

DOMAIN DECOMPOSITION FOR LOCAL SURROGATE MODELS OF PARAMETRIC SYSTEMS

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CIMNE[®]
INTERNATIONAL CENTRE
FOR NUMERICAL METHODS
IN ENGINEERING



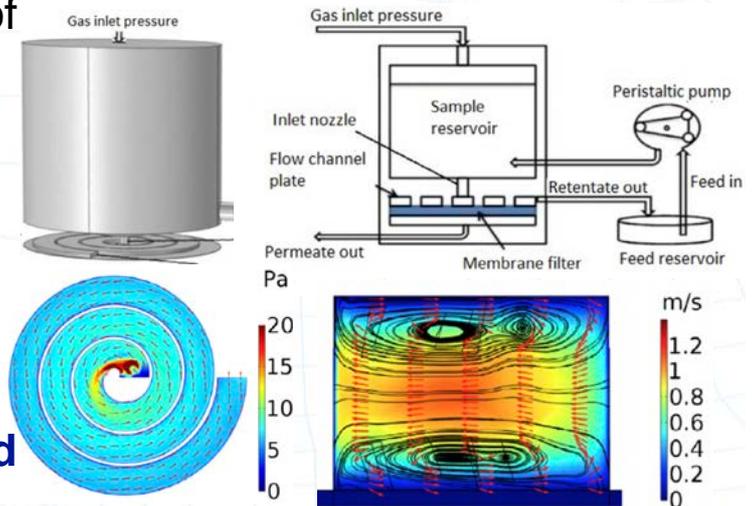
Towards digital twins of water filtration systems...

Goal: Virtual prototyping of **membranes** for **conception**, **design**, **optimisation**, and **operation** of **micro-filtration** systems



Requirements for **digital twins** of water purification systems:

- Incorporate user-defined/uncertain **parameters** (materials, geometry, functioning conditions, ...).
- Encapsulate the underlying **physics** to be **interpretable**.
- Be compatible with **established solution** strategies in **industry**.

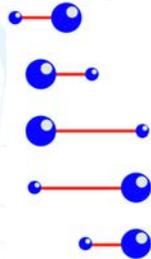
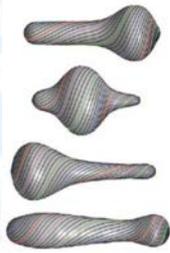


[Parasyris, Discacciati, Das. Appl Math Model 2020]

Parametric design and optimisation

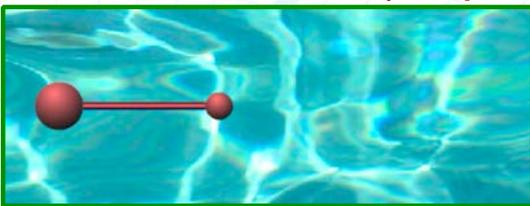
PMPY microswimmer: simplified model of euglenoid movement

- Parametrised geometry



[Arroyo, Heltai, Millán, DeSimone. PNAS 2012]

[Avron, Kenneth, Oaknin. New J Phys 2005]



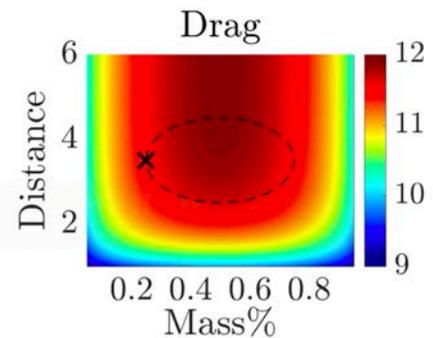
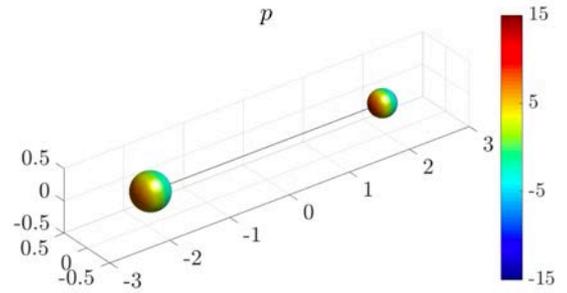
Mass% = 0.268

0.05 0.95

Distance = 3.873

1 6

- Trajectory A
- Trajectory B
- Trajectory C



[Sevilla, Borchini, Giacomini, Huerta. CMAME, 2020]

[Giacomini, Borchini, Sevilla, Huerta. Finite Elem Anal Des, 2021]

What are the computational bottlenecks?

- Multiple scenarios to be tested (many parameters)

→ High dimensional problems

- Large-scale systems

- Complex models (possibly, multi-physics)

→ Demanding spatial solves

How to reduce the cost of constructing digital twins?

- ➔ Local surrogate models
- ➔ Data augmentation
- ➔ Multi-fidelity approaches
- ➔ ...

Local Surrogate Models via Overlapping Domain Decomposition

with Loughborough University



Marco
Discacciati



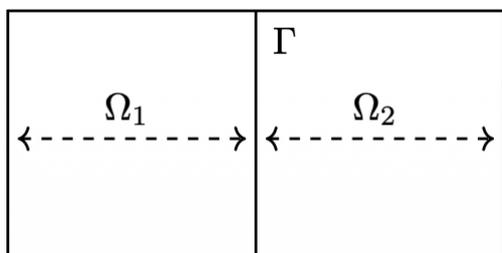
Ben
Evans

Parametric multi-domain formulations

For each value of the parameter:

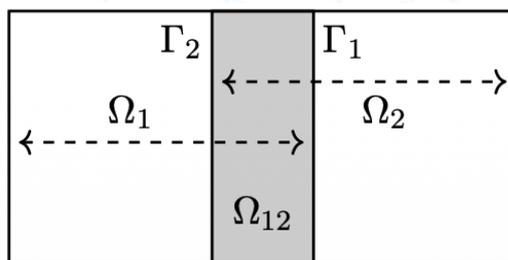
$$\begin{aligned}
 -\nabla \cdot (K(\mu)\nabla u(\mu)) &= s(\mu) & \text{in } \Omega \\
 u(\mu) &= 0 & \text{on } \partial\Omega
 \end{aligned}
 \longrightarrow
 \begin{aligned}
 -\nabla \cdot (K_i(\mu)\nabla u_i(\mu)) &= s_i(\mu) & \text{in } \Omega_i \quad (i = 1, 2) \\
 u_i(\mu) &= 0 & \text{on } \partial\Omega_i \cap \partial\Omega
 \end{aligned}$$

Non-overlapping



$$\begin{aligned}
 K_1(\mu)\nabla u_1(\mu) \cdot \mathbf{n} \\
 = K_2(\mu)\nabla u_2(\mu) \cdot \mathbf{n} & \text{ on } \Gamma \\
 u_1(\mu) = u_2(\mu) & \text{ on } \Gamma
 \end{aligned}$$

Overlapping



$$\begin{aligned}
 u_1(\mu) = u_2(\mu) & \text{ in } \Omega_{12} \\
 \text{or}
 \end{aligned}$$

$$u_1(\mu) = u_2(\mu) \text{ on } \Gamma_1 \cup \Gamma_2$$

[Discacciati, Gervasio, Quarteroni. SICON 2013]

Alternating Schwarz method

For each value of the parameter, solve:

$$\begin{pmatrix} A_{\Omega_1} & A_{\Gamma_1} & 0 & 0 \\ 0 & I_{\Gamma_1} & -R_{\Omega_2 \rightarrow \Gamma_1} & 0 \\ 0 & 0 & A_{\Omega_2} & A_{\Gamma_2} \\ -R_{\Omega_1 \rightarrow \Gamma_2} & 0 & 0 & I_{\Gamma_2} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{\Omega_1}(\bar{\mu}) \\ \mathbf{u}_{\Gamma_1}(\bar{\mu}) \\ \mathbf{u}_{\Omega_2}(\bar{\mu}) \\ \mathbf{u}_{\Gamma_2}(\bar{\mu}) \end{pmatrix} = \begin{pmatrix} \mathbf{s}_{\Omega_1}(\bar{\mu}) \\ \mathbf{0} \\ \mathbf{s}_{\Omega_2}(\bar{\mu}) \\ \mathbf{0} \end{pmatrix}$$

Schur complement leading to the interface system

$$\begin{pmatrix} I_{\Gamma_1} & R_{\Omega_2 \rightarrow \Gamma_1} A_{\Omega_2}^{-1} A_{\Gamma_2} \\ R_{\Omega_1 \rightarrow \Gamma_2} A_{\Omega_1}^{-1} A_{\Gamma_1} & I_{\Gamma_2} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{\Gamma_1}(\bar{\mu}) \\ \mathbf{u}_{\Gamma_2}(\bar{\mu}) \end{pmatrix} = \begin{pmatrix} R_{\Omega_2 \rightarrow \Gamma_1} A_{\Omega_2}^{-1} \mathbf{s}_{\Omega_2}(\bar{\mu}) \\ R_{\Omega_1 \rightarrow \Gamma_2} A_{\Omega_1}^{-1} \mathbf{s}_{\Omega_1}(\bar{\mu}) \end{pmatrix}$$

Solution of local FEM problems can become unaffordable in a parametric setting!

