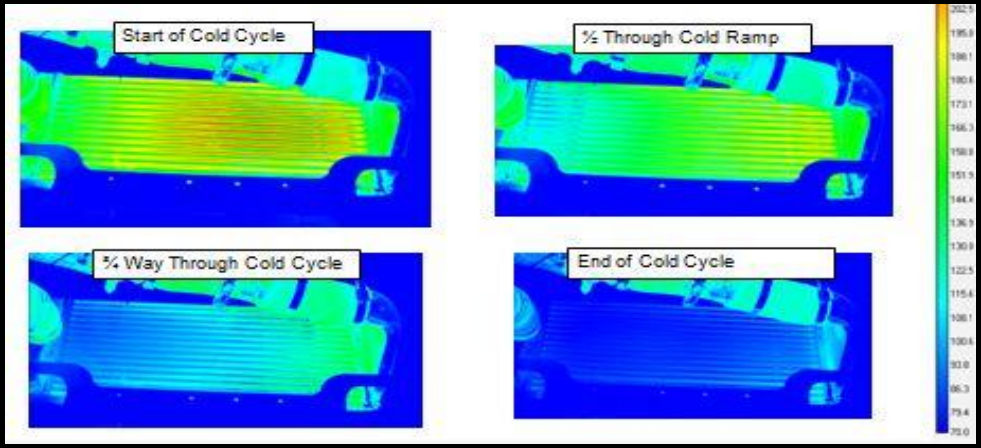


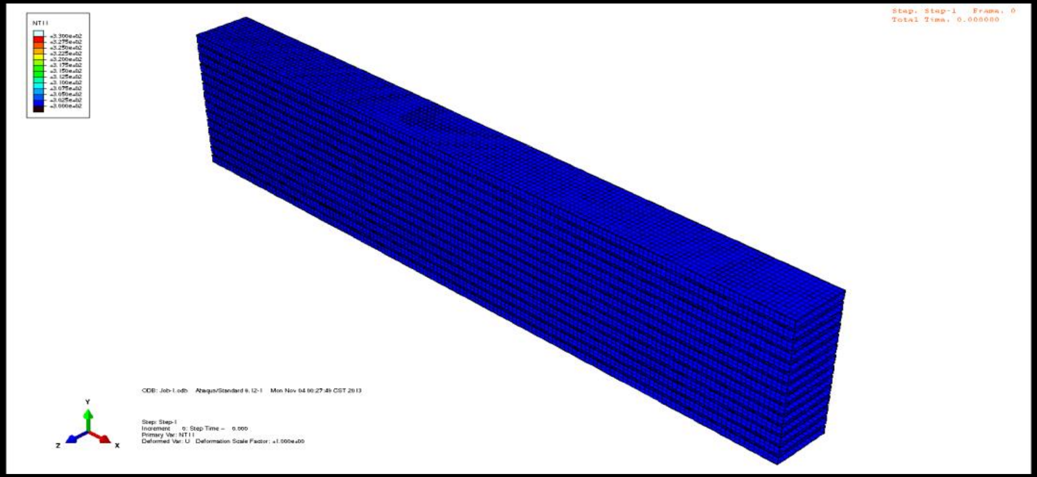
CFD Analysis of turbulent fluid flow through CAC coupled with advective HT to provide thermal BC-s for FEA

Thermo-Mechanical FEA analysis of transient thermal stresses in solid part during the thermal cycle

The history of thermal stresses is inputted into a low cycle fatigue model to estimate the cycle life at critical points

Hybrid Experimental and Numerical Method for Thermomechanical Analysis of a Heat Exchanger





Transient thermal stress analysis of the solid structure in a heat exchanger requires a multiphysics simulation workflow involving turbulent fluid flow with advective heat combined with thermo-mechanical analysis

The present method utilizes experimental input (thermal images) into FEA program (Abaqus) to eliminate one of the physical sub-problems, i.e., fluid dynamics.

The main advantage of the method is efficiently capturing multiphysics response with a significantly reduced computational modeling.

A pending UIUC Patent !

Visco-plastic Multi-physics Modeling of Steel Solidification

Seid Korić and Brian G. Thomas

National Center for Supercomputing Applications-NCSA

Mechanical Science and Engineering-MechSE

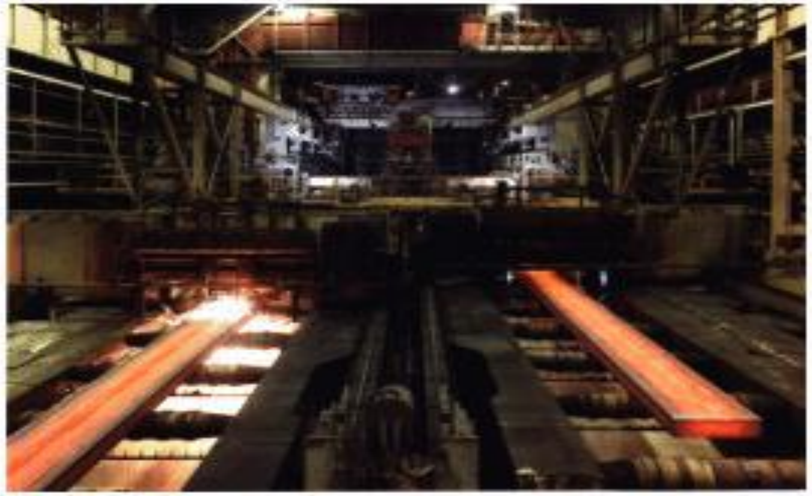
University of Illinois at Urbana-Champaign

International Symposium on Plasticity 2014

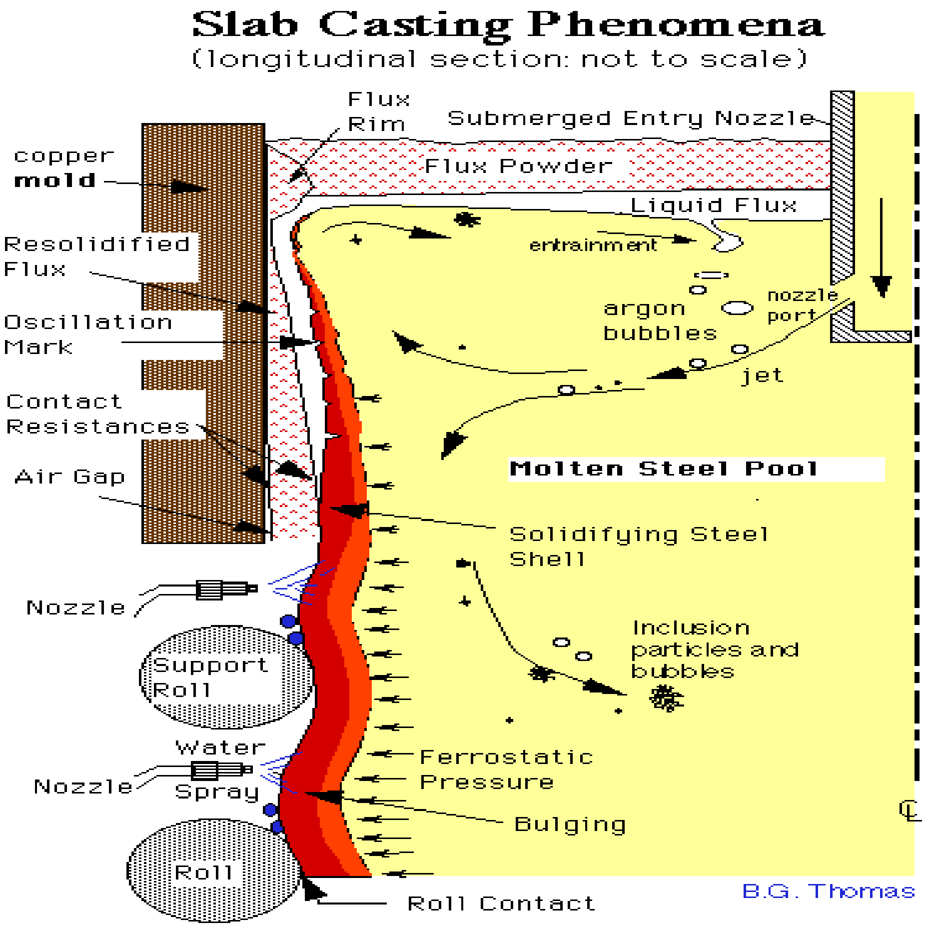
January 7, 2014

Introduction

- Many manufacturing and fabrication processes involve common solidification phenomena
- One of most important and complex among them is continuous casting
- 92% of steel today is produced through continuous casting
- Quality of continuous casting is constantly improving, but significant work is still needed to minimize defects and improve productivity
- High cost and harsh environment limit plant and lab experiments
- Better and accurate numerical modeling work is needed in simulating, optimizing and designing this process



Continuous Casting Phenomena



- **Molten steel freezes** against water-cooled walls of a copper mold to form a solid shell.
- **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.
- **Superheat flux** from turbulent fluid flow mix in liquid pool
- **Ferrostatic pressure** pushes against the shell, causing it bulge outwards.
- **Mold distortion** and **mold taper** (slant of mold walls to compensate for shell shrinkage) affects mold shape and interfacial gap size.

Objective: multiphysics approach of simulating all 3 phenomena (fluid flow, heat transfer, and stress)

Governing Equations

Solid and Mushy regions:

Heat 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 Equation

$$\nabla\cdot\boldsymbol{\sigma}(\mathbf{x})+\mathbf{b_o}=0$$

Strain Rate Decomposition

$$\dot{\boldsymbol{\varepsilon}}=\dot{\boldsymbol{\varepsilon}}_{\mathrm{el}}+\dot{\boldsymbol{\varepsilon}}_{\mathrm{ie}}+\dot{\boldsymbol{\varepsilon}}_{\mathrm{th}}$$

Liquid regions:

Energy

$$\rho\frac{Dh}{Dt}=\frac{Dp}{Dt}+k\nabla^2T-\nabla\cdot\boldsymbol{q}_{rad}+q'''+\Phi$$

Continuity

$$\nabla\cdot\mathbf{v}=0$$

Momentum

(2 extra eqs. for K and e)

$$\rho\frac{\mathrm{D}\mathbf{v}}{\mathrm{D}t}=-\nabla\mathrm{p}+\mu\nabla^2\mathbf{v}+\mathbf{B}$$

Turbulence

$$\mu_{\mathrm{T}}=\frac{\mathrm{C}\mu\rho\mathrm{k}^2}{\varepsilon}$$

Constitutive Models for Solid Steel (T<=Tsol)

Unified (Plasticity + Creep=Viscoplastic) Approach

Kozlowski Model for Austenite (Kozlowski 1991)

$$\dot{\varepsilon}(1/\sec.) = f(\%C)\left[\sigma(MPa) - f_1\left(T({}^oK)\right)\varepsilon|\varepsilon|^{f_2(T({}^oK))-1}\right]^{f_3(T({}^oK))}\exp\left(-4.465\times10^4({}^oK)/T({}^oK)\right)$$

$$f_1\left(T({}^oK)\right) = 130.5 - 5.128\times10^{-3}T({}^oK)$$

$$f_2\left(T({}^oK)\right) = -0.6289 + 1.114\times10^{-3}T({}^oK)$$

$$f_3\left(T({}^oK)\right) = 8.132 - 1.54\times10^{-3}T({}^oK)$$

$$f(\%C) = 4.655\times10^4 + 7.14\times10^4\%C + 1.2\times10^5(\%C)^2$$

Modified Power Law for Delta-Ferrite (Parkman 2000)

$$\dot{\varepsilon}(1/\sec.) = 0.1\left|\sigma(MPa)\Big/ f(\%C)\left(T({}^oK)/300\right)^{-5.52}(1+1000\varepsilon)^m\right|^n$$

$$f(\%C) = 1.3678\times10^4(\%C)^{-5.56\times10^{-2}}$$

$$m = -9.4156\times10^{-5}T({}^oK) + 0.3495$$

$$n = 1\Big/1.617\times10^{-4}T({}^oK) - 0.06166$$

Two Way Mechanical-Thermal Coupling in Solid Shell

Mechanical Solution depends on temperature field through thermal strains

$$\{\varepsilon_{th}\} = (\alpha(T)(T - T_{ref}) - \alpha(T_i)(T_i - T_{ref}))\,[1\,1\,1\,0\,0\,0]^T$$

The gap heat coefficient depends on the gap distance *d* calculated from mechanical solution

$$q_{gap} = -k\partial T / \partial n = -(h_{rad} + h_{cond})(T_{shell} - T_{mold})$$

$$\frac{1}{h_{cond}} = \frac{1}{h_{mold}} + \frac{(d_{gap} - d_{slag})}{k_{air}} + \frac{d_{slag}}{k_{slag}} + \frac{1}{h_{shell}}$$

Computational Methods Used to Solve Coupled Thermo-Mechanical Governing Equations

- **Global Solution Methods** (solving global FE equations)

