A multiprocess and multithreaded strategy for parallel proper orthogonal decomposition in a reduced order modeling framework

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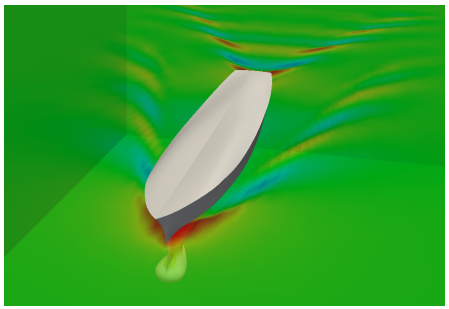
Agenda

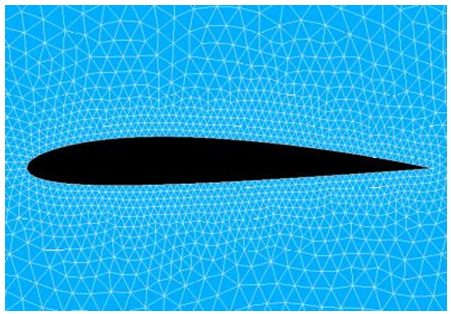
1. Reduced Basis Method
2. Parallel POD algorithms
3. Implementation and Benchmarks
4. Integration in `EZyRB` with an example

Physical Problems

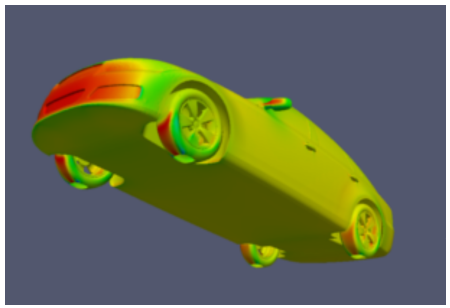
Complex phenomena described using **parametrized** **Partial Differential Equations (PDE)**



Naval Engineering



Aeronautics



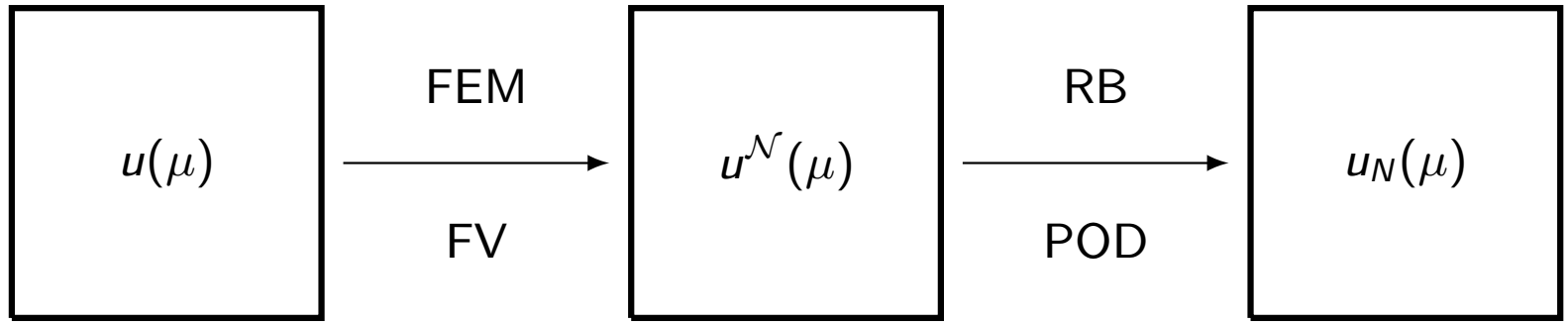
Automotive

Solving the PDEs using fine discretization like **Finite Element**, **Finite Volume**, ...

Problem: Many evaluations are expensive.

- **optimizing** the parameter (**multi query** application)
- **controlling** the parameter (**real time** application)

RB workflow



$$\text{find } u(\mu) \in \mathbb{X}: \quad a(u(\mu), v; \mu) = f(v; \mu) \quad \forall v \in \mathbb{X}.$$

Truth problem

$$\text{find } u^{\mathcal{N}}(\mu) \in \mathbb{X}^{\mathcal{N}}: \quad a(u^{\mathcal{N}}(\mu), v; \mu) = f(v; \mu) \quad \forall v \in \mathbb{X}^{\mathcal{N}}.$$

Truth solutions

$$u^{\mathcal{N}}(\mu) = \sum_{i=1}^{\mathcal{N}} u_i^{\mathcal{N}}(\mu) \cdot \varphi_i, \quad \mathbb{X}^{\mathcal{N}} = \text{span}(\varphi_1, ..., \varphi_{\mathcal{N}})$$

Goal: Approximate solution manifold

$$\mathbb{M}^{\mathcal{N}} = \{u^{\mathcal{N}}(\mu), \quad \mu \in \mathbb{P}\}$$

Reduced Space

$$\mathbb{X}_N = \text{span}(\xi_1, ..., \xi_N), \qquad N \ll \mathcal{N}$$

Reduced solutions

$$u_N(\mu) = \sum_{i=1}^{N} u_{N,i}(\mu) \cdot \xi_i$$

Reduced problem

$$\text{find } u_N(\mu) \in \mathbb{X}_N : \quad a(u_N(\mu), v; \mu) = f(v; \mu) \quad \forall v \in \mathbb{X}_N$$

POD basis generation

The POD is a method to find the optimal orthogonal space in a linear manner.

- Set based approach $\Xi_{train} = \{\mu_1, ..., \mu_{n_{train}}\}$
- $\mathbb{X}_{n_{train}} = \text{span}\left\{u^{\mathcal{N}}(\mu) | \mu \in \Xi_{train}\right\}$

Eigen value problem (EVP)

$$C(v) = \frac{1}{n_{train}} \sum_{m=1}^{n_{train}} \left(v, u^{\mathcal{N}}(\mu_m)\right)_{\mathbb{X}} u^{\mathcal{N}}(\mu_m), \quad v \in \mathbb{X}_{n_{train}}$$

$$\left(C(\xi_n), u^{\mathcal{N}}(\mu_m)\right)_{\mathbb{X}} = \lambda_n \left(\xi_n, u^{\mathcal{N}}(\mu_m)\right)_{\mathbb{X}}, \quad 1 \leq m \leq n_{train}$$

POD error

$$\frac{1}{n_{train}} \sum_{\mu \in \Xi_{train}} \inf_{w_N \in \mathbb{X}_{n_{train}}} \|u^{\mathcal{N}}(\mu) - w_N\|_{\mathbb{X}}^2 = \sum_{n=N+1}^{n_{train}} \lambda_n$$

- Truncate all modes $> N$

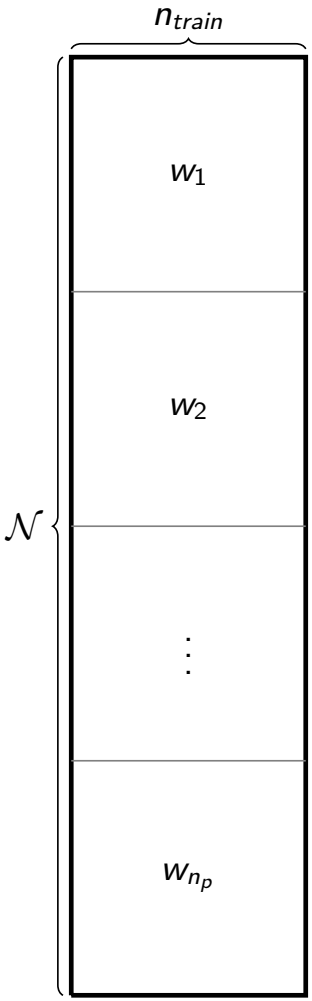
Snapshot Matrix

$$\mathcal{W} = \begin{bmatrix} | & | & & | \\ \underline{u}^{\mathcal{N}}(\mu_1) & \underline{u}^{\mathcal{N}}(\mu_2) & \dots & \underline{u}^{\mathcal{N}}(\mu_{n_{train}}) \\ | & | & & | \end{bmatrix}$$

