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Stress Analysis of Dendritic Microstructure During Solidification

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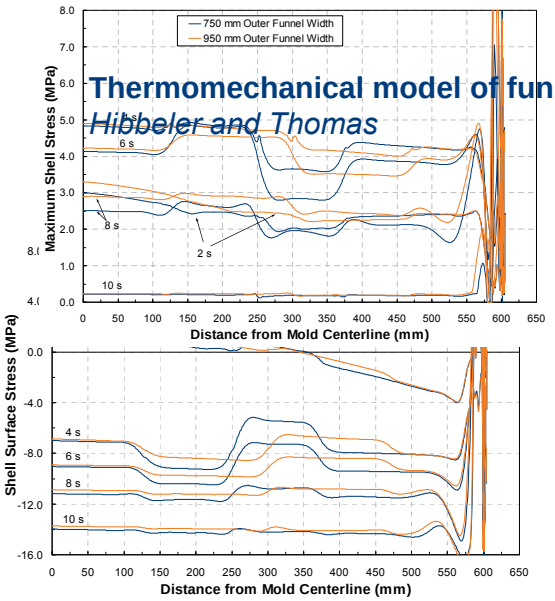
Introduction

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

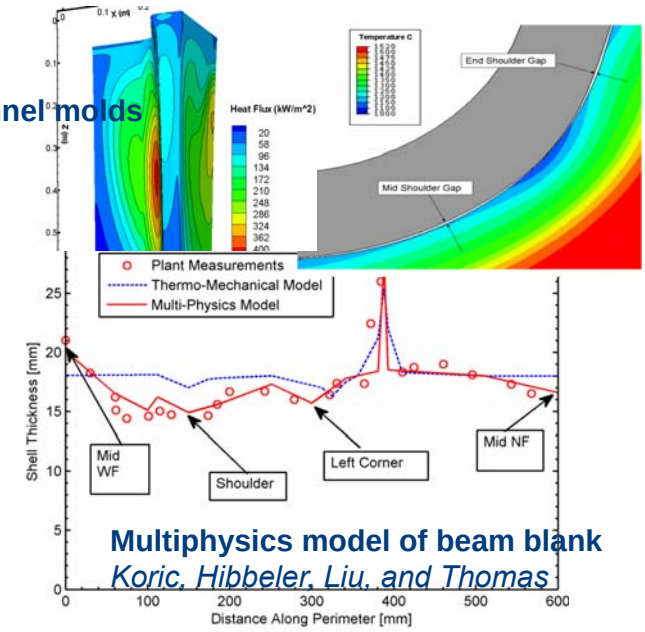
Previous Work

Large Scales

- Simulations of entire caster



Thermomechanical model of funnel molds
Hibbeler and Thomas



Multiphysics model of beam blank
Koric, Hibbeler, Liu, and Thomas

Previous Work

Intermediate Scales

- Detailed simulation of a surface defect

$$\varepsilon_c = \frac{0.02821}{\dot{\varepsilon}^{0.3131} \cdot \Delta T_B^{0.8638}}$$

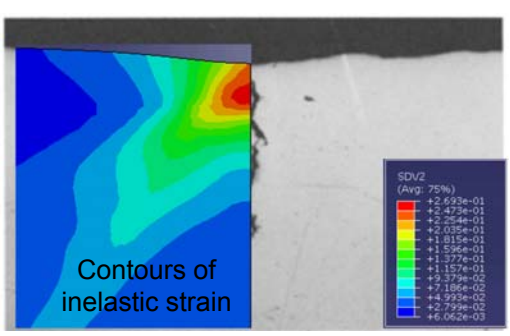
Won *et al.*, *MMTB* 2000

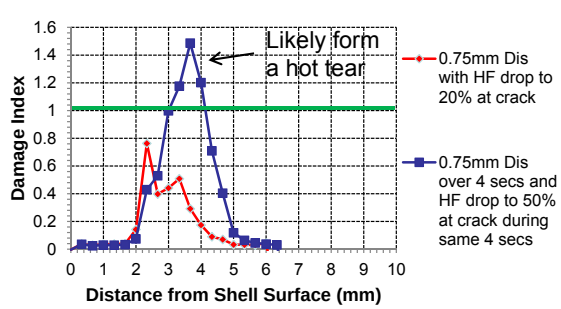
$$\Delta T_B = T(f_s = 99\%) - T(f_s = 90\%)$$

$$\dot{\varepsilon} = \frac{\varepsilon(f_s = 99\%) - \varepsilon(f_s = 90\%)}{t(f_s = 99\%) - t(f_s = 90\%)}$$

