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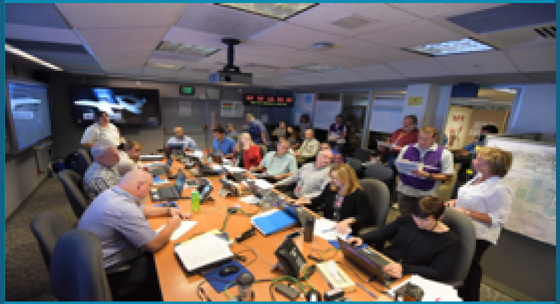
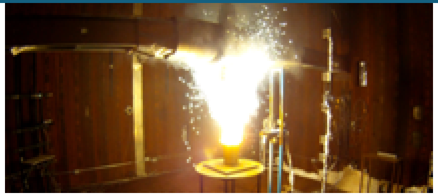
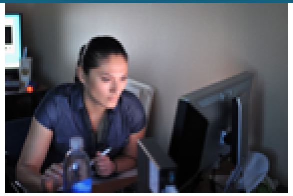
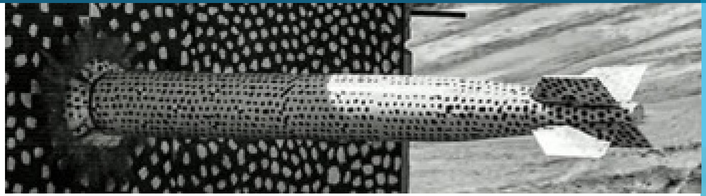
Variations on the theme of interfaces









17th U. S. National Congress on Computational Mechanics

Albuquerque, New Mexico, July 23-27, 2023

Minisymposium on Computational Interface and Contact Mechanics

In honor of our colleague and collaborator K. Chad Sockwell, who passed away unexpectedly in May of 2022

PRESENTED BY

Pavel Bochev

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Roadmap

- This talk will survey a body of work performed at Sandia over the past decade or so.
- The common theme for this work is ” interface problems”
- The variations are a result of discretizing the interface:
  - Discretized interfaces are spatially coincident (but can have non-matching grids)
    - Focus on partitioned schemes derived from monolithic formulations of the coupled problem
  - Discretized interface are spatially non-coincident
    - Focus on coupling algorithms that can handle gaps and overlaps between interfaces

Thanks to my collaborators

- J. Cheung — Millennium Space Systems, A Boeing Company,
- A. DeCastro — Clemson University/SNL
- M. Gunzburger — UT Austin
- P. Kuberry — SNL
- M. Perego — SNL
- K. Peterson — SNL
- C. Sockwell — SNL
- I. Tezaur — SNL

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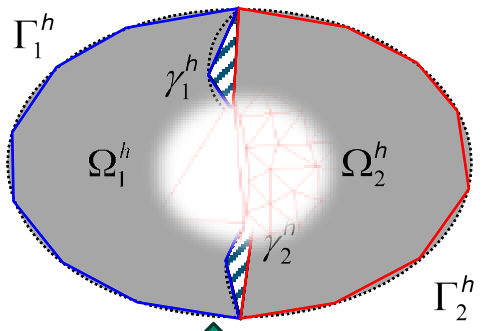
The theme and the variations

Problems with (physical or numerical) interfaces

$\dot{u}_1 + L_1 u_1 = f_1$ in Ω_1 $\dot{u}_2 + L_2 u_2 = f_2$ in Ω_2	Subdomain equations
$u_1 = u_2$ on γ	Continuity of states
$-F_1 = F_2$ on γ	Continuity of fluxes

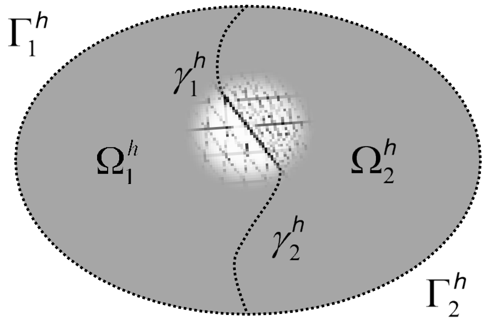
Spatially non-coincident interfaces

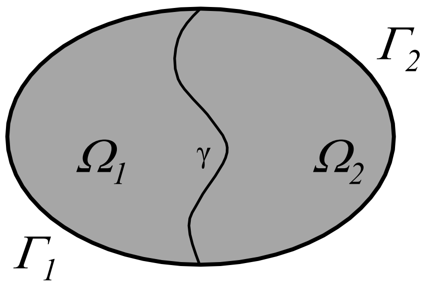
- Interface is physical or numerical, e.g., due to meshing
- **Separate meshing** creates 2 distinct, **non-coincident** versions of the same interface.
- Property-preserving data transfer between non-coincident interfaces remains a challenge.
- Existing approaches involve complex mesh manipulations.



Partitioned schemes based on monolithic formulations

- Interface is physical, e.g., material property.
- Mesh is **interface-fitted** but not necessarily matching.
- A partitioned scheme is developed from a well-posed monolithic formulation of the coupled problem
- Subdomain problems solved independently by different codes.





Basic types of partitioned methods (PM)

PM having an "iterative" basis

$$\dot{u}_1 + L_1 u_1 = f_1 \;\text{ in }\; \Omega_1$$

u_2 or F_2 $\qquad$ u_1 or F_1

$$\dot{u}_2 + L_2 u_2 = f_2 \;\text{ in }\; \Omega_2$$

- Mathematically equivalent to a single step of an iterative method, e.g., fixed point, non-overlapping Schwarz, etc.
- Small number of steps ⇒ stability & accuracy issues
- Common mitigation strategies: optimized, Robin-like transmission conditions (J. Banks), Anderson acceleration (R.Pawlowski, CASL)

A. de Boer, A. van Zuijlen, H. Bijl, Review of coupling methods for non-matching meshes, CMAME 196 (2007). *Domain Decomposition Methods: recent advances and new challenges in engineering*.

PM having a "monolithic" basis

$$\dot{u}_1 + L_1 u_1 = f_1 \;\text{ in }\; \Omega_1$$

$$\dot{u}_2 + L_2 u_2 = f_2 \;\text{ in }\; \Omega_2$$

$$\langle u_1 - u_2, \lambda \rangle_\gamma = 0 \;\text{ on }\; \gamma$$

- Use Lagrange multipliers to enforce continuity of states
- Lead to semi-discrete problems that are Hessenberg index-2 DAE

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

y - differential variable
z - algebraic variable
g - algebraic constraint

Note: g does not depend on z!

- Not "compatible" with explicit time integration: it "deletes" the constraint
- Resulting PM methods not truly explicit and resemble projection methods
- Have "hidden" constraints and are more difficult to solve

K. C. Park, C. A. Felippa, R. Ohayon, Partitioned formulation of internal fluid–structure interaction problems by localized Lagrange multipliers, CMAME 190 (2001).

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Explicit synchronous partitioned scheme (ESPS)

ESPS has a "monolithic" basis and comprises the following steps:

Step 1: reduce the DAE index of the monolithic problem

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

Hessenberg index-2

Hessenberg index-1

where the Jacobian $\partial_z g$ is non-singular

Step 2: eliminate the algebraic variable

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

$0 = g(t,y,z)$ defines an **implicit** function $z(t,y)$

Step 3: apply explicit time integration

$$\begin{aligned} y_1^{n+1} &= f_1\big(t, y^n, z(t^n, y^n)\big) \\ y_2^{n+1} &= f_2\big(t, y^n, z(t^n, y^n)\big) \end{aligned}$$

- Subdomain equations can be solved independently!
- Explicit time integration effectively decouples the system
- Remains equivalent to the parent monolithic problem
- No splitting error!

- 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.

Model Solid-Solid Interaction and Transmission Problems

SSI **TP**

Subdomain equations

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

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

Initial conditions

$$\begin{aligned} \boldsymbol{u}_i(0,\boldsymbol{x}) &= \boldsymbol{u}_0(\boldsymbol{x})\big|_{\Omega_i} \quad \text{in } \Omega_i \\ \dot{\boldsymbol{u}}_i(0,\boldsymbol{x}) &= \dot{\boldsymbol{u}}_0(\boldsymbol{x})\big|_{\Omega_i} \quad \text{in } \Omega_i \end{aligned} \quad i=1,2;$$

$$\varphi_i(\boldsymbol{x},0) = \varphi_{i,0}(\boldsymbol{x}) \quad \text{in} \quad \Omega_i \quad i=1,2;$$

Coupling conditions

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

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

Monolithic problem (weak form)

$$\textit{seek } \{\boldsymbol{u}_1,\boldsymbol{u}_2,\boldsymbol{t}\} \in \mathbf{H}^1_\Gamma(\Omega_1)\times\mathbf{H}^1_\Gamma(\Omega_2)\times\mathbf{H}^{-1/2}(\gamma) \textit{ such that}$$

$$\begin{aligned} (\ddot{\boldsymbol{u}}_1,\boldsymbol{v}_1)_{0,\Omega_1} + \langle\boldsymbol{t},\boldsymbol{v}_1\rangle_\gamma &= (\boldsymbol{f}_1,\boldsymbol{v}_1)_{0,\Omega_1} - (\sigma_1(\boldsymbol{u}_1),\varepsilon(\boldsymbol{v}_1))_{0,\Omega_1} && \forall\boldsymbol{v}_1\in\mathbf{H}^1_\Gamma(\Omega_1) \\ (\ddot{\boldsymbol{u}}_2,\boldsymbol{v}_2)_{0,\Omega_2} - \langle\boldsymbol{t},\boldsymbol{v}_2\rangle_\gamma &= (\boldsymbol{f}_2,\boldsymbol{v}_2)_{0,\Omega_2} - (\sigma_2(\boldsymbol{u}_2),\varepsilon(\boldsymbol{v}_2))_{0,\Omega_2} && \forall\boldsymbol{v}_2\in\mathbf{H}^1_\Gamma(\Omega_2) \\ \langle\boldsymbol{u}_1-\boldsymbol{u}_2,\boldsymbol{s}\rangle_\gamma &= 0 && \forall\boldsymbol{s}\in\mathbf{H}^{-1/2}(\gamma) \end{aligned}$$

$$\textit{seek } \{\varphi_1,\varphi_2,\lambda\} \in H^1_\Gamma(\Omega_1)\times H^1_\Gamma(\Omega_2)\times H^{-1/2}(\gamma) \textit{ such that}$$

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

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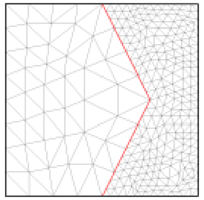
ESPS for the Solid-Solid Interaction Problem

Step 1. Spatial discretization: *seek* $\{\boldsymbol{u}_1^h, \boldsymbol{u}_2^h, \boldsymbol{t}^h\} \in S_{1,\Gamma}^h \times S_{2,\Gamma}^h \times G_\gamma^h$ *such that*

$$\begin{aligned}
(\ddot{\boldsymbol{u}}_1^h, \boldsymbol{v}_1^h)_{0,\Omega_1} + (\boldsymbol{t}^h, \boldsymbol{v}_1^h)_{0,\gamma} &= (\boldsymbol{f}_1, \boldsymbol{v}_1^h)_{0,\Omega_1} - (\sigma_1(\boldsymbol{u}_1^h), \varepsilon(\boldsymbol{v}_1^h))_{0,\Omega_1} && \forall \boldsymbol{v}_1^h \in S_{1,\Gamma}^h \\
(\ddot{\boldsymbol{u}}_2^h, \boldsymbol{v}_2^h)_{0,\Omega_2} - (\boldsymbol{t}^h, \boldsymbol{v}_2^h)_{0,\gamma} &= (\boldsymbol{f}_2, \boldsymbol{v}_2^h)_{0,\Omega_2} - (\sigma_2(\boldsymbol{u}_2^h), \varepsilon(\boldsymbol{v}_2^h))_{0,\Omega_2} && \forall \boldsymbol{v}_2^h \in S_{2,\Gamma}^h \\
(\boldsymbol{u}_1^h - \boldsymbol{u}_2^h, \boldsymbol{s}^h)_{0,\gamma} &= 0 && \forall \boldsymbol{s}^h \in G_\gamma^h
\end{aligned}$$

$$\begin{aligned}
M_1\ddot{\mathbf{u}}_1 + G_1^T\mathbf{t} &= \mathrm{f}_1(\mathbf{u}_1) \\
M_2\ddot{\mathbf{u}}_2 - G_2^T\mathbf{t} &= \mathrm{f}_2(\mathbf{u}_2) \\
G_1\mathbf{u}_1 - G_2\mathbf{u}_2 &= 0
\end{aligned}$$



We assume spatially coincident interfaces (no gaps or overlaps) but allow non-matching grids.

