

Meta-Programming and Hybrid Parallel Strategies for Solving PDEs: An FDM and PINN Comparison ^{1, 2}

Seminar Presentation III

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¹full docs: <https://liyihai.com/html/index.html>

²repository: <https://github.com/liyihai-official/Final-Project>

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Introduction

Recap - Deep Neural Network

Kolmogorov PDEs

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

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

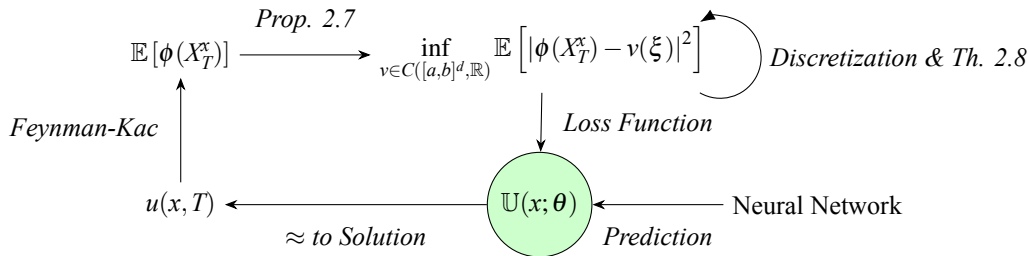


Figure: Deep Neural Network (DNN) Methodology of Solving Kolmogorov PDEs **[FIRST]**

Introduction

Recap - Physics Informed Neural Network

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 .

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

Define $f(t, x)$ to be given by $f(t, x) = u_t(t, x) + \Gamma[u; \lambda]$ (3)

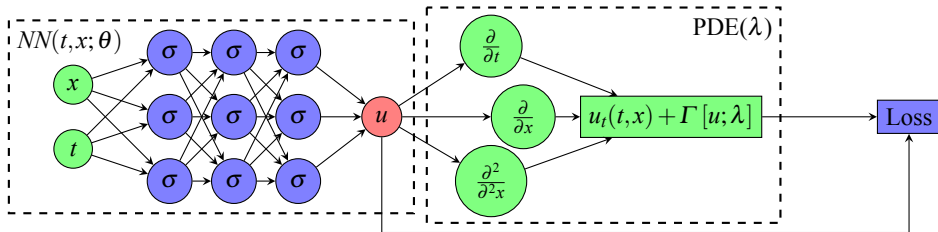


Figure: PINN, with 3 fully connected hidden layers

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

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.

However, there were many obstacles including:

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

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General Form of problem

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

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

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

Boundary Conditions

The Dirichlet and Von Neumann boundary conditions are formed as

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

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

Thermal Conduction Systems

Heat Equation 2D

The function

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

is the solution of 2D Heat Equation 7 below

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

Thermal Conduction Systems

Heat Equation 3D

The function

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

is the solution of 3D Heat Equation 9 below

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

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N-dimension Matrix

Challenges

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.

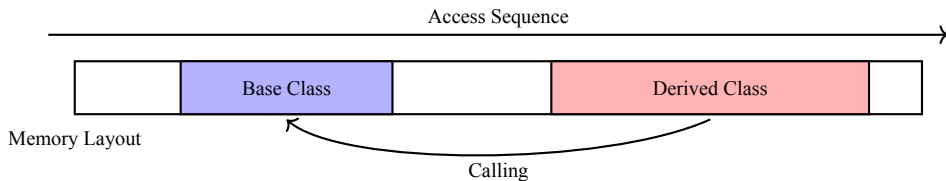


Figure: Derived Class calling members in Base class, timing is not predictable.

- 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.

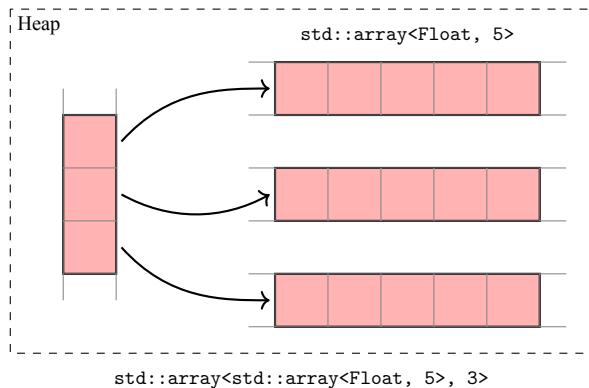


Figure: Using nested `std::array<T, N>` to store 2D array data.

