Adaptive modeling for coupling methods

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Outline

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2. Introduction to adaptive modeling
3. Example: Stokes/Navier-Stokes
4. Concurrent coupling method based on the Arlequin framework
5. Adaptive approach(es)
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Multiphysics Coupled Problems: Micro-fluidics

Structure of the Electric Double Layer (EDL) between the fluid and the wall.
Under the effect of an electric field tangent to the wall, charged particles are subjected to an electric force and thus move in the direction of the electric field.

Garg, Prudhomme, van der Zee, Carey, 2013 (Submitted).

Coupled model (simplified):

\[-\nabla \cdot (\sigma_c \nabla \phi) = 0 \quad \text{in} \ \Omega\]
\[-\mu \Delta u + \nabla p = 0 \quad \text{in} \ \Omega\]
\[\nabla \cdot u = 0 \quad \text{in} \ \Omega\]

Boundary conditions:

\[n \cdot (\sigma_c \nabla \phi) = 0 \quad \text{on} \ \Gamma_w\]
\[\phi = g \quad \text{on} \ \Gamma_{io}\]
\[u + \lambda \nabla \phi = 0 \quad \text{on} \ \Gamma_w\]
\[u \cdot t = 0 \quad \text{on} \ \Gamma_{io}\]
\[n \cdot (\sigma \cdot n) = 0 \quad \text{on} \ \Gamma_{io}\]
Micro-Fluidic Flows

\[ u + \lambda \nabla \phi = 0 \]

\[ \Rightarrow \]

\[ u \cdot t + \lambda \partial_t \phi = 0 \]
\[ u \cdot n + \lambda \partial_n \phi = 0 \]

\[ \Rightarrow \]

\[ u \cdot t + \lambda \partial_t \phi = 0 \]
\[ u \cdot n = 0 \]
Micro-Fluidic Flows

Strong form of adjoint problem:

\[-\nabla \cdot (\sigma_c \nabla \varphi^*) = 0 \quad \text{in } \Omega\]
\[-\Delta w^* + \nabla p^* = k\alpha \quad \text{in } \Omega\]
\[\nabla \cdot w^* = 0 \quad \text{in } \Omega\]

with three boundary conditions on \(\Gamma_{io}\):

\[\varphi^* = 0 \quad \text{on } \Gamma_{io}\]
\[w^* \cdot t = 0 \quad \text{on } \Gamma_{io}\]
\[n \cdot (\sigma^* \cdot n) = k \quad \text{on } \Gamma_{io}\]

and three BCs on \(\Gamma_w\):

\[n \cdot (\sigma_c \nabla \varphi^*) + \nabla \Gamma_w \cdot ((\lambda t \cdot (\sigma^* \cdot n))t) = 0 \quad \text{on } \Gamma_w\]
\[w^* = 0 \quad \text{on } \Gamma_w\]
Adjoint velocity $u^*$ (in $y$ direction). It is mainly different from zero inside the vertical channel indicating that the primal solution needs to be accurate in that region.

Adjoint potential $\phi^*$. Note that $\phi^*$ almost vanishes everywhere except at the corners and along the middle section of the top wall.
Micro-Fluidic Flows

Adaptive mesh obtained using adjoint-based error estimates. Note that the elements get refined almost exclusively near the corners due to the singularities in the primal velocity and adjoint potential.

Convergence plots for the relative error in QoI using uniform and adjoint based refinements.
Catenary (linearized) model:

\[-Tu'' = -\rho g, \quad \text{in } \Omega = (0, 1)\]
\[u = u_0, \quad \text{at } x = 0\]
\[u = u_1, \quad \text{at } x = 1\]

This is actually an approximation of the nonlinear catenary model:

\[-Tu'' = -\sqrt{1 + u'^2} \rho g, \quad \text{in } \Omega = (0, 1)\]
\[u = u_0, \quad \text{at } x = 0\]
\[u = u_1, \quad \text{at } x = 1\]

The linearized model may provide a poor approximation in the case of large deflections in the chain.
1. Base model

Find \( u \in U \) s.t.
\[
B(u; v) = F(v) \quad \forall v \in V
\]
- Is believed to capture the events of interest but is intractable.
- Is never "solved"; is only a datum for assessing other models.