Truth solution

$$u^{\mathcal{N}}(\mu) = \sum_{i=1}^{\mathcal{N}} u_i^{\mathcal{N}}(\mu)\varphi_i, \qquad \underline{u}^{\mathcal{N}}(\mu) = \begin{pmatrix} u_1^{\mathcal{N}}(\mu) \\ \vdots \\ u_{\mathcal{N}}^{\mathcal{N}}(\mu) \end{pmatrix}$$

Structure of the snapshot matrix



Partitioning cases

- Domain decomposition
- Manually blocked

Proper Orthogonal Decomposition

EVP

- Solving eigen value problem (EVP) of the snapshot matrix

$$\mathcal{W}^T\mathcal{W} = VDV^T$$

$$U = \mathcal{W}VD^{-\frac{1}{2}}$$

SVD

- Singular Value Decomposition (SVD) of the snapshot matrix

$$\mathcal{W} = USV^T$$

Relation singular values and eigen values

$$\mathcal{W}^T\mathcal{W} = (USV^T)^T USV^T = VSU^T USV^T = VS^2V^T$$

The left singular are computed with

$$U = \mathcal{W}VS^{-1}$$

Parallel SVD approach introduced by Beattie, Borggaard and Iliescu in 2007

Singular Value Decomposition (SVD) of the snapshot Matrix W

$$\mathcal{W} = USV^T$$

U are the POD modes.

Compute SVD of the local snapshot matrices $\mathcal{W} = [W_1^T ... W_{n_p}^T]^T$

$$\text{svd}(W_k) = [U, S, \boldsymbol{V_k}]$$

Compress local right singular vectors $\boldsymbol{V_k}$ using SVD

$$\hat{\mathcal{V}} = [V_1 ... V_{n_p}] \qquad \text{svd}(\hat{\mathcal{V}}) = [\mathcal{T}, \mathcal{M}, \boldsymbol{\mathcal{V}}]$$

Compute left singular vectors

$$\text{svd}(\mathcal{W}\mathcal{V}) = [\boldsymbol{\mathcal{U}}, \mathcal{S}, \mathcal{Z}]$$

Parallel EVP

We compute

$$\mathcal{W}^T\mathcal{W} = VDV^T$$

The left singular are computed with

$$U = \mathcal{W}VD^{-\frac{1}{2}}$$

Expensive operations
dimension $\mathcal{N}$

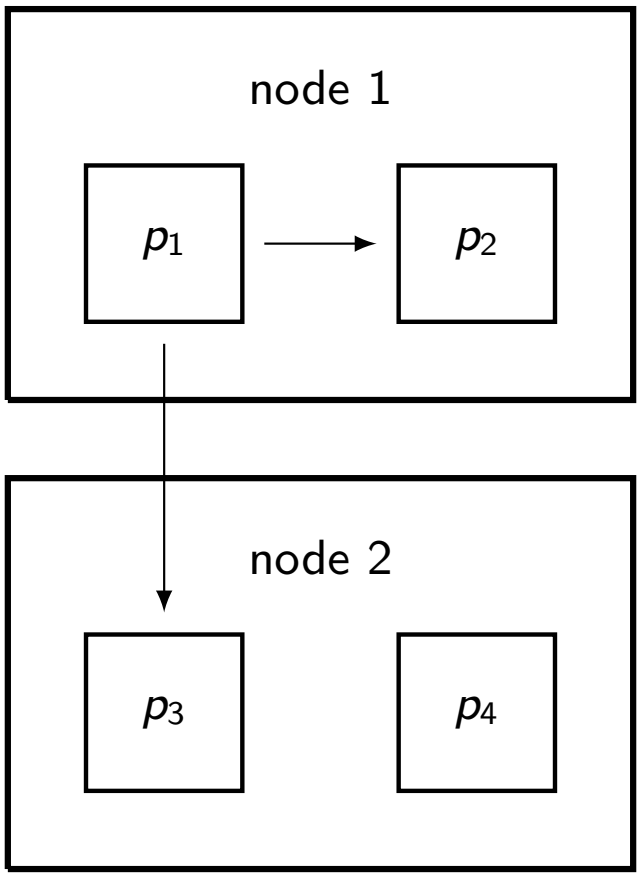
- $\mathcal{W}^T\mathcal{W}$
- $U = \mathcal{W}VD^{-\frac{1}{2}}$

Cheap operations
dimension n_{train}

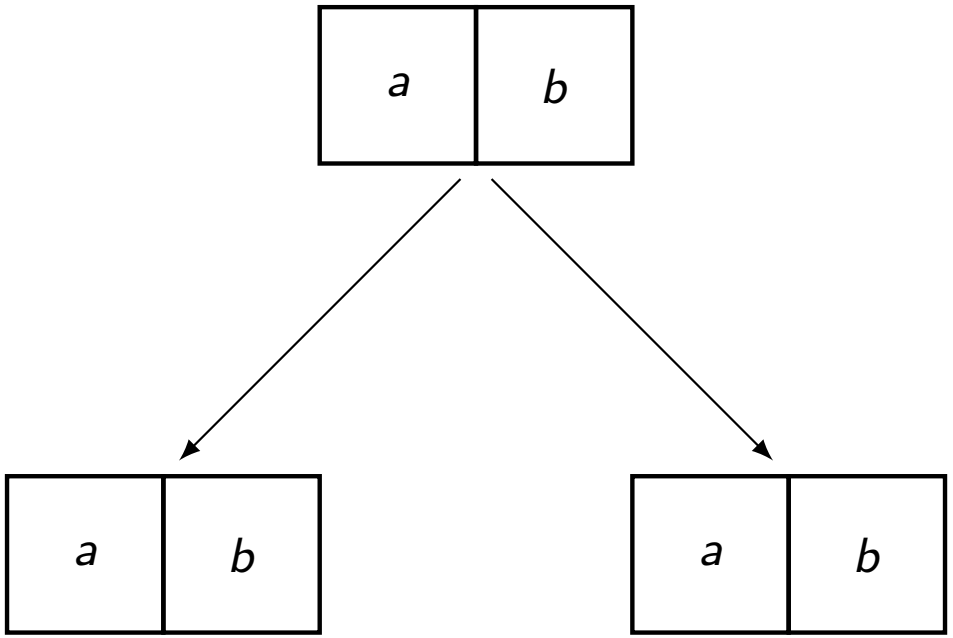
- $\mathcal{W}^T\mathcal{W} = VDV^T$ (solving EVP)
- $VD^{-\frac{1}{2}}$

MPI - Message Passing Interface

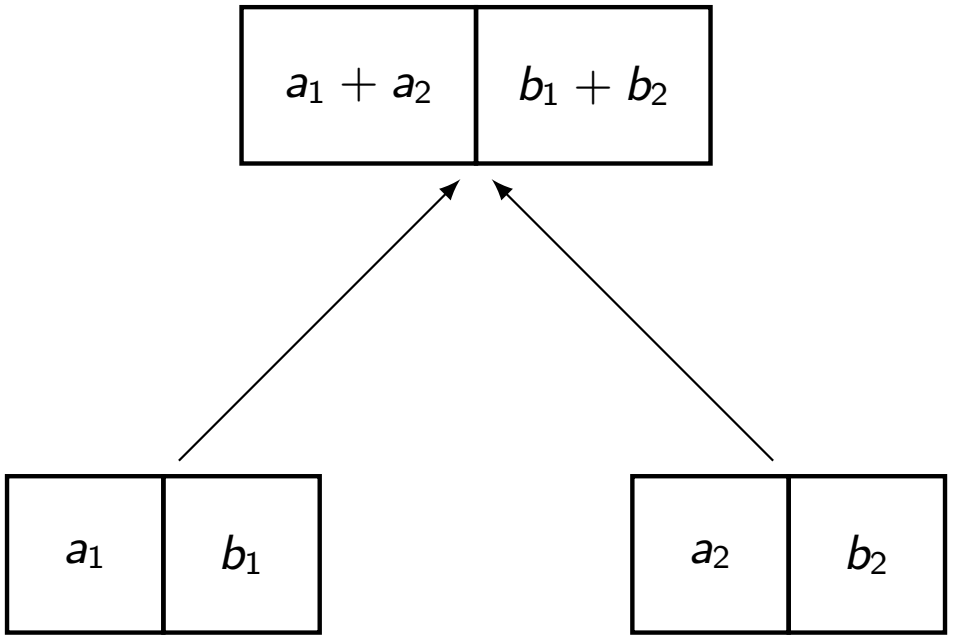
- A standard for a library interface for parallel programs.
- **process-based**: interface to send message from one process to another process.
- **distributed memory**: every memory has its own virtual memory.



