CCC Report
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New Computational Resources and Stress Model Validation

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Objectives

- A pioneer attempt to predict the coupled evolution of temperature, shape, stress and strain distribution in the solidifying shell in continuous casting mold by using commercial multipurpose finite element package

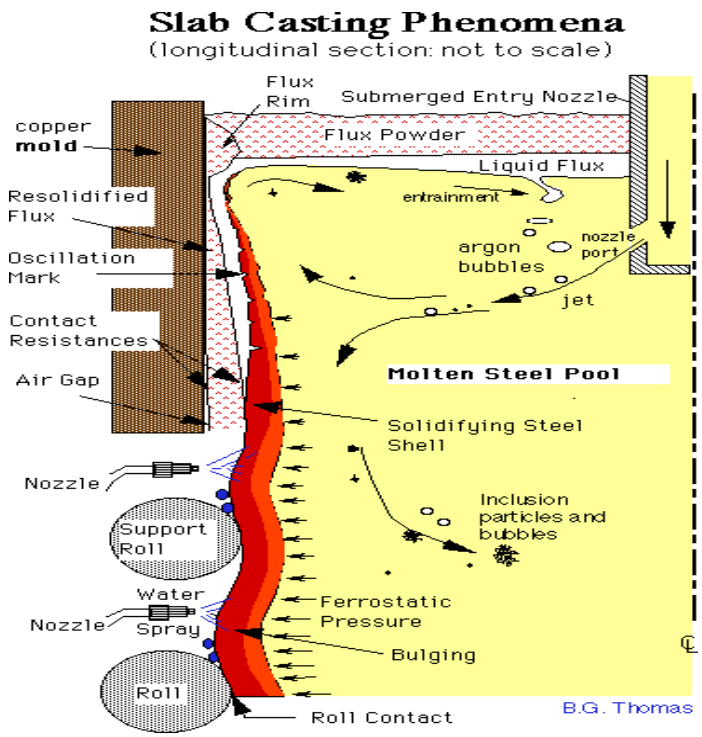
- The recent increase in computational speed and capabilities of commercial finite element software make this task feasible and desirable.

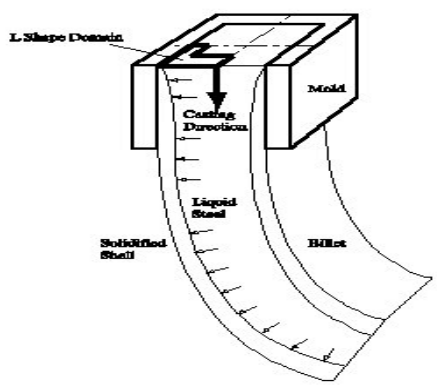
- Will validate the model with available analytical solution and then add more complexity to the model from real plant measurements and finally compare and benchmark the results with in-house code

- ABAQUS™ claims that it can solve the most challenging nonlinear problems. Will check this statement by applying Abaqus to our complex phenomena.

- Even Though ABAQUS offers the user a wide range of capabilities, it is relatively simple to use,it has imbedded pre and post processing tools, and a rich library of 2D and 3D elements. Other modelers in this field can largely benefit from this work, including our final customers – the steel industry

Basic Phenomena



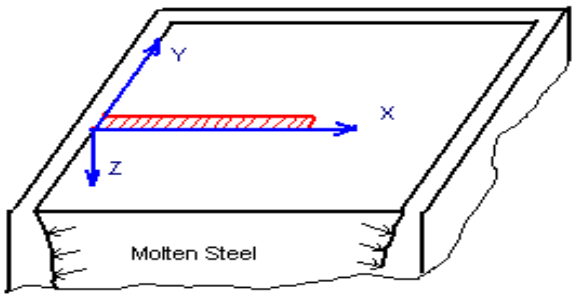


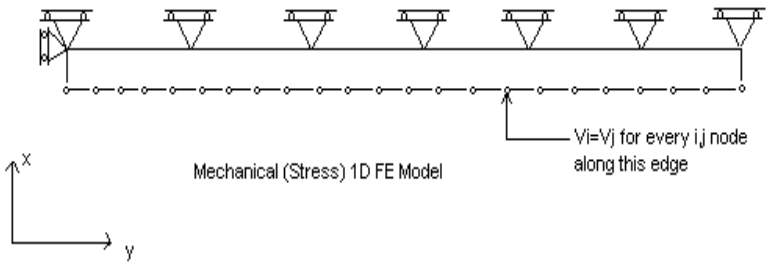
- **Initial solidification occurs at the meniscus and is responsible for the surface quality of the final product.**
- **The shell shrinks away from the mold due to thermal contraction and a gap is formed between the mold and the strand.**
- **At inner side of the strand shell the ferrostatic pressure 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.**

