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Deal.II Matrix Free Solver for Advection-Diffusion-Reaction

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Mathematical Background

Advection-Diffusion-Reaction

Problem

$$\begin{cases} -\nabla \cdot (\mu \nabla u) + \beta \cdot \nabla u + \gamma u = f & \text{in } \Omega \\ u = g & \text{on } \Gamma_D \subset \partial\Omega \\ \nabla u \cdot \vec{n} = h & \text{on } \Gamma_N = \partial\Omega \backslash \Gamma_D \end{cases}$$

Weak Formulation

$$\text{Find } u \in V \quad a(u,v) = f(v) - a(R_g, v) \quad \forall v \in V$$

$$\text{where:} \qquad a(u,v) = \underbrace{\int_\Omega \mu \nabla u \cdot \nabla v}_{\text{diffusion}} + \underbrace{\int_\Omega (\beta \cdot \nabla u) v}_{\text{advection}} + \underbrace{\int_\Omega \gamma u v}_{\text{reaction}}$$

$$f(v) = \int_\Omega f v + \int_{\Gamma_N} h v$$

Mathematical Background

Matrix-Free discretization

$$(A_k)_{ij} = \int_k [\mu \nabla \varphi_j \nabla \varphi_i] + [\beta \cdot \nabla \varphi_j \varphi_i] + [\gamma \varphi_j \varphi_i]$$

$$(A_k)_{ij} \approx \sum_{q=1}^{N_q} [\mu(\nabla \varphi_j(x_q) \cdot \nabla \varphi_i(x_q)) + \beta \cdot \nabla \varphi_j(x_q) \varphi_i(x_q) + \gamma \varphi_j(x_q) \varphi_i(x_q)] \, |J_q| w_q$$

$$(A_k)_{ij} \approx \sum_{q=1}^{N_q} \nabla \varphi_i(x_q) \underbrace{[\mu J_q w_q]}_{D_\mu} \nabla \varphi_j(x_q) + \sum_{q=1}^{N_q} \varphi_i(x_q) \underbrace{[\beta J_q w_q]}_{D_\beta} \nabla \varphi_j(x_q) + \sum_{q=1}^{N_q} \varphi_i(x_q) \underbrace{[\gamma J_q w_q]}_{D_\gamma} \varphi_j(x_q)$$

$$A_k = \underbrace{B^T D_\mu B}_{\text{Diffusion}} + \underbrace{B^T D_\beta K}_{\text{Advection}} + \underbrace{K^T D_\gamma K}_{\text{Reaction}}$$

$$B_{qj} = \nabla \phi_j(x_q) \qquad B, K \in \mathbb{R}^{N_q \times N_{\text{DoF}}}$$

$$K_{qj} = \phi_j(x_q) \qquad D_\mu, D_\beta, D_\gamma \in \mathbb{R}^{N_q \times N_q}$$

Mathematical Background

Non-Homogeneous lifting

Deal.ii Matrix-Free classes **do not** natively support **non-homogeneous problems**...

Our solution:

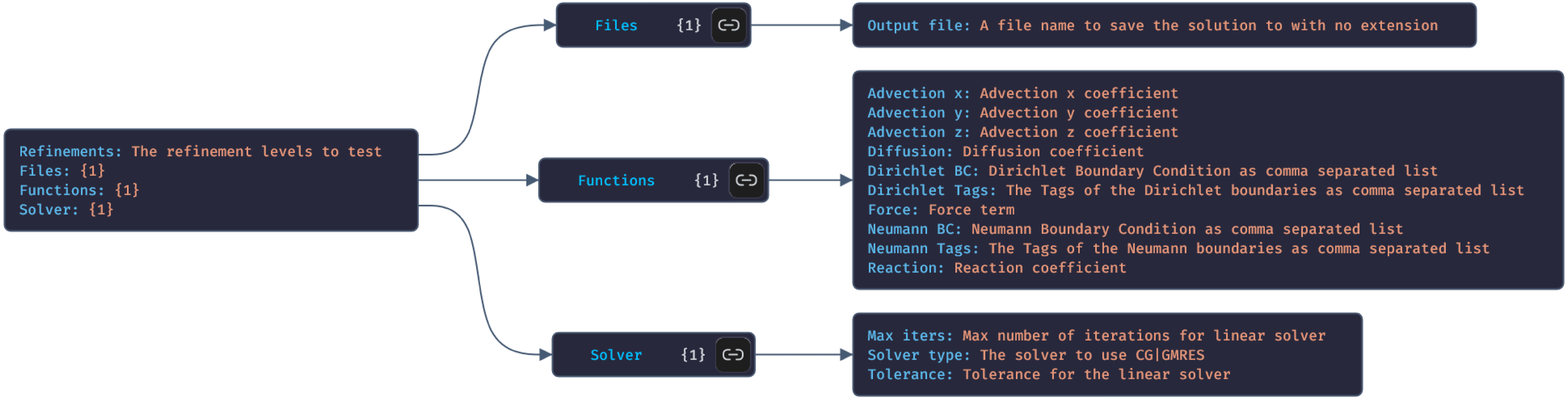
$$\text{Solve for } Au_0 = \hat{f}$$

$$\text{Where } \hat{f} = f - Au_g \text{ and } u_g = \begin{cases} g & \text{on the boundary nodes} \\ 0 & \text{elsewhere} \end{cases}$$

Project Architecture

Problem definition system

Parameters File (.prm)



Project Architecture

Solver classes

Parameters File (.prm)

Matrix-Based Solver

ADRMBProblem<dim>

→ Multigrid
→ deal.II Jacobi Smoother
→ CG / GMRES

Matrix-Free Solver

ADRProblem<dim>

→ Multigrid
→ Custom Jacobi Smoother
→ CG / GMRES
\+ SIMD Instructions

Usage example

```
Utilities::MPI::MPI_InitFinalize mpi_init(argc, argv,1);
MatrixBasedADR::ADRMBProblem<3> adr_problem;
adr_problem.run("../input/params/pb_3d_mb.prm");
```

Project Architecture

Documentation

Matrix-Free ADR Solver

Implementation of a Matrix-Free solver library for ADR problems

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- ► Matrix-Free FEM Solver for the Advectio
- ► Namespaces
- ► Classes
- ► Files

Matrix-Free FEM Solver for the Advection-Diffusion-Reaction Equation

A finite element solver for the advection-diffusion-reaction (**ADR**) equation in 2D/3D using deal.II. Compares a **matrix-free** approach (sum factorization + SIMD vectorization + geometric multigrid) against a traditional **matrix-based** approach (sparse matrix assembly) in terms of performance and memory usage.