Step 2. Index reduction: Assume $\boldsymbol{u}_0(\boldsymbol{x}^-) = \boldsymbol{u}_0(\boldsymbol{x}^+)$ and $\dot{\boldsymbol{u}}_0(\boldsymbol{x}^-) = \dot{\boldsymbol{u}}_0(\boldsymbol{x}^+)$ on $\boldsymbol{\gamma}$.

$$u_1(\boldsymbol{x},t) = u_2(\boldsymbol{x},t) \longrightarrow \ddot{u}_1(\boldsymbol{x},t) = \ddot{u}_2(\boldsymbol{x},t)$$

$$\begin{aligned}
M_1\ddot{\mathbf{u}}_1 + G_1^T\mathbf{t} &= \mathrm{f}_1(\mathbf{u}_1) \\
M_2\ddot{\mathbf{u}}_2 - G_2^T\mathbf{t} &= \mathrm{f}_2(\mathbf{u}_2) \\
G_1\ddot{\mathbf{u}}_1 - G_2\ddot{\mathbf{u}}_2 &= 0
\end{aligned}$$

It is easy to check that this problem has the Hessenberg Index-1 structure: set

$$\begin{cases} y = (u_1, u_2); \\ z = \mathbf{t}, \end{cases} \quad \text{and} \quad \begin{cases} f(t,y,z) = \begin{pmatrix} M_1^{-1}\left(\mathbf{f}_1(\mathbf{u}_1) - G_1^T\mathbf{t}\right) \\ M_2^{-1}\left(\mathbf{f}_2(\mathbf{u}_2) + G_2^T\mathbf{t}\right) \end{pmatrix} \\ g(t,y,z) = S\mathbf{t} - G_1M_1^{-1}\mathbf{f}_1(\mathbf{u}_1) + G_2M_2^{-1}\mathbf{f}_2(\mathbf{u}_2) \\ S = G_1M_1^{-1}G_1^T + G_2M_2^{-1}G_2^T \end{cases}$$

$$\begin{aligned}
\ddot{y} &= f(t,y,z) \\
0 &= g(t,y,z)
\end{aligned}$$

ESPS for the Solid-Solid Interaction Problem

Step 3. Reduction of the DAE to the underlying ODE: lumped mass matrix case

Monolithic problem assumes a form where

$$\left[\begin{array}{ccc:cc} M_{1,\gamma} & 0 & G_1^T & 0 & 0 \\ 0 & M_{2,\gamma} & -G_2^T & 0 & 0 \\ G_1 & -G_2 & 0 & 0 & 0 \\ \hdashline 0 & 0 & 0 & M_{1,0} & 0 \\ 0 & 0 & 0 & 0 & M_{2,0} \end{array}\right] \left[\begin{array}{c} \ddot{\mathbf{u}}_{1,\gamma} \\ \ddot{\mathbf{u}}_{2,\gamma} \\ \mathbf{t} \\ \hdashline \ddot{\mathbf{u}}_{1,0} \\ \ddot{\mathbf{u}}_{2,0} \end{array}\right] = \left[\begin{array}{c} \mathbf{f}_{1,\gamma}(\mathbf{u}_1) \\ \mathbf{f}_{2,\gamma}(\mathbf{u}_2) \\ 0 \\ \hdashline \mathbf{f}_{1,0}(\mathbf{u}_1) \\ \mathbf{f}_{2,0}(\mathbf{u}_2) \end{array}\right]$$

Interface blocks

are **completely separated** from the

interior blocks

Form the Schur complement of the upper left 2x2 block in the decoupled interface system

$$\left[\begin{array}{cc:c} M_{1,\gamma} & 0 & G_1^T \\ 0 & M_{2,\gamma} & -G_2^T \\ \hdashline G_1 & -G_2 & 0 \end{array}\right] \left[\begin{array}{c} \ddot{\mathbf{u}}_{1,\gamma} \\ \ddot{\mathbf{u}}_{2,\gamma} \\ \hdashline \mathbf{t} \end{array}\right] = \left[\begin{array}{c} \mathbf{f}_{1,\gamma}(\mathbf{u}_1) \\ \mathbf{f}_{2,\gamma}(\mathbf{u}_2) \\ \hdashline \mathbf{0} \end{array}\right]$$

Note: solvability of the Schur complement requires G_1 *and* G_2 to have full column ranks

and solve the resulting equation for the interface force:

$$\left(G_1 M_{1,\gamma}^{-1} G_1^T + G_2 M_{2,\gamma}^{-1} G_2^T\right) \mathbf{t} = \left(G_1 M_{1,\gamma}^{-1} \mathbf{f}_{1,\gamma}(\mathbf{u}_1) - G_2 M_{2,\gamma}^{-1} \mathbf{f}_{2,\gamma}(\mathbf{u}_2)\right)$$

ESPS for the Solid-Solid Interaction Problem

Step 3. Reduction of the DAE to the underlying ODE: consistent mass matrix case

Monolithic problem assumes a form where

$$\left[\begin{array}{ccc:cc} M_{1,\gamma} & 0 & G_1^T & M_{1,\gamma 0} & 0 \\ 0 & M_{2,\gamma} & -G_2^T & 0 & M_{2,\gamma 0} \\ G_1 & -G_2 & 0 & 0 & 0 \\ \hdashline M_{1,0\gamma} & 0 & 0 & M_{1,0} & 0 \\ 0 & M_{2,0\gamma} & 0 & 0 & M_{2,0} \end{array}\right] \left[\begin{array}{c} \ddot{\mathbf{u}}_{1,\gamma} \\ \ddot{\mathbf{u}}_{2,\gamma} \\ \mathbf{t} \\ \hdashline \ddot{\mathbf{u}}_{1,0} \\ \ddot{\mathbf{u}}_{2,0} \end{array}\right] = \left[\begin{array}{c} \mathbf{f}_{1,\gamma}(\mathbf{u}_1) \\ \mathbf{f}_{2,\gamma}(\mathbf{u}_2) \\ 0 \\ \hdashline \mathbf{f}_{1,0}(\mathbf{u}_1) \\ \mathbf{f}_{2,0}(\mathbf{u}_2) \end{array}\right]$$

Interface blocks

are **not separated** from the

interior blocks

Step 3a. "Static condensation" of the interior variables

$$\left[\begin{array}{cc:c} A_1 & 0 & G_1^T \\ 0 & A_2 & -G_2^T \\ \hdashline G_1 & -G_2 & 0 \end{array}\right] \left[\begin{array}{c} \ddot{\mathbf{u}}_{1,\gamma} \\ \ddot{\mathbf{u}}_{2,\gamma} \\ \hdashline \mathbf{t} \end{array}\right] = \left[\begin{array}{c} \widetilde{\mathbf{f}}_{1,\gamma}(\mathbf{u}_1) \\ \widetilde{\mathbf{f}}_{2,\gamma}(\mathbf{u}_2) \\ \hdashline 0 \end{array}\right]$$

Step 3b. Form Schur complement and solve for **t**

$$\left(G_1 A_{1,\gamma}^{-1} G_1^T + G_2 A_{2,\gamma}^{-1}\right) \mathbf{t} = \left(G_1 A_{1,\gamma}^{-1} \widehat{\mathbf{f}}_{1,\gamma}(\mathbf{u}_1) - G_1 A_{2,\gamma}^{-1} \widehat{\mathbf{f}}_{2,\gamma}(\mathbf{u}_2)\right)$$

Modified mass and force terms

$$A_i = M_{i,\gamma} - M_{i,\gamma 0} M_{i,0}^{-1} M_{i,0\gamma} \qquad \widehat{\mathbf{f}}_{i,\gamma}(\boldsymbol{\varphi}_i) = \mathbf{f}_{i,\gamma}(\boldsymbol{\varphi}_i) - M_{i,\gamma 0} M_{i,0}^{-1} \mathbf{f}_{i,0}(\boldsymbol{\varphi}_i)$$

ESPS for the Solid-Solid Interaction Problem

Step 4. Explicit time discretization of the underlying ODE: $\ddot{D}^{n+1}(\mathbf{u}_i) \approx \ddot{\mathbf{u}}(t^{n+1})$

We obtain two independent sets of fully discrete equations on each subdomain:

$$\begin{bmatrix} M_{i,\gamma} & 0 \\ 0 & M_{i,0} \end{bmatrix} \begin{bmatrix} \ddot{D}^{n+1}\mathbf{u}_{i,\gamma} \\ \ddot{D}^{n+1}\mathbf{u}_{i,0} \end{bmatrix} = \begin{bmatrix} \mathbf{f}^n_{i,\gamma} + (-1)^i G_i^T \mathbf{t}^n \\ \mathbf{f}_{i,0} \end{bmatrix}$$

Lumped mass matrix case

$$\begin{bmatrix} M_{i,\gamma} & M_{i,\gamma 0} \\ M_{i,0\gamma} & M_{i,0} \end{bmatrix} \begin{bmatrix} \ddot{D}^{n+1}\mathbf{u}_{i,\gamma} \\ \ddot{D}^{n+1}\mathbf{u}_{i,0} \end{bmatrix} = \begin{bmatrix} \mathbf{f}^n_{i,\gamma} + (-1)^i G_i^T \mathbf{t}^n \\ \mathbf{f}^n_{i,0} \end{bmatrix}$$

Consistent mass matrix case

- Time discretization **both discretizes** the system in time and **decouples** the subdomain equations
- As long as time step is within the stability region of the time integrator, the partitioned scheme is stable
- Not subject to splitting errors characteristic of iterative partitioned methods
- The **only error** incurred is the **time discretization** error

Here we use the second central difference $\ddot{D}^{n+1}(\mathbf{u}_i) = (\mathbf{u}_i^{n+1} - 2\mathbf{u}_i^n + \mathbf{u}_i^{n-1})/\Delta t^2$

ESPS analysis

Hessenberg Index-1 DAE requires a non-singular Jacobian $\partial_z g$. For ESPS we have that

$$g(t,y,z) = S\mathbf{t} - G_1 M_1^{-1}\mathbf{f}_1(\mathbf{u}_1) + G_2 M_2^{-1}\mathbf{f}_2(\mathbf{u}_2)$$

$$\Longrightarrow \quad \partial_z g = S \quad \text{where} \quad S = G_1 M_1^{-1} G_1^T + G_2 M_2^{-1} G_2^T$$

$\Longrightarrow$

well-posedness of ESPS requires a non-singular Schur complement S.

Variational approach: the matrices in S are generated by two bilinear forms forming a "mixed problem"

$$a(\boldsymbol{u}_1^h, \boldsymbol{u}_2^h; \boldsymbol{v}_1^h, \boldsymbol{v}_2^h) = (\boldsymbol{u}_1^h, \boldsymbol{v}_1^h)_{0,\Omega_1} + (\boldsymbol{u}_2^h, \boldsymbol{v}_2^h)_{0,\Omega_2} \quad \text{and} \quad b(\boldsymbol{v}_1^h, \boldsymbol{v}_2^h; \boldsymbol{t}^h) = (\boldsymbol{v}_1^h - \boldsymbol{v}_2^h, \boldsymbol{t}^h)_{0,\gamma}$$

$\Longrightarrow$ To show that the Schur complement S is non-singular we use Brezzi's saddle-point theory:

1. $a(\cdot,\cdot)$ is coercive on $Z = \{(\boldsymbol{v}_1, \boldsymbol{v}_2) | b(\boldsymbol{v}_1, \boldsymbol{v}_2; \mathbf{t}) = 0 \; \forall \mathbf{t}\}$.

Trivially satisfied because

$$a(\boldsymbol{v}_1^h, \boldsymbol{v}_2^h; \boldsymbol{v}_1^h, \boldsymbol{v}_2^h) = \|\boldsymbol{v}_1^h\|_{0,\Omega_1}^2 + \|\boldsymbol{v}_2^h\|_{0,\Omega_2}^2 = |||\boldsymbol{v}_1^h; \boldsymbol{v}_2^h|||^2$$

is a norm on $S_{1,\Gamma}^h \times S_{2,\Gamma}^h$

2. $b(\cdot,\cdot)$ satisfies the inf-sup condition

$$\sup_{\{\boldsymbol{v}_1^h; \boldsymbol{v}_2^h\} \in X \times X} \frac{b(\boldsymbol{v}_1^h, \boldsymbol{v}_2^h; \boldsymbol{s}^h)}{|||\boldsymbol{v}_1^h; \boldsymbol{v}_2^h|||} \geq \beta \|\boldsymbol{s}^h\|_Y$$

ESPS analysis

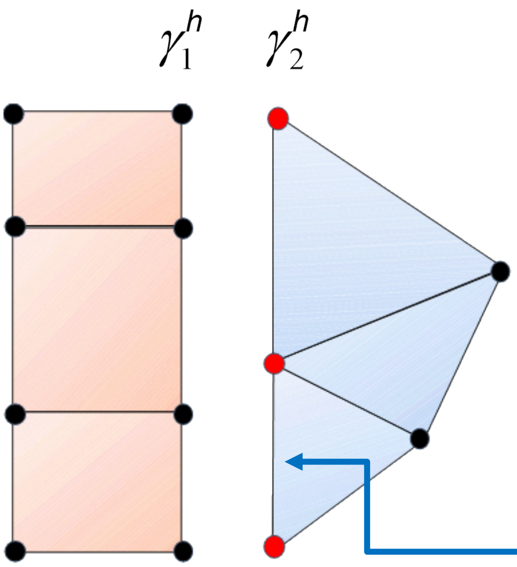
Lemma: Assume that the Lagrange multiplier space G^h_γ is such that there is an operator $Q : G^h_\gamma \mapsto S^h_{1,\Gamma} \times S^h_{2,\Gamma}$

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

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.

