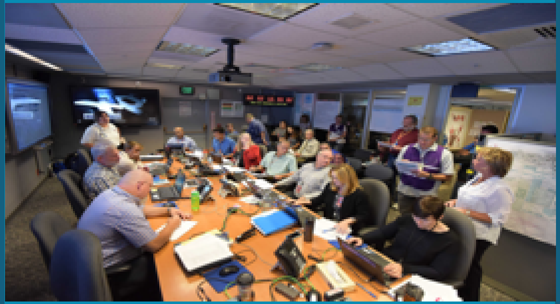
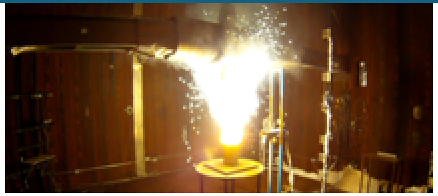
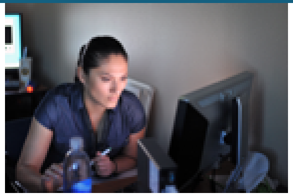
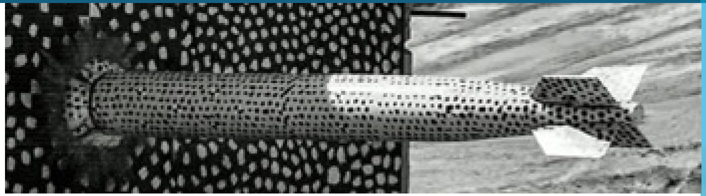
SAND2024-08595C

Explicit synchronous partitioned scheme for coupled reduced order models based on composite reduced bases









WCCM 2024 / PANACM 2024

Vancouver, British Columbia, July 21-26, 2024

Mini-symposium in memory of Prof. J. Tinsley Oden

PRESENTED BY

Pavel Bochev

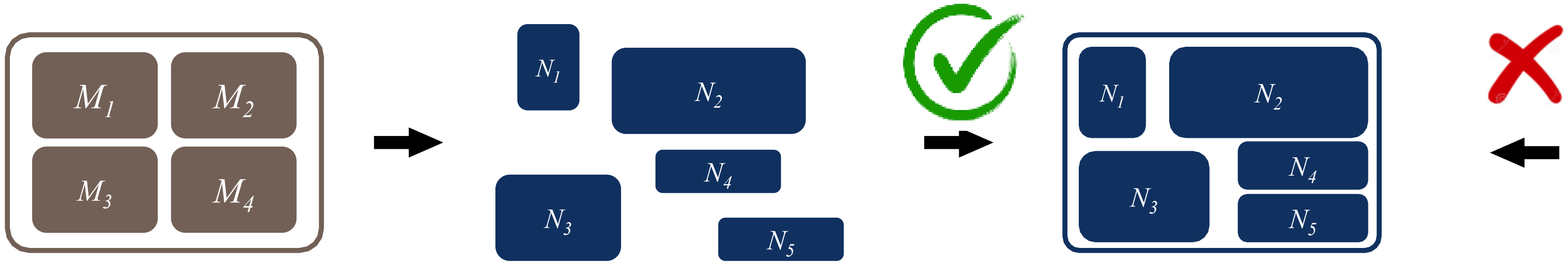
Amy De Castro, Paul Kuberry, Irina Tezaur

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

SAND2023-06581C

Why non-conventional computational methods?

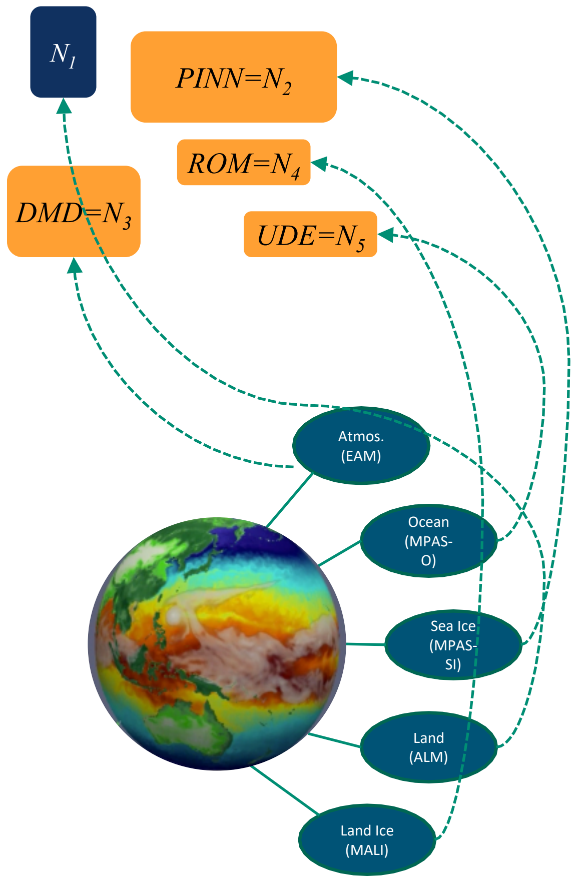
Current modeling and simulation workflows for coupled multiphysics problems are designed for traditional numerics



Complex System Model
- PDEs, ODEs
- Nonlocal, integral,…

Traditional Methods
- mesh-based (FE, FV, FD),
- meshless (SPH, MLS),…

Coupled Numerical Model
- Coupling based on rigorous mathematical theories



Interest in non-conventional data-driven models is increasing due to their valuable advantages:

- Improved computational efficiency via incorporation of cheap reduced order models (ROM)
- Reduced end-to-end simulation times by learning models directly from data
- Improved physical fidelity & predictiveness via data-driven discovery of hidden physics

However, plug-and-play integration of such models lacks the necessary theoretical and practical foundations

- In this talk we extend our Explicit Synchronous Partitioned Scheme (ESPS) for multi-material interface problems to the coupling of Reduced Order Models (ROM) with other ROMs and/or FEMs.