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Mathematical Formulation

Strong form

$$\begin{cases} -\nabla \cdot (\mu \nabla u) + \beta \cdot \nabla u + \gamma u = f & \text{in } \Omega \subset \mathbb{R}^d, \quad d \in \{1,2,3\} \\ u = g & \text{on } \Gamma_D \subset \partial\Omega \\ \nabla u \cdot \vec{n} = h & \text{on } \Gamma_N = \partial\Omega \setminus \Gamma_D \end{cases}$$

where μ is the diffusion coefficient, β is the advection coefficient, γ is the reaction coefficient, and f is the forcing term.

Weak form

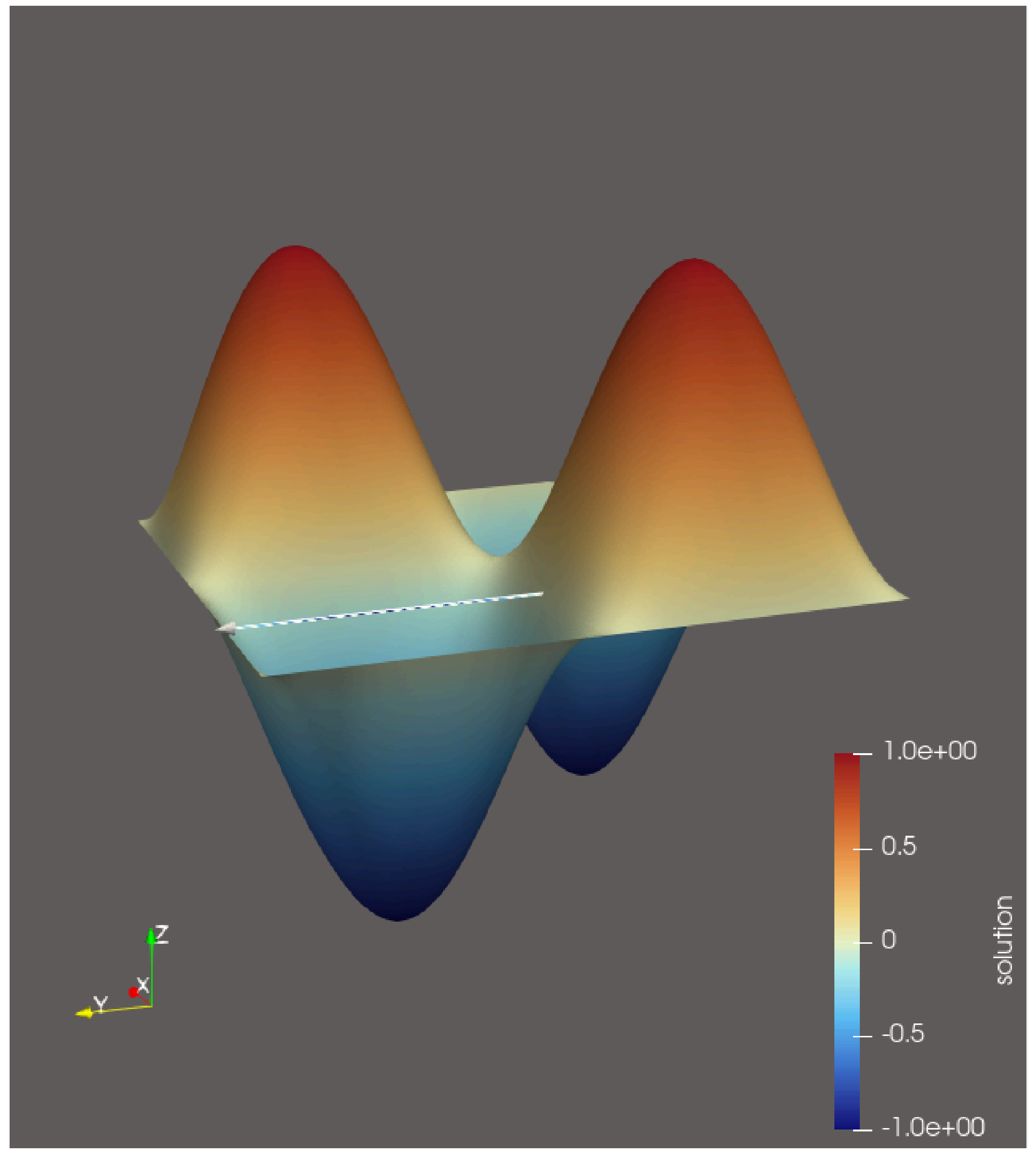
