CCC Annual Report

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Mechanical Behavior of the Mushy Zone of Solidifying Steel

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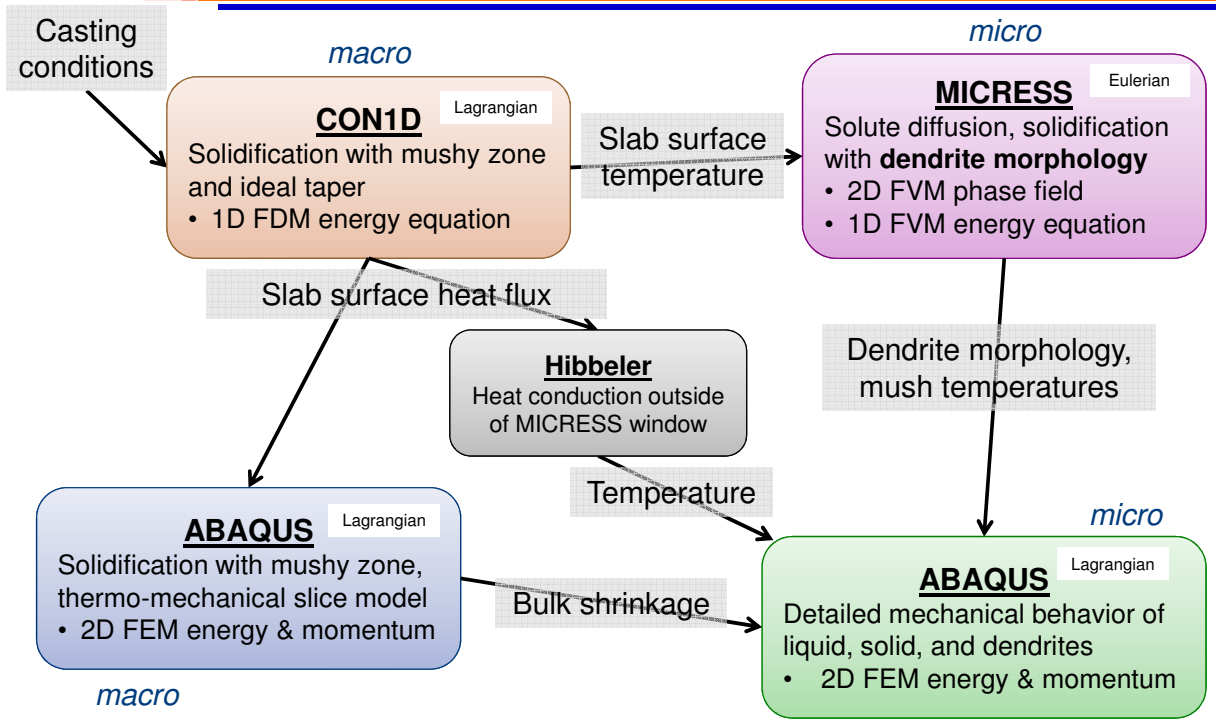
Introduction

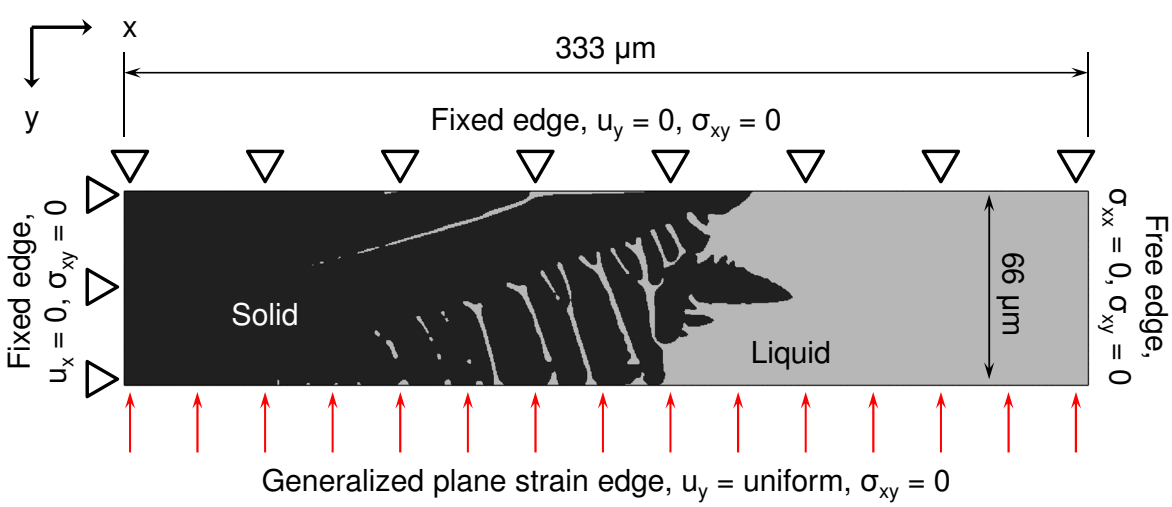
- Hot tearing is a solidification defect that leads to poor product quality at best and a breakout at worst
- The averaging in traditional **macro-scale** models – **mushy zones** – prevents study of the details of hot tear formation and propagation
- This work explores hot tears with a **micro-scale** model – of the **dendrites** themselves – by combining macro-scale information with a detailed model of the morphology of the solidification front

