Meta-Programming and Hybrid Parallel Strategies for Solving PDEs: An FDM and PINN Comparison [1, 2]

Seminar Presentation III

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Coláiste na Tríonóide, Baile Átha Cliath

[1] Full docs: `https://liyihai.com/html/index.html`

[2] Git repository: `https://github.com/liyihai-official/Final-Project`

Outline

Outline

Kolmogorov PDEs

Solving $u(x,T)$, for $\mathbb{R}^1 \ni T > 0$, $x \in \mathbb{R}^d$, $t \in [0,T]$, $u(t,x) = u \in \mathbb{R}^1$, $\mu(x) \in \mathbb{R}^d$, $\sigma(x) \in \mathbb{R}^{d\times d}$,

$$u_t = \frac{1}{2}\,\mathrm{Trace}_{\mathbb{R}^d}\left[\sigma(x)\,[\sigma(x)]^*\,\mathrm{Hess}_x u\right] + \langle \mu(x), \nabla_x u\rangle_{\mathbb{R}^d} \tag{1}$$

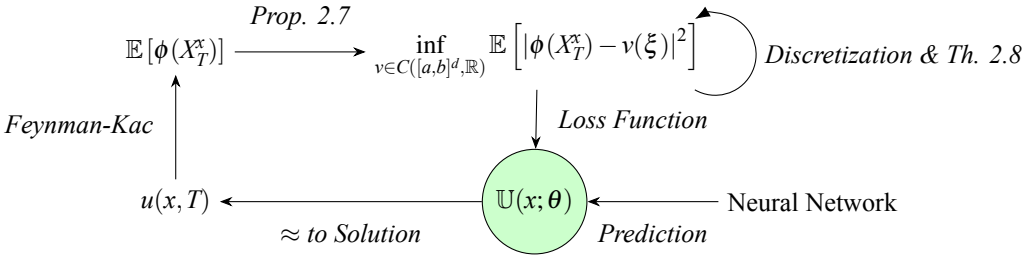

Figure: Deep Neural Network (DNN) Methodology of Solving Kolmogorov PDEs [**FIRST**]

General Form of PDEs

– $u(t,x)$ denotes with the target function, $x \in \mathbb{R}^d$.

– $\Gamma[\,\cdot\,;\lambda]$ is a non-linear operator parameterized by λ.

$$u_t(t,x) + \Gamma[u;\lambda] = 0 \tag{2}$$

Define $f(t,x)$ to be given by

$$f(t,x) = u_t(t,x) + \Gamma[u;\lambda] \tag{3}$$

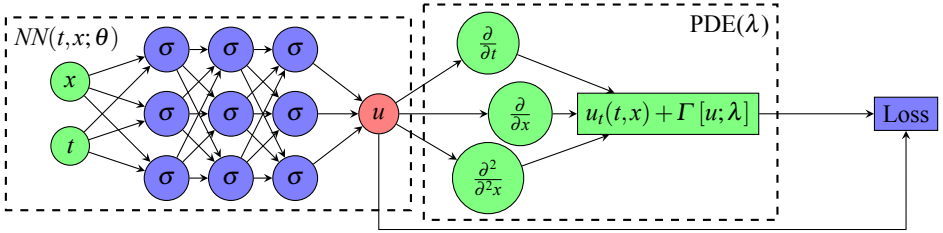

Figure: PINN, with 3 fully connected hidden layers

Comparing With Finite Difference Time Domain Method (FDTD)

1. Deep Neural Network [**FIRST**]
   - Gives lower quality approximations.
   - Takes longer time to train.
   - Possible to solve high dimension PDEs
2. Physics Informed Neural Network
   - Gives higher quality approximations.
   - Takes longer time to train.
   - Has more flexible way to get results.
   - Possible to solve high dimension PDEs

Objectives

This project focused on following objectives:

1. Implement FDTD and PINN in `C++/C`.
2. Implement FDTD hybrid parallel version using `MPI/OpenMP`.
3. Implement PINN GPU parallel version using `Libtorch/CUDA`.
4. Evaluate the efficiency and accuracy of FDTDs and PINNs.

Challanges

However, there were many obstacles including:

1. Portability, Continuity.
2. Overlapping Communication and Computation.
3. Unnecessary intra-node communication
4. Communication Overhead.
5. Scalability Issues.
6. Memory Management.

Outline

General Form of problem

The PDE parametrized by number λ and an operator $\mathscr{N}[\cdot;\lambda]$, and assume the variable x is a 2D or 3D spatio-vector which is written in

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,\vec{x}) + \mathscr{N}[u;\lambda] = 0 \\ u(0,\vec{x}) = \varphi(\vec{x}) \end{cases} \tag{4}$$

where φ is the initial condition, and $\vec{x} \in \Omega, t \in [0,+\infty)$.

Boundary Conditions

The Dirichlet and Von Neurmann boundary conditions are formed as

$$\begin{cases} u(t,\vec{x}) = g(t,\vec{x}) \\ \dfrac{\partial u}{\partial \vec{n}} = g(t,\vec{x}) \end{cases} \tag{5}$$

where $\vec{n}$ is the normal vector on $\overline{\Omega}$ the boundary of domain Ω.