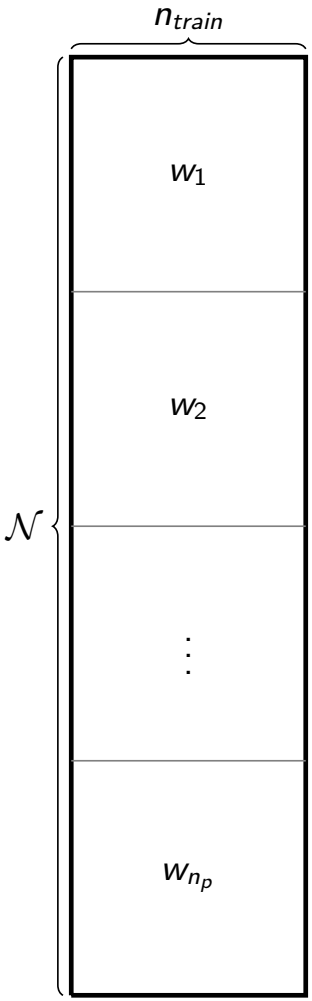
MPI_Bcast



MPI_Reduce with MPI_sum

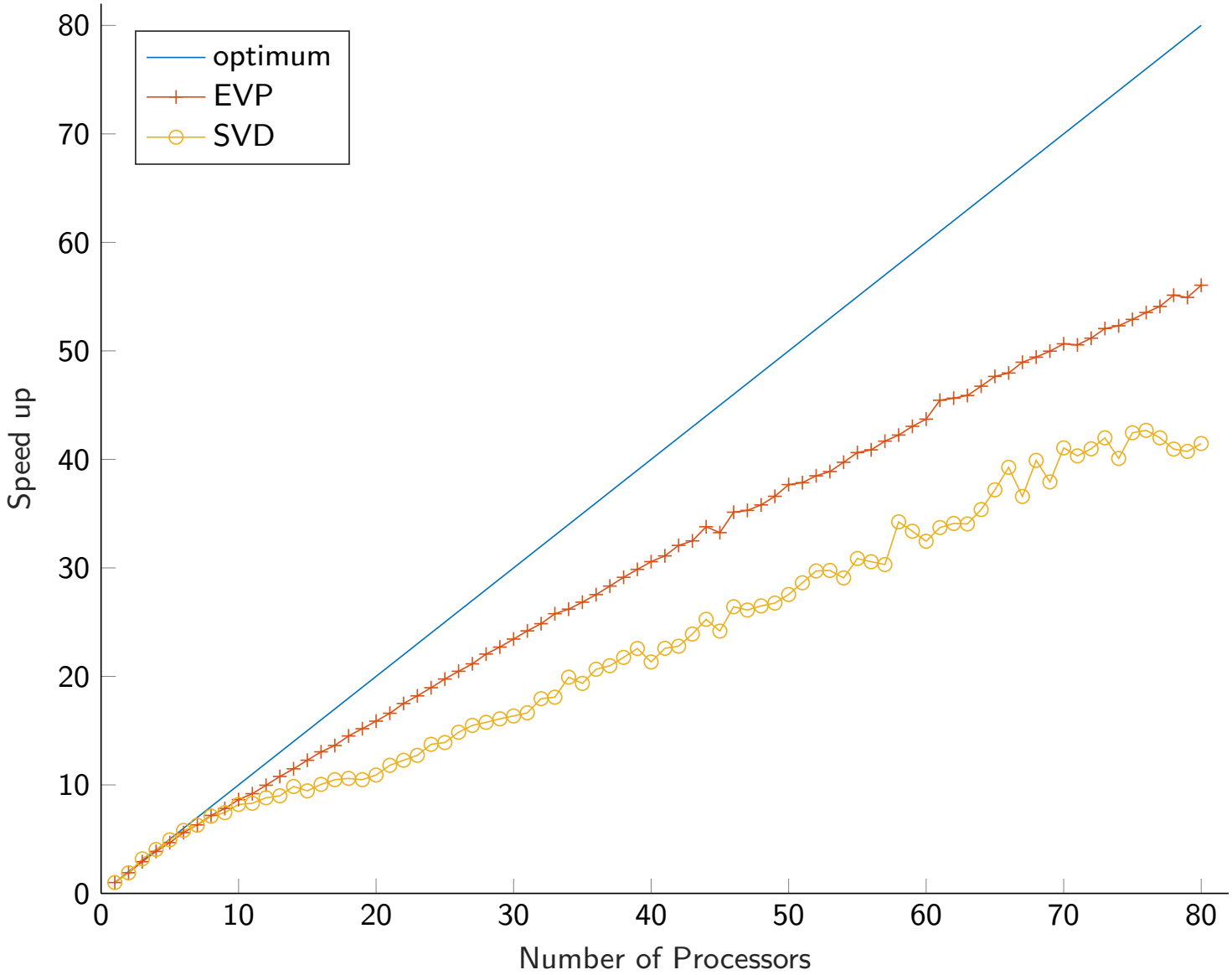


Partitioning of the Snapshot matrix

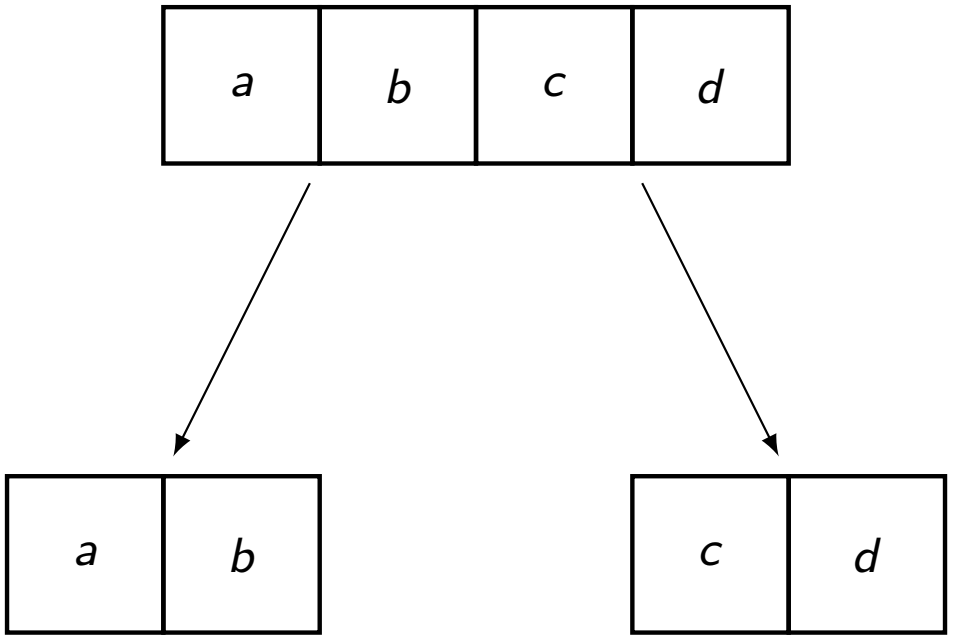


1. compute local correlation matrix $w_i^T w_i$
2. reduce local correlation matrices to get global correlation matrix C
3. Solve EVP $C = VDV^T$
4. compute $VD^{-\frac{1}{2}}$
5. Broadcast $VD^{-\frac{1}{2}}$ to every processor
6. $u_i = w_i \cdot VD^{-\frac{1}{2}}$