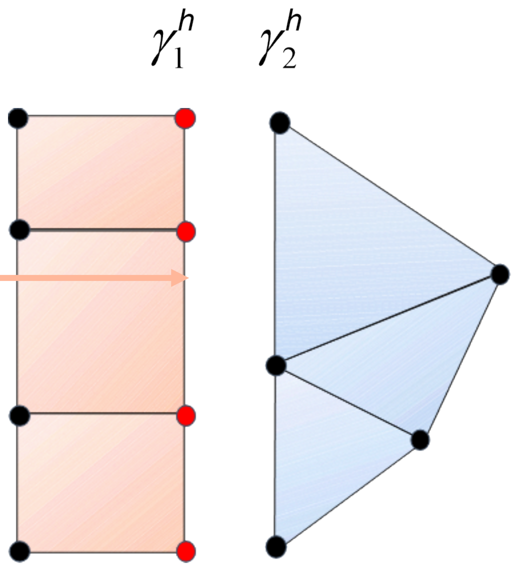
A **sufficient condition** for the existence of the operator Q is the following **Trace Compatibility Condition**:

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



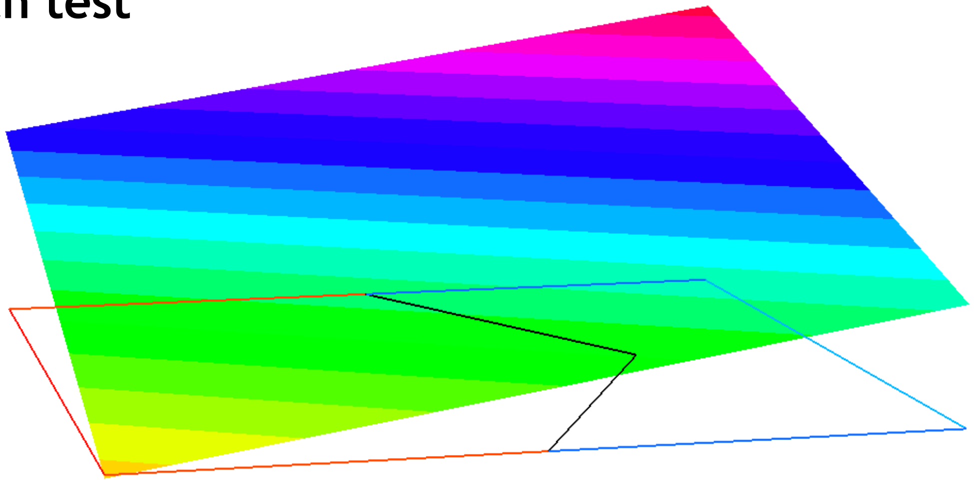
Lemma. Assume that $h_1 \le h_2$ and let $\rho = h_2/h_1 > 1$.

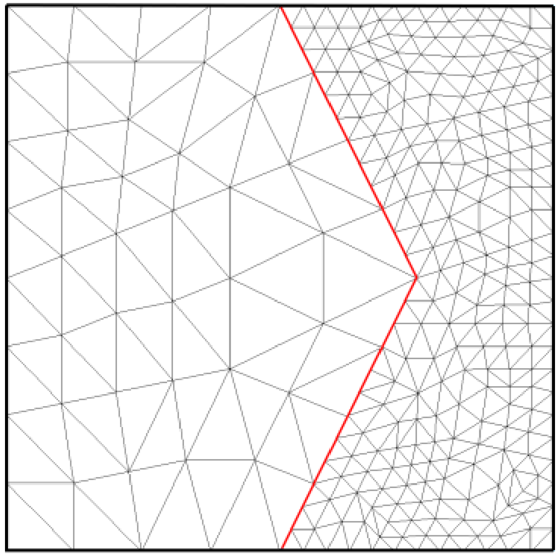
1. If the Lagrange multiplier space $G^h_\gamma = G^h_1$ then $\kappa(S) \le C\rho^{d-1}$
2. If the Lagrange multiplier space $G^h_\gamma = G^h_2$ then $\kappa(S) \le C\rho^{d}$



Numerical examples: Solid-Solid Interaction (SSI)

Patch test





Linear Elasticity

$$\ddot{\boldsymbol{u}}_i - \nabla \cdot \boldsymbol{\sigma}_i(\boldsymbol{u}_i) = \boldsymbol{f}_i$$

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

$$\lambda_i = 400 \quad \text{and} \quad \mu_i = 400$$

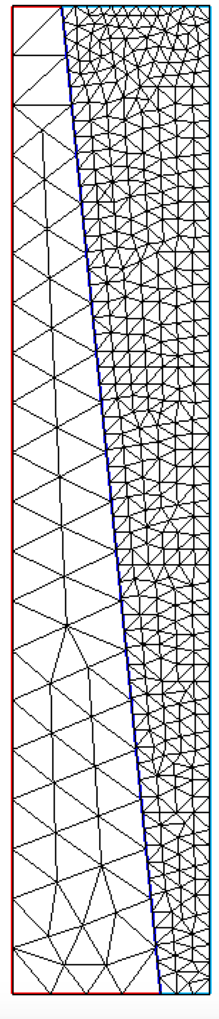
Manufactured Solution

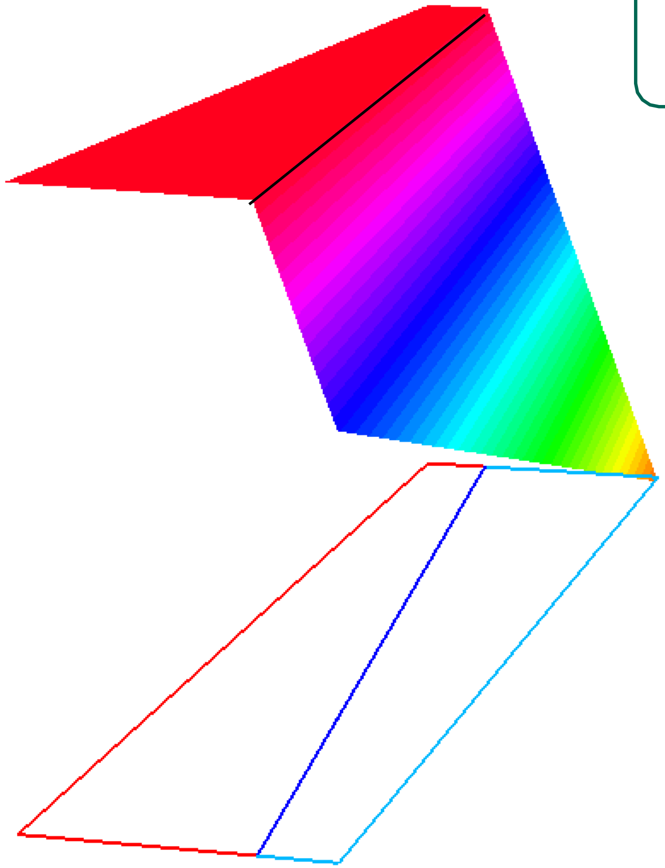
$$\boldsymbol{u}(\boldsymbol{x}) = (3x + 5y, 8x - 4.3y)$$

Error Norm	IVR(L1)	IVR(L2)	IVR(L12)
$L^2(0,T;L^2(\Omega))$	5.166e-04	1.468e-06	2.223e-15
$L^2(0,T;H^1(\Omega))$	1.683e-02	2.679e-05	3.412e-14
LM mesh:	coarser	finer	common

Numerical examples: Solid-Solid Interaction (SSI)

Discontinuous patch test





Manufactured Solution

$$\boldsymbol{u}_1(\boldsymbol{x}) = \left(\frac{-0.9 + x + 0.1y}{0.15}, \frac{18 - 20x - 2y}{0.15}\right)$$

$$\boldsymbol{u}_2(\boldsymbol{x}) = \left(100\left(\frac{-0.9 + x + 0.1y}{0.15}\right) - 99), 100\left(\frac{18 - 20x - 2y}{0.15}\right) + 1980\right)$$

$$\ddot{\boldsymbol{u}}_i - \nabla \cdot \boldsymbol{\sigma}_i(\boldsymbol{u}_i) = \boldsymbol{f}_i$$

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

$$\lambda_1 = 40 \quad \text{and} \quad \mu_1 = 40$$
$$\lambda_2 = 0.4 \quad \text{and} \quad \mu_2 = 0.4$$

Error Norm	IVR(L1)	IVR(L2)	IVR(L12)
$L^2(0,T;L^2(\Omega))$	1.093e-04	5.418e-07	4.832e-13
$L^2(0,T;H^1(\Omega))$	4.591e-02	1.083e-04	6.658e-11
LM mesh:	coarser	finer	common

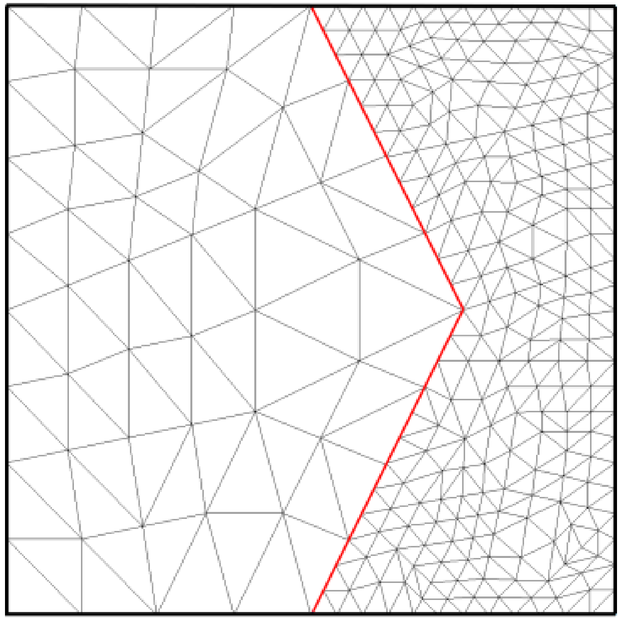
Numerical examples: Solid-Solid Interaction (SSI)

Convergence

$$\ddot{\boldsymbol{u}}_i - \nabla \cdot \boldsymbol{\sigma}_i(\boldsymbol{u}_i) = \boldsymbol{f}_i$$
$$\boldsymbol{\sigma}_i(\boldsymbol{u}_i) = \lambda_i(\nabla \cdot \boldsymbol{u}_i)I + 2\mu_i \boldsymbol{\varepsilon}_i(\boldsymbol{u}_i)$$
$$\lambda = 0.864198 \quad \text{and} \quad \mu = 0.37037$$

Manufactured Solution

$$\boldsymbol{u}(\boldsymbol{x}, t) = (3\sin(x)\sin(y)\cos(t), \sin(x)\sin(y)t)$$



$L^2(\Omega)$ Error

$h_{min}(\Omega_1)$	$h_{min}(\Omega_2)$	Δt	IVR(1)	IVR(2)	IVR(12)
0.378545	0.113981	0.00371833	0.0146414	0.0146403	0.0146404
0.220723	0.0672413	0.00185917	0.00353829	0.00349268	0.00349301
0.107240	0.0359195	0.00101409	0.00095948	0.000854641	0.000854613
0.0514682	0.0196624	0.00053119	0.00033852	0.000217698	0.000217665
0.0277461	0.00957506	0.00024789	0.000141964	5.53096e-05	5.52471e-05
Rate			1.73	2.08	2.08

$H^1(\Omega)$ Error

LM mesh:			coarser	finer	common
$h_{min}(\Omega_1)$	$h_{min}(\Omega_2)$	Δt	IVR(1)	IVR(2)	IVR(12)
0.378545	0.113981	0.00371833	0.341327	0.340643	0.340643
0.220723	0.0672413	0.00185917	0.16736	0.16385	0.163848
0.107240	0.0359195	0.00101409	0.094672	0.081204	0.0812045
0.0514682	0.0196624	0.00053119	0.0701869	0.0404745	0.0404726
0.0277461	0.00957506	0.00024789	0.0576898	0.0204939	0.0204888
Rate			0.657	1.05	1.05

Numerical examples: Transmission Problem (TP)

Discontinuous patch test

Advection Diffusion

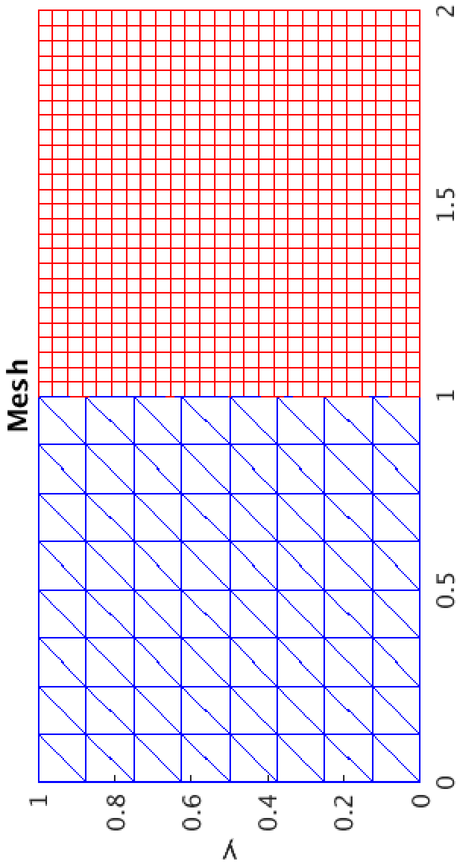
$$\dot{\varphi}_i - \nabla \cdot (\epsilon \nabla \varphi_i - \mathbf{u}\varphi_i) = f_i$$

