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Optimization-Based Modeling

A new strategy for predictive simulations of multiscale, multiphysics problems

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Outline

- **What is an optimization-based modeling (OBM)?**
- **A generic multiphysics OBM framework**
- **Application to Atomistic-to-Continuum (AtC) coupling**
  - Optimization-based formulation of AtC (OB-AtC)
  - Analysis of OB-AtC
  - Preliminary results

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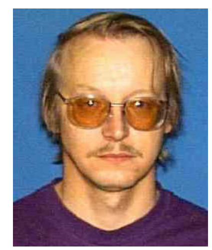

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A Metaphor

Suppose you want to solve these problems:

P1 = Airplane

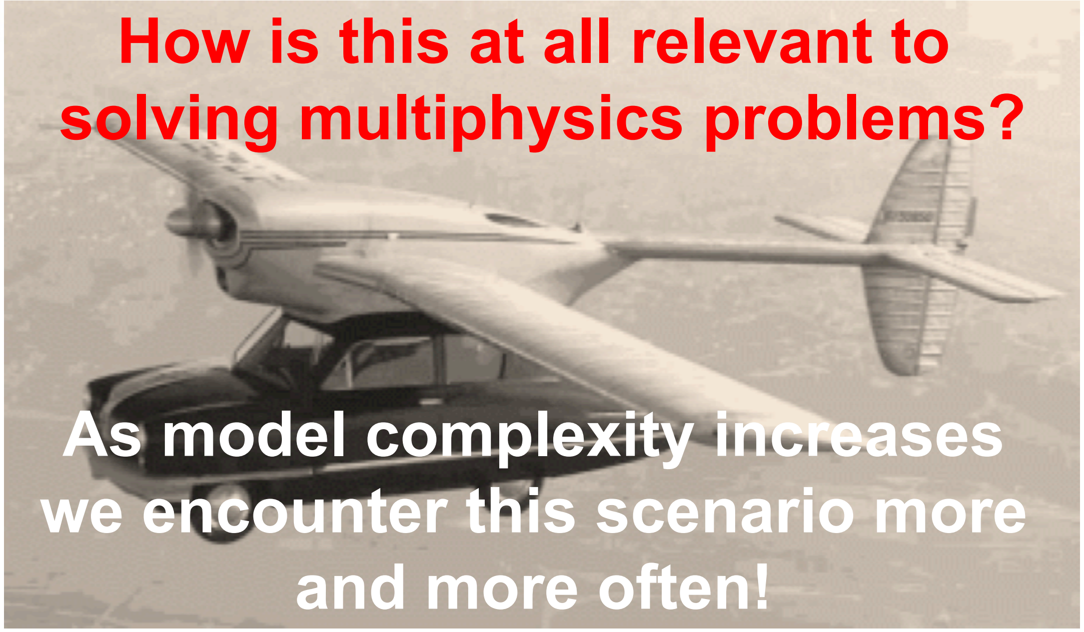
P2 = Car

There are many excellent solutions to each problem!

A Metaphor

Now, suppose you want to solve the **composite problem** P=P1+P2.

Even though there are far better solutions for P1 and P2



most likely we will end up with this

Lesson 1: Good solutions are **easier to find** for **the constituent components**

Lesson 2: Merging them into a **good solution** for the composite problem is hard!

Multiphysics & multiscale challenges

Typically L_1 and L_2 have different **mathematical structures**

$(L_1 \,\&\, L_2)(u) = f$	Goal: stable, accurate, discrete model, which preserves key physical properties	$(L_1 \,\&\, L_2)^h(u^h) = f^h$
$L_1^h \quad L_2^h$	Stable compatible methods may exist for L_1 and L_2 but not for the composite problem:	$(L_1 \,\&\, L_2)^h \neq L_1^h \,\&\, L_2^h$
$\left(L_1^h\right)^{-1} \quad \left(L_2^h\right)^{-1}$	Efficient solvers may exist for L_1 and L_2 but not for the composite problem	$\left((L_1 \,\&\, L_2)^h\right)^{-1} = ?$