Benchmarks

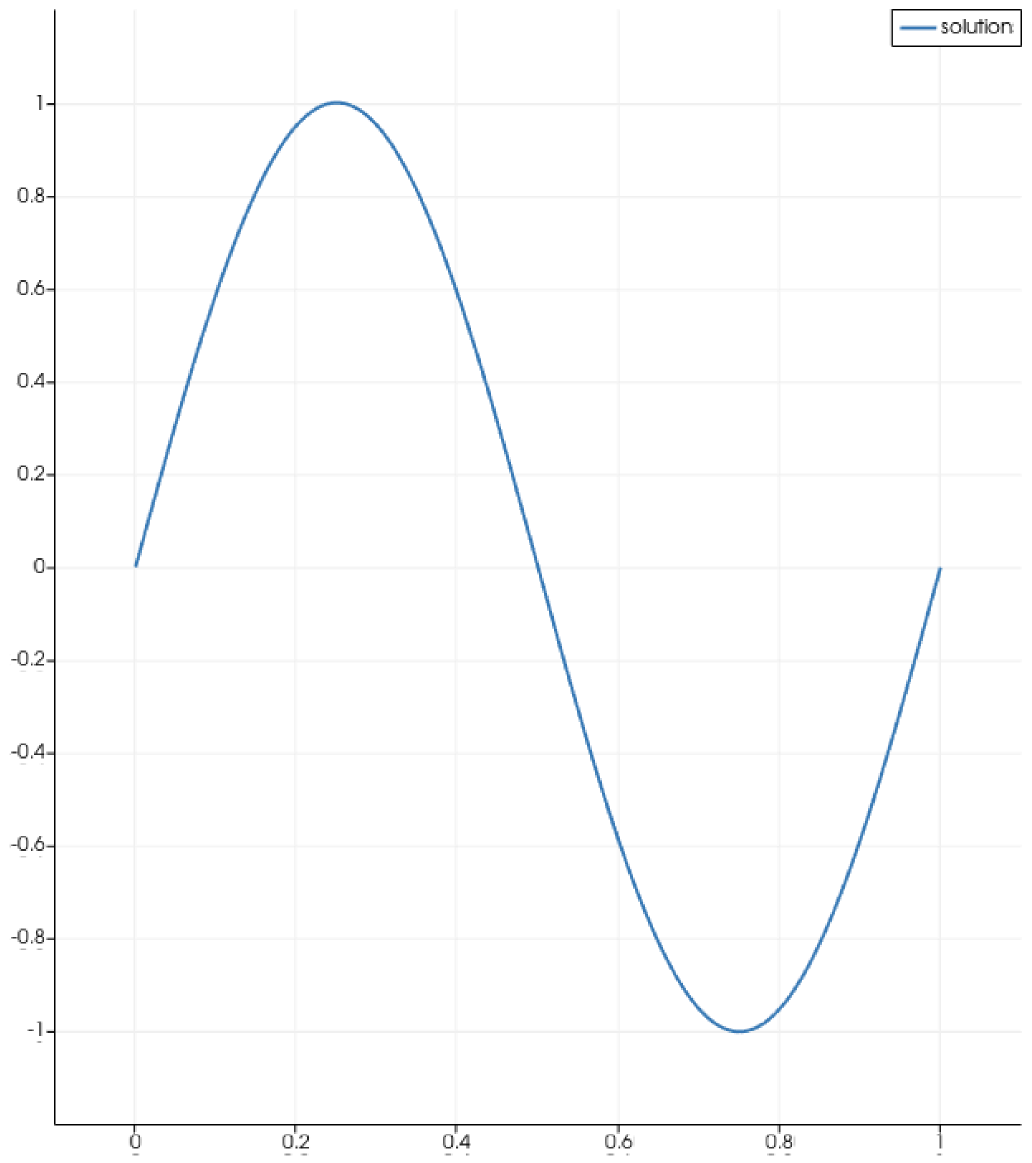
Homogeneous Dirichlet Boundary Conditions

Running on: Intel i7-14700HX @ 5.3GHz
20 Cores | **28 Threads**

2D $u_{ex} = sin(2\pi x)sin(2\pi y) \quad \Omega = [0, 1]^2$

$$\beta_{\text{small}} = [0.1 \quad 0.3]^T$$
$$\beta_{\text{medium}} = [10 \quad 30]^T$$
$$\beta_{\text{big}} = [20 \quad 60]^T$$





Matrix free solver, **Single** rank

Ref.	**DoF**	Small **Time (s)**	Medium **Time (s)**	Big **Time (s)**
5	4225	0.54	0.62	0.94
6	16641	2.04	2.43	3.46
7	66049	8.41	9.64	14.40
8	263169	35.74	44.12	57.82

