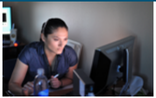
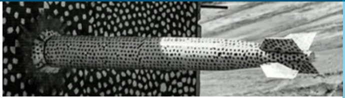
-9026C

Sandia National Laboratories

Formulation of Partitioned Schemes with Non-Standard Computational Models





Authors: Amy de Castro, Paul Kuberry, Irina Tezaur, and Pavel Bochev

Presented by:

Amy de Castro

Center for Computing Research
Sandia National Laboratories

CCR Center for Computing Research

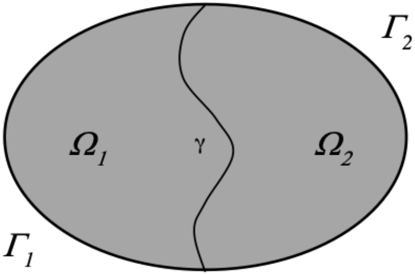
U.S. DEPARTMENT OF ENERGY NNSA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell

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

Motivation and model transmission problem

Motivation and Overview



- Couple conventional FEMs with projection-based ROMs to increase computational efficiency
- Monolithic framework: use Schur complement to approximate interface flux, explicit time integration decouples the subdomain problems at each time step
- Compare performance of FEM-FEM, ROM-FEM and ROM-ROM couplings with a model transmission problem

Model transmission problem: advection-diffusion

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

- φ_i: unknown scalar field
- $F_i(\varphi_i) = \kappa_i \nabla \varphi_i - \mathbf{u}\varphi_i$: total flux function
- κ_i: non-negative diffusion coefficient
- $\mathbf{u}$: given velocity field

Enforce continuity of states and of total flux along the interface:

$$\varphi_1(\mathbf{x}, t) - \varphi_2(\mathbf{x}, t) = 0 \quad \text{and} \quad F_1(\mathbf{x}, t) \cdot \mathbf{n}_\gamma = F_2(\mathbf{x}, t) \cdot \mathbf{n}_\gamma \quad \text{on } \gamma \times [0,T]$$

Weak formulation

Use a Lagrange multiplier to enforce state continuity interface condition: $\lambda = F_1 \cdot \mathbf{n}_\gamma = F_2 \cdot \mathbf{n}_\gamma$.

Seek $\{\varphi_1, \varphi_2, \lambda\} \in V := H^1_\Gamma(\Omega_1) \times H^1_\Gamma(\Omega_2) \times H^{-1/2}_\Gamma(\gamma)$, *such that*

$$(\dot{\varphi}_1, \nu)_{\Omega_1} + (\kappa_1 \nabla \varphi_1, \nabla \nu)_{\Omega_1} - (\mathbf{u}\varphi_1, \nabla \nu)_{\Omega_1} + (\lambda, \nu)_\gamma = (f_1, \nu)_{\Omega_1}, \quad \forall \nu \in H^1_\Gamma(\Omega_1)$$

$$(\dot{\varphi}_2, \eta)_{\Omega_2} + (\kappa_2 \nabla \varphi_2, \nabla \eta)_{\Omega_2} - (\mathbf{u}\varphi_2, \nabla \eta)_{\Omega_2} - (\lambda, \eta)_\gamma = (f_2, \eta)_{\Omega_2}, \quad \forall \eta \in H^1_\Gamma(\Omega_2)$$

$$(\varphi_1, \mu)_\gamma - (\varphi_2, \mu)_\gamma = 0, \qquad \forall \mu \in H^{-1/2}(\gamma)$$

Decoupled subdomain equations

Knowing λ allows decoupling of the subdomain equations.