N-dimension Matrix

Solution

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

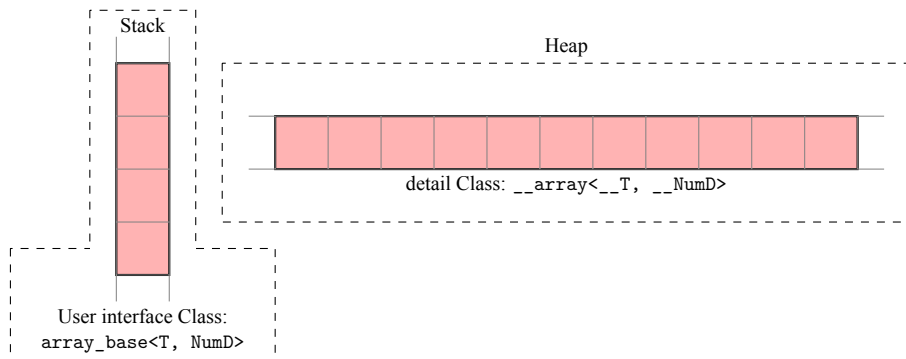


Figure: The solution of N-dimension Matrix, using detail Class, user interface Class

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.

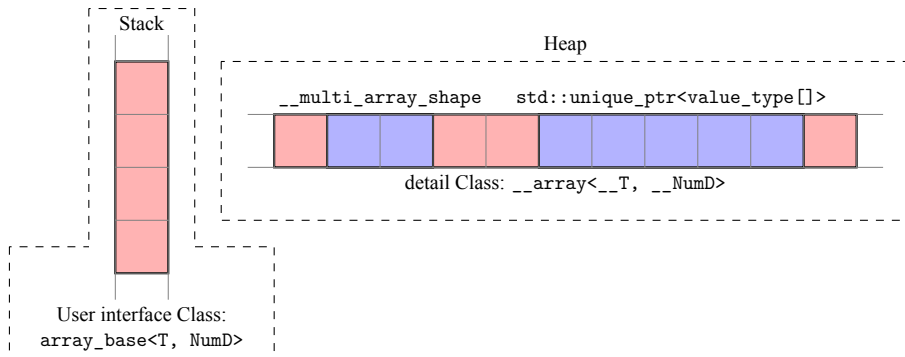


Figure: The solution of N-dimension Matrix, using detail Class, user interface Class and a shape management structure.

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.

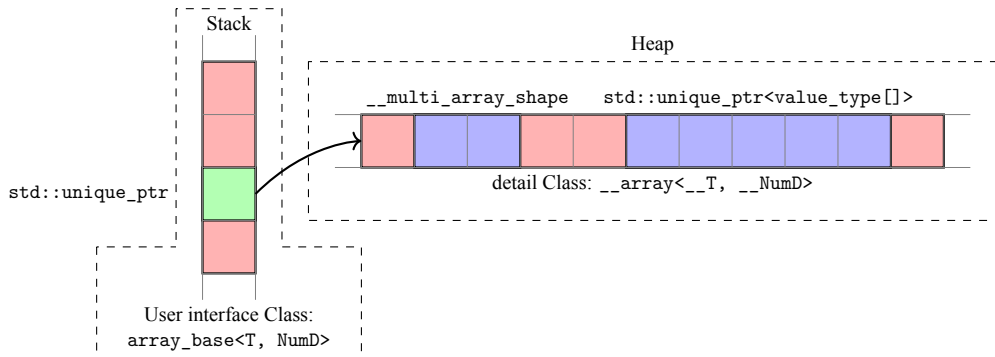


Figure: The solution of N-dimension Matrix, using detail Class, user interface Class and a shape management structure.

Parallelization of N-dimension Arrays

MPI Environment

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.

Parallelization of N-dimension Arrays

MPI Environment

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

Parallelization of N-dimension Arrays

MPI Topology - Challenges

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.