The dominant strategy for the past 30 years, based on first-order-accurate operator splitting and decoupled nonlinear methods, is approaching a **point of diminishing returns** because it

1) Lacks the stability properties for simulations over dynamic scales of interest,
2) Often relies on heuristics to control the splitting errors
3) Is prone to non-intuitive instabilities and fragile solutions

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Preservation of Physical Properties

Challenges:

$\partial_t u = Lu$	Many physical properties are not preserved automatically under discertization, even with stabilization/regularization	$\partial_t u^h = L^h u^h$
$\underline{C} \le Cu \le \overline{C}$	In multiphysics codes the solution is input for another physics component	~~$\underline{C} \le Cu^h \le \overline{C}$~~
$Bu = b$	Automatic preservation of maximum principle, local and global bounds, is required for robust, predictive simulations	~~$Bu^h = b$~~ ....

- **Preservation of structure:** "**easy**" - requires "**discrete vector calculus**"
- **Preservation of features**: "**hard**" - **burdens** discretization with tasks it is not well-equipped to handle and **imposes restrictions** on grid and variables

Optimization-based modeling (OBM)

Our strategy: use optimization and control ideas to

☛ **Synthesize multiphysics models** from models for their constituent components

☛ **Build multiphysics solvers** from solvers for the constituent components

☛ **Preserve physical properties** that are difficult to impose directly in the discretization

Potential payoffs

✔ **Mathematically rigorous** operator splitting and reconnection process through **reformulation into an equivalent optimization problem:**

- Elimination or reduction of splitting errors
- Precise stability and accuracy conditions obviate need for heuristics.

✔ **Relieve discretization** from difficult tasks such as preservation of physical properties

- natural incorporation of physical properties as optimization constraints

✔ **Generality**: applicable to FE, FV and FD, particle methods, arbitrary grids…

✔ **Enable code reuse:** solvers, optimization tools,…

OBM in a nutshell

Generic optimization "harness"

			objective	$\rightarrow$	u (state)
minimize	$J(u)+\frac{\varepsilon}{2}\|\theta\|^2$	$\leftarrow$	regularization	$\rightarrow$	θ (control)
subject to	$L(u,f;\theta)=0$	$\leftarrow$	equality	$\rightarrow$	constraints
	$\underline{C} \le Cu \le \overline{C}$	$\leftarrow$	inequality		

Key question: how to reformulate (map) a given problem into an optimization problem

3 basic steps:

(1) identify **states & controls**;

(2) identify **objective**;

(3) identify **constraints:**

Preservation of properties as an optimization problem: basic idea

Objective	Target	Constraints
minimize the distance between the solution and a suitable ***target***	**stable and accurate** solution, not required to posses all desired physical properties	provided by the desired **physical properties**
$\left\| u^h - u^T \right\|$	$\partial_t u^T = L^h u^T$	$\underline{C} \le C u^h \le \overline{C}$ $B u^h = b$ ....

Related work

- "*Optimization-based synchronous remap (FCR)*", Liska et al JCP, 2010
- "*Optimization-based remap",* Bochev, Ridzal, Scovazzi, Shashkov JCP, 2011, FCT Book 2012
- "*Optimization-based transport*", Parts 1-3, Bochev, Peterson, Ridzal, Young, LNCS 2012
- "*Enforcing DMP for 2nd order elliptic problems*", Liska, Shashkov, Comm. Comp. Phys, 2008
- "*Enforcement of constraints and DMP in VMS*", Evans, Hughes, Sangali, CMAME 2009

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Preservation of properties as an optimization problem: advantages

Generic formulation

$$\partial_t u = Lu$$
$$\underline{C} \le Cu \le \overline{C}$$
$$\ldots\ldots\ldots\ldots$$

→

$$\text{minimize} \quad \frac{1}{2}\left\| u^h - u^{\mathsf{T}} \right\|^2$$
$$\text{subject to} \quad \begin{cases} \underline{C} \le Cu^h \le \overline{C} \\ \ldots\ldots\ldots\ldots \\ \partial_t u^{\mathsf{T}} = L^h u^{\mathsf{T}} \end{cases}$$