The function

$$u(t,x,y) = x + y - xy,\ \forall \alpha \in \mathbb{R}^1 \tag{6}$$

is the solution of 2D Heat Equation 7 below

$$\begin{aligned}
&\frac{\partial u}{\partial t} = \alpha \left(\frac{\partial u^2}{\partial^2 x} + \frac{\partial u^2}{\partial^2 y} \right) && (x,y) \in \Omega,\ t \in [0,+\infty) \\
&u(0,x,y) = \varphi(x,y) = 0 && (x,y) \in \Omega \\
&u(t,x,y) = g(x,y) = \begin{cases} y,\ x = 0, y \in (0,1) \\ 1,\ x = 1, y \in (0,1) \\ x,\ y = 0, x \in (0,1) \\ 1,\ y = 1, x \in (0,1) \end{cases} && t \in [0,+\infty)
\end{aligned} \tag{7}$$

The function

$$u(t,x,y,z) = x+y+z-2xy-2xz-2yz+4xyz,\ \forall \alpha \in \mathbb{R}^1 \tag{8}$$

is the solution of 3D Heat Equation 9 below

$$\begin{aligned}
&\frac{\partial u}{\partial t} = \alpha\left(\frac{\partial u^2}{\partial^2 x}+\frac{\partial u^2}{\partial^2 y}+\frac{\partial u^2}{\partial^2 z}\right) && (x,y,z)\in\Omega,\ t\in[0,+\infty)\\
&u(0,x,y,z) = \varphi(x,y,z) = 0 && (x,y,z)\in\Omega \qquad (9)\\
&u(t,x,y,z) = g(x,y,z) = \begin{cases} y+z-2yz, & x=0,\\ 1-y-z+2yz, & x=1,\\ x+z-2xz, & y=0,\\ 1-x-z+2xz, & y=1,\\ x+y-2xy, & z=0,\\ 1-x-y+2xy, & z=1 \end{cases} && t\in[0,+\infty)
\end{aligned}$$

Outline

STL provides containers `std::array` and `std::vector` for creating one-dimension array.
There are two way for dealing with high-dimension data:

1. Nesting the one dimension arrays or vectors.
2. Hierarchy approach, designing derived classes of one-dimension array base class.

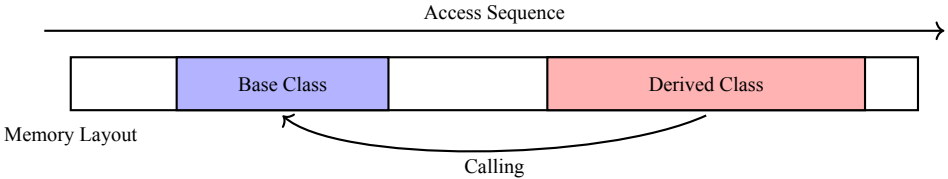

Figure: Derived Class calling members in Base class, timing is not predictable.

1. Nesting multi-dimension array has non-contiguous memory layout.
2. Derived class needs more time to access members in base class.
3. Poor cache utilization leads to poor performance.
4. MPI type create requires contiguous memory layout.

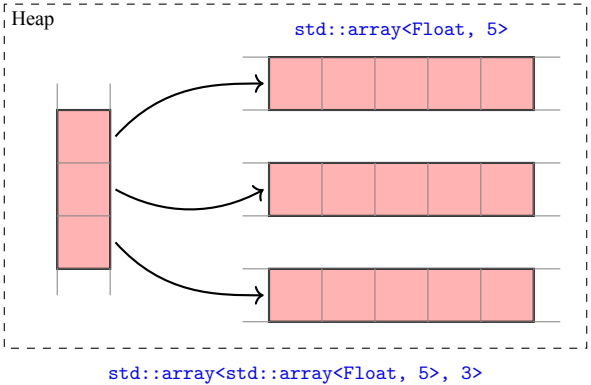

Figure: Using nested `std::array<T, N>` to store 2D array data.

N-dimension Matrix
Solution

- Separate into two detail and user interface objects adhering RAII rules.

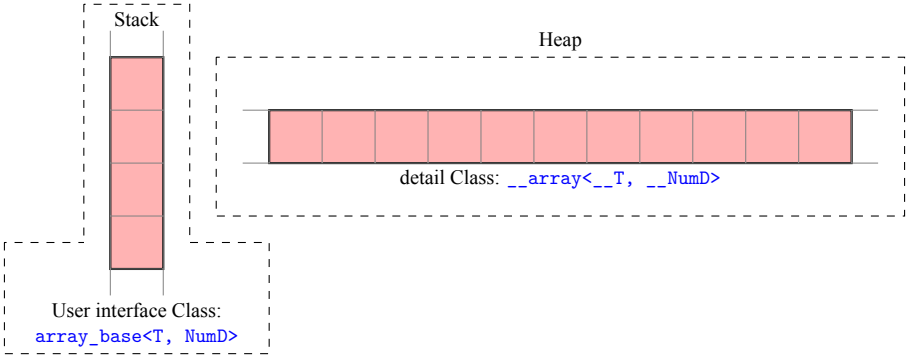

Figure: The solution of N-dimension Matrix, using detail Class, user interface Class

N-dimension Matrix
Solution

- Separate into two detail and user interface objects adhering RAII rules.
- An external small `__multi_array_shape` object defines the routines for accessing the elements.

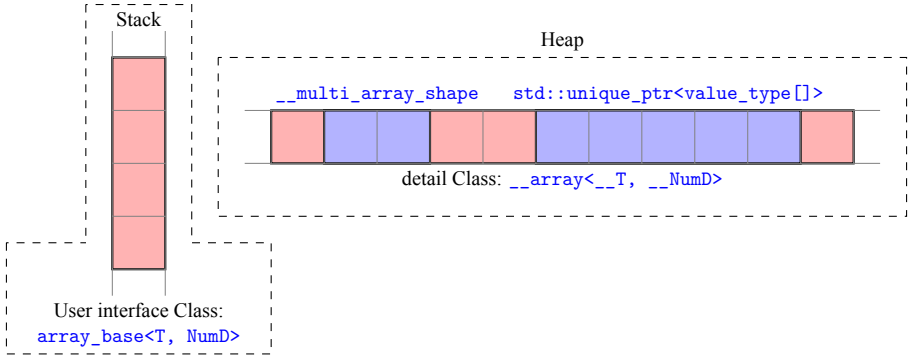

Figure: The solution of N-dimension Matrix, using detail Class, user interface Class and a shape management structure.