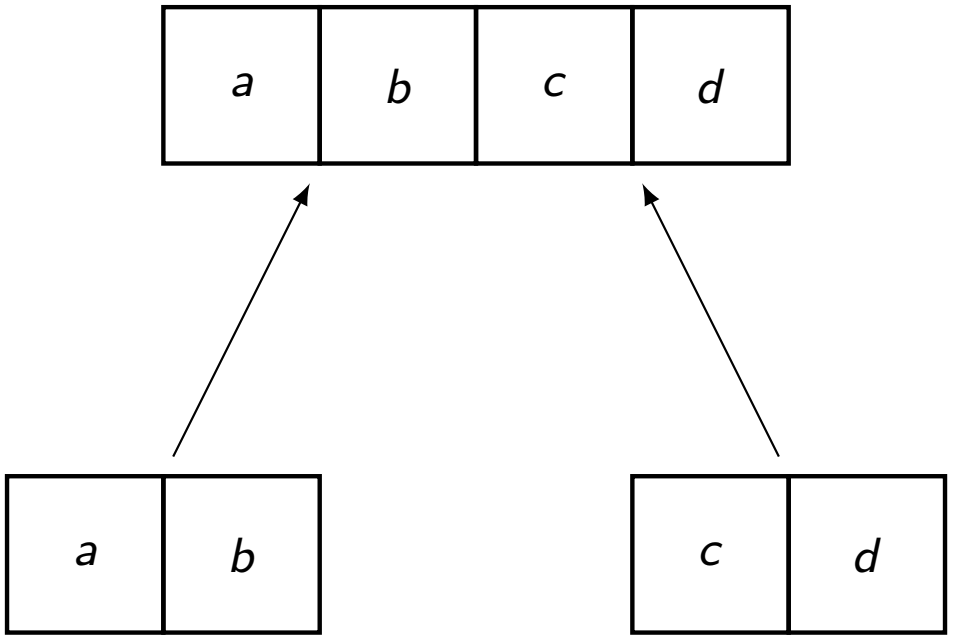
Snapshot matrix is already distributed random $10^7 \times 300$ matrix



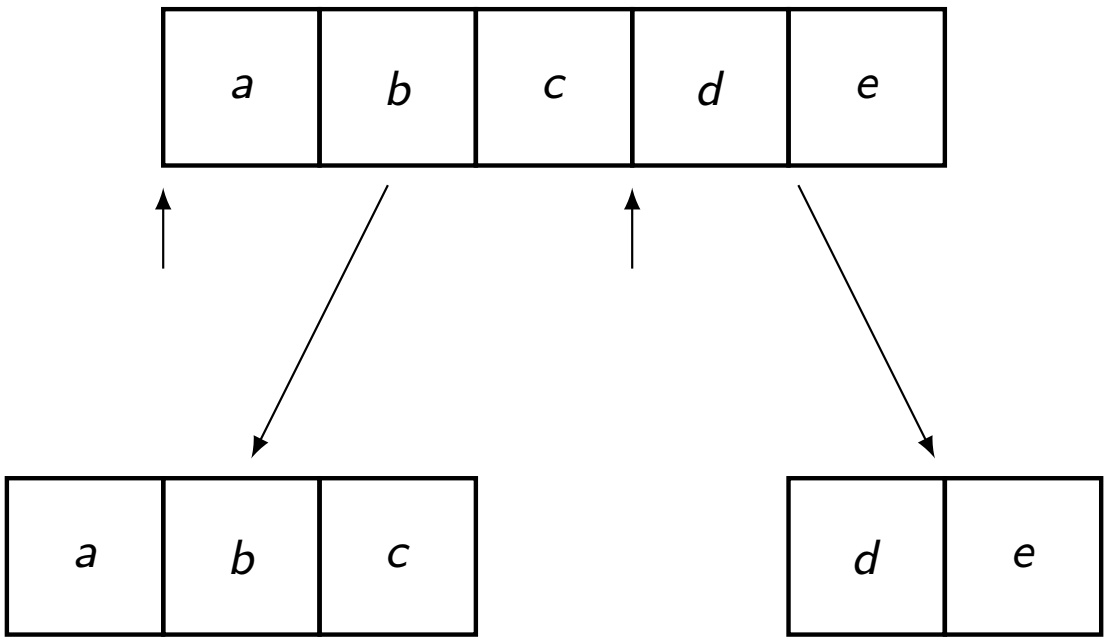
MPI_Scatter



MPI_Gather

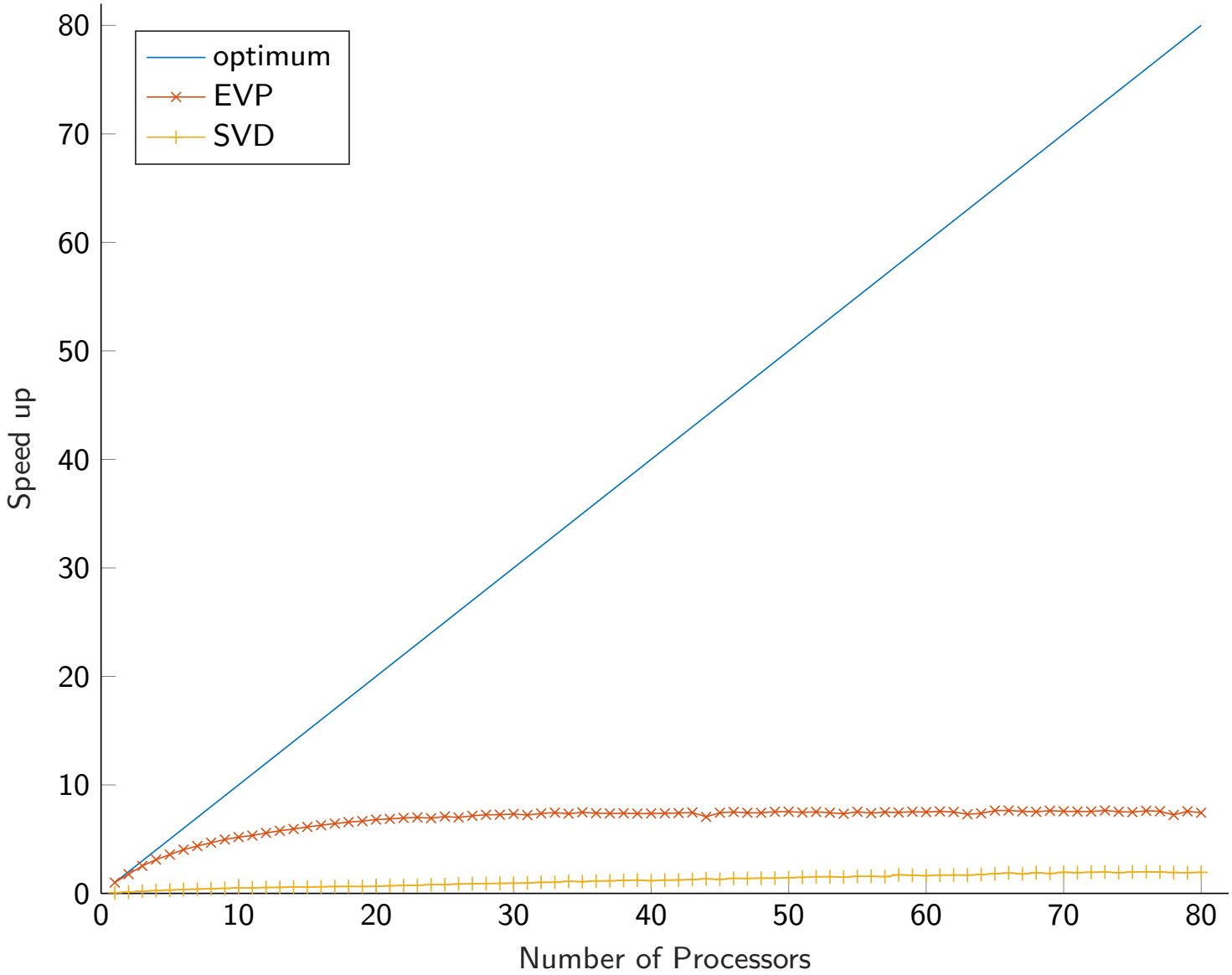


MPI_Scatterv and MPI_Gatherv



sendcount = [3,2], displacement = [0,3]

