Computational Methods for Multi-Physics Simulation of Melting in Steelmaking

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Abstract

Industrial iron and steel production accounts for approximately 8% of global carbon dioxide (CO_2) emissions. Pathways to decarbonize include replacing fossil fuels in iron ore reduction and electrifying steelmaking processes. The pellets produced by the Hydrogen Direct Reduced Iron (H_2-DRI) process, have property differences from those produced in conventional DRI processes. These differences may impact melting in electric arc furnaces (EAF) and other downstream processes. The physical properties of iron pellets vary significantly during heating, complicating predictions of their behavior. In this project, we develop computational methods, including fluid flow and convective thermal transport around pellets. We also examine conduction and phase changes within the pellets as they impact the melting process. We use adaptive mesh refinement (AMR) methods to investigate 1) the changing size of a pellet and 2) the complex dynamics between the pellet and surrounding fluids, such as molten slag. We base our simulations on the AMReX-incflo module, which allows large-scale Navier-Stokes simulations while resolving the changing particle size during melting. As we advance our numerical tools, we anticipate improved understandings of the dynamics of H_2-DRI melting. In turn, it will support accelerating the adoption of low-carbon technologies in the steelmaking industry.

Steelmaking processes

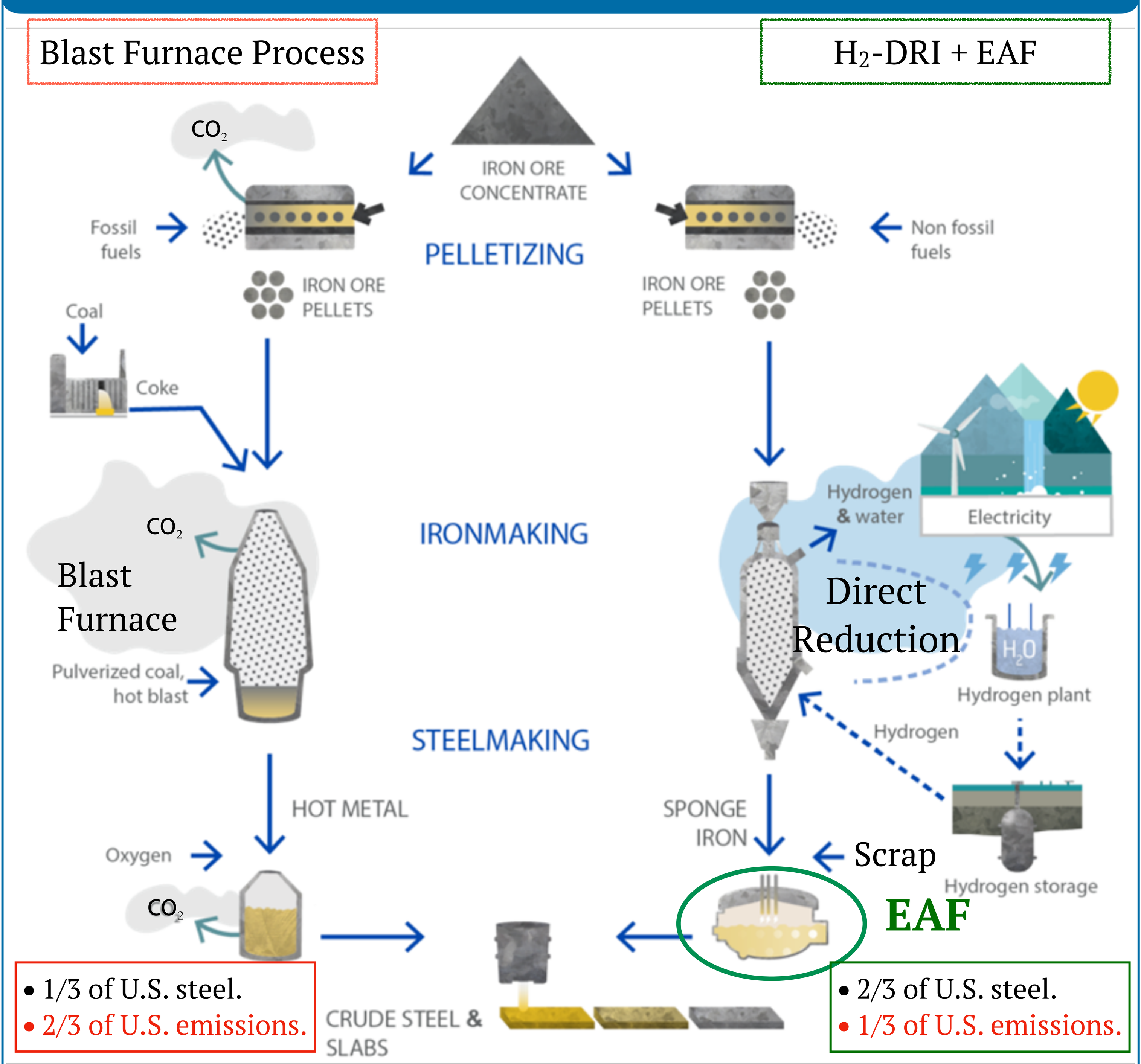


Image: HYBRIT brochure (https://www.hybritdevelopment.se/en/media/hybrit-brochure-english/)

Iron pellet in EAF

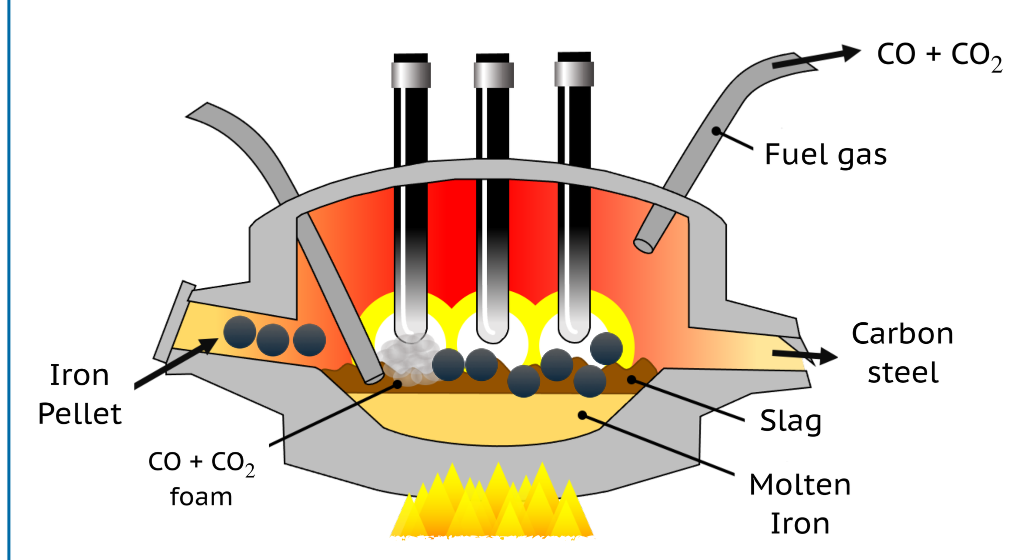


Image: R. Bell (NREL)

- With traditional BOF, we create about 1.7-2.0 tons of CO_2 to produce 1 ton of steel.
- H_2 DR pellet production and melting must be proved. Some experiments show that H_2DR pellet melts slowly.
  → CO_2 emission could be reduced to 1/10th!
- The direct reduction process would require more electricity than a blast furnace.
  → Depending on a pellet's composition and its melting time.

