AM5035 High Performance Computing Lab

Project

Phase-Field modeling of solidification in MPI(C++).

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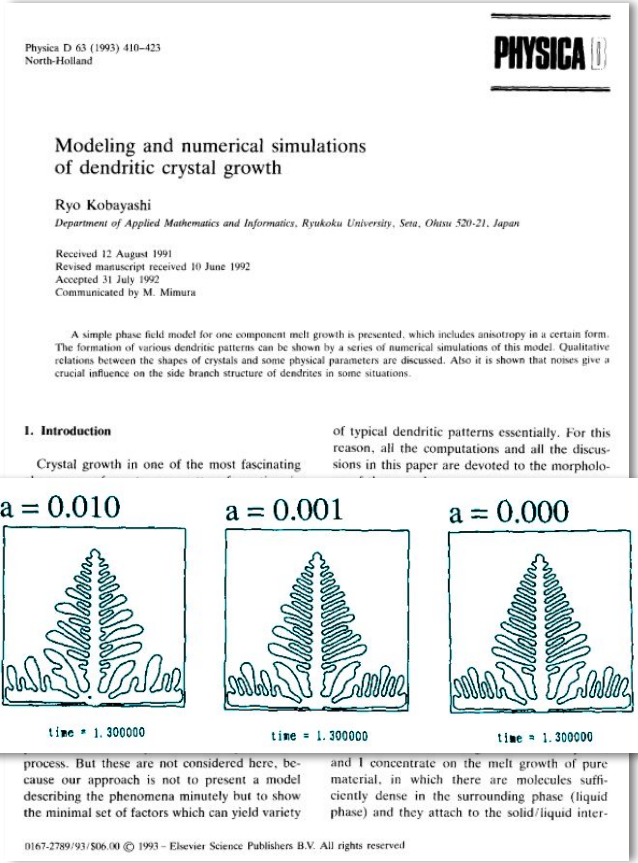
MM19B029

Abstract

We will numerically solve the anisotropic dendritic growth during solidification using the Phase-Field method. The mathematical model of the phenomenon is derived from the work of Kobayashi[1]. The PDEs will be solved within the finite-difference approximation on a 5 point stencil. The program will be written in `C++` and `MPI`(Message Passing Interface) will be used for parallel data and functional processing.

Anisotropic solidification

- A crystal grows under the influence of two prime forces:
    1. **Thermodynamic** driving force for solidification (undercooling)
    2. **Surface tension** of the solid-liquid interface (interfacial energy)
- Nucleation of dendrites is assumed in this model.
- The model also assumes pure material.
- The process limiting the growth rate of crystals is the rate of removal of latent heat from the interface.



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PHYSICA D

Modeling and numerical simulations of dendritic crystal growth

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A simple phase field model for one component melt growth is presented, which includes anisotropy in a certain form. The formation of various dendritic patterns can be shown by a series of numerical simulations of this model. Qualitative relations between the shapes of crystals and some physical parameters are discussed. Also it is shown that noises give a crucial influence on the side branch structure of dendrites in some situations.

1. Introduction

Crystal growth in one of the most fascinating

of typical dendritic patterns essentially. For this reason, all the computations and all the discussions in this paper are devoted to the morpholo-

process. But these are not considered here, because our approach is not to present a model describing the phenomena minutely but to show the minimal set of factors which can yield variety

and I concentrate on the melt growth of pure material, in which there are molecules sufficiently dense in the surrounding phase (liquid phase) and they attach to the solid/liquid inter-

Kobayashi dendrite growth model

Order parameter:	1. Phase identifier 0 = solid 1 = liquid 2. Temperature 0 = melting point
Type:	Both Non-conserved.
Evolution equation:	Allen-Cahn.
Boundary conditions	Dirichlet boundary conditions on all sides
Symmetry:	Hexagonal