2. Quantities of Interest

Given \( Q : U \rightarrow \mathbb{R} \), find \( Q(u) \)

3. Surrogate models

Find \( u_0 \in U_0 \) s.t.
\[
B_0(u_0; v) = F_0(v) \quad \forall v \in V_0
\]
- Must be tractable.
- Ideally captures coarser scales of the phenomena (may involve fine and coarse scale components).

4. Modeling Error

\[
\mathcal{E} = Q(u) - Q(\pi u_0)
\]
where \( \pi : U_0 \rightarrow U \)
Error Representation

\[ \mathcal{E} = Q'(\pi u_0; u - \pi u_0) + \Delta Q = B'(\pi u_0; u - \pi u_0, p) + \Delta Q \]
\[ = B(u; p) - B(\pi u_0; p) - \Delta B + \Delta Q \]
\[ = F(p) - B(\pi u_0; p) + \Delta Q - \Delta B \]
\[ \equiv R(\pi u_0; p) \]
\[ \equiv \Delta \]

where “adjoint” problem is defined as:

Find \( p \in V \) such that \( B'(\pi u_0; v, p) = Q'(\pi u_0; v), \quad \forall v \in V \)

and

\[ \Delta_B = \int_0^1 B''(\pi u_0 + se; e, e, p)(1 - s)ds \]
\[ \Delta_Q = \int_0^1 Q''(\pi u_0 + se; e, e)(1 - s)ds \]
Adaptive Modeling

Adjoint Problem:

\[ B'(u; v, p) = Q'(u; v), \quad \forall \ v \in U \]

\[
B'(u; v, p) = \lim_{\theta \to 0} \frac{B(u + \theta v; p) - B(u; p)}{\theta} \\
Q'(u; v) = \lim_{\theta \to 0} \frac{Q(u + \theta v) - Q(u)}{\theta}
\]

Theorem: If \( u \) is a solution of the base model and \( u_0 \) an arbitrary member of \( U \), then:

\[
Q(u) - Q(\pi u_0) = R(\pi u_0; p) + \Delta
\]

where \( \Delta \) is a remainder involving terms of \( O(\|u - u_0\|^r) \), \( r \geq 2 \) and

\[
R(\pi u_0; p) = F(p) - B(\pi u_0; p)
\]

\[
B'(\pi u_0; v, p) = Q'(\pi u_0; v), \quad \forall \ v \in U
\]

Example: Stokes & Navier-Stokes

Navier-Stokes

\[ u \cdot \nabla u - \nabla \cdot \sigma(u, p) = 0 \text{ in } \Omega^n \]
\[ \nabla \cdot u = 0 \text{ in } \Omega^n \]
\[ u = g \text{ on } \partial\Omega_D \cap \partial\Omega^n \]
\[ \sigma(u, p) \cdot n^n = h \text{ on } \partial\Omega_N \cap \partial\Omega^n \]

Stokes

\[ -\nabla \cdot \sigma(u, p) = 0 \text{ in } \Omega^s \]
\[ \nabla \cdot u = 0 \text{ in } \Omega^s \]
\[ u = g \text{ on } \partial\Omega_D \cap \partial\Omega^s \]
\[ \sigma(u, p) \cdot n^s = h \text{ on } \partial\Omega_N \cap \partial\Omega^s \]

Geometry

\[ \Omega^s \]
\[ \Omega^n \]
\[ \partial\Omega_D \]
\[ \partial\Omega_N \]
\[ \Sigma \]