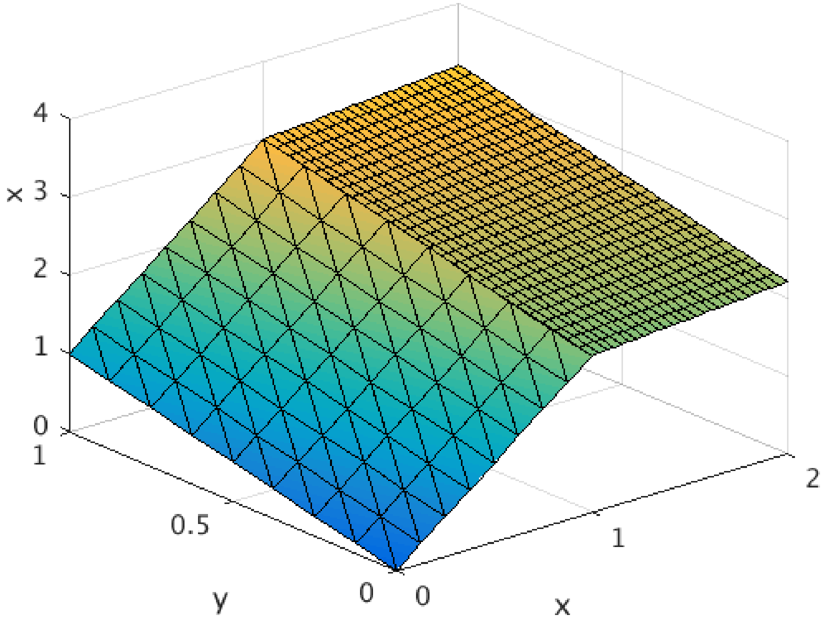
$$\epsilon_1 = 0.01 \qquad \epsilon_2 = 0.1$$

Manufactured Solution

$$\varphi_1(\mathbf{x}, t) = 2x + y$$

$$\varphi_2(\mathbf{x}, t) = 0.2x + y + 1.8$$





Pure Diffusion $\quad \mathbf{u}_1 = \mathbf{u}_2 = 0$

Error Norm	IVR(1)	IVR(2)	IVR(12)
$L^2(\Omega)$	1.899e-04	3.963e-07	4.365e-14
$H^1(\Omega)$	7.510e-03	8.674e-06	1.920e-12

LM mesh: coarser finer common

Moderate Advection $\quad \mathbf{u}_1 = \mathbf{u}_2 = (-\sin(\pi/6), \cos(\pi/6))$

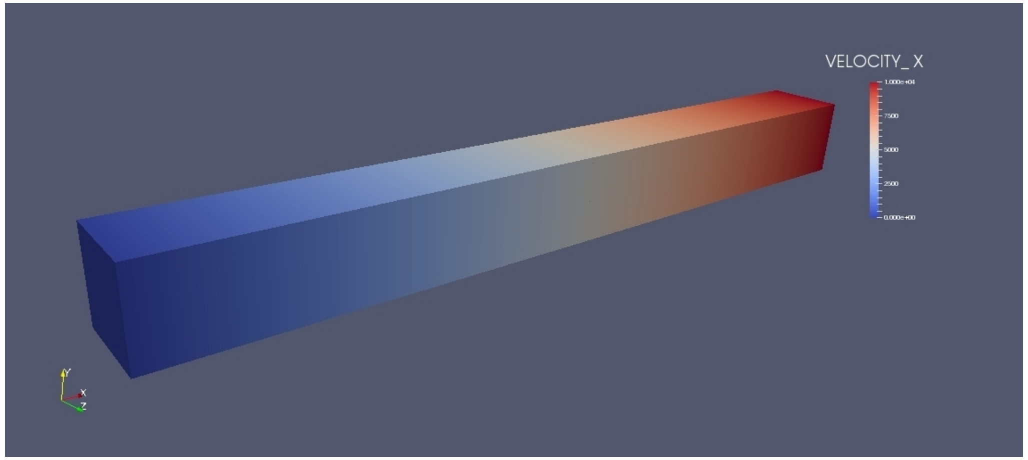
Error Norm	IVR(1)	IVR(2)	IVR(12)
$L^2(\Omega)$	1.269e-02	2.003e-05	1.700e-13
$H^1(\Omega)$	5.098e-01	3.573e-04	5.149e-12

ESPS implementation in production codes

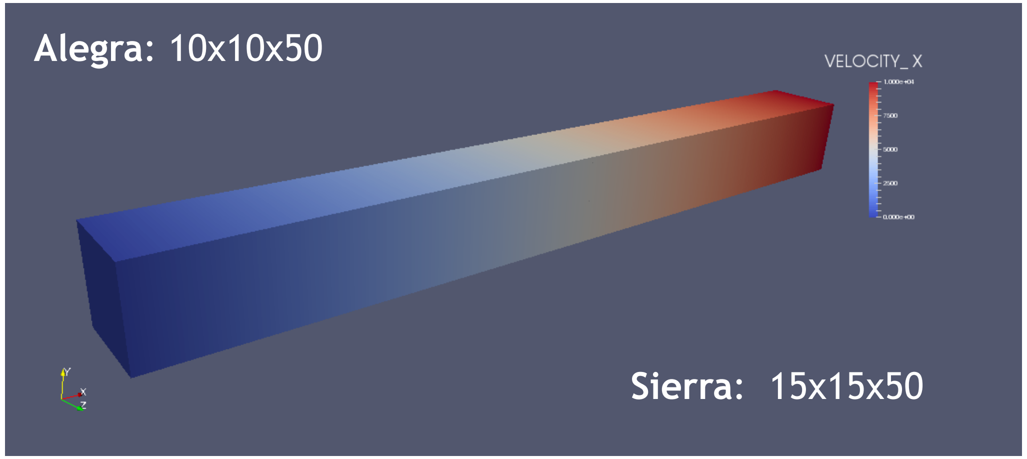
ESPS has been deployed in Sandia's Forte software to couple Alegra and Sierra SM codes.

Consistency test

Exact →



Forte →



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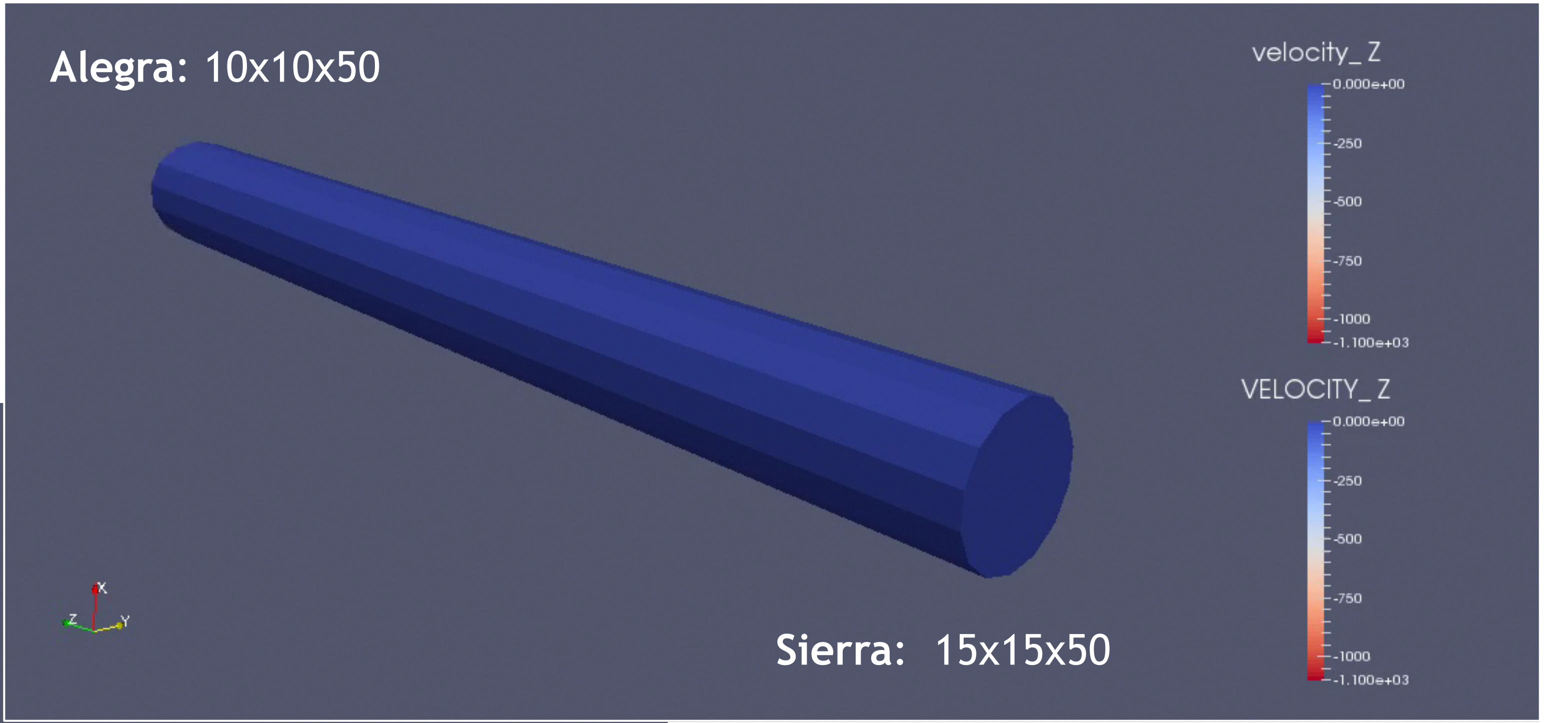
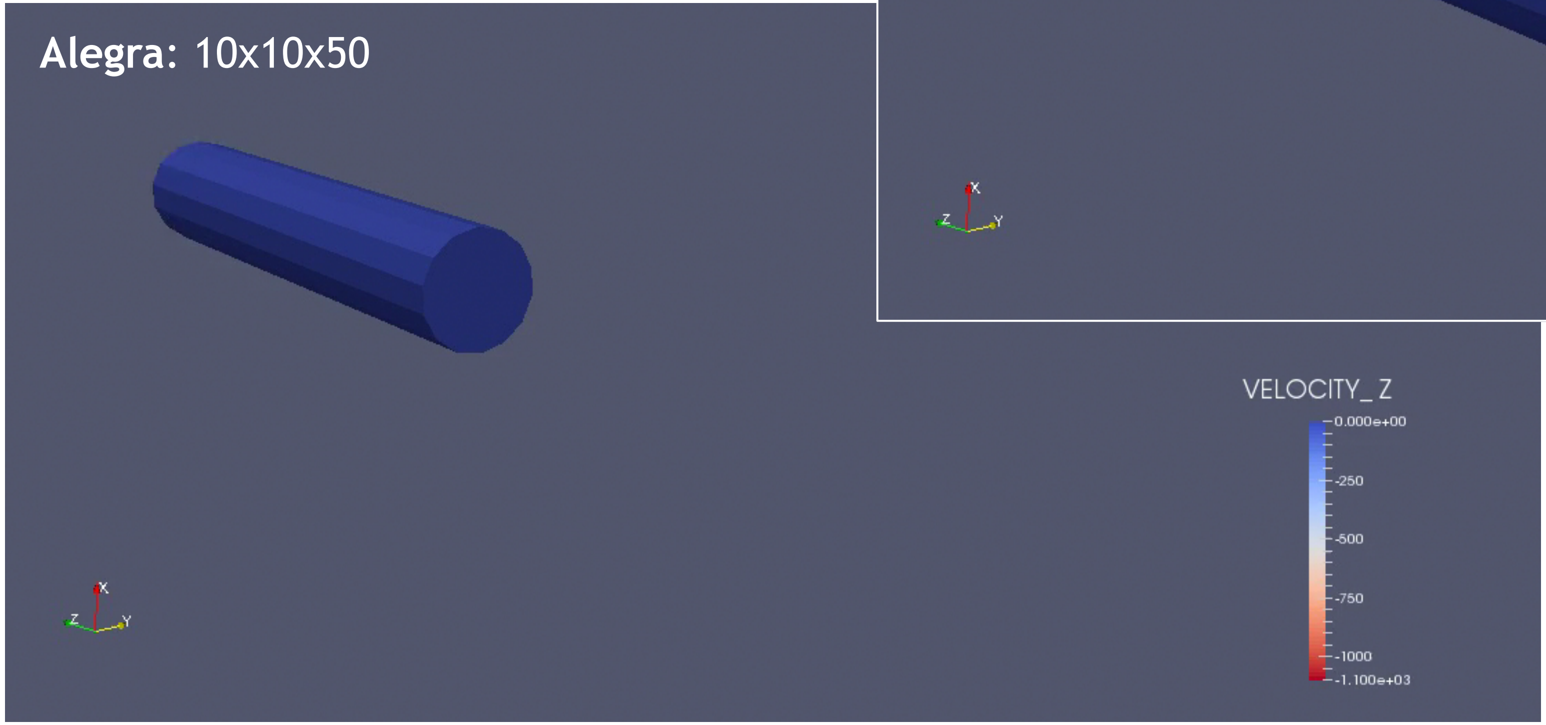
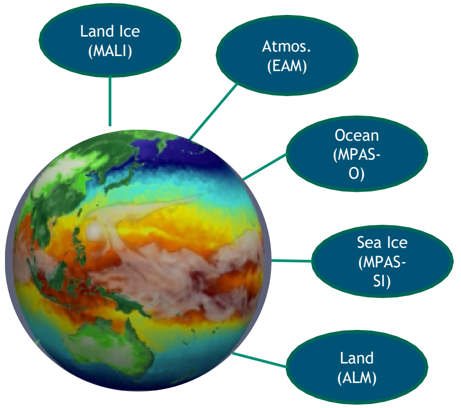
ESPS implementation in production codes

