Adaptive modeling for coupling methods

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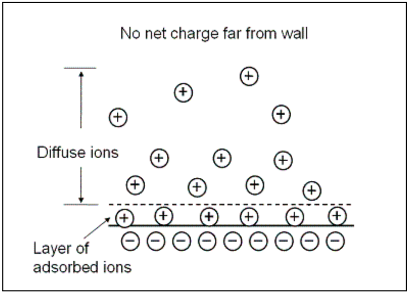
Outline

1. Multiphysics coupled problems: Micro-fluidics
2. Introduction to adaptive modeling
3. Example: Stokes/Navier-Stokes
4. Concurrent coupling method based on the Arlequin framework
5. Adaptive approach(es)
6. Concluding Remarks

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).

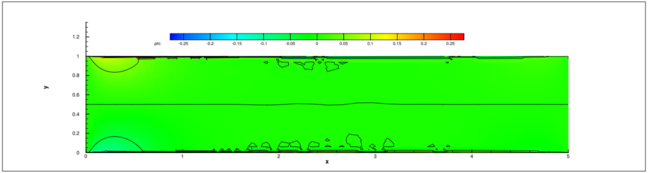
Coupled model (simplified):

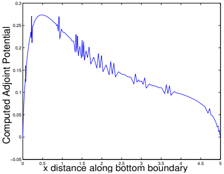
$$\boxed{\begin{aligned} -\nabla \cdot (\sigma_c \nabla \phi) = 0 &\quad \text{in } \Omega \\ -\mu \Delta u + \nabla p = 0 &\quad \text{in } \Omega \\ \nabla \cdot u = 0 &\quad \text{in } \Omega \end{aligned}}$$

Boundary conditions:

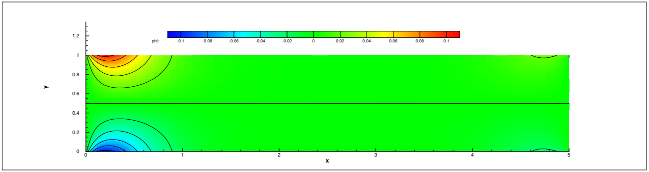
$$\boxed{\begin{aligned} n \cdot (\sigma_c \nabla \phi) = 0 &\quad \text{on } \Gamma_w \\ \phi = g &\quad \text{on } \Gamma_{io} \\ u + \lambda \nabla \phi = 0 &\quad \text{on } \Gamma_w \\ u \cdot t = 0 &\quad \text{on } \Gamma_{io} \\ n \cdot (\boldsymbol{\sigma} \cdot n) = 0 &\quad \text{on } \Gamma_{io} \end{aligned}}$$

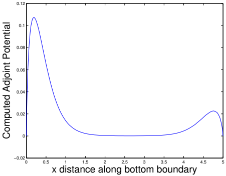
Micro-Fluidic Flows





$$\boxed{u + \lambda \nabla \phi = 0} \quad \Rightarrow \quad \boxed{\begin{aligned} u \cdot t + \lambda \partial_t \phi &= 0 \\ u \cdot n + \lambda \partial_n \phi &= 0 \end{aligned}} \quad \Rightarrow \quad \boxed{\begin{aligned} u \cdot t + \lambda \partial_t \phi &= 0 \\ u \cdot n &= 0 \end{aligned}}$$





Micro-Fluidic Flows

Strong form of adjoint problem:

$$\boxed{\begin{aligned} -\nabla\cdot(\sigma_c\nabla\varphi^*) &= 0 && \text{in } \Omega \\ -\Delta w^* + \nabla p^* &= k\boldsymbol{\alpha} && \text{in } \Omega \\ \nabla\cdot w^* &= 0 && \text{in } \Omega \end{aligned}}$$

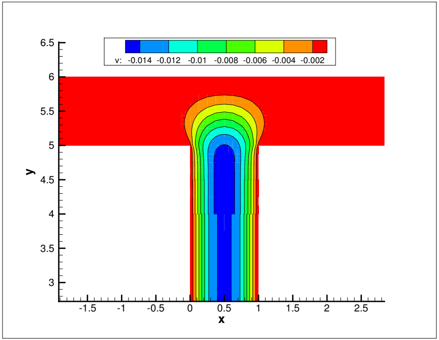
with three boundary conditions on Γ_{io}:

$$\begin{aligned} \varphi^* &= 0 && \text{on } \Gamma_{io} \\ w^*\cdot t &= 0 && \text{on } \Gamma_{io} \\ n\cdot(\boldsymbol{\sigma}^*\cdot n) &= k && \text{on } \Gamma_{io} \end{aligned}$$