Each subdomain problem is a well-posed mixed boundary value problem with a Neumann condition on γ provided by λ:

$$\left.\begin{aligned} \dot{\varphi}_i - \nabla \cdot F_i(\varphi_i) &= f_i \qquad \text{on } \Omega_i \times [0,T] \\ \varphi_i &= g_i \qquad \text{on } \Gamma_i \times [0,T] \\ F_i(\varphi_i) \cdot \mathbf{n}_i &= (-1)^i \lambda \qquad \text{on } \gamma \times [0,T] \end{aligned}\right. \qquad i = 1, 2\,.$$

Semi-discrete formulation

Let $V^h \subset V$ be a conforming finite element space spanned by a basis $\{\nu_i, \eta_j, \mu_k\}$; $i = 1, \ldots, N_1$; $j = 1, \ldots, N_2$; $k = 1, \ldots, N_\gamma$. Discretizing the weak formulation yields a Differential Algebraic Equation (DAE) system:

Semi-discrete formulation

Let $V^h \subset V$ be a conforming finite element space spanned by a basis $\{\nu_i, \eta_j, \mu_k\}$; $i = 1, \ldots, N_1$; $j = 1, \ldots, N_2$; $k = 1, \ldots, N_\gamma$. Discretizing the weak formulation yields a Differential Algebraic Equation (DAE) system:

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

where for $r = 1, 2$

- M_r: mass matrices
- $\overline{\mathbf{f}}_r(\mathbf{\Phi}_r) = \mathbf{f}_r - (D_r + A_r)\mathbf{\Phi}_r$
- D_r, A_r: matrices for diffusive and advective flux terms
- G_r: matrices enforcing the (weak) continuity of the states

  $(G_1)_{i,j} = (\nu_j, \mu_i)_\gamma$; $(G_2)_{i,j} = (\eta_j, \mu_i)_\gamma$

Explicit partitioned scheme: IVR

IVR method: eliminate then discretize

Goal: Express $\boldsymbol{\lambda}$ as an implicit function of the states
Differentiate the state continuity equation to reduce to an Index-1 Hessenberg DAE:

$$\dot{y} = f(t, y, z)$$
$$0 = g(t, y, z)$$

with $y = (\boldsymbol{\Phi}_1, \boldsymbol{\Phi}_2)$ the differential variable, $z = \boldsymbol{\lambda}$ the algebraic variable

$$f(t, y, z) = \begin{pmatrix} M_1^{-1}\left(\bar{\mathbf{f}}_1(\boldsymbol{\Phi}_1) - G_1^T \boldsymbol{\lambda}\right) \\ M_2^{-1}\left((\bar{\mathbf{f}}_2(\boldsymbol{\Phi}_2) + G_2^T \boldsymbol{\lambda}\right) \end{pmatrix}$$

and

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

Decoupling and time discretization

$S = G_1 M_1^{-1} G_1^T + G_2 M_2^{-1} G_2^T$: Schur complement from the FEM-FEM system. Nonsingular under certain conditions for G_i.

The equation $g(t, y, z) = 0$ defines z as an implicit function of the differential variable.
This decouples the system into 2 ODEs:

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

Apply an explicit time integration scheme to solve them independently.

ROM Construction

Creating a ROM

Goal: Extend the IVR scheme to a ROM-FEM coupling. Want a reduced order basis matrix $\tilde{U}$ on Ω_1 such that $\mathbf{\Phi}_1 = \tilde{U}\boldsymbol{\varphi}_R + \boldsymbol{\beta}$.

1. Obtain m snapshots in time of the original FE solution on Ω_1
2. Create a matrix X whose columns are the m snapshots
3. Dirichlet BCs: define $\boldsymbol{\beta}_k$ as a vector whose free coefficients (nodes on the interior or γ) are zero and whose Dirichlet coefficients are the nodal values of the boundary data at time t_k. Form adjusted matrix, X_0, by subtracting $\boldsymbol{\beta}_k$ from the k^{th} column of X. (Effectively zeros out Dirichlet rows of X).
4. Compute the SVD of the adjusted matrix, $X_0 = U_0\Sigma_0V_0^T$.
5. Create $\tilde{U}_0$ by removing columns of U_0 corresponding to singular values less than a tolerance δ.

Extension of IVR to a ROM-FEM coupling

ROM-FEM system to DAE

Assume time-independent Dirichlet conditions for the following.