Benchmarks

Homogeneous Dirichlet Boundary Conditions

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20 Cores | 28 Threads

2D $u_{ex} = sin(2\pi x)sin(2\pi y) \quad \Omega = [0,1]^2$

$$\beta_{\text{small}} = [0.1 \quad 0.3]^T$$
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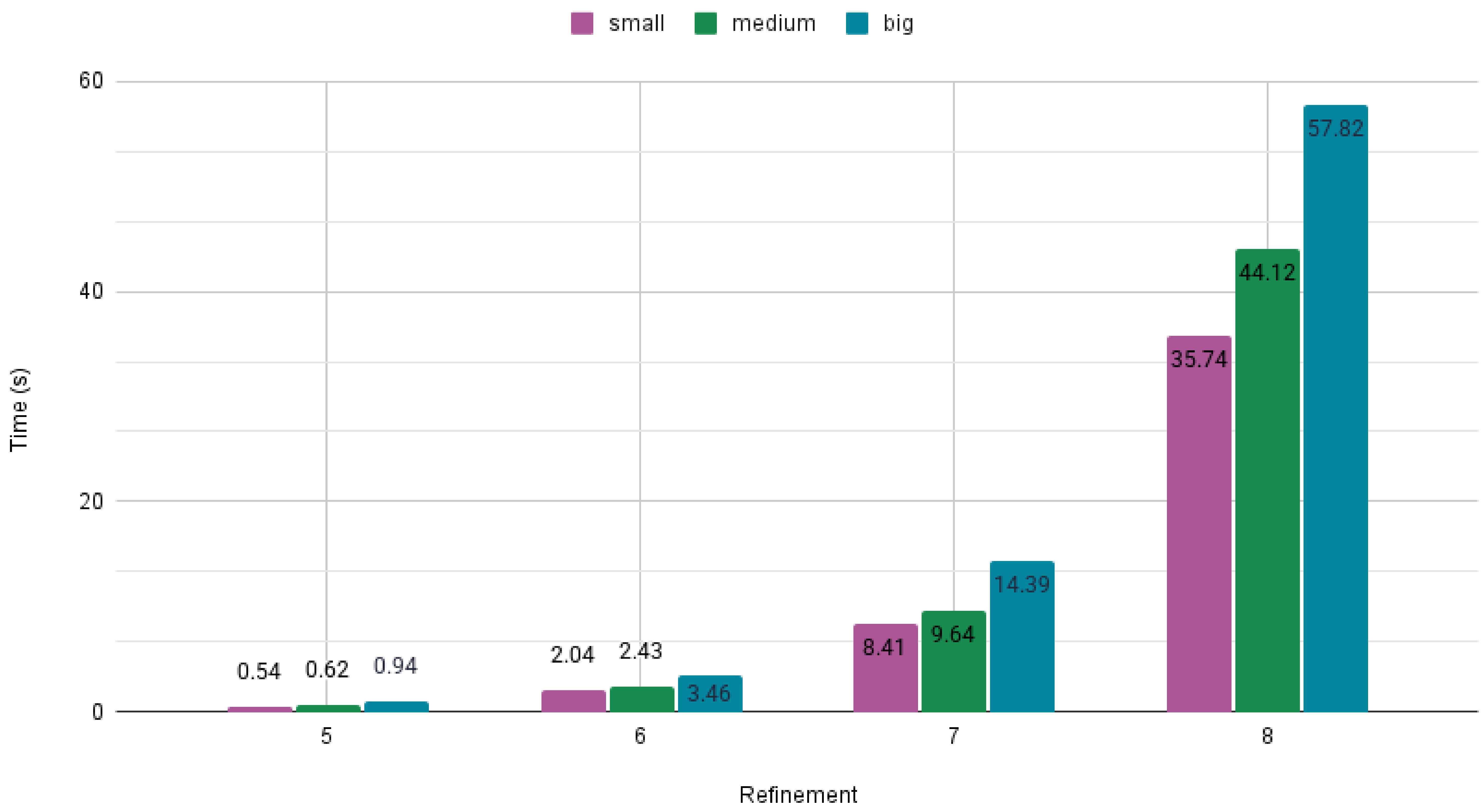


$\|\beta\| \ll \mu \implies$ A symmetric Jacobi is a good Smoother

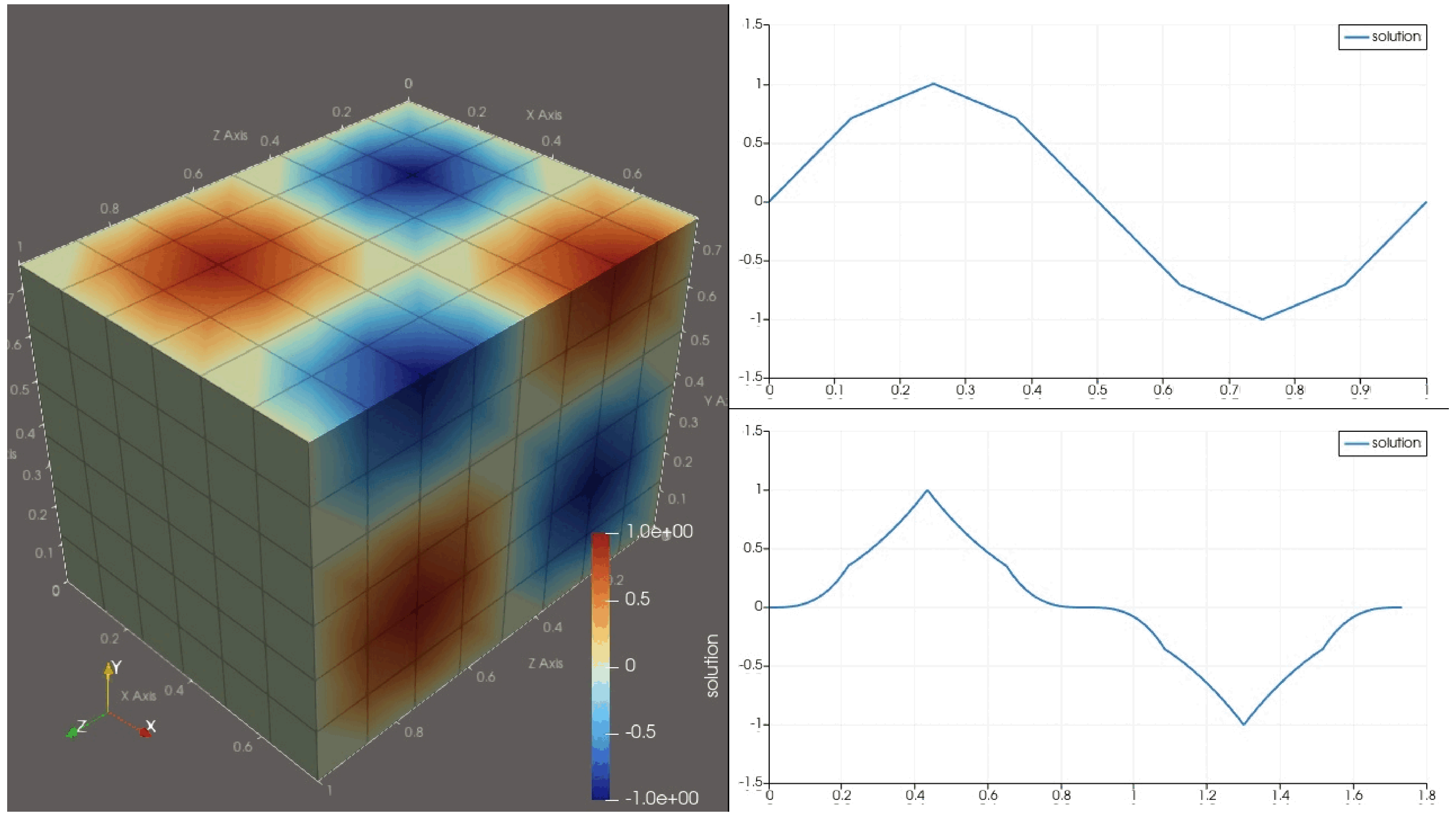
$\|\beta\| \gg \mu \implies$ A not symmetric Jacobi is not a good Smoother