E3SM Energy Exascale Earth System Model

SAND2023-06581C

The Explicit Synchronous Partitioned Scheme (ESPS)

Model multi-material interface (transmission) problem

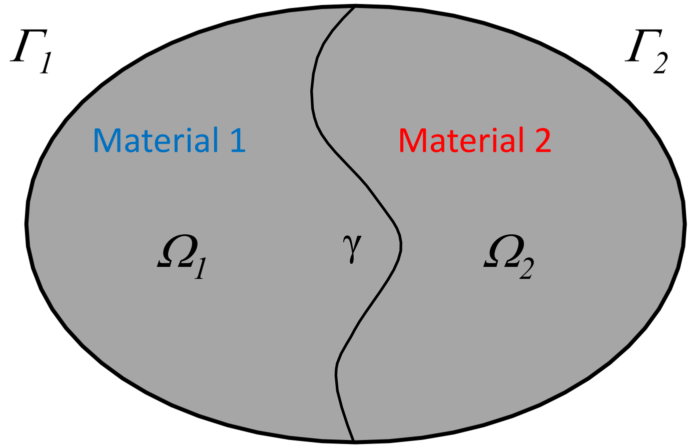
$$\begin{aligned} \dot{\varphi}_i - \nabla \cdot F_i(\varphi_i) &= f_i \quad \text{in} \quad \Omega_i \times [0,T] \\ \varphi_i &= g_i \quad \text{in} \quad \Gamma_i \times [0,T] \end{aligned} \qquad i = 1,2$$

$$F_i(\varphi_i) = \epsilon_i \nabla \varphi_i - \boldsymbol{u}\varphi_i$$

Subdomain equations

$$\begin{aligned} \varphi_1(\boldsymbol{x},t) - \varphi_2(\boldsymbol{x},t) &= 0 \\ F_1(\boldsymbol{x},t)\cdot \boldsymbol{n}_\gamma &= F_2(\boldsymbol{x},t)\cdot \boldsymbol{n}_\gamma \end{aligned} \quad \text{on} \quad \gamma \times [0,T].$$

Coupling conditions



Step 1: Define a monolithic, semi-discrete in time formulation using Lagrange multipliers

$$\begin{aligned} (\dot{\varphi}_1^h, \psi_1^h)_{0,\Omega_1} + (\lambda^h, \psi_1^h)_{0,\gamma} &= (f_1, \psi_1^h)_{0,\Omega_1} - (F_1(\varphi_1^h), \nabla\psi_1^h)_{0,\Omega_1} & \forall \psi_1^h \in S_{1,\Gamma}^h \\ (\dot{\varphi}_2^h, \psi_2^h)_{0,\Omega_2} - (\lambda^h, \psi_2^h)_{0,\gamma} &= (f_2, \psi_2^h)_{0,\Omega_2} - (F_2(\varphi_2^h), \nabla\psi_2^h)_{0,\Omega_2} & \forall \psi_2^h \in S_{2,\Gamma}^h \\ (\varphi_1^h - \varphi_2^h, \mu^h)_{0,\gamma} &= 0 & \forall \mu^h \in G_\gamma^h. \end{aligned}$$

$$\begin{aligned} M_1 \dot{\boldsymbol{\Phi}}_1 + G_1^T \boldsymbol{\lambda} &= \bar{\mathbf{f}}_1(\boldsymbol{\Phi}_1) \\ M_2 \dot{\boldsymbol{\Phi}}_2 - G_2^T \boldsymbol{\lambda} &= \bar{\mathbf{f}}_2(\boldsymbol{\Phi}_2) \\ G_1 \boldsymbol{\Phi}_1 - G_2 \boldsymbol{\Phi}_2 &= \mathbf{0}, \end{aligned}$$

$$\begin{aligned} \dot{y}_1 &= f_1(t,y,\lambda) \\ \dot{y}_2 &= f_2(t,y,\lambda) \\ 0 &= g(t,y) \end{aligned}$$

y - differential variable
λ - algebraic variable
g - algebraic constraint

Leads to a Hessenberg index-2 DAE

- Difficult to solve due to “hidden constraints
- Incompatible with explicit time integration: it “deletes” the constraint
- Resulting partitioned methods not truly explicit and resemble projection methods

The Explicit Synchronous Partitioned Scheme (ESPS)

Step 2: Reduce the DAE index

$$\begin{aligned} M_1\dot{\mathbf{\Phi}}_1 + G_1^T\boldsymbol{\lambda} &= \bar{\mathbf{f}}_1(\mathbf{\Phi}_1) \\ M_2\dot{\mathbf{\Phi}}_2 - G_2^T\boldsymbol{\lambda} &= \bar{\mathbf{f}}_2(\mathbf{\Phi}_2) \\ G_1\mathbf{\Phi}_1 - G_2\mathbf{\Phi}_2 &= \mathbf{0}, \end{aligned} \quad \rightarrow \quad \begin{aligned} M_1\dot{\mathbf{\Phi}}_1 + G_1^T\boldsymbol{\lambda} &= \bar{\mathbf{f}}_1(\mathbf{\Phi}_1) \\ M_2\dot{\mathbf{\Phi}}_2 - G_2^T\boldsymbol{\lambda} &= \bar{\mathbf{f}}_2(\mathbf{\Phi}_2) \\ G_1\dot{\mathbf{\Phi}}_1 - G_2\dot{\mathbf{\Phi}}_2 &= 0\ . \end{aligned}$$

Hessenberg index-2 | Hessenberg index-1

$$\begin{aligned} \dot{y}_1 &= f_1(t,y,\lambda) \\ \dot{y}_2 &= f_2(t,y,\lambda) \\ 0 &= g(t,y) \end{aligned} \quad \rightarrow \quad \begin{aligned} \dot{y}_1 &= f_1(t,y,\lambda) \\ \dot{y}_2 &= f_2(t,y,\lambda) \\ 0 &= g(t,y,\lambda) \end{aligned}$$

Step 3: Eliminate the algebraic variable

$$\begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix} \begin{bmatrix} \dot{\mathbf{\Phi}}_1 \\ \dot{\mathbf{\Phi}}_2 \end{bmatrix} = \begin{bmatrix} \bar{\mathbf{f}}_1(\mathbf{\Phi}_1) - G_1^T\boldsymbol{\lambda}(\mathbf{\Phi}_1,\mathbf{\Phi}_2) \\ \bar{\mathbf{f}}_2(\mathbf{\Phi}_2) + G_2^T\boldsymbol{\lambda}(\mathbf{\Phi}_1,\mathbf{\Phi}_2) \end{bmatrix} \quad \leftarrow$$

- Assume the Jacobian $\partial_\lambda g$ is non-singular. Then, $0 = g(t,y,\lambda)$ defines an implicit function $\lambda(t,y)$.

Step 4: Apply explicit time integration

$$y_1^{n+1} = f_1\big(t, y^n, \lambda(t^n, y^n)\big)$$

$$y_2^{n+1} = f_2\big(t, y^n, \lambda(t^n, y^n)\big)$$

- Subdomain equations can be solved independently!
- Explicit time integration effectively decouples the system
- Remains equivalent to the parent monolithic problem
- No splitting error! Similar ideas used in HATI schemes:

K. Peterson, P. Bochev, and P. Kuberry. Explicit synchronous partitioned algorithms for interface problems based on Lagrange multipliers. Computers & Mathematics with Applications, 78(2):459 – 482, 2019

A. Gravouil and A. Combescure. Multi-time-step explicit–implicit method for non-linear structural dynamics. International Journal for Numerical Methods in Engineering, 50(1):199–225, 2001.