Parallelization of N-dimension Arrays

MPI Topology - Solution

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

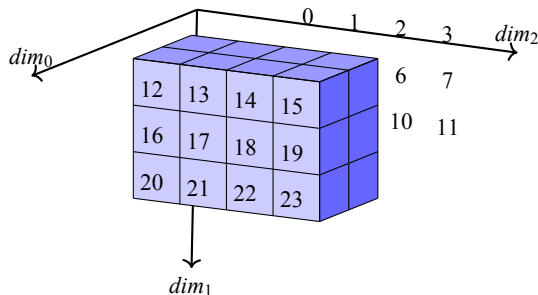


Figure: The Schematic representation of the MPI Cartesian topology scheme of 24 processors on 3 dimension space, which has a $2 \times 3 \times 4$ grid of processes

Parallelization of N-dimension Arrays

MPI Topology - Solution

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

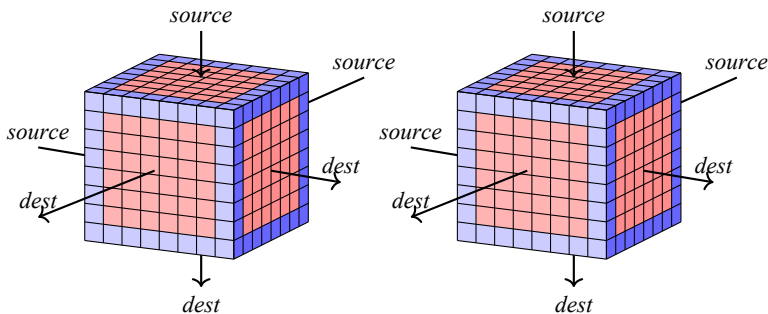


Figure: Representation of a 3D MPI Communication Scheme of 2 among 24 processes between 3 dimension sub-arrays.

Parallelization of N-dimension Arrays

MPI Topology - Solution

- 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.

Parallelization of N-dimension Arrays

MPI Topology - Solution

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

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N-dimension Boundary and Initial Conditions Challenges

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

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

Challenges

- ❶ PDE solver of Heat Equations in different dimension space have similar parameters and features, type-field solution lead to code redundancy.
- ❷ Applying MPI communications between local arrays, avoiding overhead.
- ❸ Three type of strategies:
 - ❶ Pure MPI parallel
 - ❷ Master-only, no overlapping hybrid parallel.
 - ❸ Master-only, communication/computation (comm./comp.) overlapping hybrid parallel.

virtual function is resolved at run-time, 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 overriding functions in derived class on every dimension.

N-dimension PDE solvers

Solutions

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

N-dimension PDE solvers

Solutions

- ③ Three type of strategies
 - ① Pure MPI parallel

N-dimension PDE solvers

Solutions

- ③ Three type of strategies
 - ① Master-only, no overlapping hybrid parallel.

N-dimension PDE solvers

Solutions

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

PINN Model

Challenges

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

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

- 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.

PINN Model

Solution

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

- 1 Pytorch C++ API: Libtorch.

to reproduce the Python version of PINN.

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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

Non-unified Memory Access (NUMA) node Topology:

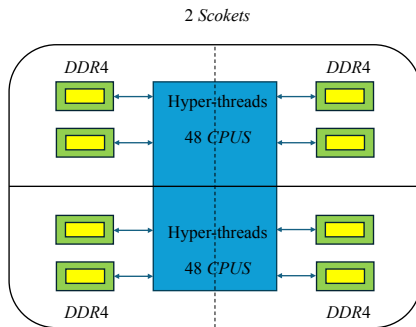
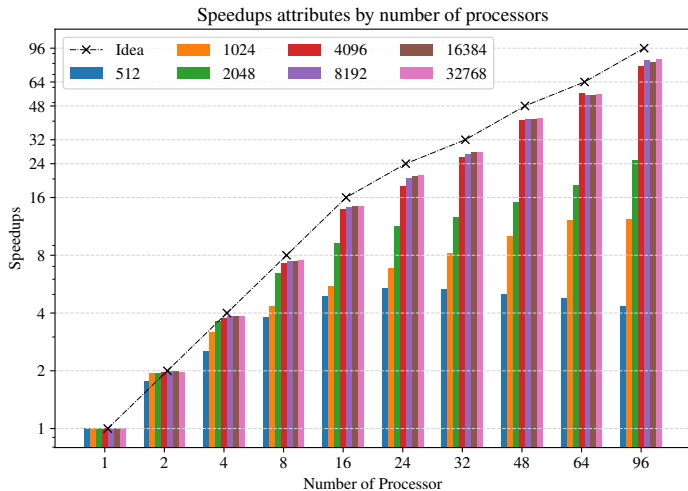