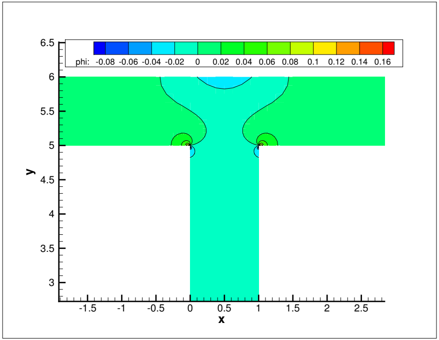
and three BCs on Γ_w:

$$\begin{aligned} n\cdot(\sigma_c\nabla\varphi^*) + \nabla_{\Gamma_w}\cdot\Big(\big(\lambda t\cdot(\boldsymbol{\sigma}^*\cdot n)\big)t\Big) &= 0 && \text{on } \Gamma_w \\ w^* &= 0 && \text{on } \Gamma_w \end{aligned}$$

Micro-Fluidic Flows

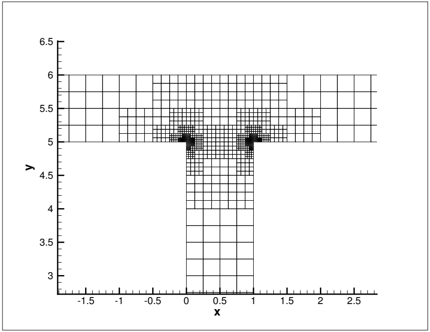


Adjoint velocity u^* (in y direction). It is mainly different from zero inside the vertical channel indicating that the primal solution needs to be accurate in that region.

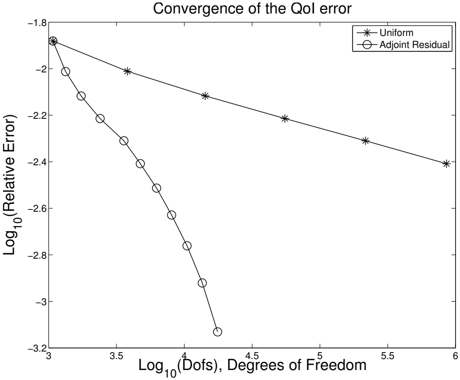


Adjoint potential ϕ^*. Note that ϕ^* almost vanishes everywhere except at the corners and along the middle section of the top wall.

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.

Introduction

Catenary (linearized) model:

$$\boxed{\begin{aligned} -Tu'' &= -\rho g, \quad \text{in } \Omega = (0,1) \\ u &= u_0, \quad \text{at } x = 0 \\ u &= u_1, \quad \text{at } x = 1 \end{aligned}}$$

This is actually an approximation of the nonlinear catenary model:

$$\boxed{\begin{aligned} -Tu'' &= -\sqrt{1+u'^2}\rho g, \quad \text{in } \Omega = (0,1) \\ u &= u_0, \quad \text{at } x = 0 \\ u &= u_1, \quad \text{at } x = 1 \end{aligned}}$$

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

Base Model and Surrogate Model

1. Base model*

Find $u \in U$ s.t.

$$B(u;v) = F(v)\ \forall v \in V$$

- 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 $Q : U \longrightarrow \mathbb{R}$,

find $Q(u)$

3. Surrogate models

Find $u_0 \in U_0$ s.t.

$$B_0(u_0;v) = F_0(v)\ \forall v \in V_0$$

- 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 $\pi : U_0 \longrightarrow U$

Error Representation

$$\boxed{\begin{aligned}\mathcal{E} = Q'(\pi u_0; u - \pi u_0) + \Delta_Q &= B'(\pi u_0; u - \pi u_0, p) + \Delta_Q \\ &= B(u;p) - B(\pi u_0; p) - \Delta_B + \Delta_Q \\ &= \underbrace{F(p) - B(\pi u_0; p)}_{\equiv \mathcal{R}(\pi u_0; p)} + \underbrace{\Delta_Q - \Delta_B}_{\equiv \Delta}\end{aligned}}$$

where “adjoint” problem is defined as:

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

and

$$\Delta_B = \int_0^1 B''(\pi u_0 + se; e, e, p)(1-s)ds$$

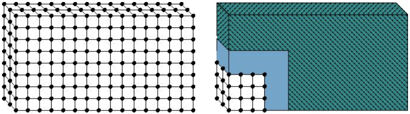
$$\Delta_Q = \int_0^1 Q''(\pi u_0 + se; e, e)(1-s)ds$$

Adaptive Modeling

Adjoint Problem:

$$\boxed{B'(u;v,p) = Q'(u;v), \ \forall\, v \in U}$$

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



Base (u) and surrogate models (u_0)

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

$$\boxed{Q(u) - Q(\pi u_0) = \mathcal{R}(\pi u_0;p) + \Delta}$$

where Δ is a remainder involving terms of $\mathcal{O}(\|u-u_0\|^r), \ r \geq 2$ and

$$\boxed{\mathcal{R}(\pi u_0;p) = F(p) - B(\pi u_0;p)}$$

$$\boxed{B'(\pi u_0;v,p) = Q'(\pi u_0;v), \ \forall\, v \in U}$$

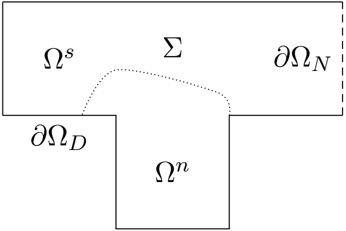
Oden, Prudhomme, *J. Comp. Phys.* (2002).
Oden, Prudhomme, Romkes, and Bauman, *SIAM J. Sci. Comput.* (2006).