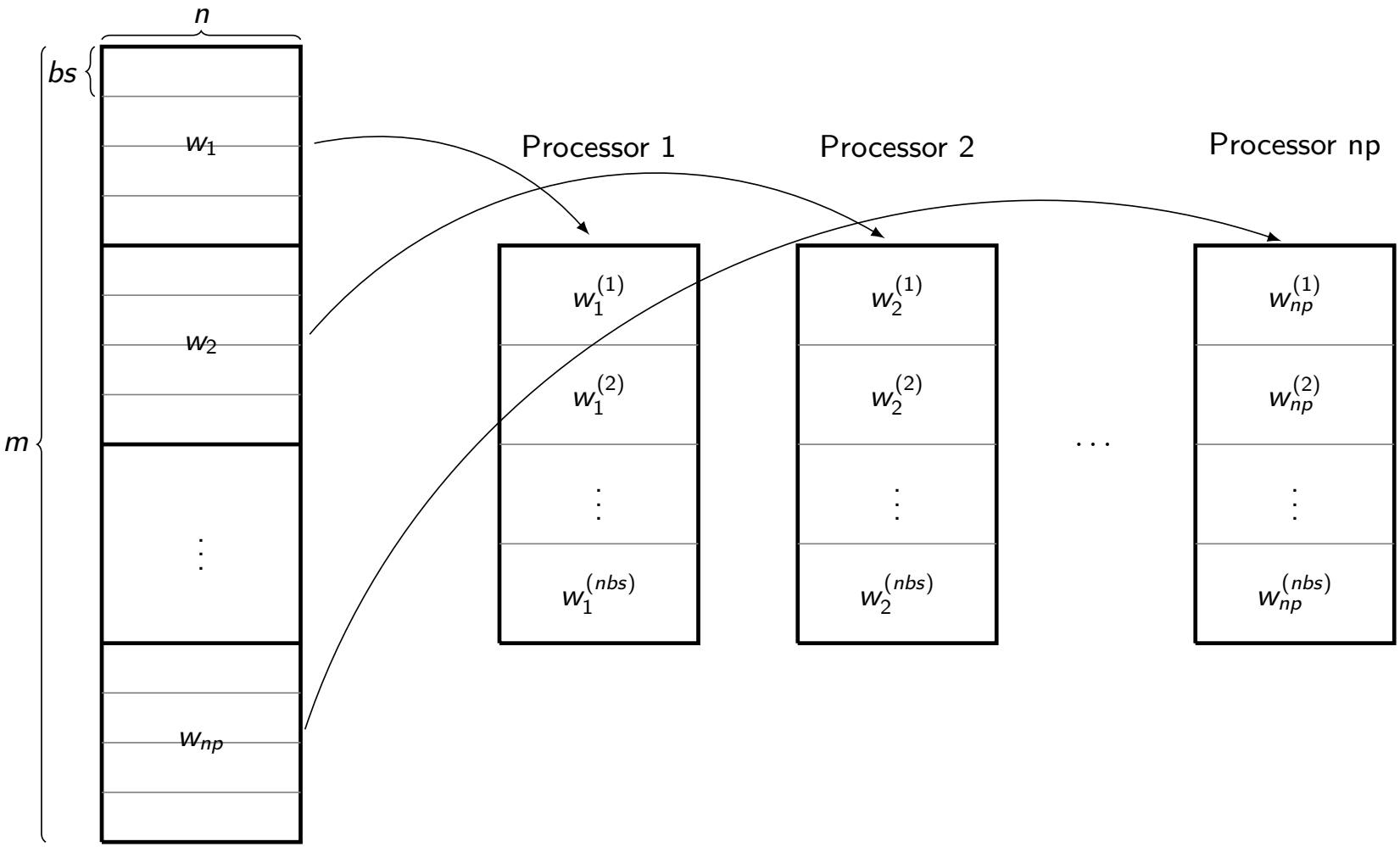
With scattering and gathering of $\mathcal{W}$ random $10^7 \times 300$ matrix



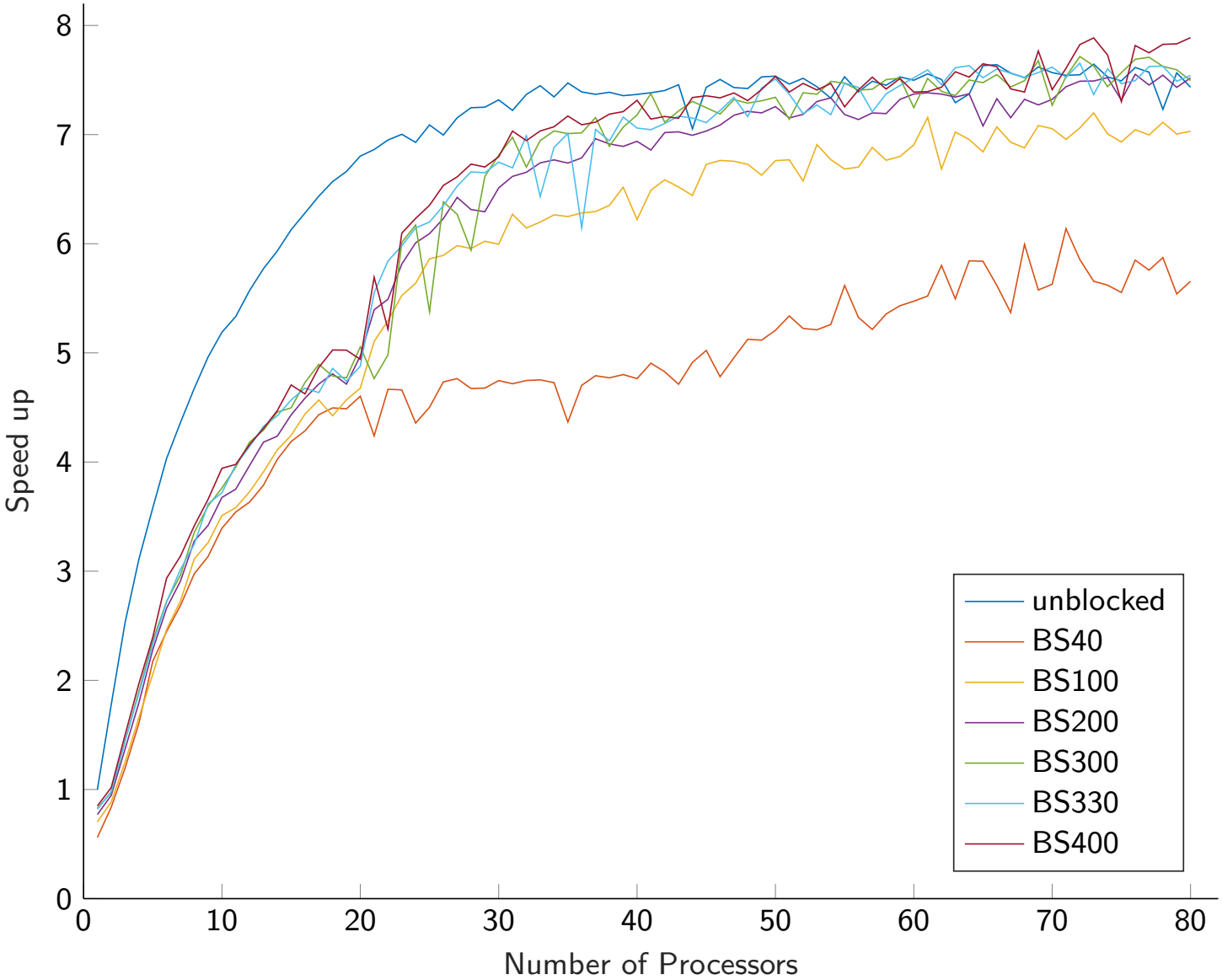
MPI I functions

- I functions provide non bocking communication
- communication is not blocking processor
- communication buffer should not be used while communication
- MPI_Scatterv ⇒ MPI_Iscatterv
- MPI_Gatherv ⇒ MPI_Igatherv

