6th NCSA Blue Waters Symposium,
Sunriver, Oregon, June 04-07, 2018

Multiphase Turbulent Flow Modeling of Steel Continuous Casting with Electro-Magnetic Systems to Minimize Surface Defects

Illinois General Project:
Multiphysics Modeling of Steel Continuous Casting

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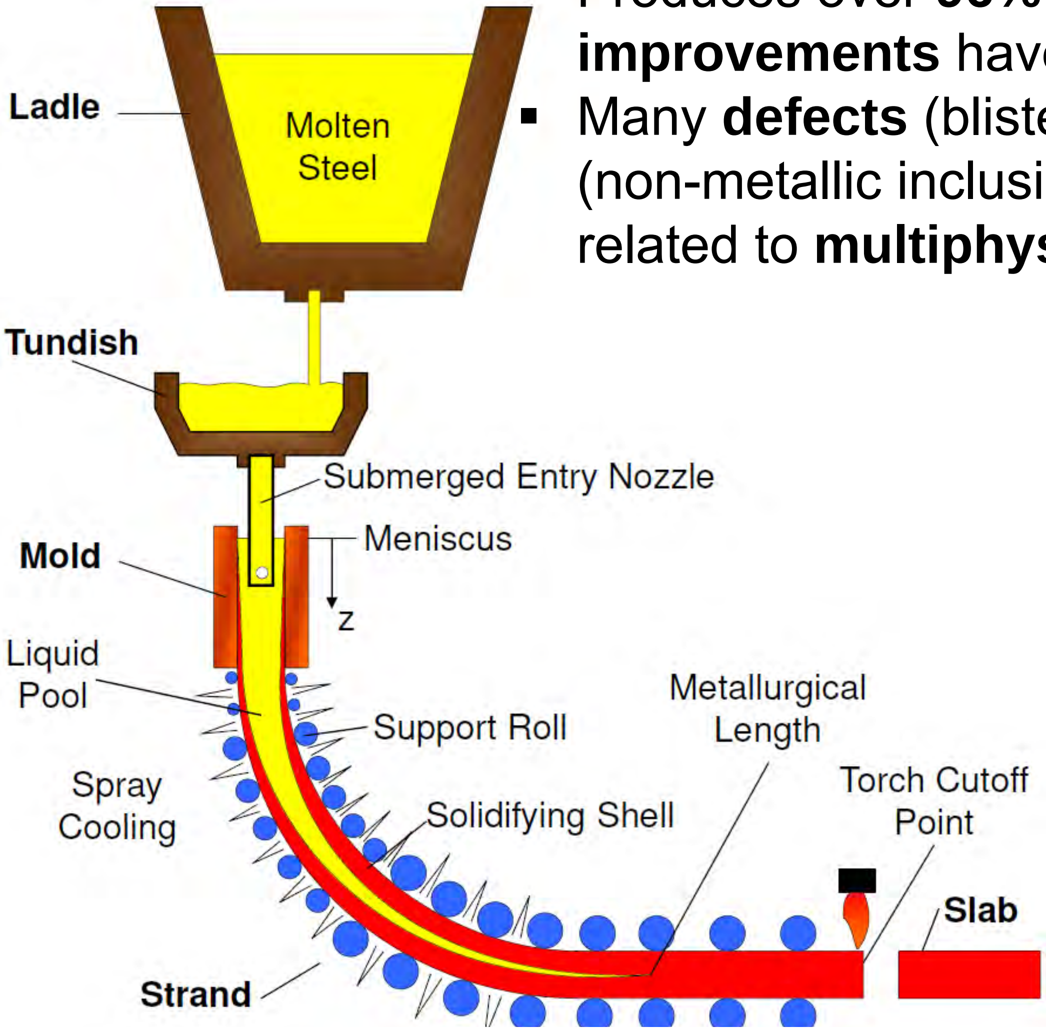
Recent Publications Acknowledging Blue Waters (2017-2018)

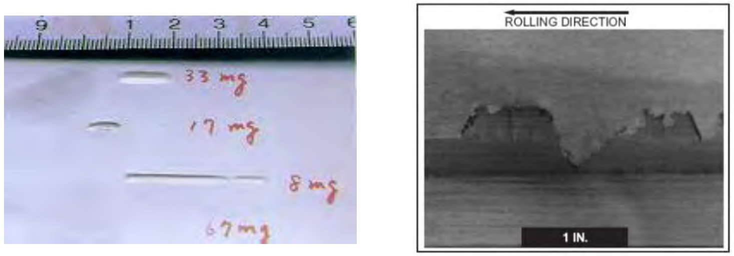
1) Thomas, B. G., S-M. Cho, S. P. Vanka, H. Yang, M. Zappulla, A. Taha, and S. Koric: “Transient Multiphase Flow Phenomena and Defect Formation in Steel Continuous Casting”, Blue Waters Annual Report book, 2017, ed. B. Jewett, University of Illinois, Urbana, IL, 2017, pp. 160-161.
2) Jin, K., S. P. Vanka, and B.G. Thomas: “Large Eddy Simulations of Argon Bubble Transport and Capture in Mold Region of a Continuous Steel Caster”, Proc. TFEC2017, Las Vegas, NV, 2017
3) Jin, K., S. P. Vanka, and B.G. Thomas: “Large Eddy Simulations of the Effects of EMBr and SEN Submergence Depth on Turbulent Flow in the Mold Region of a Steel Caster”, *Metallurgical and Materials Transaction B*, vol. 48B (2017), pp. 162-178.
4) Yang, H., S. P. Vanka, and B. G. Thomas, Hybrid Eulerian Eulerian Discrete Phase Model of Turbulent Bubbly Flow, *Proceeding of the ASME IMECE 2017*, 2017.
5) Zappulla, M. L. S. and B. G. Thomas, Thermal-Mechanical Model of Depression Formation in Steel Continuous Casting, *Proceeding of TMS 2017*, 2017.
6) Cho, S-M., B. G. Thomas, S-H. Kim, S-W. Han, and Y-J. Kim, Effect of EMLS Moving Magnetic Field on Transient Slab-Mold Flow, *CCC Annual Report*, 2017.
7) Kim, H-S., S-M. Cho, S-H. Kim, and B. G. Thomas, Mold Flow and Shell Growth in Large-Section Bloom Casting using CON1D, *CCC Annual Report*, 2017.
8) Yang, H., S. P. Vanka, and B. G. Thomas, Hybrid Model of Multiphase Flow Including Gas Pockets, Gas Bubbles, Breakup and Coalescence, *CCC Annual Report*, 2017.
9) Jin, K., S. P. Vanka, and B. G. Thomas, Large Eddy Simulations of Electromagnetic Braking Effects on Argon Bubble Transport and Capture in a Steel Continuous Casting Mold, *Metallurgical and Materials Transaction B*, vol. 49B (2018), pp. 1360-1377.
10) Yang, H., S. P. Vanka, and B. G. Thomas, A Hybrid Eulerian-Eulerian Discrete-Phase Model of Turbulent Bubbly Flow, *Journal of Fluids Engineering*, 2018, DOI: 10.1115/1.4039793.
11) Yang, H., S. P. Vanka, and B. G. Thomas, Modeling of Argon Gas Behavior in Continuous Casting of Steel, *Proceeding of TMS 2018*, 2018.
12) Zappulla, M. L. S. and B. G. Thomas, Surface Defect Formation in Steel Continuous Casting, *Proceeding of THERMEC’2018*, 2018, Accepted.
13) Cho, S-M. and B G. Thomas, “Effect of Nozzle Port Angle on Transient Flow Variations during Continuous Steel-Slab Caster”, *Metallurgical and Materials Transaction B,* in preparation
14) CCC Annual Reports, August, 2018, pending

Introduction I: Continuous Casting (CC) of Steel & Defects

- Produces over **96% of steel** in the world*), so **small improvements** have **large impact on steel industries**
- Many **defects** (blister (gas bubble defect) and sliver (non-metallic inclusion defect), depression, crack) related to **multiphysics phenomena** in mold



<Schematic of steel continuous casting>



Blister (coil)

Sliver (coil)

Depression (slab)

longitudinal crack (slab)

<CC Defects >

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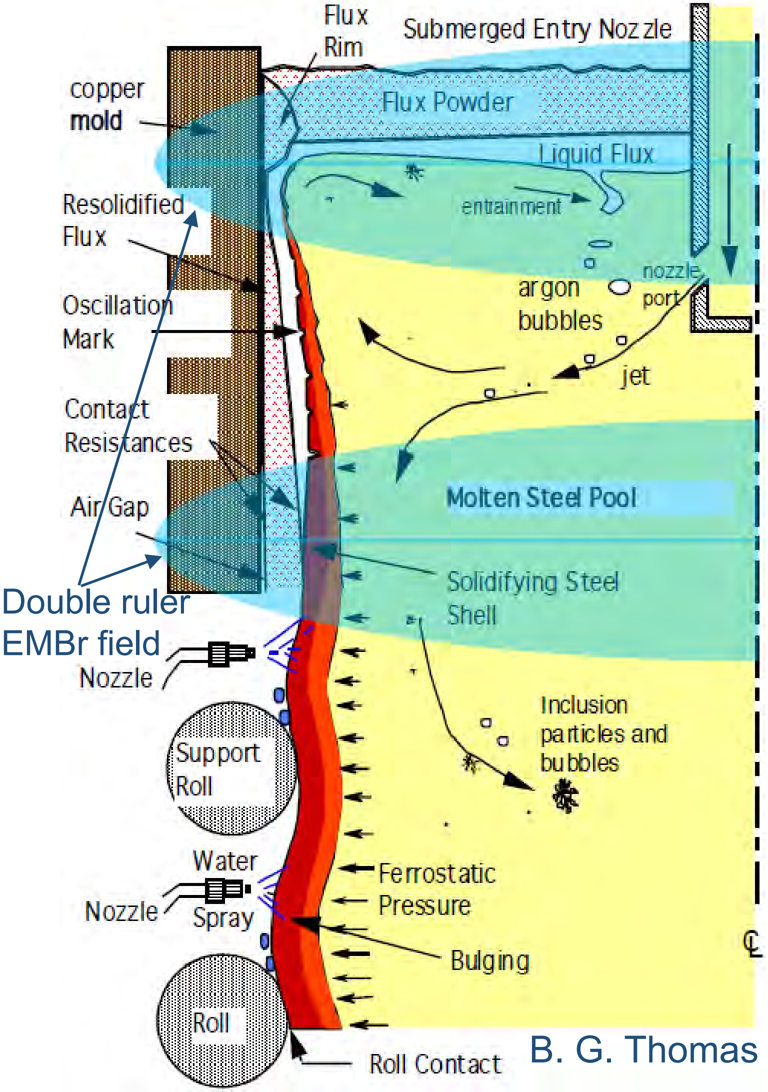
*) World Steel Association, Steel Statistical Yearbook 2017