Benchmarks

Homogeneous Dirichlet Boundary Conditions

Running on: Intel i7-14700HX @ 5.3GHz
20 Cores | 28 Threads

3D $u_{ex} = sin(2\pi x)sin(2\pi y)sin(2\pi z) \quad \Omega = [0,1]^3 \quad \beta = [0.1 \quad 0.2 \quad 0.1]^T$



Matrix Free vs **Matrix Based**, **Single** rank

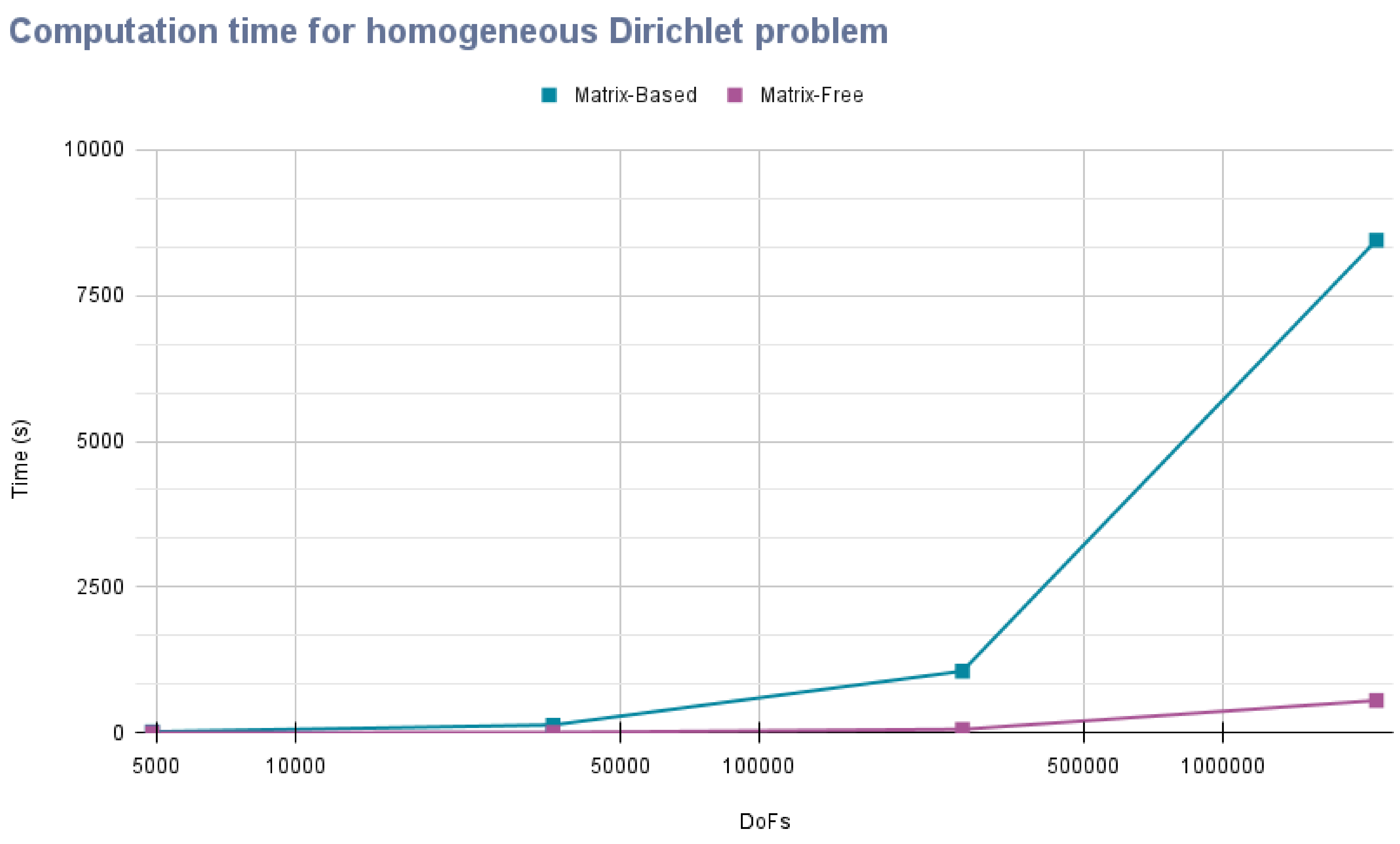
DoF	Matrix Based **Time (s)**	Matrix Free **Time (s)**	Matrix Based **Memory (MB)**	Matrix free **Memory (MB)**
4913	17.14	0.83	4.94	1.28
35937	133.98	6.76	38.29	9.92
274625	1057.77	58.54	301.82	78.26
2146689	8448.95	553.39	2396.80	622.17

