Transient Multiphysics Simulations on Blue Waters and Their Applications in Improvement of Steel Continuous Casting

Illinois General Project:
Fluid-Flow and Stress Analysis of Steel Continuous Casting

Seong-Mook Cho¹ (Co-PI and Presenter) and Brian G. Thomas¹,² (PI)

1. Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign
2. Department of Mechanical Engineering, Colorado School of Mines
Acknowledgements

- Blue Waters / National Center for Supercomputing Applications (NCSA) at UIUC
- Co-PIs at U-Illinois: Kai Jin (previous Ph.D. Student), S.P. Vanka (Emeritus Professor of Mechanical Engineering), Hyunjin Yang (Ph.D. Student), Matthew Zappulla (previous M.S. Student), Xiaolu Yan (M.S. Student)
- Co-PIs at NCSA: Ahmed Taha (Technical Program Manager), Seid Koric (Adjunct Associate Professor)
- ANSYS. Inc. for Fluent-HPC License Allocation
- Continuous Casting Consortium at UIUC and Continuous Casting Center at CSM Members (ABB, AK Steel, ArcelorMittal, Baosteel, JFE Steel Corp., Magnesita Refractories, Nippon Steel and Sumitomo Metal Corp., Nucor Steel, Postech/Posco, SSAB, ANSYS/Fluent)
- National Science Foundation (Grant Nos. 11-30882 and 15-63553)
Introduction I: Continuous Casting of Steel

- Produces over 95% of steel in the world[^1], so small improvements have large impact
- Many defects (blister (gas bubble defect) and sliver (non-metallic inclusion defect), etc) related to multiphysics phenomena in mold
- Harsh environment makes experiments difficult; computer models allow process to be understood and improved

[^1]: Steel Statistical Yearbook 2014. (World Steel Association, Brussels, Belgium, 2014)
Introduction II: Complex Phenomena in CC

- Turbulent multiphase flow
- Heat transfer & solidification
- Steel/slag interface & surface tension
- Nucleation, collision, growth of steel crystals, bubbles & inclusions
- Transport & removal of particles
- Multiphase thermodynamics
- Mass transfer & segregation
- Deformation & stress
- Microstructure evolution
- Precipitate particles
- Embrittlement & cracks
- Multiple time & size scales
- MagnetoHydroDynamics (MHD)
Instability at liquid mold flux/molten steel interface, can *entrain liquid mold flux* into molten steel pool, and produce *capture into steel shell*, resulting in surface or internal defects.

- **Argon bubbles** make mold flow more complex and may be *entrapped with non-metallic inclusions by solidifying steel shell*, which can be defects.

- **Meniscus freezing** and **hook formation**, affected by fluid flow with superheat transportation, govern steel *solidification* and produce other defects.

1. Surface fluctuation
2. Meniscus freezing, hook formation
3. Vortex Formation
4. Shear layer instability
5. Upward flow
6. Argon bubble interactions/slag foaming
7. Slag crawling
8. Surface wave instability
9. Surface balding

< Slag entrainment mechanisms[^2-4] >


10μm

Alumina cluster

Alumina dendrite

Bubble with inclusions

Slag inclusions

< Bubbles and Inclusions entrapped by steel shell[^1] >
Computational Models on Blue Waters

- **Why computational model:** limitation of experiments on quantifying and understanding complex multiphysics phenomena related to defect formation in CC, and improving CC process

- **Why Blue Waters**
  - High-resolution (< 1mm length scale) prediction of multiphysics phenomena in huge domain (eg. 0.2 m X 1.9 m X 4.6 m)
  - Speed-up breakthrough (over ~3357X) on computing

- **Applied models:** ANSYS FLUENT (commercial CFD code) and CUFLOW (in-house multi-GPU based code)
  - Turbulence models: Large Eddy Simulation (LES), Reynolds-Averaged Navier-Stokes (RANS) model (standard k-ε)
  - Second-phase models: Volume Of Fluid (VOF), Lagrangian Discrete Phase Model (DPM)
  - MagnetoHydroDynamics (MHD) model
  - Heat transfer model
  - Particle capture model (based on local force balances on particles at solidification front)
CUFLOW Configuration