Introduction II: Complex Multiphysics Phenomena in CC

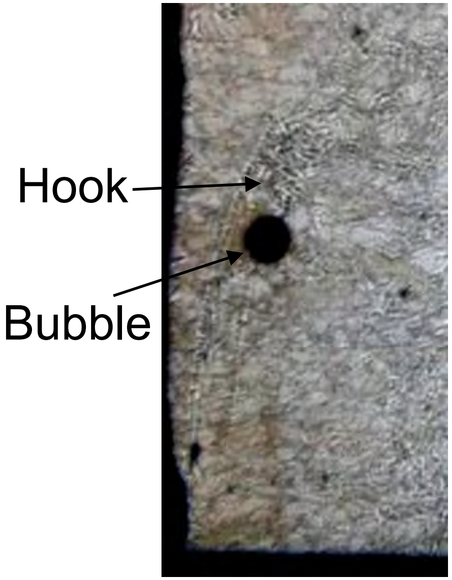


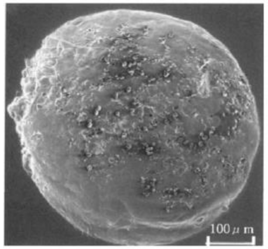
B. G. Thomas

<Schematic of phenomena in mold>

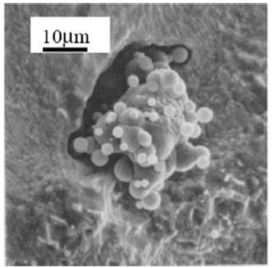
- Turbulent multiphase flow
- Heat transfer & solidification
- Steel/slag interface & surface tension
- Nucleation, collision, growth of steel crystals, bubbles & inclusions
- Transport & removal of particles
- Multiphase thermodynamics
- Mass transfer & segregation
- Deformation & stress
- Microstructure evolution
- Precipitate particles
- Embrittlement & cracks
- MagnetoHydroDynamics (MHD)

Introduction III: Defect Formation Mechanisms in CC



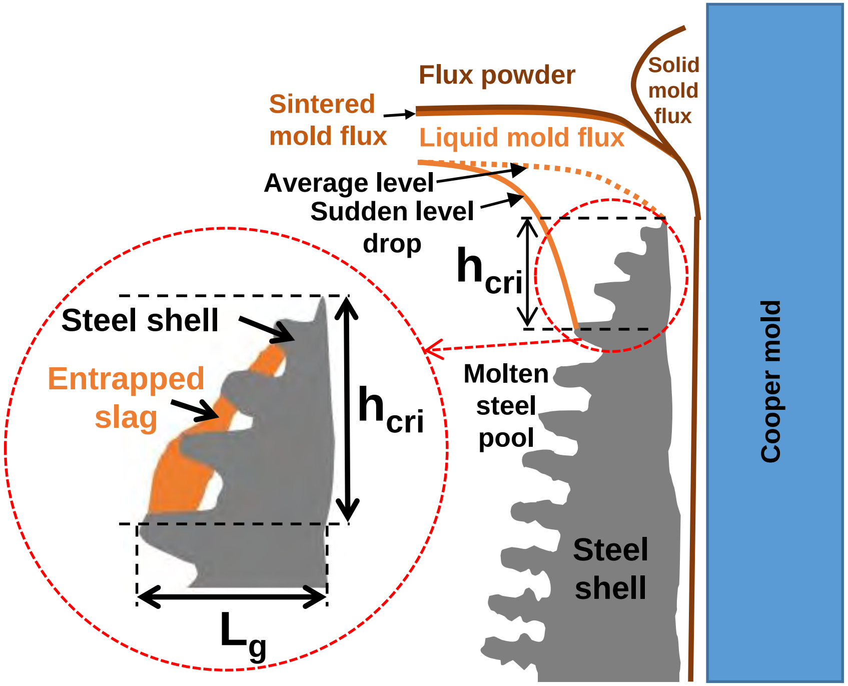


Bubble with inclusions



Alumina cluster

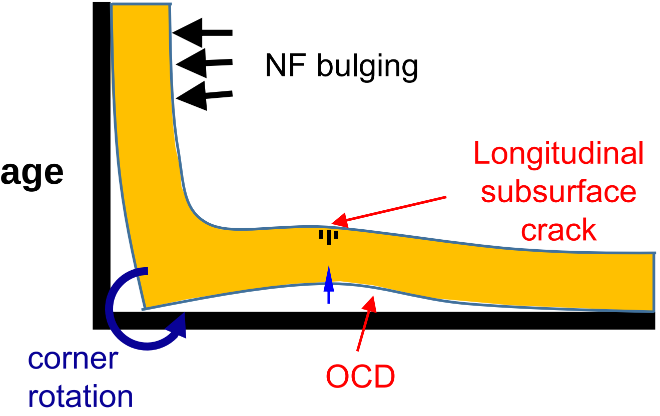
<Bubble and inclusion capture into steel shell>



Slag inclusions

<Slag entrapment into steel shell by surface level fluctuations>

Mold taper < shell shrinkage



<Depression and longitudinal subsurface crack formation*)>

*) B. G. Thomas, et al., ISS Transactions, Vol. 23, No. 4, 1996, pp. 57-70

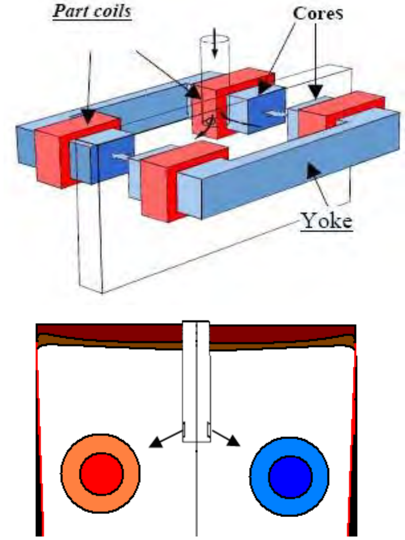
Introduction IV: Electro-Magnetic Systems

- **Magnetic fields greatly alter steel flow in the mold**
  - Control surface turbulence, deep inclusion penetration, and internal microstructure

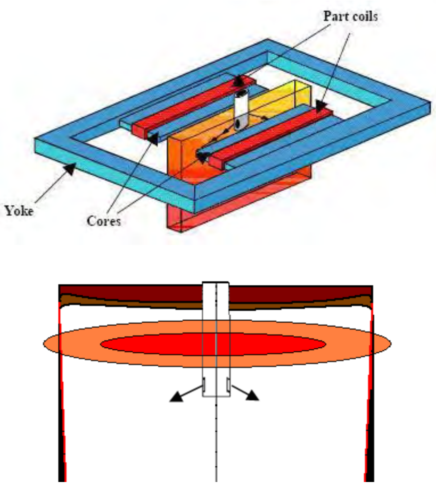
Electro-Magnetic Stirrer (EMS (AC)):

- Electro-Magnetic Level Stabilizer (EMLS): decelerate
- Electro-Magnetic Accelerator (EMLA): accelerate
- Electro-Magnetic Rotating Stirrer (EMRS): rotate

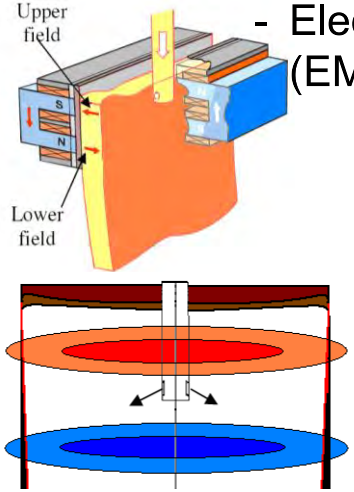
Electro-Magnetic Braking (EMBr (DC)): braking: slow down flow



Local EMBr

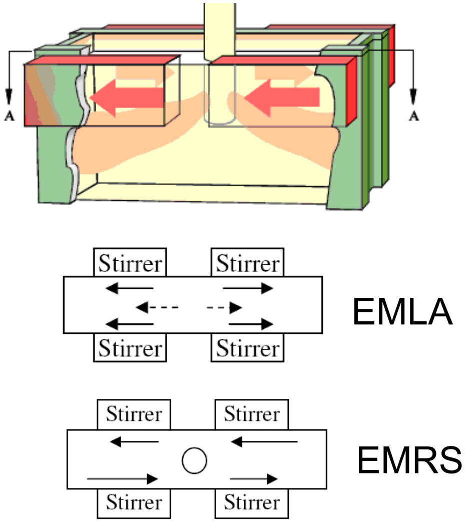


Single-ruler EMBr



“FC-Mold”, ABB

Double-ruler EMBr



Moving field

Computational Models on Blue Waters

- **Why computational model**: harsh environment with numerous process conditions make experiments difficult to quantify and understand complex multiphysics phenomena related to defect formation in CC and improve the process.

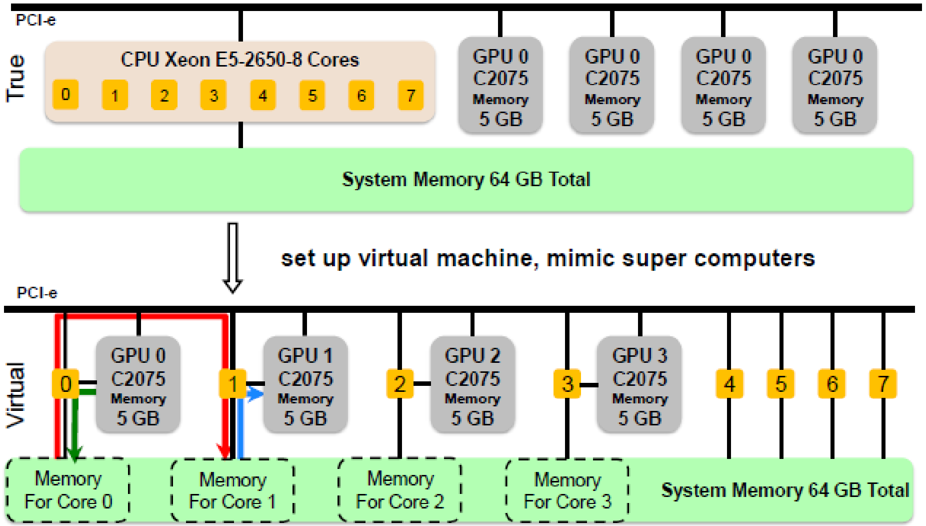
- **Why Blue Waters**
  - High-resolution (< 50μm length-scale and 5e-04s time-scale) prediction of multiphysics phenomena in huge domain (> $2m^3$).
  - Speed-up breakthrough (over ~3000×) on Blue Waters computing.