Surrogate-based alternating Schwarz method

For each value of the parameter, solve:

$$\begin{pmatrix} A_{\Omega_1} & A_{\Gamma_1} & 0 & 0 \\ 0 & I_{\Gamma_1} & -R_{\Omega_2 \rightarrow \Gamma_1} & 0 \\ 0 & 0 & A_{\Omega_2} & A_{\Gamma_2} \\ -R_{\Omega_1 \rightarrow \Gamma_2} & 0 & 0 & I_{\Gamma_2} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{\Omega_1}(\bar{\mu}) \\ \mathbf{u}_{\Gamma_1}(\bar{\mu}) \\ \mathbf{u}_{\Omega_2}(\bar{\mu}) \\ \mathbf{u}_{\Gamma_2}(\bar{\mu}) \end{pmatrix} = \begin{pmatrix} \mathbf{s}_{\Omega_1}(\bar{\mu}) \\ \mathbf{0} \\ \mathbf{s}_{\Omega_2}(\bar{\mu}) \\ \mathbf{0} \end{pmatrix}$$

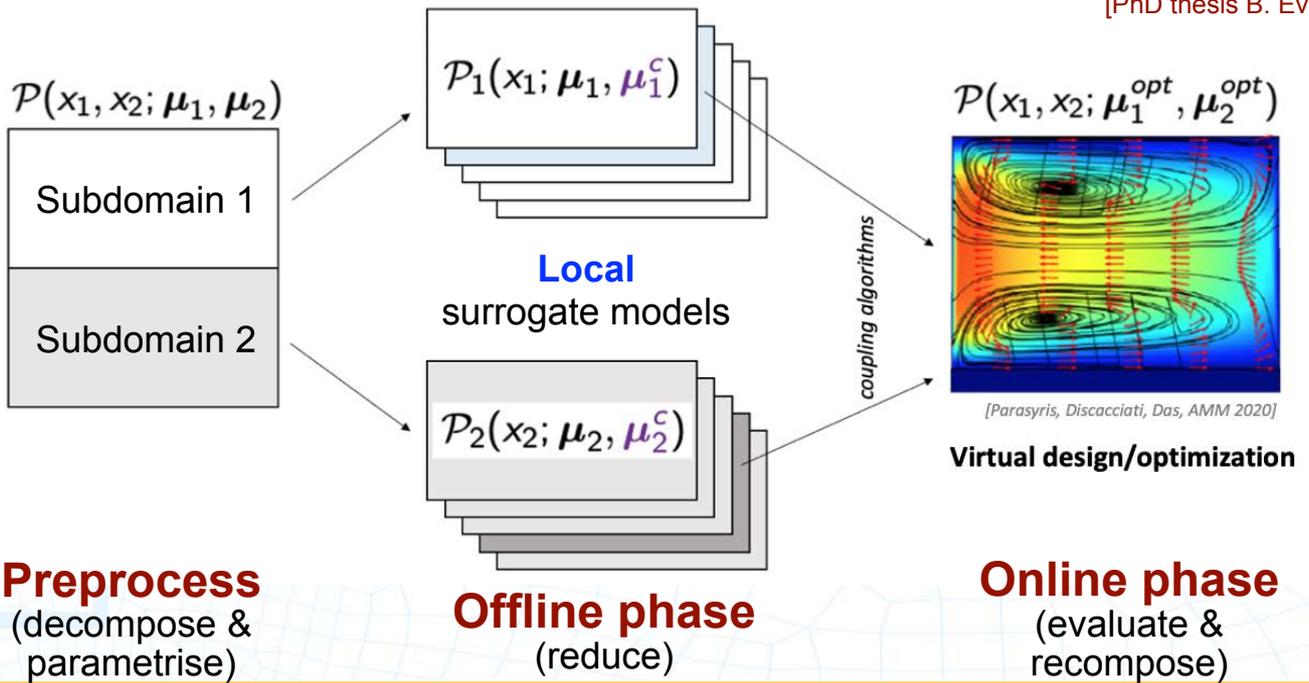
Schur complement leading to the interface system

$$\begin{pmatrix} I_{\Gamma_1} & R_{\Omega_2 \rightarrow \Gamma_1} A_{\Omega_2}^{\text{PGD}} \\ R_{\Omega_1 \rightarrow \Gamma_2} A_{\Omega_1}^{\text{PGD}} & I_{\Gamma_2} \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} = \begin{pmatrix} R_{\Omega_2 \rightarrow \Gamma_1} \mathbf{u}_{2,\text{PGD}}^s(\bar{\mu}) \\ R_{\Omega_1 \rightarrow \Gamma_2} \mathbf{u}_{1,\text{PGD}}^s(\bar{\mu}) \end{pmatrix}$$

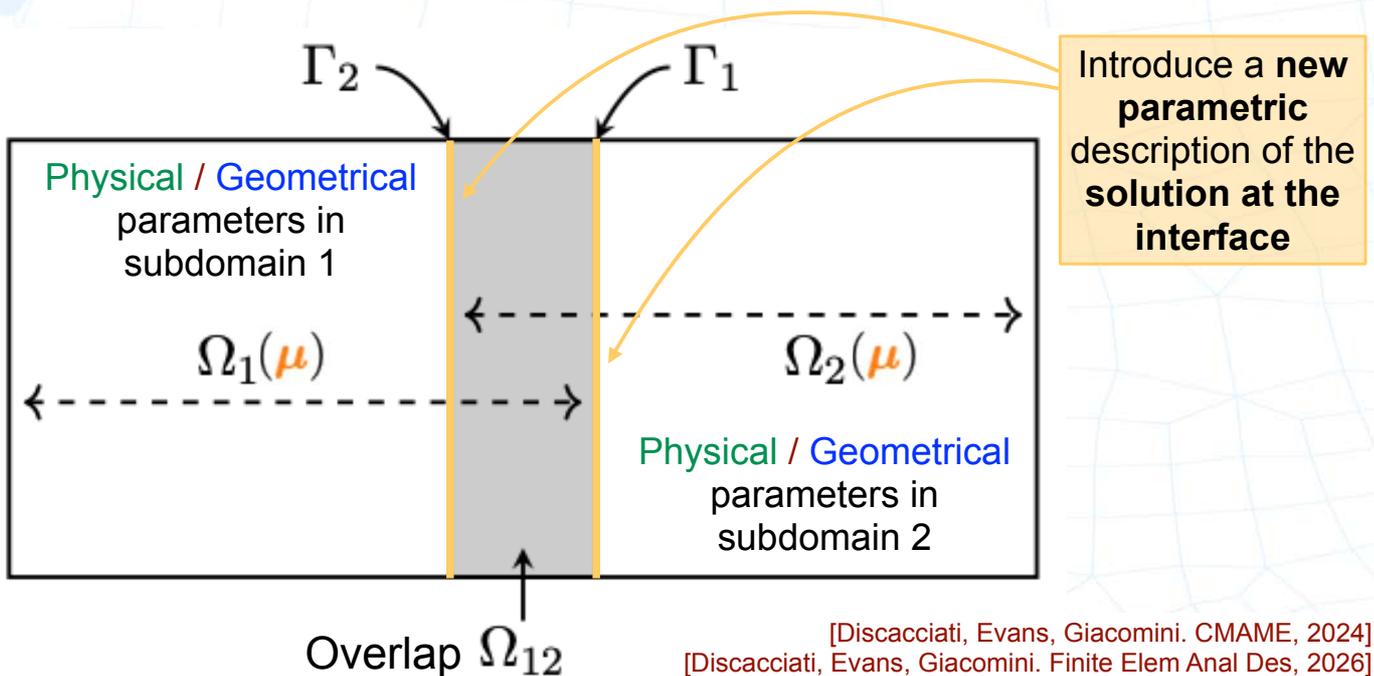
Replace by means of a previously surrogate model (**inexpensive evaluation!**)

Decompose > Reduce > Recompose

[PhD thesis B. Evans]