Phase evolution:

$$\tau\frac{\partial\phi}{\partial t} = \frac{\partial}{\partial y}\left(\epsilon\frac{\partial\epsilon}{\partial\theta}\frac{\partial\phi}{\partial x}\right) - \frac{\partial}{\partial y}\left(\epsilon\frac{\partial\epsilon}{\partial\theta}\frac{\partial\phi}{\partial y}\right) + \nabla.(\epsilon^2\nabla\phi) + \phi(1-\phi)(\phi - \frac{1}{2} + m)$$

Epsilon is the symmetry parameter. Constant.
Tau is a constant that determines the change in phi.

$$m(T) = \frac{\alpha}{\pi}\arctan\left[\gamma(T_{eq} - T)\right]$$

$$\epsilon = \bar{\epsilon}\sigma(\theta) \qquad \sigma(\theta) = 1 + \delta\cos j(\theta - \theta_0) \qquad \theta = \arctan\left(\frac{\partial\phi/\partial y}{\partial\phi/\partial x}\right)$$

delta is the strength of anisotropy ; **j** is the symmetry parameter.

Temperature evolution: $\frac{\partial T}{\partial t} = \nabla^2 T + \kappa\frac{\partial\phi}{\partial t}$ **Kappa** is the heat of solidification.

Need for Parallelization

1. **Improved Computational Efficiency:**
   Parallelization enables the simultaneous execution of the PDE kernel on multiple subdomains of the system thus increasing computational efficiency.

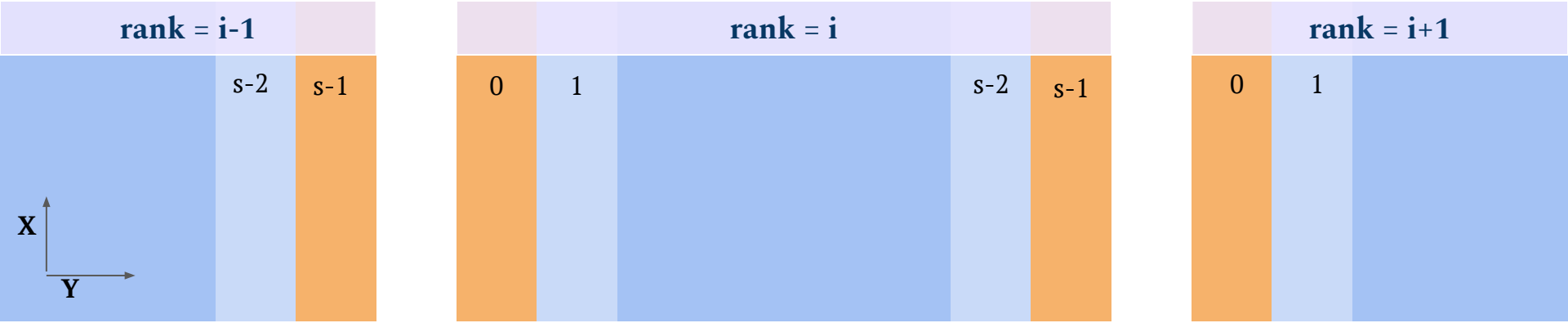
2. **Scalability:**
   Parallelization provides scalability, allowing our simulations to be performed on increasingly larger scales within relatively smaller execution times.

3. **Parameter Exploration and Sensitivity Analysis:**
   Parallelization facilitates conducting parameter explorations and sensitivity analyses efficiently. By running multiple simulations simultaneously with different parameter values, we can study the behavior and sensitivity of the physical system to various factors.

4. **Handling High-Dimensional Problems:**
   Parallelization helps reduce the computational burden associated with high-dimensional simulations.