- Define $\tilde{M}_1 := \tilde{U}_0^T M_1 \tilde{U}_0$and $\tilde{G}_1^T := \tilde{U}_0^T G_1^T$
- Substitute $\tilde{U}_0 \boldsymbol{\varphi}_R + \boldsymbol{\beta}$ for $\mathbf{\Phi}_1$ and multiply the first equation by $\tilde{U}_0^T$

$$\tilde{M}_1 \dot{\boldsymbol{\varphi}}_R + \tilde{G}_1{}^T \boldsymbol{\lambda} = \tilde{U}_0^T \overline{\mathbf{f_1}}(\tilde{U}_0 \boldsymbol{\varphi}_R + \boldsymbol{\beta})$$

$$M_2 \dot{\mathbf{\Phi}}_2 - G_2^T \boldsymbol{\lambda} = \overline{\mathbf{f}}_2(\mathbf{\Phi}_2)$$

$$\tilde{G}_1 \dot{\boldsymbol{\varphi}}_R - G_2 \dot{\mathbf{\Phi}}_2 = 0$$

ROM-FEM system to DAE

Assume time-independent Dirichlet conditions for the following.

- Define $\tilde{M}_1 := \tilde{U}_0^T M_1 \tilde{U}_0$and $\tilde{G}_1^T := \tilde{U}_0^T G_1^T$
- Substitute $\tilde{U}_0 \boldsymbol{\varphi}_R + \boldsymbol{\beta}$ for $\boldsymbol{\Phi}_1$ and multiply the first equation by $\tilde{U}_0^T$

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

The ROM-FEM monolithic system is an index-1 DAE:

$$f(t, y, z) = \begin{pmatrix} \tilde{M}_1{}^{-1} \left(\tilde{U}_0^T \overline{\mathbf{f}}_1 (\tilde{U}_0 \boldsymbol{\varphi}_R + \boldsymbol{\beta}) - \tilde{G}_1{}^T \boldsymbol{\lambda} \right) \\ M_2^{-1} \left((\overline{\mathbf{f}}_2(\boldsymbol{\Phi}_2) + G_2^T \boldsymbol{\lambda} \right) \end{pmatrix}$$

and

$$g(t, y, z) = \tilde{S} \boldsymbol{\lambda} - \tilde{G}_1 \tilde{M}_1{}^{-1} \left(\tilde{U}_0^T \overline{\mathbf{f}}_1 (\tilde{U}_0 \boldsymbol{\varphi}_R + \boldsymbol{\beta}) \right) + G_2 M_2^{-1} \overline{\mathbf{f}}_2(\boldsymbol{\Phi}_2)$$

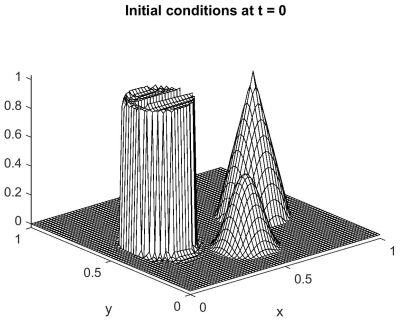
ROM-FEM and ROM-ROM extension

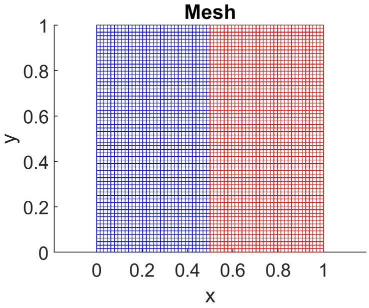
- Requires the Jacobian $\partial_z g = \tilde{S}$ to be nonsingular for all t. Analytically proven for FEM-FEM coupling under certain conditions for the Lagrange multiplier space, empirically observed for ROM-FEM.