Figure: NUMA topology of single node on Cluster

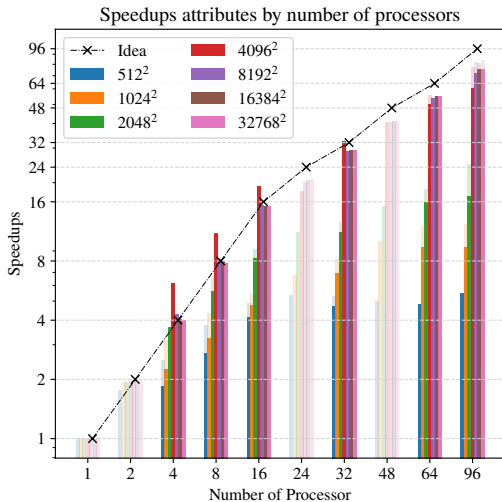
Single Node Scaling Tests

Strong Scaling - pure MPI

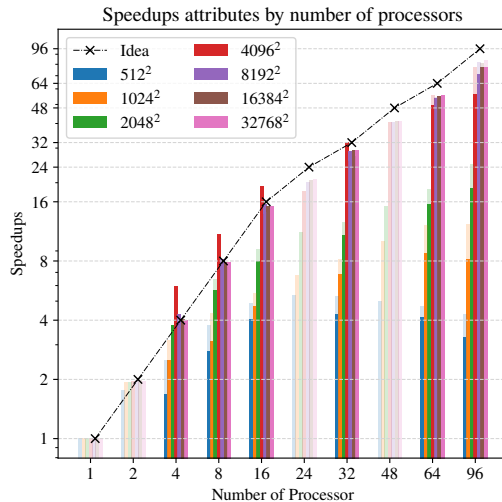


Single Node Scaling Tests

Strong Scaling - MPI/OpenMP Hybrid



(a) No overlapping comm./comp.



(b) With overlapping comm./comp.