Program Validation and Preliminary Results

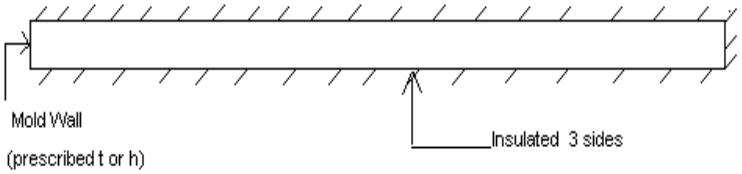
1D Solidification Stress Problem

- **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-Prefect Plastic material behavior**





Mechanical (Stress) 1D FE Model



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 B&W Analytical and Abaqus Numerical Solutions

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^3]	7500.
Poisson's Ratio	0.3	
Liquidus Temp	[^{o} C]	1494.48
Solidus Temp	[^{o} C]	1494.38
Initial Temp	[^{o} C]	1495.
Latent Heat	[J/kgK]	272000.
Number of Elements		300.
Uniform Element Length [mm]		0.1

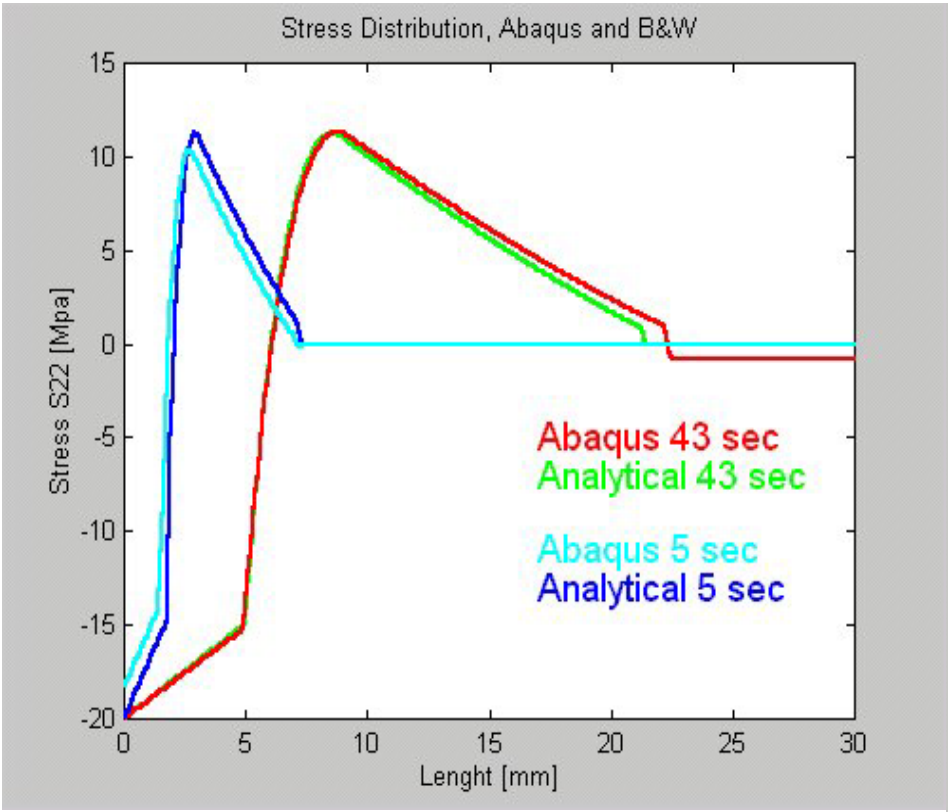
Artificial and non-physical thermal BC from B&W (slab surface quenched to 1000C), replaced by a convective BC with h=220000 [W/m^{2}K]