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

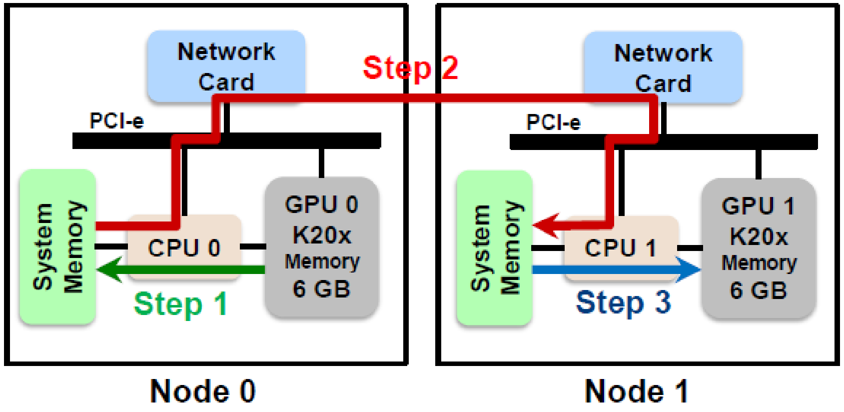
CUFLOW Configuration

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

	PC - 4GPU Workstation	Blue Waters Supercomputer
#of Nodes	1	4224
Node CPU	Xeon E5-2650v2 Ivy Bridge, 2.60 GHz, 8 cores	AMD 6276, 2.3 GHz, 16 cores
GPU/Node	4 × Nvidia Tesla C2075, 4 × **5 GB**, 575 MHz	1 × Nvidia Tesla K20x, 1 × **6 GB**, 732 MHz



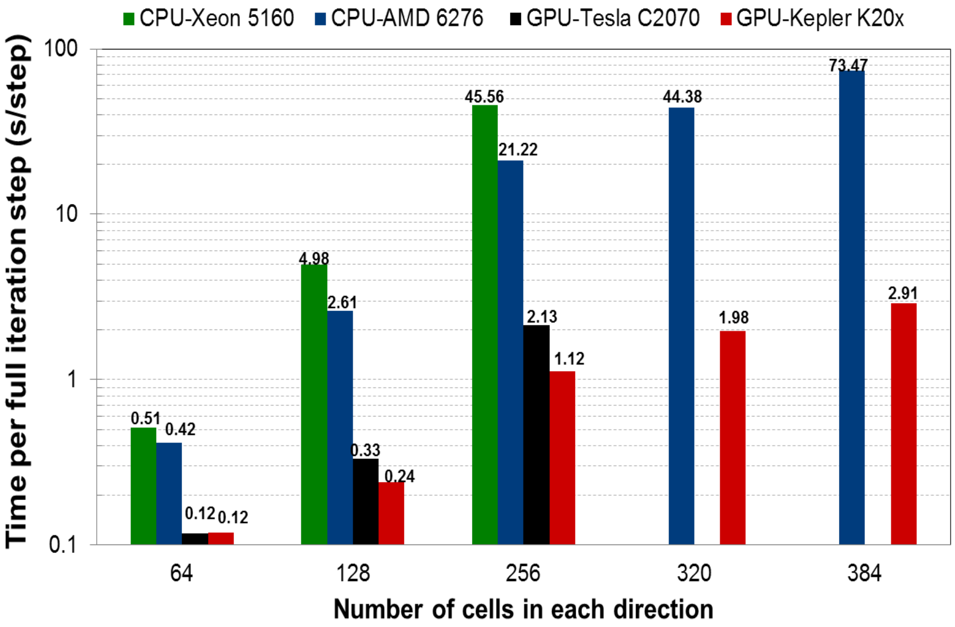
<Configuration of 4 GPU workstation>

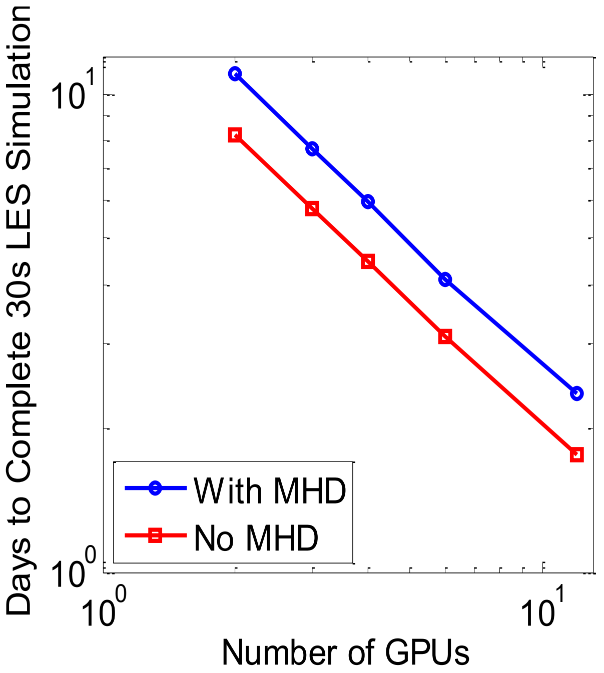


Three Steps: cudaMemcpy(…), MPI_Send(…) and MPI_Recv(…), cudaMemcpy(…)

<Configuration of BW nodes showing 2 nodes>

CUFLOW on Blue Waters XK Node





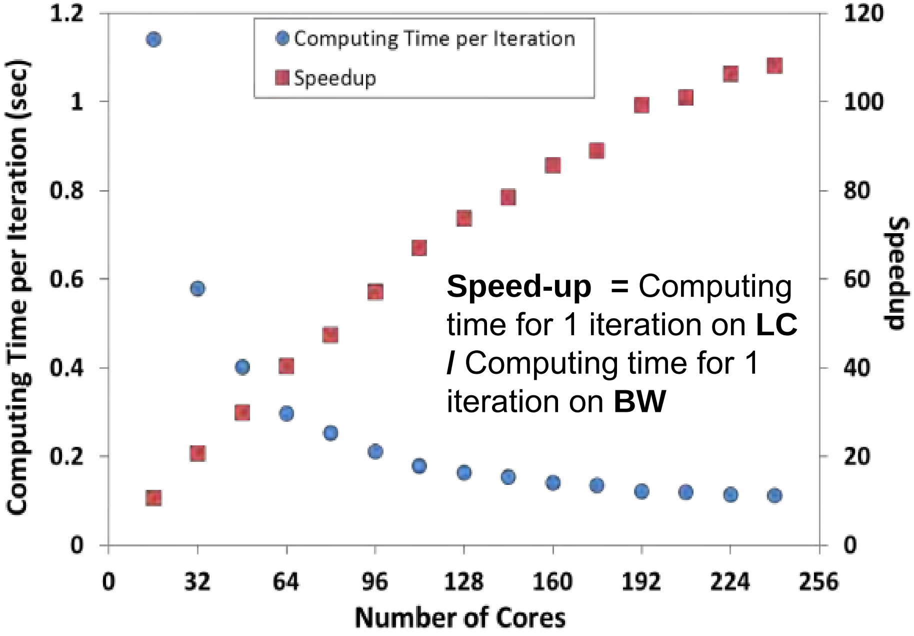
<PPE solver performance on Blue Waters CPU and GPU>

<Estimated time for 30s LES simulation of caster with 14.1 million cells>

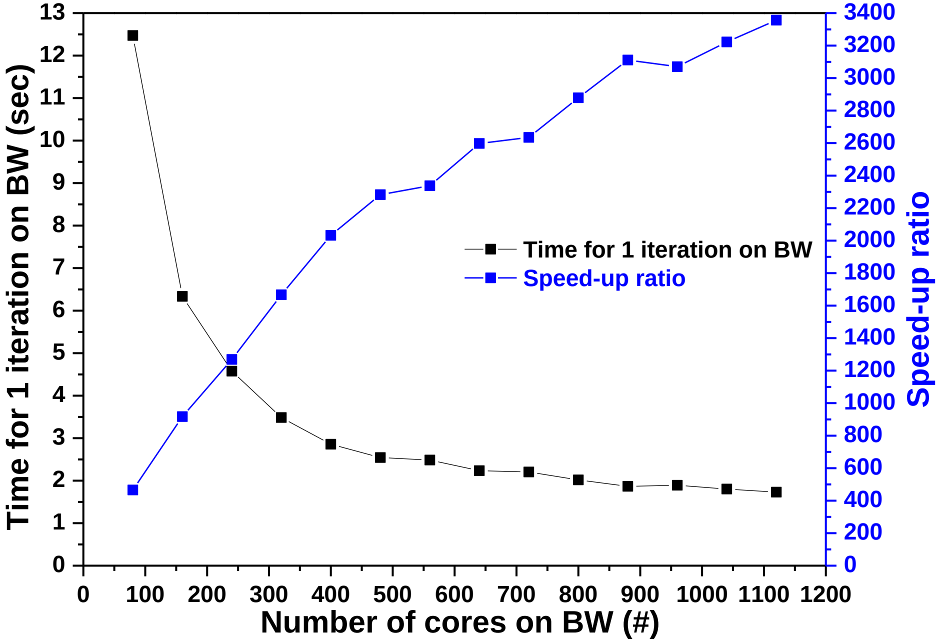
- Both CPU and GPU versions of in-house code CUFLOW were developed and tested on Blue Waters XK node.
- The **multi-GPU based CUFLOW on Blue Waters XK node**, which has K20x GPU as co-processors, shows **good speed up**.