Objectives

$$\nabla \cdot \mathbf{u} = 0$$

$$\rho c_p \left(\frac{\partial \phi(\mathbf{x}, t)}{\partial t} + \mathbf{u} \cdot \nabla \phi(\mathbf{x}, t) \right) = \left(\nabla \cdot k \nabla \right) \phi(\mathbf{x}, t)$$

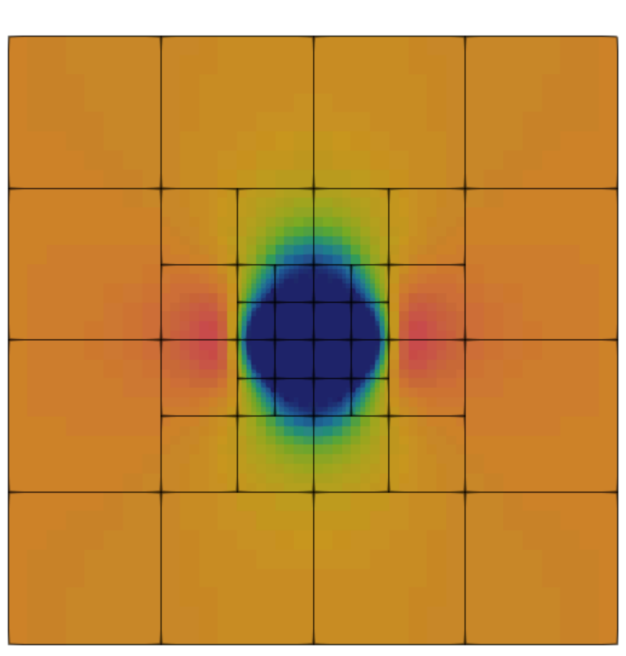
- Consider incompressible & Non-conservative tracer equations to solve for ϕ and $\mathbf{u}$.
- ρ, c_p, k are temperature dependent.
- We first examined the computational capability by separating the conduction from flow momentum:

$$\rho c_p \frac{\partial \phi(\mathbf{x}, t)}{\partial t} = \left(\nabla \cdot k \nabla \right) \phi(\mathbf{x}, t)$$

- We simulate a multi-phase model between liquid and solid for an iron pellet and surrounding fluid.
- We would like to obtain
  i) Volume & Radius of each phase:
  → molten/solid slag & molten/solid iron (Fe)
  ii) Melting time of solid slag and Fe

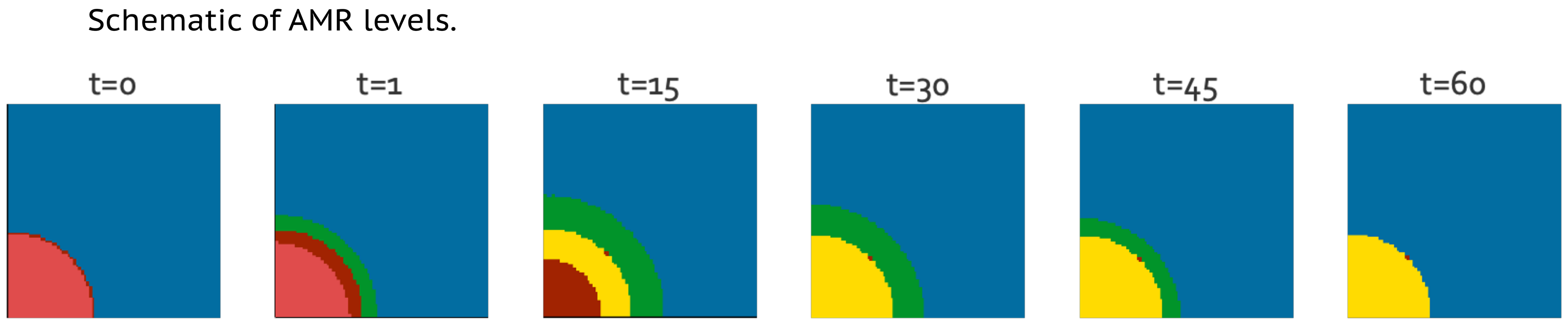
$\mathbf{u}$ = Velocity, ϕ = Temperature, t = Time, ρ = Density, k = Conductivity, c_p = Specific heat

Computational tools: AMReX



Schematic of AMR levels.