Interface conditions

\[ \gamma^s u = \gamma^n u \text{ on } \Sigma \]
\[ \sigma \cdot n^s = -\sigma \cdot n^n \text{ on } \Sigma \]
Example: Stokes & Navier-Stokes

- \( Q \) = averaged vorticity in lower right corner of cavity.
- Adjoint equations:

\[
\begin{align*}
    u_0 \cdot \nabla z_u + z_u \cdot \nabla u_0 - \nabla \cdot \sigma(z_u, z_p) &= k(v, q) \quad \text{in} \; \Omega \\
    \nabla \cdot z_u &= 0 \quad \text{in} \; \Omega \\
    z_u &= 0 \quad \text{on} \; \partial \Omega_D \\
    \sigma(z_u, z_p) \cdot n &= 0 \quad \text{on} \; \partial \Omega_N
\end{align*}
\]

- Residual:

\[
R((u_0, p_0); (v, q)) = - \int_{\Omega} (u_0 \cdot \nabla)u_0 \cdot v \; dx
\]

- Error estimate: \( E_Q \approx -R((u_0, p_0); (z_u, z_p)) = - \int_{\Omega} (u_0 \cdot \nabla)u_0 \cdot z_u \; dx \)
Example: Stokes & Navier-Stokes

True solution at Re = 1000 (velocity magnitude and streamlines)
Example: Stokes & Navier-Stokes

Stokes solution \( (\varepsilon_Q = 1.73 \times 10^0) \)
Example: Stokes & Navier-Stokes

Coupled solution after iteration # 12 ($\mathcal{E}_Q = -7.24 \times 10^{-3}$)
Example: Stokes & Navier-Stokes

Dual solution (velocity magnitude)
Example: Stokes & Navier-Stokes

Relative error $\epsilon_Q$ in QoI vs. percent of elements “refined”
Nano-manufacturing Process

Continuum models are unable to simulate roughness.

A molecular approach is suited for simulating roughness.
1D Spring Model

- $N$ linear springs $(k_i, \ell_i)$, $i = 1, \ldots, N$ and $N + 1$ particles with positions $x_i$ and displacements $z_i$, $i = 0, \ldots, N$.

- Quadratic potential:

  $$W = \frac{1}{2} \sum_{i=1}^{N} k_i \left[ (x_i - x_{i-1}) - l_i \right]^2 = \frac{1}{2} \sum_{i=1}^{N} k_i (w_i - w_{i-1})^2$$

- Assume periodic distribution with springs $(k_1, \ell)$ and $(k_2, \ell)$. 
1D Continuum Model

1D linear elasticity model

Let $\Omega = (0, L)$ with $L = \sum_{i=1}^{N} \ell_i$.

$$-(Eu')' = 0, \quad \text{in } \Omega, \quad u(0) = 0, \quad Eu'(L) = T$$

Homogenization based on “Representative Volume Element”:

$$E = \frac{k_1 k_2}{k_1 + k_2} \frac{(l_1 + l_2)}{A}$$

(We take $A = 1$ here)
Coupling Strategy

Concurrent multiscale simulation
Large and small scales models are solved simultaneously
Coupling Method by the Arlequin Framework

- Partition of energies.
- Weight coefficients may be chosen constant, linear, cubic in overlap region.
- Coupling through Lagrange multipliers.
- Resulting mixed problem is well-posed.

Coupling of Molecular and Continuum Models

Find \((u, w) \in V_c \times V_d\) such that:

\[
(u, w) = \operatorname{argmin}_{(v, z) \in V_c \times V_d} \left[ E_c(v) + E_d(z) \right]
\]

\(v = \Pi z\) in \(\Omega_o\)

where:

\[
\Pi : V_d \longrightarrow H^1(\Omega_o) \quad \text{(interpolation)}
\]

\[
E_c(v) = \frac{1}{2} \int_{\Omega_c} \alpha_c \, v'^2 \, dx
\]

\[
E_d(z) = \frac{1}{2} \sum_{i=1}^{M} \alpha_d k_i (z_i - z_{i-1})^2 - f z_M
\]

