physics-AI For CFD Simulations: SciML

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Outline

What is the Czochralski (CZ) Process?

- Dominant method for single-crystal silicon growth
- Used in semiconductor and photovoltaic industries

CZ Furnace Schematic

CZ Furnace: Crucible, Melt, Heater, Crystal Pulling

Crystal Growth Physics

- Solidification at melt–crystal interface
- Strong heat extraction through crystal
- Melt flow affects dopant and defect transport

Why Modeling is Difficult

- Strong thermal–fluid coupling
- High Rayleigh number convection
- Thin boundary layers
- Multi-physics and multi-scale nature

Axisymmetric Approximation

- Nearly rotationally symmetric geometry
- Reduces 3D problem to 2D (r, z)

Computational Domain

Axisymmetric Melt Domain in (r, z)

Boundary Identification

Crucible Wall, Free Surface, Crystal Interface

Physical Assumptions

- Incompressible Newtonian melt
- Laminar, steady-state flow
- Constant material properties
- Boussinesq approximation

Continuity Equation

$$\frac{1}{r}\frac{\partial}{\partial r}(r u_r) + \frac{\partial u_z}{\partial z} = 0$$

Radial Momentum Equation

$$u_r \partial_r u_r + u_z \partial_z u_r = -\frac{1}{\rho} \partial_r p + \nu \left(\nabla^2 u_r - \frac{u_r}{r^2} \right)$$

Axial Momentum Equation

$$u_r \partial_r u_z + u_z \partial_z u_z = -\frac{1}{\rho} \partial_z p + \nu \nabla^2 u_z + g\beta(T - T_0)$$

Energy Equation

$$u_r \partial_r T + u_z \partial_z T = \alpha \nabla^2 T$$

Thermal–Fluid Coupling

- Temperature $\rightarrow$ buoyancy force
- Velocity $\rightarrow$ heat advection
- Strong nonlinear feedback loop

Rayleigh Number

$$\mathrm{Ra} = \frac{g\beta\Delta T L^3}{\nu\alpha}$$

- Measures strength of natural convection

High Rayleigh Number Regime

- Thin thermal and velocity boundary layers
- Strong nonlinear advection
- Major source of instability for PINNs

Standard PINN Concept

- Neural network approximates PDE solution
- Physics enforced via residual minimization

PINN Inputs and Outputs

- Inputs: (r, z)
- Outputs: u_r, u_z, p, T

Spatial Information (SI) Embedding

- Coordinates injected into hidden layers
- Preserves geometric sensitivity
- Improves boundary-layer resolution

Adaptive Loss Balancing

- Separate losses for each equation
- Trainable weights
- Prevents gradient domination

PINN Loss Function Structure

$$\mathcal{L} = \lambda_c \mathcal{L}_c + \lambda_m \mathcal{L}_m + \lambda_e \mathcal{L}_e + \lambda_b \mathcal{L}_b$$

Continuity Loss

$$\mathcal{L}_c = \frac{1}{N}\sum_i \left| \frac{1}{r}\partial_r(ru_r) + \partial_z u_z \right|^2$$

Momentum Loss

$$\mathcal{L}_m = \|\mathcal{R}_{u_r}\|^2 + \|\mathcal{R}_{u_z}\|^2$$

- Enforces Navier–Stokes equations

Energy Loss

$$\mathcal{L}_e = \frac{1}{N} \sum_i \left| u_r \partial_r T + u_z \partial_z T - \alpha \nabla^2 T \right|^2$$

Boundary Condition Loss

$$\mathcal{L}_b = \|u - u_{BC}\|^2 + \|T - T_{BC}\|^2$$

Why Adaptive Weighting Matters

- Different PDEs have different stiffness
- High-Ra momentum residuals dominate gradients
- Learned weights improve conditioning

Motivation for XPINN

- Global PINNs struggle with large domains
- Boundary layers are spatially localized

XPINN Concept

- Decompose domain into subdomains
- One neural network per subdomain
- Interface conditions enforce consistency

XPINN Domain Decomposition

Melt Domain Split into Multiple Subdomains

Interface Loss Terms

$$\mathcal{L}_{\text{int}} = \|u^{(1)} - u^{(2)}\|^2 + \|\nabla u^{(1)} - \nabla u^{(2)}\|^2$$

Why XPINN Improves Stability

- Localizes stiffness
- Reduces spectral bias
- Mimics FEM element locality

Training Data

- No experimental or CFD data
- Physics-only collocation points

Reference Solution

- COMSOL Multiphysics
- Weak-form finite element solver

Velocity Comparison

COMSOL vs PINN Velocity Contours

Temperature Comparison

COMSOL vs PINN Temperature Contours

Error Metrics

- Relative L_2 norms
- Improved PINN outperforms standard PINN

Key Conclusions

- Improved PINNs handle thermal–fluid coupling
- SI embedding improves spatial accuracy
- XPINNs improve stability at high Ra
- Results comparable to COMSOL

Future Work

- Transient growth
- Rotation and Marangoni effects
- Real-time process optimization

Thank You