Preprocess: decompose into parametric subdomains



Offline: define a parametric subproblem

In each subdomain, solve the **linear** elliptic PDE:

$$\begin{aligned}
 L(u_i(\boldsymbol{\mu}); \boldsymbol{\mu}) &= s_i(\boldsymbol{\mu}) && \text{in } \Omega_i, \\
 u_i(\boldsymbol{\mu}) &= g_i^D(\boldsymbol{\mu}) && \text{on } \Gamma_i^D, \\
 \nu(\boldsymbol{\mu}) \nabla u_i(\boldsymbol{\mu}) \cdot \mathbf{n} &= g_i^N(\boldsymbol{\mu}) && \text{on } \Gamma_i^N, \\
 u_i(\boldsymbol{\mu}) &= \lambda_i && \text{on } \Gamma_i,
 \end{aligned}$$

$$\lambda_i = \lambda_i(\mathbf{x}) = \sum_{q=1}^{N_{\Gamma_i}} \Lambda_i^q \eta_i^q(\mathbf{x})$$

User-defined spatial functions (**FEM basis**)

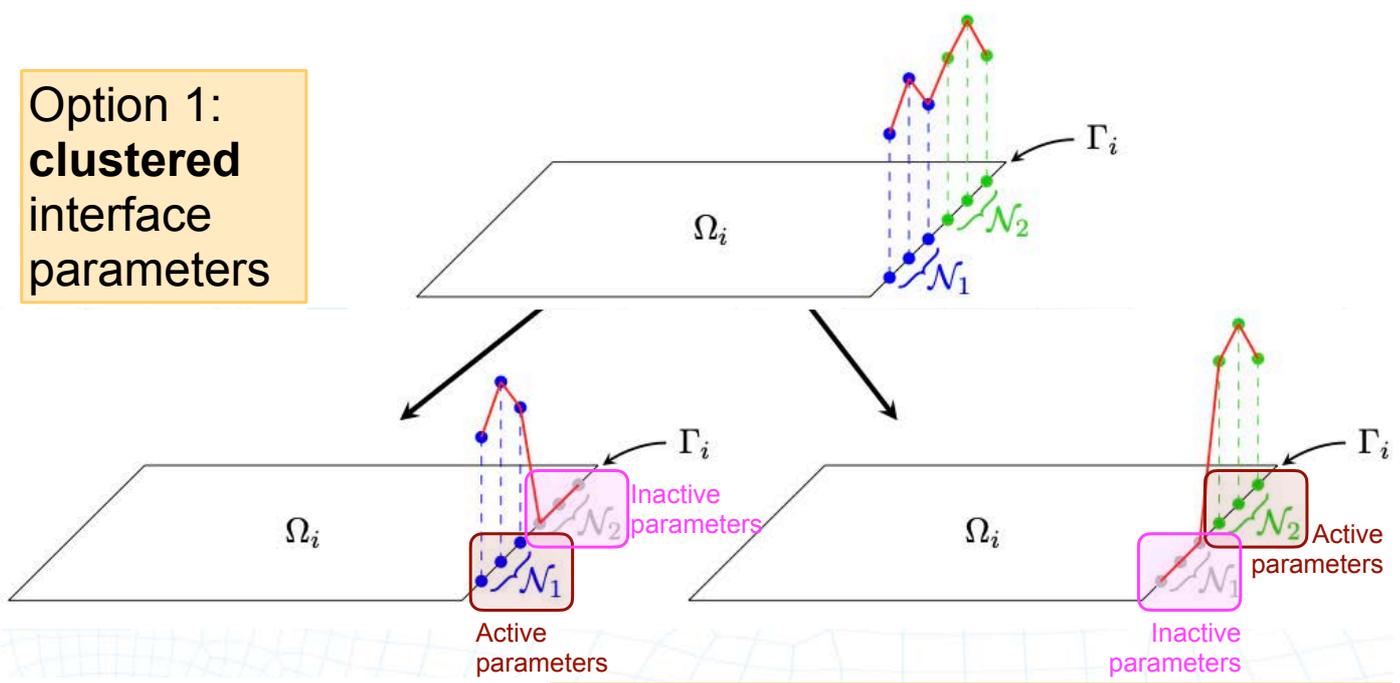
New set of **parameters**
(To be determined **online**)

Less DOFs in space but **higher dimensional** problem!

[Discacciati, Evans, Giacomini. CMAME, 2024]
 [Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

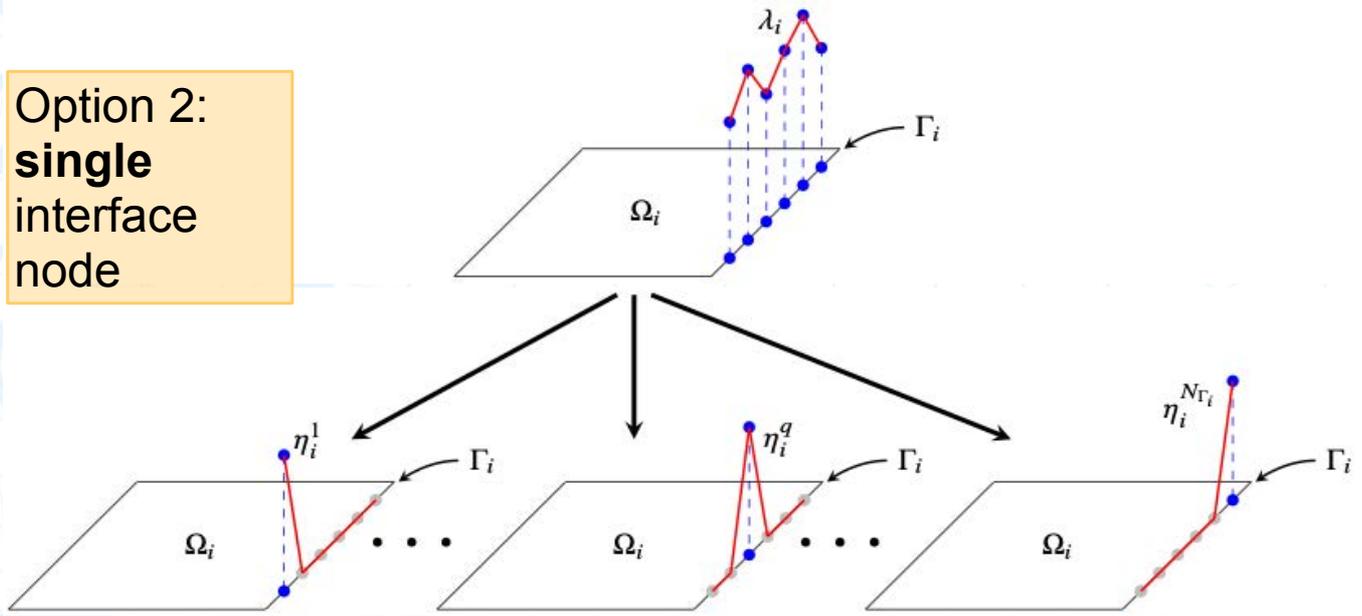
Offline: reduce the dimensionality

Option 1:
clustered
interface
parameters



Offline: reduce the dimensionality

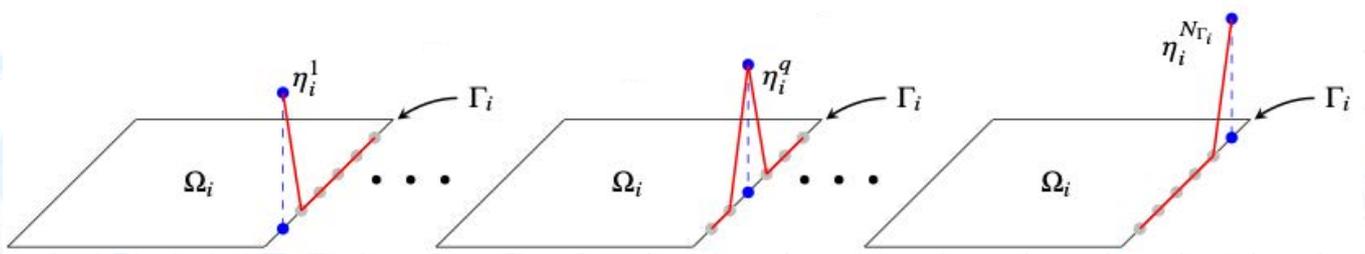
Option 2:
single
 interface
 node



[Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

Offline: construct a PGD local surrogate model

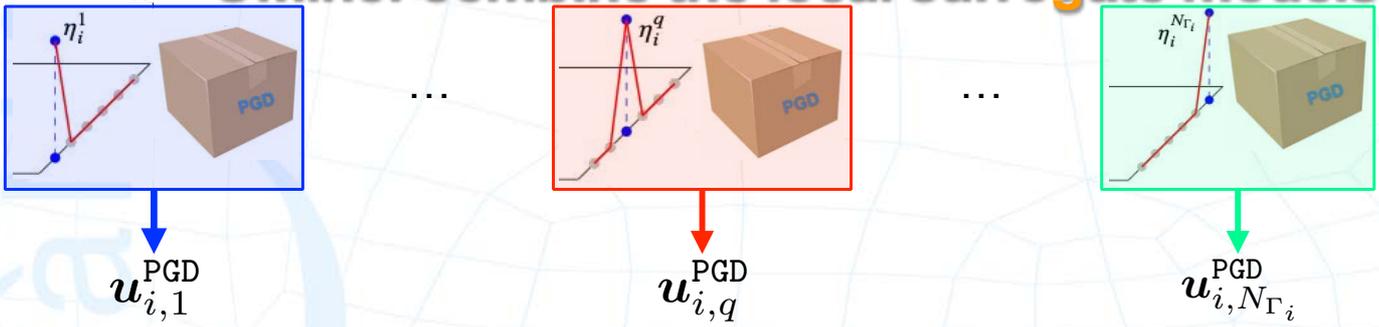
In each subdomain, construct N_{Γ_i} local surrogate models, each associated with the non-zero BC on one node of the interface.