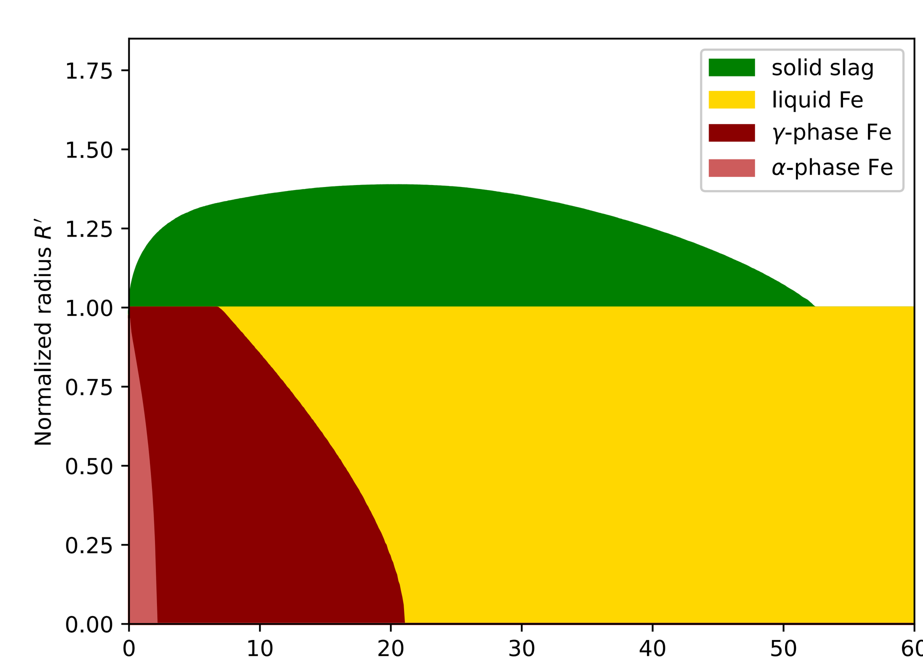
- AMReX is an open-source library for building massively parallel block-structured adaptive mesh refinement (AMR) applications developed at LBNL.
- We use the 'incflo' module in AMReX-Fluids.
  → Finite Volume Method base solver.
- By refining the grid cells near the liquid-solid interface, we can capture phase variation more accurately and efficiently.