Example: Stokes & Navier-Stokes

Navier-Stokes

$$\boxed{\begin{aligned} u\cdot\nabla u - \nabla\cdot\sigma(u,p) &= 0 \ \text{ in } \ \Omega^n \\ \nabla\cdot u &= 0 \ \text{ in } \ \Omega^n \\ u &= g \ \text{ on } \ \partial\Omega_D \cap \partial\Omega^n \\ \sigma(u,p)\cdot n^n &= h \ \text{ on } \ \partial\Omega_N \cap \partial\Omega^n \end{aligned}}$$

Geometry



Stokes

$$\boxed{\begin{aligned} -\nabla\cdot\sigma(u,p) &= 0 \ \text{ in } \ \Omega^s \\ \nabla\cdot u &= 0 \ \text{ in } \ \Omega^s \\ u &= g \ \text{ on } \ \partial\Omega_D \cap \partial\Omega^s \\ \sigma(u,p)\cdot n^s &= h \ \text{ on } \ \partial\Omega_N \cap \partial\Omega^s \end{aligned}}$$

Interface conditions

$$\boxed{\begin{aligned} \gamma^s u &= \gamma^n u \ \text{ on } \ \Sigma \\ \sigma\cdot n^s &= -\sigma\cdot n^n \ \text{ on } \ \Sigma \end{aligned}}$$

Example: Stokes & Navier-Stokes

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

$$\boxed{\begin{aligned} u_0 \cdot \nabla z_u + z_u \cdot \nabla u_0 - \nabla \cdot \sigma(z_u, z_p) = k(v,q) \ \ \text{in} \ \ \Omega \\ \nabla \cdot z_u = 0 \ \ \text{in} \ \ \Omega \\ z_u = 0 \ \ \text{on} \ \ \partial\Omega_D \\ \sigma(z_u, z_p) \cdot n = 0 \ \ \text{on} \ \ \partial\Omega_N \end{aligned}}$$

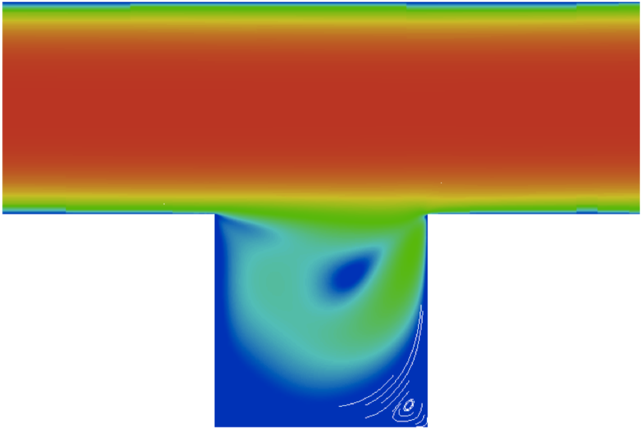
- Residual:

$$\boxed{\mathcal{R}((u_0, p_0); (v,q)) = -\int_\Omega (u_0 \cdot \nabla) u_0 \cdot v \, dx}$$

- Error estimate: $\mathcal{E}_Q \approx -\mathcal{R}((u_0, p_0); (z_u, z_p)) = -\int_\Omega (u_0 \cdot \nabla) u_0 \cdot z_u \, dx$

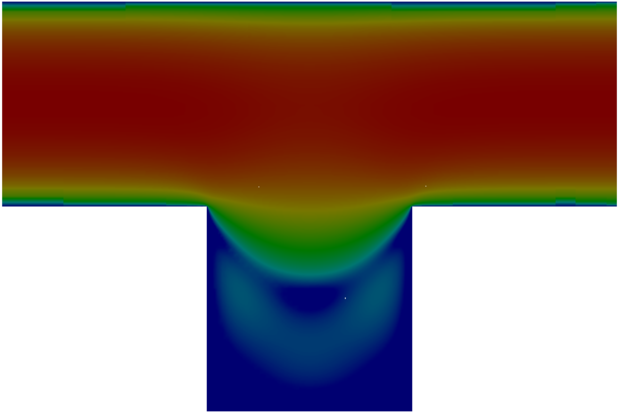
Example: Stokes & Navier-Stokes

True solution at Re = 1000 (velocity magnitude and streamlines)