Modeling Approach



Microscale Domain and BC

200,000 4-node elements, 0.3-μm square



Out-of-plane assumption: generalized plane strain u_z = uniform

Phase field calculated with MICRESS by B. Boettger

Explicit Finite Element Method

Get accelerations from force balance

$$\nabla \cdot \boldsymbol{\sigma} + \boldsymbol{b} = \rho \boldsymbol{a} \qquad \Rightarrow \boldsymbol{a}^n = \boldsymbol{M}^{-1}(\boldsymbol{F}_{ext}^n - \boldsymbol{F}_{int}^n)$$

Integrate to get half-step velocity

$$\boldsymbol{v}^{n+\frac{1}{2}} = \boldsymbol{v}^{n-\frac{1}{2}} + \boldsymbol{a}^n \frac{\Delta t^{n+1} + \Delta t^n}{2}$$

Integrate at half-step to get displacement

$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^n + \boldsymbol{v}^{n+\frac{1}{2}} \Delta t^{n+1}$$

Critical time step

$$\Delta t < \frac{L_{min}}{c_d}$$

L_{min} Smallest element characteristic length

Dilational wave speed (approx. 1000 m/s)

$$c_d = \sqrt{\frac{\hat{\lambda} + 2\hat{\mu}}{\rho}}$$

$\hat{\mu}$ Effective shear modulus

$\hat{\lambda}$ Effective Lame constant

Efficiencies from:

- No Newton iterations (no matrix solve)
- Lumped mass matrix (no matrix solve)
- Mass scaling – make density large to increase critical step size

Koric, Hibbeler, Thomas
IJNME 2009

Modeling Issues

- ABAQUS/Explicit has trouble with the formation of the first solid material, but the explanation is more evident than with ABAQUS/Standard:
  - The large step-change in stiffness causes the critical time step to be violated

- The mass scaling must be readjusted, ***frequently***, to account for the change in stiffness as temperature and phase evolve

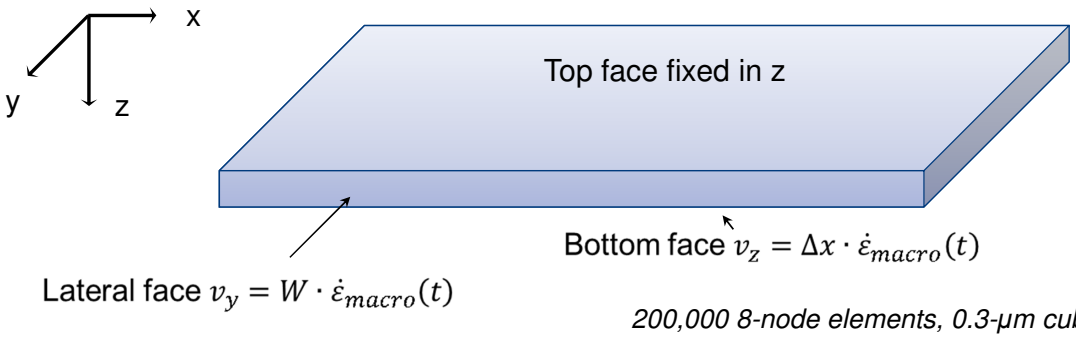
$$\hat{\lambda} + 2\hat{\mu} = \frac{\Delta p}{\Delta \varepsilon_{dil}} + \frac{2}{3}\frac{\Delta \boldsymbol{s} : \Delta \boldsymbol{e}}{\Delta \boldsymbol{e} : \Delta \boldsymbol{e}}$$