$$\mathbf{u}_{i,j}(\mathbf{x}, \boldsymbol{\mu}) \simeq \mathbf{u}_{i,j}^{\text{PGD}}(\mathbf{x}, \boldsymbol{\mu}) = \sum_{m=1}^n \sigma_u^m \mathbf{f}_u^m(\mathbf{x}) \phi^m(\boldsymbol{\mu}) \quad j = 1, \dots, N_{\Gamma_i}$$

[Discacciati, Evans, Giacomini. CMAME, 2024]
 [Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

Offline: combine the local surrogate models



Retrieve the surrogate model for subdomain Ω_i

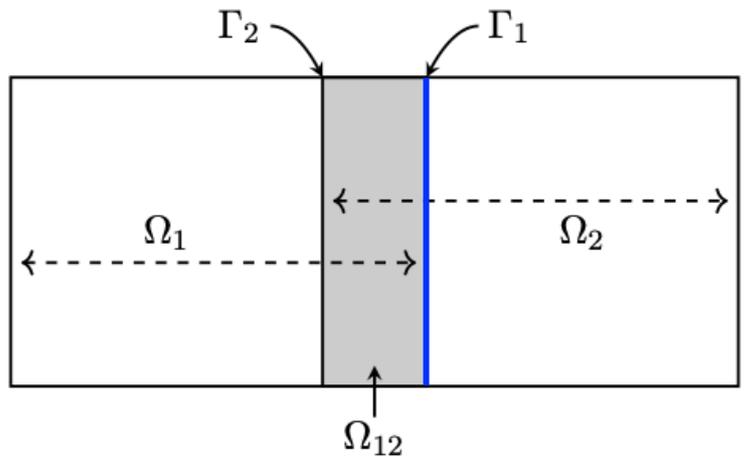
$$\mathbf{u}_i^{\text{PGD}}(\mathbf{x}, \boldsymbol{\mu}, \Lambda_i) = \sum_{q=1}^{N_{\Gamma_i}} \Lambda_i^q \mathbf{u}_{i,q}^{\text{PGD}}(\mathbf{x}, \boldsymbol{\mu})$$

Because of linearity of the PDE!

[Discacciati, Evans, Giacomini. CMAME, 2024]
 [Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

Online: parametric overlapping Schwarz

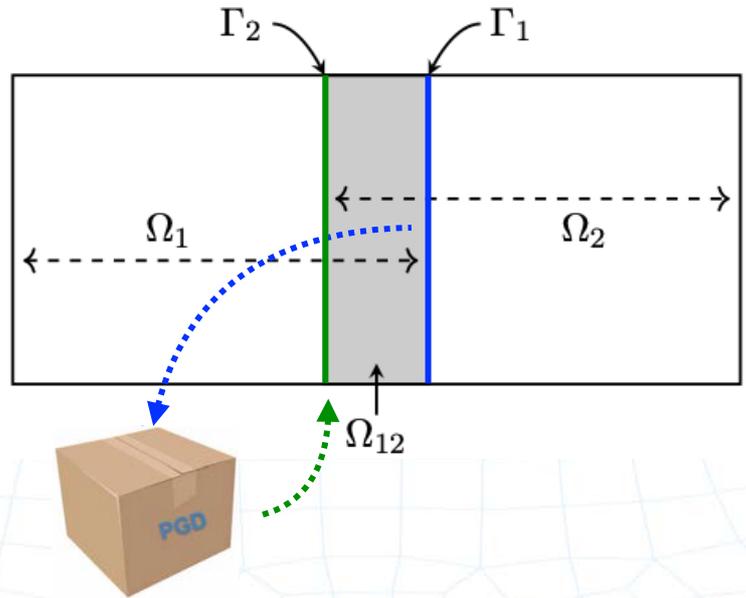
1. Fix a set of **boundary parameters** Λ_1 describing the solution on Γ_1



[Discacciati, Evans, Giacomini. CMAME, 2024]
 [Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

Online: parametric overlapping Schwarz

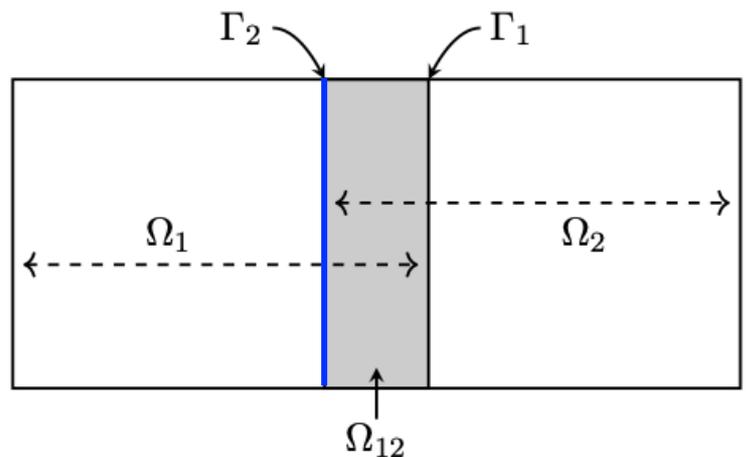
1. Fix a set of **boundary parameters** Λ_1 describing the solution on Γ_1
2. Evaluate the **PGD solution** u_1^{PGD} on Γ_2



[Discacciati, Evans, Giacomini. CMAME, 2024]
 [Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

Online: parametric overlapping Schwarz

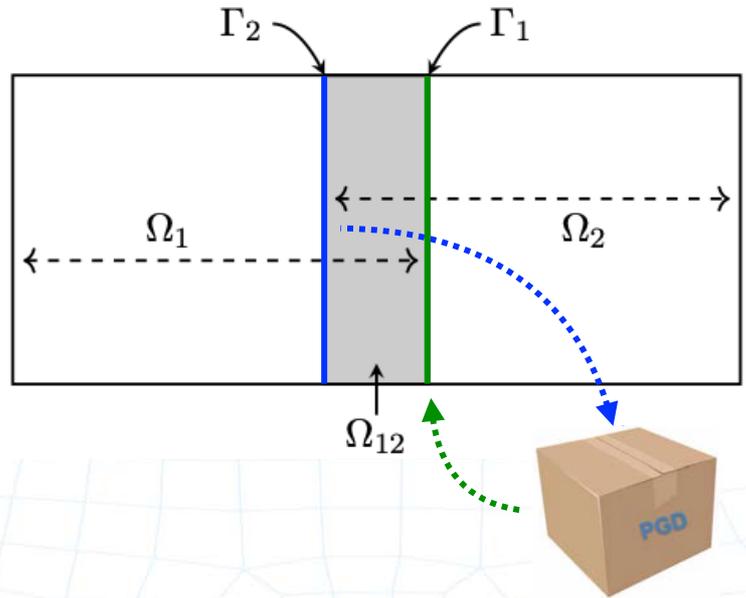
1. Fix a set of **boundary parameters** Λ_1 describing the solution on Γ_1
2. Evaluate the **PGD solution** u_1^{PGD} on Γ_2
3. Extract the **boundary parameters** Λ_2 on Γ_2



[Discacciati, Evans, Giacomini. CMAME, 2024]
 [Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

Online: parametric overlapping Schwarz

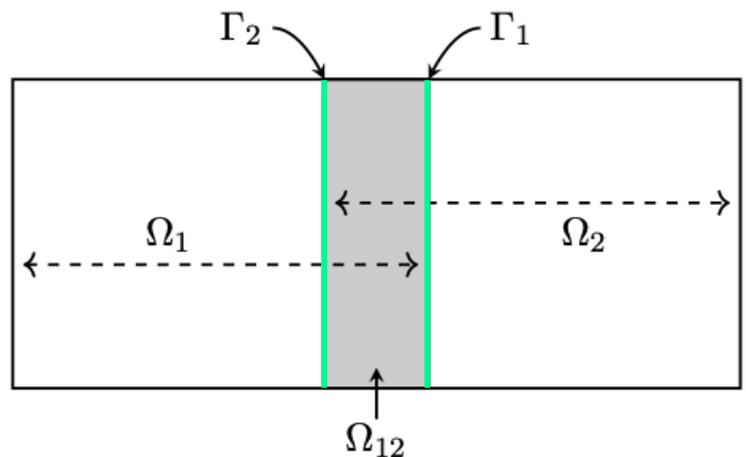
1. Fix a set of **boundary parameters** Λ_1 describing the solution on Γ_1
2. Evaluate the **PGD solution** u_1^{PGD} on Γ_2
3. Extract the **boundary parameters** Λ_2 on Γ_2
4. Evaluate the **PGD solution** u_2^{PGD} on Γ_1



[Discacciati, Evans, Giacomini. CMAME, 2024]
 [Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

Online: parametric overlapping Schwarz

1. Fix a set of **boundary parameters** Λ_1 describing the solution on Γ_1
2. Evaluate the **PGD solution** u_1^{PGD} on Γ_2
3. Extract the **boundary parameters** Λ_2 on Γ_2
4. Evaluate the **PGD solution** u_2^{PGD} on Γ_1
5. Check **convergence** and go to 1.