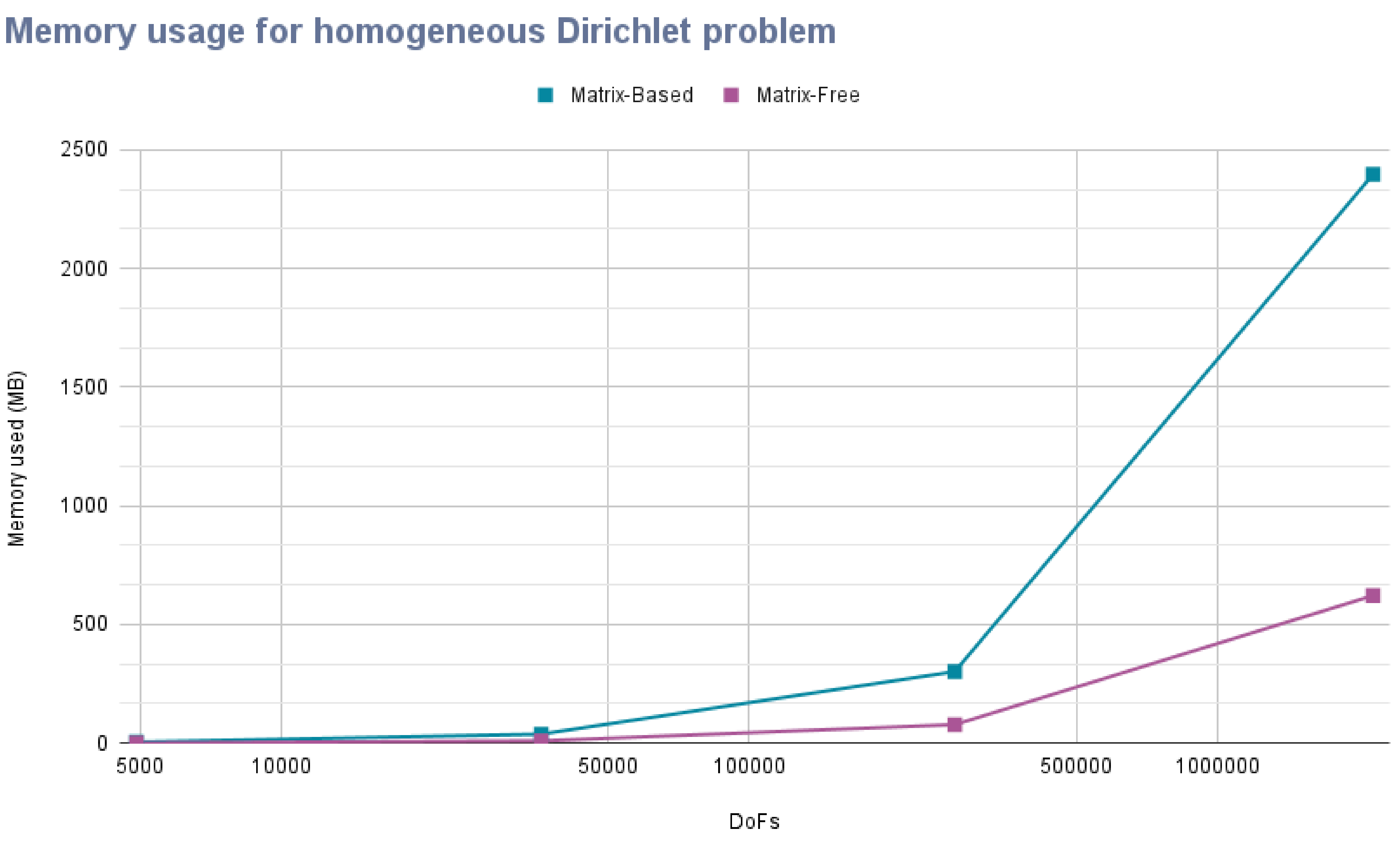
Benchmarks

Homogeneous Dirichlet Boundary Conditions

Running on: Intel i7-14700HX @ 5.3GHz
20 Cores | 28 Threads

3D $u_{ex} = sin(2\pi x)sin(2\pi y)sin(2\pi z)$ $\Omega = [0,1]^3$ $\beta = \begin{bmatrix} 0.1 & 0.2 & 0.1 \end{bmatrix}^T$





Benchmarks

Homogeneous Dirichlet Boundary Conditions

Running on: Intel i7-14700HX @ 5.3GHz
20 Cores | 28 Threads

3D $u_{ex} = sin(2\pi x)sin(2\pi y)sin(2\pi z)$ $\Omega = [0,1]^3$ $\beta = \begin{bmatrix} 0.1 & 0.2 & 0.1 \end{bmatrix}^T$

Matrix Free solver **Parallel Speedup**

Type	MPI Ranks	Time (s)	Memory (MB)
Matrix based	1	1075.50	8448.95
Matrix free	1	64.74	553.39
Matrix free	4	18.43	156.02
Matrix free	8	11.08	109.64
Matrix free	16	8.52	106.66
Matrix free	20	7.73	98.9715