Δp	Pressure stress increment
$\Delta \varepsilon_{dil}$	Dilational strain increment
$\Delta \boldsymbol{s}$	Deviatoric stress increment
$\Delta \boldsymbol{e}$	Deviatoric strain increment

Modeling Issues

- Imposing the generalized plane strain constraint prevents parallelization (in ABAQUS/Explicit)
- Efficient solution to this problem is to calculate the shrinkage in a macroscale model (with mush) and impose time-dependent boundary conditions

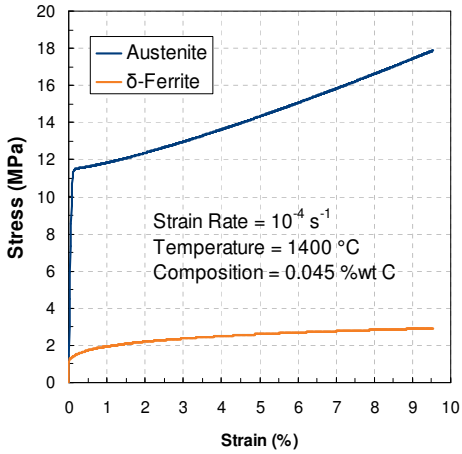
Other BCs mimic 2D case



200,000 8-node elements, 0.3-μm cube

Material Models

- Liquid:
  - Nearly-incompressible Newtonian fluid
- Solid
  - Zhu (ferrite) or Kozlowski III (austenite)



$$\dot{\varepsilon}(s^{-1}) = 0.1\left|\sigma / f(C)(T/300)^{-5.52}(1+1000\varepsilon)^{m}\right|^{n}$$

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

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

$$n = 1/1.617\times10^{-4}T - 0.06166$$

Zhu

$$\dot{\varepsilon}(s^{-1}) = f(C)\left[\sigma - f_1(T)\varepsilon\left|\varepsilon\right|^{f_2(T)-1}\right]^{f_3(T)}\exp\left(-\frac{4.465\times10^{4}(K)}{T}\right)$$