Partitioning for non-blocking communication



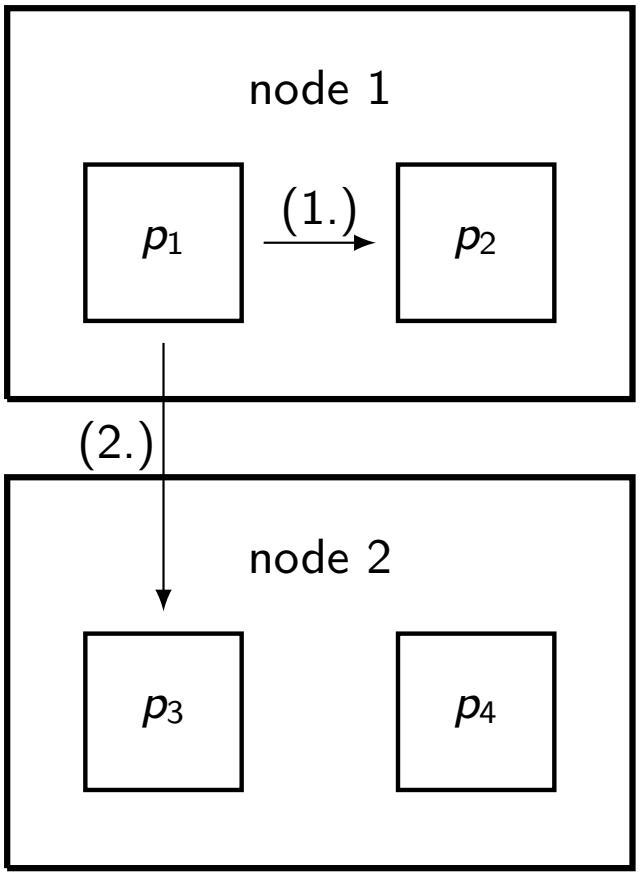
Different block sizes random $10^7 \times 300$ matrix



Increasing waiting time

- We measured the waiting time
- Waiting time increased from 0.0062 to 0.0263 (magnitude of 10)
- Possible reason: **too many communications**
- Possible solution: **reduce** MPI communications

MPI communication



1. **Copy** operation in memory
2. **Sending** operation via network

MPI & OpenMP

MPI

- Process Based
- Communication on one node is copying

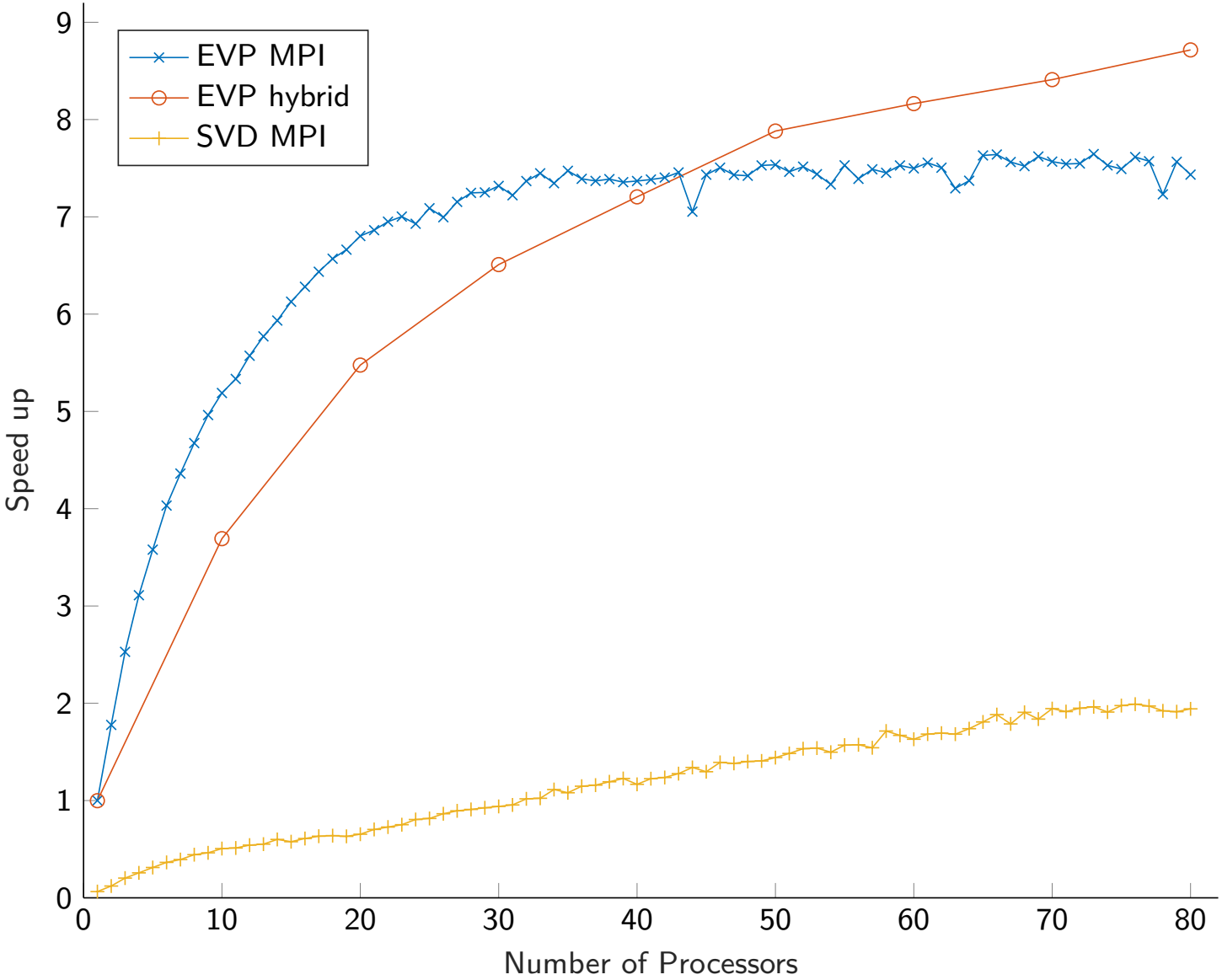
OpenMP

- Thread based
- shared memory

Hybrid implementation

- MPI for communication between nodes and processors
- OpenMP parallelization on nodes