$$\varepsilon_{dmg} = \varepsilon(f_s = 99\%) - \varepsilon(f_s = 90\%)$$

$$D = \varepsilon_{dmg} / \varepsilon_c$$





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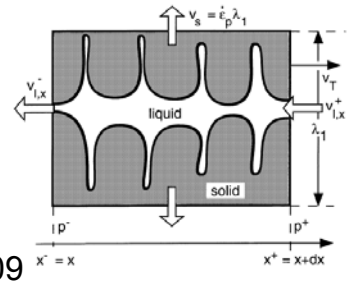
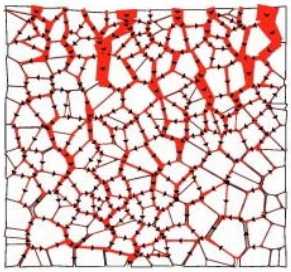
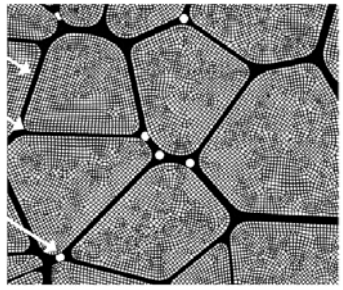
Previous Work

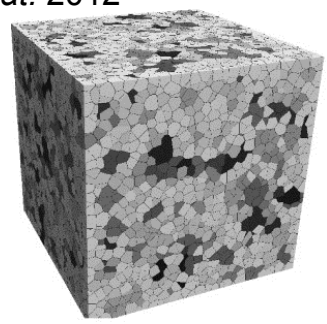
Small Scales

- Semi- or Analytical models
  - Rappaz, Drezet, and Gremaud, *MMTA* 1999
  - Monroe and Beckerman, *MSEA* 2005
- Mushy zone RVE models
  - Vernede, Dantzig, and Rappaz, *Acta Mat.* 2009
  - Phillion, Cockcroft, and Lee, *MSMSE* 2009
  - Sistaninia, Phillion, Drezet, and Rappaz, *Acta Mat.* 2012









Previous Work

Room for Improvement

- Previous work covers mostly:
  - Aluminum alloys
  - Equiaxed/globular grains
  - Mushy zone frozen in time
  - Macro- or meso-scale – need liquid+solid averaging
  - Oversimplified material models – solid, liquid or both
- Present work is concerned with:
  - Commercial steel alloys
  - Entire solidification history – surface and columnar zones
  - Microscale – no averaging
  - Proper material models
  - Relate microscale information to macroscale quantities

Background

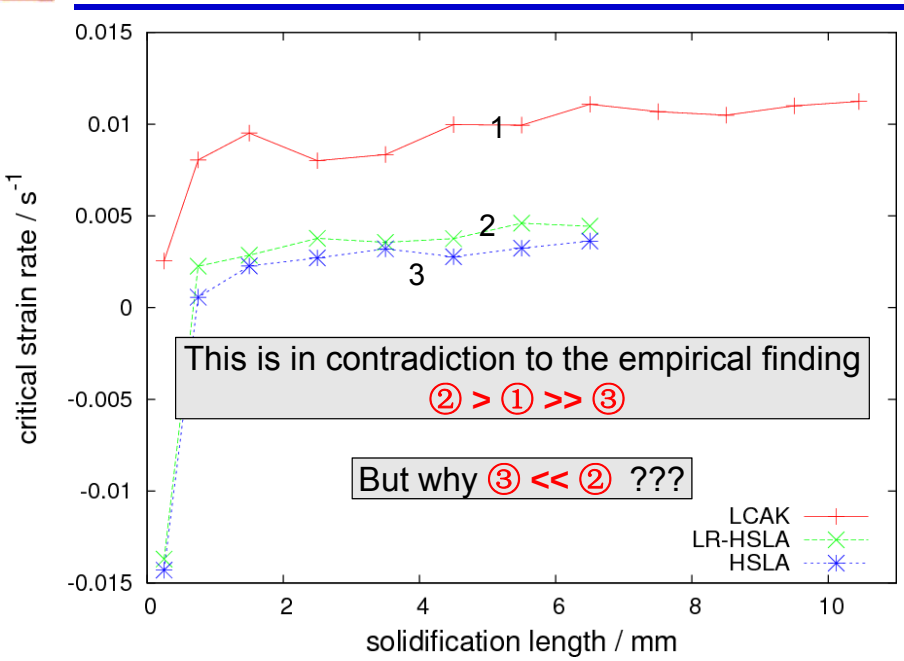
- Different break-out risk is observed during production, which is believed to be due to hot cracking in the first solid shell inside the caster: ② > ① >> ③

Table 1: Typical chemical composition of three steel grades

Steel grade	C (wt %)	Mn (wt %)	V (wt %)	Nb (wt %)	N (ppm) aim	N (ppm) max
① LCAK	0.045	0.22	-	-	-	50
② LR-HSLA	0.045	0.8	0.04	0.013	80	100
③ HSLA	0.045	0.8	0.13	0.013	130	150