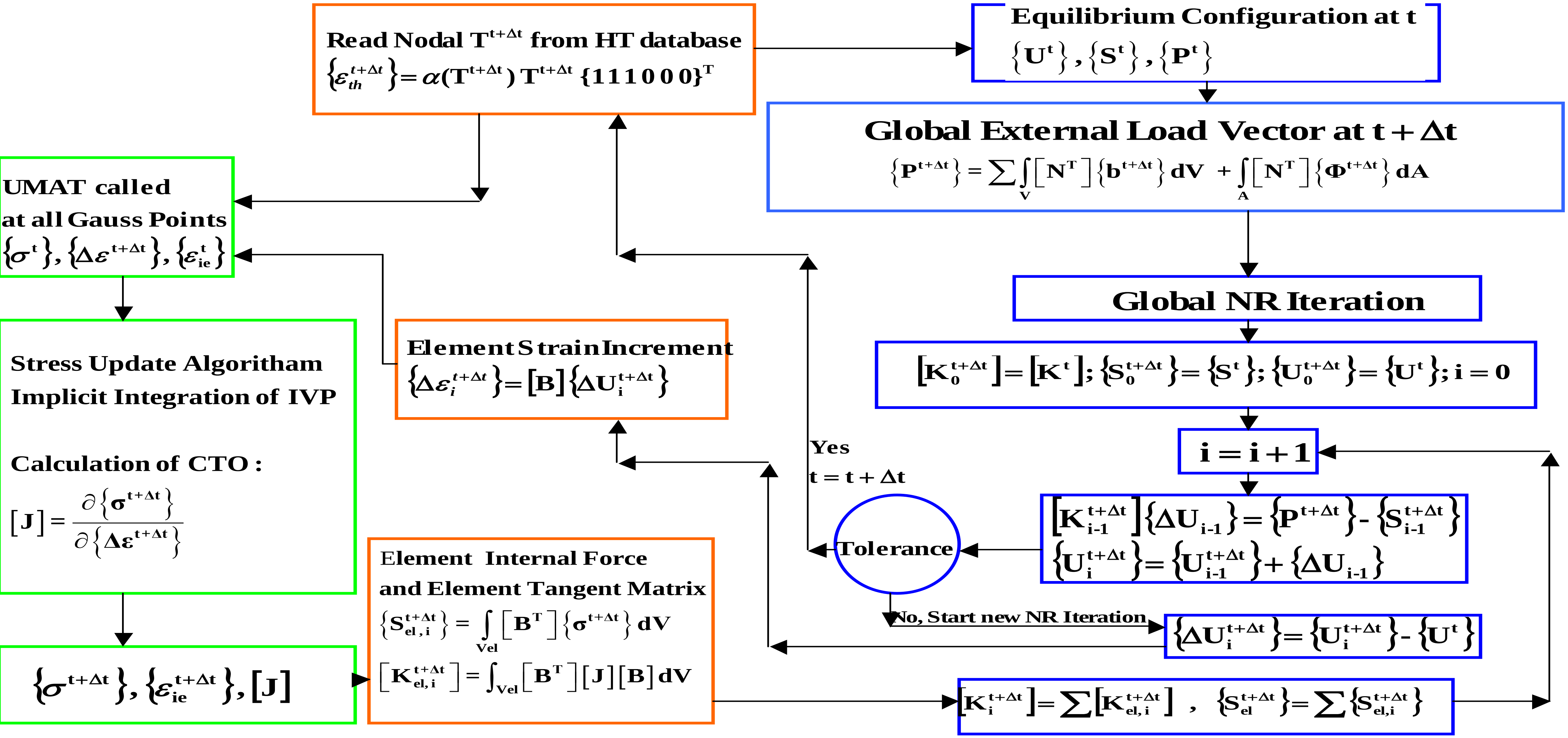
  - Full Newton-Raphson (Abaqus)

- **Local Integration Methods** (on every material points integrating constitutive laws) [IJNME Koric,2006 & 2010]

  -Fully Implicit followed by local bounded NR, for solid regions.

  -Radial Return Method for Rate Independent Plasticity, for non solid regions.

Model Details: Non-Linear FEM Solution Strategy (in Abaqus with UMAT)



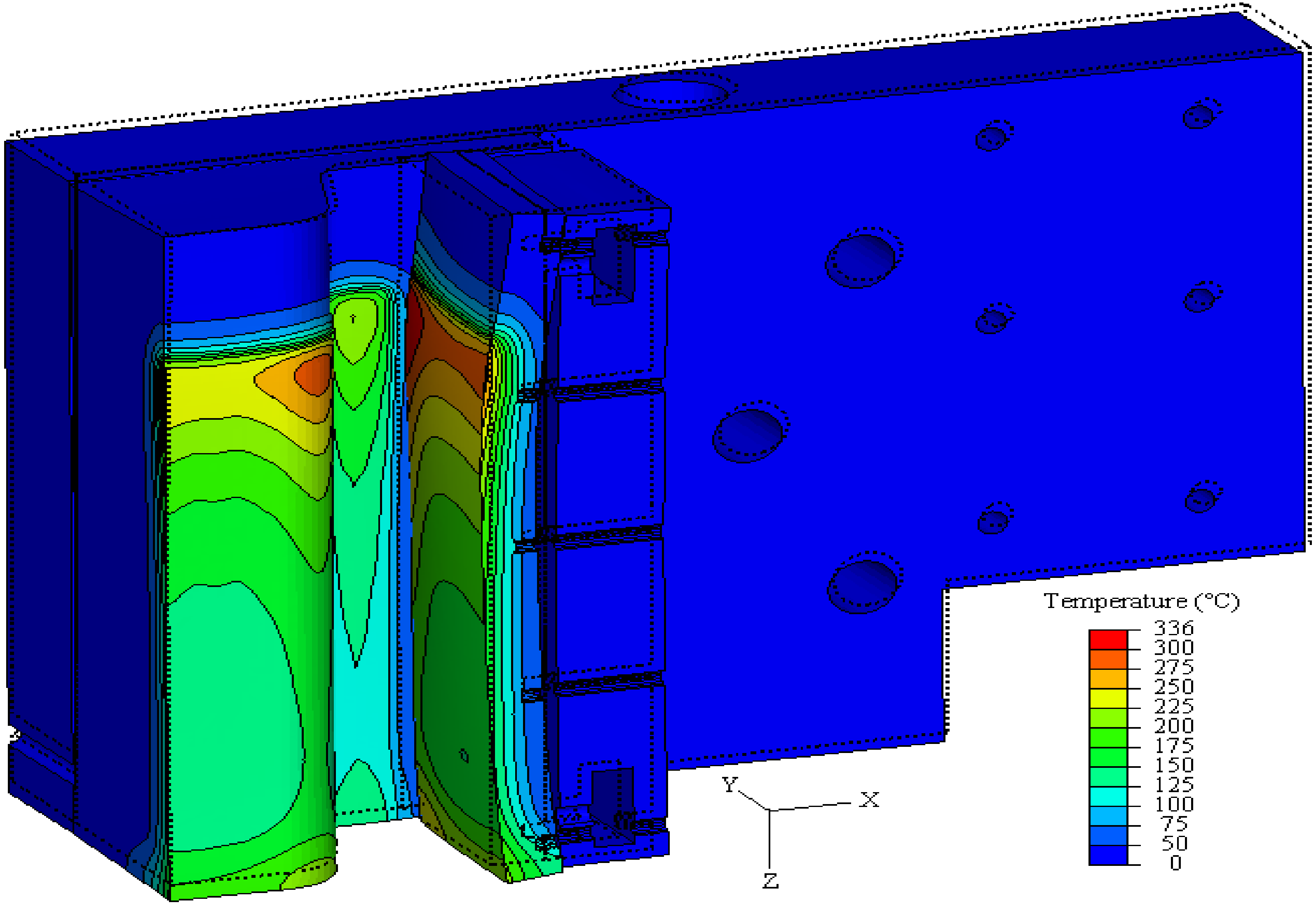
Koric & Thomas, Int J Num Meths Eng, 2006

Continuous Casting of Beam Blanks

Seimens VAI in Continuous Bloom/Beam Blank Casting Solutions

Thermal distortion of Mold

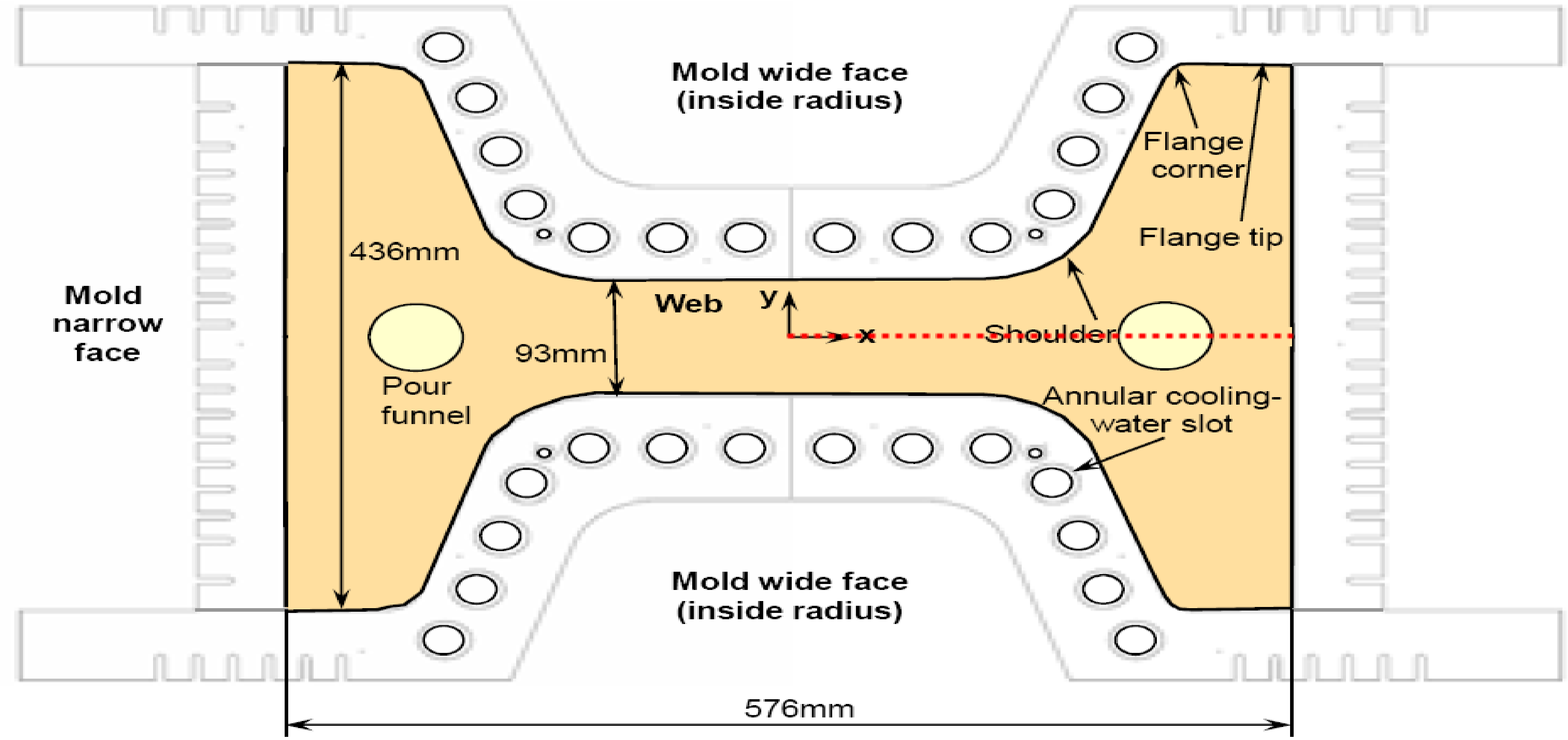
(Complex Geometry but “Easy” Physics)



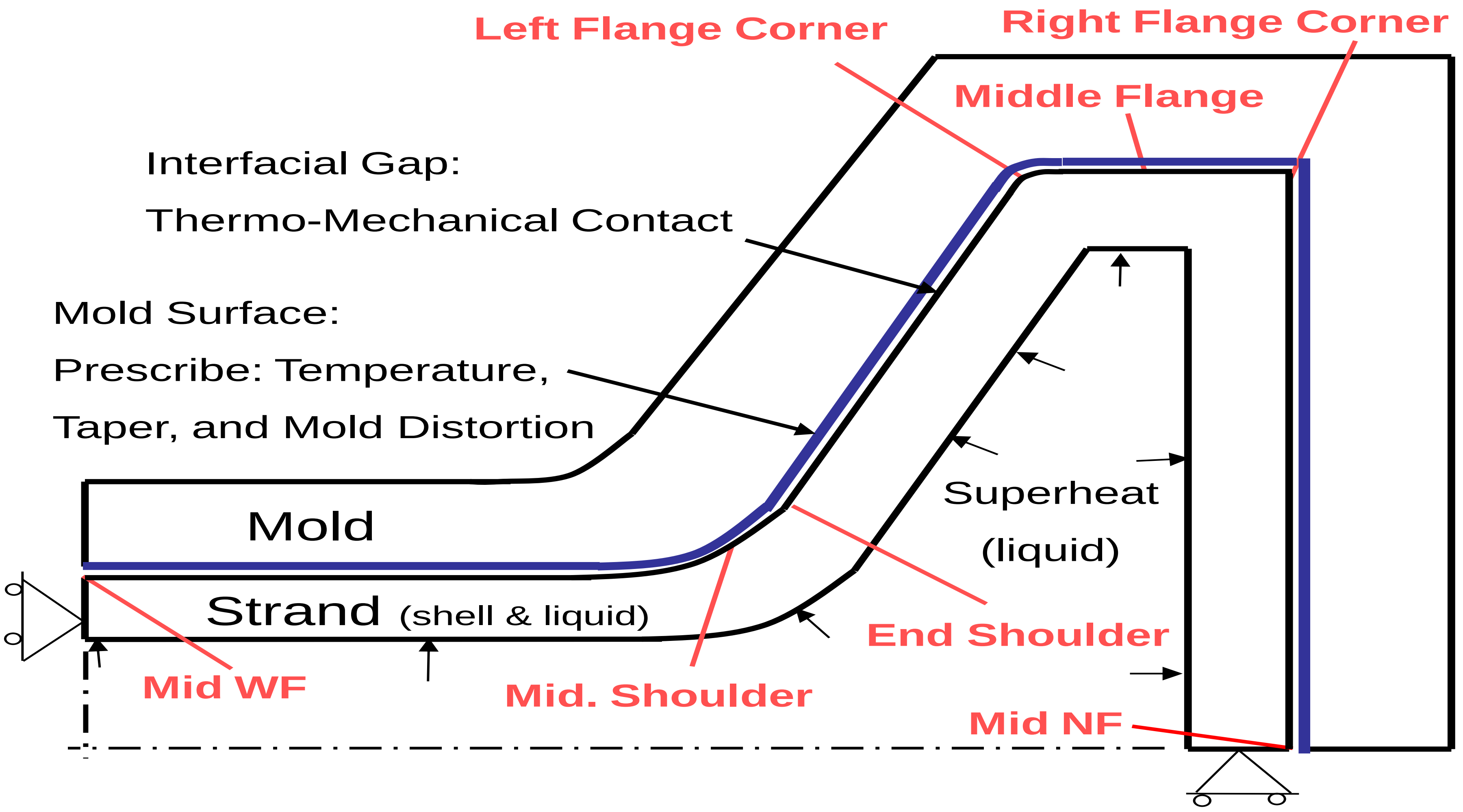
L. Hibbeler, 2008

Coupled Thermo-Mechanical Model of Beam Blank Casting

Incrementally-Coupled 2-D Generalized Plane Strain Thermo-Mechanical Model
Casting Speed 0.889 m/min
Working Mold Length 660.4 mm