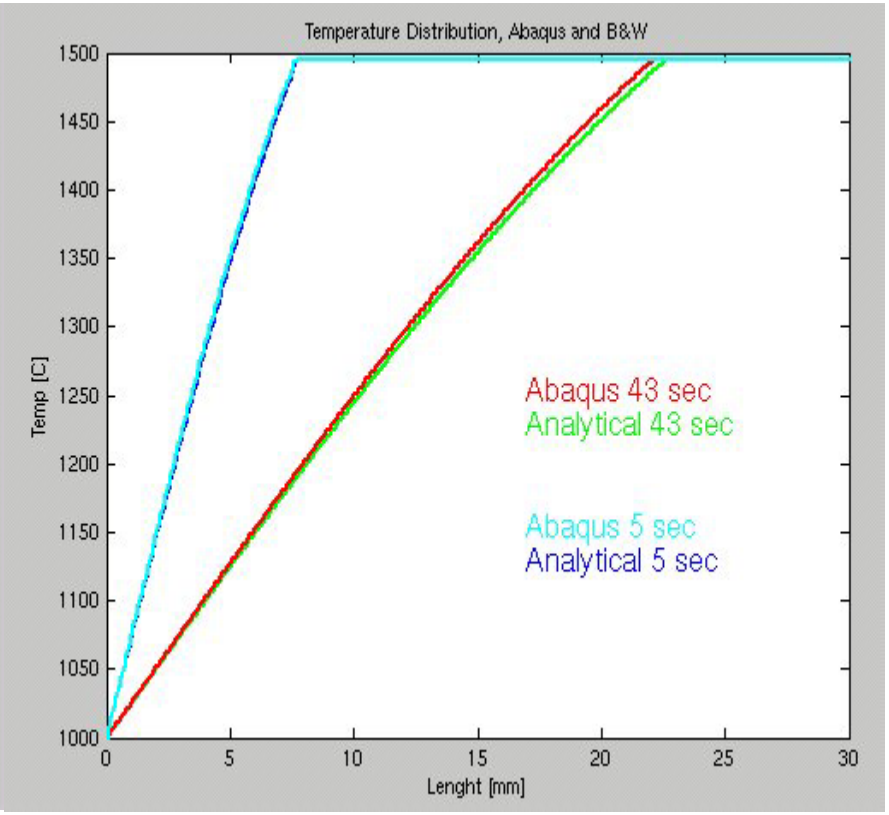
Simple calculation to get h, from surface energy balance at initial instant of time:

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

Temperature and Stress Distributions for 1D Solidification

Abaqus and Analytical (Weiner-Boley)Solutions



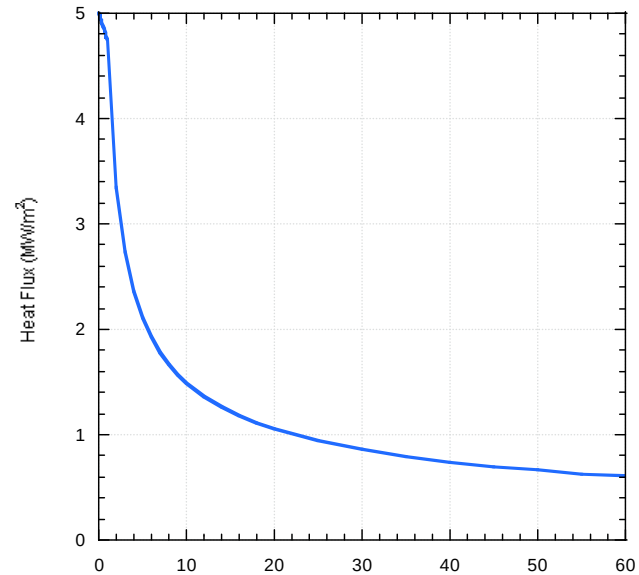


- **The numerical representations from MATLAB and Abaqus produces almost identical results**
- **Model is numerically consistent and has acceptable mesh**