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

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

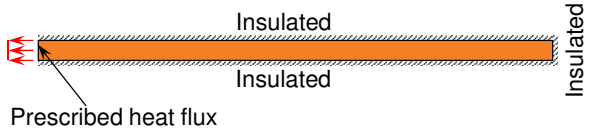
$$f_3(T) = 8.132 - 1.54\times10^{-3}T$$

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

Kozlowski

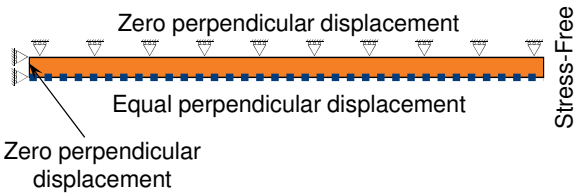
Macroscale Slice Model

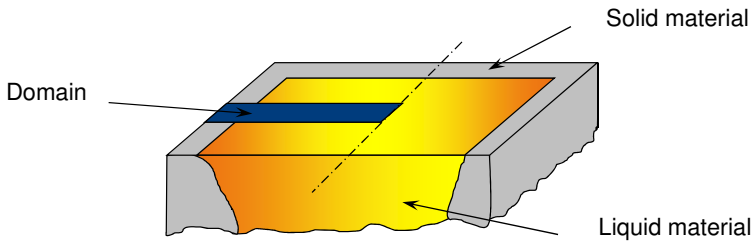
Thermal Boundary Conditions



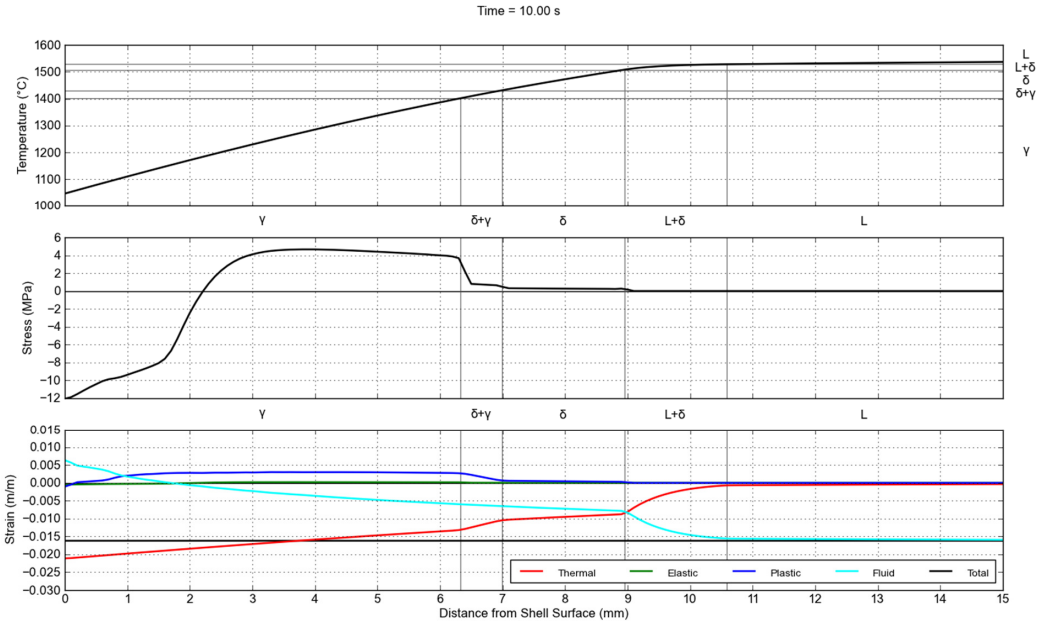
- Material properties from CON1D
- Mushy zone solidification

Mechanical Boundary Conditions

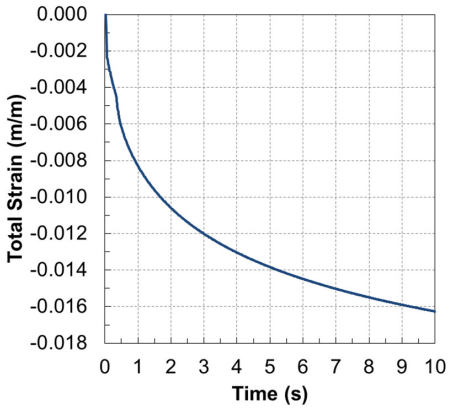


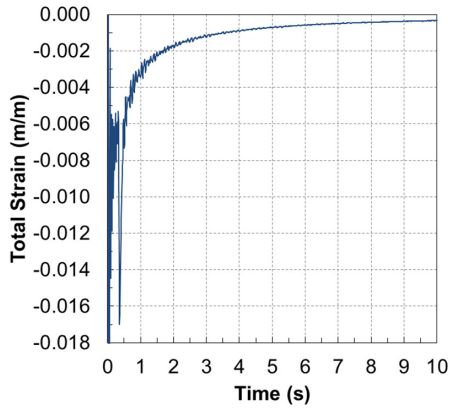


Macroscale Model Results



Macroscale Total Strain





- Extract the total strain and its rate from the macroscale model
- Use piecewise approximation to eliminate noise from solidifying nodes

$$\dot{\varepsilon} = 0 \qquad 0\ \text{s} \leq t \leq 0.03\ \text{s}$$

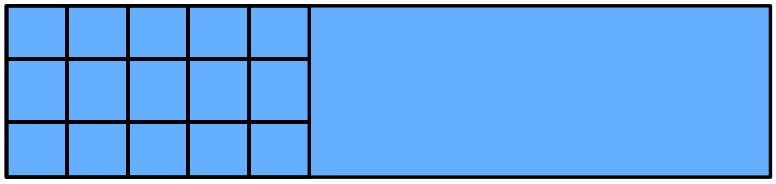
$$\dot{\varepsilon} = -0.1135\,t + 0.0035 \qquad 0.03\ \text{s} \leq t \leq 0.05\ \text{s}$$

$$\dot{\varepsilon} = -0.0076\,t + 0.0020 \qquad 0.05\ \text{s} \leq t \leq 0.34\ \text{s}$$

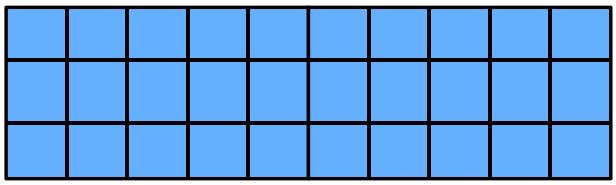
$$\dot{\varepsilon} = -0.0030\ln(t) - 0.0083 \qquad 0.34\ \text{s} \leq t \leq 10.0\ \text{s}$$

Descriptions of Motion

- MICRESS uses a moving Eulerian (spatial) description, where the mesh follows the solidification front of stationary material