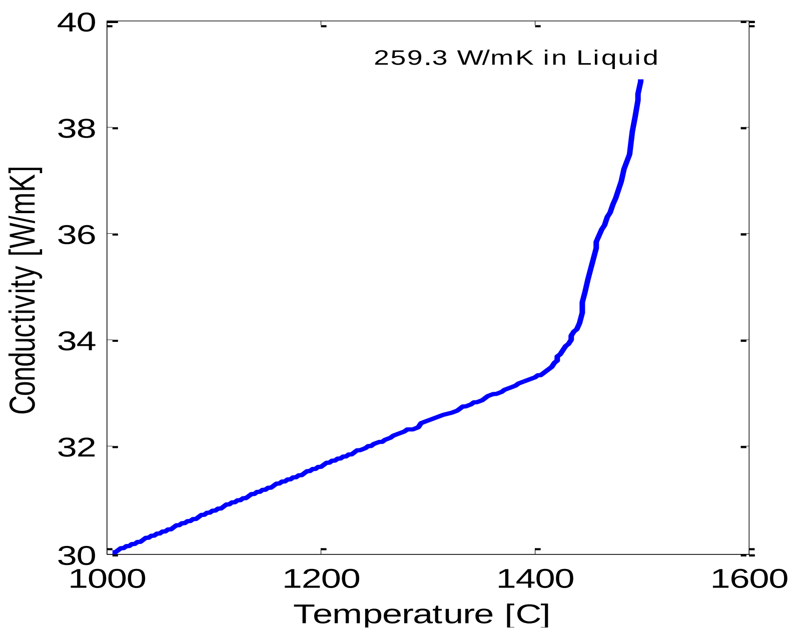
Shell model domain with thermo-mechanical boundary conditions

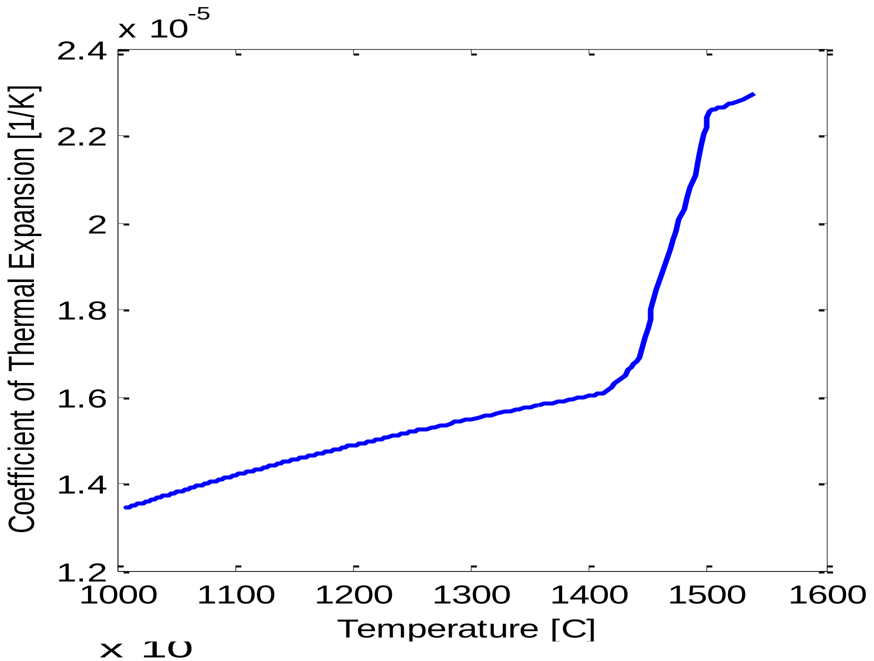


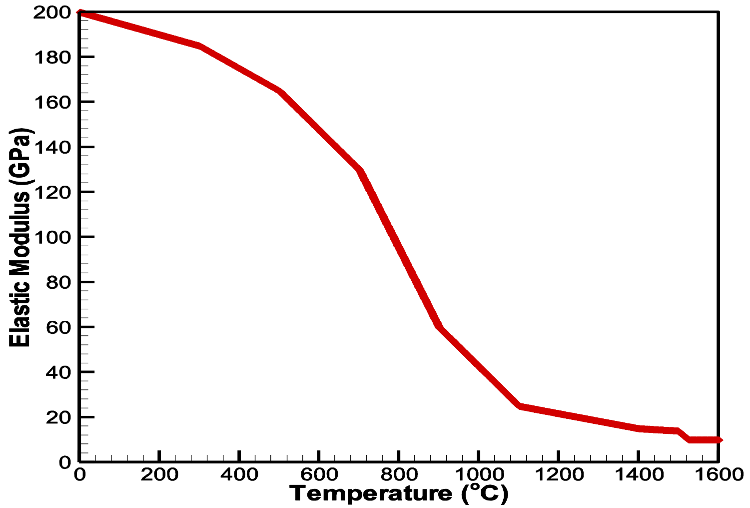
Model of Solidifying Steel Shell of 2D Beam Blank Coupled Thermo-Mechanical Model

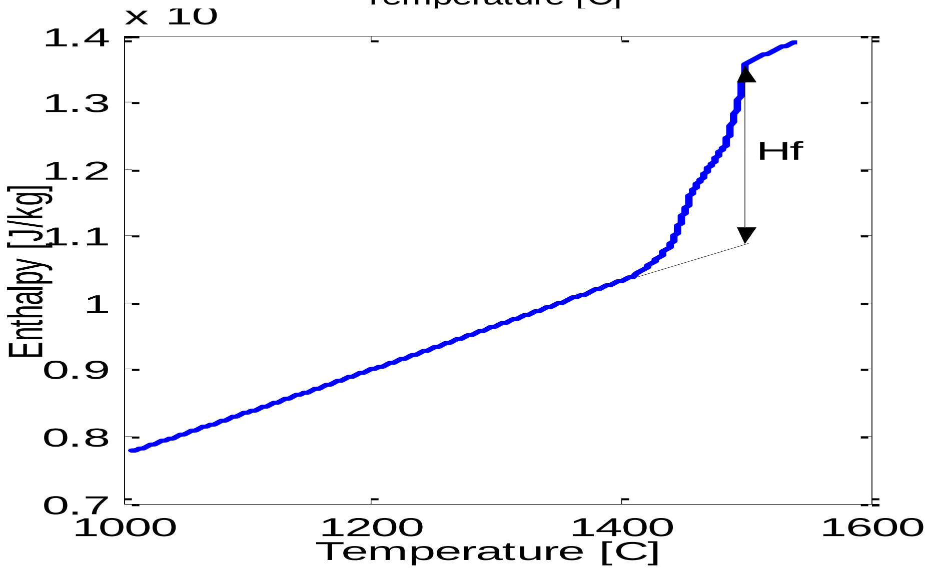
- Complex geometries produce additional difficulty in numerical modeling.
- Austenite and delta-ferrite viscoplastic constitutive laws integrated in UMAT - Material Nonlinearity.
- Temperature dependant material properties for 0.07 %C steel grade – Nonlinear Material Properties.
- GAPCON subroutine modeling interfacial heat transfer
- Softened mechanical contact with friction coefficient 0.1-Boundary Nonlinearity.
- DLOAD subroutine modeling Ferrostatic pressure.