N-dimension Matrix
Solution

- Separate into two detail and user interface objects adhering RAII rules.
- An external small `__multi_array_shape` object defines the routines for accessing the elements.
- Smart pointer, ensure memory's contiguous layout and safety.

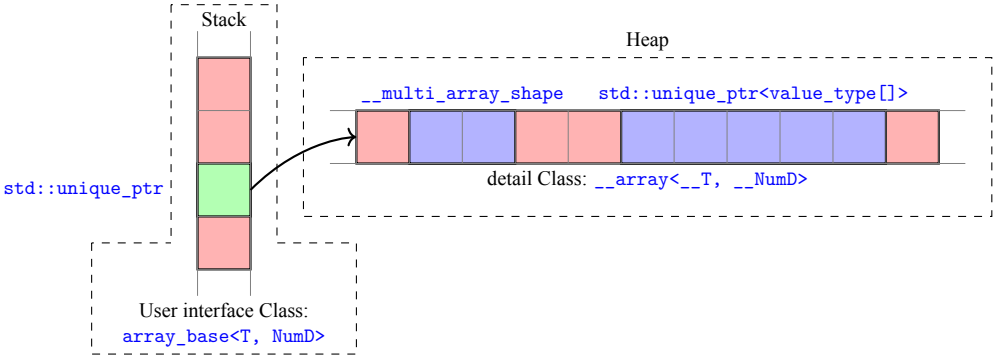

Figure: The solution of N-dimension Matrix, using detail Class, user interface Class and a shape management structure.

The hybrid PDE solver requires the MPI supports multi-threads on each processes.

- High-level libraries like Boost.MPI
  1. have better MPI resource management and other basic communication features.
  2. only provide limited useful features for latter PDE solvers.
  3. lead to lower performance than low-level OpenMPI.

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- High-level libraries like Boost.MPI
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  2. only provide limited useful features for latter PDE solvers.
  3. lead to lower performance than low-level OpenMPI.

- I developed an environment class for MPI
  1. better resource management than raw MPI.
  2. provides basic features exclusively for this project.

Distributed N-dimension arrays are created based on MPI N-dimension Cartesian topology.

Distributed N-dimension arrays are created based on MPI N-dimension Cartesian topology.

1. Ghost communication is required in overlapping of MPI communication and local computation.
2. Parallel I/O is needed for debugging and storing results.
3. Topology information will be frequently used in PDE solver.

1. An MPI Topology class defines the distribution details of N-dimension array.

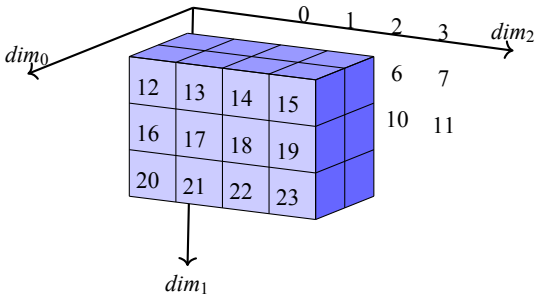

Figure: The Schematic representation of the MPI Cartesian topology scheme of 24 processors on 3 dimension space, which has a $2 \times 3 \times 4$ grid of processes

2. Using `MPI_Type_create_subarray` for creating Ghost MPI datatype for communication.

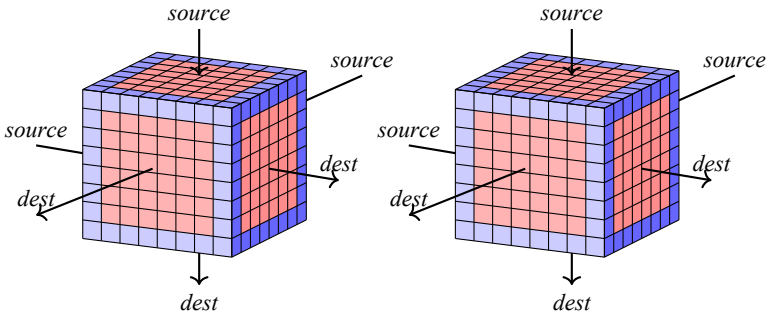

Figure: Representation of a 3D MPI Communication Scheme of 2 among 24 processes between 3 dimension sub-arrays.

3. Cartesian array has members Topology class and N-dimension array class, to ensure they are closely located on memory.
4. The external functions provide gather-based I/O and MPI I/O for handling different scenarios.
   - gather-based function is designed for small scale problem,
     it collects all data included with the boundaries to the root process, and use the I/O of N-dimension array.
   - MPI I/O function is designed for handling large scale problem,
     it only collects the internal bulk without boundary.

5. User interface class unified features for both topology and array classes.
6. Separate into two detail and user interface objects adhering RAII rules.