\(\Omega_c\) (continuum model)
\(\Omega_d\) (molecular model)
\(\Omega_o = \Omega_c \cap \Omega_d\) (Overlap)

\(V_c = \{ v \in H^1(\Omega_c); \, v(0) = 0 \}\)

\(V_d = \mathbb{R}^M\) \(\, (M \ll N)\)

Partition of unity:

\[
\alpha_c + \alpha_d = 1
\]

\[
\alpha_c \leq 1
\]

\[
\alpha_d \leq 1
\]
Mesh Dependent Coupling

Coupling term:

\[ C(\mu, (u, w)) = \int_{\Omega_o} \beta_0 \mu(u - \Pi w) + \beta_1 \mu'(u - \Pi w)' \, dx, \quad \mu \in M = H^1(\Omega_o) \]

\[ \min_{(v, z) \in V_c \times V_d} \max_{\lambda \in M} \left[ E_c(v) + E_d(z) + C(\lambda, (v, z)) \right] \]

Find \((u, w) \in V_c \times V_d, \lambda \in M\) such that:

\[ a((u, w), (v, z)) + C(\lambda, (v, z)) = f z_M \quad \forall (v, z) \in V_c \times V_d \]

\[ C(\mu, (u, w)) = 0 \quad \forall \mu \in M \]

\[ a((u, w), (v, z)) = \int_{\Omega_o} \alpha_c Eu'v' \, dx + \sum_{i=1}^{M} \alpha_d k_i (w_i - w_{i-1}) (z_i - z_{i-1}) \]

**Theorem:** Let \(\beta_1 > 0\). Then, the above problem is well-posed.
Discretization of Arlequin method: Examples

LM meshsize = $h$ (cont. model)
$H^1$ norm coupling
$\alpha$ linear

LM meshsize = $\epsilon$ (RVE)
$H^1$ norm coupling
$\alpha$ linear

LM meshsize = $l$ (part. model)
$H^1$ norm coupling
$\alpha$ constant

LM meshsize = $h$ (cont. model)
$H^1$ norm coupling
$\alpha$ linear
Mesh-independent coupling

\[ C(\mu, (u, w)) = \beta_0 \overline{\mu} (u - \Pi w) + \beta_1 \int_{\Omega_o} \mu^* (u - \Pi w)^* dx \]

Prudhomme, Bouclier, Chamoin, Ben Dhia, and Oden, *LNCSE* (2011)
Mesh Independent Coupling

\[
b(\mu, (u, w)) = \beta_0 \bar{\mu}(v - \Pi z) + \beta_1 \int_{\Omega_o} \mu^*(v - \Pi z)^* dx
\]

\[
\bar{v} = \frac{1}{|\Omega_o|} \int_{\Omega_o} v dx
\]

\[
v^*(x) = \begin{cases} 
\frac{1}{\varepsilon} \int_{x_a}^{x_a + \varepsilon} v' dy = \frac{1}{\varepsilon} [v(x_a + \varepsilon) - v(x_a)] & \forall x \in [x_a, x_a + \varepsilon/2] \\
\frac{1}{\varepsilon} \int_{x_a}^{x_a + \varepsilon/2} v' dy = \frac{1}{\varepsilon} [v(x + \varepsilon/2) - v(x - \varepsilon/2)] & \forall x \in (x_a + \varepsilon/2, x_b - \varepsilon/2) \\
\frac{1}{\varepsilon} \int_{x_b - \varepsilon}^{x_b} v' dy = \frac{1}{\varepsilon} [v(x_b) - v(x_b - \varepsilon)] & \forall x \in [x_b - \varepsilon/2, x_b]
\end{cases}
\]

Note: \( \varepsilon \) is the size of the Representative Volume Element.
Numerical Examples - 1D

