Domain decomposition for physics-data combined neural network based parametric reduced order modelling

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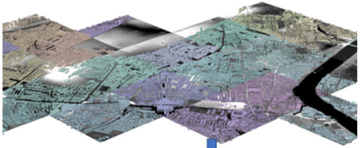
Reduced Order Modelling

High dimensional, non-linear physical system

10^6—10^9



Simulation

Reduced representation

Aerospace engine design, computational fluid dynamics (CFD) and porous media and so on.
Needs repeated simulations for 10,000-100,000times

$$\begin{bmatrix} B^{POD} & C^{POD} \\ (C^{POD})^T & 0 \end{bmatrix} \begin{bmatrix} \alpha^{u,n+1} \\ \alpha^{p,n+1} \end{bmatrix} = \begin{bmatrix} B'^{POD} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \alpha^{u,n} \\ \alpha^{p,t} \end{bmatrix} + \begin{bmatrix} s^{POD} \\ 0 \end{bmatrix}$$

10^1—10^2 dimensional size

Parallel computing

$$\begin{bmatrix} B & C \\ C^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} B' & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}^{n} \\ p^{n} \end{bmatrix} + \begin{bmatrix} s \\ 0 \end{bmatrix}$$

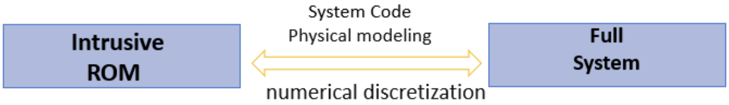
discretised NS equations 10^6—10^9

ROM : Three types

- Intrusive ROM: Integrate with physics model

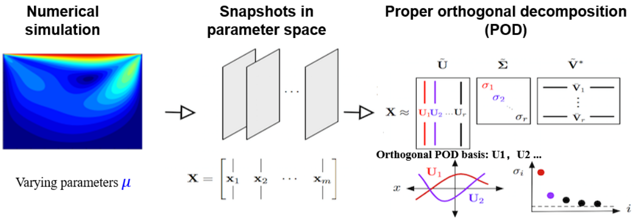
$$\mathcal{F}(\mathbf{u}(\mathbf{x},t),\mathbf{x},t,\mu)=s(\mathbf{x},t,\mu). \tag{1}$$

  - Difficult to implement, modify and extend



- Non-intrusive ROM: Independent of physical system
  - black box
  - Lack of rigorous error analysis
- Physics-Data combined ROM : Integrate with physics model and data model

Parametric reduced-order modelling via POD



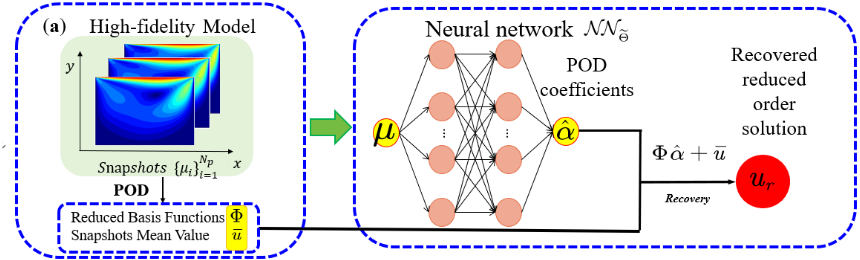
- Reduced-order solution:

$$\mathbf{u}_r(\mu) = \sum_{i=1}^{M} \alpha_i \mathbf{U_i} = \mathbf{U}\alpha. \tag{2}$$

- Substituting the Reduced-order solution (2) into Full order model (1), we can obtain reduced model

$$\mathbf{U}^T \mathcal{F}(\mathbf{U}\alpha\;, \mathbf{x}, t, \mu) = \mathbf{U}^T s(\mathbf{x}, t, \mu).$$