  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 Δt=0.0005s)

ANSYS FLUENT HPC on Blue Waters XE Node



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



- Lab Computer (LC) calculation: Dell T7600 (Intel ® Xeon ® X5650 @ 2.67GHz, RAM 48.0 GB, using 6 cores
- Lab Computer (LC) calculation: Dell T7600 (Intel ® Xeon ® CPU E5-2603 @ 1.80GHz, RAM 40.0 GB, using 6 cores

<RANS coupled with Eulerian model in domain of ~0.7 million hexahedral cells>

<LES coupled with VOF in domain of ~22 million hexahedral cells>

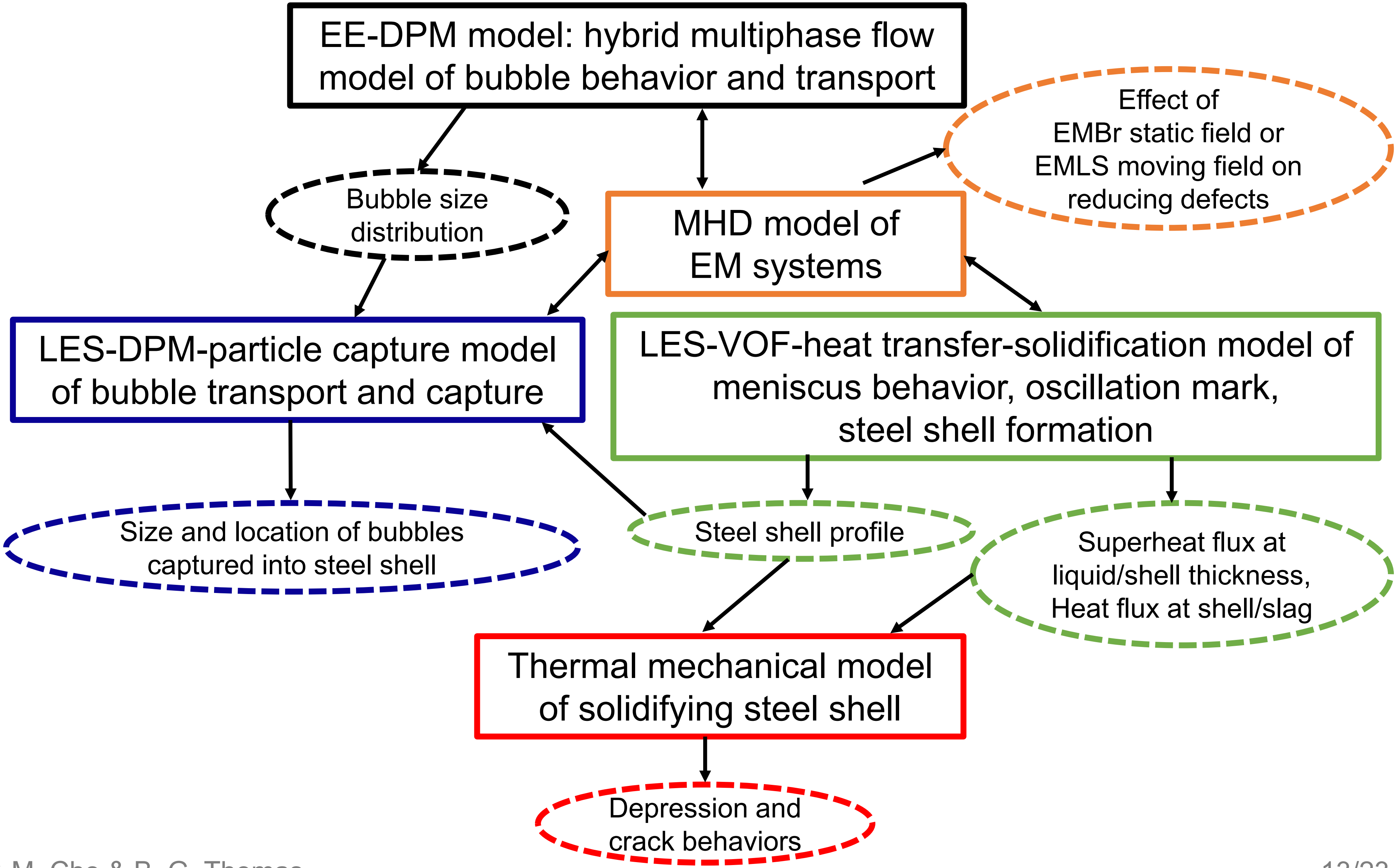
- LES multiphase simulation on BW 70 XE nodes (1120 cores) runs ~ **3357 times faster** than on LC: one iteration requires ~1.7 s of wall clock time. one the other hand, on LC, the same simulation requires ~ 5808 s of wall-clock time.
- Fluent HPC on BW XE node shows speed-up breakthrough; getting much more efficiency for much finer mesh domain with smaller time-scale.

Research Scope with Blue Waters

- **Objectives:**
  - Develop comprehensive, sophisticated, computationally-intensive multiphysics models of steel CC.
  - Get insights into defect formation mechanisms: bubble defect, slag inclusion defect, hook, crack, depression, etc.
  - Suggest optimal process conditions for better product quality: bubble injection, EMS strength, mold oscillating method, mold taper.

- **Topics:**
  - Bubble behavior and size distribution: EE-DPM hybrid multiphase model
  - Argon bubble transport and capture in mold with Electro-Magnetic Braking (EMBr): LES-DPM-MHD-Particle capture model
  - Effect of EMLS Moving Magnetic Field on transient mold flow and bubble transport: LES-DPM-MHD model
  - Steel Solidification, Erosion, Oscillation Mark, Macrosegregation in Mold: LES-VOF-heat transfer-solidification model

Flow Chart of Multiphysics Models



EE-DPM model: hybrid multiphase flow model of bubble behavior and transport

Bubble size distribution

MHD model of EM systems

Effect of EMBr static field or EMLS moving field on reducing defects

LES-DPM-particle capture model of bubble transport and capture

LES-VOF-heat transfer-solidification model of meniscus behavior, oscillation mark, steel shell formation

Size and location of bubbles captured into steel shell

Steel shell profile

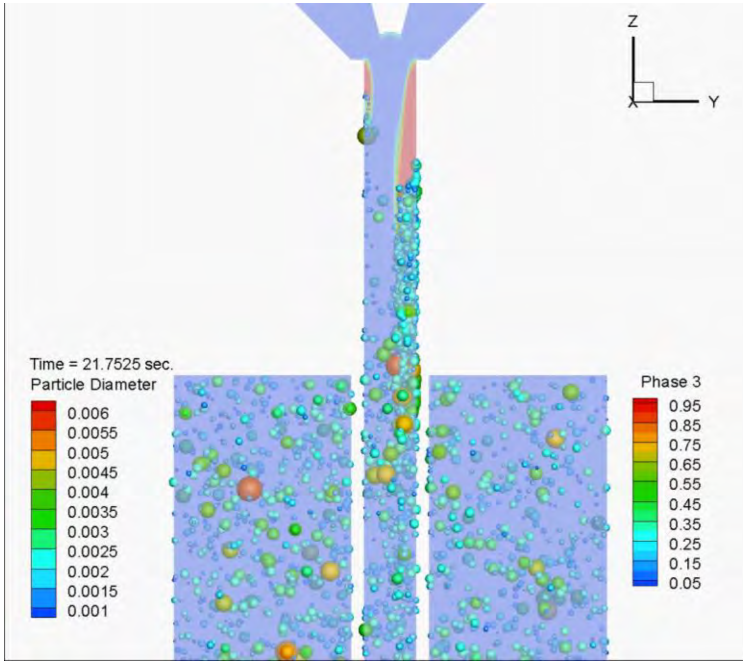
Superheat flux at liquid/shell thickness, Heat flux at shell/slag

Thermal mechanical model of solidifying steel shell

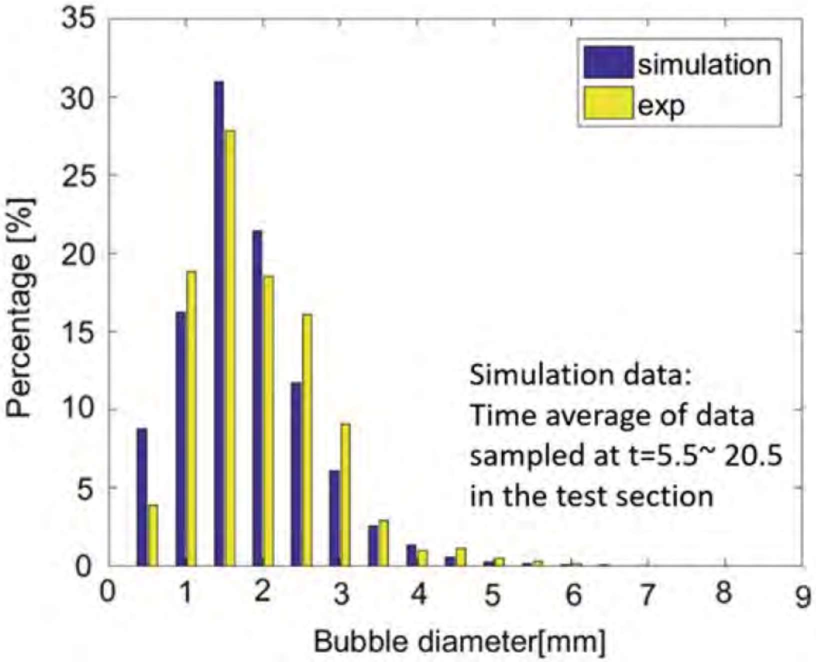
Depression and crack behaviors

Bubble Behavior and Size Distribution

- **EE-DPM Hybrid multiphase flow model**: Eulerian-Eulerian (EE) coupled simultaneously with Discrete Phase Model (DPM)
- Bubble behavior including gas pocket formation, shearing off, volumetric expansion, breakup, coalescence, transport and bubble size distribution.



<Predicted bubble behavior and size distribution in nozzle and mold>



<Comparison of predicted bubble size distribution with measurements>

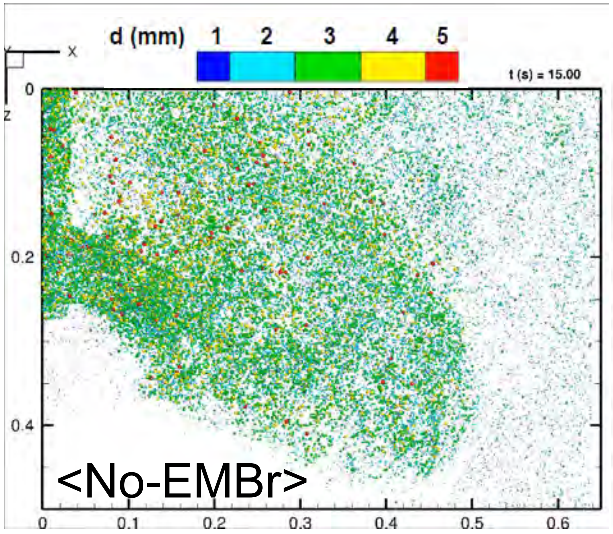
- The hybrid model was validated via measurements and ready to be applied for real caster case (molten steel-argon gas system)

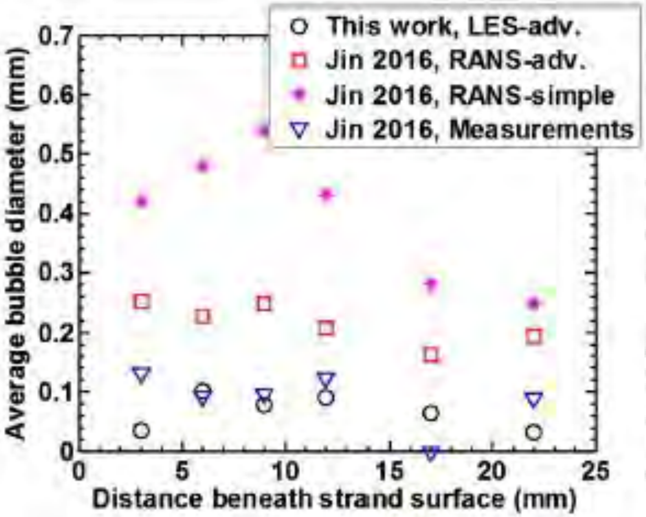
*)Yang, H. et. al.: *Proceeding of TMS 2018*, 2018.