SAND2023-06581C

ESPS analysis

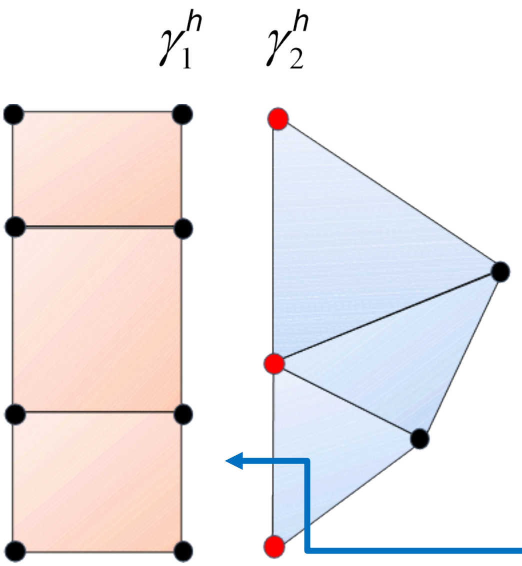
Lemma: Assume that the Lagrange multiplier space G_γ^h is such that there is an operator $Q : G_\gamma^h \mapsto S_{1,\Gamma}^h \times S_{2,\Gamma}^h$

$$\|s^h\|_{0,\gamma} \le C_1 \left(s^h, (Qs^h)_1 - (Qs^h)_2\right)_{0,\gamma} \quad \forall s^h \in G_\gamma^h, \text{ and } |||Q(s^h)||| \le C_2 h_\gamma^\alpha \|s\|_{0,\gamma}, \quad \alpha \ge 0$$

Then $b(\cdot,\cdot)$ satisfies the inf-sup condition, $G^T = (G_1^T, G_2^T)$ has full column rank, and the Schur complement $S = G_1 M_1^{-1} G_1^T + G_2 M_2^{-1} G_2^T$ is SPD.

A sufficient condition for the existence of the operator Q is the following Trace Compatibility Condition:

Every Lagrange multiplier is a trace of a finite element function from one of the two sides of the interface.

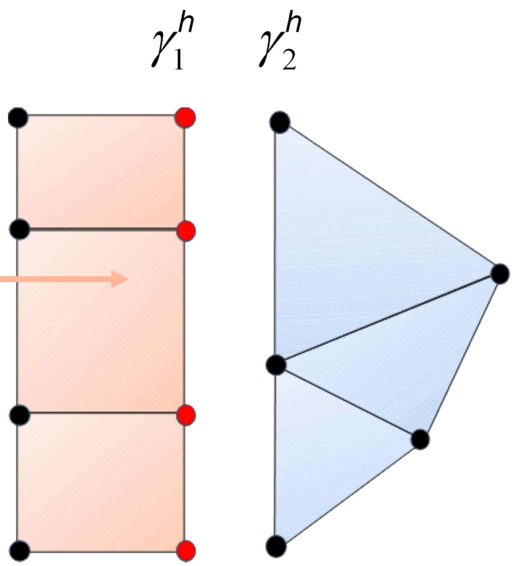


Lemma. Assume that $h_1 \le h_2$ and let $\rho = h_2/h_1 > 1.$

finer

1. If the Lagrange multiplier space $G_\gamma^h = G_1^h$ then $\kappa(S) \le C\rho^{d-1}$
2. If the Lagrange multiplier space $G_\gamma^h = G_2^h$ then $\kappa(S) \le C\rho^{d}$

coarser



SAND2023-06581C

How can non-conventional methods improve ESPS?

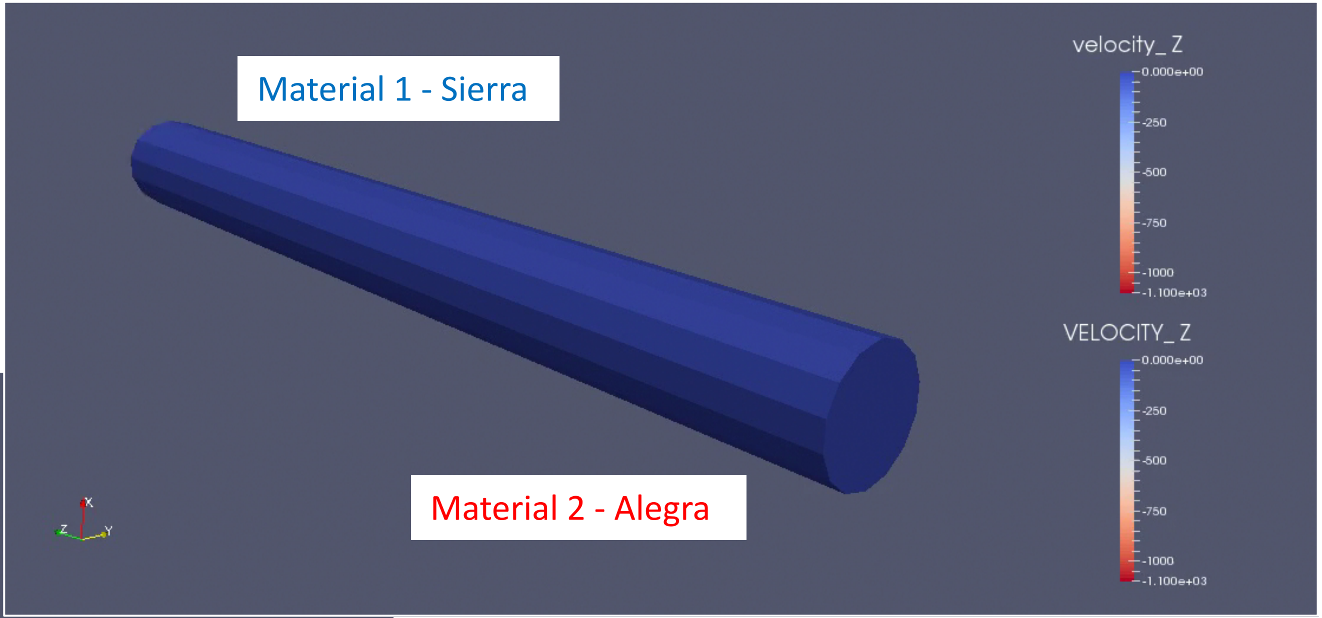
Production implementation of ESPS solves a coupled structure-structure interaction problem with two different materials modeled by Sierra SM and Alegra, resp.