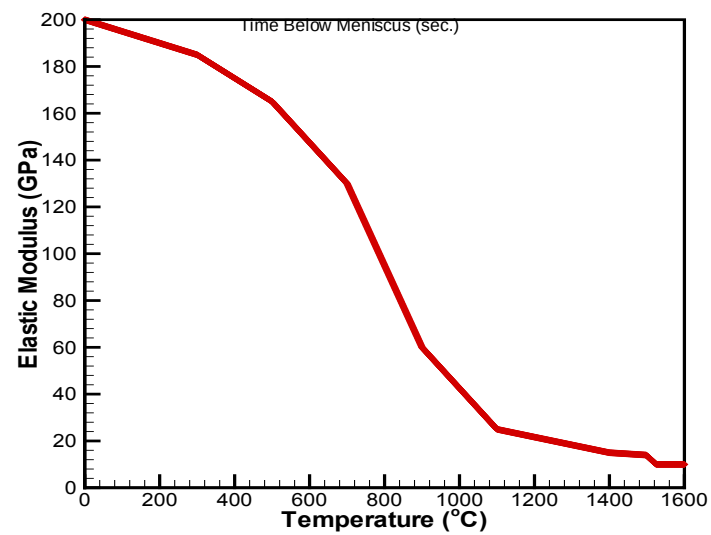
Add more complexity (physics) to the Abaqus model by means of user subroutines

Applied instantaneous Heat Flux from a real plant measurements:

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



Elastic modulus decreases as temperature increase:



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

$$\dot{\varepsilon} = \begin{cases} 10^{-11}(|\sigma| - \sigma_{yield})^2 & if \quad |\sigma| > \sigma_{yield} \\ 0 & if \quad |\sigma| \le \sigma_{yield} \end{cases}$$

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

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

where

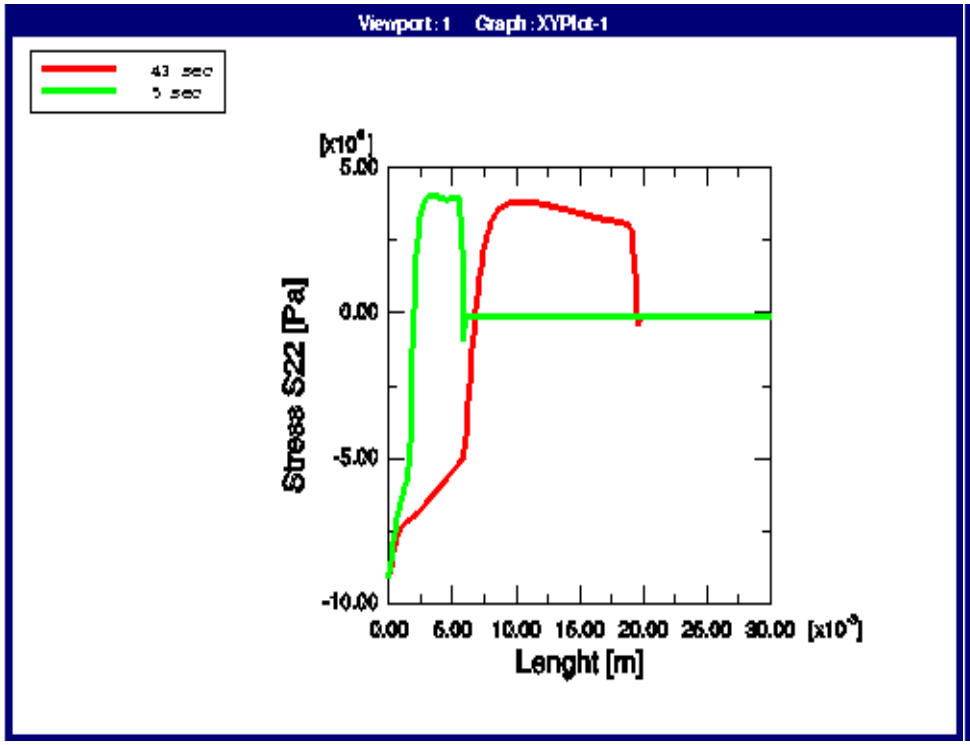
$$f_1\left(T\left({}^oK\right)\right) = 130.5 - 5.128\times10^{-3}T\left({}^oK\right)$$