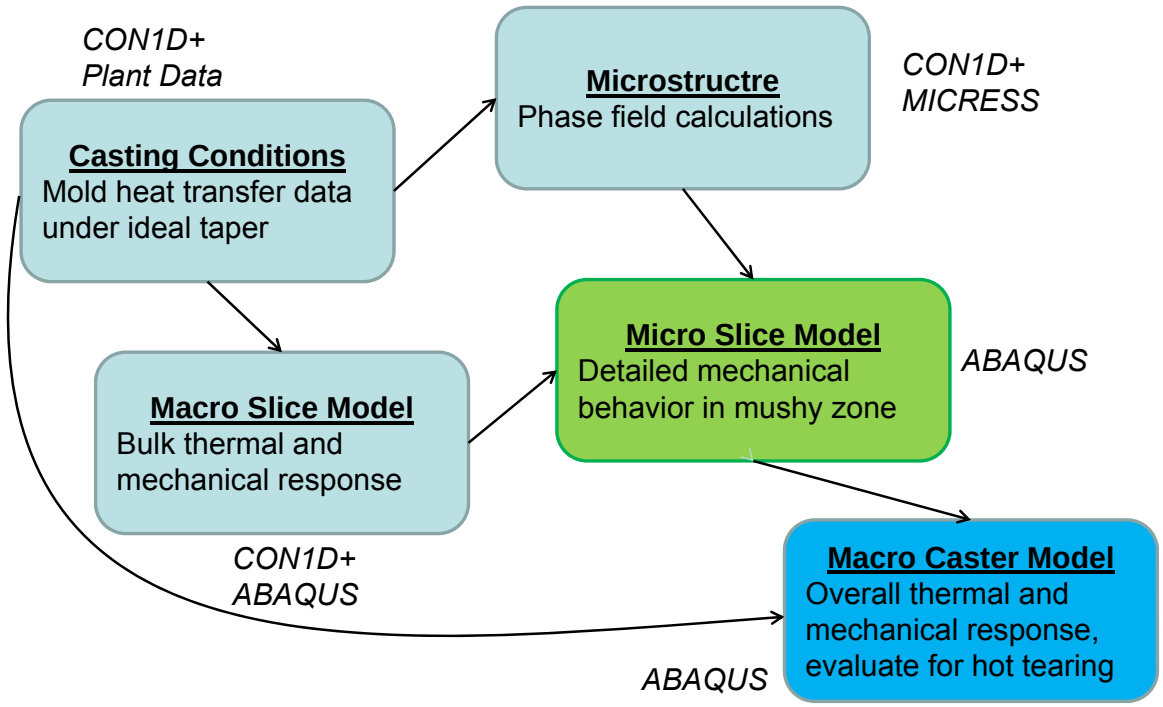
B. Boettger *et al.*, MCWASP XIII

RDG Criterion for Steels



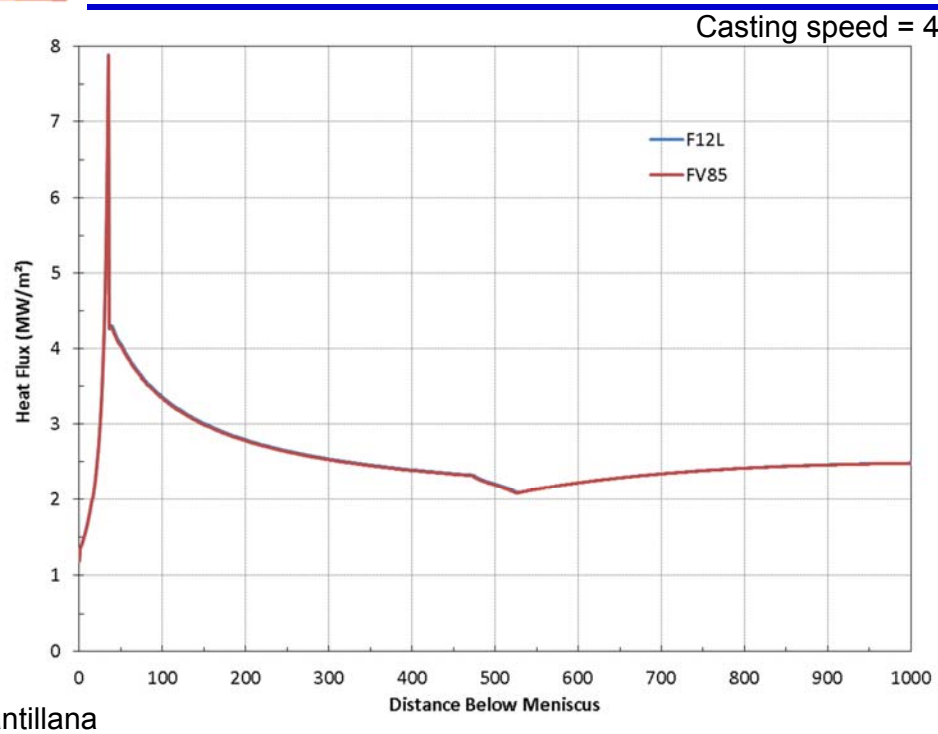
B. Boettger *et al.*, MCWASP XIII

Modeling Approach



Calibrated Heat Flux Profile

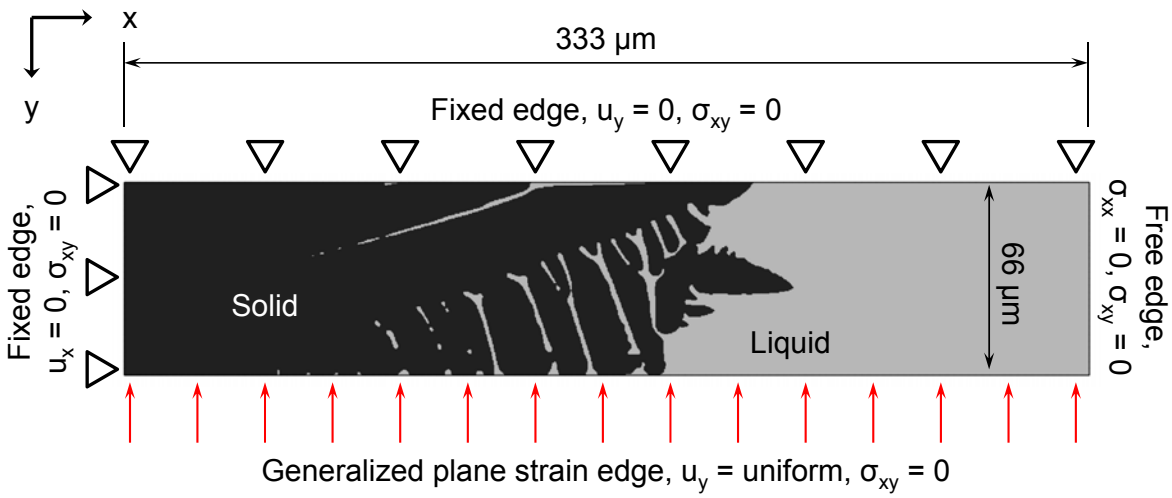
Casting speed = 4.8 m/min



B. Santillana

Microscale Domain

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 FEM

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

Modeling Issues

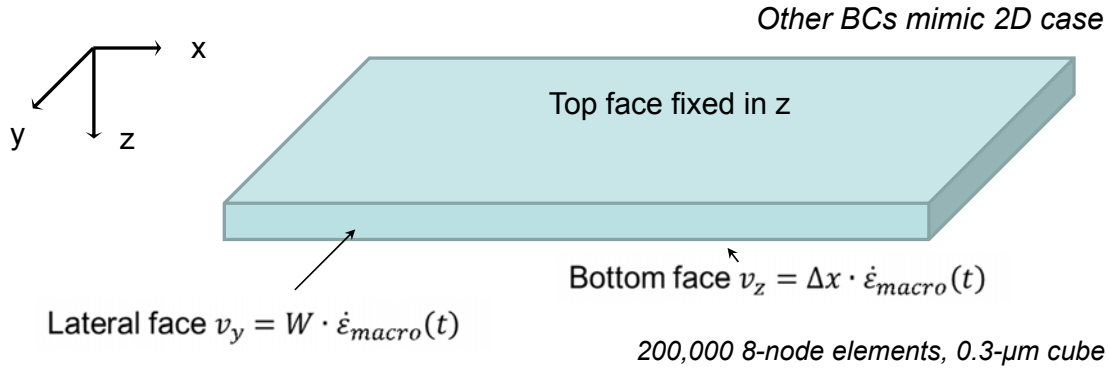
- Using the "traditional" quasi-static approach, the 2D simulation with previously-described conditions **always** crashes with the formation of solid material

- An alternative approach, which explicitly integrates the full force balance, is more numerically stable
  - Mass scaling technique increases critical time step size
  - Explicit marching scales well across processors
  - No generalized plane strain elements; must work in 3D
  - See (Koric, Hibbeler, and Thomas, IJNME 2009) for more detail

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 and impose time-dependent boundary conditions