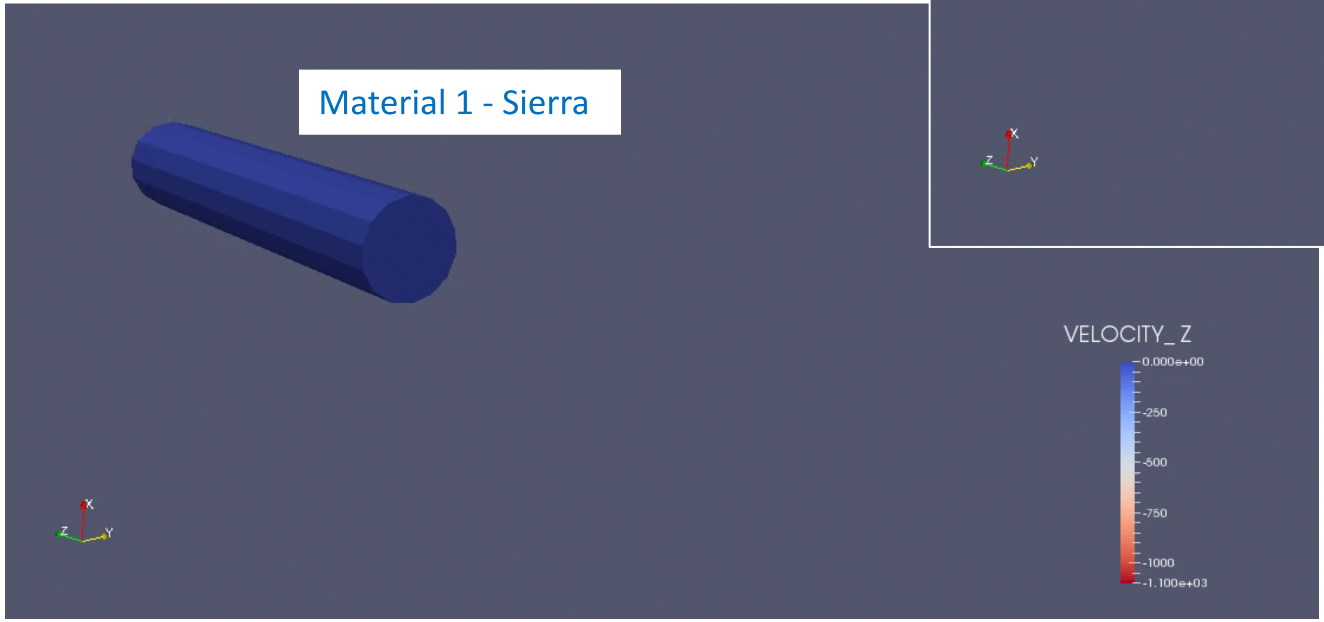
Axial pulse bar test

$$
\left.\begin{aligned}
\ddot{\boldsymbol{u}}_i - \nabla \cdot \sigma_i(\boldsymbol{u}_i) &= \boldsymbol{f}_i \quad \text{in } \Omega_i \times [0,T] \\
\boldsymbol{u}_i &= \boldsymbol{g}_i \quad \text{on } \Gamma_i \times [0,T]
\end{aligned}\right., \quad i = 1,2
$$

$$
\sigma_i(\boldsymbol{u}_i) = \lambda_i(\nabla \cdot \boldsymbol{u}_i)I + 2\mu_i\varepsilon(\boldsymbol{u}_i)
$$

$$
\left.\begin{aligned}
\boldsymbol{u}_1(\boldsymbol{x},t) &= \boldsymbol{u}_2(\boldsymbol{x},t) \\
\sigma_1(\boldsymbol{x},t)\cdot\boldsymbol{n}_\gamma &= \sigma_2(\boldsymbol{x},t)\cdot\boldsymbol{n}_\gamma
\end{aligned}\right. \quad \text{on} \quad \gamma \times [0,T].
$$





Material 2 requires a much finer mesh than Material 1. Replacing the FE code for Material 2 (and/or Material 1) by computationally efficient ROM can speed up the simulation.

SAND2023-06581C

Model Order Reduction (MOR) for Parametric PDEs (μPDEs)

Basic idea: the solution $u(\boldsymbol{\mu})$ of the μPDE: $\dot{u} + L(u, \boldsymbol{\mu}) = f;\ \ \boldsymbol{\mu} \in \boldsymbol{R}^p$ is often a "nice" function of $\boldsymbol{\mu}$.

- A good approximation for $u(\boldsymbol{\mu})$ can be computed from snapshots $u(\boldsymbol{\mu}_i)$ sampling the parameter space

A proper orthogonal decomposition (POD) Galerkin projection approach

Step 1: compute a reduced basis (RB)

- Collect n snapshots $\mathbf{u}_i$ (coefficients of $u(\boldsymbol{\mu}_i)$) and compute the SVD:
- Given tolerance $\delta > 0$ choose d such that $\dfrac{\sum_{j=1}^{d} \sigma_j^2}{\sum_{j=1}^{n} \sigma_j^2} \geqslant 1 - \delta$
- Define the RB as the d left singular vectors, i.e., the matrix $\widetilde{U}$

$$S = [\mathbf{u}_1, \cdots, \mathbf{u}_n] = U \Sigma V^T$$

$$S = [\overbrace{\widetilde{U}}^{d} \mid \widetilde{U}_{\mathrm{trun}}] \begin{bmatrix} \widetilde{\Sigma}^T & 0 \\ 0 & \widetilde{\Sigma}^T_{\mathrm{trun}} \end{bmatrix} \begin{bmatrix} \widetilde{V}^T \\ \widetilde{V}^T_{\mathrm{trun}} \end{bmatrix}$$

$$S \approx \tilde{S} = \widetilde{U} \widetilde{\Sigma} \widetilde{V}^T$$

Low-rank approximation of S

Step 2: Galerkin projection onto the reduced basis

$a(u, v) = f(v)$ for all $v \in V$ → $K\mathbf{u} = \mathbf{f}$ → $\mathbf{u} = \widetilde{U}\mathbf{a}$ → $\widetilde{U}^T K \widetilde{U} \mathbf{a} = \widetilde{U}^T \mathbf{f}$ $d \ll m$