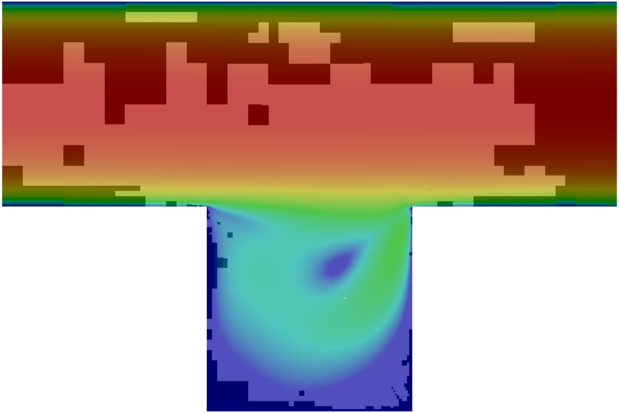
Example: Stokes & Navier-Stokes

Stokes solution ($\mathcal{E}_Q$ = 1.73 $\times$ 10^0)



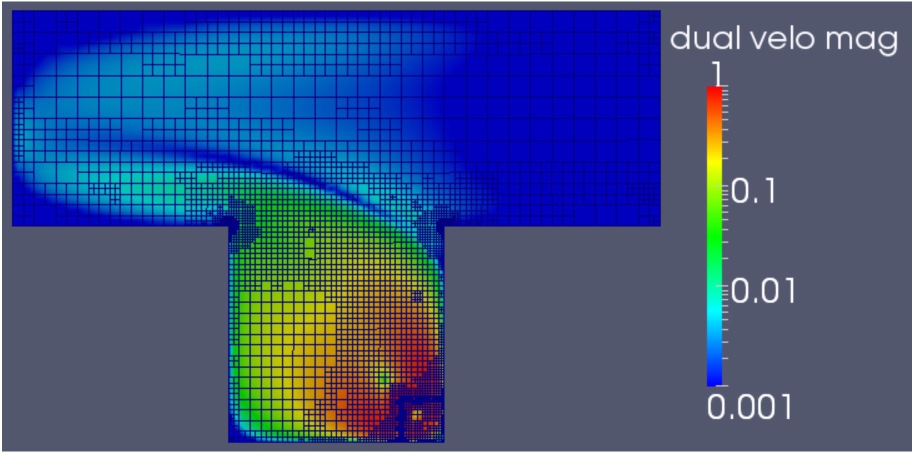
Example: Stokes & Navier-Stokes

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



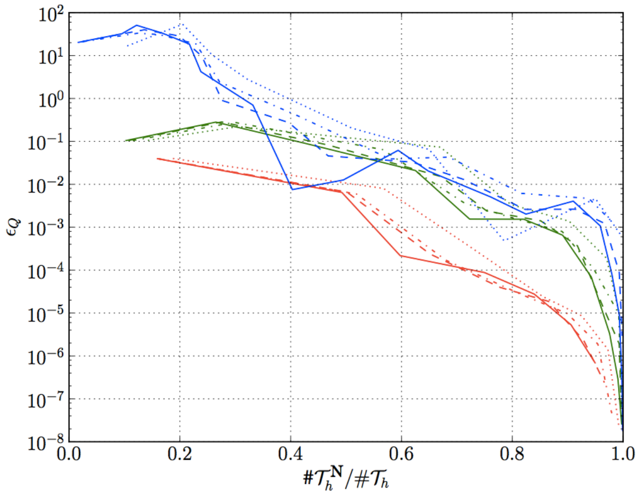
Example: Stokes & Navier-Stokes

Dual solution (velocity magnitude)



Example: Stokes & Navier-Stokes

Relative error ϵ_Q in QoI vs. percent of elements “refined”

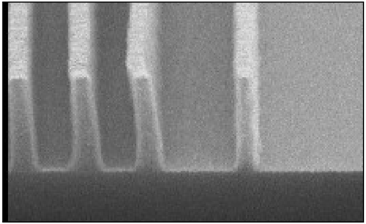


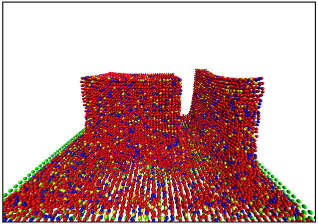
Re =10

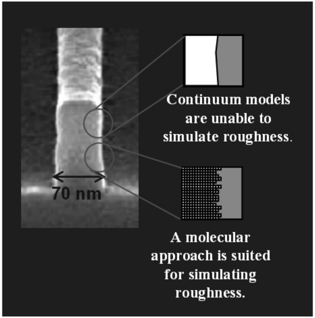
Re =100

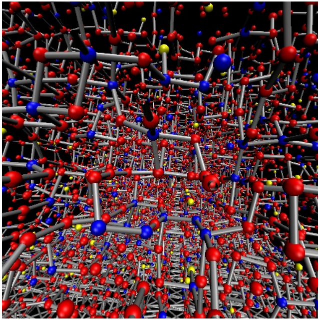
Re =1000

Nano-manufacturing Process

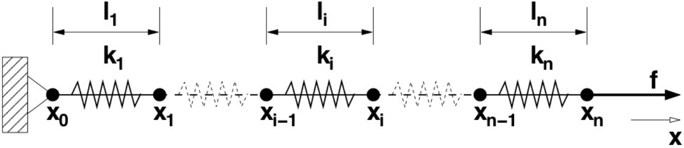








1D Spring Model



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

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

- Assume periodic distribution with springs (k_1, ℓ) and (k_2, ℓ).