Parallelization

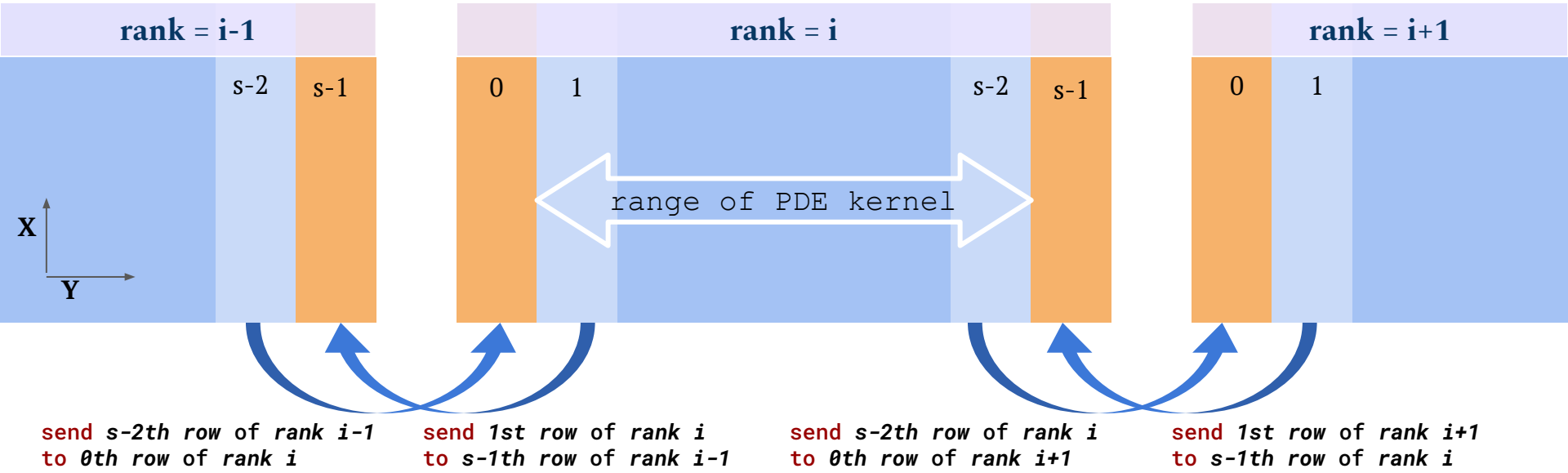
The entire simulation domain is divided along the Y-axis. Local and Global indexes are defined for initiation and syncing subdomain boundaries.