Axial pulse bar test





ESPS extension to non-standard coupling conditions



E3SM Energy Exascale Earth System Model

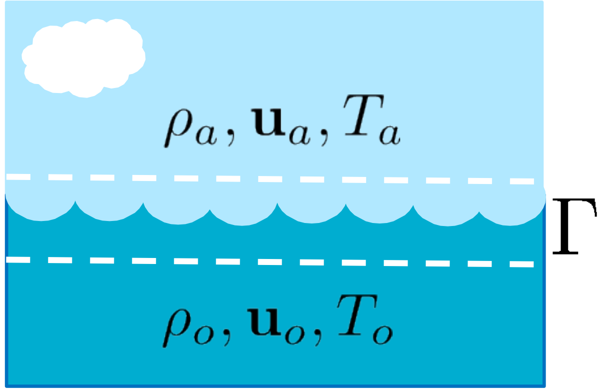
Earth system models

- Coupled ocean-atmosphere problem with velocity and temperature states
- Ocean-atmosphere fluxes defined by a parameterization of the surface layers
- Results in the "bulk" coupling conditions

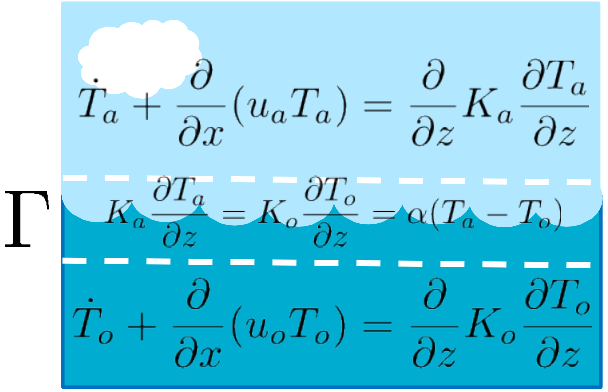
Lemarié, Blayo, Debreu (2015) *Proc. Comp. Sci.*; M. Gross, *et al.* (2018) *MWR*

$$\rho_a \nu_a \frac{\partial \mathbf{u}_a}{\partial z} = \rho_o \nu_o \frac{\partial \mathbf{u}_o}{\partial z} = \boldsymbol{\tau} \quad \text{on } \Gamma \qquad \boldsymbol{\tau} = \rho_a C_\tau \|[\![\mathbf{u}]\!]\| [\![\mathbf{u}]\!] \qquad [\![\mathbf{u}]\!] = \mathbf{u}_a - \mathbf{u}_o \quad \text{on } \Gamma$$

$$\rho_a K_a \frac{\partial T_a}{\partial z} = \rho_o K_o \frac{\partial T_o}{\partial z} = Q_{net} \quad \text{on } \Gamma \qquad Q_{net} = \mathcal{R} + \rho_a C_Q \|[\![\mathbf{u}]\!]\| [\![T]\!] \qquad [\![T]\!] = T_a - T_o \quad \text{on } \Gamma$$



We consider the temperature equation with a prescribed velocity



- ESPS requires a monolithic system in which the flux is one of the variables
- For standard coupling conditions the flux is the Lagrange multiplier
- This is not the case for the bulk condition where the flux and the state are connected
- To get the desired monolithic formulation with the bulk condition:
  - Directly introduce the flux as a new variable λ
  - Close the system by adding the bulk condition as a third equation

ESPS with the bulk condition

The strong monolithic problem: system of 3 equations

Equations

Atmosphere

$$\dot{T}_a + \frac{\partial}{\partial x}(u_a T_a) = \frac{\partial}{\partial z} K_a \frac{\partial T_a}{\partial z} \quad \text{in } \Omega_a$$

$$K_a \frac{\partial T_a}{\partial z} = \lambda \quad \text{on } \Gamma$$

Ocean

$$\dot{T}_o + \frac{\partial}{\partial x}(u_o T_o) = \frac{\partial}{\partial z} K_o \frac{\partial T_o}{\partial z} \quad \text{in } \Omega_o$$

$$K_o \frac{\partial T_o}{\partial z} = -\lambda \quad \text{on } \Gamma$$

Neumann BC

Bulk condition

$$\lambda = \alpha(T_a - T_o) \quad \text{on } \Gamma$$

Semi-discrete monolithic problem: has the structure of a "stabilized" mixed formulation

$$\begin{aligned} M_a \dot{\mathbf{T}}_a + G_a^T \boldsymbol{\lambda} &= \mathbf{f}_a(\mathbf{T}_a) \\ M_o \dot{\mathbf{T}}_o - G_o^T \boldsymbol{\lambda} &= \mathbf{f}_o(\mathbf{T}_o) \\ \alpha G_a \mathbf{T}_a - \alpha G_o \mathbf{T}_o - \widehat{M}_\Gamma \boldsymbol{\lambda} &= 0 \end{aligned}$$

- The interface equation is not a result of using a Lagrange multiplier
- It relates λ to $\mathbf{T}_a$ and $\mathbf{T}_o$ but not their time derivatives
- We can't use the Schur complement as in the standard interface case

Simple solution: Discretize in time, then solve the fully discrete problem for the flux λ

$$\begin{aligned} M_a \left(\frac{\mathbf{T}_a^{n+1} - \mathbf{T}_a^n}{\Delta t}\right) + G_a^T \boldsymbol{\lambda} &= \mathbf{f}_a(\mathbf{T}_a^n) \\ M_o \left(\frac{\mathbf{T}_o^{n+1} - \mathbf{T}_o^n}{\Delta t}\right) - G_o^T \boldsymbol{\lambda} &= \mathbf{f}_o(\mathbf{T}_o^n) \\ \alpha G_a \mathbf{T}_a^{n+1} - \alpha G_o \mathbf{T}_o^{n+1} - \widehat{M}_\Gamma \boldsymbol{\lambda} &= 0 \end{aligned}$$

$$\boldsymbol{\lambda} = \left(\Delta t G_a^T A_a^{-1} G_a + \Delta t G_o^T A_o^{-1} G_o - \frac{\widehat{M}_\Gamma}{\alpha}\right)^{-1} \left(G_a^T A_a^{-1} \hat{\mathbf{g}}_a(\mathbf{T}_a^n) - G_o^T A_o^{-1} \hat{\mathbf{g}}_o(\mathbf{T}_o^n)\right)$$

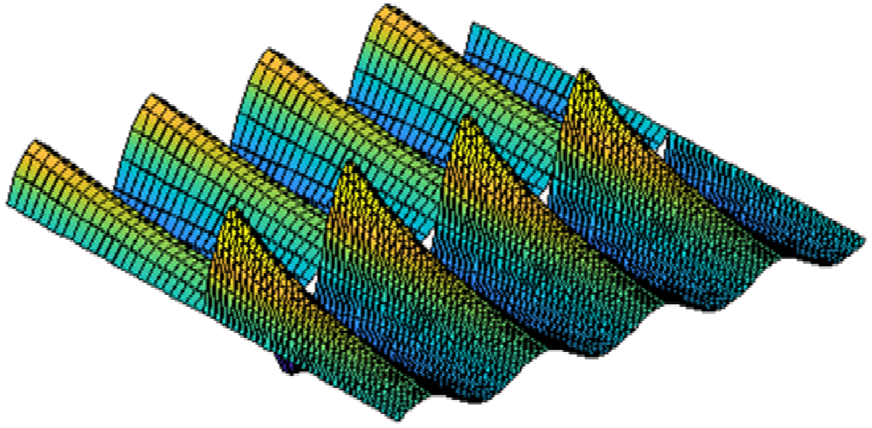
With explicit time stepping only involves information from old time step!

K. C. Sockwell, K. Peterson, P. Kuberry, P. Bochev, and N. Trask. Interface flux recovery coupling method for the ocean–atmosphere system. Results in Applied Mathematics, 8:100110, 2020

ESPS with the bulk condition: numerical results

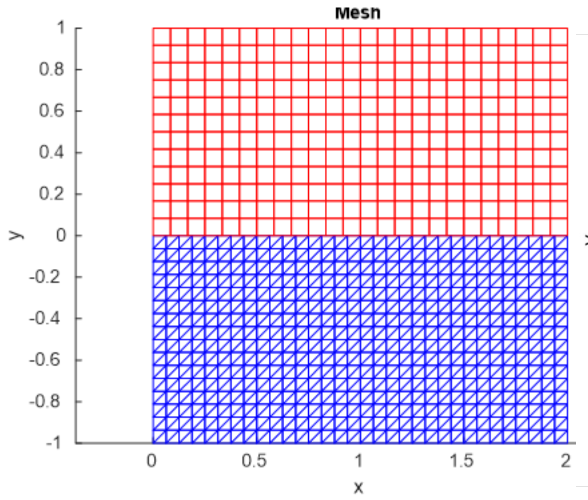
Manufactured solution (temperature equation + velocity field)

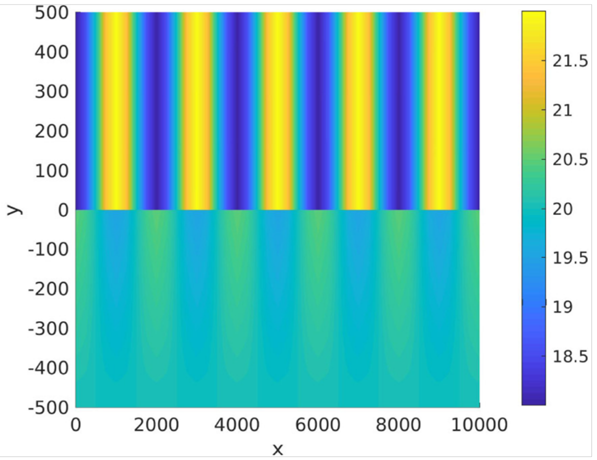
- A wave in the horizontal direction with a discontinuity across the interface.
- Test case models the heat exchange between the ocean and atmosphere.



Mesh (Ω_o)	Mesh (Ω_a)	Δt	BIVR(λ_o)	BIVR(λ_a)
16×8	12×6	1.33e-02	2.09e-00	2.09e-00
32×16	24×12	6.67e-03	3.40e-01	3.40e-01
64×32	48×24	3.32e-03	6.18e-02	6.18e-02
128×64	96×48	1.66e-03	1.30e-02	1.30e-02
Rate	-	-	2.25	2.25

Mesh (Ω_o)	Mesh (Ω_a)	Δt	BIVR(λ_o)	BIVR(λ_a)
16×8	12×6	1.33e-02	5.66e01	5.66e01
32×16	24×12	6.67e-03	2.78e01	2.78e01
64×32	48×24	3.32e-03	1.37e01	1.37e01
128×64	96×48	1.66e-03	6.84e00	6.84e00
Rate	-	-	1.01	1.01





K. C. Sockwell, K. Peterson, P. Kuberry, P. Bochev, and N. Trask. Interface flux recovery coupling method for the ocean–atmosphere system. Results in Applied Mathematics, 8:100110, 2020

ESPS extension to reduced order models.

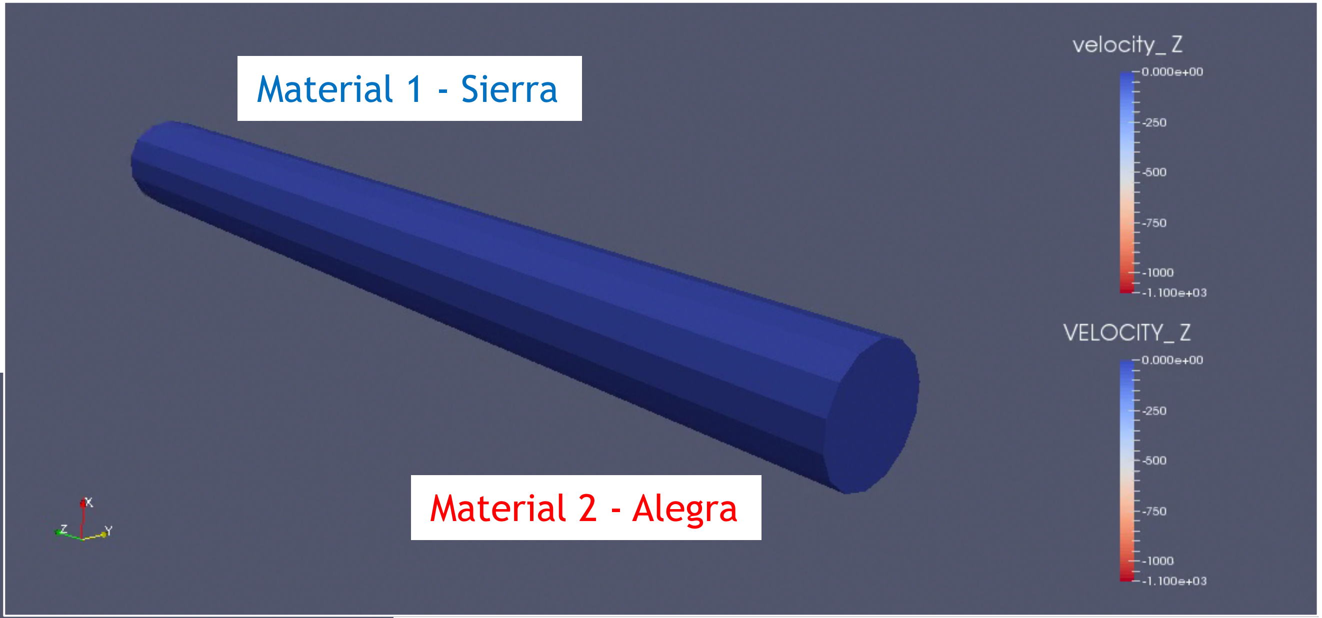
Recall the production implementation of ESPS, which solves a coupled structure-structure interaction problem with two different materials modeled by Sierra SM and Alegra, resp.