Realistic Temperature-Dependant Material Properties









Steel Phase Fractions

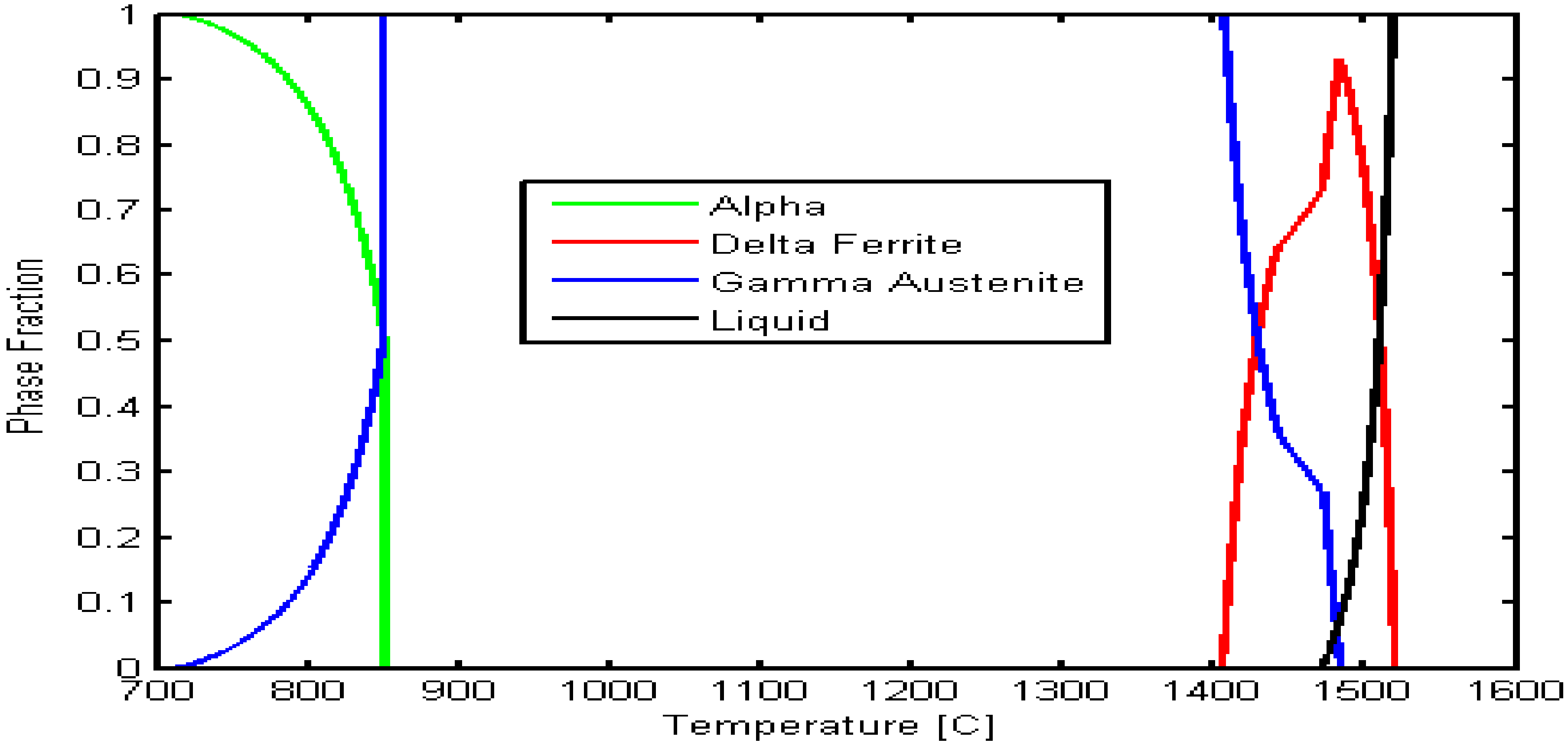
Steel Grade: 0.07 %C

Tsol = 1471.9 C

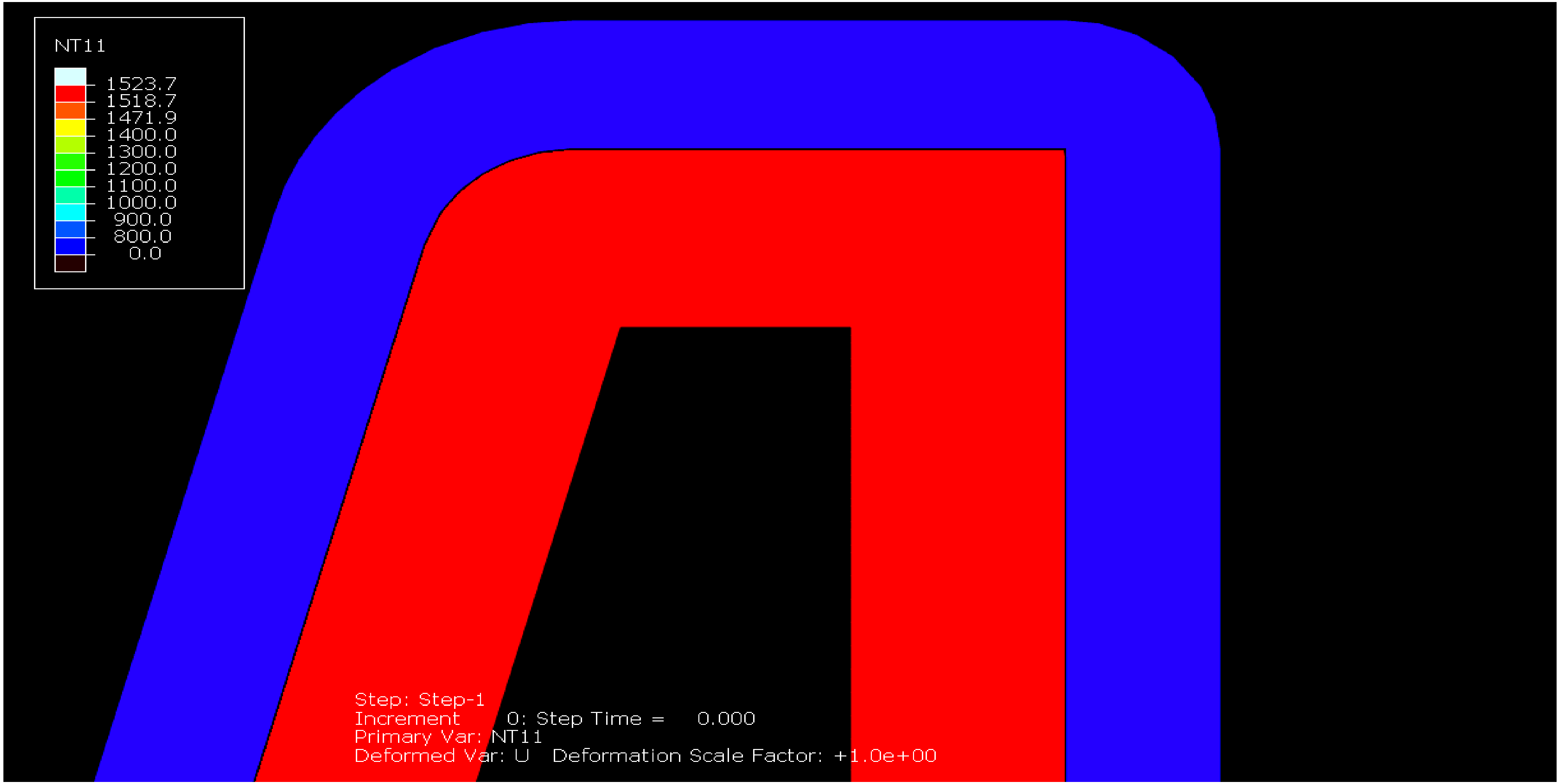
Tliq = 1518.7 C

Tinit = 1523.7 C

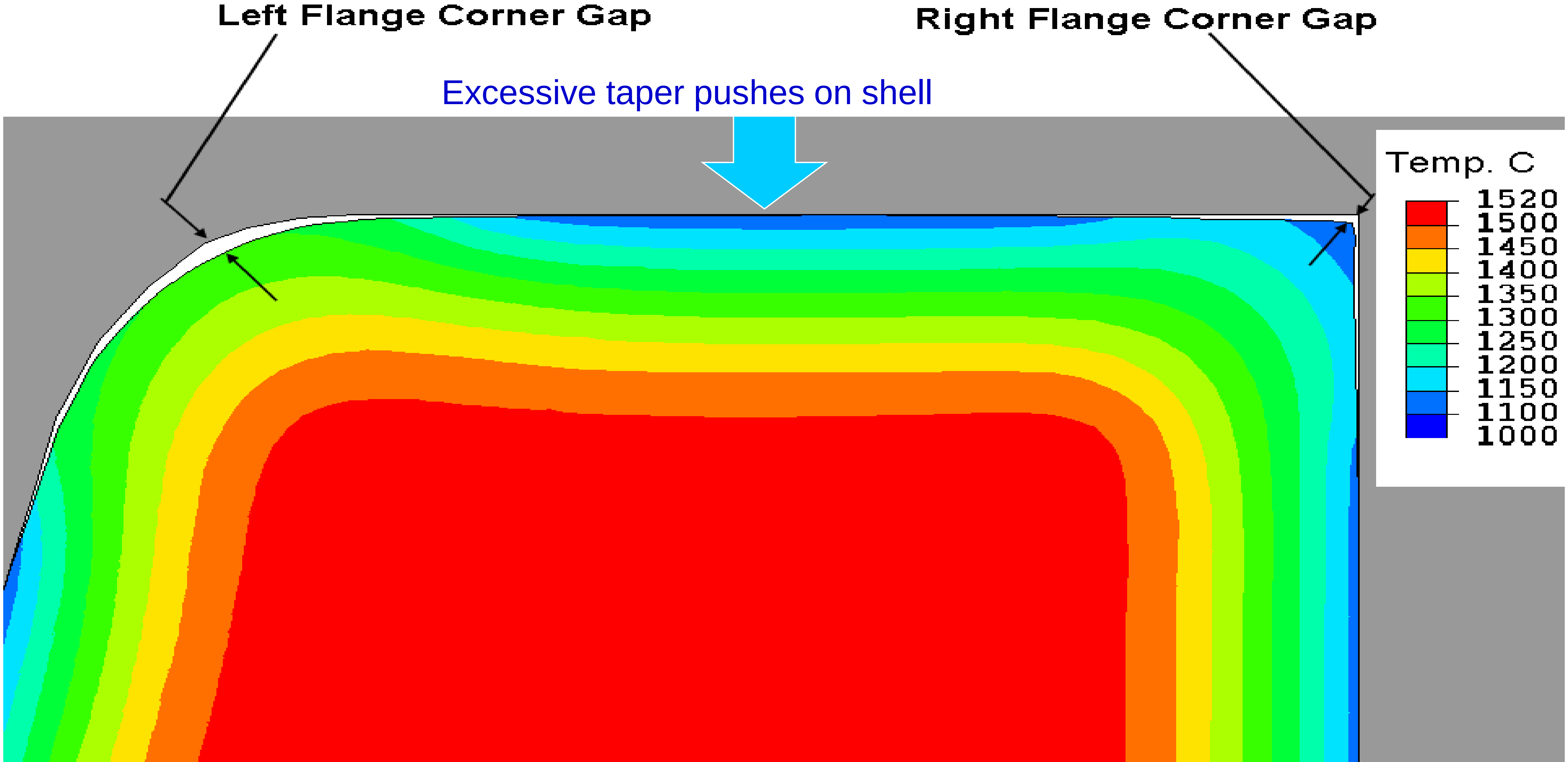
$T_{10\%delta}$ = 1409.2 C



Shell Solidification and Shrinkage

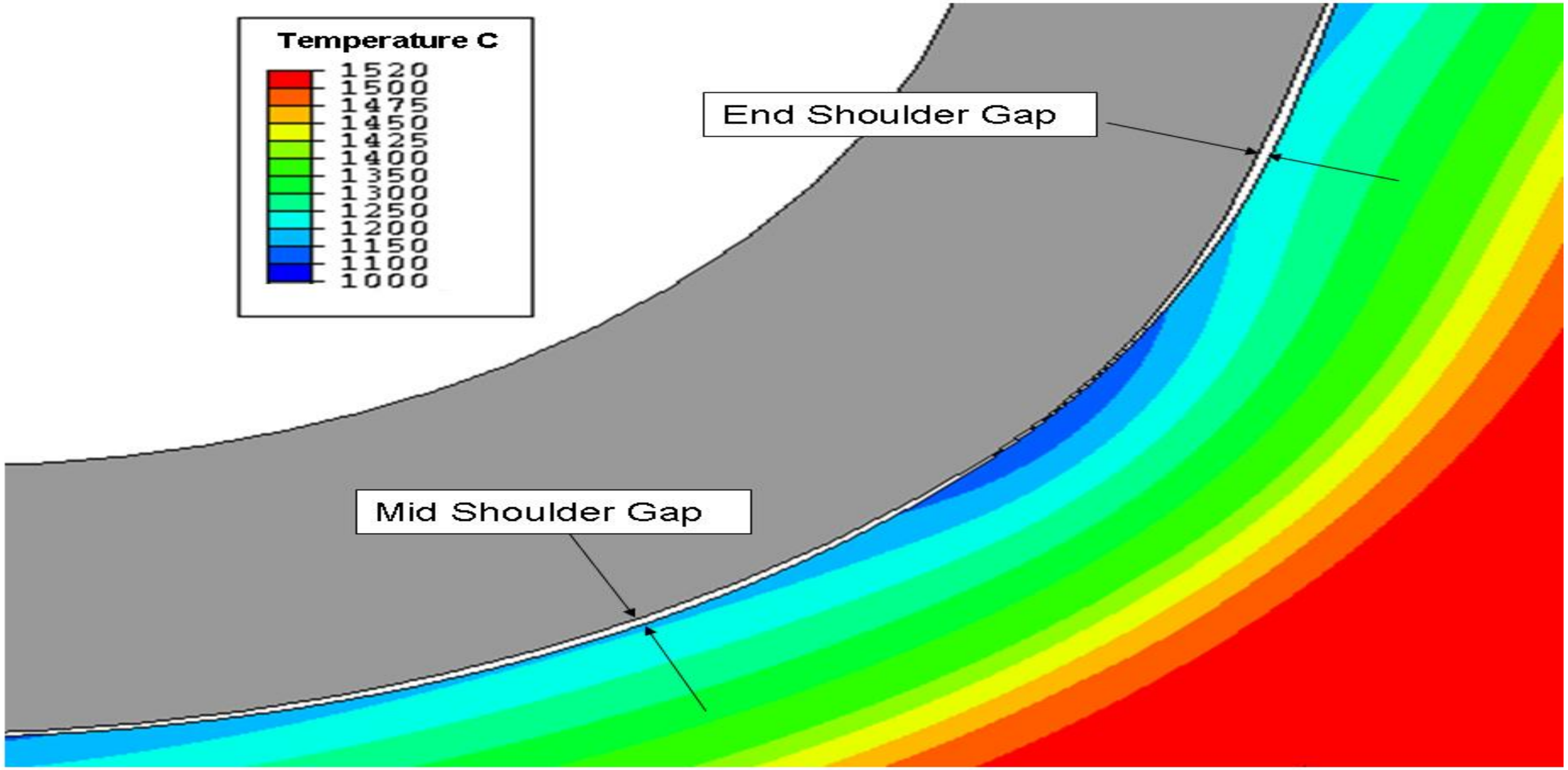


Shell Solidification and Shrinkage

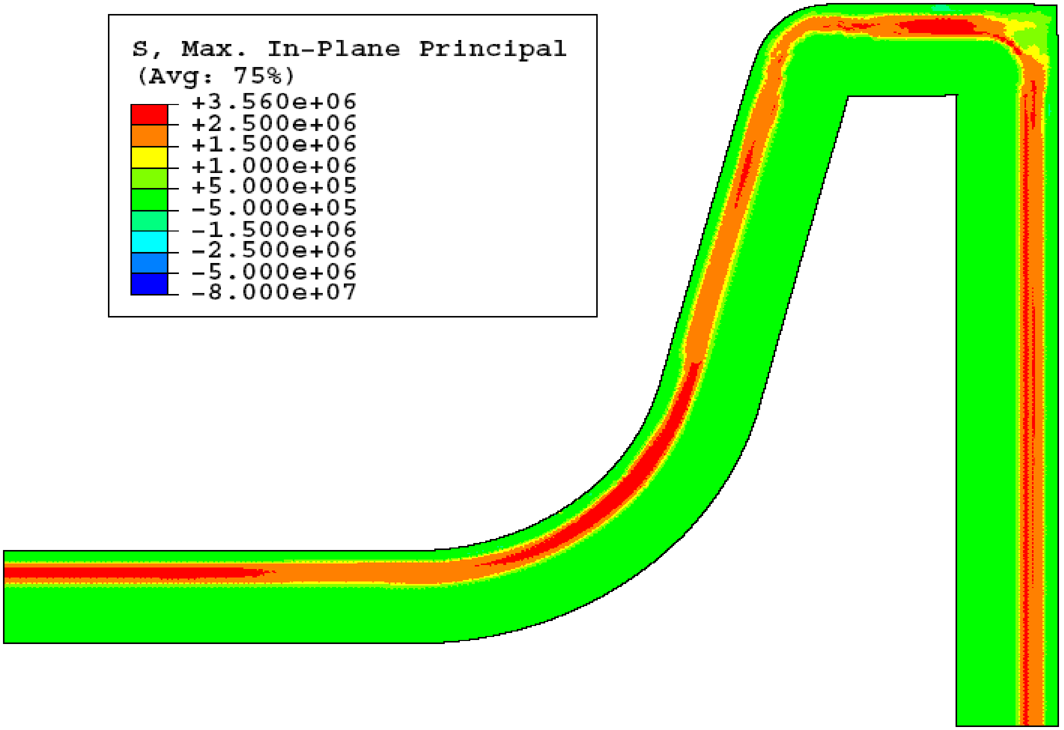


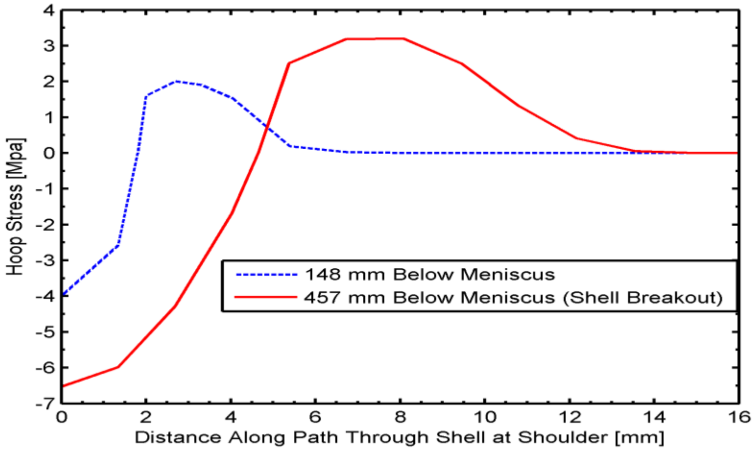
Shoulder Shell Temperature Contour 457 mm down the mold

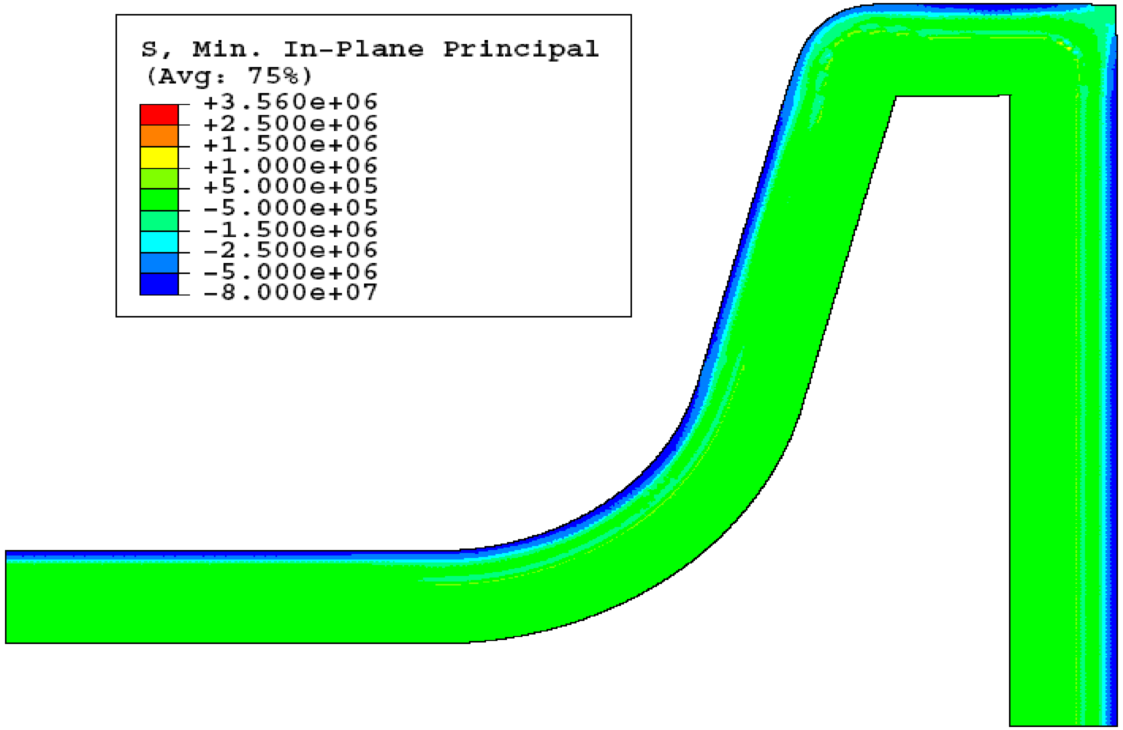
Hot shell pushed down by mid flange is bending and opening gaps at the shoulder region