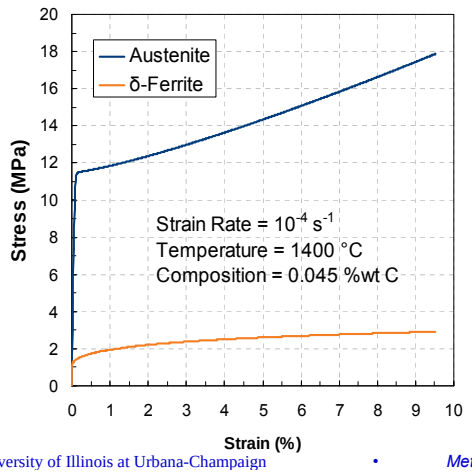
Other BCs mimic 2D case



200,000 8-node elements, 0.3-μm cube

Material Models

- Liquid:
  - Elastic, perfectly plastic (500 Pa yield stress)
  - To be improved to Newtonian fluid (viscosity increases critical Δt)
- Solid: Zhu (ferrite) or Kozlowski III (austenite)



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

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

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

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

Zhu

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

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

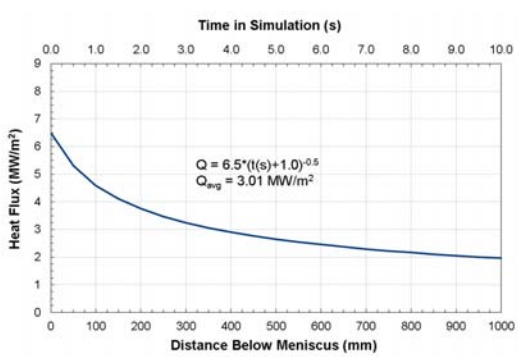