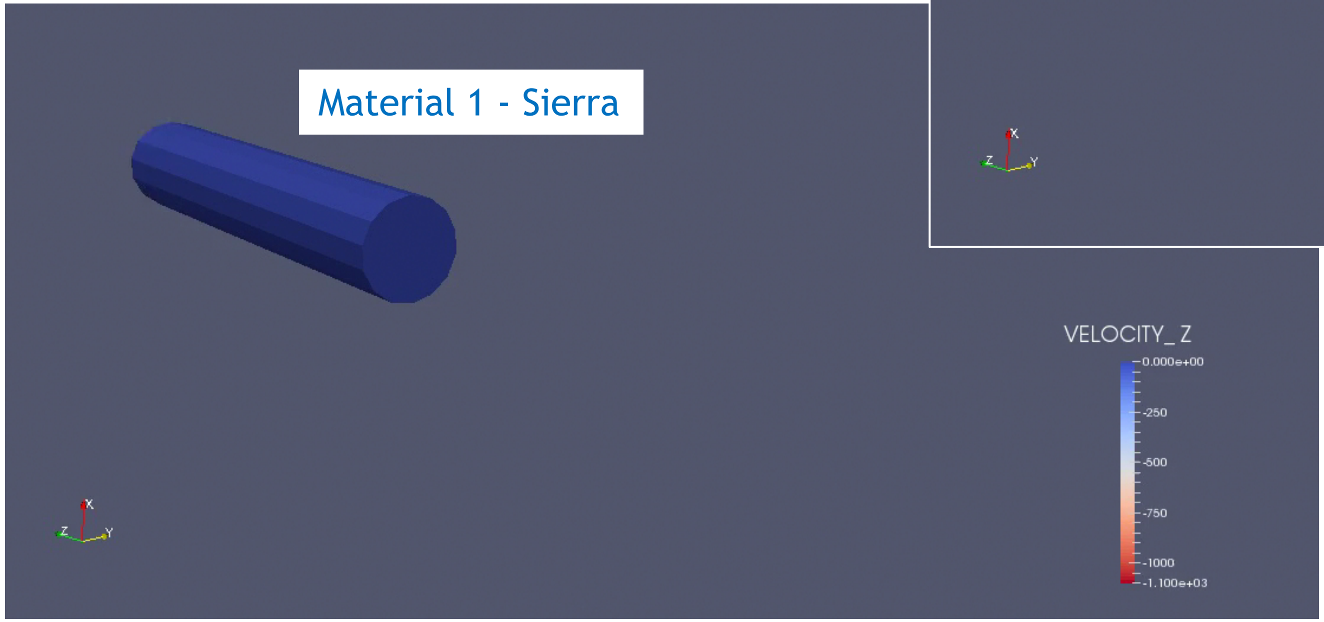
$$\left.\begin{aligned} \ddot{\boldsymbol{u}}_i - \nabla\cdot\sigma_i(\boldsymbol{u}_i) &= \boldsymbol{f}_i \quad \text{in } \Omega_i \times [0,T] \\ \boldsymbol{u}_i &= \boldsymbol{g}_i \quad \text{on } \Gamma_i \times [0,T] \end{aligned}\right., \quad i = 1,2$$

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

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

Axial pulse bar test





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.

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: $S = [\mathbf{u}_1, \cdots, \mathbf{u}_n] = U\Sigma V^T$
- Given tolerance $\delta > 0$ choose d such that $\dfrac{\sum_{j=1}^{d} \sigma_j^2}{\sum_{j=1}^{n} \sigma_j^2} \geqslant 1 - \delta$

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

- Define the RB as the d left singular vectors, i.e., the matrix $\tilde{U}$

$S \approx \tilde{S} = \tilde{U}\tilde{\Sigma}\tilde{V}^T$ Low-rank approximation of S

Step 2: Galerkin projection onto the reduced basis

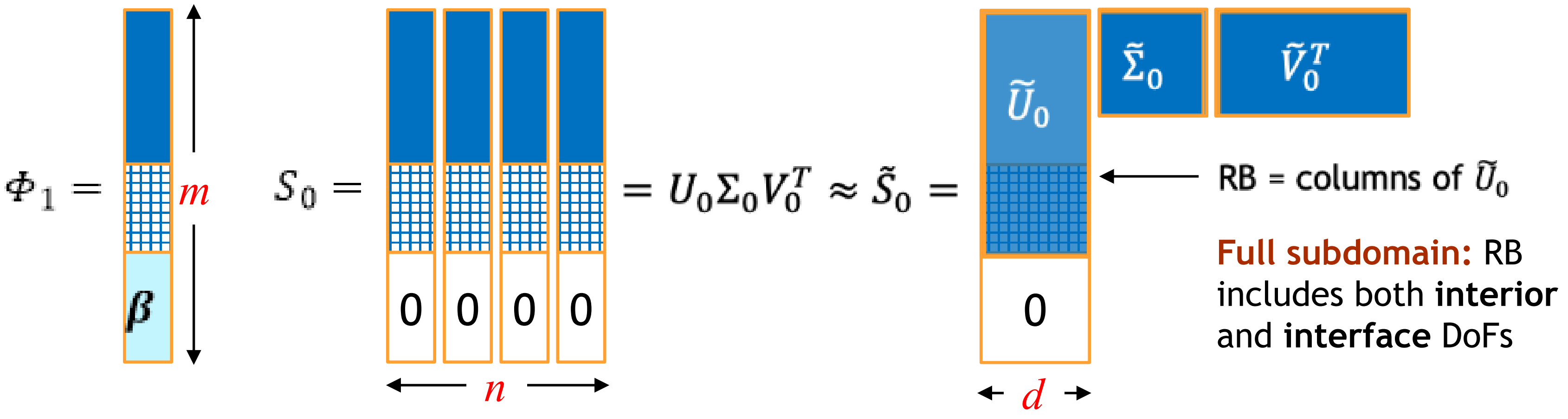
$a(u, v) = f(v)$ for all $v \in V$ → $K\mathbf{u} = \mathbf{f}$ → $\mathbf{u} = \tilde{U}\mathbf{a}$ → $\tilde{U}^T K \tilde{U}\mathbf{a} = \tilde{U}^T\mathbf{f}$ $\quad d \ll m$

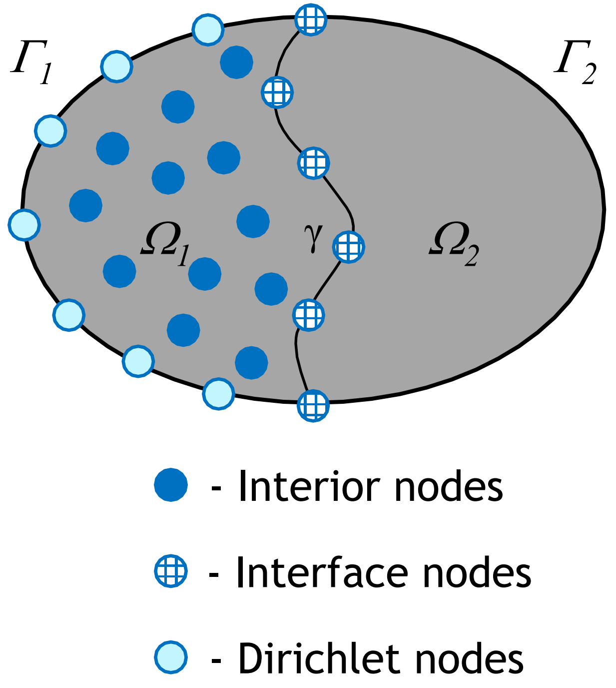
Full Order Model (FOM): $m \times m$ Reduced Order Model (ROM): $d \times d$

ESPS extension to ROM+ROM and ROM+FEM couplings

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

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





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

RB projection:

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

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

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

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

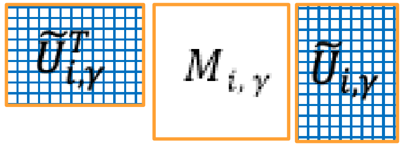
$$\left[\begin{array}{ccc:cc} M_{1,\gamma} & 0 & G_1^T & 0 & 0 \\ 0 & M_{2,\gamma} & -G_2^T & 0 & 0 \\ G_1 & -G_2 & 0 & 0 & 0 \\ \hdashline 0 & 0 & 0 & M_{1,0} & 0 \\ 0 & 0 & 0 & 0 & M_{2,0} \end{array}\right]$$

Interface blocks are separated from the interior blocks

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

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

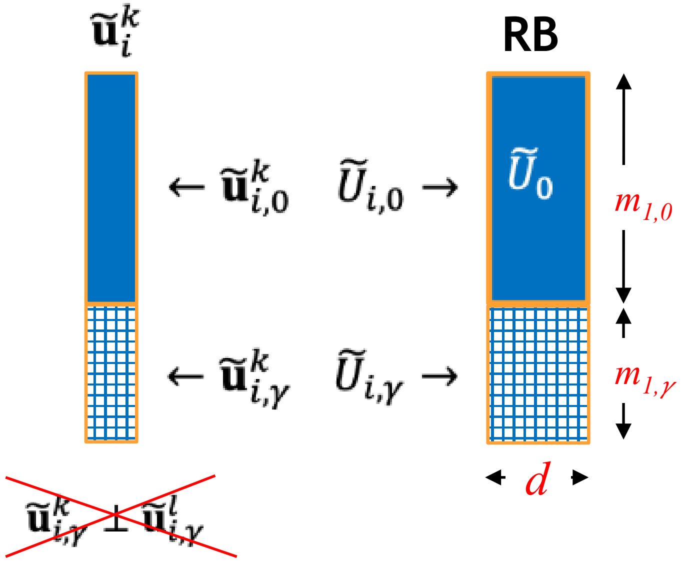
$$\widetilde{M}_{i,\gamma} = \widetilde{U}_{i,\gamma}^T M_{i,\gamma} \widetilde{U}_{i,\gamma}$$



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

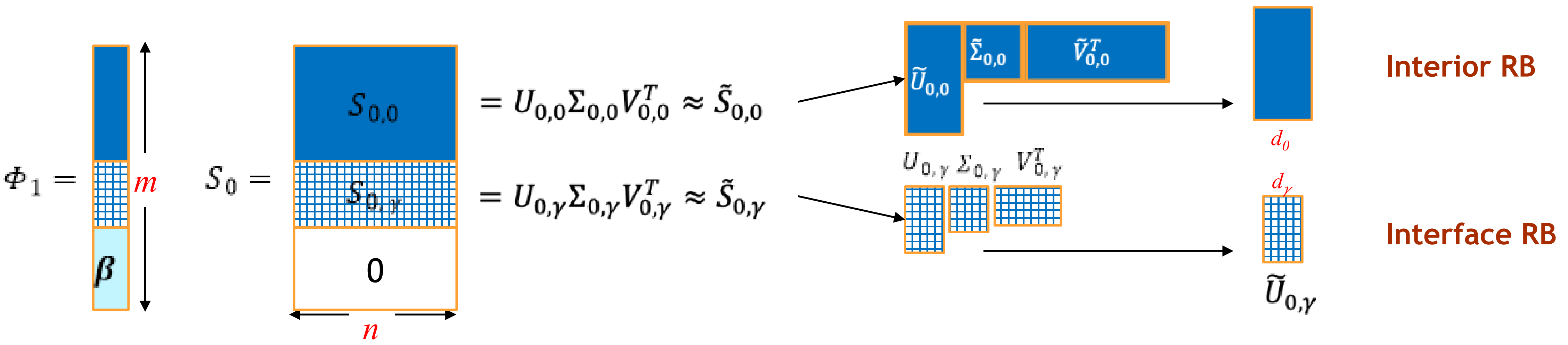
However, their parts $\tilde{\mathbf{u}}_{i,\gamma}^k$ and $\tilde{\mathbf{u}}_{i,\gamma}^k$ corresponding to interface DoFs are not! They can be almost linearly dependent