Principal Stresses 457 mm Below Meniscus

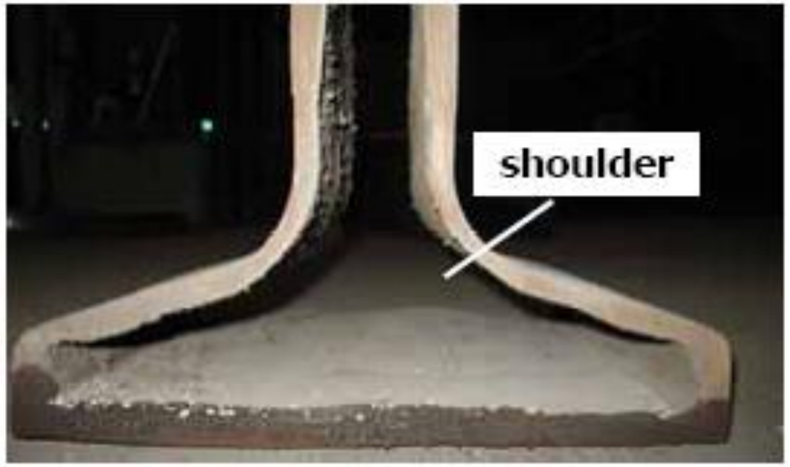


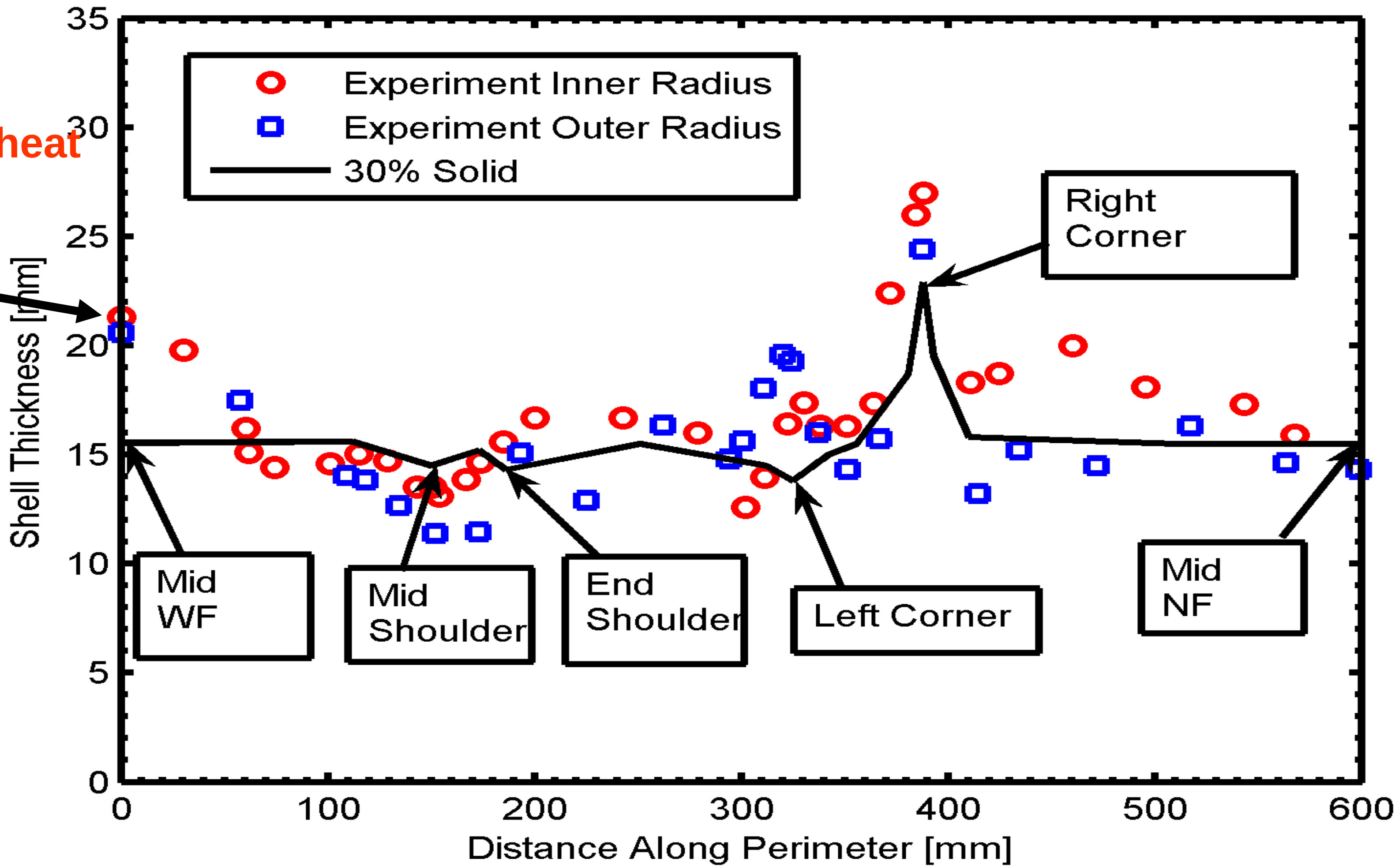




Breakout Shell Thickness Comparison Between Model and Plant Data

Mismatch here due to uneven superheat distribution !





Incorporating CFD Superheat Results via Enhanced Latent Heat

Problem: Can not apply superheat fluxes on moving solidifying front whose position is a part of solution ?

Solution: Apply additional latent heat to account for superheat flux delivered from liquid pool calculated from:

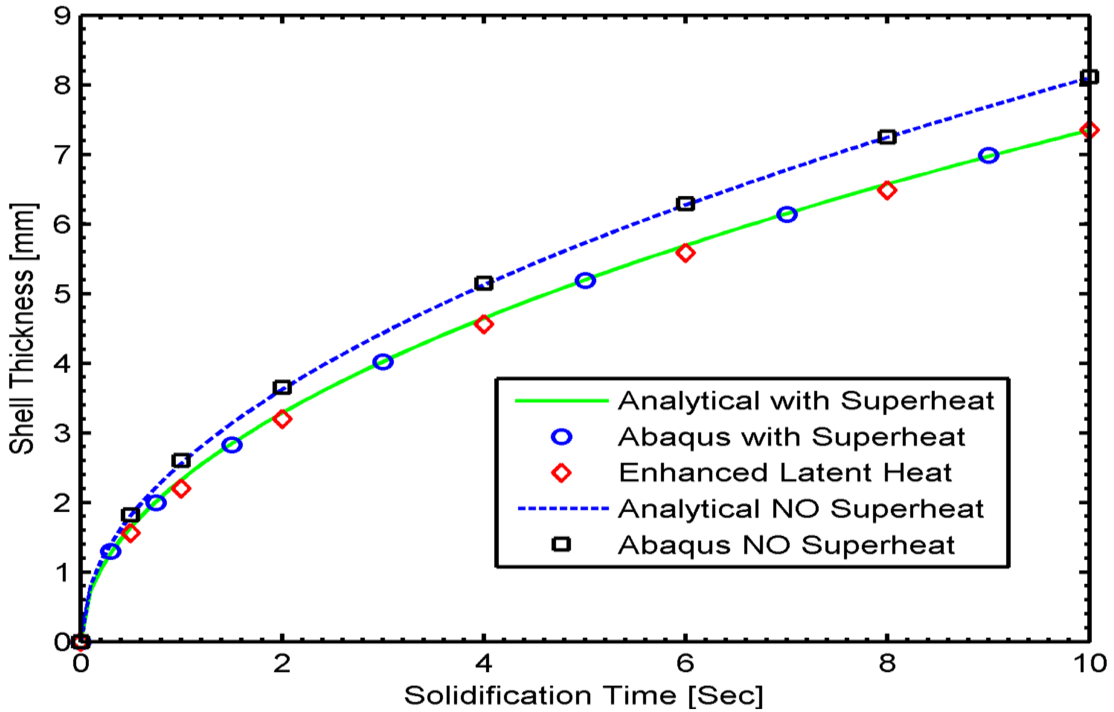
$$\Delta H_f = \frac{q''_{super}}{\rho_s \, v}$$

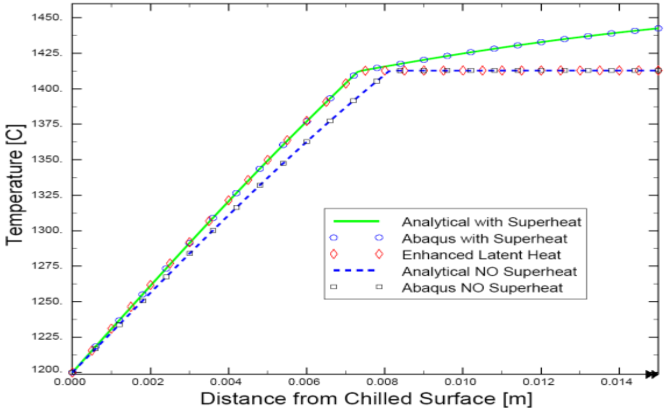
Instantaneous velocity *v* is estimated from analytical or numerical solutions

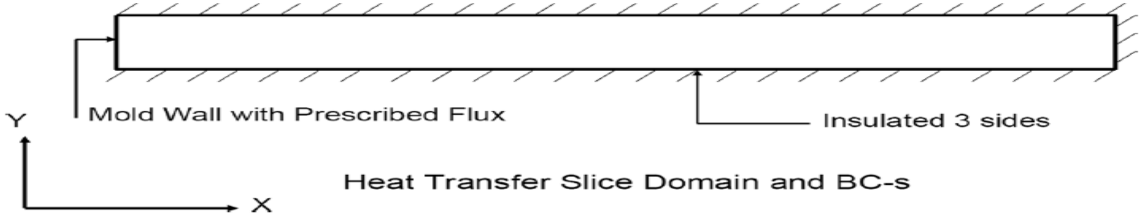
A thermal user subroutine UMATHT was created to implement the enhanced latent heat method into Abaqus

S. Koric, B.G Thomas, V.R. Voller ,Numerical Heat Transfer B, 2010

Validation: Shell Thickness History and Temperature Profiles at 2 sec







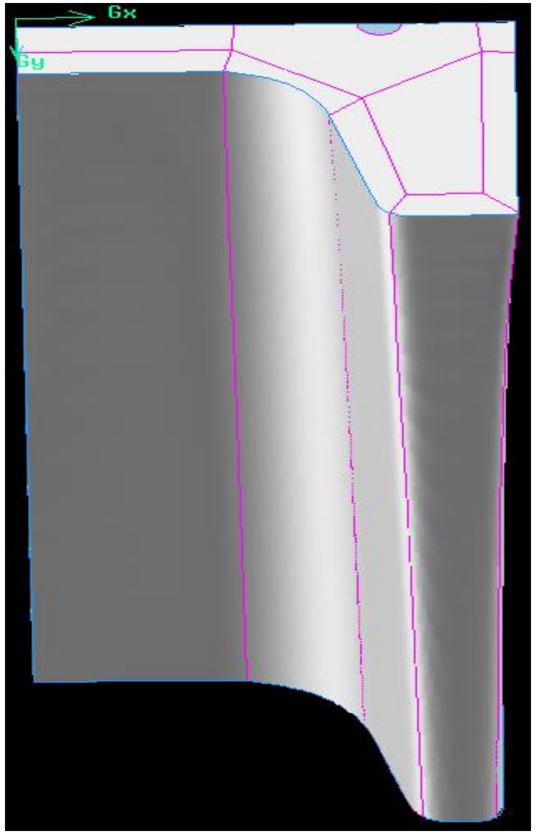
1D Solidifying Slice with stagnant fluid in liquid phase, the analytical solution exists

