Fast prediction of transport structures in bulk single crystal growth by Physics Informed Neural Networks

Yasunori Okano[1]*, Yuto Takehara[1], Sadik Dost[2]
*lead presenter: okano.yasunori.es@osaka-u.ac.jp
1 Osaka University, Japan
2 University of Victoria, Canada

Introduction

In bulk single crystal growth, the understanding of transport structures in the growth melt, such as fluid flow, and temperature and concentration distributions, is essential for the growth of high-quality crystals. Direct observation of such transport structures during growth is difficult. Modelling by Computational Fluid Dynamics (CFD) offers a powerful tool for this purpose and provides essential insight to control these transport structures in the melt. However, predictions by CFD requires long computations giving rise to a high computational cost. To overcome this difficulty, we proposed a new technique, "Physics Informed Neural Networks (PINNs)[1]" for fast predictions.

Numerical method

Because PINN learns the governing equations and the boundary conditions, PINN has advantages such as (1) exact results which can be achieved by CFD, and (2) quick predictions which can be obtained by Neural Networks. In this study, PINN is constructed as shown in Fig. 1. In the model, the governing equations are *momentum*, *continuity*, and *energy* equations with the *Poisson* equation of the electrical potential. The input parameters are x = (x, y, z, T_l, T_r, T_h, h), where x, y, and z are the cartesian coordinates and T_l, T_r, T_h the obtained temperatures at the bottom center of the crucible, the surface edge, and the bottom edge of the melt, respectively. h is the melt height.

Results

Figure 2 shows the temperature field, and the streamlines colored by the magnitude of the melt flow obtained by CFD and PINNs. As shown in the figure, the predicted distributions by PINNs are consistent with the results by CFD. The CPU and GPU times for CFD and PINNs were about 3 hours and about 0.1 s, respectively. Because PINN is a mesh-free method, variation of the calculation domain, such as melt depth variation, accompanying crystal growth can become available without mesh reconstruction.

Conclusion and Future work

PINNs that can quickly and exactly predict transport phenomena in crystal growth was successfully developed. In future the effect of rotation will be included for an optimal control.

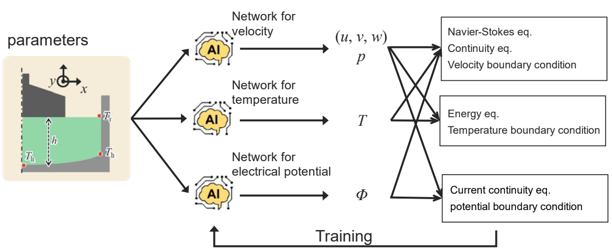

Fig. 1. The architecture of PINNs.

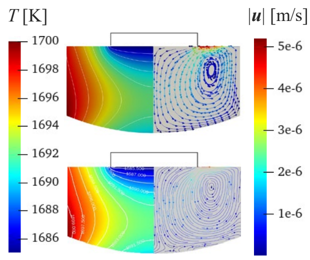

Fig. 2. The temperature (left) and melt flow velocity (right) distributions by CFD (top) and PINNs (bottom).

[1] Raissi M, et al. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. J. Comput. Phys. 2019;378:686-707.