$$f_2(T)=-0.6289+1.114\times10^{-3}T$$

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

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

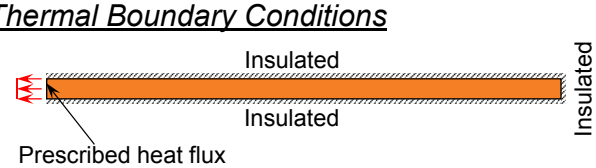
Kozlowski

Macroscale Model

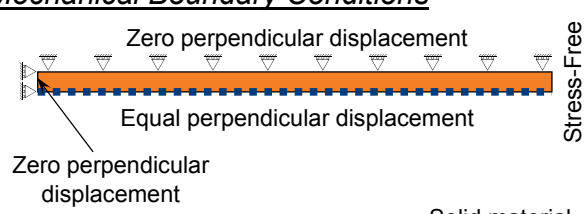


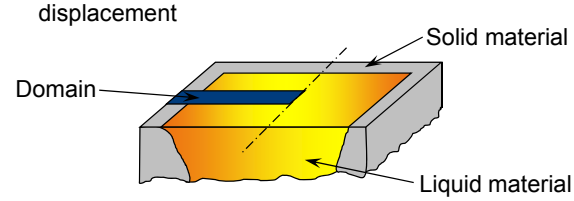
Material properties from CON1D

Thermal Boundary Conditions

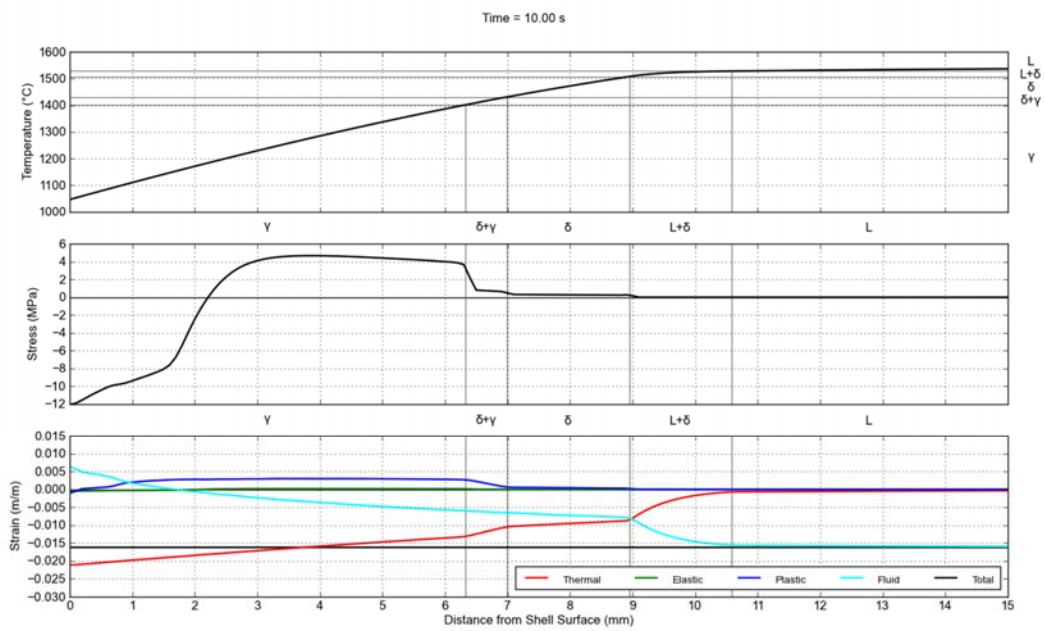


Mechanical Boundary Conditions



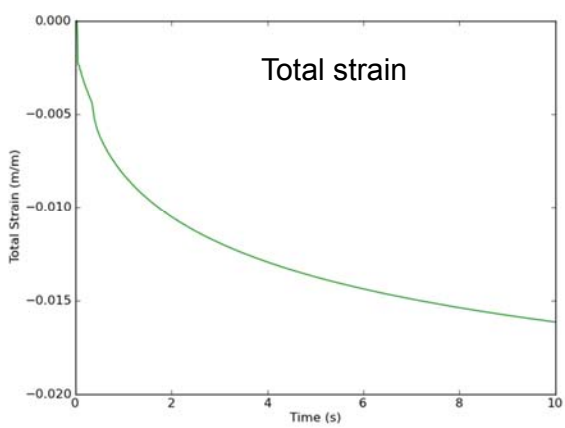


Macroscale Model – Results

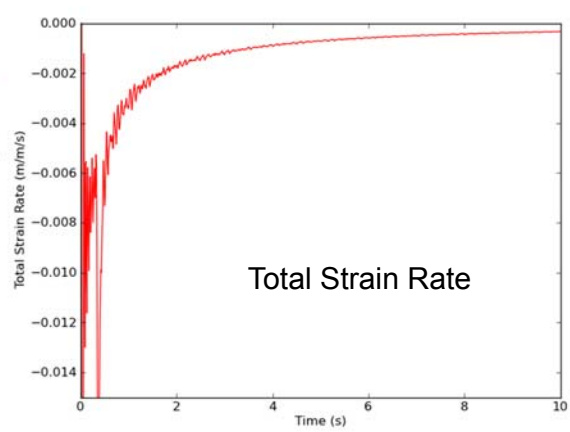


Macroscale Strain History

Input this data into microscale model



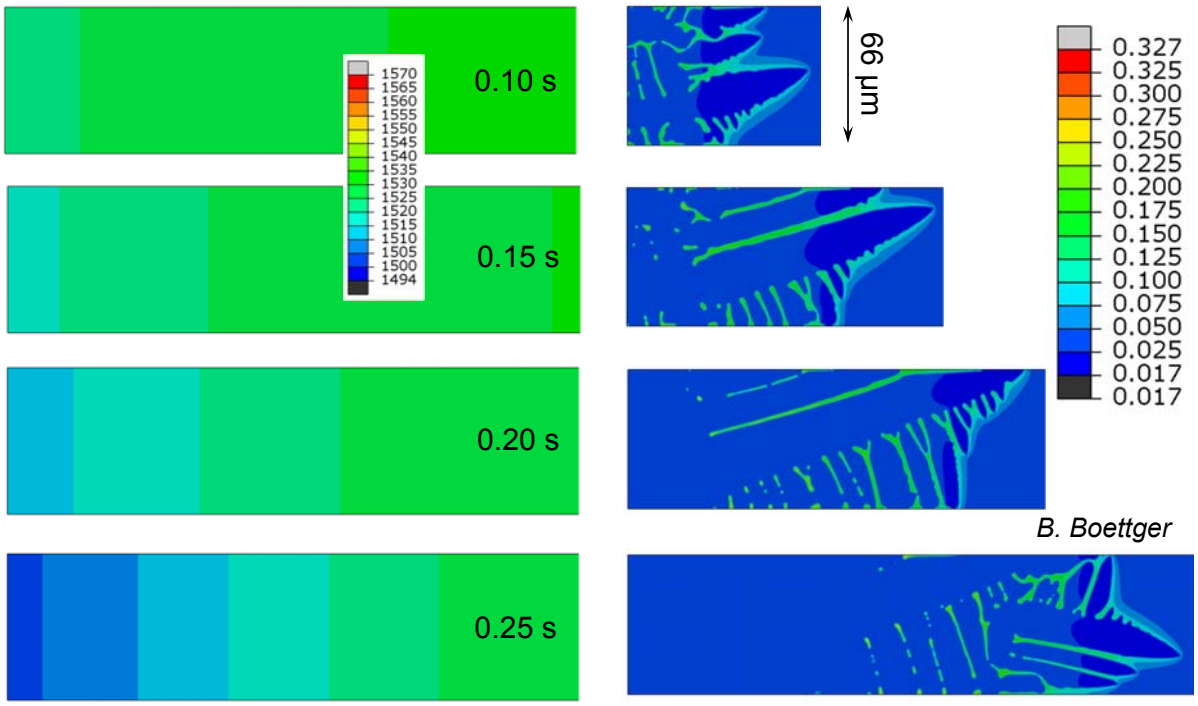
Noise corresponds to nodes turning solid