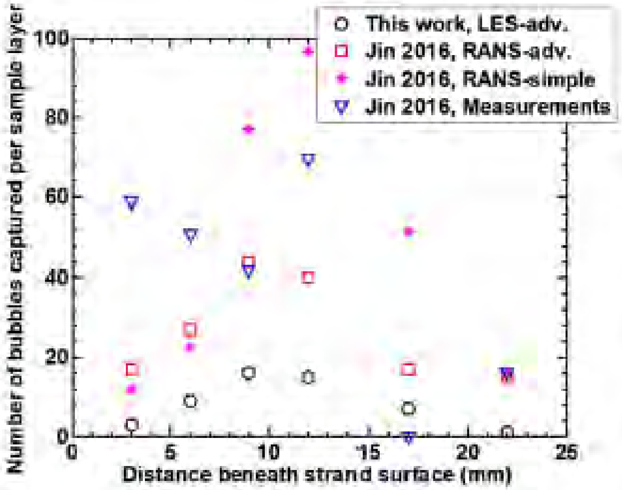
Bubble Transport and Capture in Mold with and without EMBr

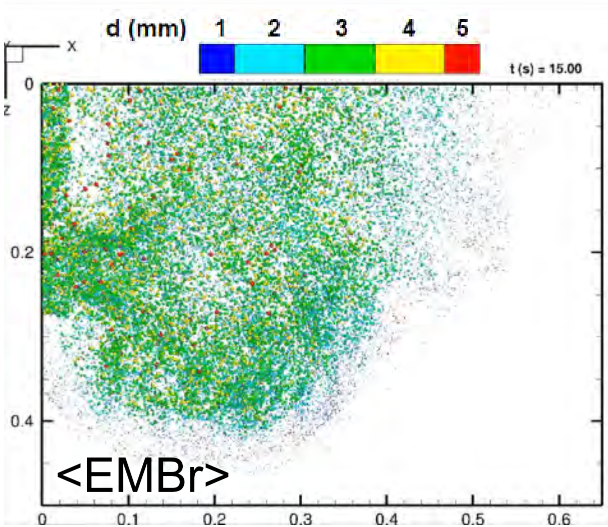
- **LES coupled with DPM, particle capture model, and MHD model**

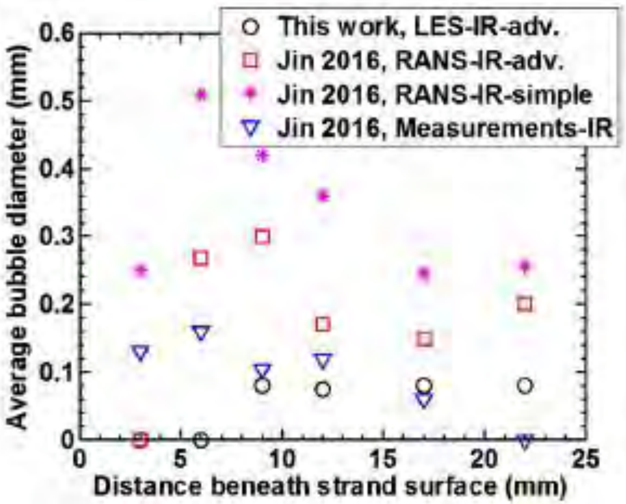
*) Jin, K. et. al.: *MMTB*, vol. 49B (2018), pp. 1360-1377.

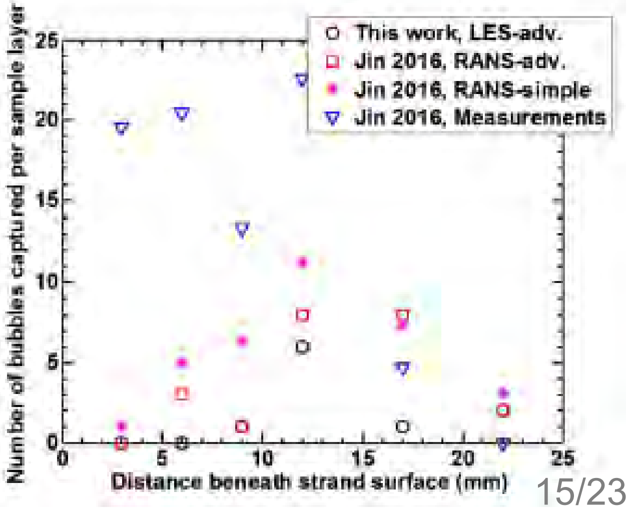








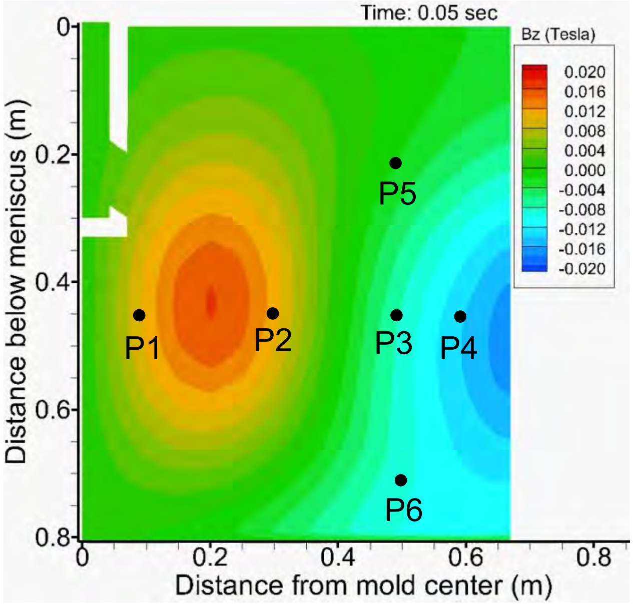




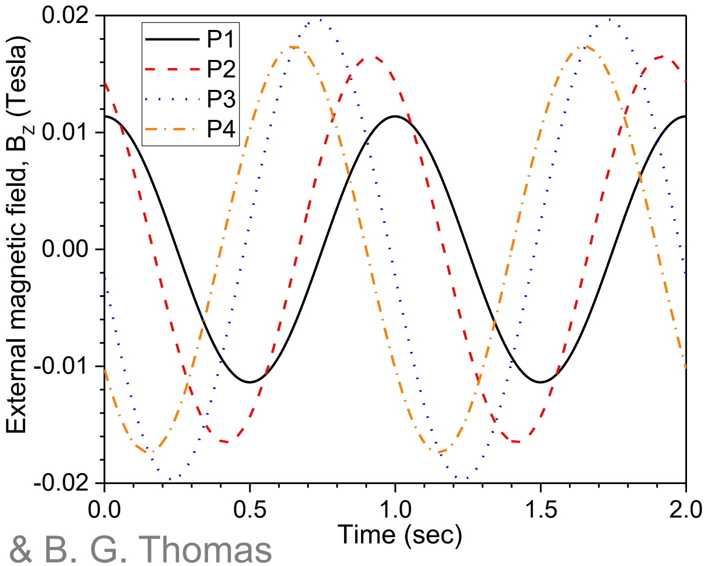
EMLS Moving Magnetic Field

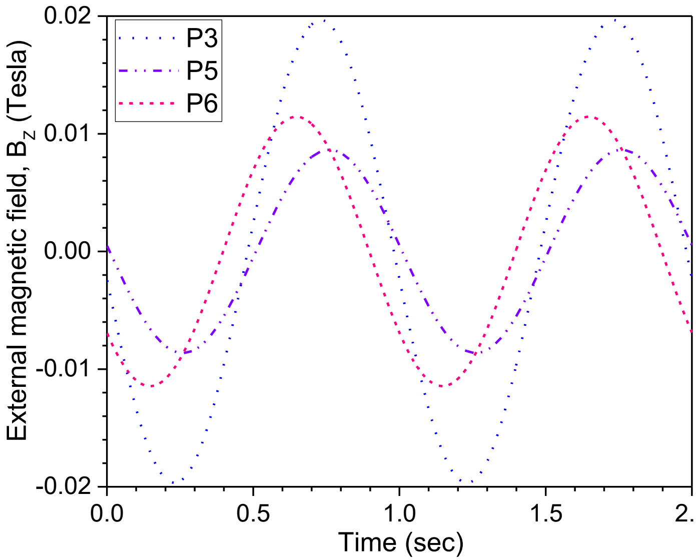
B_z

Point coordinates	(x (mm), y(mm))
P1	(100, 450)
P2	(300, 450)
P3	(500, 450)
P4	(600, 450)
P5	(500, 200)
P6	(500, 700)



- Frequency of local EMLS field: 1Hz.
- EMLS field has strong phase shift at 2Hz, which creates moving field across mold width.
- In width direction: EMLS field amplitude gets smaller from NF towards SEN.
- In casting direction: EMLS field drastically changes amplitude