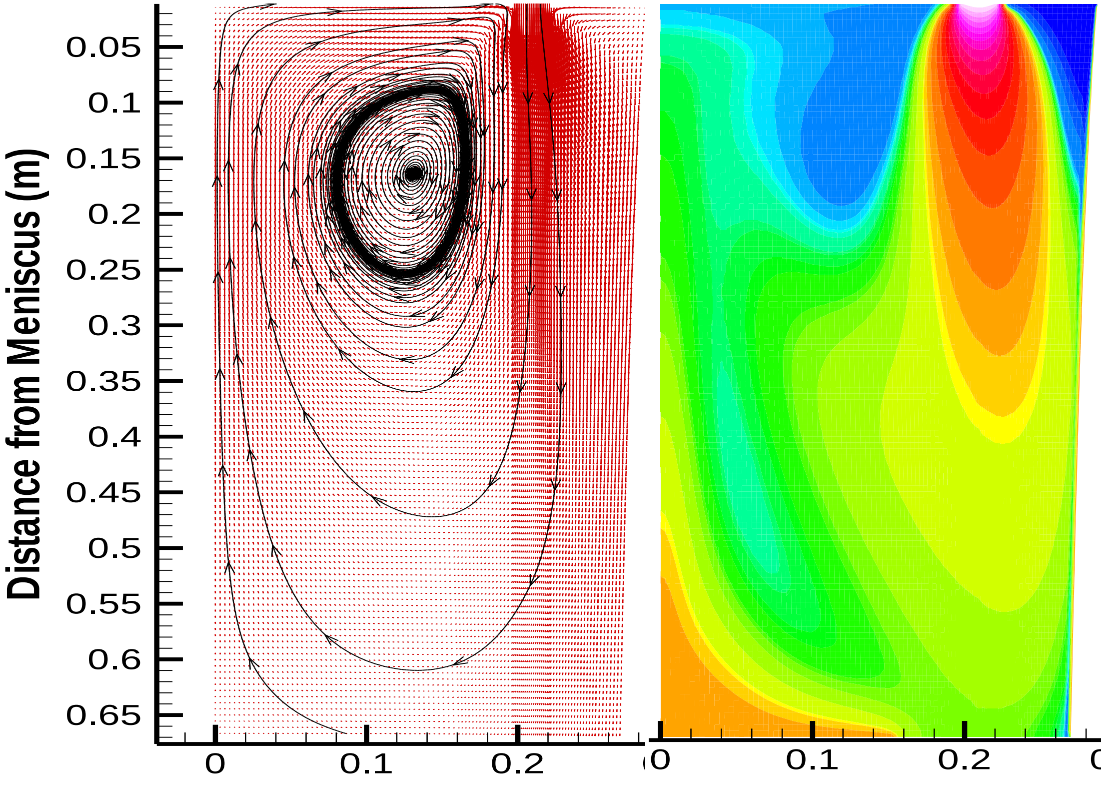
Start with Tinit >Tliq. Calculate Temperature distribution using built-Abaqus HT, and record superheat flux history at Tliq (solidifying front)

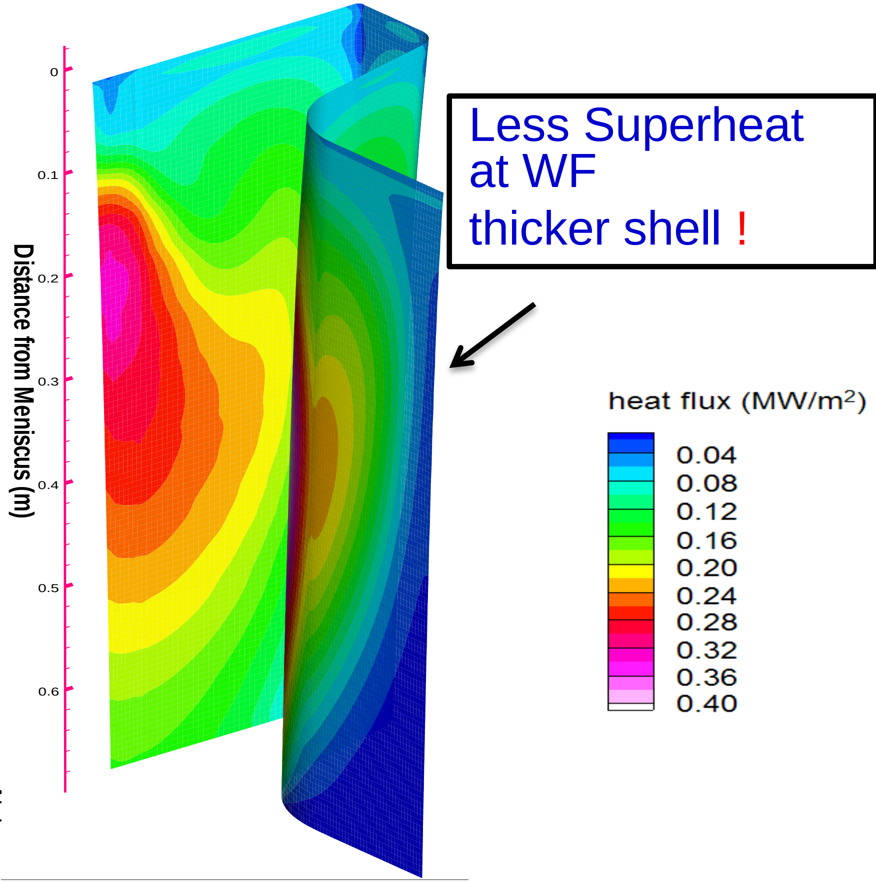
Rerun with Tinit=Tliq linking Abaqus with UMATH (that converts superheat fluxes into enhanced latent heat)

Add super-heat free solution too

Turbulent Flow & Superheat Calculations (Fluent)







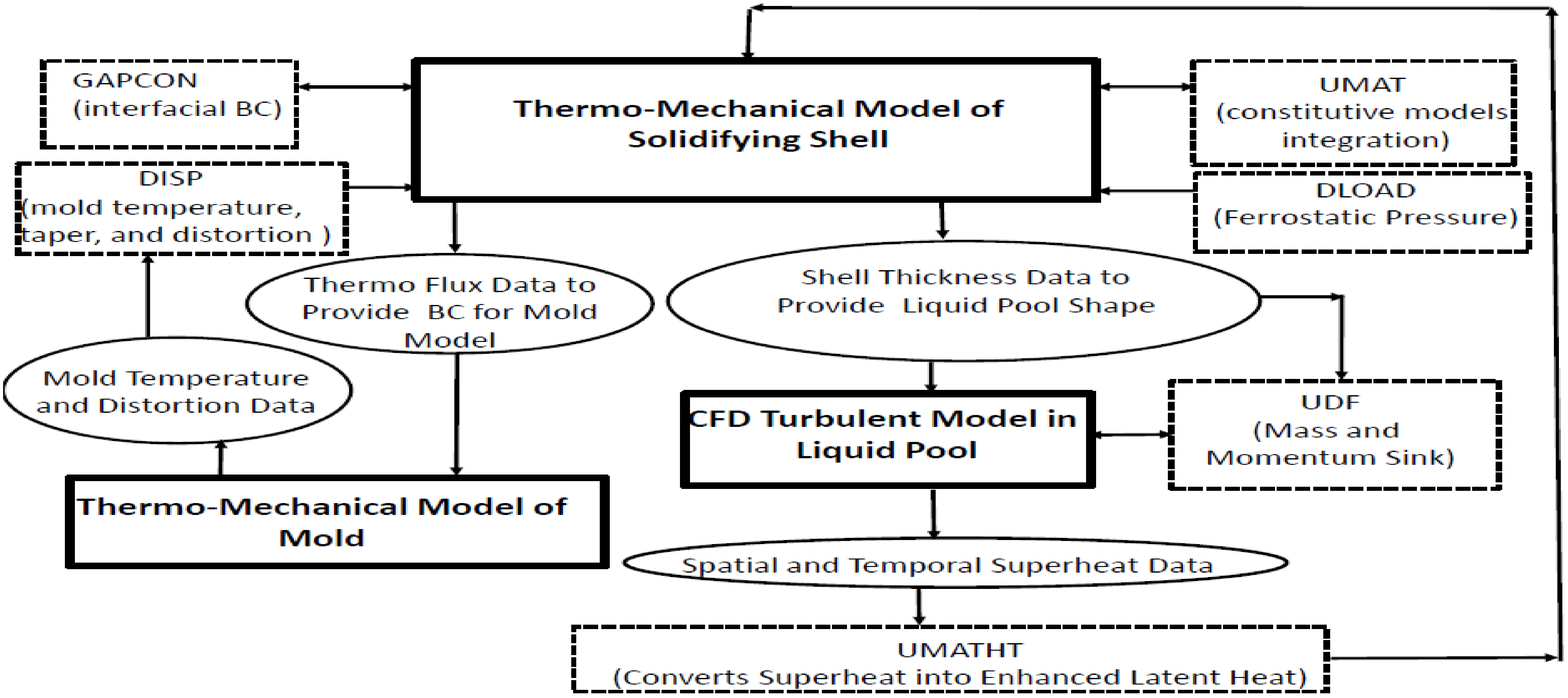
Domain

Velocity

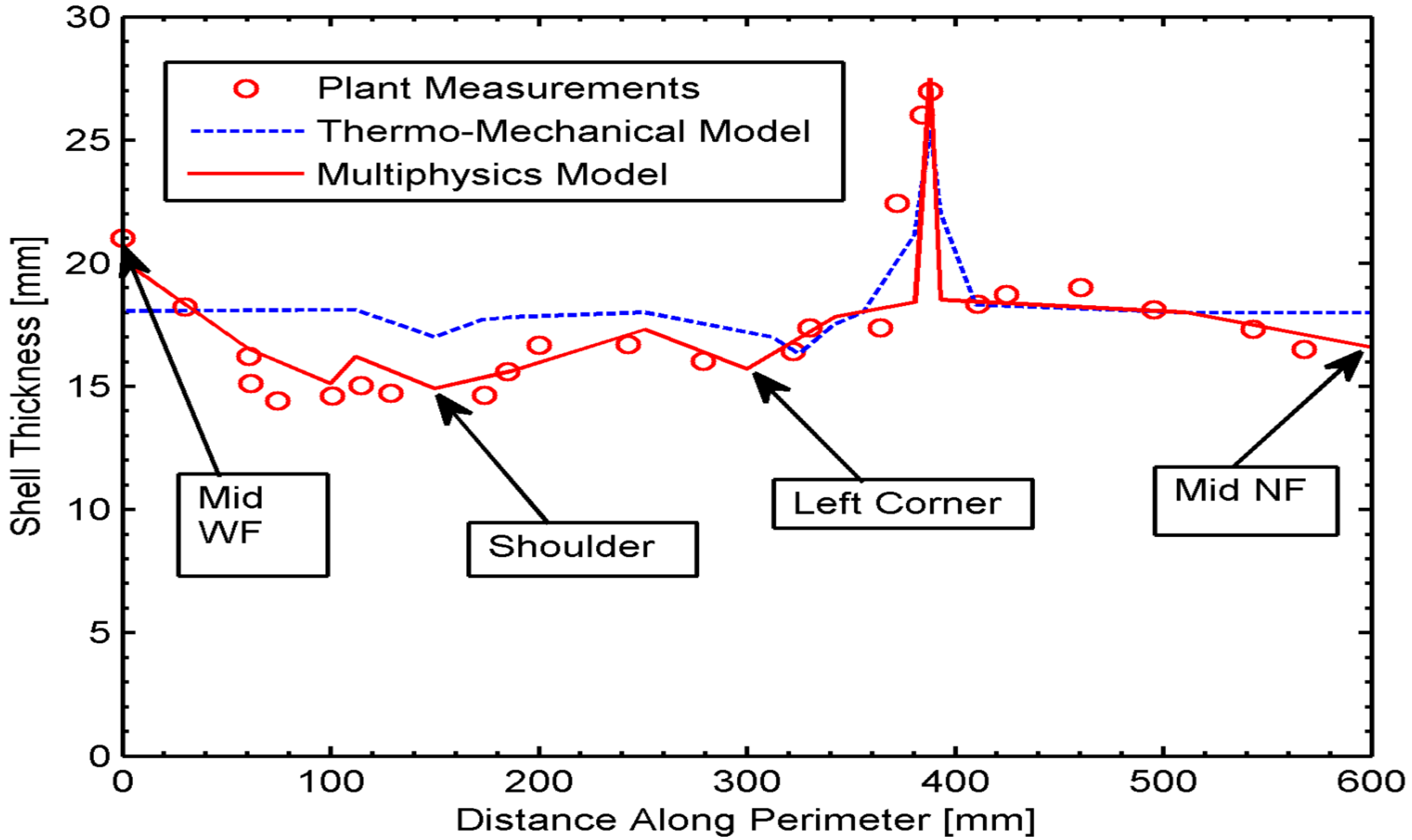
Temperature

Superheat Flux

Flowchart for Multiphysics Solution Strategy



New Shell Thickness Comparison



S. Koric, L. C. Hibbeler, R. Liu, B.G Thomas, Numerical Heat Transfer B, 2010

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- Steel Dynamics Structural and Rail Mill
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Multiscale Modeling of Bone Fracture and Strength

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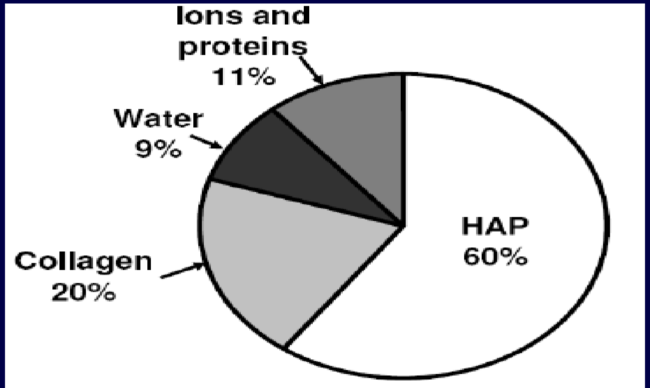
Tim Rossman and Dragomir Daescu– Mayo Clinic

November 11, 2015

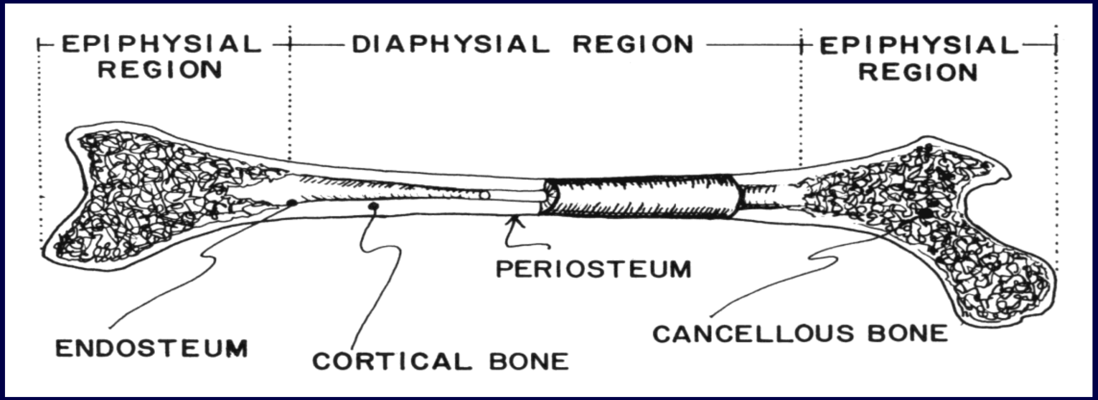
Bone: An Introduction

- Bone is a (nano)composite material
  - Collagen – soft and deformable
  - Minerals – stiff, strong, but brittle (nanoscale)
  - Non-collagenous proteins
  - Fluids
  - Cells