Component of strain perpendicular to solidification direction

Microscale Domain

Temperature and Carbon Concentration



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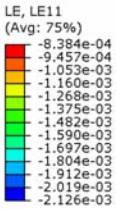
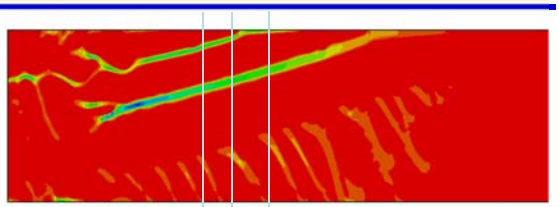
Microscale Deformation

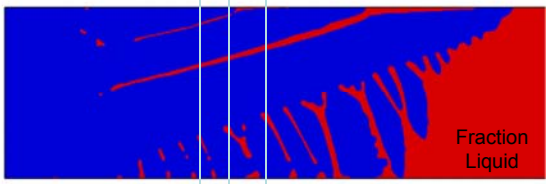
Preliminary Results

Total strain in vertical direction

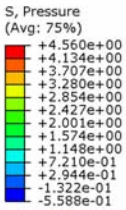


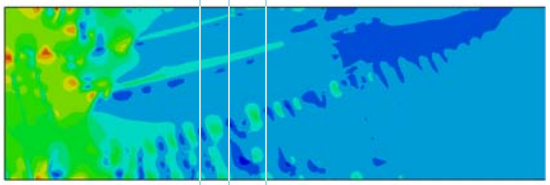


- Strain concentrations in liquid regions
  - Most motion occurs in liquid
- Peak negative pressure in roots of secondary arms
  - Insufficient feeding can lead to porosity