[Discacciati, Evans, Giacomini. CMAME, 2024]
 [Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

Encapsulated Proper Generalised Decomposition

[Ammar, Mokdad, Chinesta, Keunings. J Nonnewton Fluid Mech 2006]
 [Díez, Zlotnik, García-González, Huerta. ACME, 2020]

- The **commercial/industrial software** selected by the user for the spatial problem is used to **preprocess data** for the construction of the discrete high-dimensional parametric problem.

$$\mathbf{u}_{i,j}^{\text{PGD}}(\mathbf{x}, \boldsymbol{\mu}) = \sum_{m=1}^n \sigma_u^m \mathbf{f}_u^m(\mathbf{x}) \phi^m(\boldsymbol{\mu}) = \sum_{m=1}^n \sigma_u^m \mathbf{f}_u^m(\mathbf{x}) \prod_{k=1}^{n_{\text{pa}}} \phi_k^m(\mu_k)$$

Discretised using finite elements, finite volumes, ... according to the format of the **selected spatial solver**.

Discretised using **pointwise collocation**.

- Vectors and matrices of the spatial component of the high-dimensional problem are extracted from the spatial solver.

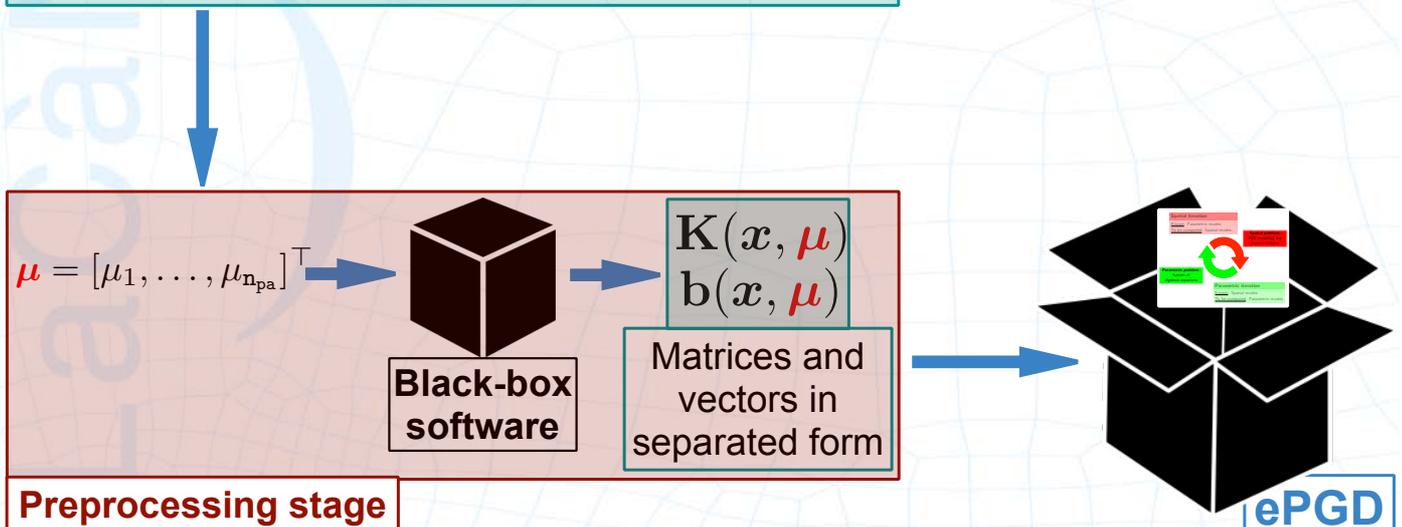
$$\mathbf{K}(\mathbf{x}, \boldsymbol{\mu}) \mathbf{u}(\mathbf{x}, \boldsymbol{\mu}) = \mathbf{b}(\mathbf{x}, \boldsymbol{\mu})$$

Encapsulated Proper Generalised Decomposition

[Díez, Zlotnik, García-González, Huerta. ACME, 2020]

Parametric system

$$\mathbf{K}(\mathbf{x}, \boldsymbol{\mu}) \mathbf{u}(\mathbf{x}, \boldsymbol{\mu}) = \mathbf{b}(\mathbf{x}, \boldsymbol{\mu})$$



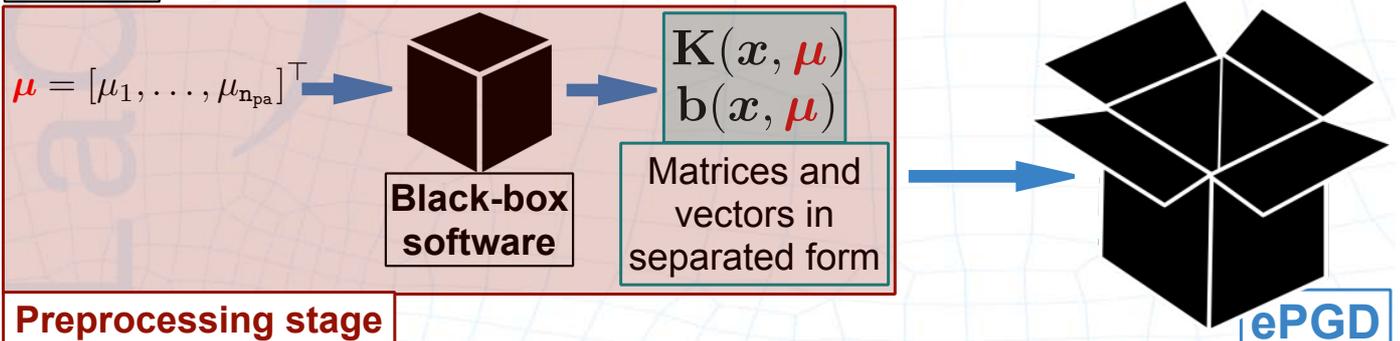
Encapsulated Proper Generalised Decomposition

[Díez, Zlotnik, García-González, Huerta. ACME, 2020]

- ePGD offers a **seamless implementation of PGD** for the end user (invisible greedy and ADI routines).
- Suitable for **commercial and industrial environment**.
- Generic implementation **independent of the spatial solver**.

VPS/Pam-Crash [Rocas, García-González, Zlotnik, Larráyo, Díez. FINEL 2021]

NASTRAN [Cavaliere, Zlotnik, Sevilla, Larrayoz, Díez. CMAME 2022]



The notion of separated tensor

Parametric model problem

$$-\nabla \cdot ((1 + \mu x) \nabla u) = s(\mu), \quad \text{in } \Omega \quad \Omega = (0, 2) \times (0, 1) \quad \mathcal{I} = [1, 50]$$

$$u = 0, \quad \text{on } \partial\Omega \quad s(\mu) = b_s^1(x) + \mu b_s^2(x) + \mu^2 b_s^3(x)$$

Parametric weak form

Parametric modes: vectors discretised in \mathcal{I} with pointwise collocation

$$\xi_\nu^1 \int_\Omega \nabla v \cdot \nabla u \, d\Omega + \xi_\nu^2 \int_\Omega x \nabla v \cdot \nabla u \, d\Omega = \xi_s^1 \int_\Omega v b_s^1(x) \, d\Omega + \xi_s^2 \int_\Omega v b_s^2(x) \, d\Omega + \xi_s^3 \int_\Omega v b_s^3(x) \, d\Omega$$