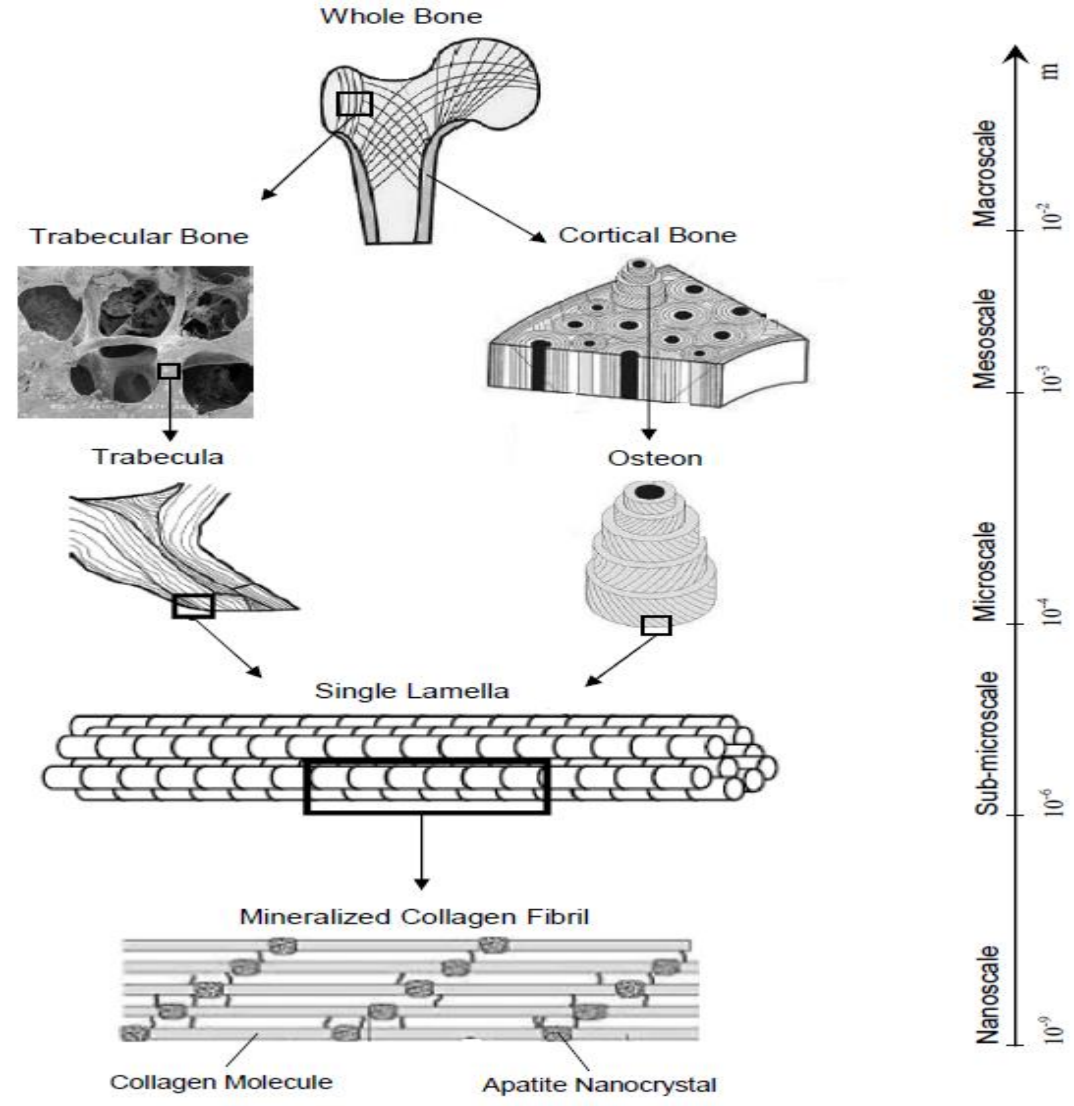


- Bone has a complex, hierarchical and heterogeneous structure at several different length scales

- Bone is a biological material: a living tissue with evolving structure (due to mechanical, biological & chemical factors)
  - age, diet, medications, hormones, exercise, disease



Hierarchical Structure of Bone



- Macroscale (whole bone)
- Mesoscale **(0.5 – 10 cm) –** cortical & trabecular bone
- Microscale **(10 – 500 μm) –** single osteon or trabecula
- Sub-microscale **(1 – 10 μm) –** single lamella
- Nanoscale **(below 1 μm) –** collagen fibrils, apatite crystals

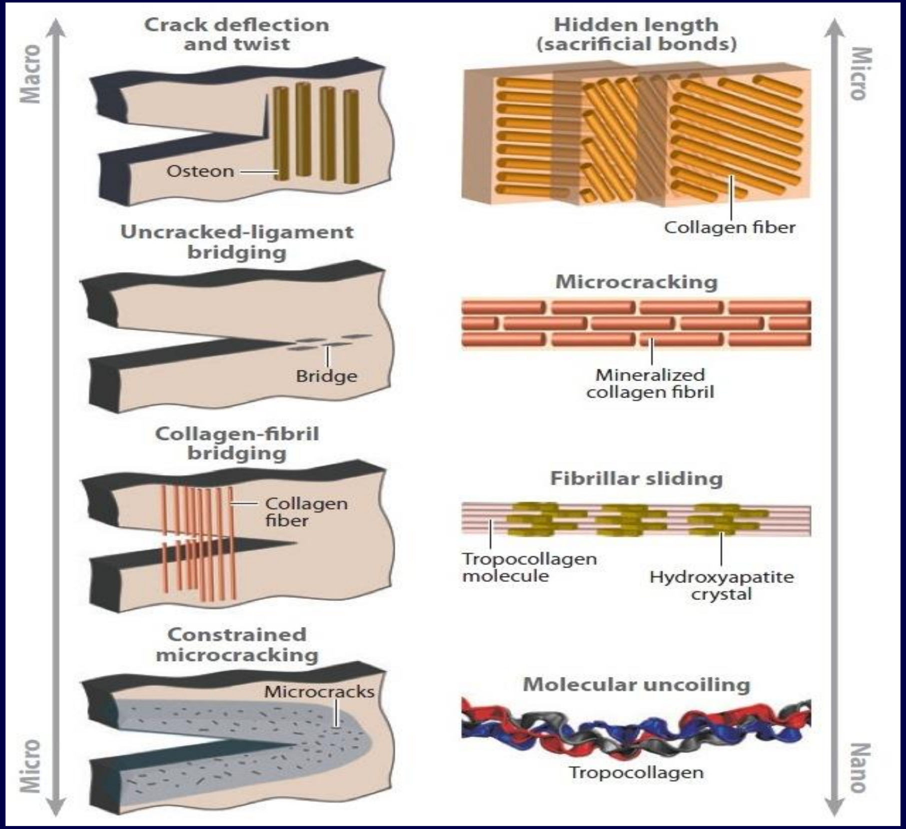
Why study bone and bone as a multiscale material?

Motivation

Bone fracture – outstanding clinical problem

a) Fracture due to high force impact or repeated loads.
b) Pathologic fracture (minimal trauma injury, **osteoporosis**).

Fracture is a multiscale phenomenon



Launey et al., Annu. Rev. Mater. Res. 2010. 40:25–53

Research Objectives

To create an experimentally-based multiscale model to predict elasticity, fracture and strength of bone.

- Determine multiscale structure-composition-property relations for bone (orthopedics, bioinspiration);

- Develop predictive tools for assessing bone quality
  (healthy, diseased, developing, aging, effect of medications, exercise, diet, and other factors)

HPC at NCSA is crucial for these computations due to the size and complexity of bone's structure FEA models and multiple nonlinearities

Multiscale Modeling of Bone - Methods

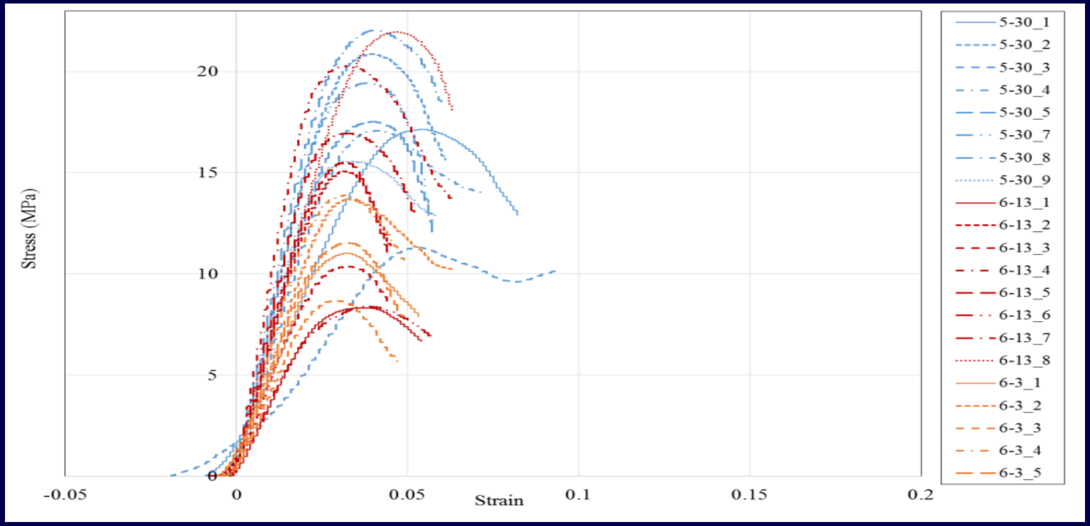
- Computational softwares:
- Molecular dynamics : NAMD, CHARMM, LAMMPS
- Finite element method: Abaqus

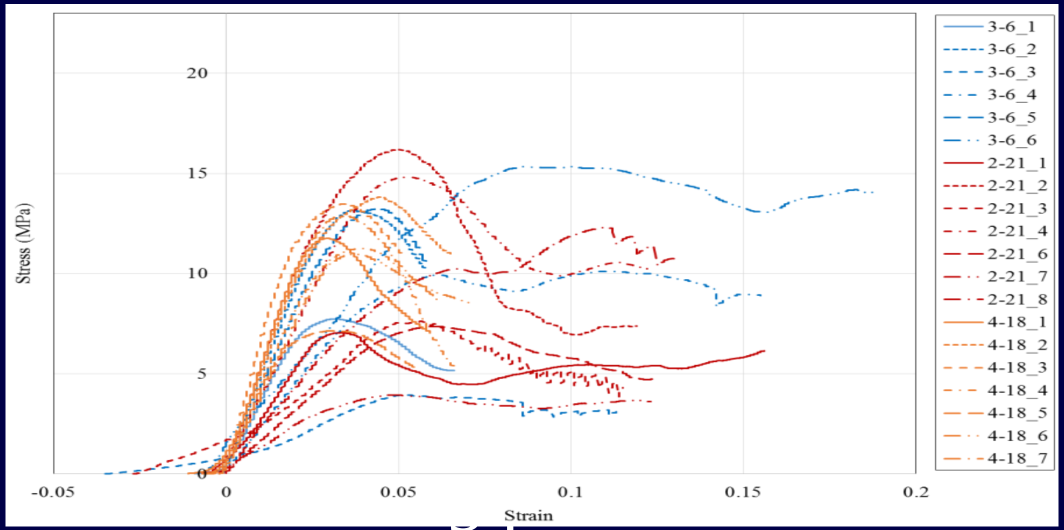
- Nanostructure (Collagen fibrils, apatite, water, other proteins)
- Sub-microstructure (single lamella, network of fibrils)
- Microstructure (lamellae in different orientations)
- Mesostructure (cortical and trabecular bone)
- Macroscale (whole bone)

- Computational Approaches:
- Hierarchical: Output at one scale - input for next scale
- Multiscale: Coupling of scales

Experimental program
(Woowon Lee)

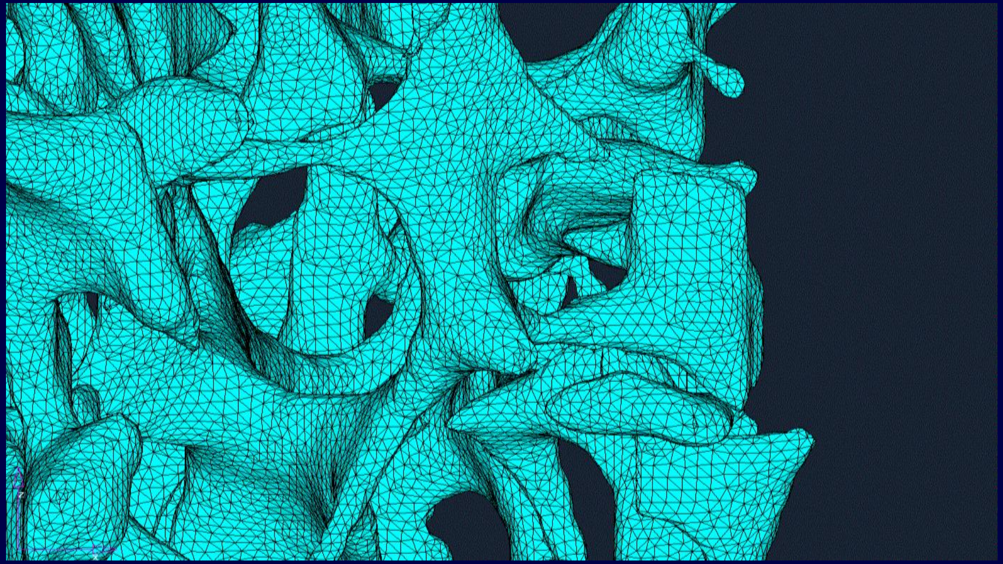
- 85 cylindrical sample of six-month old porcine trabecular bone from femur were prepared
- Bone samples were frozen for different periods:
- The samples were ~ 4 mm by ~8 mm cylinders
- 3D images of bone samples were prepared using MicroCT
- Compression test was performed on the samples until failure

