Solidification Stress Model in Abaqus

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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.
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

- **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 dependent 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
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:

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

where,

\[
\{\sigma\} = \begin{bmatrix} \sigma_x & \sigma_y & \sigma_z & \tau_{xy} \end{bmatrix}^T
\]

\[
\{\varepsilon\} = \begin{bmatrix} \varepsilon_x & \varepsilon_y & \varepsilon_z & \varepsilon_{xy} \end{bmatrix}^T
\]

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

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

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

Incremental Total Strain

\[
\{\Delta \varepsilon\} = \{\Delta \varepsilon_e\} + \{\Delta \varepsilon_{th}\} + \{\Delta \varepsilon_{el}\}
\]
Constants Used in Abaqus Numerical Solution of B&W Analytical Test Problem

<table>
<thead>
<tr>
<th>Property</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conductivity</td>
<td>[W/mK]</td>
<td>33.</td>
</tr>
<tr>
<td>Specific Heat</td>
<td>[J/kg/K]</td>
<td>661.</td>
</tr>
<tr>
<td>Thermal Linear Exp.</td>
<td>[1/k]</td>
<td>2.E-4</td>
</tr>
<tr>
<td>Density</td>
<td>[kg/m³]</td>
<td>7500.</td>
</tr>
<tr>
<td>Poisson’s Ratio</td>
<td></td>
<td>0.3</td>
</tr>
<tr>
<td>Liquidus Temp</td>
<td>[° C]</td>
<td>1494.48</td>
</tr>
<tr>
<td>Solidus Temp</td>
<td>[° C]</td>
<td>1494.38</td>
</tr>
<tr>
<td>Initial Temp</td>
<td>[° C]</td>
<td>1495.</td>
</tr>
<tr>
<td>Number of Elements</td>
<td></td>
<td>300.</td>
</tr>
<tr>
<td>Uniform Element Length [mm]</td>
<td></td>
<td>0.1</td>
</tr>
</tbody>
</table>

Artificial and non-physical thermal BC from B&W (slab surface quenched to 1000°C), replaced by a convective BC with \( h = 220000 \) [W/m²K]

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

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

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

Elastic modulus decreases as temperature increase:
The only difference between solid and liquid is a large creep rate in the liquid

\[ \varepsilon = \begin{cases} 10 \quad (|\sigma| - \sigma_{\text{yield}}) & \text{if} \quad |\sigma| > \sigma_{\text{yield}} \\ 0 & \text{if} \quad |\sigma| \leq \sigma_{\text{yield}} \end{cases} \]

(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:

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

where

\[ f_1\left(\circ\ K\right) = 130.5 - 5.128 \times 10^{-3} T\left(\circ\ K\right) \]
\[ f_2\left(\circ\ K\right) = -0.6289 + 1.114 \times 10^{-3} T\left(\circ\ K\right) \]
\[ f_3\left(\circ\ K\right) = 8.132 - 1.54 \times 10^{-3} T\left(\circ\ K\right) \]
\[ f\left(\%C\right) = 4.655 \times 10^4 + 7.14 \times 10^4 \%C + 1.2 \times 10^5 \left(\%C\right)^2 \]
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

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

Distance from slab surface (mm)

Y-Stress (MPa)

Abaqus results

CON2D results

43s => 1 m/min

Distance from slab surface (mm)
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

Read Nodal $T^{t+\Delta t}$ from HT database
\[ \{\varepsilon_{\text{th}}^{t+\Delta t}\} = \alpha (T^{t+\Delta t}) T^{t+\Delta t} \{111000\}^T \]

Equilibrium Configuration at
\[ \{U^t\}, \{S^t\}, \{P^t\} \]

Global External Load Vector at $t + \Delta t$
\[ \{P^{t+\Delta t}\} = \sum_i \int [N^T] [b^{t+\Delta t}] dV + \int [B^T] [S] [\varepsilon_{\text{th}}^{t+\Delta t}] dV + \int [N^T] [\Phi^{t+\Delta t}] dA \]

Global NR Iteration

Yes
$t = t + \Delta t$

Element Strain Increment
\[ \{\Delta \varepsilon_i^{t+\Delta t}\} = [B] \{\Delta U_i^{t+\Delta t}\} \]

Element Internal Force and Element Tangent Matrix
\[ \{S_i^{t+\Delta t}\} = -\sum_i [B^T] [\sigma^{t+\Delta t}] dV \]
\[ [K_i^{t+\Delta t}] = \int_{\text{vel}} [B^T] [J] [B] dV \]

UMAT called at all Gauss Points
\[ \{\sigma^t\}, \{\Delta \varepsilon^{t+\Delta t}\}, \{\varepsilon_i^t\} \]

Constitutive Model Integration using 2 level Implicit Scheme from CON2D

Calculation of CTO:
\[ [J] = \frac{\partial \{\sigma^{t+\Delta t}\}}{\partial \{\Delta \varepsilon^{t+\Delta t}\}} \]

\[ \{\sigma^{t+\Delta t}\}, \{\varepsilon_i^{t+\Delta t}\}, [J] \]

No, Start new NR Iteration

Yes
\[ i = i + 1 \]

\[ \{K_i^{t+\Delta t}\} \{\Delta U_i^{t+\Delta t}\} = \{P^{t+\Delta t}\} - \{S_i^{t+\Delta t}\} \]
\[ \{U_i^{t+\Delta t}\} = \{U_i^{t+\Delta t}\} + \{\Delta U_i^{t+\Delta t}\} \]

Tolerance

\[ \{\Delta U_i^{t+\Delta t}\} = \{U_i^{t+\Delta t}\} - \{U^t\} \]

\[ K_i^{t+\Delta t} = \sum [K_i^{t+\Delta t}] \]
\[ \{S_i^{t+\Delta t}\} = \sum [S_i^{t+\Delta t}] \]
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

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**Stress \( \sigma_y \) Distribution at 8.6 sec**

![Stress Distribution Chart](chart.png)
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

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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

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

NCSA machine room expansion
  – capacity to 20 TF and expandable
  – dedicated September 5, 2001

University of Illinois at Urbana-Champaign  •  Metals Processing Simulation Lab  •  Seid Koric
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 21st Century, a story of TeraGrid

Computing Resources: Anytime, Anywhere

Qwest 40 Gb/s Backbone

Abilene

TeraGrid Backbone

Chicago

Indianapolis

Urbana

Los Angeles

San Diego

I-WIRE

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OC-48 (2.5 Gb/s, Abilene)
Multiple 10 GbE (Qwest)
Multiple 10 GbE (I-WIRE Dark Fiber)

StarLight
International Optical Peering Point
(see www.startap.net)

Qwest 40 Gb/s Backbone

Abbreviations:
- ANL: Argonne National Laboratory
- I-WIRE: Illinois Network for Research and Education
- UIUC: University of Illinois at Urbana-Champaign
- NCSA: National Center for Supercomputing Applications
- NW Univ: Northwestern University
- Ill Inst of Tech: Illinois Institute of Technology
- Univ of Chicago
- NCSA/UIUC
- $7.5M Illinois DWDM Initiative

Multiple Carrier Hubs

Starlight / NW Univ

I-WIRE

Multiple Carrier Hubs

Ill Inst of Tech

Univ of Chicago

NCSA/UIUC

Metals Processing Simulation Lab

Seid Koric
Some CSM and CFD Applications on NCSA machines

Reference: Bob Wilhelmson (NCSA)
Severe Weather Forecast
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