\mathbf{K}^1
 \mathbf{K}^2
 \mathbf{b}^1
 \mathbf{b}^2
 \mathbf{b}^3

Spatial modes: matrices and vectors discretised in Ω with black-box solver

Separated tensor
 $\mathbf{K}(x, \mu)$

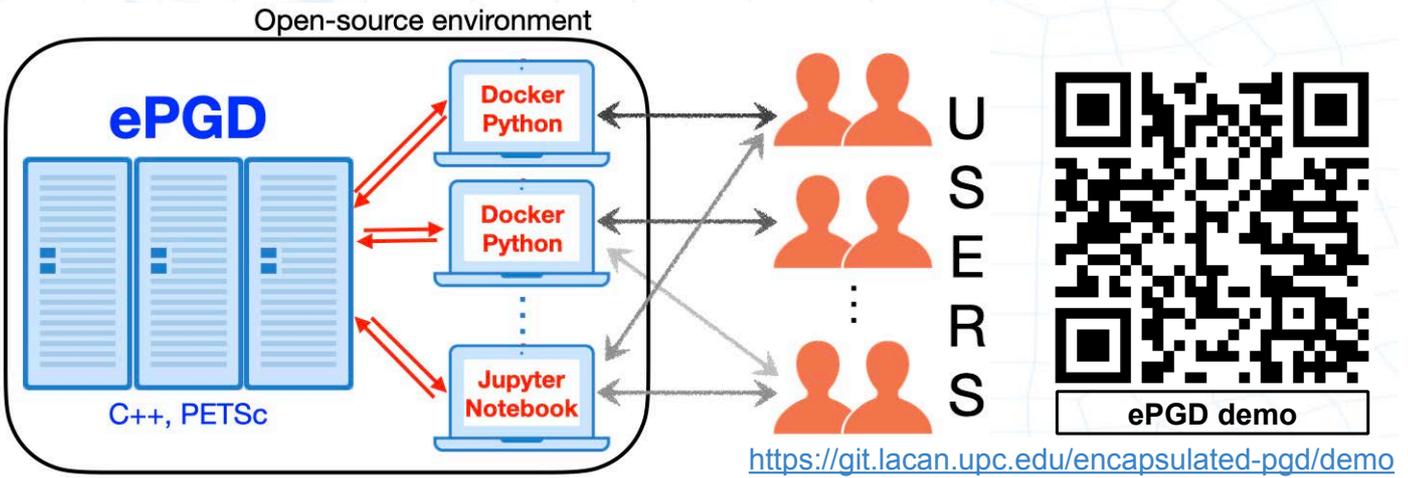
Separated tensor
 $\mathbf{b}(x, \mu)$



Prueba de Concepto
PDC2021-121554-C21

The ePGD library

- **Open-source** environment.
- **Efficient** core routines implemented in **C++**, linked with **PETSc**.
- **User-friendly** interface in **Python**.

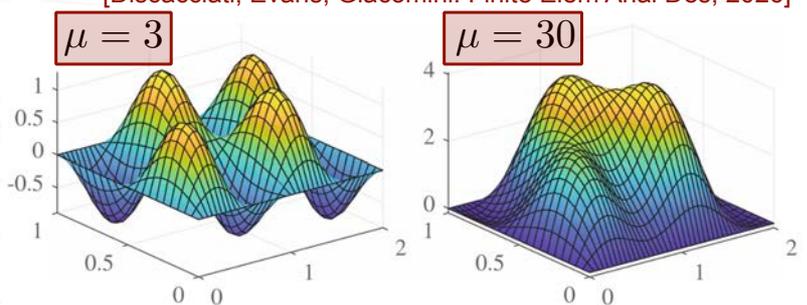


A synthetic example

[Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

$$-\nabla \cdot ((1 + \mu x) \nabla u(\mu)) = s(\mu) \quad \text{in } \Omega,$$

$$u(\mu) = 0 \quad \text{on } \partial\Omega,$$



- **Domain:** $\Omega = (0, 2) \times (0, 1)$
- **Decomposition:** $\Omega_1 = (0, 1 + nh_x) \times (0, 1)$
 $\Omega_2 = (1 - nh_x, 2) \times (0, 1)$
- **Parametric domain:** $\mu \in \mathcal{P} = [1, 50]$
- **Discretisation:** \mathcal{Q}_1 finite elements

Overlap: $2nh_x$

$h_\mu = h_\Lambda = 10^{-3}$
 $h_x = 5 \times 10^{-2}$

[Discacciati, Evans, Giacomini. CMAME, 2024]

A synthetic example

[Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

Problem setup:

- 2 spatial dimensions
- 1 parameter μ
- 19 parametric nodes at the interface

	Number of clustered interface parameters	Number of subproblems	Dimension of subproblems	Offline time (s)
Single interface node	-	19	3	5.66
Clustered interface parameters	1	19	4	9.80
	3	7	6	112.14
	5	4	8	482.68

A synthetic example

[Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

Problem setup:

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- 1 parameter μ
- 19 parametric nodes at the interface

Space of the solution of dimension 22

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A synthetic example

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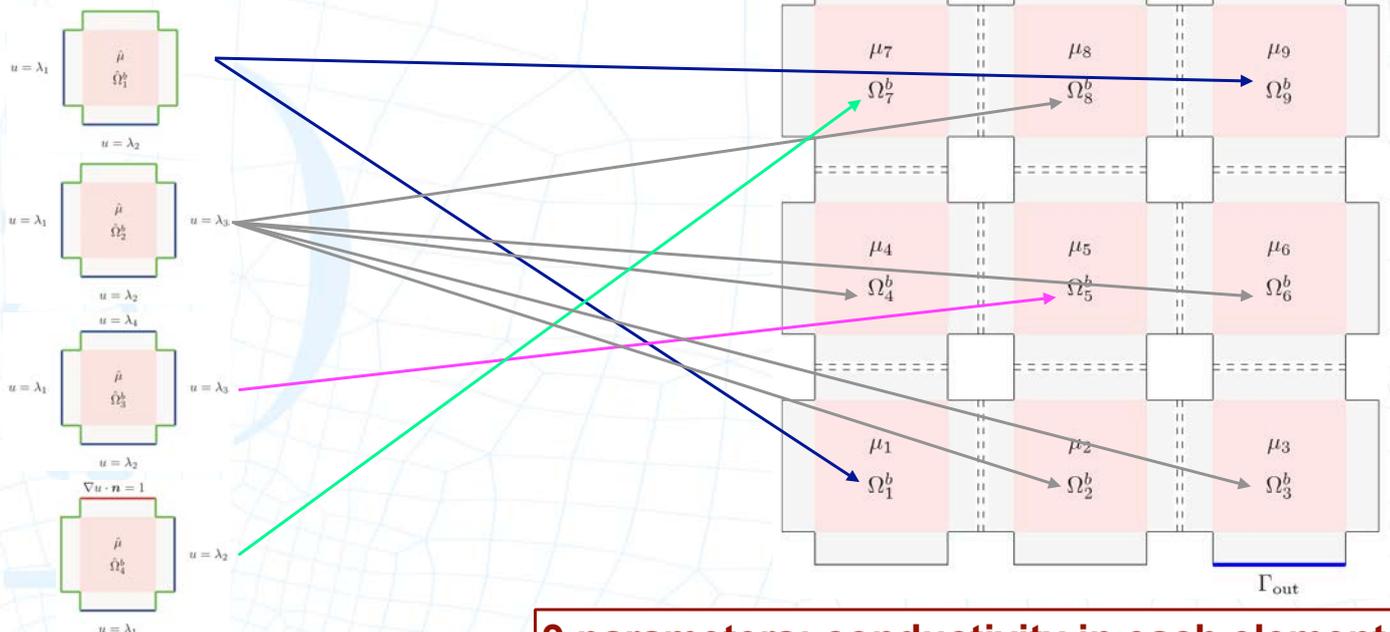
- 2 spatial dimensions
- 1 parameter μ
- 19 parametric nodes at the interface

Accuracy comparable in all cases

	Number of clustered interface parameters	Number of subproblems	Dimension of subproblems	Offline time (s)	Number of GMRES iterations (online)
Single interface node	-	19	3	5.66	9
Clustered interface parameters	1	19	4	9.80	13
	3	7	6	112.14	16
	5	4	8	482.68	18

A thermal problem with parametrised conductivity

- Four elemental subdomains:

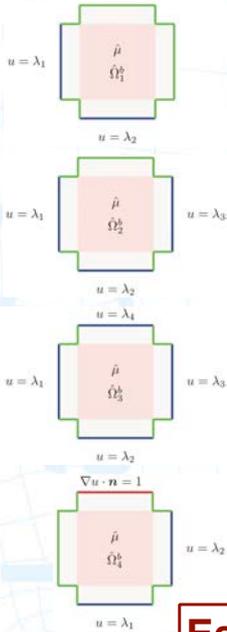


[Eftang, Patera. IJNME 2013]