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

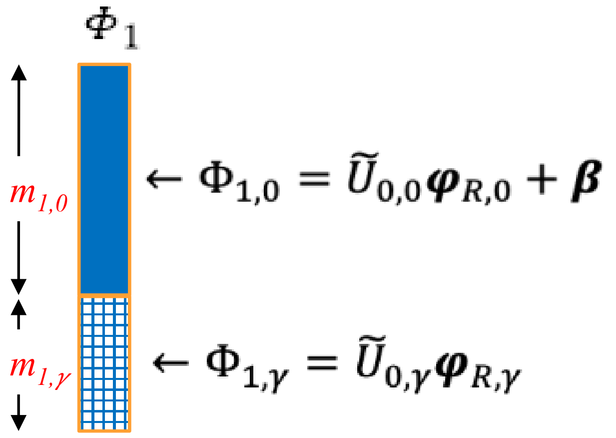


Solution: a Composite Reduced Basis Implementation

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

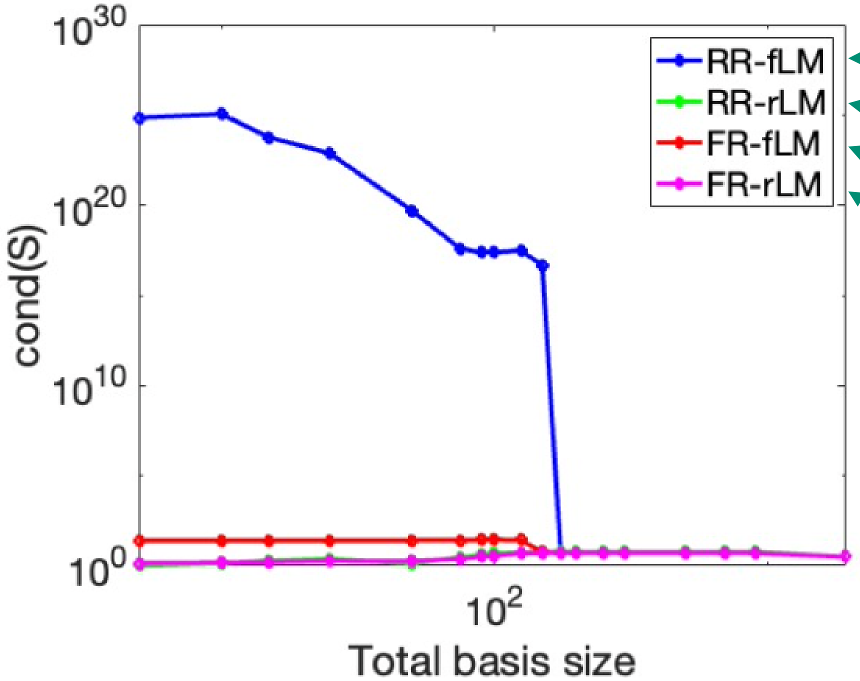
$$\tilde{S} = \tilde{G}_1 \tilde{M}_{1,\gamma}^{-1} \tilde{G}_1^T + G_2 M_{2,\gamma}^{-1} G_2^T$$

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



ROM+ROM: full subdomain basis **violates** TCC

ROM+ROM: composite RB **satisfies** TCC

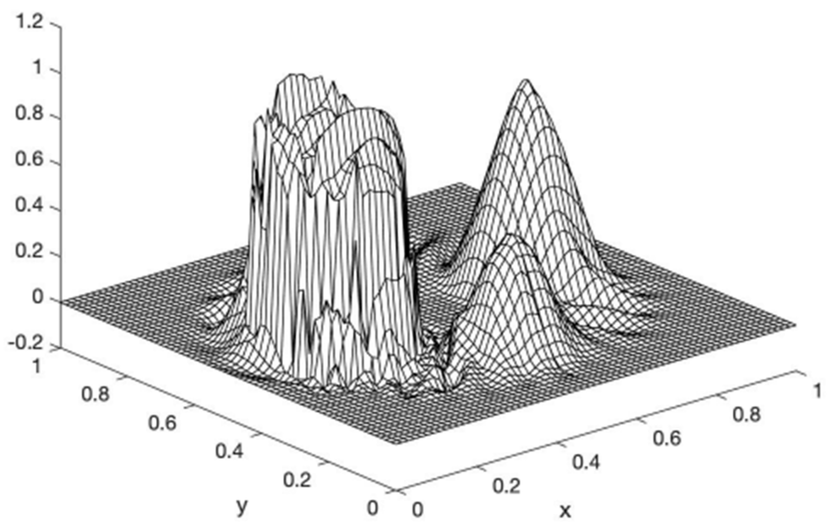
ROM+FOM: interface FEM from the FEM side **satisfies** TCC

ROM+FOM: interface RB from the ROM side **satisfies** TCC

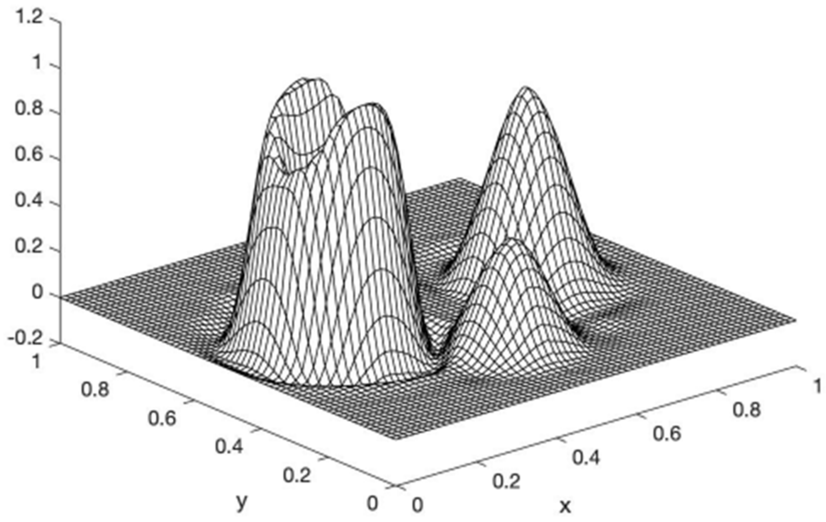
A. DeCastro, P. Bochev, P. Kuberry, and I. Tezaur. Explicit synchronous partitioned scheme for coupled reduced order models based on composite reduced bases. CMAME. In revision.

Numerical example

Full subdomain RB ROM-ROM



Composite RB ROM-ROM



$d = 50$ modes in each subdomain

FOM: 4225 DOFs

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

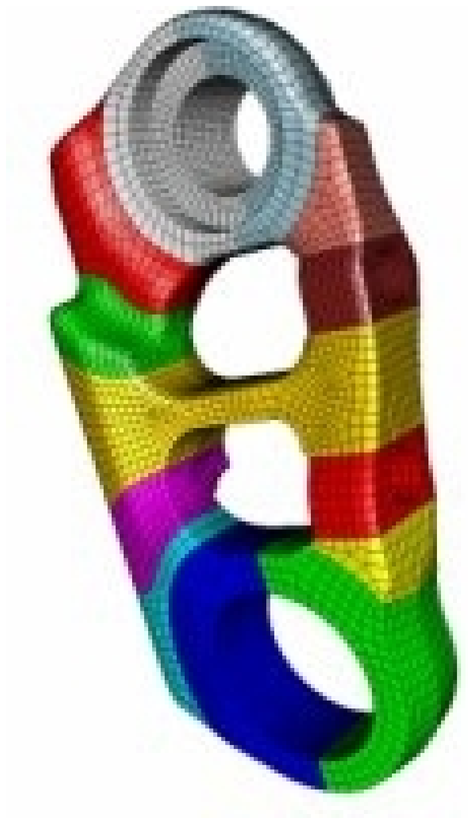
In each subdomain

- Composite RB improves conditioning of the Schur complement
- Allows accurate results with smaller total number of modes

Spatially non-coincident interfaces: where do they come from?

Separate subdomain meshing can create 2 non-coincident versions of the interface

I. Interface problems where subdomain equations are solved by different codes
II. Meshing of complex geometries may requires breaking up the part into simpler pieces

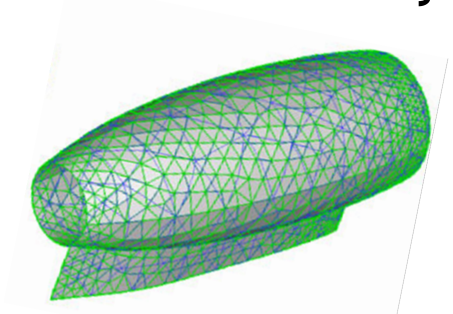


http://cubit.sandia.gov

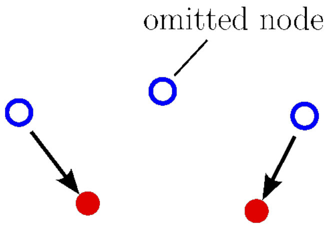
Challenges

- Traditional mortars not appropriate: duplicate interface typically requires some sort of master-slave identification and appropriate formulation of data transfers between them
- Data transfers between non-coincident interfaces present theoretical and practical difficulties

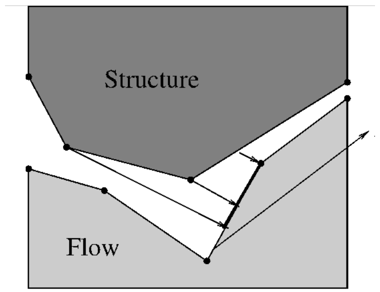
Some of the commonly used data transfer strategies:



Common refinement
Complex intersections



Nearest Neighbor
Omitted nodes



Nearest Projection
Elements not covered

X. Jiao and M. T. Heath. Common-refinement-based data transfer between non-matching meshes in multiphysics simulations. IJNME, 61(14):2402- 2427, 2004.
A. de Boer, A. van Zuijlen, and H. Bijl. Review of coupling methods for non-matching meshes. CMAME 196(8):1515 – 1525, 2007.

Optimization-based coupling approach for non-coincident interfaces

We couch the coupling into a constrained optimization problem

Advantages:

- Physical properties can be distributed between the objective and the constraints.
- Physics-motivated constraints/objectives can be defined on non-coincident interfaces!
- Can avoid complex and/or expensive mesh operations at every time step

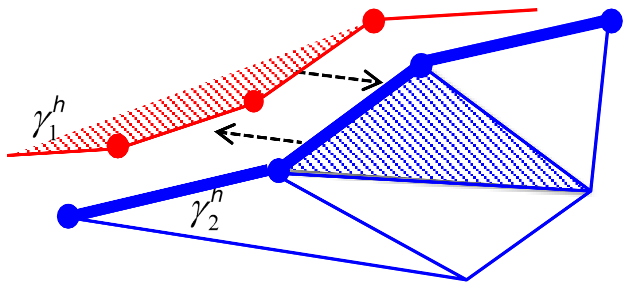
Objective: minimize the quadratic functional

$$J(\phi_1,\phi_2;\theta_1,\theta_2)=\frac{1}{2}\left(\int_{\gamma_1^h}\mathbf{n}_1\cdot\nabla\phi_1\,ds+\int_{\gamma_2^h}\mathbf{n}_2\cdot\nabla\phi_2\,ds\right)^2 \xrightarrow{\text{Flux continuity}} \mathbf{n}_1\cdot\nabla\phi_1=\mathbf{n}_2\cdot\nabla\phi_2 \quad \text{on } \gamma$$

$$+\frac{1}{2}\left(\|\phi_1-E(\phi_2)\|_{\gamma_1^h}^2+\|\phi_2-E(\phi_1)\|_{\gamma_2^h}^2\right) \xrightarrow{\text{State continuity}} \phi_1=\phi_2 \quad \text{on } \gamma$$

$$+\frac{\delta}{2}\left(\|\theta_1\|_{\gamma_1^h}^2+\|\theta_2\|_{\gamma_2^h}^2\right) \longrightarrow \text{control penalty}$$

Extension operators $E:\gamma_i^h\rightarrow\gamma_j^h$



- Polynomial extension
- Meshfree (GMLS), etc.