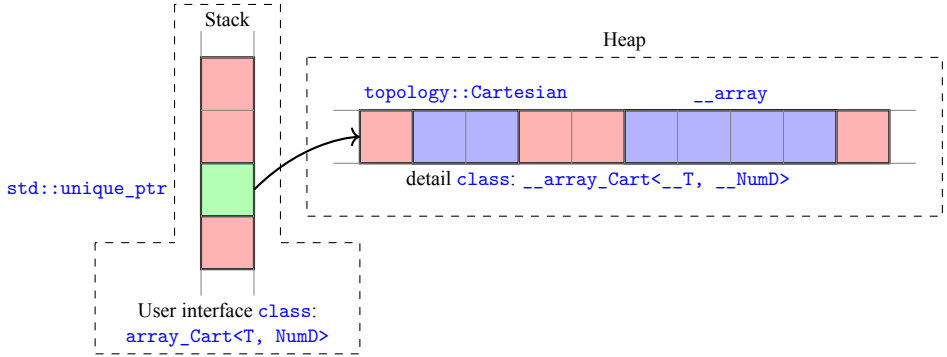

Figure: The solution of distributed N-dimension Array, using detail `class`, user interface `class` and a Cartesian topology `class`.

Outline

Outline

N-dimension Boundary and Initial Conditions
Challanges

1. Mathematical function needs be discretized and distributed as well.
2. Initial and Dirichlet boundary conditions only applies once.
3. Von Neumann boundary condition participates the evolving process in FDM.
4. Need to access the data.

N-dimension Boundary and Initial Conditions
Solution

1. Use `lambda` function to construct classes.
2. Creating external classes for each conditions as the `friend` classes of PDE solver classes.
3. Set `Bool` vectors help to determine the status of conditions and type of boundary conditions.

N-dimension PDE solvers
Challanges

1. PDE solver of Heat Equations in different dimension space have similar parameters and features, but type-field solution lead to code redundancy.
2. Applying MPI communications between local arrays, avoiding overhead.

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2. Applying MPI communications between local arrays, avoiding overhead.
3. Three type of strategies:
    1. Pure MPI parallel
    2. Master-only, no overlapping hybrid parallel.
    3. Master-only, communication/computation (comm./comp.) overlapping hybrid parallel.

`virtual` function is resolved at run-time though `vtable`, and only lose up to about 25% efficiency in terms of the function call mechanism,

1. Create an abstract Heat base class of Heat Equation, and `override` functions in derived class on every dimension.

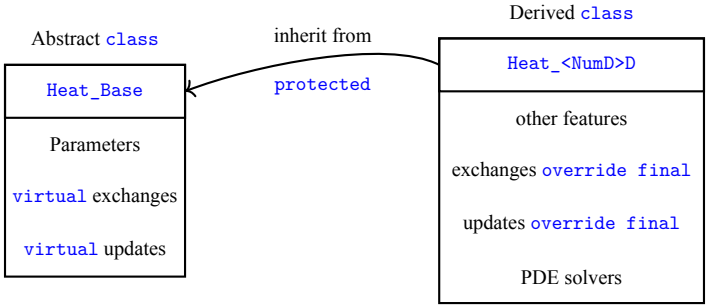

Figure: Abstract inheritance scheme representation.

The MPI Remote Memory Access (MPI-RMA) operations require hardware support to gain the benefits, so:

2. MPI communications are implemented in
   - non-blocking using `MPI_Isend`/`MPI_Irecv`.
   - blocking using `MPI_Sendrecv`

Outline

3. Three type of strategies
   1. Pure MPI parallel

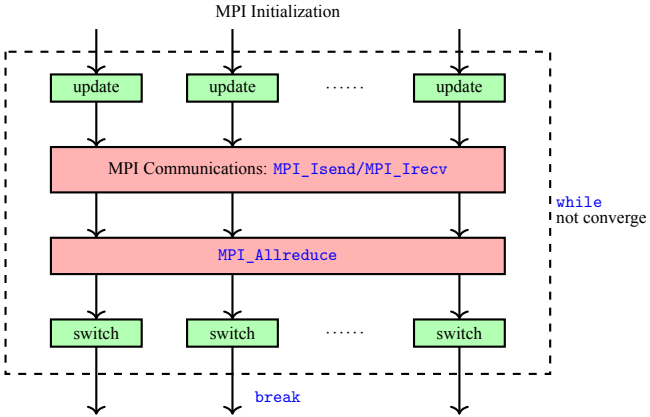

Figure: Scheme Representation: flow chart of Pure MPI model

- Three type of strategies
  1. Master-only, no overlapping hybrid parallel.