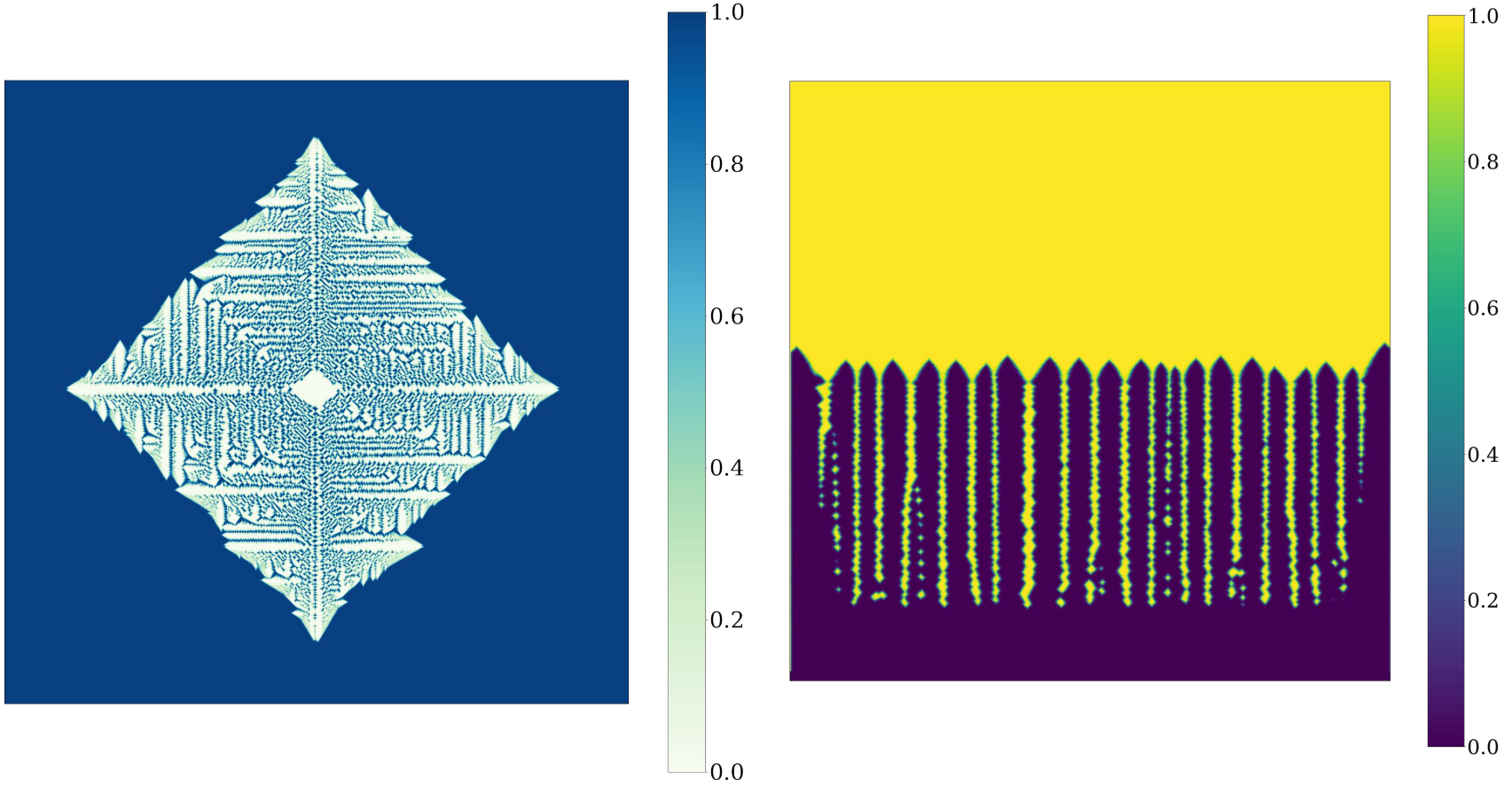
`subdomain size = s such that s-2 = DOMAIN_SIZE_Y / no. of processors`