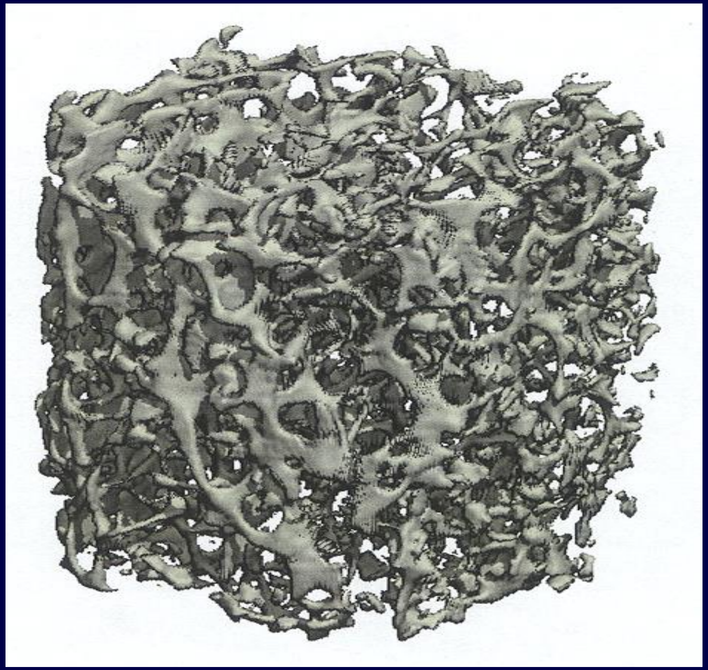




Mesostructure – Trabecular bone

- MicroCT imaging
  - Output
    - microCT data
    - .stl file
    - Nodes and 2D tetrahedral surfaces
    - Over 6,000,000 finite elements

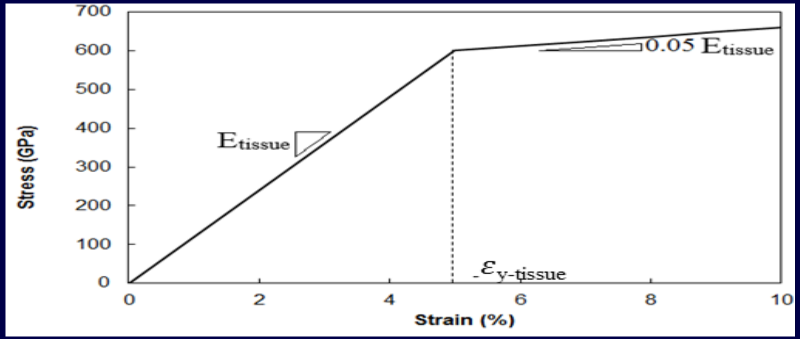




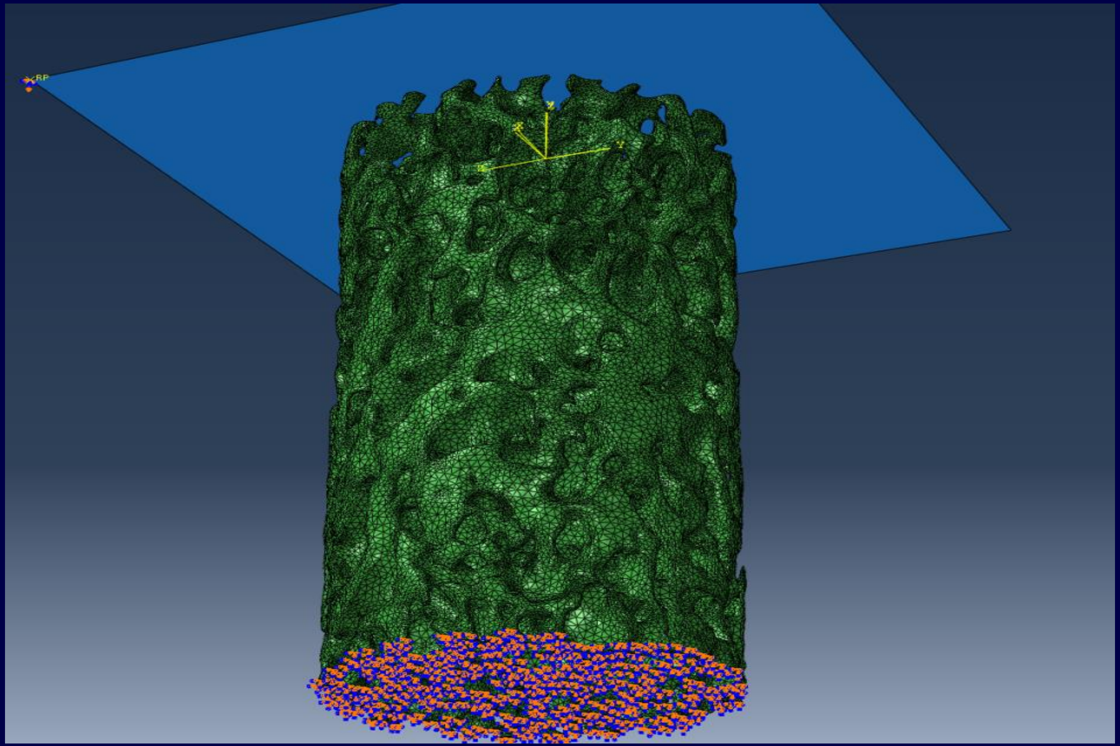
Trabecular Bone Architecture

- Porosity
- 3D Complex Domain
- Trabecula thickness
- Fractal dimension
- Density

- Meshing
  - Hypermesh 6.0
  - 6+ million elements, 1.5+ million nodes
  - Solid tetrahedral elements

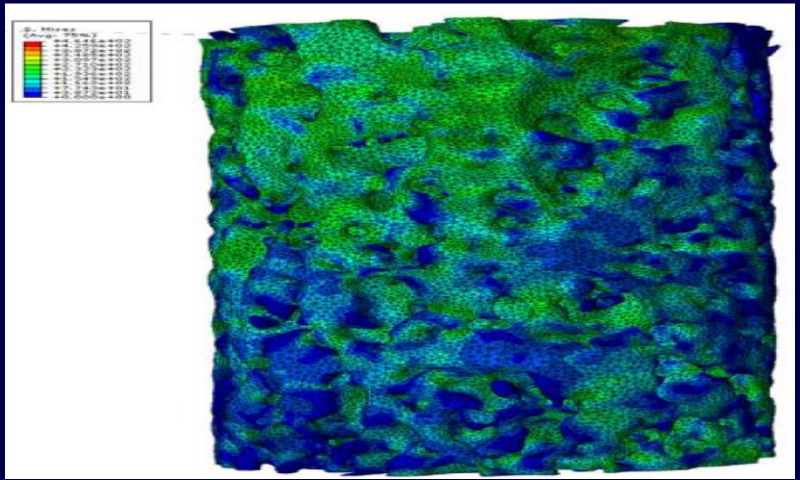


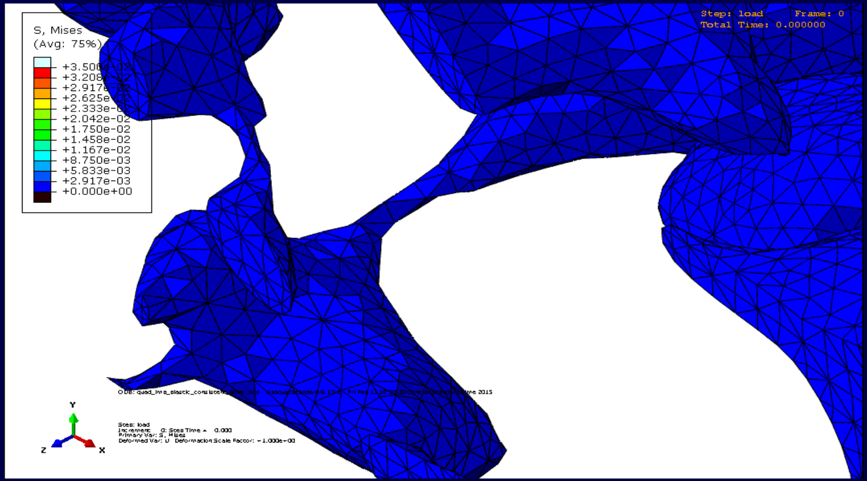
- Solver & Post-Processor
  - Abaqus (material + geometrical+ contact nonlinearities)
    - Volume stress/strain/energy averages
    - Apparent properties
    - Stress-strain response

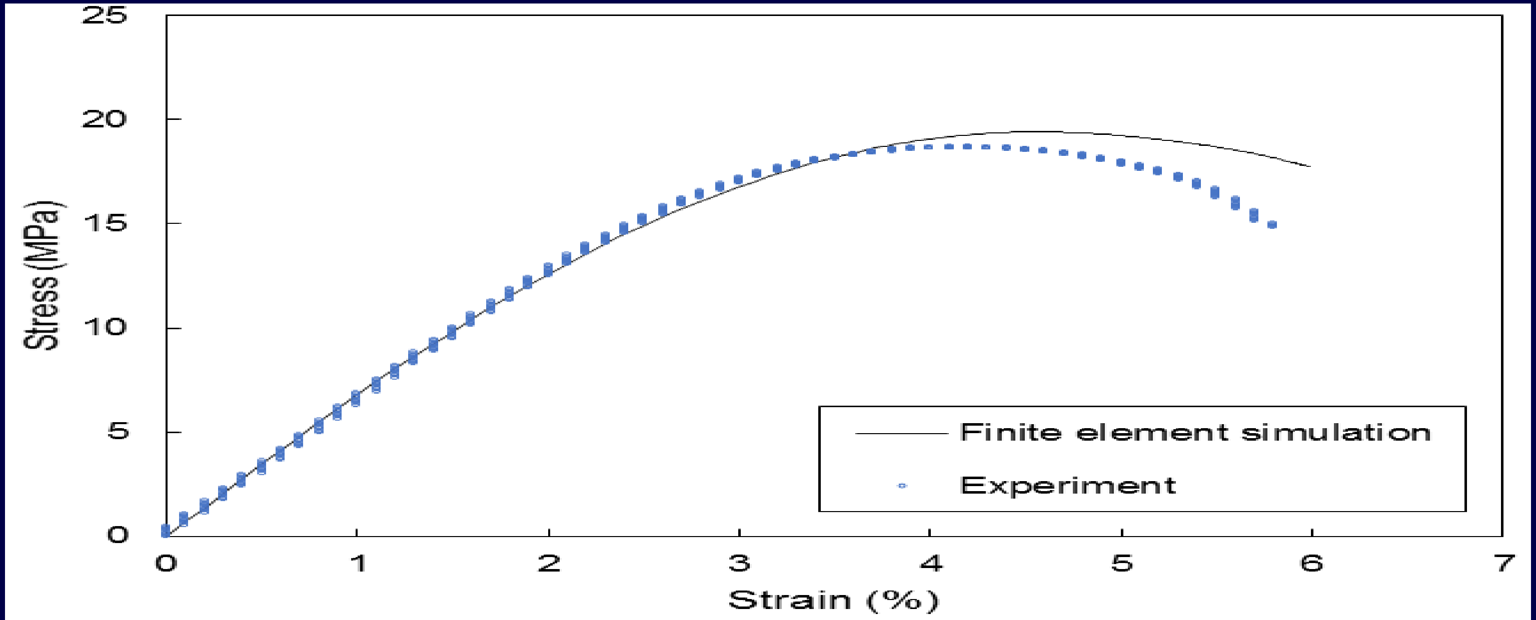


- Boundary Conditions
- Top surface
  - Applied normal displacement
  - zero shear traction
- Bottom surface
  - zero normal displacement
  - zero shear traction
- Side surfaces
  - Zero traction boundary conditions

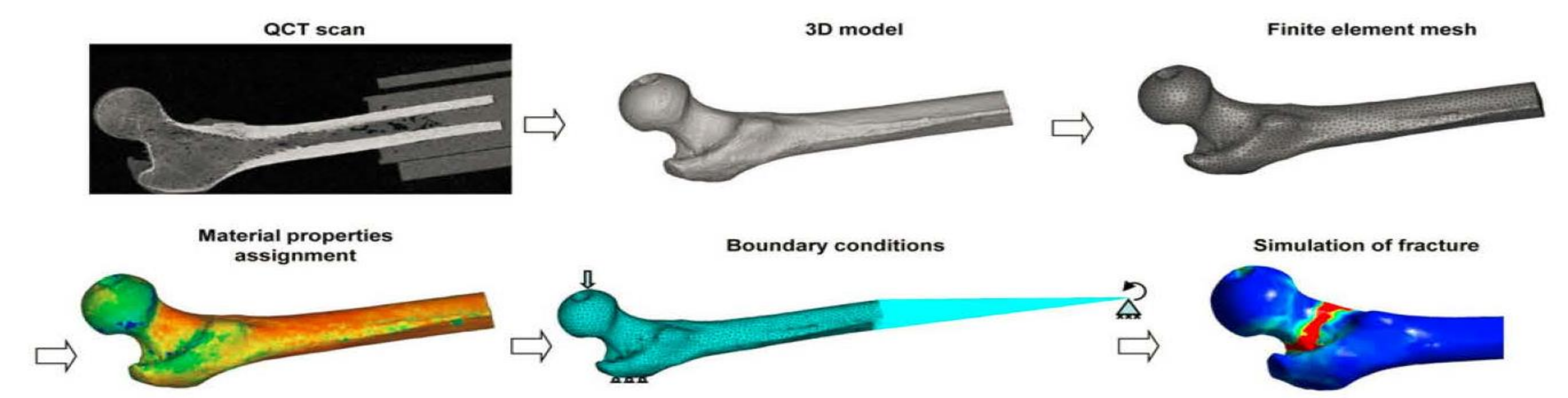
FEA vs. Experiment







Macroscale - Whole Bone



Dragomir-Daescu *et al*. Annals Biomed Eng, 2011

QCT/FEA modeling:

- QCT scan segmented to obtain a 3D model.
- Model meshed with finite elements in Ansys, converted to Abaqus at NCSA
- Spatial Material properties assigned to the Macroscale FEA model based on effective anisotropic properties obtained from the mesoscale models.
- Boundary conditions and damage applied to simulate fracture.

Thank you