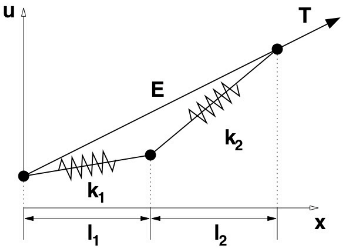
1D Continuum Model

1D linear elasticity model

Let $\Omega = (0, L)$ with $L = \sum_N \ell_i$.

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

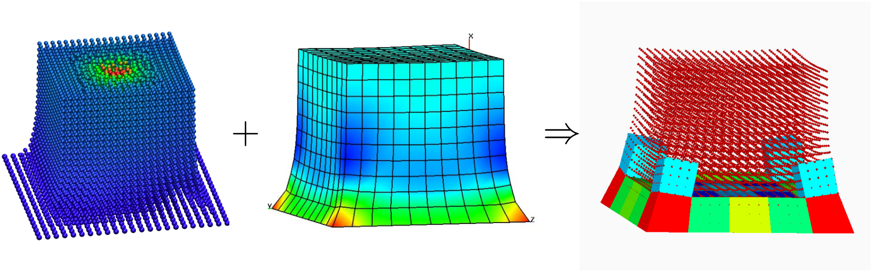
Homogenization based on “Representative Volume Element”:



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

(We take $A = 1$ here)

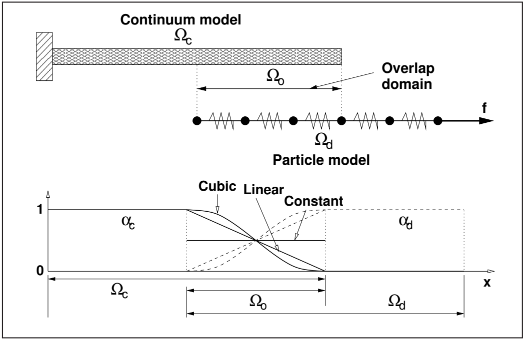
Coupling Strategy



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.

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*Ben Dhia, *Comptes Rendus de l'Académie des Sciences* (1998)
Xiao and Belytschko, *IJNME* (2004)
Bauman, Ben Dhia, Elkhodja, Oden, and Prudhomme, *Comput. Mechanics* (2008)

Coupling of Molecular and Continuum Models

Ω_c (continuum model)

Ω_d (molecular model)

$\Omega_o = \Omega_c \cap \Omega_d$ (Overlap)

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

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

Partition of unity:

$$\alpha_c + \alpha_d = 1$$

$$\alpha_c \leq 1$$

$$\alpha_d \leq 1$$

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

$$\boxed{(u, w) = \underset{\substack{(v,z) \in V_c \times V_d \\ v = \Pi z \text{ in } \Omega_o}}{\operatorname{argmin}} \Big[E_c(v) + E_d(z) \Big]}$$

where:

$$\begin{cases} \Pi : V_d \longrightarrow H^1(\Omega_o) \quad \text{(interpolation)} \\ E_c(v) = \dfrac{1}{2} \displaystyle\int_{\Omega_c} \alpha_c E v'^2 dx \\ E_d(z) = \dfrac{1}{2} \displaystyle\sum_{i=1}^{M} \alpha_d k_i (z_i - z_{i-1})^2 - f z_M \end{cases}$$

Mesh Dependent Coupling

Coupling term:

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

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

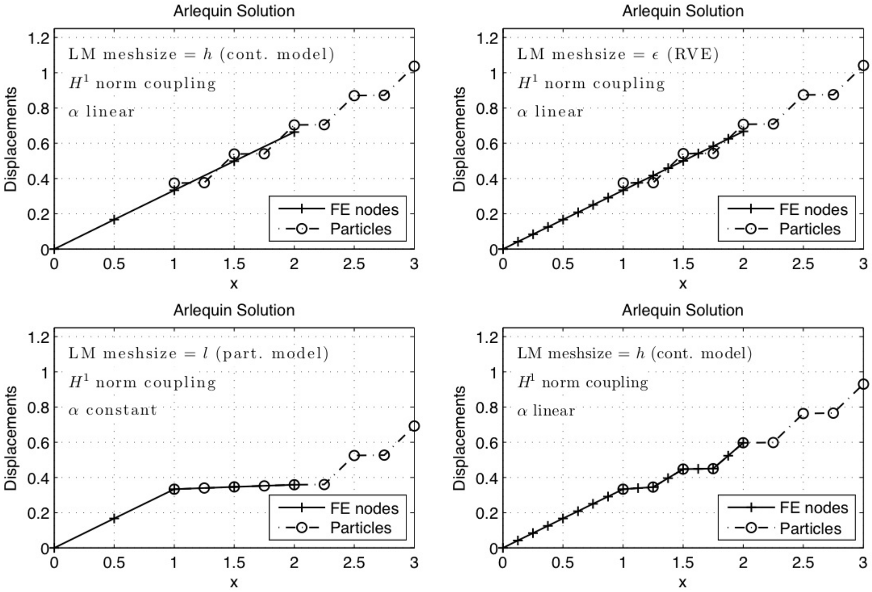
Find $(u,w) \in V_c \times V_d$, $\lambda \in M$ such that:

$$\begin{aligned} a((u,w),(v,z)) + C(\lambda,(v,z)) &= f z_M && \forall (v,z) \in V_c \times V_d \\ C(\mu,(u,w)) &= 0 && \forall \mu \in M \end{aligned}$$

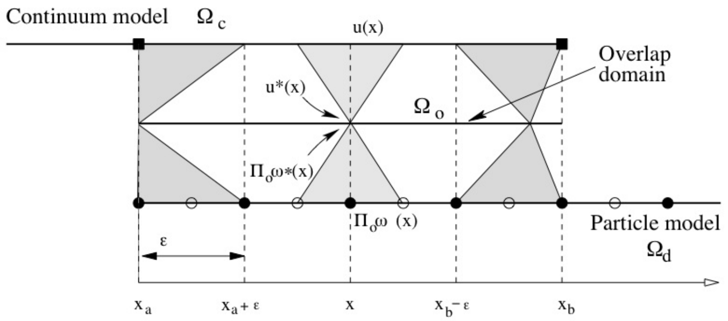
$$a\left((u,w),(v,z)\right) = \int_{\Omega_c} \alpha_c E u' v' dx + \sum_{i=1}^{M} \alpha_d k_i (w_i - w_{i-1})(z_i - z_{i-1})$$

Theorem: Let $\beta_1 > 0$. Then, the above problem is well-posed.

Discretization of Arlequin method: Examples



Mesh-independent coupling



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

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

Mesh Independent Coupling

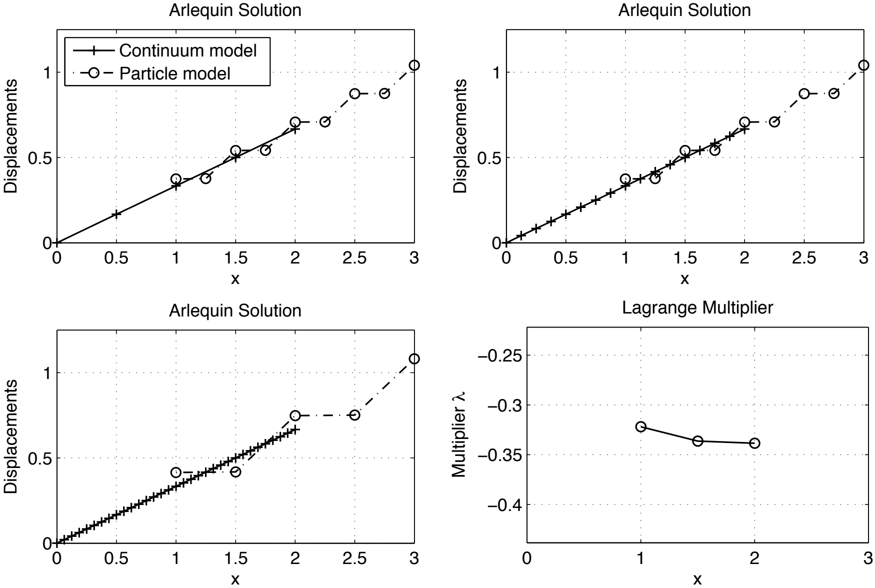
$$\boxed{b(\mu,(u,w)) = \beta_0 \overline{\mu}\,\overline{(v-\Pi z)} + \beta_1 \int_{\Omega_o} \mu^*(v-\Pi z)^* dx}$$