Full Order Model (FOM): $m \times m$

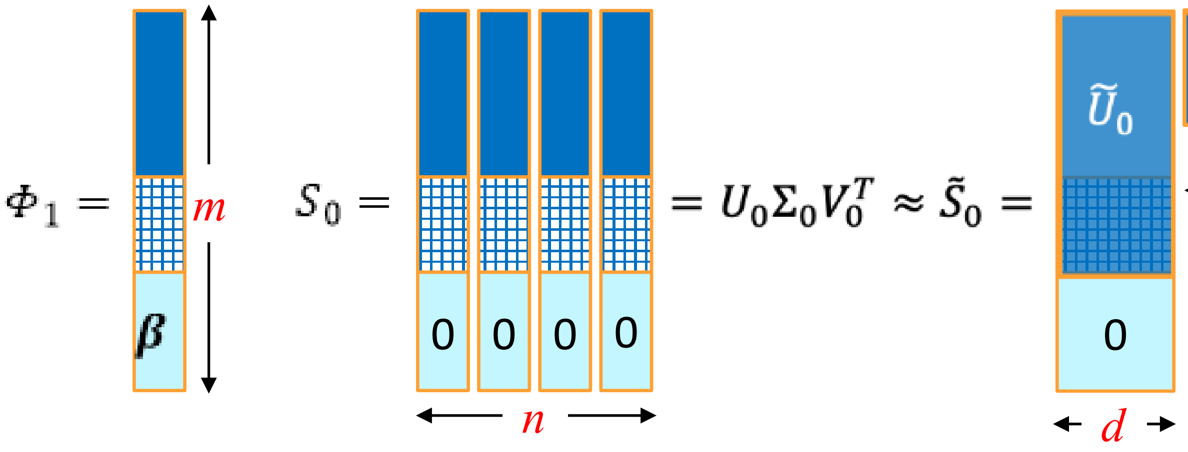
Reduced Order Model (ROM): $d \times d$

SAND2023-06581C

ESPS extension to ROM+ROM and ROM+FEM couplings

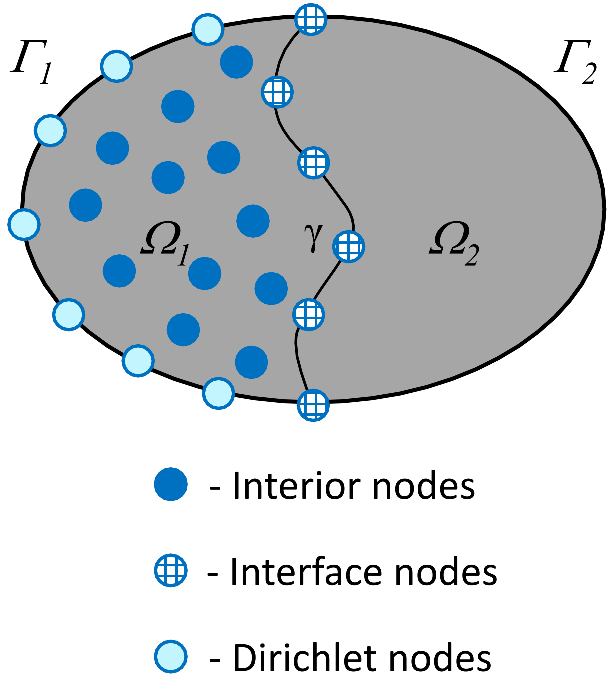
Full subdomain RB are commonly used in Domain Decomposition for ROM. Can they work for us?

A full subdomain RB formulation. Inhomogeneous Dirichlet conditions $\beta(x,t)$



RB = columns of $\tilde{U}_0$

Full subdomain: RB includes both interior and interface DoFs



ROM-FEM coupled problem. (ROM-ROM very similar)

RB projection:

$$\mathbf{\Phi}_1 = \widetilde{U}_0 \boldsymbol{\varphi}_R + \boldsymbol{\beta}$$

$$\begin{aligned}
\widetilde{M}_1 \dot{\boldsymbol{\varphi}}_R + \widetilde{G}_1^T \boldsymbol{\lambda} &= \widetilde{U}_0^T \overline{\mathbf{f}}_1(\widetilde{U}_0 \boldsymbol{\varphi}_R + \boldsymbol{\beta}) \\
M_2 \dot{\mathbf{\Phi}}_2 - G_2^T \boldsymbol{\lambda} &= \overline{\mathbf{f}}_2(\mathbf{\Phi}_2) \\
\widetilde{G}_1 \dot{\boldsymbol{\varphi}}_R - G_2 \dot{\mathbf{\Phi}}_2 &= 0,
\end{aligned}$$

$$\widetilde{M}_1 := \widetilde{U}_0^T M_1 \widetilde{U}_0$$
$$\widetilde{G}_1^T := \widetilde{U}_0^T G_1^T.$$

SAND2023-06581C

Full subdomain RB formulation: issues.

Key issue: the Schur complement is not provably non-singular!

- To understand the problem, consider the lumped mass matrix case and the ROM-ROM coupling

$$\left[\begin{array}{ccc|cc} M_{1,\gamma} & 0 & G_1^T & 0 & 0 \\ 0 & M_{2,\gamma} & -G_2^T & 0 & 0 \\ G_1 & -G_2 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & M_{1,0} & 0 \\ 0 & 0 & 0 & 0 & M_{2,0} \end{array}\right]$$

Interface blocks

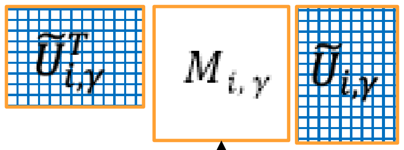
are separated from the

interior blocks

The ROM-ROM Schur complement uses only the interface mass matrices

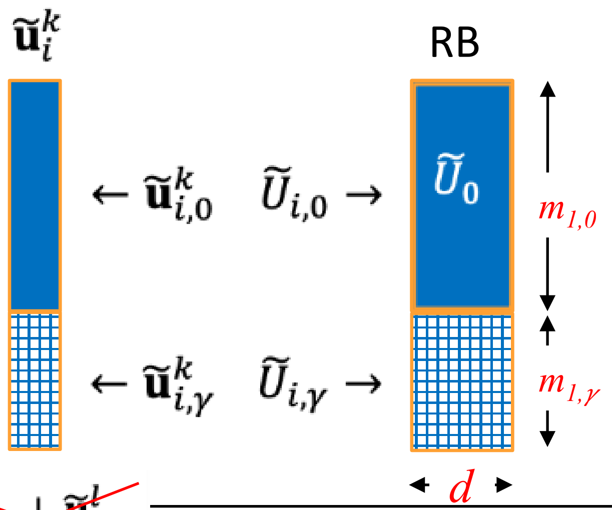
$$\tilde{S} = \tilde{G}_1 \tilde{M}_{1,\gamma}^{-1} \tilde{G}_1^T + \tilde{G}_2 \tilde{M}_{2,\gamma}^{-1} \tilde{G}_2^T$$

$$\tilde{M}_{i,\gamma} = \tilde{U}_{i,\gamma}^T M_{i,\gamma} \tilde{U}_{i,\gamma}$$



- Any two columns of the RB are orthonormal by construction: $\tilde{\mathbf{u}}_i^k \perp \tilde{\mathbf{u}}_i^l$

- However, their parts $\tilde{\mathbf{u}}_{i,\gamma}^k$ and $\tilde{\mathbf{u}}_{i,\gamma}^k$ corresponding to interface DoFs are not! They can be almost linearly dependent.