Physics-Data Combined Neural Network



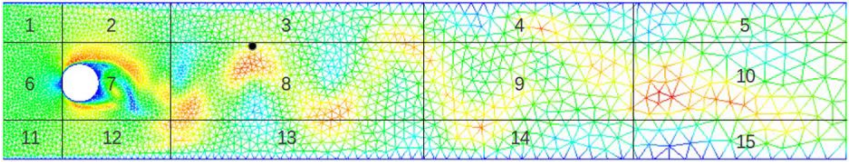
- The reduced PDEs terms contributes to the loss function

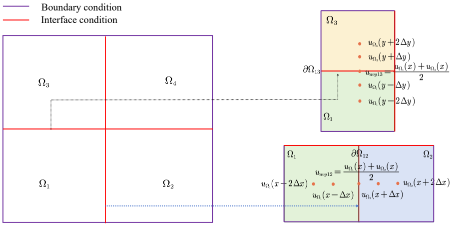
$$\mathcal{L}(\Theta) = \omega_{ib}(MSE_{IC} + MSE_{BC}) + \omega_{PDE} MSE_{PDE}. \tag{3}$$

- In this equation

$$MSE_{IC} = \frac{1}{N_r}\sum_{i=1}^{N_r}\left\|\mathcal{I}(\mathbf{u}_r;\mu_i) - \mathbf{u_0}(\mu_i)\right\|_2^2, MSE_{BC} = \frac{1}{N_r}\sum_{i=1}^{N_r}\left\|\mathcal{B}(\mathbf{u}_r;\mu_i) - \mathbf{u_b}(\mu_i)\right\|_2^2, MSE_{PDE} = \frac{1}{N_r}\sum_{i=1}^{N_r}\left\|\mathbf{U}^T(\mathcal{PDE}(\mathbf{u}_r;\mu_i) - \mathcal{S}(\mu_i))\right\|_2^2.$$

Domain Decomposition Strategy





- The average of $\mathbf{u}$ along the common interface

$$\mathbf{u}_{avgjk} = \frac{\mathbf{u}_{r,\Omega_k}(\mu_i) + \mathbf{u}_{r,\Omega_j}(\mu_i)}{2}$$

- Reduced PDEs terms along interfaces

$$\frac{\partial u_{r,\partial\Omega_{jk}}}{\partial x} = \widetilde{L}u_{r,\partial\Omega_{jk}} = \frac{-u_{r,\Omega_j}(\mathbf{x}+2\Delta\mathbf{x}) + 8u_{r,\Omega_j}(\mathbf{x}+\Delta\mathbf{x}) - 8u_{r,\Omega_k}(\mathbf{x}-\Delta\mathbf{x}) + u_{r,\Omega_k}(\mathbf{x}-2\Delta\mathbf{x})}{12\Delta x}. \quad (4)$$

Domain Decomposition Strategy

- Average term contributes to loss function along interface

$$MSE_{u_{avg}} = \frac{1}{N_r}\sum_{i=1}^{N_r}\sum_{j,k}^{\partial\Omega_{jk}\neq\varnothing}\frac{1}{|\partial\Omega_{jk}|}\left\|\mathbf{u}_{r,\Omega_{jk}}(\mu_i) - \mathbf{u}_{avgjk}(\mu_i)\right\|_2^2.$$

- Reduced PDEs terms contributes to loss function along interface

$$MSE_{u_{con}} = \frac{1}{|\partial\Omega|}\frac{1}{N_r}\sum_{i=1}^{N_r}\sum_{j,k}^{\partial\Omega_{jk}\neq\varnothing}\left\|\mathbf{U}^T\left(\mathcal{PDE}(\mathbf{u}_{r,\Omega_j}(\mu_i);\mathbf{u}_{r,\Omega_k}(\mu_i);\mathbf{u}_{avgjk}) - \mathcal{S}(\mu_i)\right)\right\|_2^2.$$