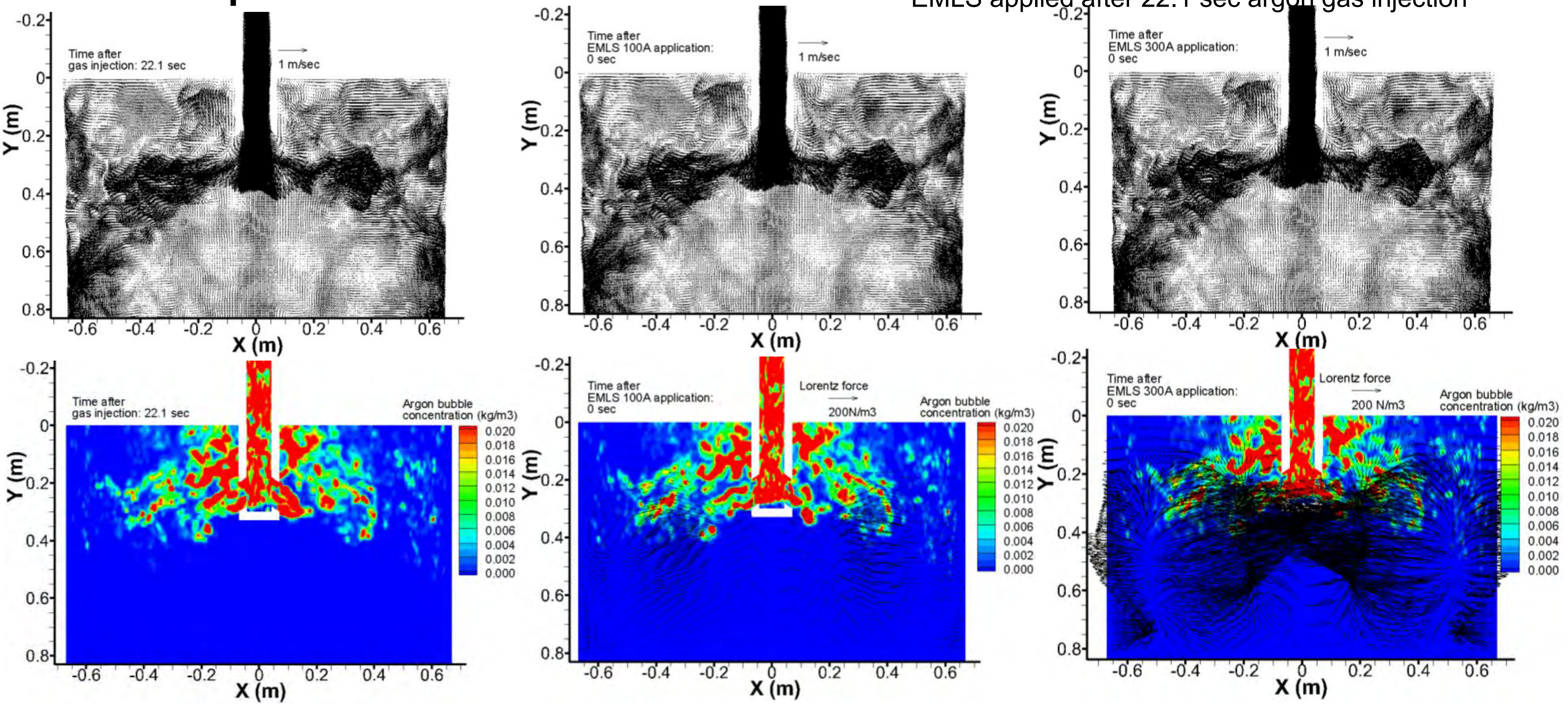




Effect of EMLS on Steel-Argon Flow and Argon Bubble Distribution

- **LES coupled with DPM and MHD model**

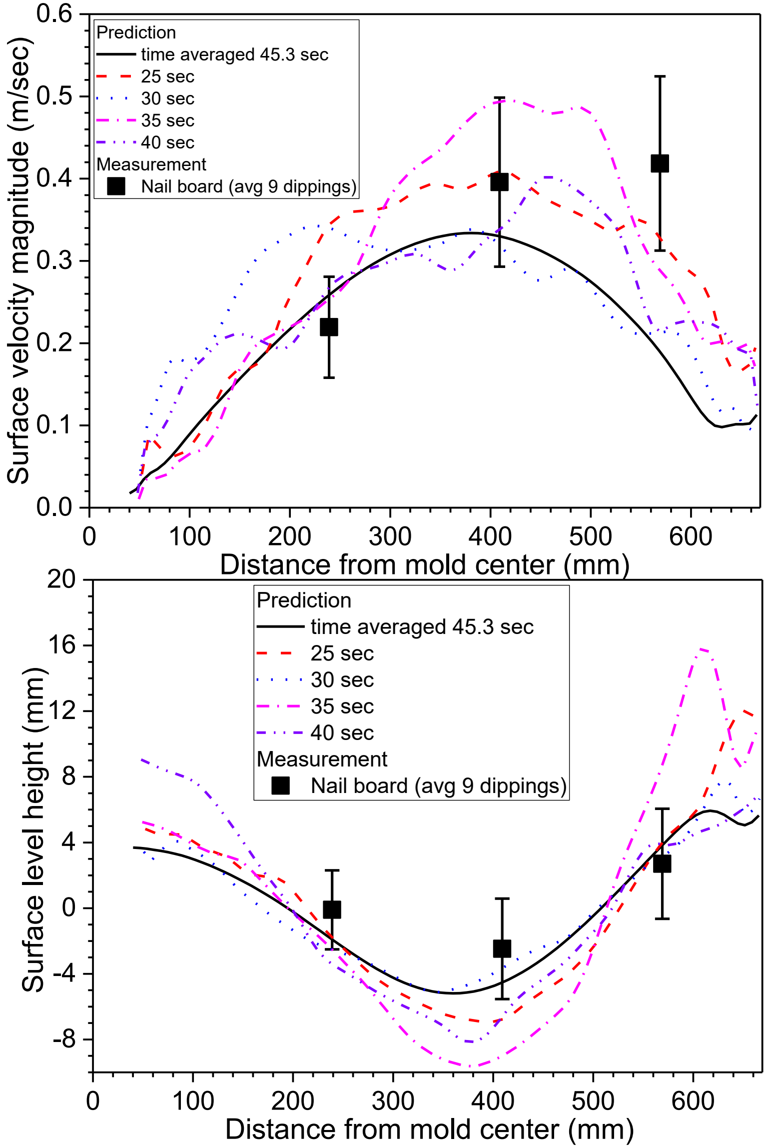
EMLS applied after 22.1 sec argon gas injection



<EMLS off> <EMLS 100A> <EMLS 300A>

- EMLS reduces jet wobbling and makes jet deflect slightly downward near Narrow Face (NF).
- Jet flow has a longer path towards mold top surface, resulting in lower and more stable surface velocity and level, which can reduce slag-entrapment defects.
- Strong Lorentz forces near NFs transport argon bubbles further away from steel shell, which decreases chances of bubble-capture defects.

EMLS Model Validation: Comparison of Surface Velocity and Level



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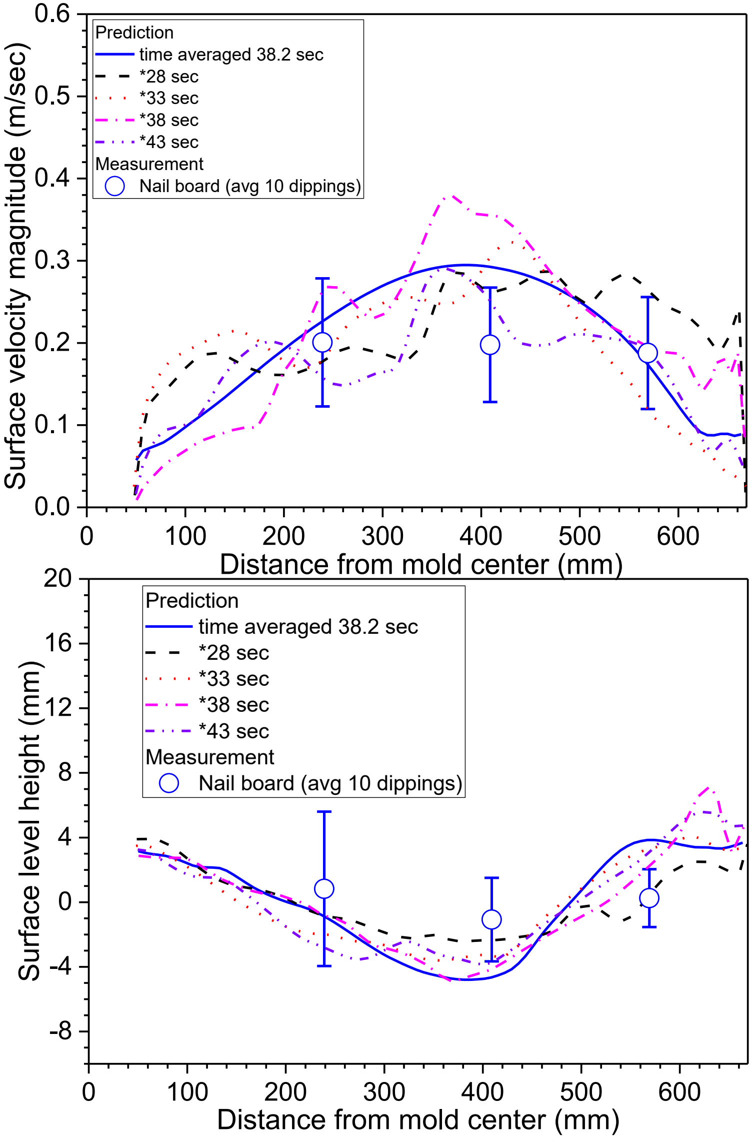