`global_X = local_x and global_Y = (s-2)*rank + local_y`

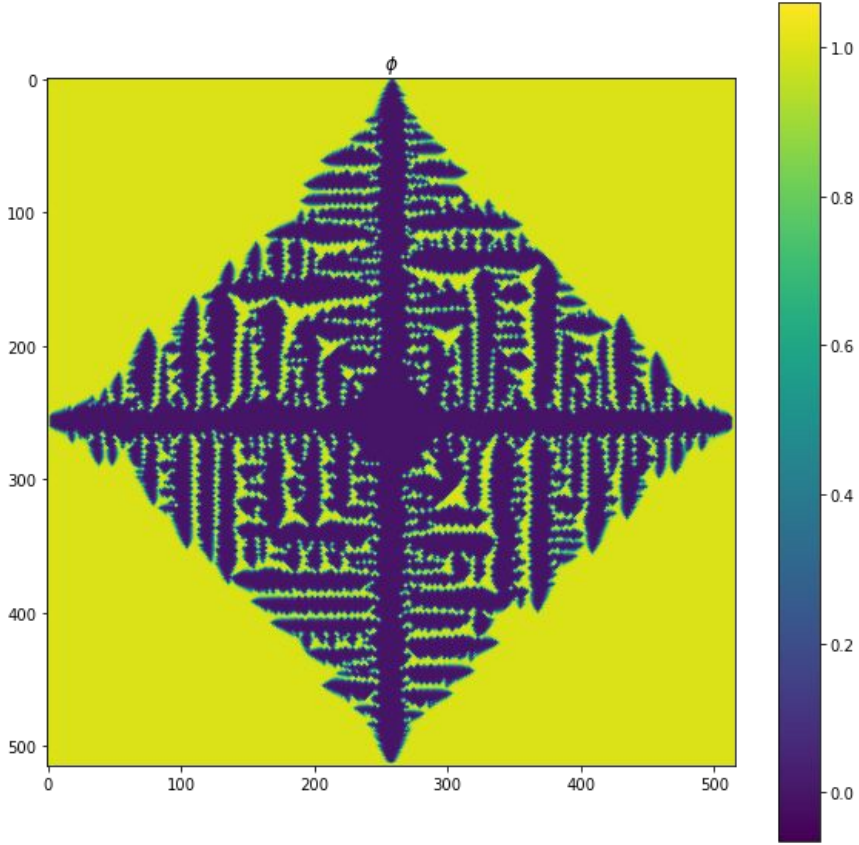
Kernel range and sync