- Two versions of CUFLOW, CPU and GPU versions
  - CPU version, run on multi-CPU PC: data communication through MPI
  - GPU version, run on multi-GPU PC and multi-CPU&GPU pair supercomputer (e.g., Blue Waters)

<table>
<thead>
<tr>
<th>PC - 4GPU Workstation</th>
<th>Blue Waters Supercomputer</th>
</tr>
</thead>
<tbody>
<tr>
<td># of Nodes</td>
<td>1</td>
</tr>
<tr>
<td>Node CPU</td>
<td>Xeon E5-2650v2 Ivy Bridge, 2.60 GHz, 8 cores</td>
</tr>
<tr>
<td>GPU/Node</td>
<td>4 × Nvidia Tesla C2075, 4 × 5 GB, 575 MHz</td>
</tr>
</tbody>
</table>

<Configuration of 4 GPU workstation>

<Configuration of BW nodes showing 2 nodes>
The in-house multi-GPU code CUFLOW has been developed and tested on Blue Waters XK node, which has Nvidia K20x GPU as co-processors, and good speed up has been obtained.

Less than 2 days are required for a 30s-LES simulation of flow in a caster domain with 14.1 million cells (based on 100 time step test run with average time step size $\Delta t=0.0005s$)

<Estimated time for 30s LES simulation of caster with 14.1 million cells$^5$>
ANSYS FLUENT on Blue Waters

- Lab Computer (LC) calculation: Dell T7600 (Intel ® Xeon ® CPU E5-2603 @ 1.80GHz, RAM 40.0 GB, using 6 cores

- Speed-up ratio = Computing time for 1 iteration on LC / Computing time for 1 iteration on BW

Speed-up test was performed for LES coupled with VOF in domain of ~22 million hexahedral cells

- With 1120 cores (70XE nodes), the simulation on BW runs ~ 3357 times faster than on our LC: one iteration on BW using 1120 cores (70 XE nodes) requires ~1.7 seconds of wall clock time. one the other hand, on the LC, the same simulation requires ~ 5808 seconds of wall-clock time for 1 iteration.

- For this case, Fluent-14.5 HPC on BW shows speed-up breakthrough with 1120 cores (70 XE nodes); getting much more efficiency for much finer mesh domain
Research Scope with Blue Waters

- **Objectives:**
  - Get insights into *multiphysics phenomena* and *defect formation*
  - Suggest *optimum CC-process conditions* to improve final steel-product quality

- **Topics:**
  - Effect of *nozzle port angle* on transient mold flow and *liquid slag/molten steel interfacial motion*\(^1,12\): LES-VOF model
  - Effect of *SEN depth* on mold flow\(^1,5,6\): LES
  - Argon bubble transport and capture in mold with *Electro-Magnetic Braking (EMBr)*\(^1,3-9,11\): LES-DPM-Particle capture model
  - Transient mold flow and superheat transfer on solidifying steel shell\(^1,2\): LES-VOF-Heat transfer model
Case 1. $+15^\circ$ (up) angle

Case 2. $-30^\circ$ (down) angle

Full domain: ~4.1 million hexahedral cells
Effect of Nozzle Port Angle: Mold Flow Pattern and Slag Entrainment

- LES coupled with VOF model for molten steel-liquid mold flux flow

**Case 1. +15° (up) angle**
- P3 (10, -600)
- P4 (10, 600)

**Case 2. -30° (down) angle**
- Point coordinate (x (m), y (m))
Effect of Nozzle Port Angle: Surface Velocity Instability (Model Validation)

Case 1. +15° (up) angle

Case 2. -30° (down) angle
Effect of Nozzle Port Angle: Surface Level Instability and Defect Formation