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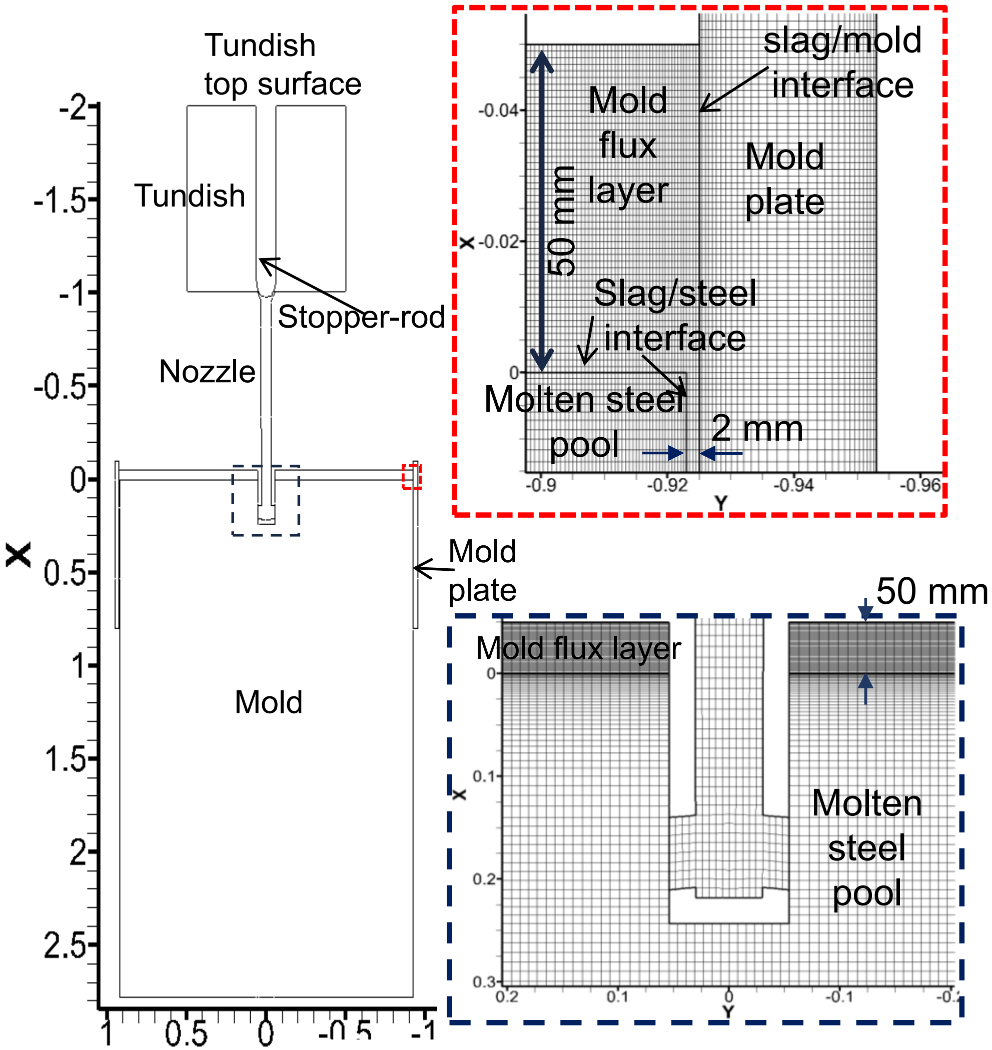
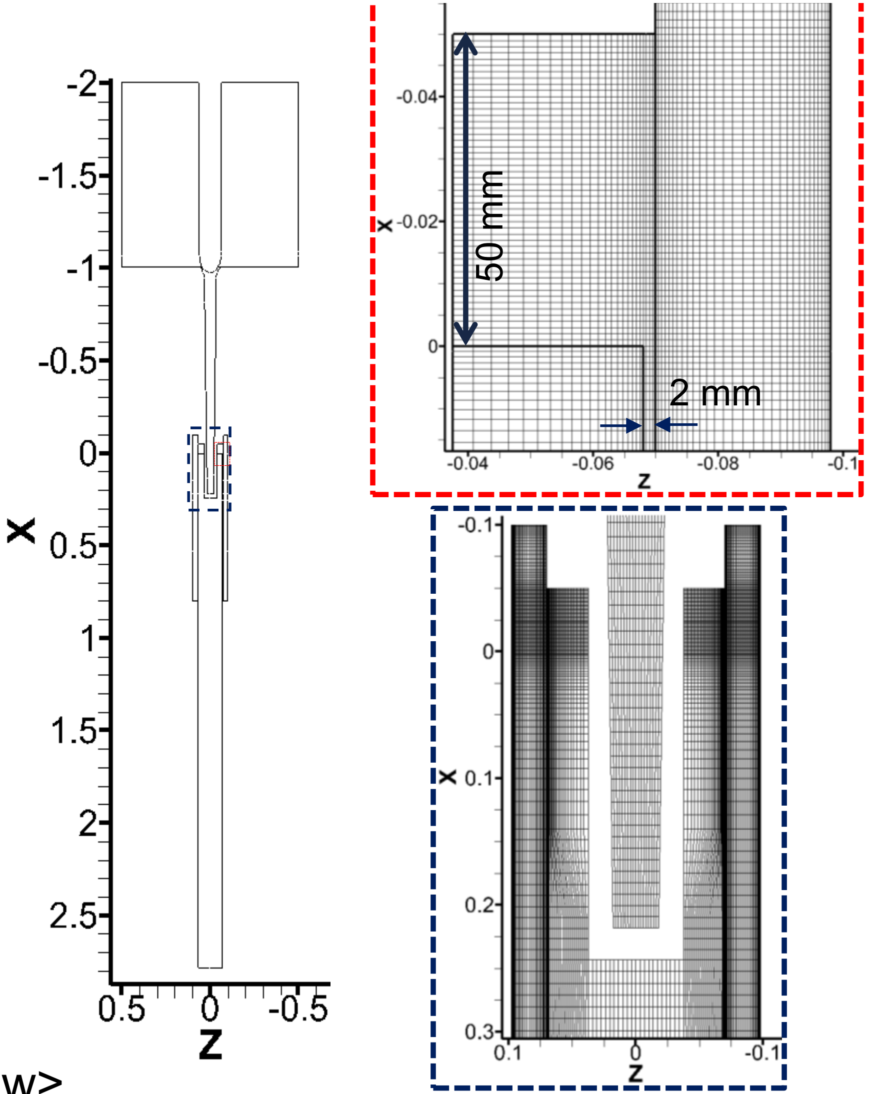
Solidification, Erosion, Oscillation Mark, Macrosegregation in Mold: Domain and Mesh

Goal: 50 µm length-scale and 5e-4 s time-scale analysis with 150 million hexahedral mapped computational cells



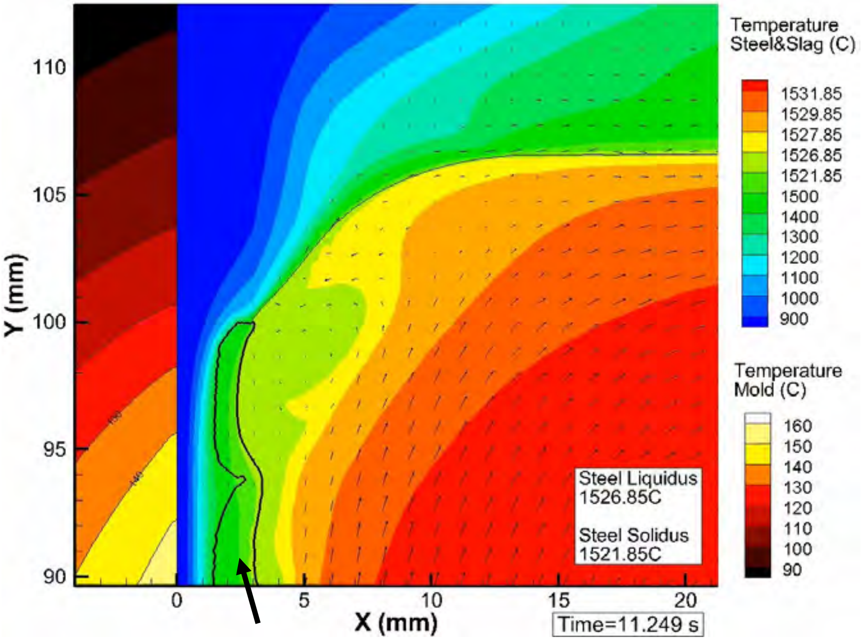
<Center-middle plane: front view>



<Center-middle plane: side view>

*)Research collaboration with NCSA

Transient 2-D Model Results and 3-D Model Setup

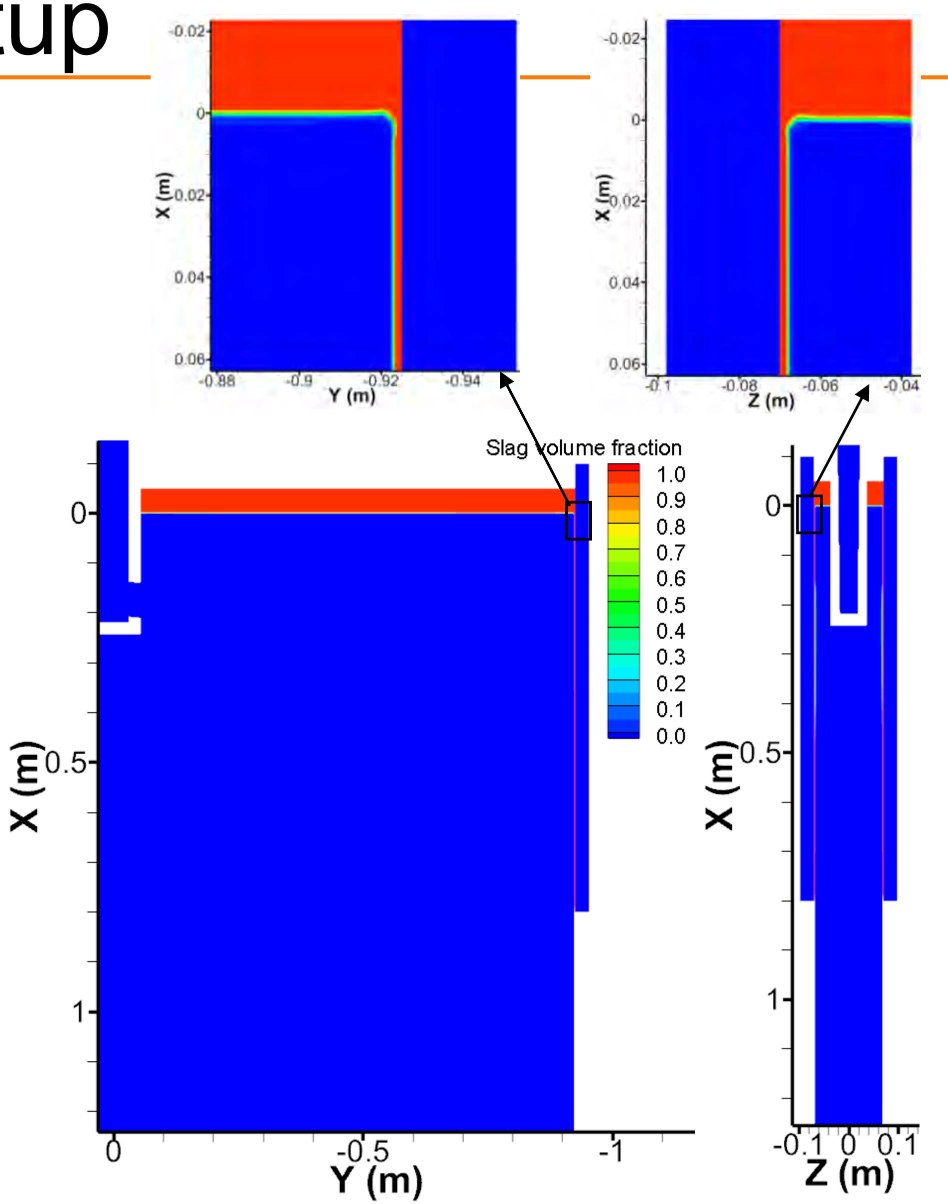


Solidifying steel shell with oscillation mark

<Temperature profile in 2-D meniscus region*)>

- Validated 2-D model is applied to 3-D domain covering all caster regions, to simulate comprehensive multiphysics phenomena.