Benchmarks

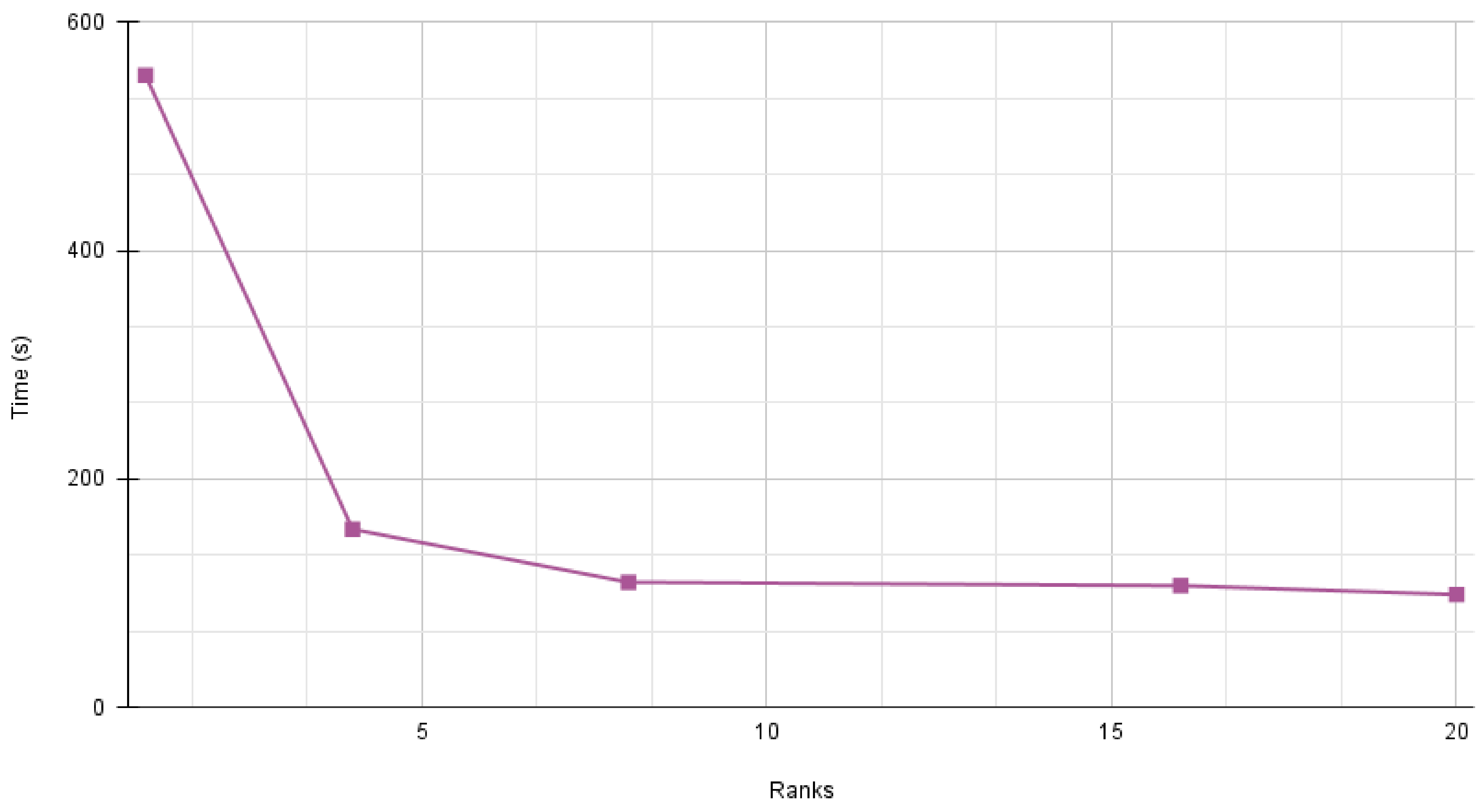
Homogeneous Dirichlet Boundary Conditions

Running on: Intel i7-14700HX @ 5.3GHz
20 Cores | **28 Threads**

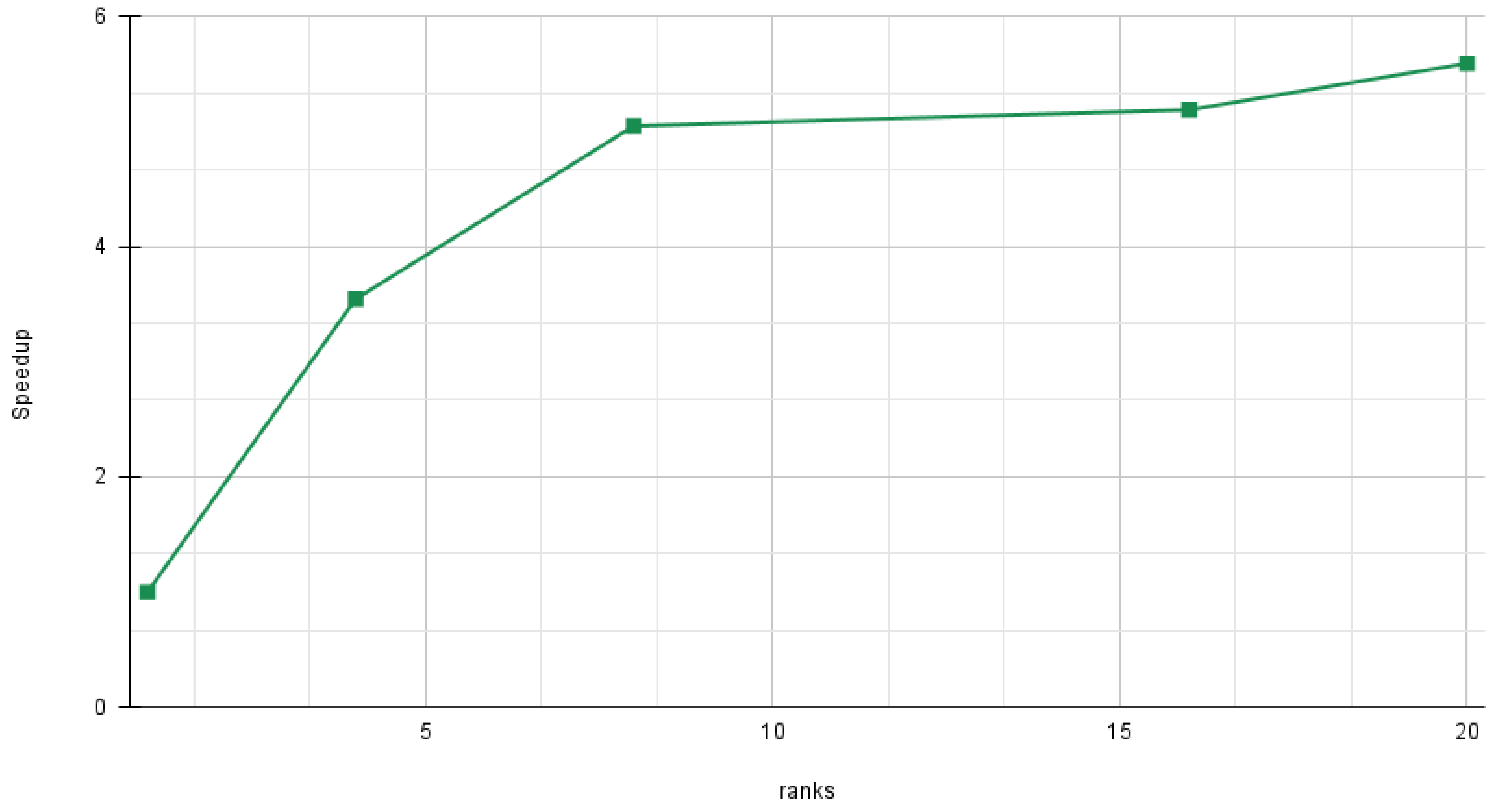
3D $u_{ex} = sin(2\pi x) sin(2\pi y) sin(2\pi z)$ $\Omega = [0, 1]^3$ $\beta = [0.1 \quad 0.2 \quad 0.1]^T$