More variations at liquid mold flux/molten steel interface in mold with upward angled nozzle port

Slag defects on final plates

Case 1. +15° (up) angle

Case 2. -30° (down) angle
Effect of SEN Depth on Mold Flow Patterns

- Increasing submergence depth decreases top-surface velocity in mold: slag entrainment caused by instability at slag/molten steel interface, could be reduced
Double Ruler ElectroMagnetic Braking (EMBr)

Meniscus flow speed controlled by the upper magnetic field
Penetration depth controlled by the lower magnetic field

Magnitude of external magnetic field (Tesla)
- 1.7E-01
- 1.5E-01
- 1.4E-01
- 1.2E-01
- 1.0E-01
- 8.5E-02
- 6.8E-02
- 5.1E-02
- 3.4E-02
- 1.7E-02
- 0.0E+00

Distance from mold top (m)

Distance from mold center (m)

Weaker

0 0.2 0.4 0.6 0.8 1.0 1.2 1.4
0 -0.2 -0.4 -0.6 -0.8

Both upper and lower ruler: DC300A

Electromagnetic force on transient flow in CC
Effect of Double Ruler EMBr on Bubble Transport and Capture in Mold

- With EMBr, less bubbles reaching NF
- Less bubbles going deep into mold
- EMBr reduces argon bubble capture into steel shell; less surface and internal defects

* K. Jin: CCC 2016 annual report
- **Temperature distribution** in mold shows transient behaviors according to **transient flow patterns**.
- Due to **spread jet flow pattern** in mold with $+15^\circ$ (up) angled nozzle port, superheat flux distribution is bigger on WF than NF shells.
- **Meniscus freezing** and **hook formation** on corner regions.

<Hook defect and bubble capture>

<Superheat flux on steel shell>
Summary

- Blue Waters supercomputing has been applied to quantify complex multiphysics phenomena related to defect formation in Continuous Casting (CC) in order to improve the process.
  - Turbulent multiphase flow: liquid mold flux/molten steel interface, molten steel-argon bubble flow
  - Particle transport and capture: argon bubble motion and capture into steel shell
  - MagnetoHydroDynamics (MHD): EMBr effect on flow pattern and argon bubble behaviors
  - Evaluation of nozzle port angle, nozzle submergence depth, and EMBr strength

- Blue Waters resources (ANSYS Fluent HPC on BW XE nodes and In-house multi-GPU code, CUFLOW on BW XK nodes) show modeling capability breakthrough (over 3000x faster) for high-resolution (less than 1mm length scale) and huge-domain simulation for CC.
Appendix I: Liquid Mold Flux/Molten Steel Interface Model: VOF

- **Volume fraction of each phase:**
  \[
  \frac{\partial \alpha_{\text{slag}}}{\partial t} + \nabla \cdot \left( \alpha_{\text{slag}} \cdot \mathbf{u}_{\text{slag}} \right) = 0
  \]
  \[
  \alpha_{\text{steel}} = 1 - \alpha_{\text{slag}}
  \]
  slag volume fraction
  steel volume fraction

- **Continuity:**
  \[
  \frac{\partial \rho_{\text{mix}}}{\partial t} + \nabla \cdot \left( \rho_{\text{mix}} \mathbf{u} \right) = \mathbf{S}_{\text{shell,mass}}
  \]
  \[
  \rho_{\text{mix}} = \alpha_{\text{steel}} \rho_{\text{steel}} + \alpha_{\text{slag}} \rho_{\text{slag}}
  \]