$$\overline{v} = \frac{1}{|\Omega_o|}\int_{\Omega_o} v dx$$

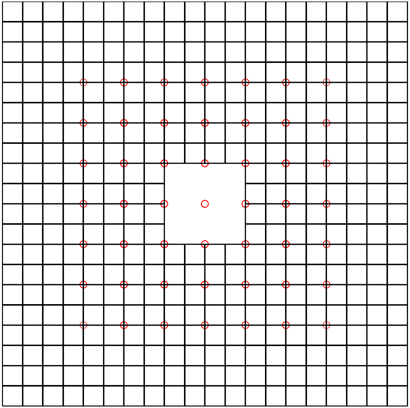
$$v^*(x) = \begin{cases} \dfrac{1}{\varepsilon}\displaystyle\int_{x_a}^{x_a+\varepsilon} v' dy = \dfrac{1}{\varepsilon}[v(x_a+\varepsilon) - v(x_a)] & \forall x \in [x_a, x_a+\varepsilon/2] \\ \dfrac{1}{\varepsilon}\displaystyle\int_{x-\varepsilon/2}^{x+\varepsilon/2} v' dy = \dfrac{1}{\varepsilon}[v(x+\varepsilon/2)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

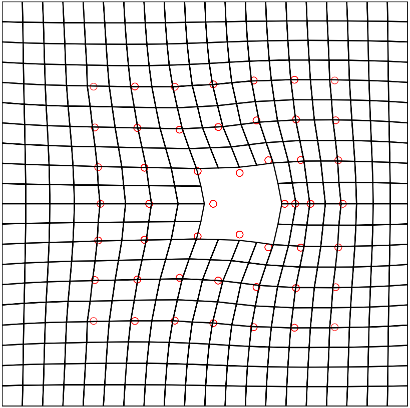
Note: ε is the size of the Representative Volume Element.

Numerical Examples - 1D



Numerical Examples - 2D





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

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

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

$$B_0(u_0; v_0) = a((u,w),(v,z)) + C(\lambda,(v,z)) + C(\mu,(u,w))$$

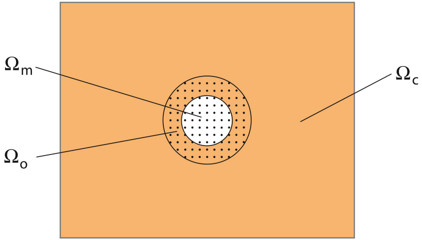
$$F_0(v_0) = \sum_{i=1}^{M} f_i \cdot v_i$$

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

Model Adaptation

Unknown parameters of Arlequin formulation:

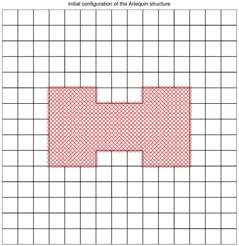
1) Size of Ω_0: is related to RVE size.
2) Size of Ω_m: depends on QoI.

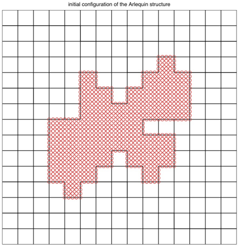


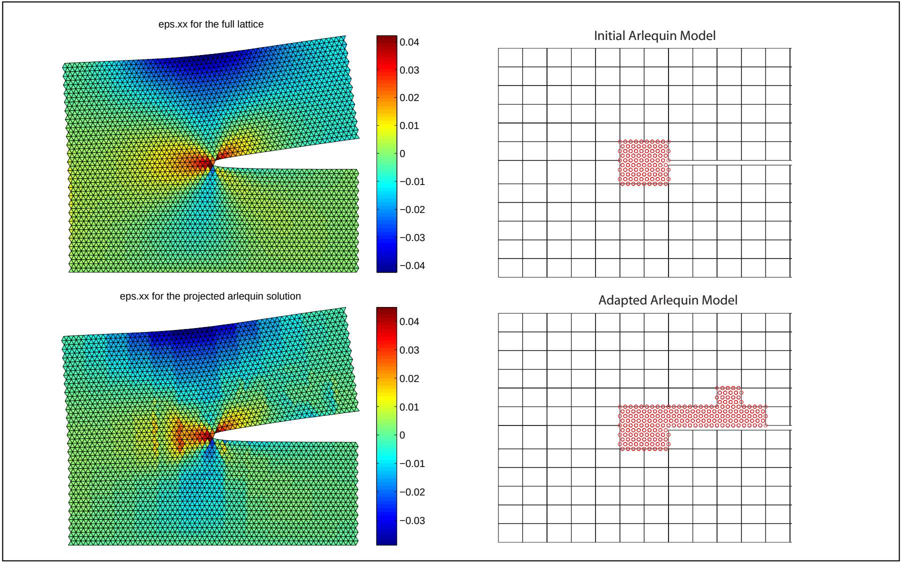
Two approaches for adaptation:

1) Error estimation of QoI.
2) Optimization approach based on parametrization of Ω_m.