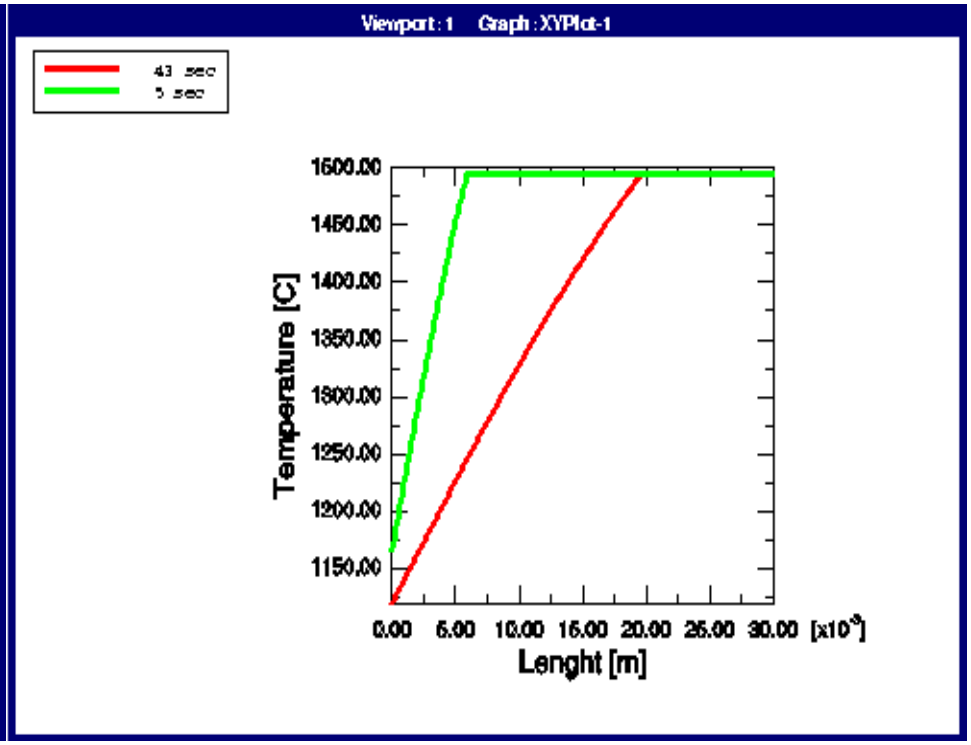
$$f_2\left(T\left({}^oK\right)\right) = -0.6289 + 1.114\times10^{-3}T\left({}^oK\right)$$