*) Blaes and Yan: CCC annual report 2016

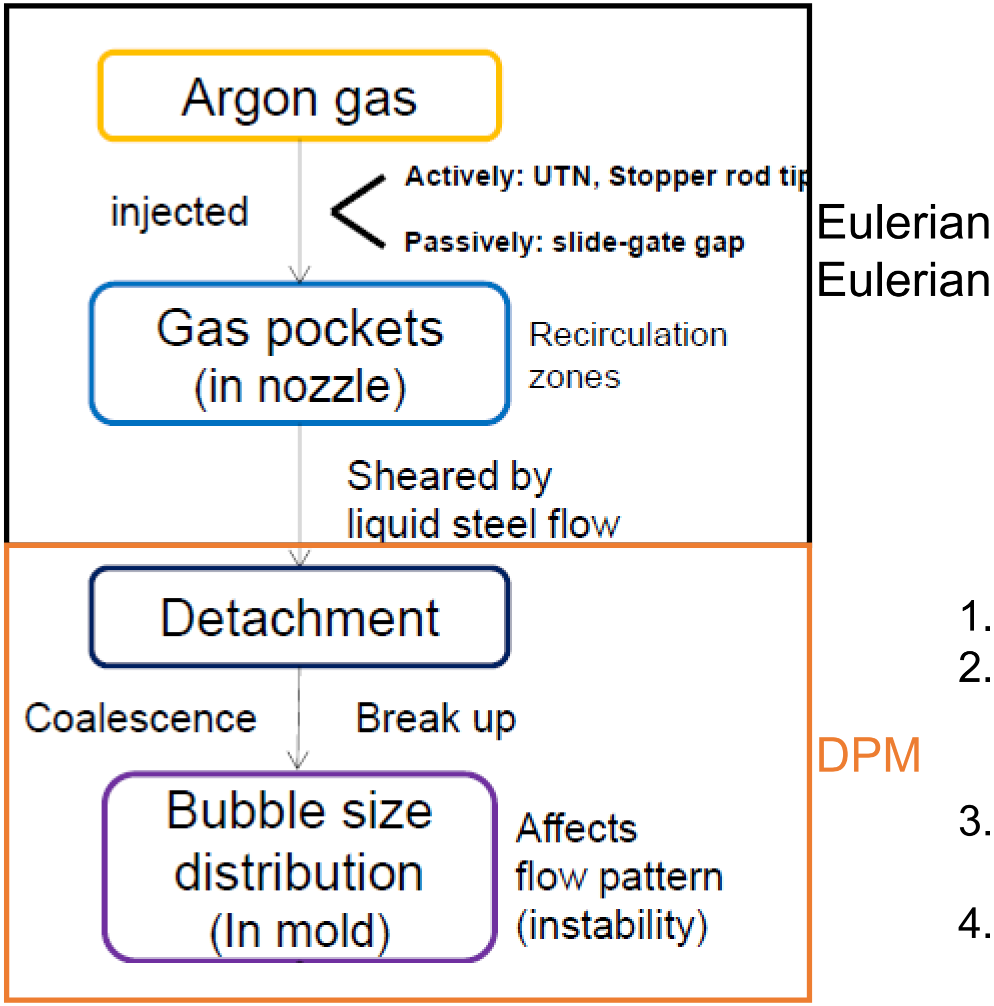


<Slag volume fraction in 3-D meniscus region>

Summary

- **Blue Waters resources (ANSYS Fluent HPC on BW XE node** and **multi-GPU based in-house code**, **CUFLOW on BW XK node) show modeling capability breakthrough** (over 3000× faster) for groundbreaking simulations with **high-resolution** (smaller than 50µm length-scale and 5e-04s time-scale) and **huge-domain** (~2m^3) for Continuous Casting (CC) of Steel**.**
- **Various multiphase flow simulations** have been conducted **to quantify complex multiphysics phenomena** related to **defect formation** and **to reduce defects by applying EM systems** as follows.
  - **Turbulent multiphase flow**: bubble behavior and size distribution, bubble transport and capture
  - **MagnetoHydroDynamics (MHD):** Effects of EMBr static magnetic field, EMLS moving magnetic field effect on flow pattern and argon bubble transport and capture.
  - **Heat transfer** and **solidification:** oscillation mark, hook, and shell thickness
  - **Thermal mechanical behavior**: depression and crack

Appendix I: Bubble Behavior Model: EE-DPM Hybrid Multiphase Model



Argon gas

injected

Actively: UTN, Stopper rod tip

Passively: slide-gate gap

Eulerian

Eulerian

Gas pockets (in nozzle)

Recirculation zones

Sheared by liquid steel flow

Detachment

Coalescence

Break up

DPM

Bubble size distribution (In mold)

Affects flow pattern (instability)

	EE model	DPM
Recirculation zone	O	O
Gas pocket formation	O	X
Shearing off	X	X
Bubble interactions	X	O

1. Run EE model and capture gas pockets.
2. Calculate detached bubble sizes by semi-analytical shearing off model: Bubbles are injected as DPM bubbles.
3. Track each bubble by DPM model as point mass.
4. Handle bubble interactions (coalescence and breakup) with semi-analytical modeling: only binary interaction.
5. Size distribution of DPM bubbles is transferred to EE model.

*) Yang: CCC annual report 2017

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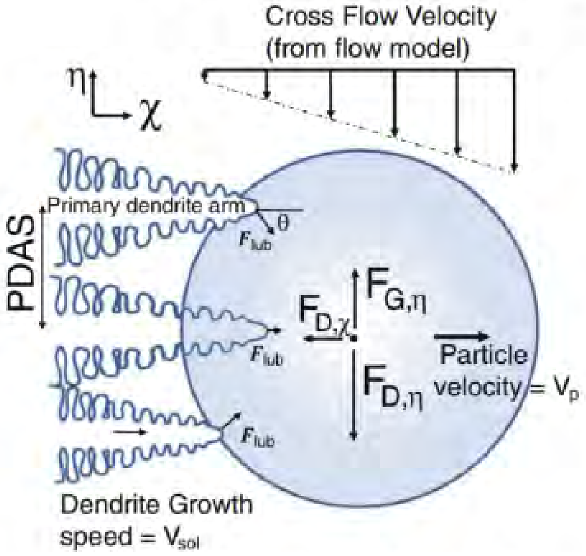
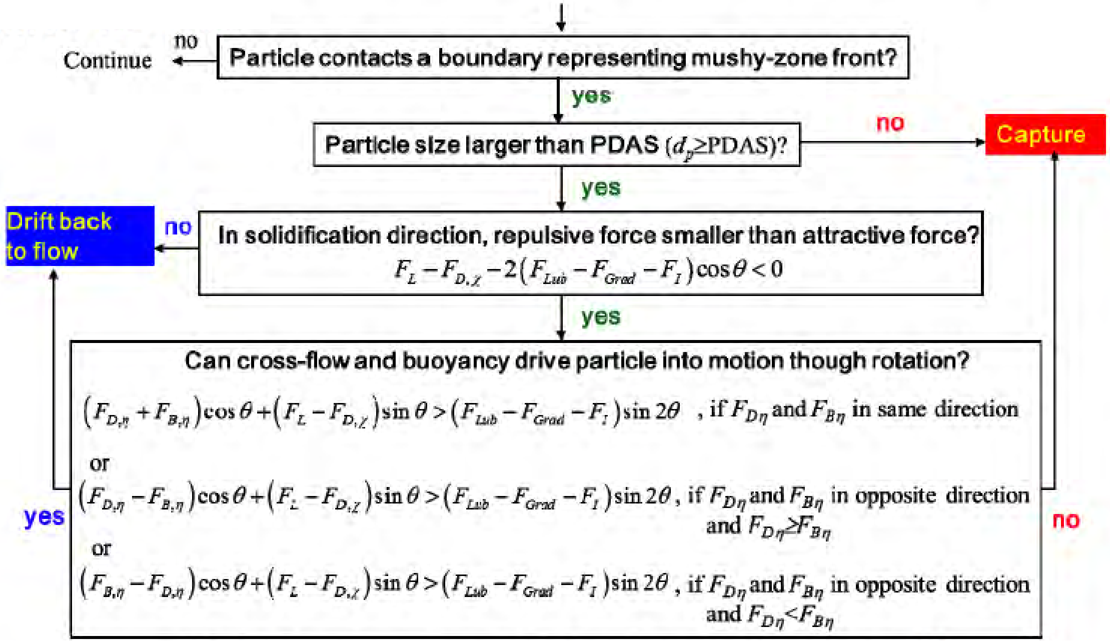
Appendix II: Advanced Particle-Capture Model for Bubble Entrapment

Advanced particle capture criterion*,**) 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>



Particle contacts a boundary representing mushy-zone front?

no → Continue

yes ↓

Particle size larger than PDAS ($d_p \geq PDAS$)?

no → Capture

yes ↓

In solidification direction, repulsive force smaller than attractive force?

$$F_L - F_{D,\chi} - 2\left(F_{Lub} - F_{Grad} - F_I\right)\cos\theta < 0$$

no → Drift back to flow

yes ↓

Can cross-flow and buoyancy drive particle into motion though rotation?

$\left(F_{D,\eta} + F_{B,\eta}\right)\cos\theta + \left(F_L - F_{D,\chi}\right)\sin\theta > \left(F_{Lub} - F_{Grad} - F_I\right)\sin 2\theta$, if $F_{D\eta}$ and $F_{B\eta}$ in same direction

or

$\left(F_{D,\eta} - F_{B,\eta}\right)\cos\theta + \left(F_L - F_{D,\chi}\right)\sin\theta > \left(F_{Lub} - F_{Grad} - F_I\right)\sin 2\theta$, if $F_{D\eta}$ and $F_{B\eta}$ in opposite direction and $F_{D\eta} \geq F_{B\eta}$

or

$\left(F_{B,\eta} - F_{D,\eta}\right)\cos\theta + \left(F_L - F_{D,\chi}\right)\sin\theta > \left(F_{Lub} - F_{Grad} - F_I\right)\sin 2\theta$, if $F_{D\eta}$ and $F_{B\eta}$ in opposite direction and $F_{D\eta} < F_{B\eta}$

yes → Drift back to flow

no → Capture

F_D: Drag force, F_B: Buoyancy force, F_L: Lift force, F_{Lub}: lubrication force, F_{Grad}: interfacial concentration gradient force, F_I: Van der Waals force

<Particle capture criterion flow chart>

*) Q. Yuan: Ph.D. Thesis, UIUC, 2004

**) B. G. Thomas, Q. Yuan, S. Mahmood, R. Liu, and R. Chaudhary: MMTB, 2004, Vol. 45, pp. 22-35