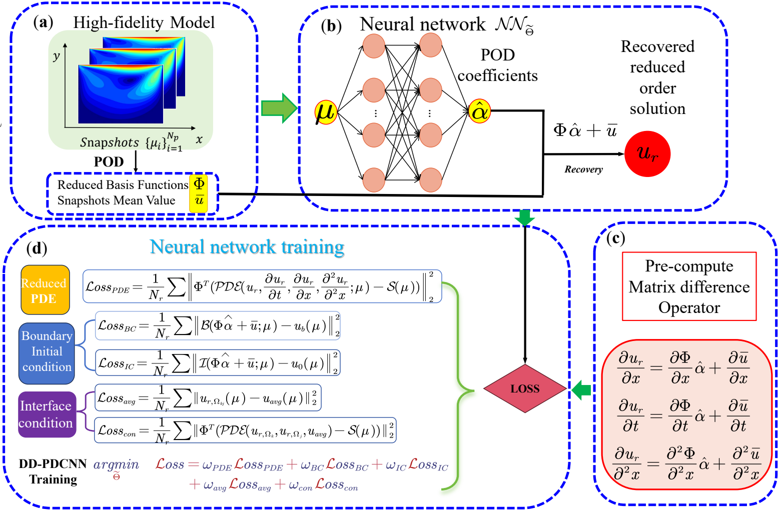
- In summary, the total loss function of DD-PDCNN is as follow

$$\mathcal{L}(\widetilde{\Theta}) = \omega_{ib}(MSE_{IC} + MSE_{BC}) + \omega_{PDE}MSE_{PDE} + \omega_{avg}MSE_{u_{avg}} + \omega_{con}MSE_{u_{con}}.$$

- Combine solutions to obtain the complete domain solution

$$\mathbf{u}_{r,\Omega} = \sum_{i=1}^{N_{sd}}\mathbf{u}_{\Omega_i}(\mu)\cdot\mathbb{I}_{\Omega_i}(x).$$

- Framwork


(a) High-fidelity Model
y
x
Snapshots $\{\mu_i\}_{i=1}^{N_p}$
POD
Reduced Basis Functions Φ
Snapshots Mean Value $\bar{u}$
(b) Neural network $\mathcal{NN}_{\tilde{\Theta}}$
μ
$\hat{\alpha}$
POD coefficients
Recovered reduced order solution
$\Phi\hat{\alpha}+\bar{u}$
Recovery
u_r
(d) Neural network training
Reduced PDE
$\mathcal{L}oss_{PDE}=\frac{1}{N_r}\sum\left\|\Phi^T(\mathcal{PDE}(u_r,\frac{\partial u_r}{\partial t},\frac{\partial u_r}{\partial x},\frac{\partial^2 u_r}{\partial^2 x};\mu)-\mathcal{S}(\mu))\right\|_2^2$
Boundary Initial condition
$\mathcal{L}oss_{BC}=\frac{1}{N_r}\sum\left\|\mathcal{B}(\Phi\hat{\alpha}+\bar{u};\mu)-u_b(\mu)\right\|_2^2$
$\mathcal{L}oss_{IC}=\frac{1}{N_r}\sum\left\|\mathcal{I}(\Phi\hat{\alpha}+\bar{u};\mu)-u_0(\mu)\right\|_2^2$
Interface condition
$\mathcal{L}oss_{avg}=\frac{1}{N_r}\sum\|u_{r,\Omega_k}(\mu)-u_{avg}(\mu)\|_2^2$
$\mathcal{L}oss_{con}=\frac{1}{N_r}\sum\|\Phi^T(\mathcal{PDE}(u_{r,\Omega_k},u_{r,\Omega_j},u_{avg})-\mathcal{S}(\mu))\|_2^2$
DD-PDCNN Training
$\underset{\tilde{\Theta}}{argmin}\ \mathcal{L}oss=\omega_{PDE}\mathcal{L}oss_{PDE}+\omega_{BC}\mathcal{L}oss_{BC}+\omega_{IC}\mathcal{L}oss_{IC}+\omega_{avg}\mathcal{L}oss_{avg}+\omega_{con}\mathcal{L}oss_{con}$
LOSS
(c)
Pre-compute Matrix difference Operator
$\frac{\partial u_r}{\partial x}=\frac{\partial\Phi}{\partial x}\hat{\alpha}+\frac{\partial\bar{u}}{\partial x}$
$\frac{\partial u_r}{\partial t}=\frac{\partial\Phi}{\partial t}\hat{\alpha}+\frac{\partial\bar{u}}{\partial t}$
$\frac{\partial u_r}{\partial^2 x}=\frac{\partial^2\Phi}{\partial^2 x}\hat{\alpha}+\frac{\partial^2\bar{u}}{\partial^2 x}$