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

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

Temperature and Stress Distribution
Elastic-visco-plastic model by Kozlowski

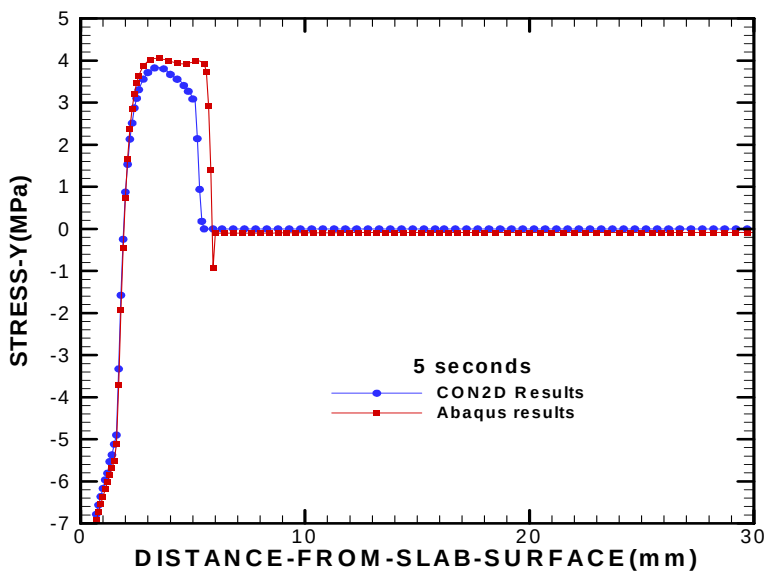


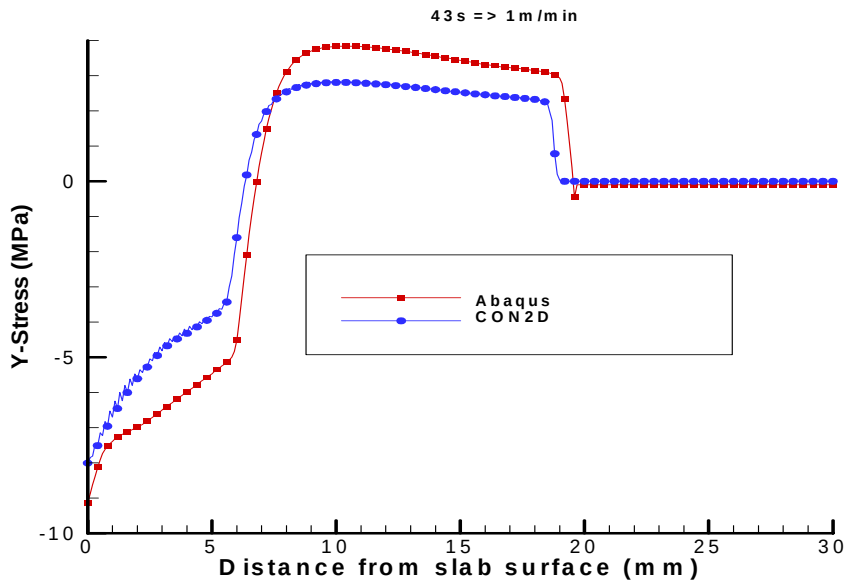


- **Different residual stress values due to different creep rate function**
- **Lower temperatures due to real flux data**

Comparison of Abaqus and CON2D for previous complex model

	CON2D	ABAQUS
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	<1Gb	6Gb
Wall clock normalized to 1Ghz	**17 minutes**	**204 minutes**



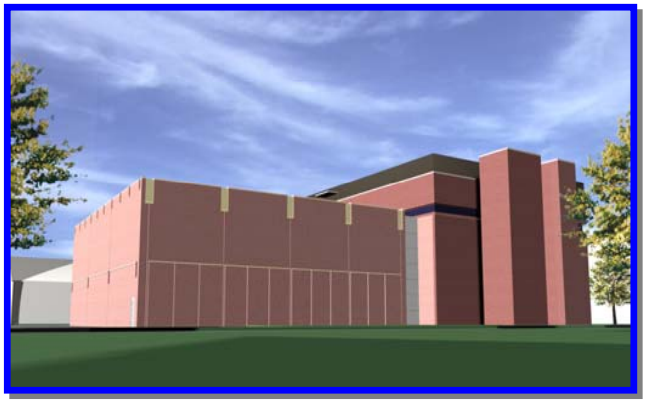


Conclusions and Future Work

- Nowadays, It is possible to perform numerical simulations of steel solidification process in the Continuous Casting Mold with multipurpose commercial finite element code-Abaqus
- 12 times more CPU and 6 times more memory resources are needed with Abaqus compared to in-house code CON2D for identical problem due to superior CON2D robust implicit-explicit integration scheme.
- Quantitatively results are matching well, qualitative differences are under investigation
- It is realistic to expect much better wall clocks both with CON2D and Abaqus on the newest NCSA High Performance Architectures (IBM Regatta, Linux IA-64 Clusters)
- If there are enough dofs, parallel Abaqus features can be applied (each increment solved in parallel)
- Move to 2D and perhaps 3D FE domains with Abaqus and to increase process understanding
- 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…
- Replace Abaqus native integration model and apply robust implict-explicit integration scheme form CON2D with another user defined subroutine UMAT

NCSA Terascale Linux Clusters

- **1 TF IA-32 Cluster of Parallel PC-s**
  - 512 1 GHz dual processor nodes
  - Myrinet 2000 interconnect between PC-s
  - 5 TB of RAID storage
- **1 TF IA-64 Cluster of Paralle Itanium PC-s**
  - 164 800 MHz dual processor nodes
  - Myrinet 2000 interconnect beween PC-s
- **Can solve a million equations with million unknowns in less then a minute by performing $17*10^9$ 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 !