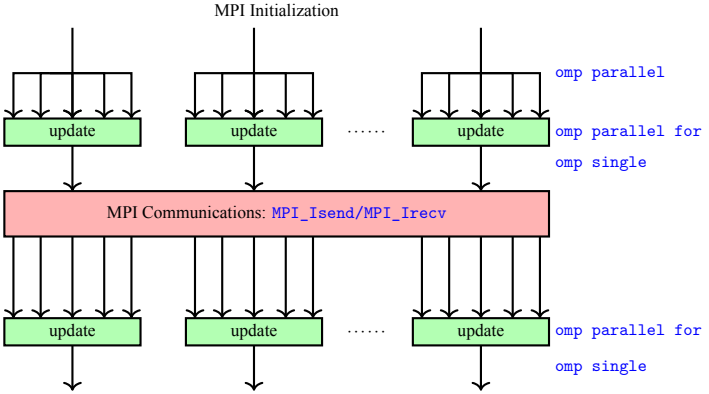

Figure: Scheme Representation: flow chart of Hybrid model, with no overlapping

3. Three type of strategies
   1. Master-only, comm./comp. overlapping hybrid parallel.

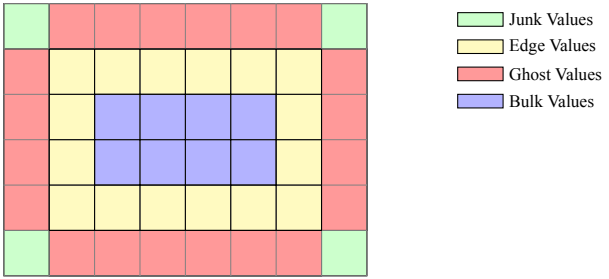

Figure: Scheme Representation: Grid 2D, type of values

3. Three type of strategies
   1. Master-only, comm./comp. overlapping hybrid parallel.

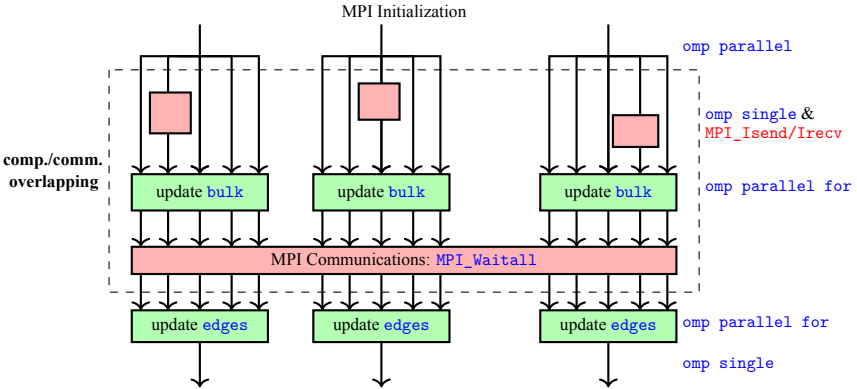

Figure: Scheme Representation: flow chart of Hybrid model, with comp./comm. overlapping

`Python` has many easy-use libraries such as `Pytorch`, `Tensorflow` and `Caffe`.

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For neural network implementations, there are some issues in practice:

1. Interpret language `Python` is significant slower than compile language `C/C++`
2. Worse resource management than `C/C++`
3. Lower security in parallel program.

For getting higher performance and better safety, I chose to use

1. Pytorch C++ API: `Libtorch`.

to reproduce the Python version of PINN.

Outline

Hardware

GPU cluster

Each node has a

- AMD Ryzen 7, 7800 X3D, with 16 CPU(s)
- NVIDIA RTX 4090, 24GB

CPU cluster

Each node has a: `Intel(R) Xeon(R) Platinum 9242 CPU 2.30Ghz with 96 CPU(s), 4 Non-unified Memory Access (NUMA) nodes, 1MB L2 cache, 35.75MB L3 cache.`

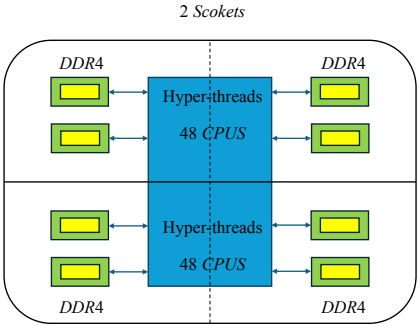
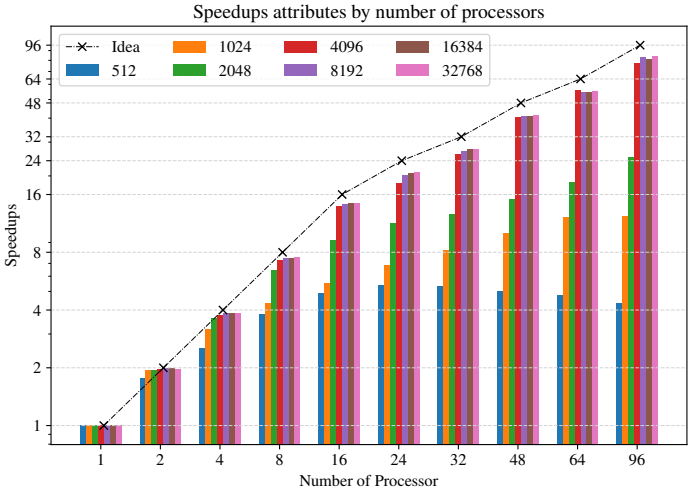


Figure: NUMA topology of single node on Cluster

Single Node Scaling Tests

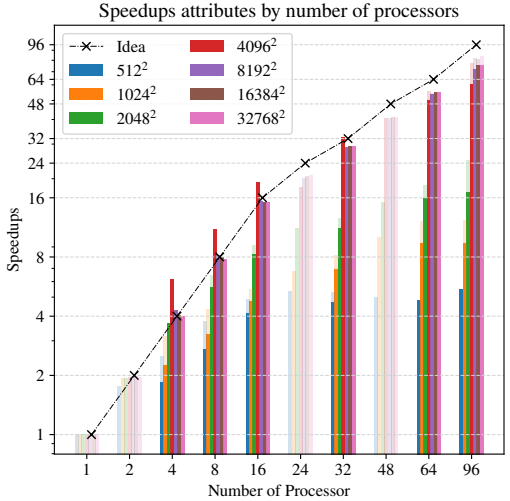
- 2D Heat Equation
- Single Precision
- Problem Size: $512^2, 1024^2, 2048^2, 4096^2, 8192^2, 16384^2, 32768^2$
- Run 5 times for each test, remove the max/mini-mum values, use the average of left 3.