Hybrid implementation random $10^7 \times 300$ matrix

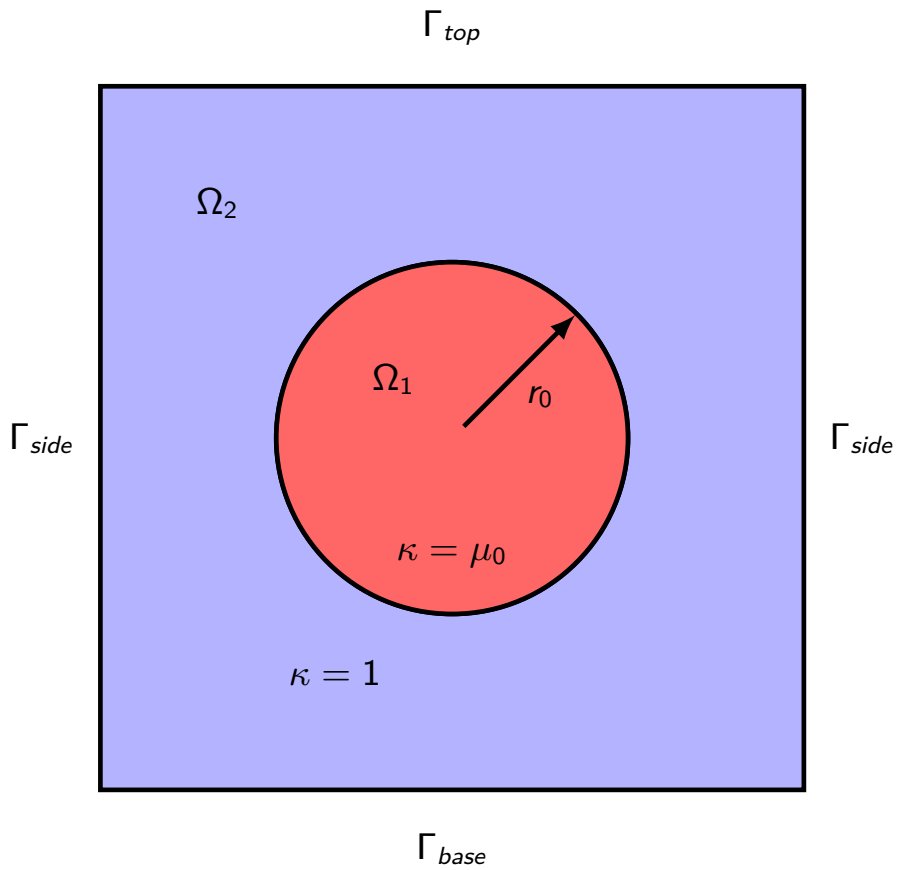


EZyRB: Easy Reduced Basis method

- Open source on `GitHub`
- Data driven reduced order modeling framework in python
- POD with interpolation (PODI)

Example Heat Conduction

$$\begin{cases} -\nabla \cdot (\kappa(x,\mu)\nabla u(x,\mu)) = 0 & \text{in } \Omega \\ u(x,\mu) = 0 & \text{on } \Gamma_{top} \\ \kappa(\mu)\nabla u(x,\mu) \cdot \mathbf{n} = 0 & \text{on } \Gamma_{side} \\ \kappa(\mu)\nabla u(x,\mu) \cdot \mathbf{n} = \mu_1 & \text{on } \Gamma_{base} \end{cases}$$



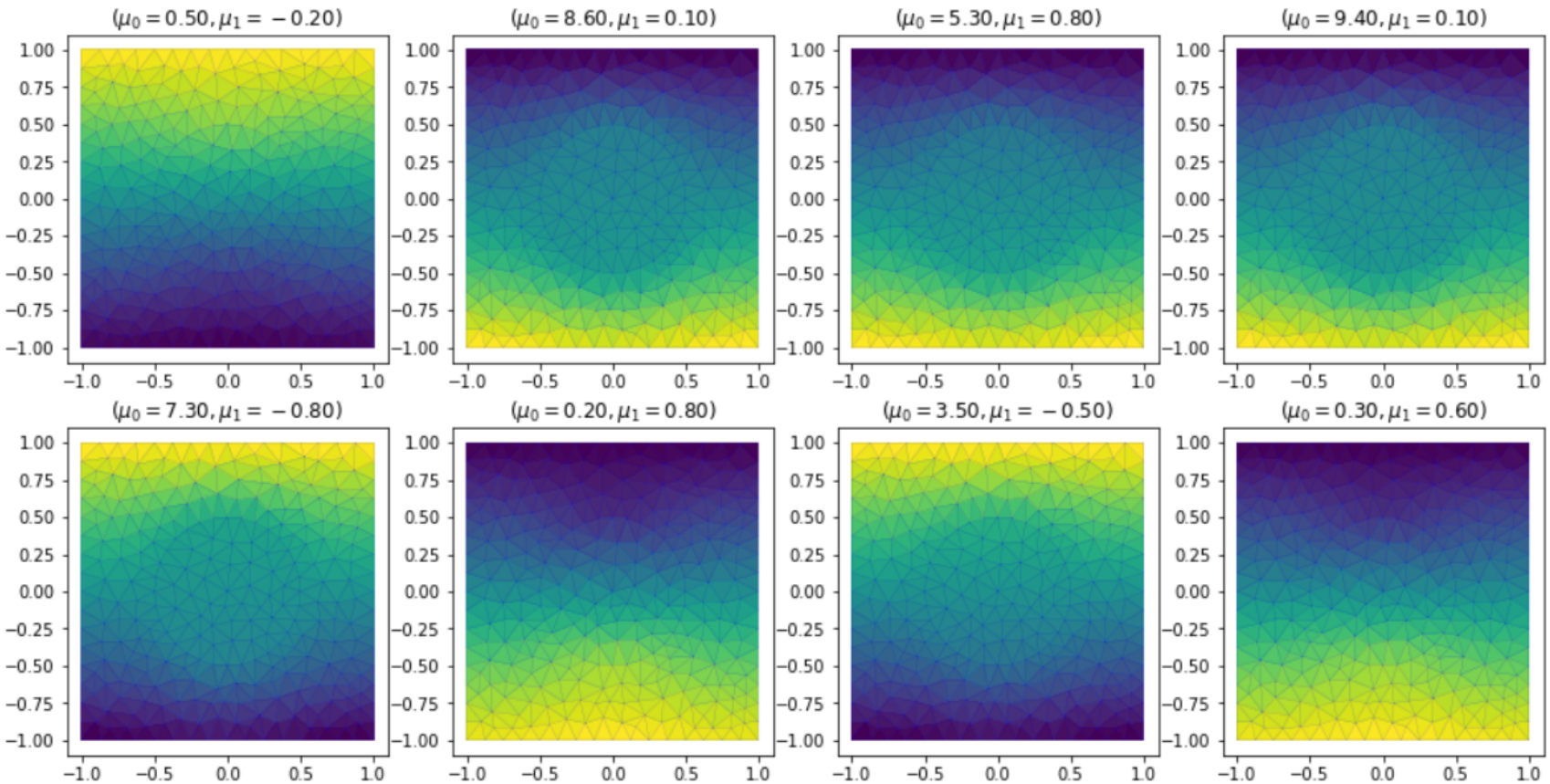
find $u(\mu) \in \mathbb{X}$:

$a(u(\mu), v; \mu) = f(v; \mu) \quad \forall v \in \mathbb{X}.$

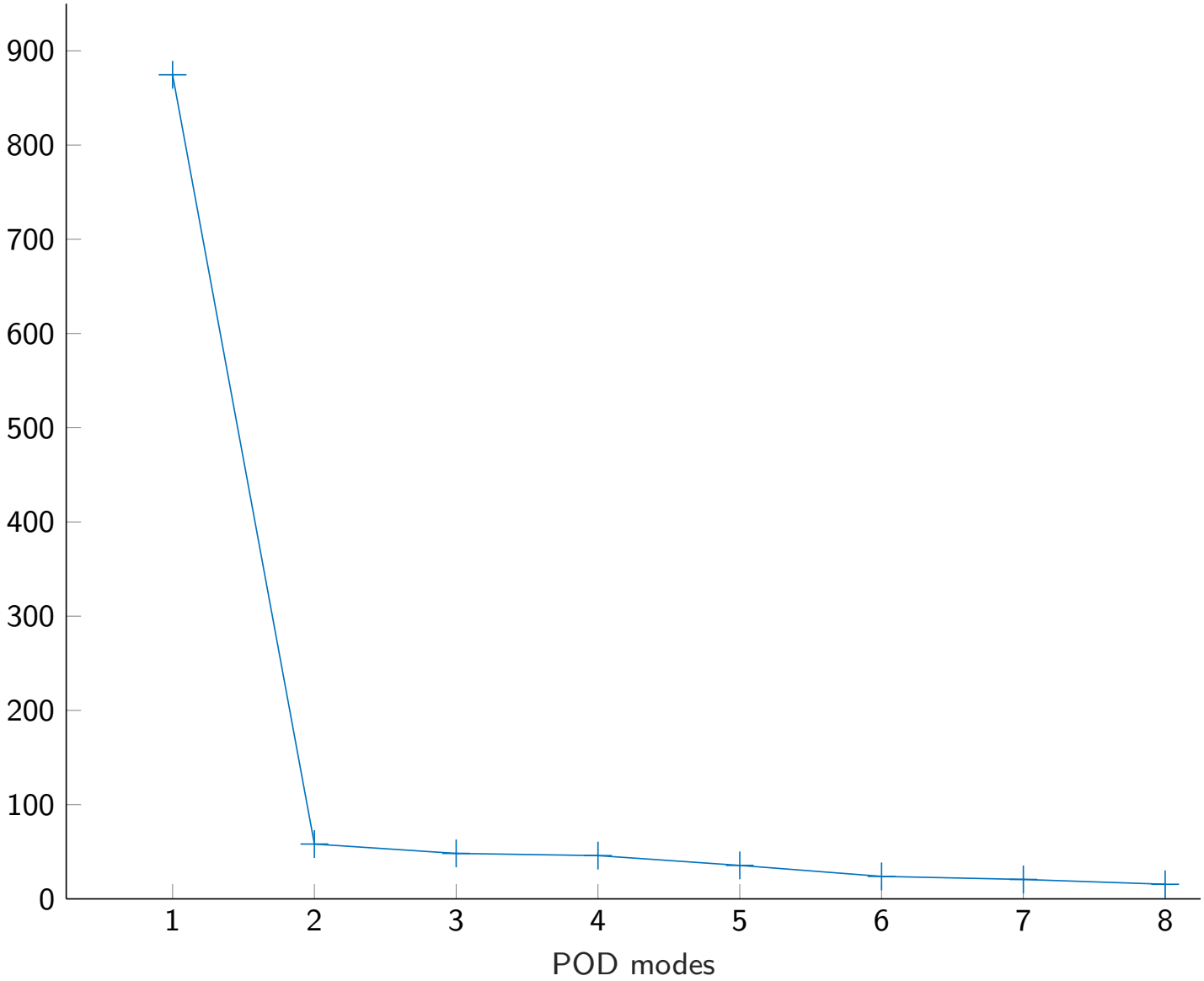
$$a(u, v; \mu) = \int_\Omega \kappa(x,\mu)\nabla u(x,\mu)\nabla v(x) dx, \qquad f(v;\mu) = \mu_1 \int_{\Gamma_{base}} v \; ds$$

Snapshots

$$\Xi_{train} = \left\{ \begin{pmatrix} 0.5 \\ -0.2 \end{pmatrix}, \begin{pmatrix} 8.6 \\ 0.1 \end{pmatrix}, \begin{pmatrix} 5.3 \\ 0.8 \end{pmatrix}, \begin{pmatrix} 9.4 \\ 0.1 \end{pmatrix}, \begin{pmatrix} 7.3 \\ -0.8 \end{pmatrix}, \begin{pmatrix} 0.2 \\ 0.8 \end{pmatrix}, \begin{pmatrix} 3.5 \\ -0.5 \end{pmatrix}, \begin{pmatrix} 0.3 \\ 0.6 \end{pmatrix} \right\}.$$



Singular values



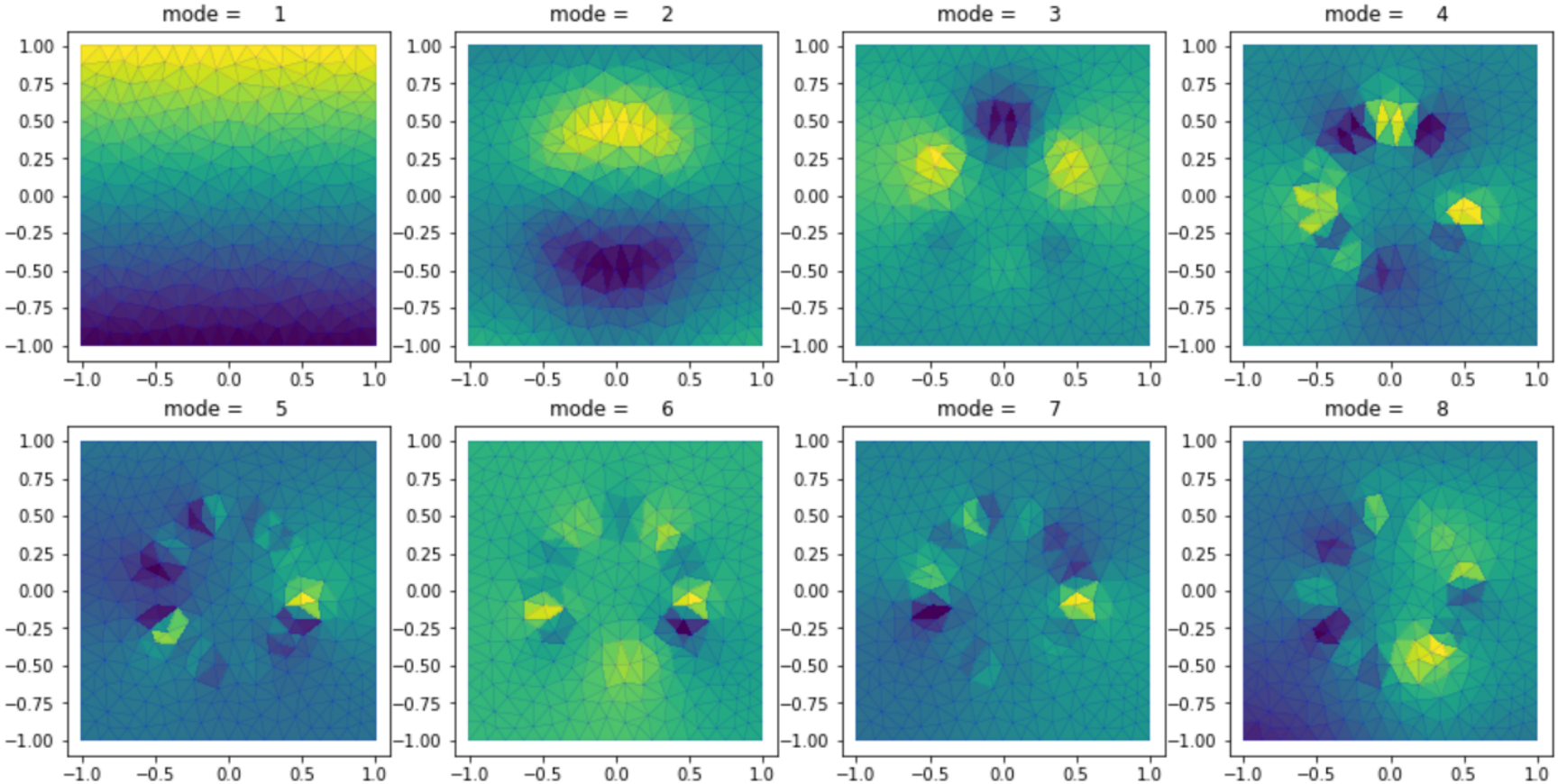
Conclusion

- We presented two algorithms to compute the POD in parallel
- EVP perfomes better than SVD due to its limited number of operations
- Distributing the snapshot matrix is a bottle neck
- We presented hybrid parallel strategy for the POD

Outlook

- The performance of the computation of the **correlation matrix** could be improved by using graphics processing units (**GPU**).

PODmodes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−0.75
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−1.0
−0.5
0.0
0.5
1.0