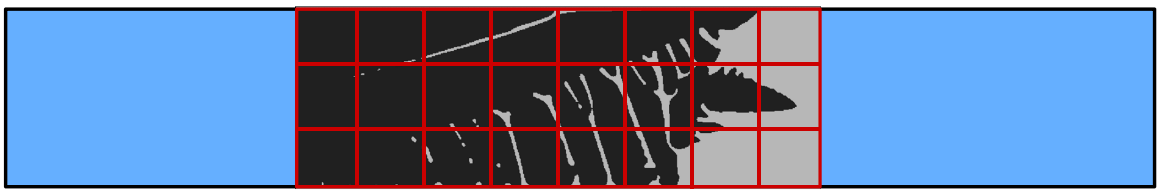


- ABAQUS uses a Lagrangian (material) description, where the mesh is fixed on the material



Eulerian—Lagrangian Conversion

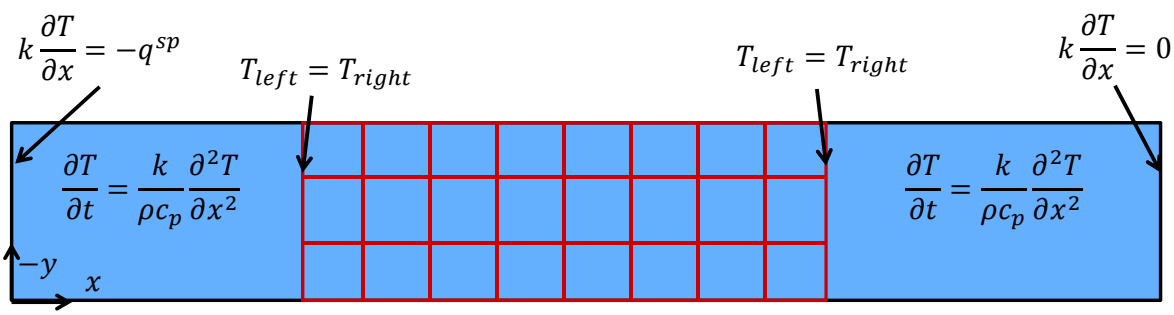
- The “window” of data from MICRESS is patched into an ABAQUS domain according to how the Eulerian simulation has moved



Fraction Solid = 1 | **MICRESS Fraction Solid = *f*(*x*,*y*)** | Fraction Solid = 0

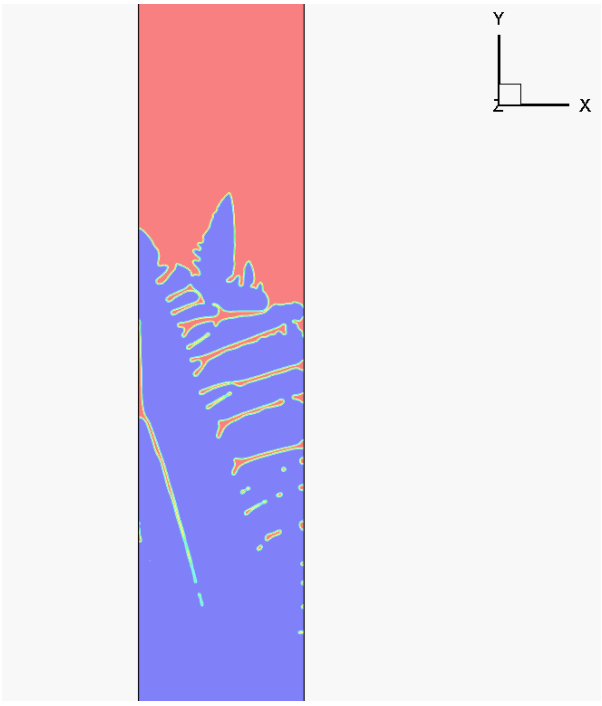
Eulerian—Lagrangian Conversion

- Outside of the MICRESS window, the 1D heat conduction equation is solved with temperature and heat flux boundaries
- In the Python script that builds the ABAQUS file
- Temperature is continuous at boundaries of MICRESS window



MICRESS Temperature = *f*(*x*)

Eulerian Dendrite Movement



Acknowledgments

- Continuous Casting Consortium Members (ABB, ArcelorMittal, Baosteel, Magnesita Refractories, Nippon Steel and Sumitomo Metal Corp., Nucor Steel, Postech/ Posco, Severstal, SSAB, Tata Steel, ANSYS/ Fluent)
- National Center for Supercomputing Applications (NCSA) at UIUC
- Dr. Bernd Boettger, ACCESS e.V.
  - See (Boettger, Apel, Santillana, and Eskin, MCWASP XIII) for more detail