- **Minimize** distance
- **Enforce** constraints
- **Define** target field

➪ **Solution is a globally optimal state**: the best possible, relative to the target, state that has the desired physical properties

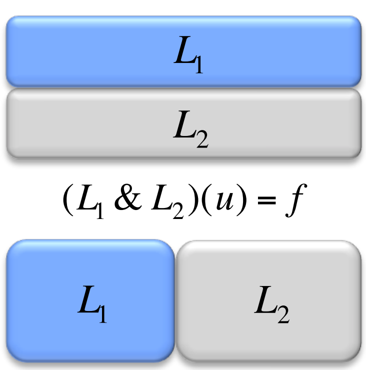
➪ **Decoupling of the target** from the enforcement of the properties allows to adapt the formulation by choosing the most appropriate target and objective for a given problem

➪ **Enforcement of properties** as constraints is impervious to grid structures and discrete field representations: enables feature preserving methods on arbitrary grids.

Multi-physics coupling as an optimization problem

Objective	Constraints	Controls
Minimize error between the states of the constituent physics components	**Enforce** constituent physics components **independently**	**Enable** variability of the states, required to minimize the **objective**

concurrent



sequential

$$\text{minimize} \quad \frac{1}{2}\left(\left\| u_1^h - u_2^h \right\|^2 + \varepsilon \left\| \theta^h \right\|^2 \right)$$

$$\text{subject to} \quad \begin{cases} L_1^h(u_1^h; \theta^h) = f_1^h \\ L_2^h(u_2^h; \theta^h) = f_2^h \end{cases}$$

"Magic" Variable

Reconcile states

Physics component #1

Physics component #2

- Sequential: "*Optimization-based domain decomposition*", M. Gunzburger, 1997
- Concurrent: "*Decomposition of everything*", J.L. Lyons, 2001, *"Additive operator-splitting"* Bochev&Ridzal, 2008-11

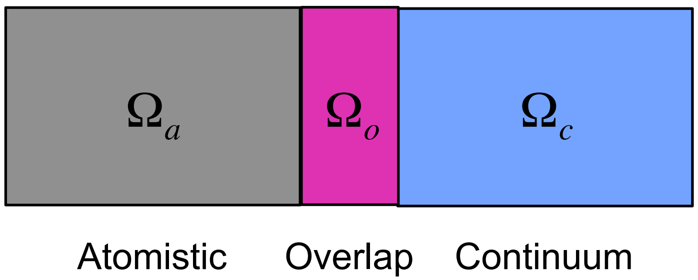
An overview of AtC coupling

AtC objectives

Combine the efficiency of continuum methods with the accuracy of (more expensive) atomistic models necessary to resolve local features such as cracks and dislocations.

Typical AtC configuration

A – atomistic operator: valid in Ω
C – continuum operator: valid in Ω_o and Ω_c
f_c – external force at continuum points
f_a – external force at atom locations



Key challenge:

- How to merge A and C into a stable and accurate AtC formulation?

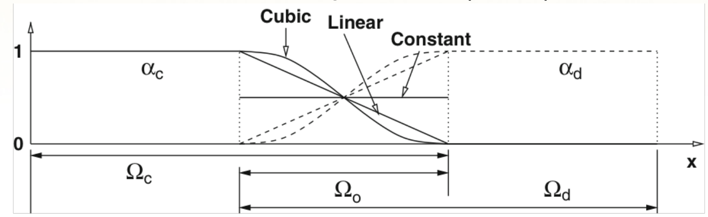
"Blending" is a dominant AtC strategy

- **Energy**: blend atomistic and continuum energy functionals over Ω_o (Arlequin, QC)
- **Force**: blend atomistic and continuum Euler-Lagrange equations over Ω_o

Drawbacks of blending

Typical energy-blended AtC method

Bauman et al, Comp. Mech. (2008) 42.