- ROM-ROM coupling: transform both subdomain equations using $\mathbf{\Phi}_1 = \tilde{U}_{1,0}\boldsymbol{\phi}_R + \boldsymbol{\beta}_1$ for the first subdomain, and $\mathbf{\Phi_2} = \tilde{U}_{2,0}\boldsymbol{\psi}_R + \boldsymbol{\beta}_2$ for the second subdomain.

Numerical examples

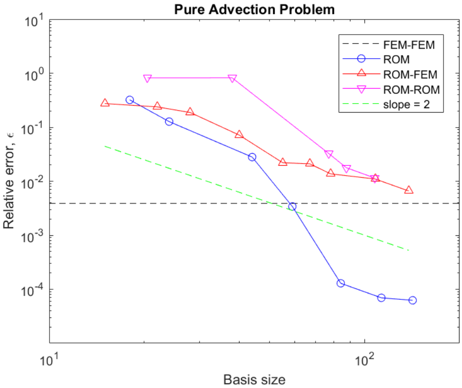
Numerical results

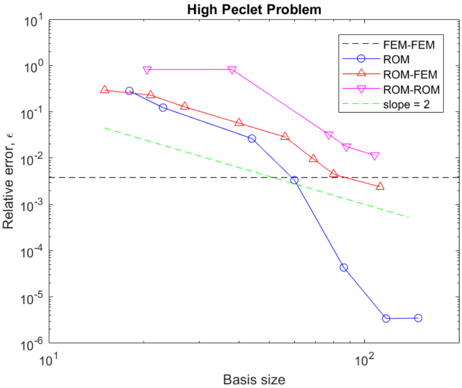




- RK4 used for time discretization; snapshots from monolithic FEM on Ω
- Rotating advection field $(0.5 - y, x - 0.5)$ for one full rotation
- 4225 DOFs in Ω, 2145 DOFs in each subdomain
- Two configurations: "pure advection": $\kappa_i = 0$, and "high Peclét": $\kappa_i = 10^{-5}$

Accuracy: relative error vs. basis size



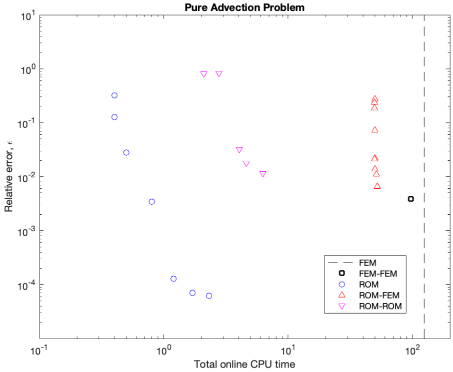


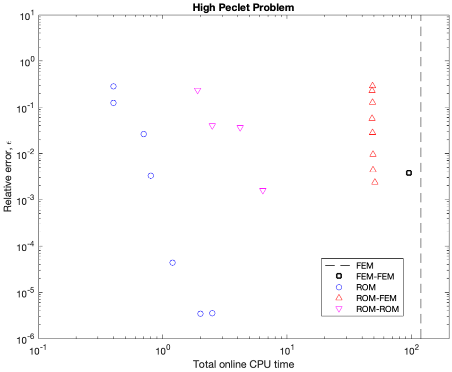
- Relative error defined as

$$\epsilon := \frac{||X_{2\pi} - F_{2\pi}||_2}{||F_{2\pi}||_2} \qquad \text{for } X \in \{R, FF, RF, RR\}.$$

- Reference solution is the global FEM solution at $t = 2\pi$

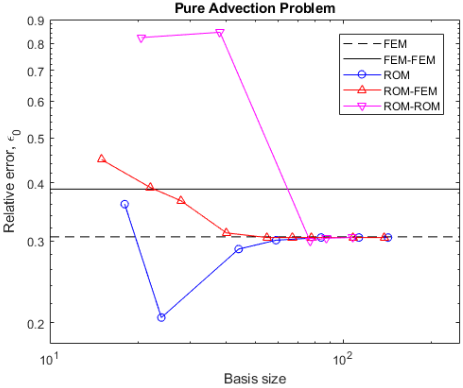
Efficiency: relative error vs. online CPU time