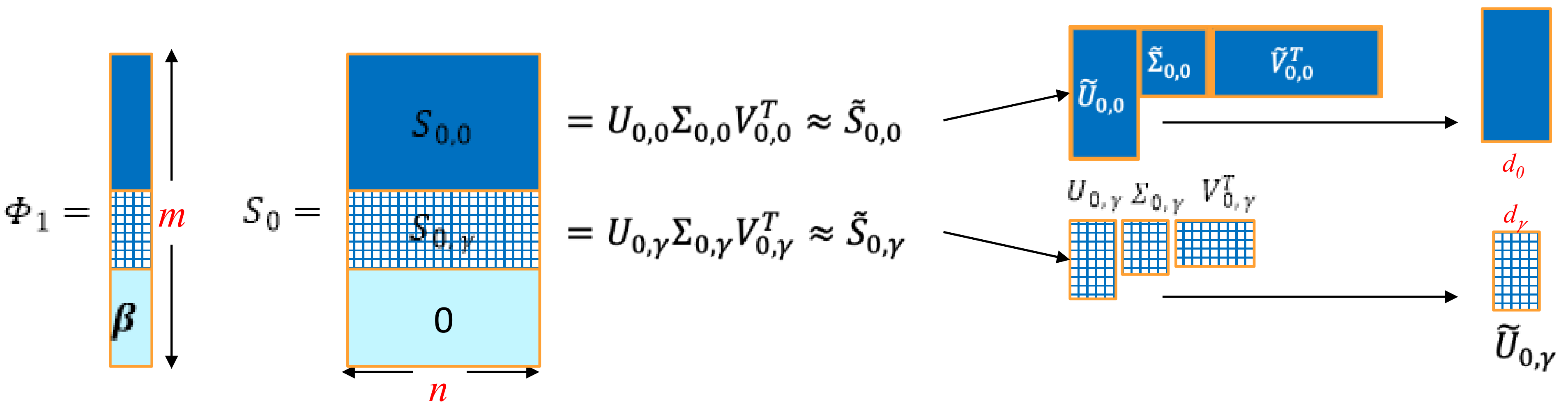
The projected mass matrix $\tilde{M}_{i,\gamma}$ is not guaranteed to be non-singular!

$\cancel{\tilde{\mathbf{u}}_{i,\gamma}^k \perp \tilde{\mathbf{u}}_{i,\gamma}^l}$

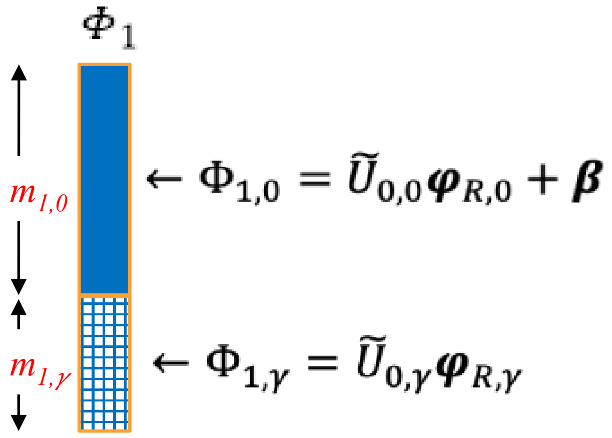
SAND2023-06581C

Solution: a Composite Reduced Basis Approach

Compute separate SVDs for the interior and the interface DoFs



ROM-FEM coupled problem defined by using separate projections for interior and interface DoFs



Projected mass matrix

$$\tilde{M}_{1,\gamma} = \tilde{U}_{1,\gamma}^T M_{1,\gamma} \tilde{U}_{1,\gamma}$$

Schur complement

$$\tilde{S} = \tilde{G}_1 \tilde{M}_{1,\gamma}^{-1} \tilde{G}_1^T + G_2 M_{2,\gamma}^{-1} G_2^T$$

orthonormal → Provably non-singular

Analysis

One can show that a version of the Trace Compatibility Condition (TCC) is sufficient for the existence of a nonsingular Schur complement for the coupled ROM+ROM and ROM+FOM formulations.

- ROM+ROM: Every RB Lagrange multiplier is a trace of a RB function from one of the two sides of the interface.
- ROM+FOM: Every Lagrange multiplier is either
  - a trace of a RB function from the ROM side of the interface, or
  - A trace of a FEM function from the FEM side of the interface

Test example: solid body rotation

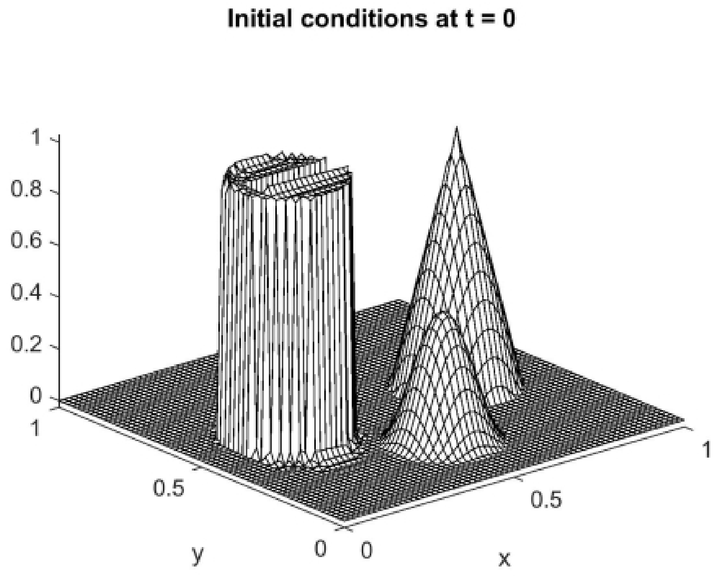
- **Advection: u** = ($0.5 - y, x - 0.5$)
- **Time scheme:** RK4

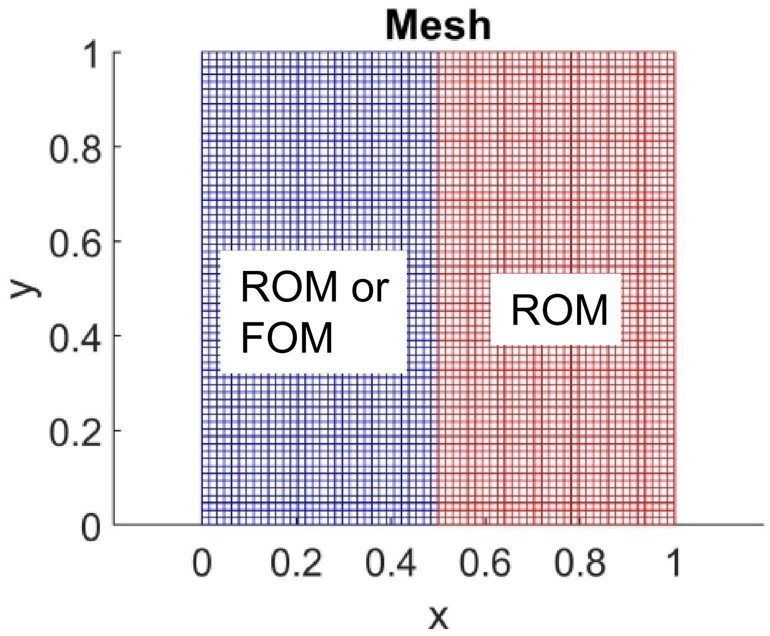
Simulation settings:

- $\varepsilon_1 = \varepsilon_2$: Single physics(DD)
- $\varepsilon_1 \neq \varepsilon_2$: Multi-physics

Snapshots:

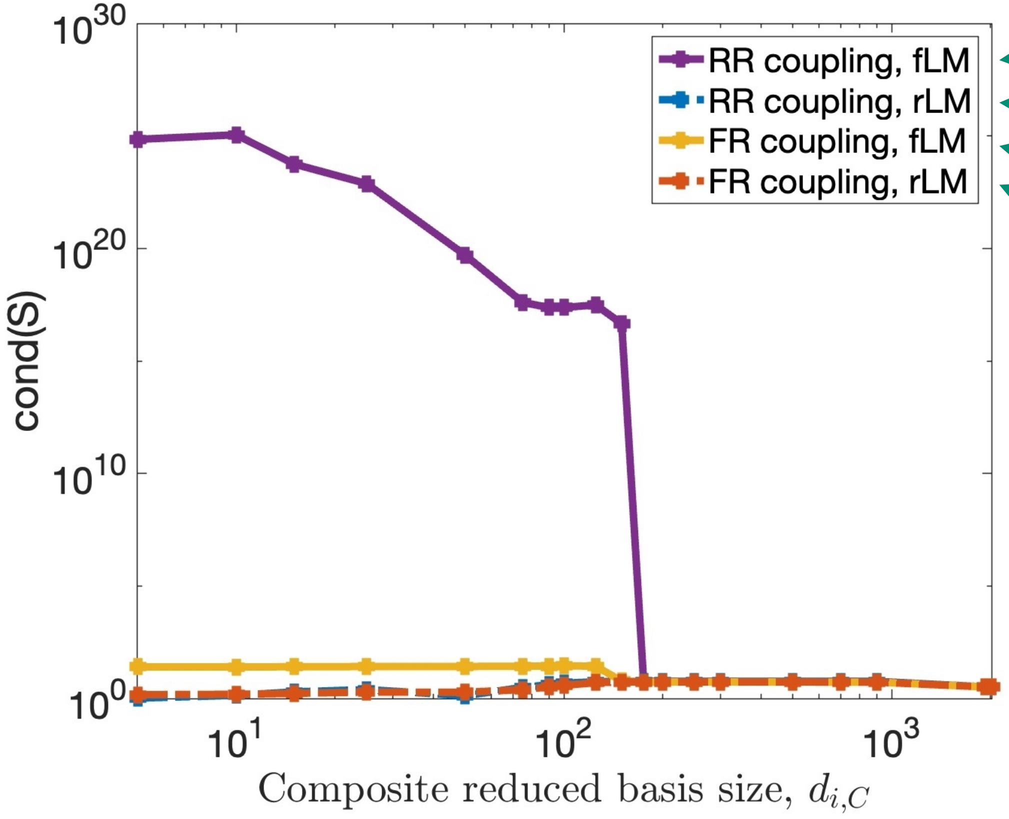
- monolithic FEM on Ω for $T_{final} = 2\pi$