Deterministic case



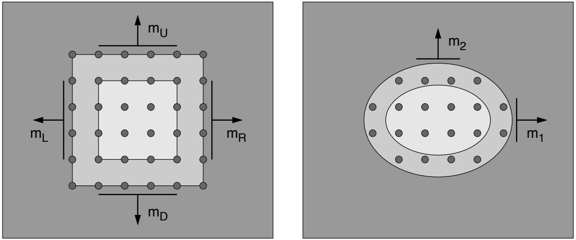




Prudhomme, Chamoin, Ben Dhia, and Bauman, “An adaptive strategy for the control of modeling error in two-dimensional atomic-to-continuum coupling simulations”, CMAME (2009).

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:

$$B_{0,m}((u_m, w_m, \lambda_m); (v, w, \mu)) = F_0(w, v, \mu), \qquad \forall (w, v, \mu) \in \mathcal{U} \times \mathcal{W} \times \mathcal{X}$$

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:

$$m^* = \underset{m}{\operatorname{argmin}} \left[\frac{1}{2} \Big(\lambda_{\text{tol}} - [Q(y) - Q(y_{0,m})] \Big)^2 \right] = \underset{m}{\operatorname{argmin}}\, J(U_m)$$

Optimal Approach

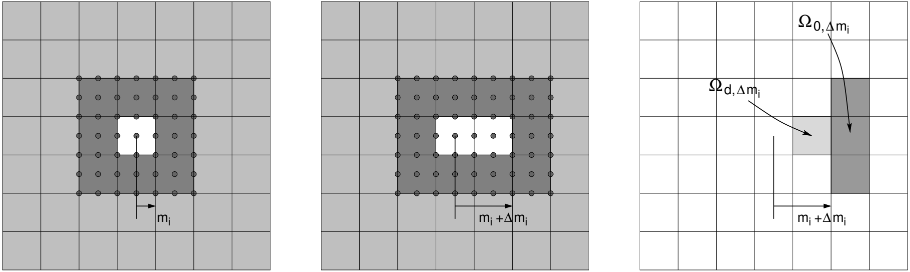
Lagrangian:

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

Saddle point (U,P,m):

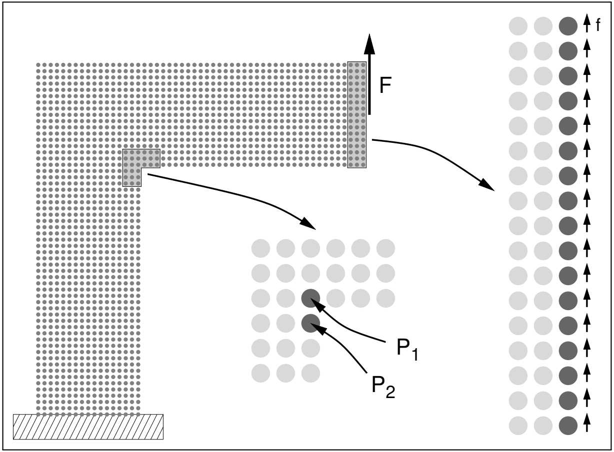
$$\left\{\begin{array}{l} \dfrac{\partial \mathcal{L}}{\partial P} = 0 \\[2ex] \dfrac{\partial \mathcal{L}}{\partial U} = 0 \\[2ex] \dfrac{\partial \mathcal{L}}{\partial m} = 0 \end{array}\right. \implies \left\{\begin{array}{ll} B_{0,m}(U;V) = F_0(V), & \forall V \in \mathcal{V} \\[2ex] B_{0,m}(V;P) = \nabla_U J(U) \cdot V, & \forall V \in \mathcal{V} \\[2ex] \nabla_m B_{0,m}(U;P) \cdot q = 0, & \forall q \in \mathcal{Q} \end{array}\right.$$

Optimal Approach

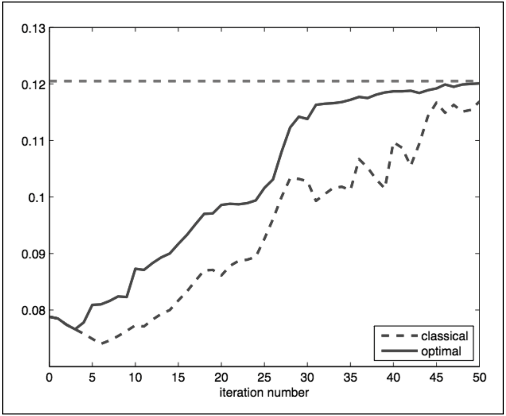


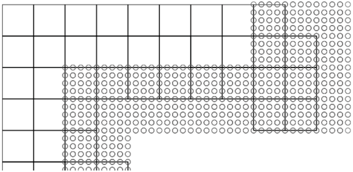
Numerical Example

A two-dimensional example: L-shaped structure

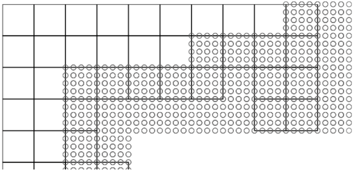


Numerical Example





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.