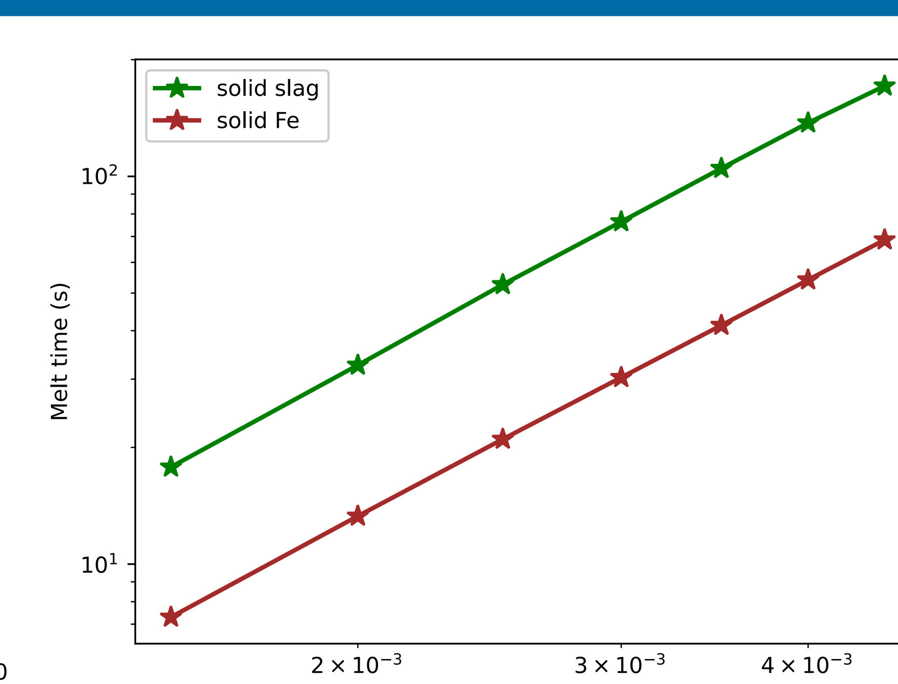


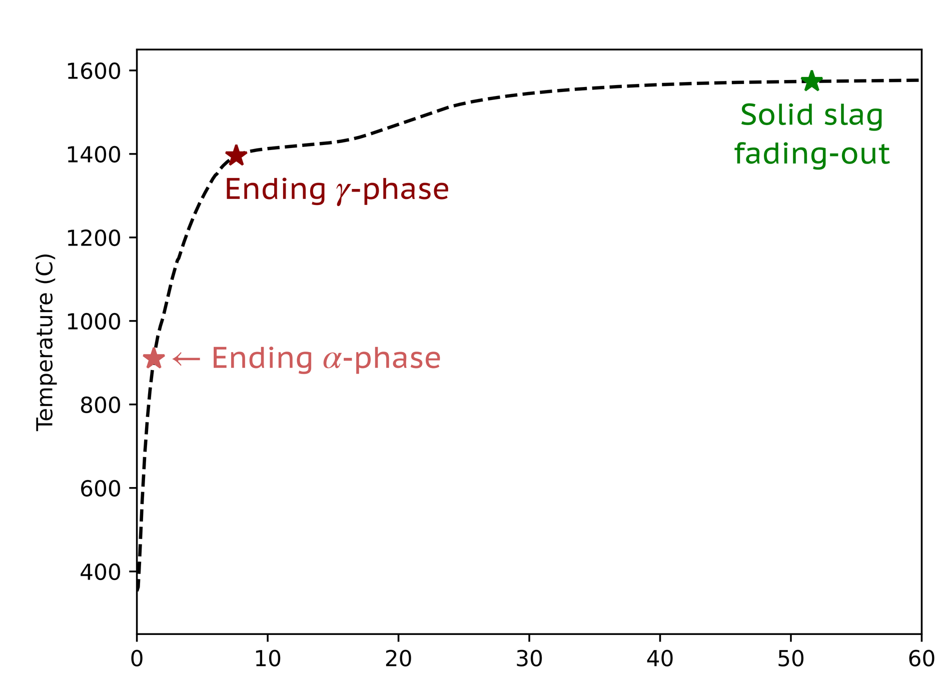
A 2-D slice a pure iron pellet model with radius of 0.0025 (m) in surrounding slag bath;
Liquid slag (blue), solid slag (green), α-phase Fe (coral), γ-phase Fe (dark red), and liquid Fe (yellow).

- The three AMR levels are based on gradients in the specific heat and temperature.
- The initial pellet temperature is 300˚C, while the bath temperature is 2000˚C.
- α-phase: Solid Fe under 910˚C. γ-phase: Solid Fe over 910˚C.

Preliminary results







- Normalized radius R' is computed with
$$R_{max} = \left(V_{max}^{Fe} \frac{3}{4\pi} \right)^{1/3},$$
where V_{max}^{Fe} = maximum volume of Fe.
- Temperature plot is obtained at the center of iron pellet over time.
- Melt time rate ∝ Pellet Radius^2

In progress & Future work

- Using AMReX-incflo module, we are integrating convection-conduction codes.
- We plan to make simulations to understand the thermo-chemical dynamics between pellets with various composition and surrounding slag bath in EAF.
- The conduction results will be presented in ASME-IMECE2024 conference.

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