- Coupling does not introduce significant overhead for high fidelity models
- Introducing a ROM on one or both sides of the coupling can reduce CPU time by 1-1.5 orders of magnitude while maintaining accuracy

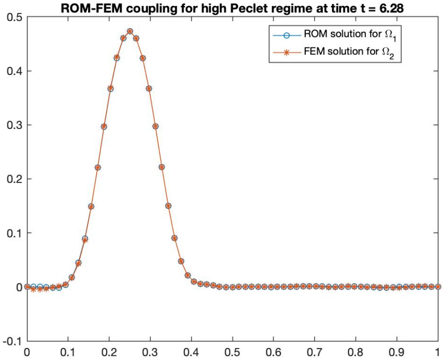
Relative errors vs. basis size for pure advection

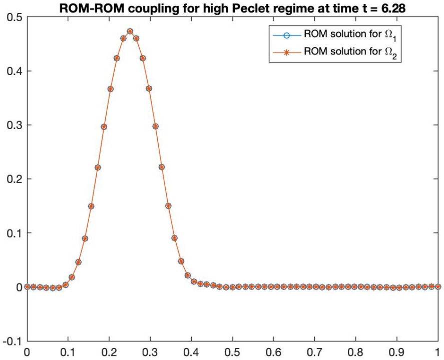


For the exact solution to the pure advection problem, ϵ_0 is identically 0.

$$\epsilon_0 := \frac{||X_0 - X_{2\pi}||_2}{||X_{2\pi}||_2} \qquad \text{for } X \in \{F, R, FF, RF, RR\}$$

High Peclét interface solutions at $t = 2\pi$

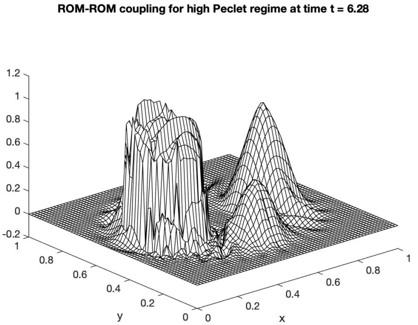




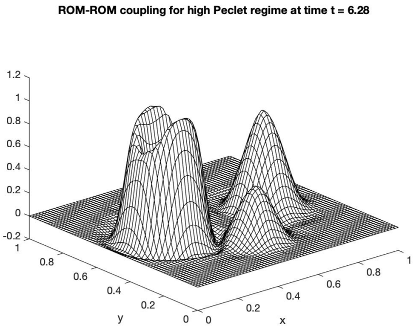
- ROM-FEM using $N_R = 80$
- ROM-ROM using $N_{R,left} = 112, N_{R,right} = 110$

Alternate formulation for ROM-ROM

- Form separate SVDs for the interface and interior DOFs, resulting in the ansatzes for $i = 1, 2$:
  - $\mathbf{\Phi}_{i,0} = \tilde{U}_{i,0}\boldsymbol{\phi}_{i,0} + \boldsymbol{\beta}_{i,0}$ and $\mathbf{\Phi}_{i,\gamma} = \tilde{U}_{i,\gamma}\boldsymbol{\phi}_{i,\gamma} + \boldsymbol{\beta}_{i,\gamma}$ (subscripts "0" and "γ" represent interior and interface DOFs, respectively)



50 modes in each subdomain



40 interior/10 interface modes in each subdomain

Conclusions

- Extended an explicit partitioned scheme to include ROM-FEM and ROM-ROM couplings
  - Lagrange multiplier (interface flux) expressed as implicit function of state solutions through Schur complement
  - Explicit time integration decouples the subdomains
- Both coupling results strongly agree with those produced by FEM-FEM coupling
- Implementing ROM in one or both subdomains reduces time/cost
- Continuing work: Extend to other discretizations or reduced models, reduced space for Lagrange multiplier, analysis for ROM-FEM and ROM-ROM cases