Single Node Scaling Tests
Strong Scaling - Pure MPI

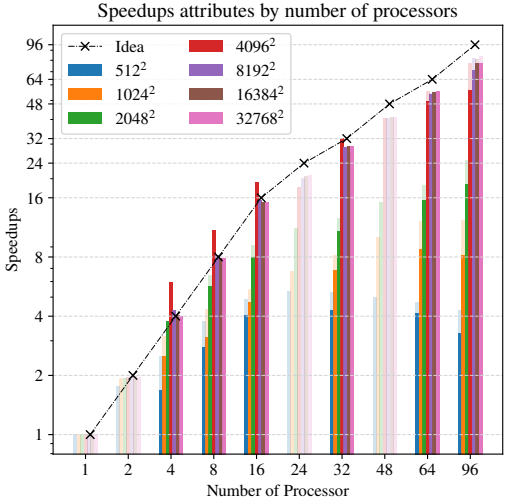


Single Node Scaling Tests

Strong Scaling - MPI/OpenMP Hybrid



(a) No overlapping comm./comp.



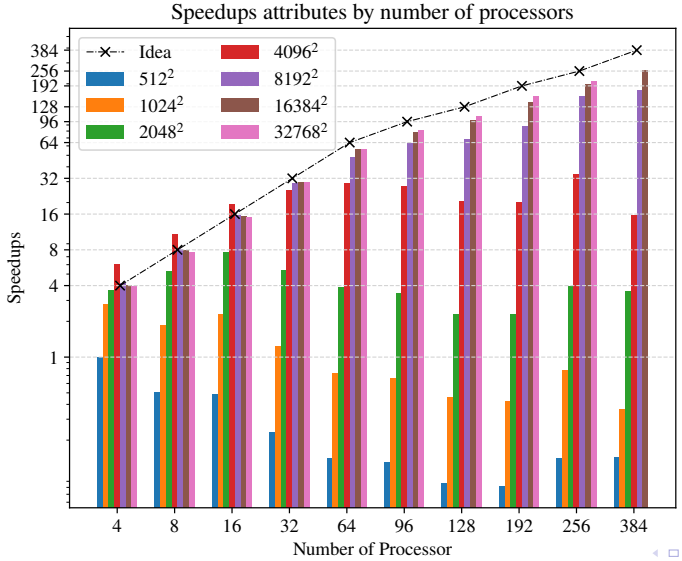
(b) With overlapping comm./comp.

Single Node Scaling Tests

Weak Scaling

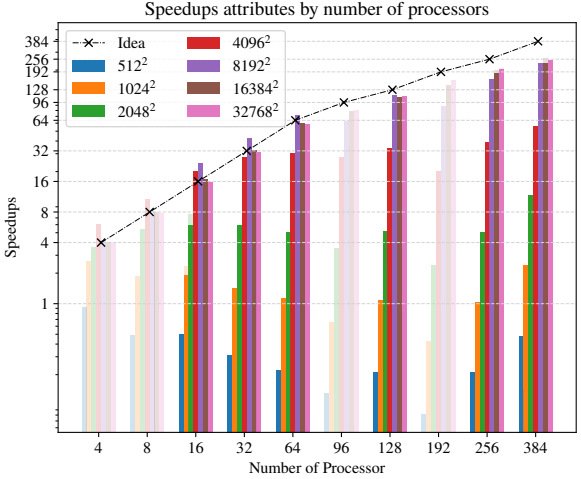
Strategy	Size	Number of CPUs			$f_p(\%)$
		4	**16**	**64**	
Pure MPI	512^2	4.006	12.497	47.849	75.1
No Overlap		2.876	11.206	42.754	67.0
With Overlap		3.173	10.818	42.282	66.2
Pure MPI	1024^2	3.838	9.304	33.707	53.2
No Overlap		3.947	12.995	33.447	54.1
With Overlap		4.024	12.932	33.361	54.0
Pure MPI	2048^2	2.376	8.245	31.203	49.0
No Overlap		3.874	8.972	31.510	49.8
With Overlap		3.740	8.989	31.430	49.7
Pure MPI	4096^2	3.543	8.245	31.203	77.5
No Overlap		3.953	13.799	49.515	78.0
With Overlap		3.948	13.800	49.989	78.7

Multi-node Scaling Tests
Strong Scaling - Pure MPI



Multi-node Scaling Tests

Strong Scaling - MPI/OpenMP Hybrid



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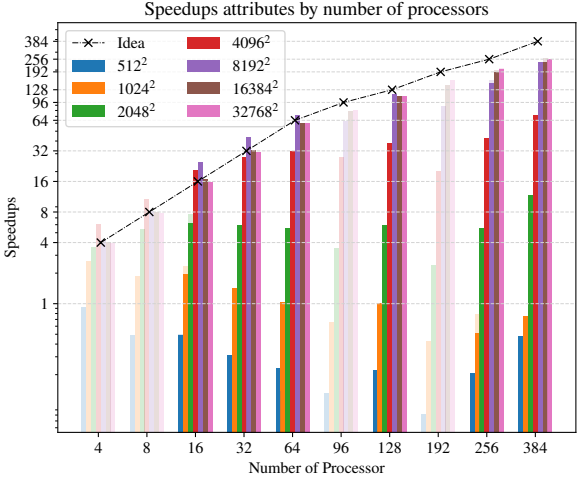
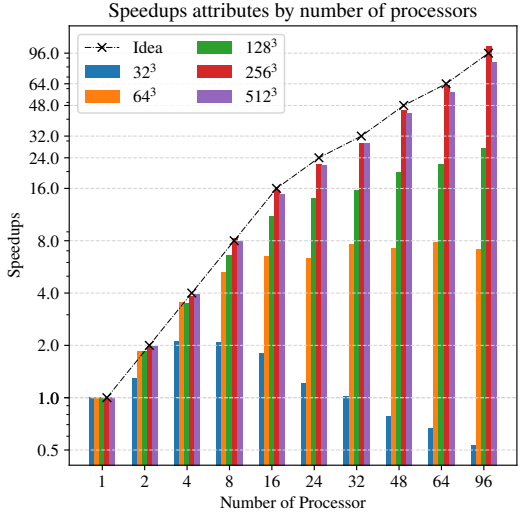