9 parameters: conductivity in each element

A thermal problem with parametrised conductivity

- Four elemental subdomains:

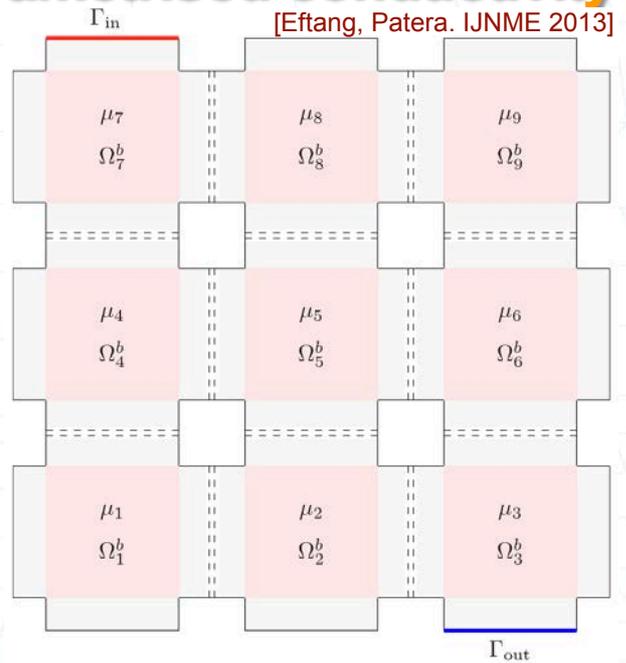


42 subproblems with 2,163 DOFs

63 subproblems with 2,142 DOFs

84 subproblems with 2,121 DOFs

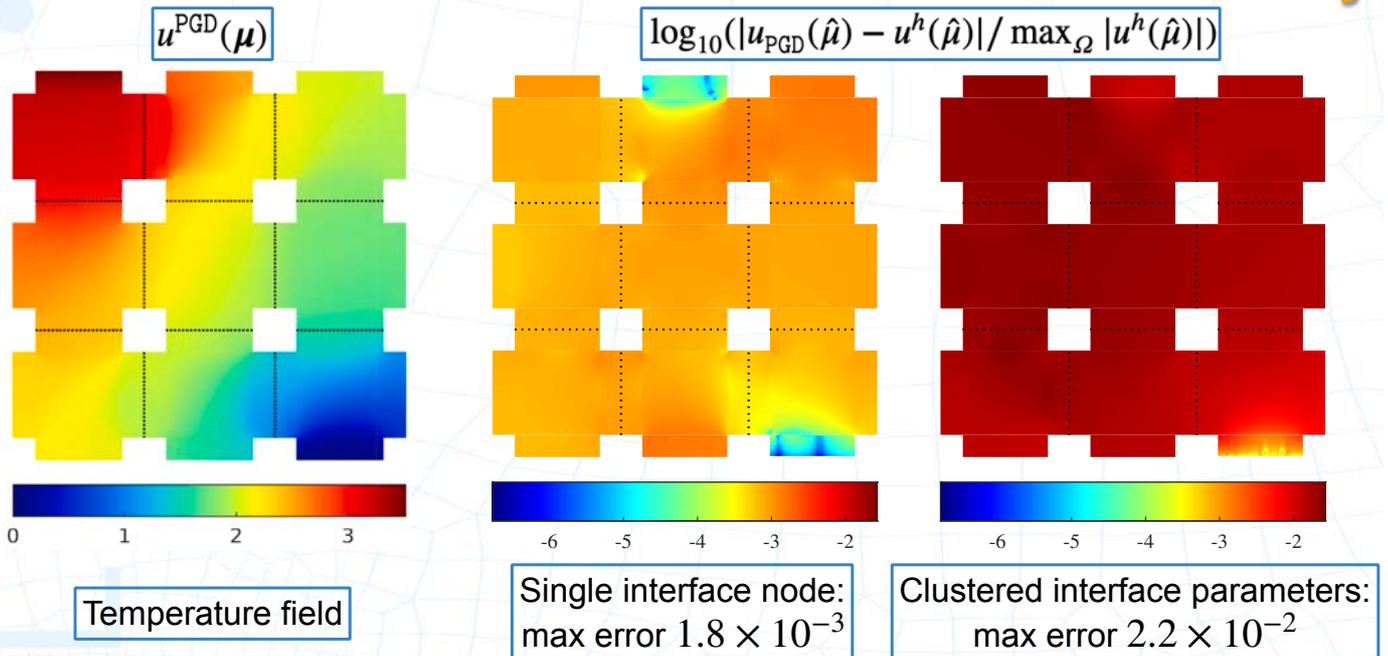
43 subproblems with 2,163 DOFs



[Eftang, Patera. IJNME 2013]

Each subproblem with 2 spatial and 1 parametric dimensions

DD-PGD accuracy



[Discacciati, Evans, Giacomini. CMAME, 2024]

DD-PGD efficiency

	Number of clustered interface parameters	Number of subproblems	Dimension of subproblems	Offline time (s)	Number of GMRES iterations	Online time (s)
Single interface node	-	231	3	36.18	93	0.47
Clustered interface parameters	3	77	6	872.38	302	157.23
Reference DD-FEM					95	414.80

DD-PGD speed-up of 882 times w.r.t. DD-FEM!

[Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

DD-PGD efficiency

	Number of clustered interface parameters	Number of subproblems	Dimension of subproblems	Offline time (s)	Number of GMRES iterations	Online time (s)
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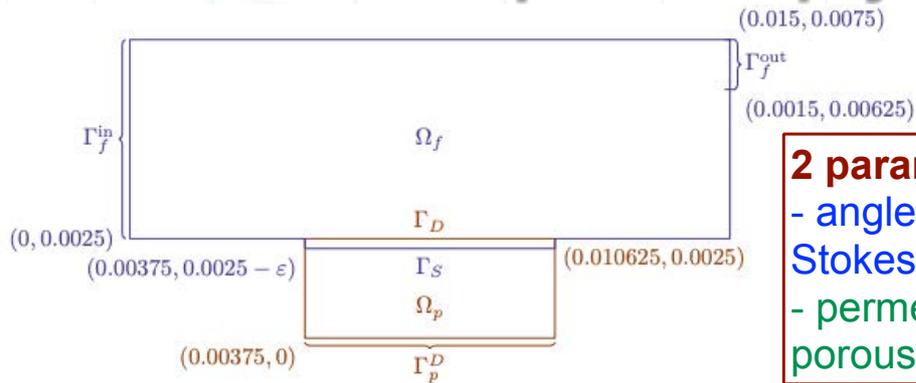
DD-PGD speed-up of 11 times w.r.t. DD-FEM!

[Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

The coupled multi-physics case

Fluid domain

Porous medium



2 parameters:
 - angle of inlet Stokes velocity
 - permeability of porous medium

Stokes equations:

$$\begin{aligned}
 -\nabla \cdot \boldsymbol{\sigma}(\mathbf{u}_f(\boldsymbol{\mu}), p_f(\boldsymbol{\mu}); \boldsymbol{\mu}) &= \mathbf{0} && \text{in } \Omega_f, \\
 \nabla \cdot \mathbf{u}_f(\boldsymbol{\mu}) &= 0 && \text{in } \Omega_f, \\
 \mathbf{u}_f(\boldsymbol{\mu}) &= \mathbf{g}_f^D(\boldsymbol{\mu}) && \text{on } \Gamma_f^{\text{in}}, \\
 \boldsymbol{\sigma}(\mathbf{u}_f(\boldsymbol{\mu}), p_f(\boldsymbol{\mu}); \boldsymbol{\mu}) \cdot \mathbf{n} &= \mathbf{0} && \text{on } \Gamma_f^{\text{out}}, \\
 \mathbf{u}_f(\boldsymbol{\mu}) &= \mathbf{0} && \text{on } \partial\Omega_f \setminus (\Gamma_f^{\text{in}} \cup \Gamma_f^{\text{out}} \cup \Gamma_S), \\
 \mathbf{u}_f(\boldsymbol{\mu}) &= \boldsymbol{\lambda}_S(\boldsymbol{\mu}) && \text{on } \Gamma_S.
 \end{aligned}$$