Matrix Free solver **Parallel Speedup**

Computation time vs Ranks



Computation time Speed up

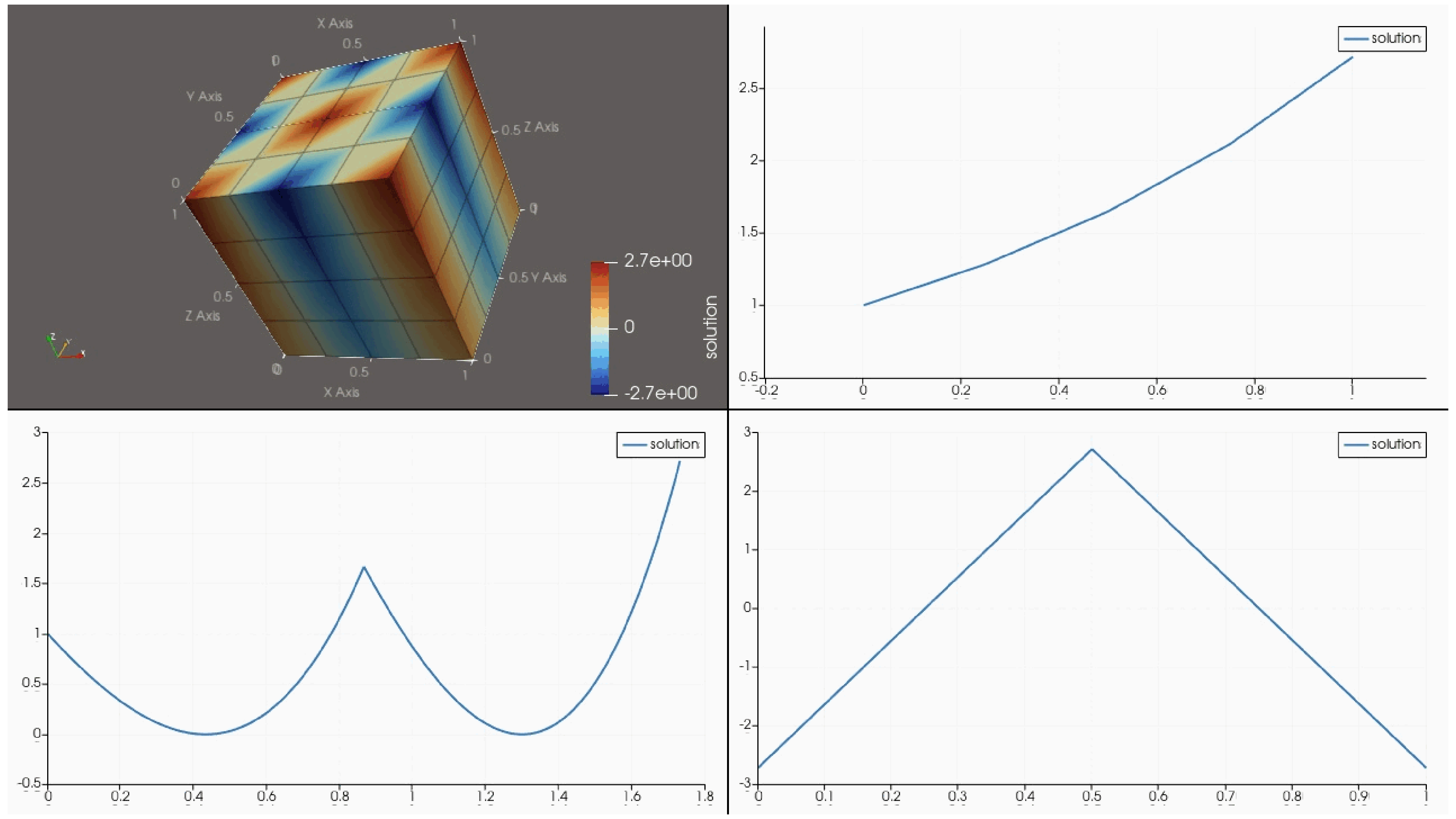


Benchmarks

Non-Homogeneous Dirichlet Boundary Conditions

Running on: Intel i7-14700HX @ 5.3GHz
20 Cores | **28 Threads**

3D $$u_{ex} = e^z \cos(2\pi x)\cos(2\pi y) \qquad \Omega = [0,1]^3$$



Matrix Free vs **Matrix Based**, **Single** rank

DoF	Matrix Based **Time (s)**	Matrix Free **Time (s)**	Matrix Based **Memory (MB)**	Matrix free **Memory (MB)**
729	2.59	0.15	0.66	0.18
4913	20.06	0.97	4.93	1.28
35937	163.84	7.19	38.29	9.91
274625	1075.50	64.74	301.81	78.26

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Deal.II Matrix Free Solver for ADR Problem

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