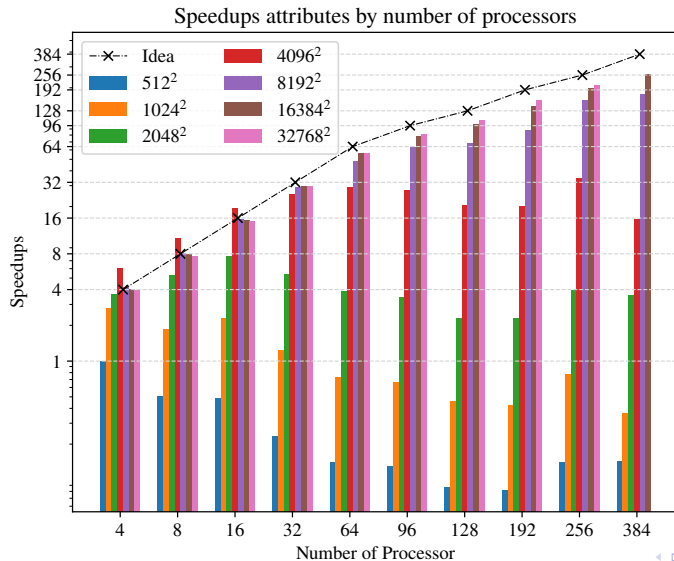
Single Node Scaling Tests

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

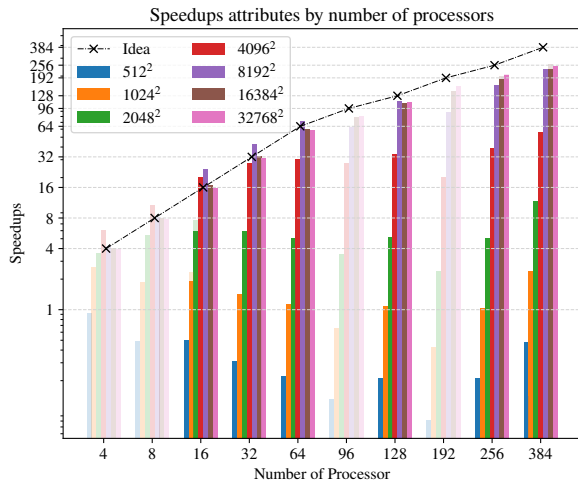
Multi-node Scaling Tests

Strong Scaling - pure MPI

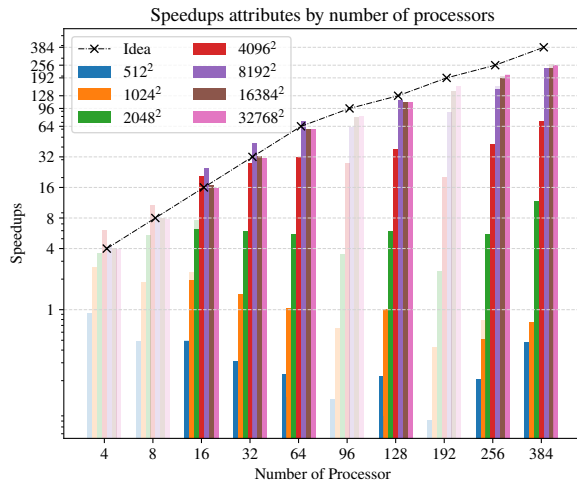


Single Node Scaling Tests

Strong Scaling - MPI/OpenMP Hybrid



(a) No overlapping comm./comp.



(b) With overlapping comm./comp.

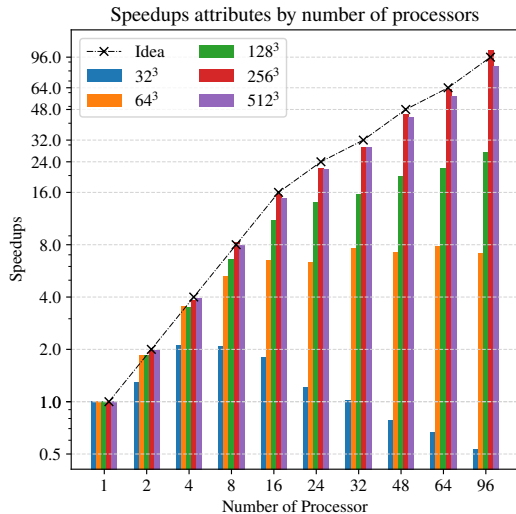
Single Node Scaling Tests

Weak Scaling

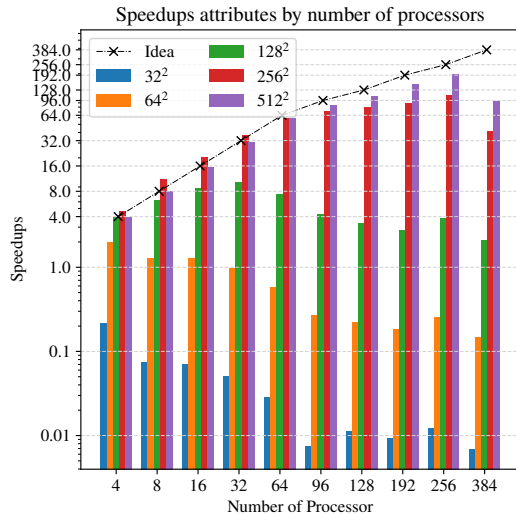
Strategy	Size	Number of CPUs				$f_p(\%)$
		4	16	64	256	
Pure MPI	512 ²	3.300	10.379	26.000	124.375	48.2
No Overlap		-	8.094	25.931	127.648	49.3
With Overlap		-	8.386	27.126	116.951	45.5
Pure MPI	1024 ²	3.848	13.037	30.143	-	49.3
No Overlap		-	13.702	44.040	-	69.8
With Overlap		-	13.834	44.090	-	69.9
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