Pressure stress



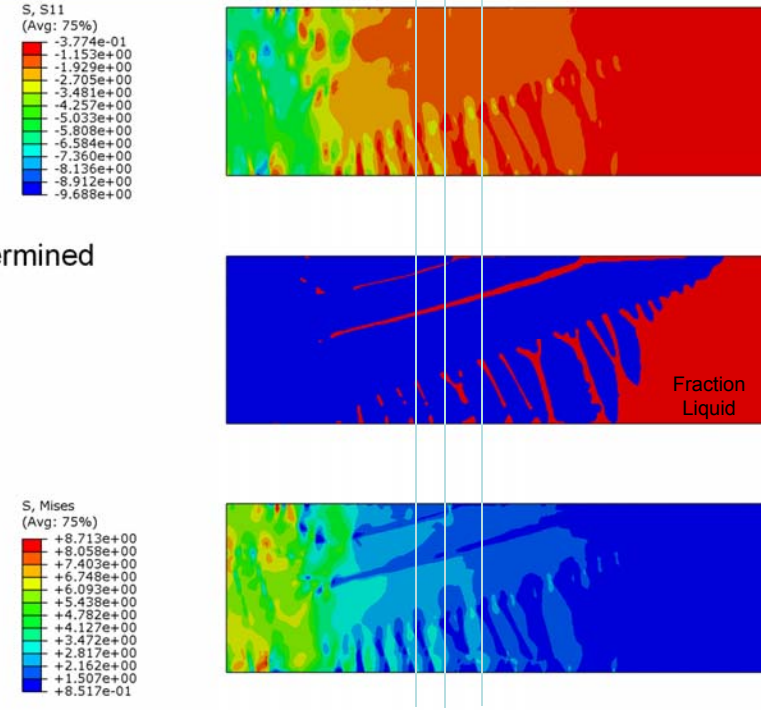


Negative pressure means material in tension

Microscale Deformation

Preliminary Results

Stress in vertical direction

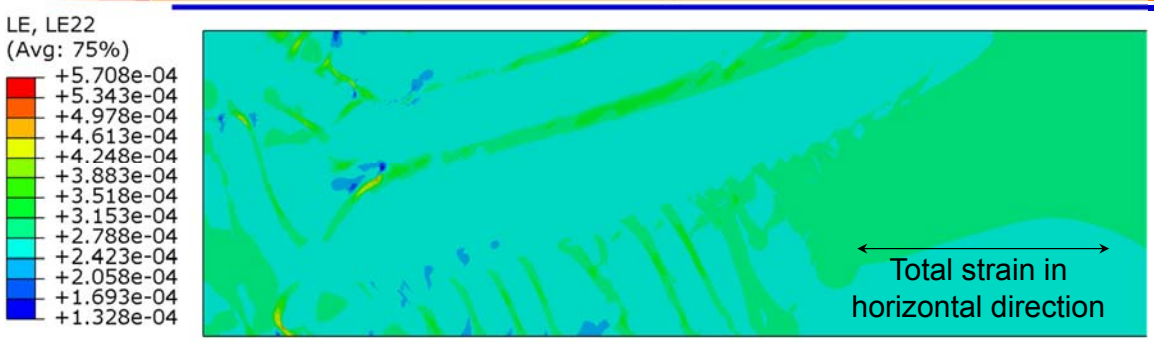


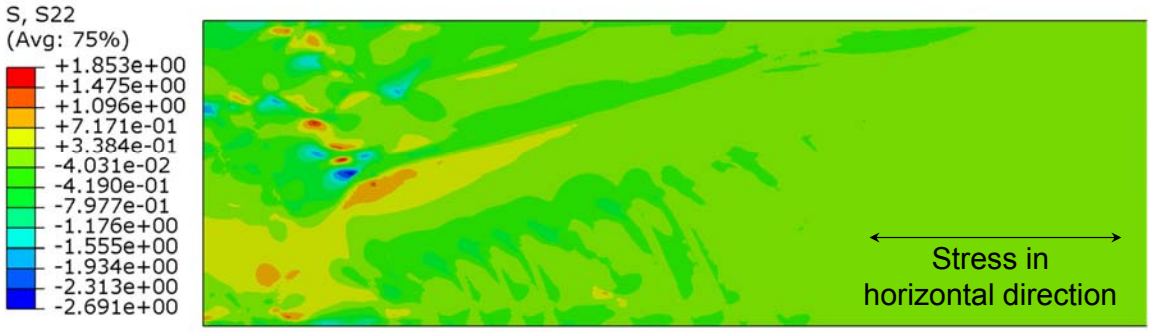
- Consequences to be determined

von Mises stress

Microscale Deformation

Preliminary Results





Modeling Issues

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

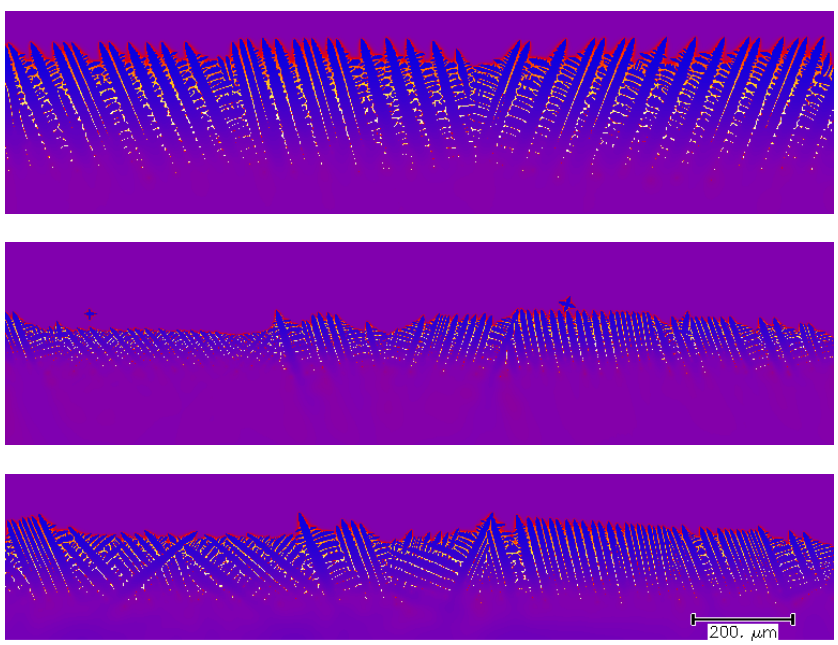
- The mass scaling must be readjusted, frequently, to account for the change in stiffness as temperature and phase evolve

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

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

Future Work

Simulations of many dendrites will reveal statistically significant data that is useable for macroscopic models



B. Boettger

Conclusions

- Modeling effort underway to predict hot tearing from small-scale phenomena
  - Preliminary efforts look promising
- Future studies based on very large phase field simulations

Acknowledgements

- Continuous Casting Consortium Members (ABB, ArcelorMittal, Baosteel, Tata Steel, Goodrich, Magnesita Refractories, Nucor Steel, Nippon Steel, Postech/Posco, SSAB, ANSYS-Fluent)
- Dr. Bernd Boettger, ACCESS e.V.
  - See (Boettger, Apel, Santillana, and Eskin, MCWASP XIII) for more detail
- National Center for Supercomputing Applications (NCSA) at UIUC – “Forge” cluster
- Dassault Systemes (ABAQUS parent company)