Numerical examples: violation of the Trace Compatibility Condition

Condition number of the Schur complement as function of reduced basis size



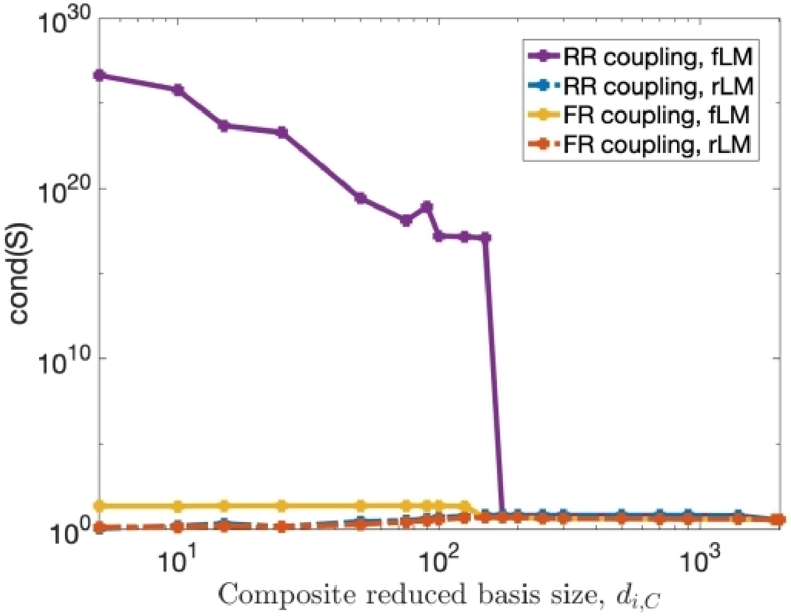
Single physics

ROM+ROM (RR): full subdomain basis violates TCC

ROM+ROM (RR): composite RB satisfies TCC

FOM+ROM (FR): interface FEM from the FEM side satisfies TCC

FOM+ROM (FR): interface RB from the ROM side satisfies TCC

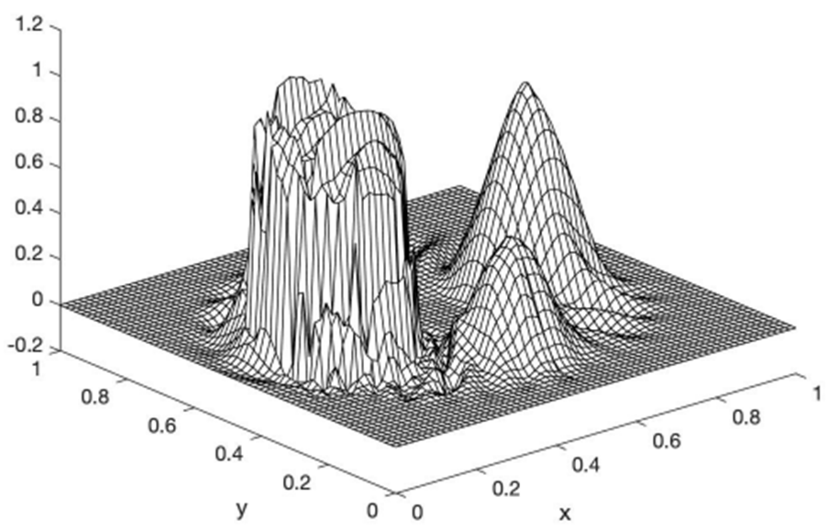


Multi-physics

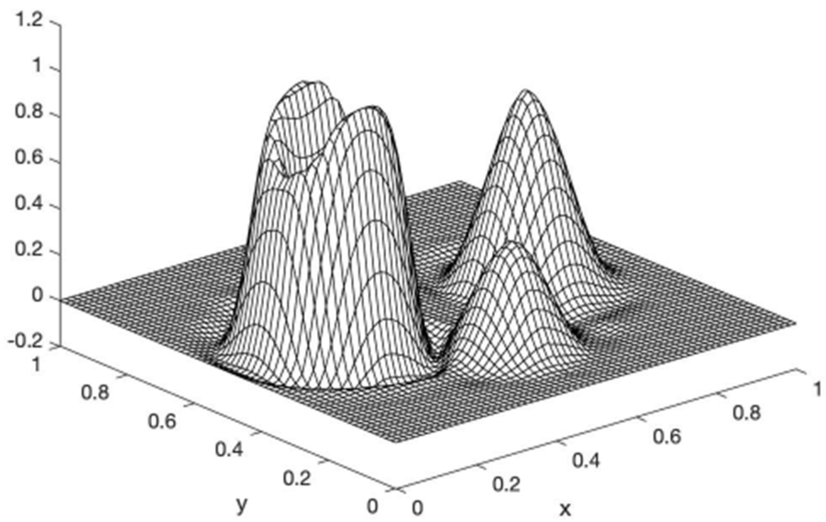
A. DeCastro, P. Bochev, P. Kuberry, and I. Tezaur. Explicit synchronous partitioned scheme for coupled reduced order models based on composite reduced bases. CMAME, 2023.

Numerical examples: violation of the Trace Compatibility Condition

Full subdomain RB ROM-ROM



Composite RB ROM-ROM



$d = 50$ modes in each subdomain

FOM: 4225 DOFs,
Subdomains: 2145 DOFs

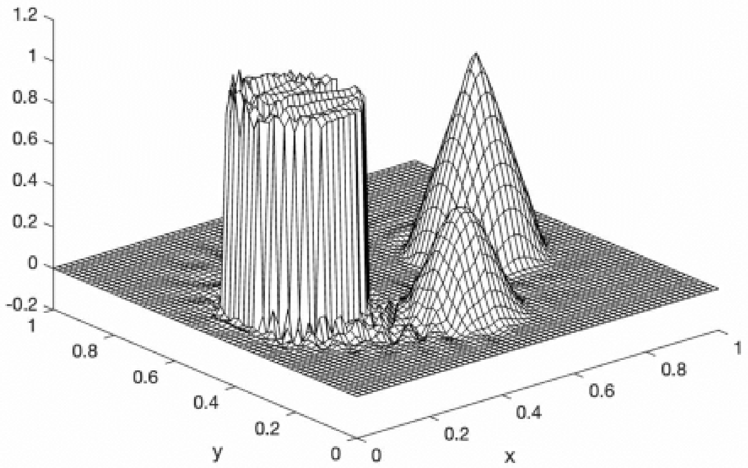
$d_{i,0} = 40$ interior modes
$d_{i,\gamma} = 10$ interface modes

In each subdomain

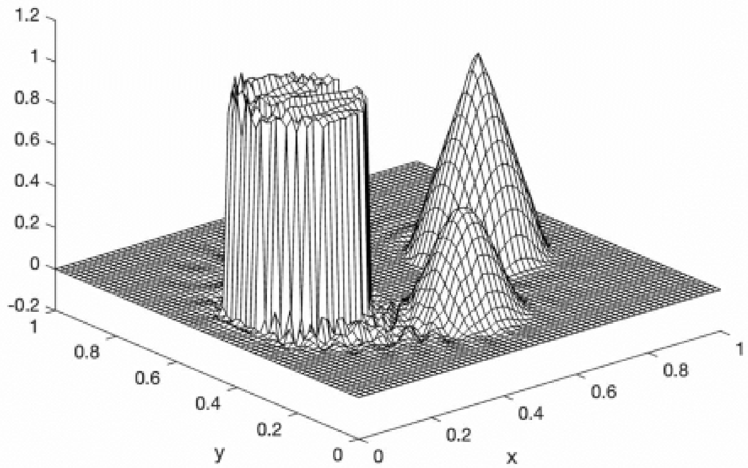
- Composite RB guarantees a non-singular Schur complement
- Allows accurate results with smaller total number of modes

Numerical examples: violation of the Trace Compatibility Condition

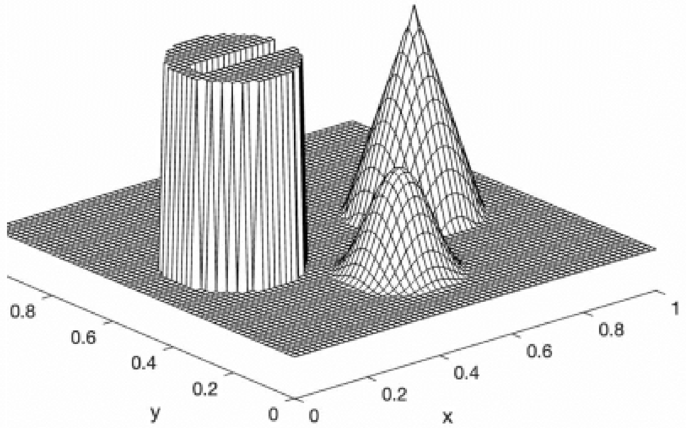
Full subdomain RB ROM-ROM



Composite RB ROM-ROM



FOM-FOM



Conclusions

We presented extension of the ESPS scheme to ROM-FEM and ROM-ROM coupling:

- Use of ROM on one or both subdomains reduces simulation time by over an order of magnitude
- Accuracy retained with a relatively small number of modes in the RB

Choice of RB basis is essential for a provably well-posed ROM-FEM and ROM-ROM couplings:

- **Full subdomain RB:**
  - Standard in many ROM+DD schemes but does not guarantee non-singular Schur complement
  - Size of the interface problem dependent on the size of the RB – governed by accuracy considerations including *all* DoFs
- **Split subdomain RB:**
  - Provably non-singular Schur complement
  - Requires two, but smaller size SVDs: cost comparable to the full subdomain case
  - Allows more flexibility by choosing RB for the interior and the interface independently

Ongoing work:

- Couplings involving equation-free, e.g., DMD sub-models
- Multi-rate & heterogeneous time integration schemes