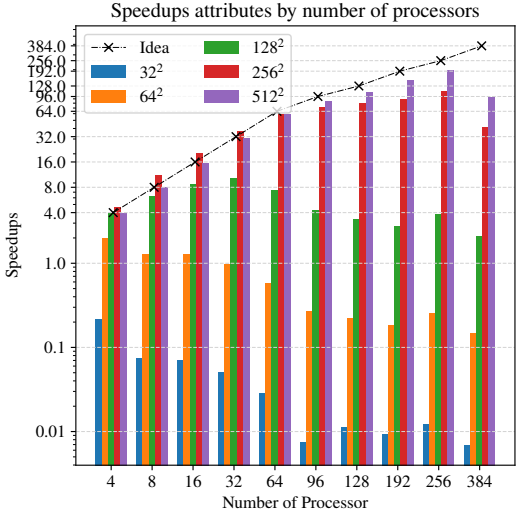
(b) With overlapping comm./comp.

Multi-node Scaling Tests
Weak Scaling

Strategy	Size	Number of CPUs				$f_p(\%)$
		4	**16**	**64**	**256**	
Pure MPI	512^2	3.300	10.379	26.000	124.375	48.2
No Overlap		-	8.094	25.931	127.648	49.3
With Overlap		-	8.386	27.126	116.951	45.5
Pure MPI	1024^2	3.848	13.037	30.143	-	49.3
No Overlap		-	13.702	44.040	-	69.8
With Overlap		-	13.834	44.090	-	69.9
Pure MPI	2048^2	3.787	9.172	32.013	-	50.6
No Overlap		-	13.936	34.368	-	55.7
With Overlap		-	14.274	34.414	-	55.9
Pure MPI	4096^2	3.884	13.859	51.041	-	80.2
No Overlap		-	15.315	53.157	-	83.8
With Overlap		-	15.294	53.401	-	84.2