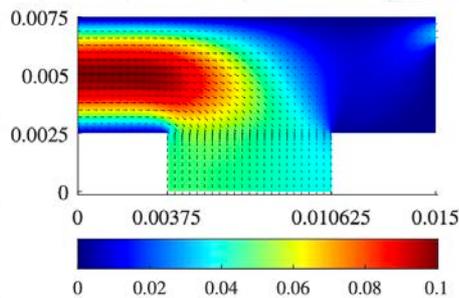
Darcy equations:

$$\begin{aligned}
 \nu(\boldsymbol{\mu}) \mathbf{K}(\boldsymbol{\mu})^{-1} \mathbf{u}_p(\boldsymbol{\mu}) + \nabla p_p(\boldsymbol{\mu}) &= \mathbf{0} && \text{in } \Omega_p, \\
 \nabla \cdot \mathbf{u}_p(\boldsymbol{\mu}) &= 0 && \text{in } \Omega_p, \\
 p_p(\boldsymbol{\mu}) &= 0 && \text{on } \Gamma_p^D, \\
 \mathbf{u}_p(\boldsymbol{\mu}) \cdot \mathbf{n} &= 0 && \text{on } \partial\Omega_p \setminus (\Gamma_p^D \cup \Gamma_D), \\
 p_p(\boldsymbol{\mu}) &= \boldsymbol{\lambda}_D(\boldsymbol{\mu}) && \text{on } \Gamma_D.
 \end{aligned}$$

Parametric Stokes-Darcy cross-flow

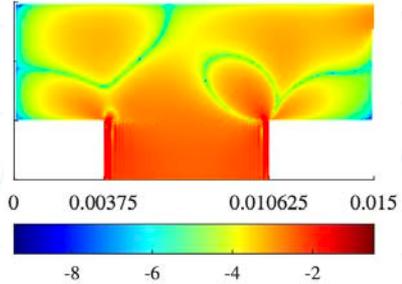
Max inlet velocity

Very permeable material



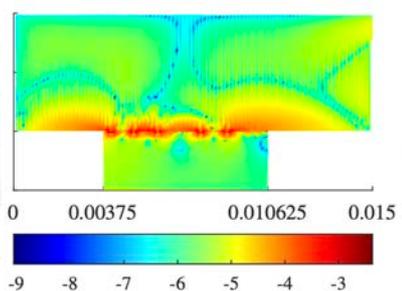
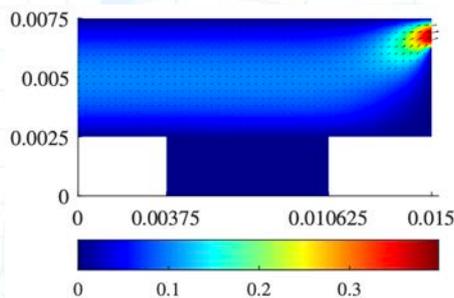
$$\|\mathbf{u}^{\text{PGD}}(\bar{\boldsymbol{\mu}})\|$$

$$\log_{10}(|\mathbf{u}^{\text{PGD}}(\bar{\boldsymbol{\mu}}) - \mathbf{u}^h(\bar{\boldsymbol{\mu}})| / \max_{\Omega} |\mathbf{u}^h(\bar{\boldsymbol{\mu}})|)$$

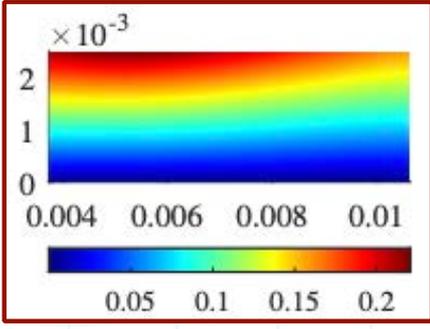
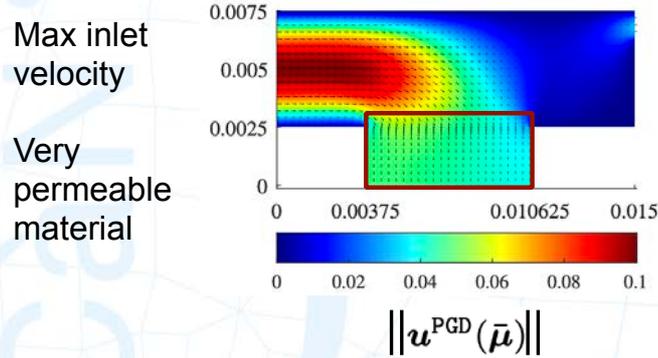


Max inlet velocity

Almost impermeable material

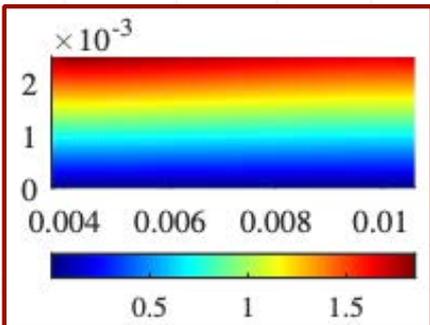
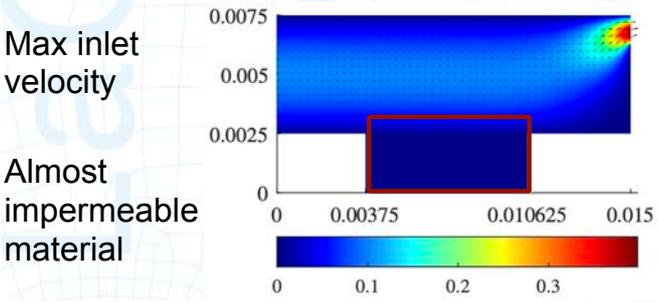


Parametric Stokes-Darcy cross-flow



Offline phase:
Local PGD
(2 spatial and 1
parametric
dimension)

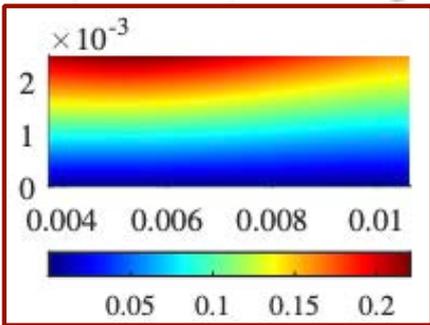
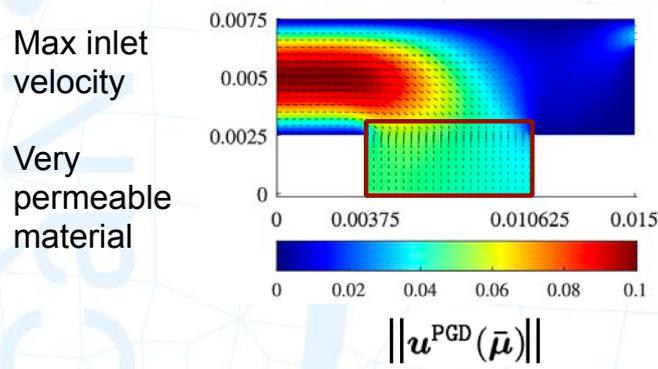
Stokes
176 modes
67 minutes



119 minutes

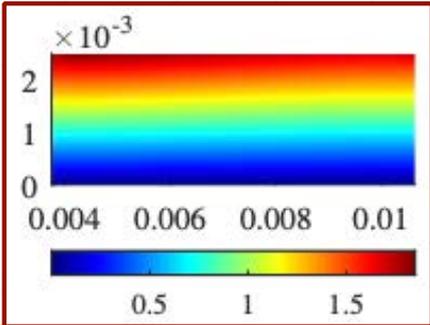
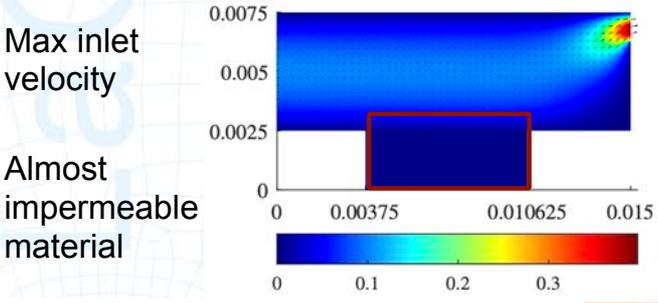
Darcy
178 modes
52 minutes

Parametric Stokes-Darcy cross-flow



Online phase:
DD-PGD
144 GMRES iter.
0.8 seconds

DD-FEM
78 GMRES iter.
24 minutes



5 DD-FEM instances are as expensive as the offline phase!

Concluding remarks

Real-time DD for parametric problems:

- **Traces of FEM functions** are used to **define parametric Dirichlet BC** in each subproblem (**no auxiliary basis functions**).
- **Physics accounted for** by the local **PGD** surrogate in each subdomain (also for **multiple physics**).
- **ePGD** provides a **non-intrusive** framework for **physics-based surrogate models**.
- **No need for Lagrange multipliers**, nor additional problems to be solved online **to glue the subdomains**.

Poisson & convection-diffusion - [Discacciati, Evans, Giacomini. CMAME, 2024]

Single VS. clustered nodes - [Discacciati, Evans, Giacomini. Finite Elem Anal Des, 2026]

Stokes & Stokes-Darcy - [Discacciati, Evans, Giacomini. arXiv:2507.06861]