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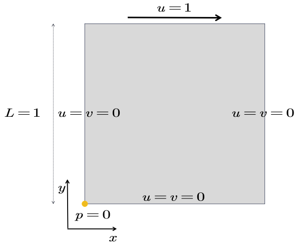
- Kovasznay flow
- Korteweg–de Vries equation
- Steady lid-driven cavity flow

Steady lid-driven cavity flow

- Navier-Stokes equations:

$$\nabla \cdot \mathbf{u} = 0,$$
$$\nabla \cdot (\mathbf{u} \otimes \mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u}$$

- Parameter Space $\mu \in [3 \times 10^{-3}, 10^{-2}]$
- Numerical solutions: Finite element simulation
- Divide the computational domain into three subdomains with interfaces at y = [0.3, 0.6]

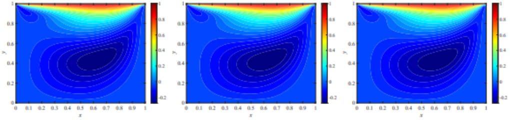


Geometry and boundary conditions of lid driven cavity

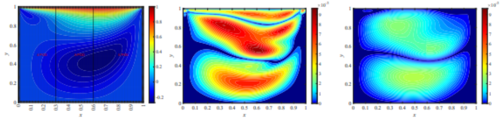
Results

- Compared to High-fidelity model and Physics-data combined ROM model

- Stream-wise Velocity for $\mu = 6 \times 10^{-3}$

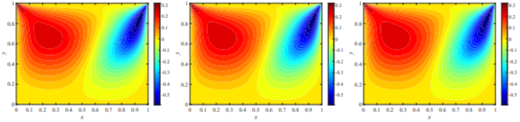


(a) High-fidelity model (b) PDCNN (c) DD-PDCNN

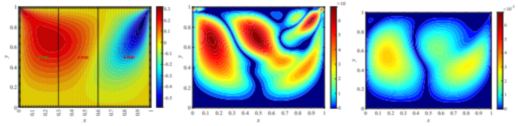


(d) POD basis functions for each subdomain (e) point-wise error of PDCNN (f) point-wise error of DD-PDCNN

- Normal-wise Velocity for $\mu = 6 \times 10^{-3}$



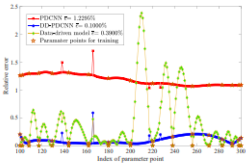
(a) High-fidelity model (b) PDCNN (c) DD-PDCNN



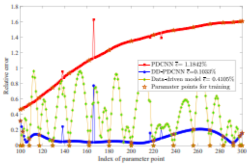
(d) POD basis functions for each subdomain (e) point-wise error of PDCNN (f) point-wise error of DD-PDCNN

Results

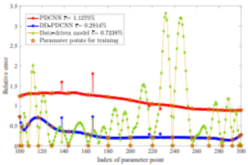
- Error



(a) Prediction relative L_2-norm error of velocity component u



(b) Prediction Relative L_2-normerror of velocity component v



(c) Prediction Relative L_2-norm error of pressure p

- Error

Subdomain	1	2	3	whole domain
Layers	3	3	3	4
Neurons	40	40	40	60
Relative L_2 error u	0.0535%	0.0567%	0.1022%	1.1842%
Relative L_2 error v	0.0638%	0.1257%	0.1065%	1.2295%
Relative L_2 error p	0.5857%	0.1240%	0.1458%	1.1275%

Conclusion and future work

- Present a novel domain decomposition method for ROM.
- Domain decomposition techniques enhance model accuracy and generalization capability
- The DD-PDCNN method can construct a reliable and general reduced-order model.
- Combine with closure modelling
- More complicated cases

Main Reference

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Thanks!