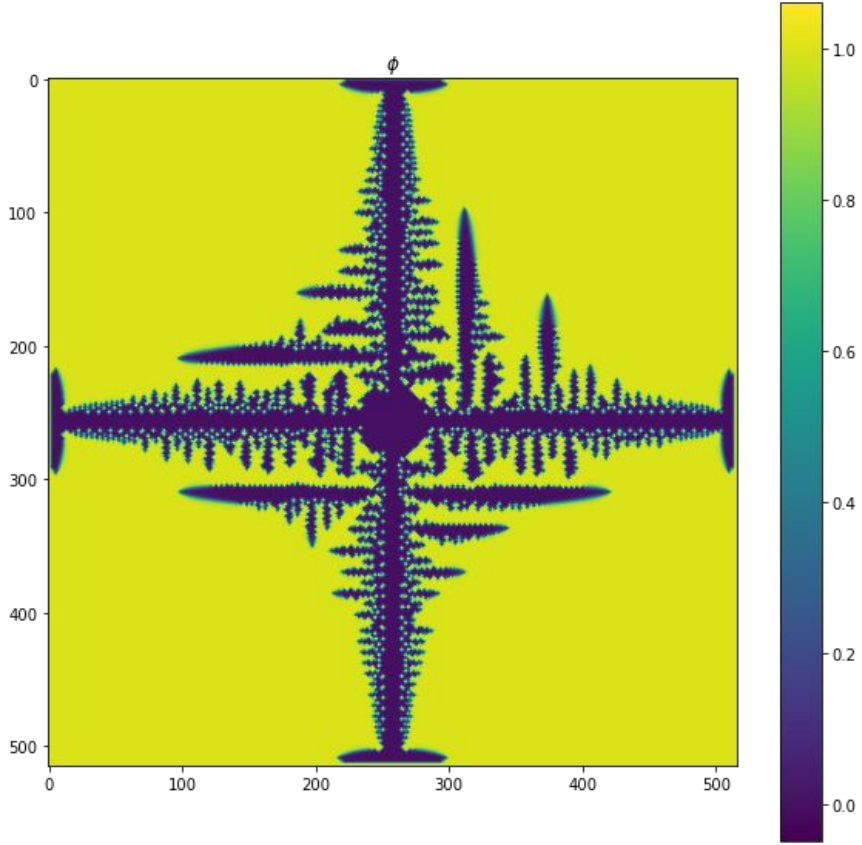


Results: anisotropic and directional

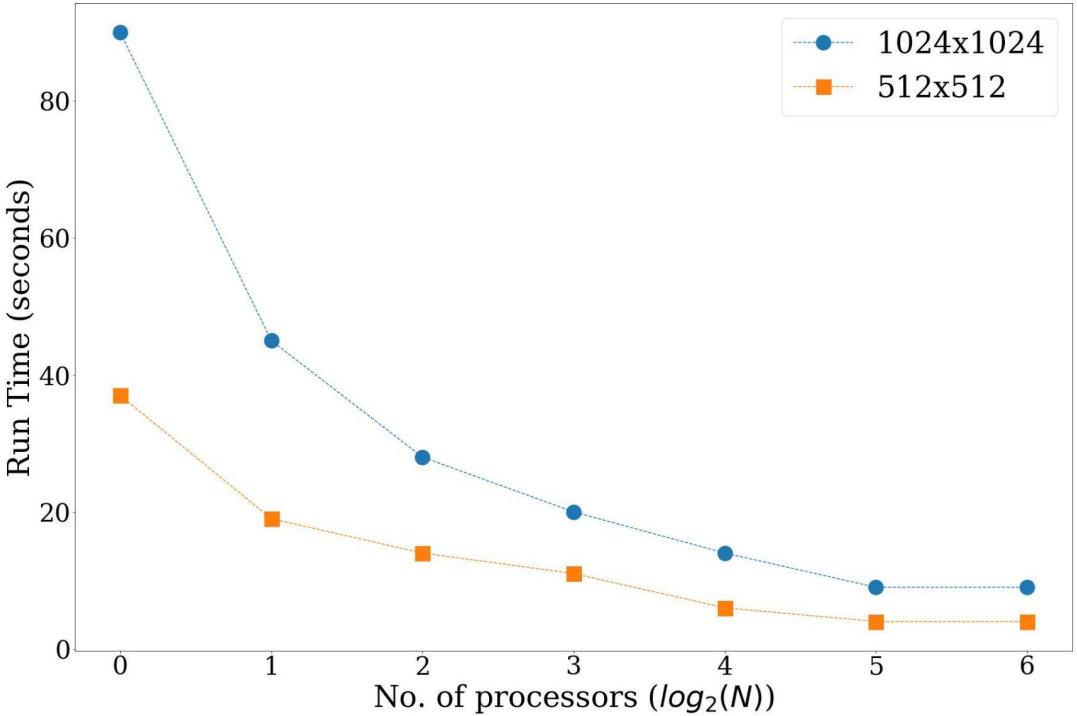


Results with varying noise.