Subject to constraints (the subdomain PDEs)

$$(\nabla\phi_i,\nabla\psi_i)_{\Omega_1}=(f,\psi_i)_{\Omega_1}+\langle\theta_i,\psi_i\rangle_{\gamma_i^h}$$

$$\begin{cases}-\nabla\cdot\nabla\phi_i=f & \text{in } \Omega_i\\ \phi_i=0 & \text{on } \Gamma_i\\ \mathbf{n}_i\cdot\nabla\phi_i=\theta_i & \text{on } \gamma_i^h\end{cases}$$

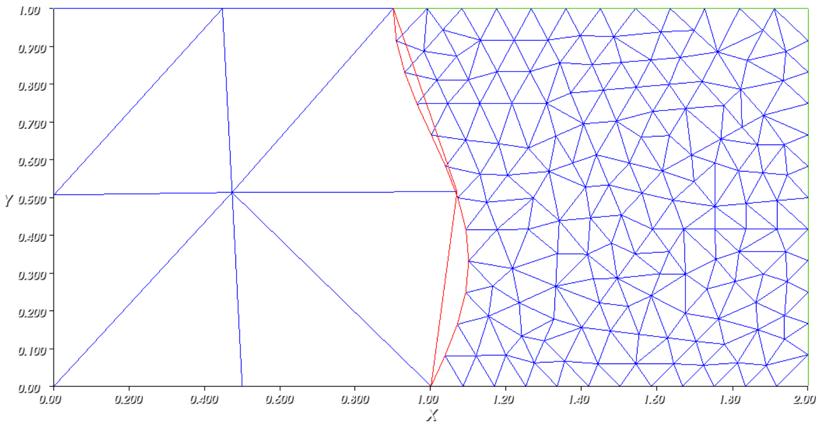
Virtual Neumann controls

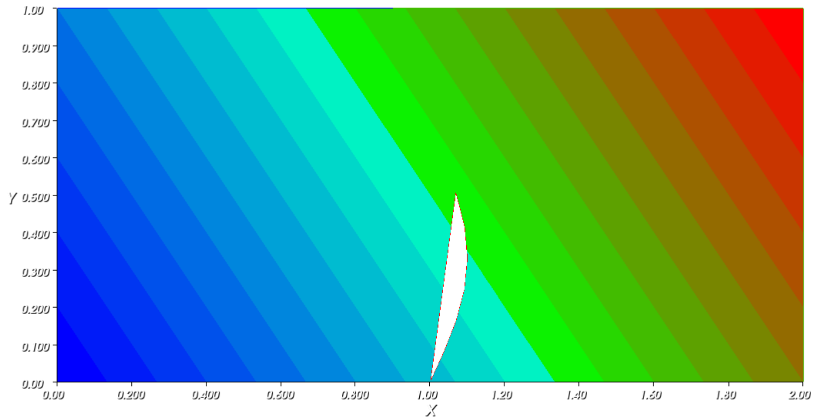
We close the subdomain problems by using a virtual control to specify a Neumann boundary condition on the interface

Properties

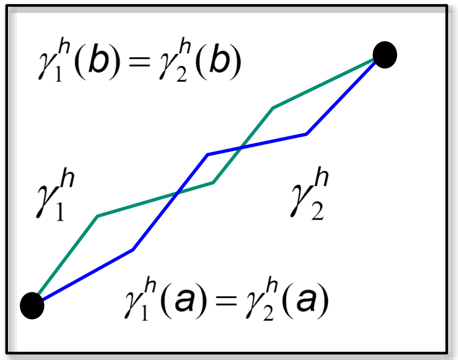
Theorem Assume that the discrete interfaces have matching boundaries. Then the optimization-based coupling formulation **recovers exactly globally linear solutions** ϕ^* of the coupled problem.

Patch test $\phi(x,y) = 3x+2y$

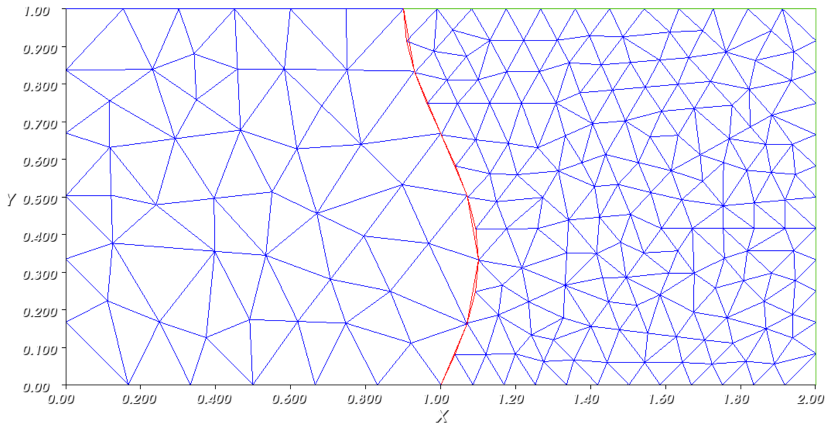


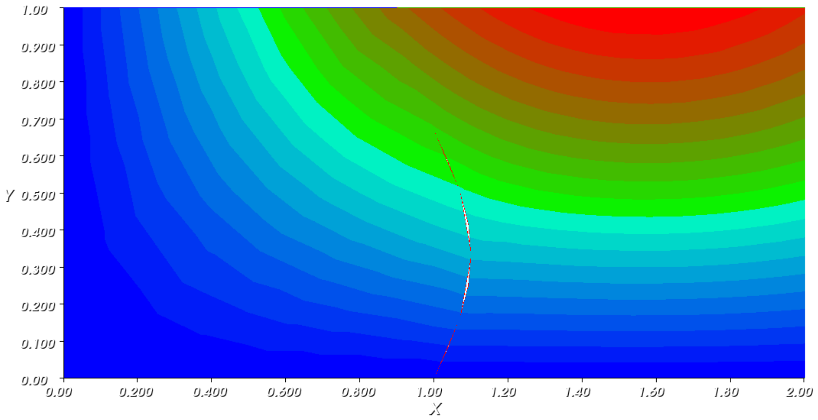


2D

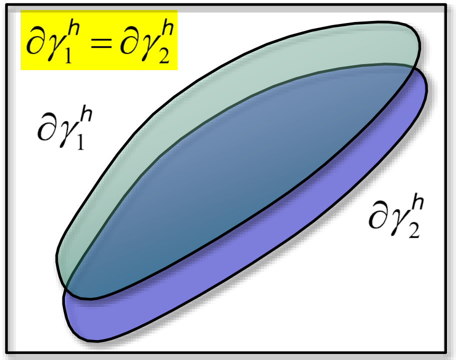


Manufactured solution $\phi(x,y) = sin(x)*sin(y)$





3D



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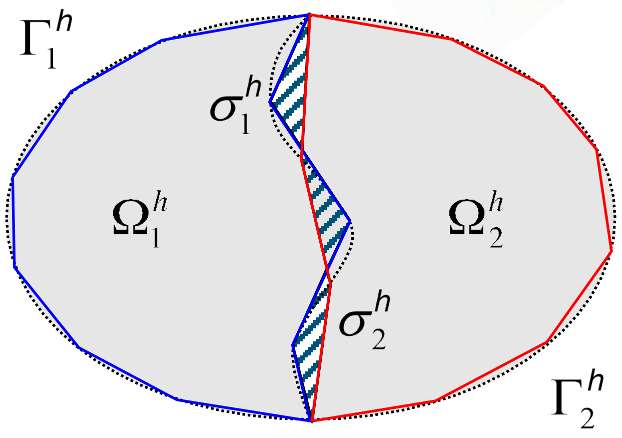
Least-squares finite element (LSFEM) formulation for mesh tying

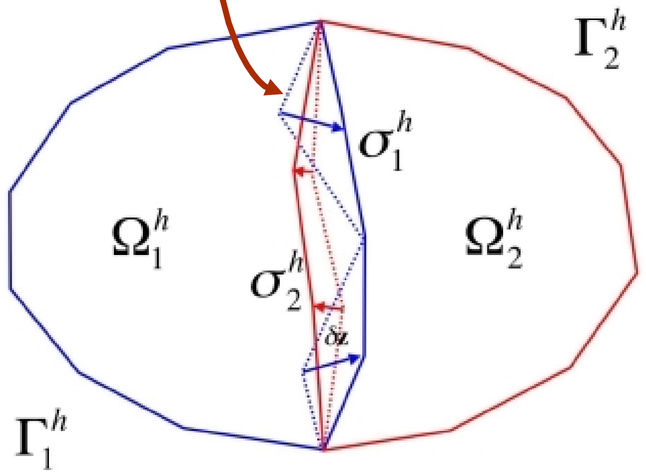
- Mesh tying is required when a complex part is meshed by breaking it into separate simpler parts
- Often the interface meshes have tiny gaps and overlaps.
- Creating watertight meshes may introduce sliver elements, which can limit explicit time steps

LSFEM offers a surprisingly effective solution for non-coincident grids



- ➪ LS are based on minimization of **artificial residual energy**, not physical energy
- ➪ Minimization of **residual energy** allows to measure energy **redundantly**
- ➪ **All that is needed is elimination of the void regions to create sufficient overlap:**
  - **– Can be done by interface perturbation or by simply extending the domains**

$$\min \frac{1}{2}\sum_i \underbrace{\left(\|\nabla\phi_i + \mathbf{v}_i\|^2_{0,\Omega_i} + \|\nabla\cdot\mathbf{v}_i - f\|^2_{0,\Omega_i}\right)}_{\text{residual energy}} + \underbrace{\omega_\phi \|\phi_1-\phi_2\|^2_{1,\Sigma} + \omega_{\mathbf{v}}\|\mathbf{v}_1-\mathbf{v}_2\|^2_{div,\Sigma}}_{\text{coupling term}}$$



Advantages

- ✓ Provably **stable** (coercive formulation)
- ✓ Provable **optimal convergence** rate
- ✓ Can pass an **arbitrary order** patch test
- ✓ Does not require expensive **mesh intersections**

Analysis: least-squares for mesh tying

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Norm-equivalence of the mesh-tying LS functional

Theorem 1 *There exist positive weights ω_ϕ, $\omega_{\mathbf{v}}$, independent of the maximum element diameter h, such that for every $\{\psi, \mathbf{v}\} \in \mathbf{H}$ there holds the lower bound*

$$J_h(\{\psi, \mathbf{v}\}; 0) \geq \frac{1}{4} |||\{\psi, \mathbf{v}\}|||^{\mathbf{2}}. \tag{17}$$

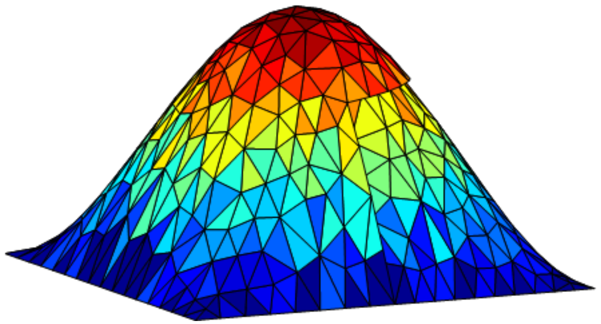
Optimal error estimates

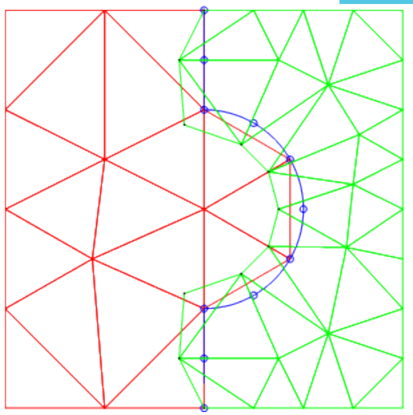
Theorem 3 *Assume that the first order system*

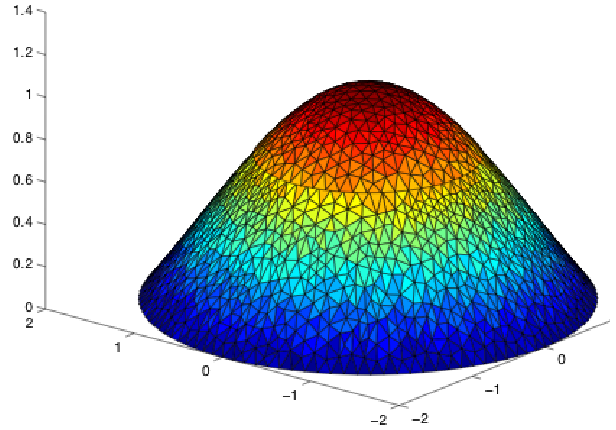
$$\begin{cases} \nabla \cdot \mathbf{u} + \phi = f \quad \text{and} \quad \nabla \phi + \mathbf{u} = 0 \quad \text{in } \Omega \\ \phi = 0 \quad \text{on } \partial\Omega \end{cases}$$

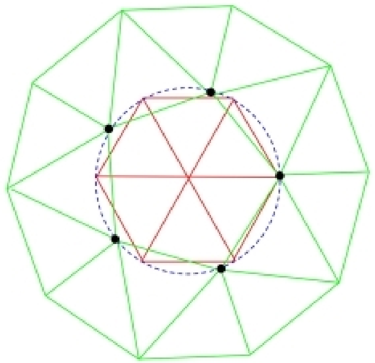
has a solution $\phi \in H_0^1(\Omega) \cap H^{r+1}(\Omega)$ and $\mathbf{u} \in H(\mathrm{div}, \Omega) \cap (H^{p+1}(\Omega))^2$. If $\{\phi^h, \mathbf{u}^h\} \in \mathbf{H}^h$ is a solution of the least-squares mesh-tying problem (12), then

$$|||\{\phi - \phi^h, \mathbf{u} - \mathbf{u}^h\}||| \leq C \left(h^r \|\phi\|_{r+1,\Omega} + h^p \|\mathbf{u}\|_{p+1,\Omega} \right). \tag{22}$$

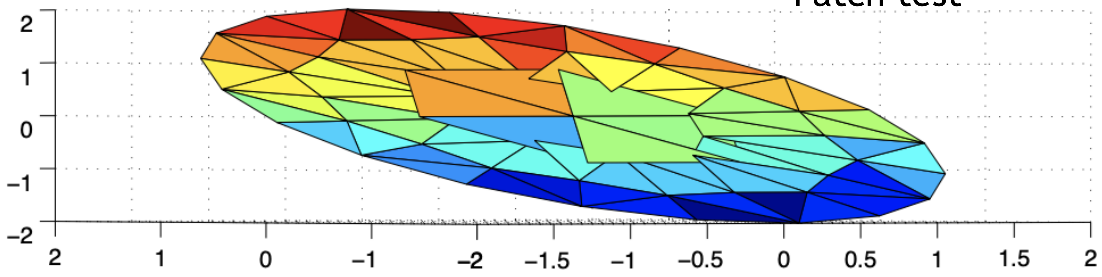








Patch test



Thank you!

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