Coupling Method

[Graphs showing Arlequin Solution and Lagrange Multiplier]
Numerical Examples - 2D

Initial configuration of the Arlequin structure

Deformed configuration of the Arlequin structure
Molecular-to-Continuum Coupling Method

**Base model**

Find \( u \in \mathbb{R}^{3N} \) such that \( B(u, v) = F(v) \), \( \forall v \in \mathbb{R}^{3N} \) where

\[
B(u; v) = \sum_{i=1}^{N} \sum_{k=1}^{N_i} \frac{\partial E_{ik}}{\partial u_i} \cdot v_i \\
F(v) = \sum_{i=1}^{N} f_i \cdot v_i
\]

**Surrogate model**

Find \( u_0 \in U_0 \) such that \( B_0(u_0, v_0) = F_0(v_0) \), \( \forall v \in U_0 \) where

\[
B_0(u_0; v_0) = a((u, w), (v, z)) + C(\lambda, (v, z)) + C(\mu, (u, w)) \\
F_0(v_0) = \sum_{i=1}^{M} f_i \cdot v_i
\]

with \( u_0 = (u, w, \lambda) \) and \( v_0 = (v, z, \mu) \)
Model Adaptation

Unknown parameters of Arlequin formulation:
1) Size of $\Omega_0$: is related to RVE size.
2) Size of $\Omega_m$: depends on QoI.

Two approaches for adaptation:
1) Error estimation of QoI.
2) Optimization approach based on parametrization of $\Omega_m$. 
Optimal Approach

Parameterization of the particle region

Ben Dhia, Chamoin, Oden, Prudhomme, *CMAME* (2011)
Optimal Approach

Arlequin Problem:

Find \((u_m, w_m, \lambda_m) \in \mathcal{U} \times \mathcal{W} \times \mathcal{X}\) such that:

\[
B_{0,m}(u_m, w_m, \lambda_m; (v, w, \mu)) = F_0(w, v, \mu),
\]

\[
\forall (w, v, \mu) \in \mathcal{U} \times \mathcal{W} \times \mathcal{X}
\]

Compact form:

Find \(U_m \in \mathcal{V}\) such that:

\[
B_{0,m}(U_m; V) = F_0(V), \quad \forall V \in \mathcal{V}
\]

Optimal control problem:

Find the set of parameters \(m^*\) such that:

\[
m^* = \arg\min_m \left[ \frac{1}{2} \left( \lambda_{tol} - [Q(y) - Q(y_{0,m})] \right)^2 \right] = \arg\min_m J(U_m)
\]
Optimal Approach

Lagrangian:

\[ \mathcal{L}(U, P, m) = J(U) - [B_{0,m}(U; P) - F_0(P)] \]

Saddle point \((U, P, m)\):

\[
\begin{align*}
\frac{\partial \mathcal{L}}{\partial P} &= 0 \\
\frac{\partial \mathcal{L}}{\partial U} &= 0 \\
\frac{\partial \mathcal{L}}{\partial m} &= 0
\end{align*}
\]

\[
\begin{align*}
B_{0,m}(U; V) &= F_0(V), \quad \forall V \in \mathcal{V} \\
B_{0,m}(V; P) &= \nabla_U J(U) \cdot V, \quad \forall V \in \mathcal{V} \\
\nabla_m B_{0,m}(U; P) \cdot q &= 0, \quad \forall q \in \mathcal{Q}
\end{align*}
\]
Optimal Approach
Numerical Example

A two-dimensional example: L-shaped structure
Numerical Example

Classical Approach

Optimal Approach
Concluding Remarks

- Model adaptivity.
- Application to the coupling of Stokes and Navier-Stokes equations.
- Concurrent coupling method based on Arlequin framework.
- Development of an adaptive schemes based on a posteriori error estimates of the modeling error with respect to quantities of interest and on an optimal approach.
- Modeling of heterogeneous molecular models such as polymeric networks.