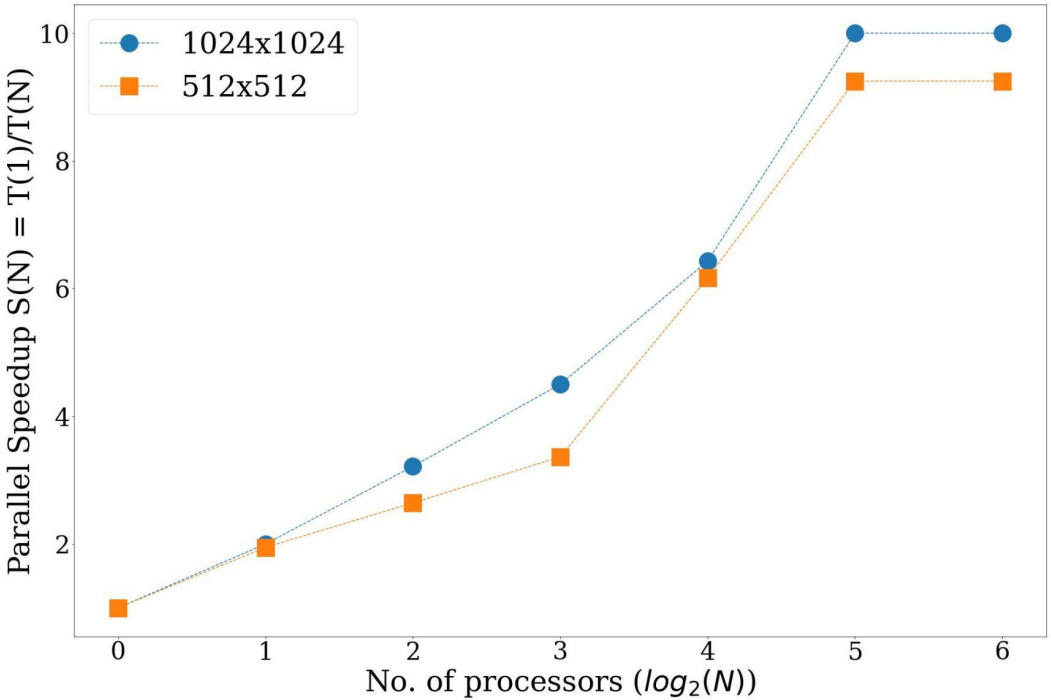




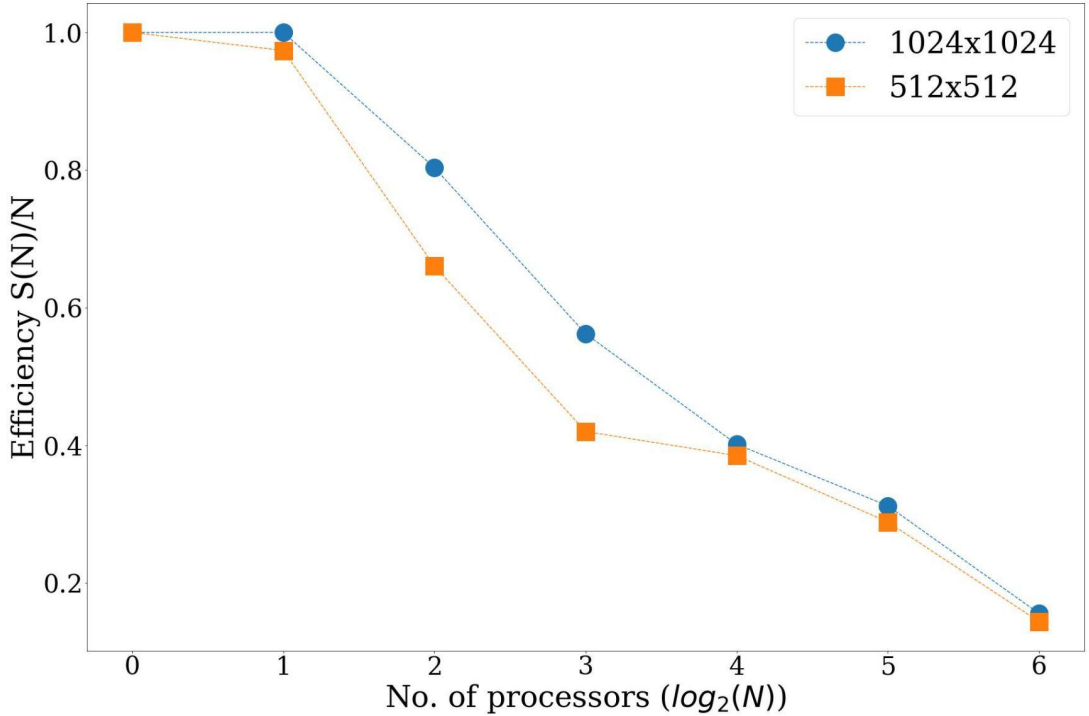
Run time


1024x1024
512x512
Run Time (seconds)
0
20
40
60
80
0
1
2
3
4
5
6
No. of processors ($log_2(N)$)

Speedup


1024x1024
512x512
Parallel Speedup S(N) = T(1)/T(N)
No. of processors ($log_2(N)$)
0
1
2
3
4
5
6
2
4
6
8
10

Efficiency


1024x1024
512x512
Efficiency S(N)/N
1.0
0.8
0.6
0.4
0.2
0
1
2
3
4
5
6
No. of processors ($log_2(N)$)

Conclusions

The following conclusions can be drawn from the speedup and efficiency plots:

- Good enough Scalability.
- Significant Communication Overhead.
- Inherent Sequential Dependencies.

Several conclusions can be drawn from the results :

- Anisotropic Solidification :
  Seen from the preferred growth directions of the dendritic arms.
- Microstructural Evolution :
  Nucleation and coarsening of dendritic arms are seen.
- Interface Morphology :
  The diffused nature of the solid liquid interface is seen.
- Solidification Conditions :
  Different morphologies obtained with varying degrees of undercooling.

References

1. Kobayashi, Ryo. 1993. “*Modeling and Numerical Simulations of Dendritic Crystal Growth.*” Physica D: Nonlinear Phenomena 63 (3–4): 410–23. link

2. Leasar, Richard. 2013. *Introduction to Computational Materials Science. Principles of Inorganic Materials Design.* 1st ed. New York: Cambridge University Press. link