- **Momentum conservation:**
  \[
  \rho_{\text{mix}} \frac{\partial \mathbf{u}}{\partial t} + \rho_{\text{mix}} \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \left[ \mu_{\text{mix}} \left( \nabla \mathbf{u} + \nabla^T \mathbf{u} \right) \right] + \rho_{\text{mix}} \mathbf{g} + \mathbf{F}_{\text{interface}} + \mathbf{S}_{\text{shell,mom}}
  \]

  \[
  \mathbf{F}_{\text{interface}} = \sigma_{\text{slag-steel}} \frac{\rho_{\text{mix}} \kappa_{\text{slag}} \nabla \alpha_{\text{slag}}}{1 \left( \rho_{\text{steel}} + \rho_{\text{slag}} \right)}
  \]
  \[
  \kappa_{\text{slag}} = \nabla \cdot \mathbf{n} \quad \mathbf{n} = \nabla \alpha_{\text{slag}}
  \]

**User Defined Function (UDF):**

- **Mass sink term to account for solidification of molten steel**: 
  \[
  \mathbf{S}_{\text{shell,mass}} = -\frac{\rho_{\text{steel}} \mathbf{u}_{\text{casting}}}{V} \mathbf{A}
  \]

- **Momentum sink term in each component direction to consider solidification of molten steel**: 
  \[
  \mathbf{S}_{\text{shell,mom,i}} = -\frac{\rho_{\text{steel}} \mathbf{u}_{\text{casting}}}{V} \mathbf{A} \mathbf{u}_i
  \]

Appendix II: Bubble Transport Model

- Two-way coupled Lagrangian particle tracking model

F_D: Drag force
F_B: Buoyancy/gravity force
F_L: Lift force
F_A: Added mass force
F_P: Pressure gradient force

\[ m_{Ar} \frac{du_{Ar}}{dt} = F_D + F_B + F_L + F_A + F_P \]

Drag coefficient:

\[ C_D = \frac{16}{Re_{Ar}} \quad (Re_{Ar} < 0.49) \]
\[ = \frac{20.68}{Re_{Ar}^{0.643}} \quad (0.49 < Re_{Ar} < 100) \]
\[ = \frac{6.3}{Re_{Ar}^{0.385}} \quad (100 < Re_{Ar}) \]
\[ = \frac{We}{3} \quad (2065.1 < We^{2.6}) \]
\[ = \frac{8}{3} \quad (8 < We) \]

\[ Re_{Ar} = \frac{\rho d_{Ar} |u - u_{Ar}|}{\mu} \]
\[ We = \frac{\rho d_{Ar} (u - u_{Ar})^2}{\sigma_{steel-argon}} \]

\[ S_{Ar} = -V^{-1}_{cell} \sum_{i=1}^{n} (F_D + F_B + F_L + F_A + F_P) \]

Appendix III: Advanced Particle-Capture Model for Bubble Entrapment

Advanced particle capture criterion\cite{1,2} when particle touches steel shell
- If particle diameter is smaller than primary dendrite arm spacing -> capture
- Else, compute 3 other forces: lubrication force, Van der Waals force, and interfacial concentration gradient force, and do force balance on particle to decide its capture

Particle touching 3 dendrite tips \cite{1}

\begin{itemize}
  \item Particle diameter smaller than primary dendrite arm spacing
  \item Compute 3 other forces: lubrication force, Van der Waals force, and interfacial concentration gradient force
  \item Do force balance on particle to decide its capture
\end{itemize}

\begin{enumerate}
  \item Q. Yuan: Ph.D. Thesis, UIUC, 2004
\end{enumerate}
Appendix IV: Nail Dipping Test

Dipping test details

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Total tests (for each IR and OR region)</td>
<td>5</td>
</tr>
<tr>
<td>interval of each test</td>
<td>1 minute</td>
</tr>
<tr>
<td>Dipping time</td>
<td>3 sec</td>
</tr>
</tbody>
</table>

Empirical equation for surface velocity magnitude[^]:

Surface velocity magnitude: \( u_s (m/s) = 0.624 \cdot (\varphi_{lump} (mm))^{-0.696} \cdot (h_{lump} (mm))^{0.567} \)

[^]: Liu et al., Proc. of TMS 2011, TMS, Warrendale, PA, USA