3D Space Heat Equation

Strong Scaling - pure MPI



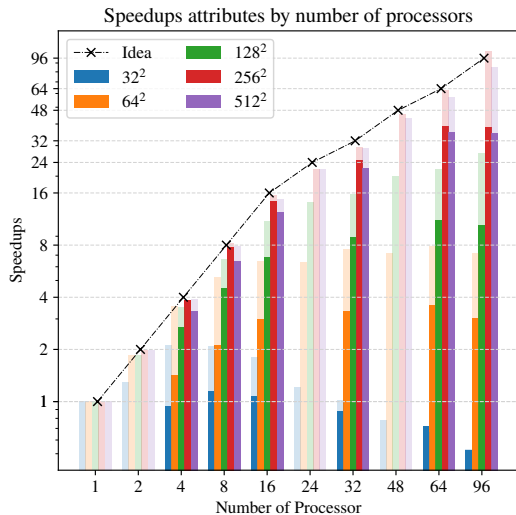
(a) Single node



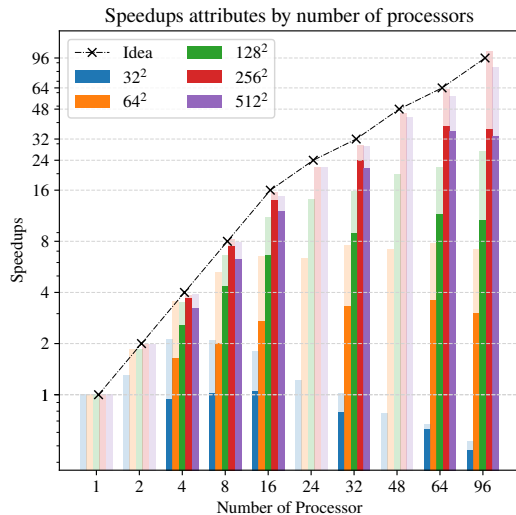
(b) Four nodes

3D Space Heat Equation

Strong Scaling - MPI/OpenMP Hybrid, Single Node



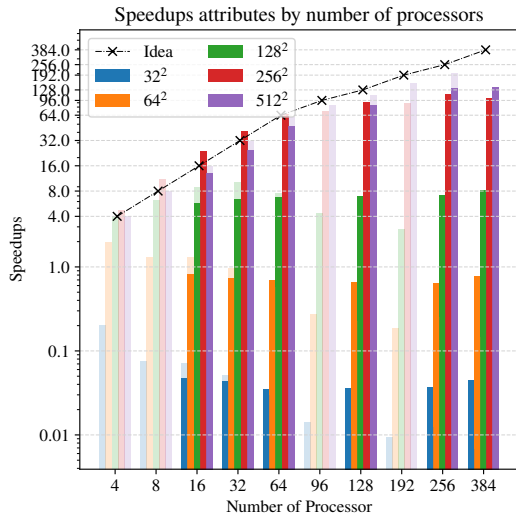
(a) Non-overlapping



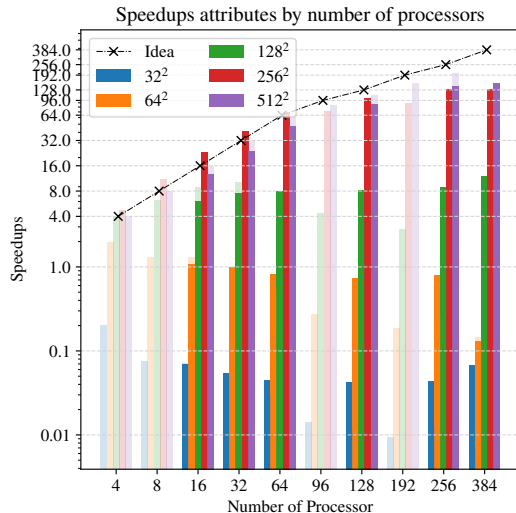
(b) With overlapping

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

PINN v.s. FDTD

Accuracy

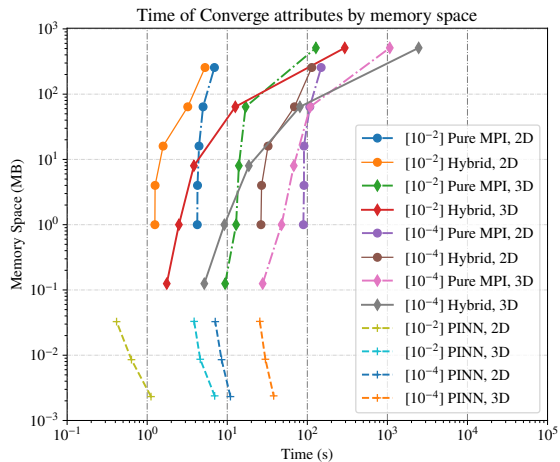
Table: Mean Square Error of Results

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

Tolerance: 10^{-4}

PINN v.s. FDTD

Memory Usage v.s. Time of Convergence



Figure

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Conclusion

Finite Difference Time Domain Method

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.

Conclusion

Physics Informed Neural Network

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.

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Further Research Directions

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

Thank you for your attention!

Any questions?