New NCSA Capabilities: Coming Soon

- 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

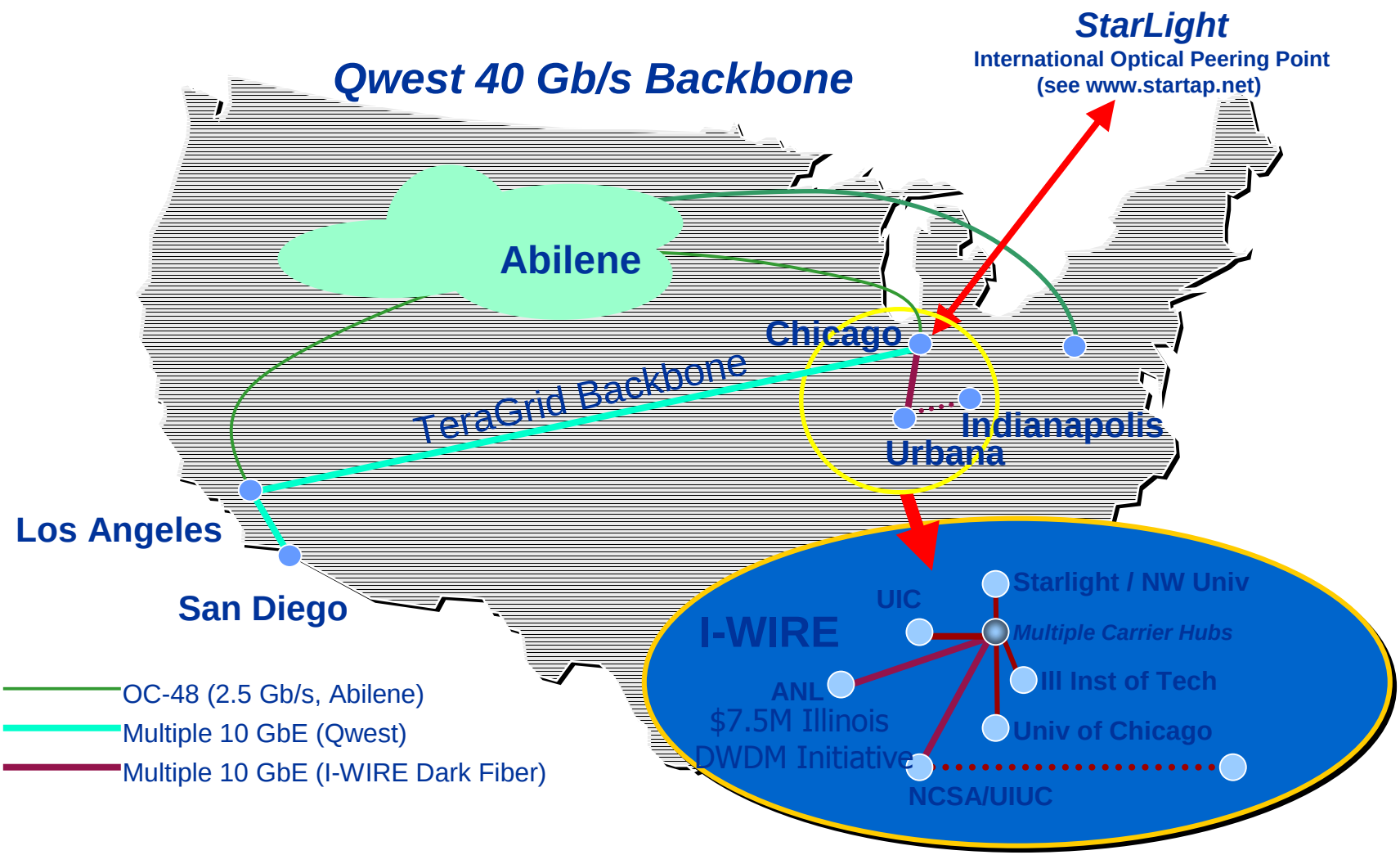
  Perfect for engineering commercial software like:

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

- Cluster expansion
  - 5 TF Pentium4 Linux cluster
- Secondary and tertiary storage
  - 500 TB secondary storage SAN
  - 3.4 PB tertiary storage

Computing in 21St Century, a story of TeraGrid

Computing Resources: Anytime, Anywhere



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