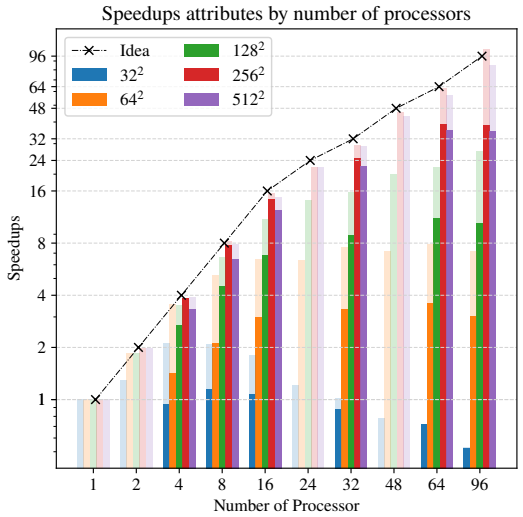
(a) Single node



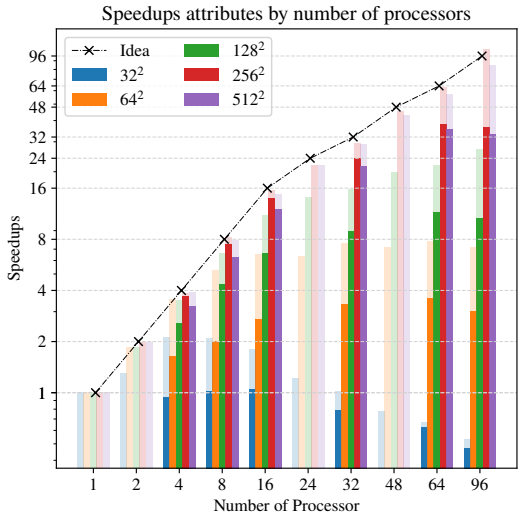
(b) Four nodes

3D Space Heat Equation

Strong Scaling - MPI/OpenMP Hybrid, Single Node



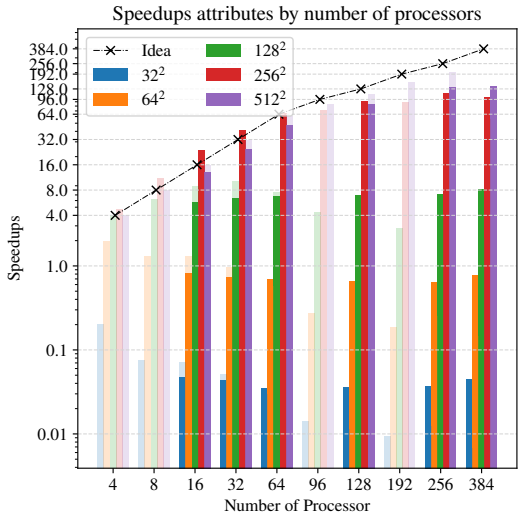
(a) Non-overlapping



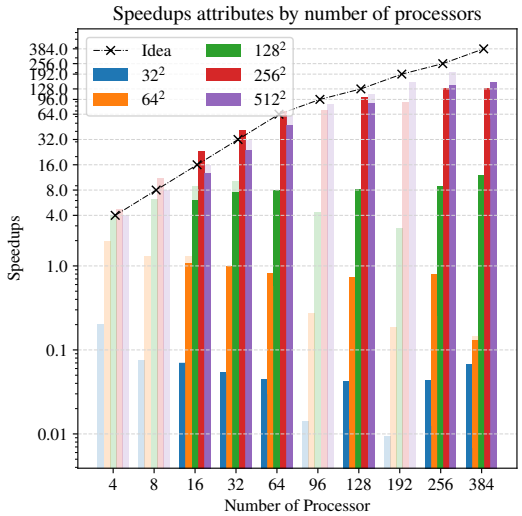
(b) With overlapping

3D Space Heat Equation

Strong Scaling - MPI/OpenMP Hybrid, Four Nodes



(a) Non-overlapping



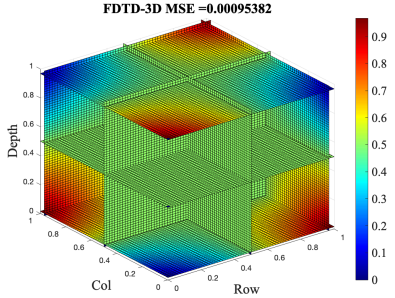
(b) With overlapping

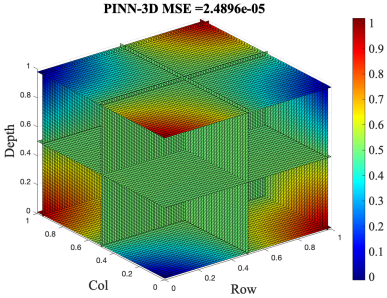
3D Space Heat Equation
Weak Scaling

Strategy	Size	Number of CPUs 8	64	$64_{\text{Multi-node}}$	$f_p(\%)$	$f_p(\%)_{\text{Multi-node}}$
Pure MPI		5.243	26.405	9.078	41.6	14.2
No Overlap	32^3	2.124	13.386	8.094	21.0	12.7
With Overlap		2.014	13.884	9.586	21.8	39.7
Pure MPI		7.937	32.034	30.106	50.8	47.1
No Overlap	64^3	5.393	20.007	33.460	31.8	52.3
With Overlap		5.200	19.558	35.254	31.1	31.6
Pure MPI		3.513	24.239	25.428	38.0	39.7
No Overlap	128^3	3.303	15.235	35.254	24.1	55.1
With Overlap		3.187	15.107	20.096	23.9	31.4

Table: Mean Square Error (MSE) of Approximations, Tolerance: 10^{-4}

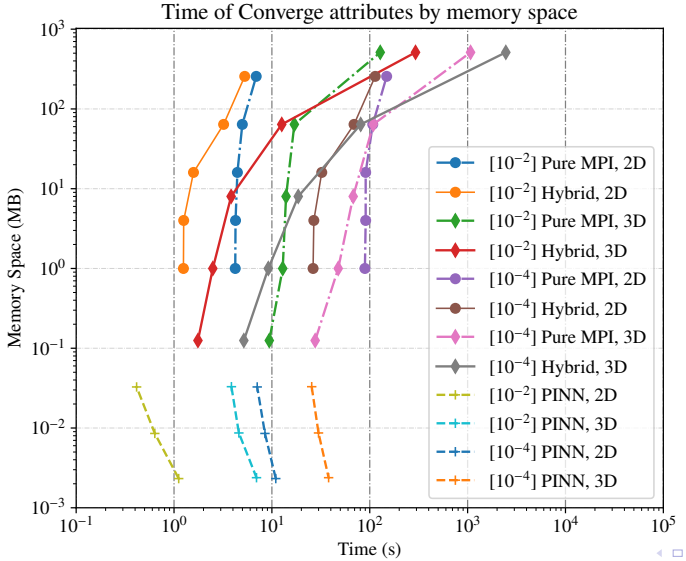
Method	Heat 2D	Heat 3D
FDTD	1.7287	953.84
PINN	13.37	24.896





PINN v.s. FDTD

Memory Usage v.s. Time of Convergence



Outline

For 2D and 3D Thermal Conduction PDE systems
I implemented the FDTD methods in fined region with three parallel models:

- Pure MPI model
  1. had best performance on single compute node overall.
  2. speedup ratio quickly drop on multi-node.
- MPI/OpenMP Hybrid models
  1. had lower performance in general.
  2. can make more use of the advantage of L3 cache.
  3. superliner speedup in certain scenario.

For 2D and 3D Thermal Conduction PDE systems
I implemented PINN models and trained on generated datasets, comparing with FDTD, the PINN

1. had identical or higher accuracy.
2. had less memory usage.
3. took shorter time to get the predictions(results).
4. had more flexibility on producing the results.

In this project, in order to overcome the obstacles, I

- Used abstract mechanisms in C++, the Meta-programming techniques, to ensure high flexibility, security.
- Used smart pointers to have better resource management.
- Tried to use hybrid parallel techniques to have better scaling performance.
- Made a comparison with the state-of-the-art PINN models.

Outline

Further Research Directions

- Resource Management
- Workload Management
- MPI/CUDA Hybrid parallel of FDTD/PINN
- Other PDE Systems
- Other Boundary Conditions

Closing Remarks [3, 4]

Thank you for your attention!

Any questions?

[3] Full docs: `https://liyihai.com/html/index.html`

[4] Git repository: `https://github.com/liyihai-official/Final-Project`