$$\begin{cases} \text{minimize} \quad \alpha E_a(u_a) + (1-\alpha) E_c(u_c) \\ \text{subject to} \ \|\Pi u_a - u_c\|_{\Omega_o} = 0 \end{cases}$$

Minimize blended energy subject to constraints **forcing the equality of the atomistic and continuum states**

- Blending of two distinct physical models is inherently **ambiguous**
- The notion of "equality" depends on the projection Π, adding **more ambiguity**
- Resulting AtC formulations typically suffer from spurious effects, e.g., **ghost forces**

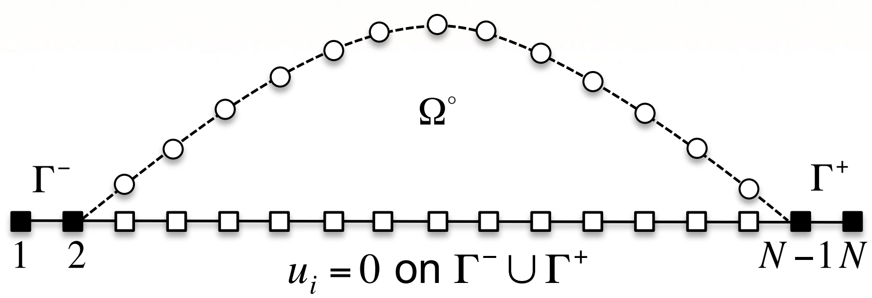
An optimization-based AtC approach

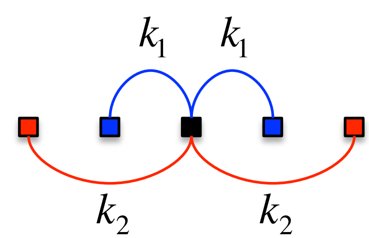
A **divide-and-conquer** strategy, which **completely separates** the atomistic and continuum models, and **reverses the roles** of constraints and objectives:

Minimize the discrepancy between the atomistic and continuum states subject to the **two models acting** independently in Ω_a and Ω_c

The global atomistic model

Linear mass-spring system with next nearest neighbor interactions





The total atomistic energy

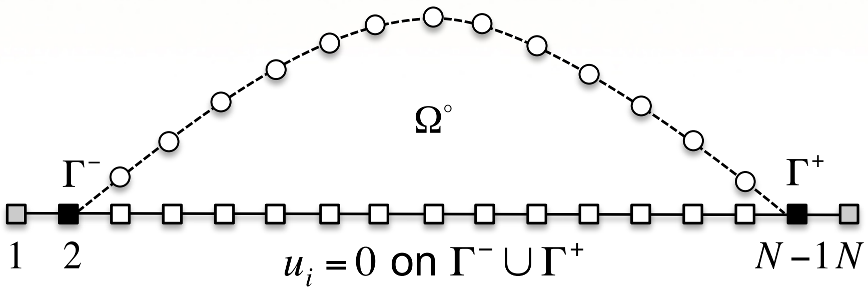
$$E^a(u) = \sum_{i=0}^{N-1} \frac{k_1}{2}(u_{i+1} - u_i)^2 + \sum_{i=1}^{N-1} \frac{k_2}{2}(u_{i+1} - u_{i-1})^2 - \left(f, u\right)_{\ell^2}$$

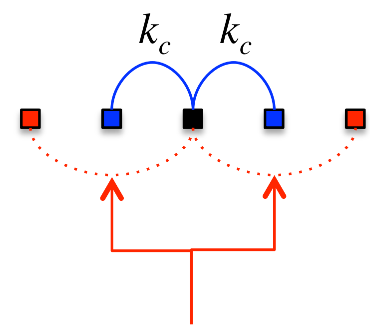
The atomistic problem

$$\tilde{u}^a = \arg\min E^a(u) \quad \Rightarrow \quad \partial E^a(\tilde{u}^a) = 0 \quad \Rightarrow \quad \begin{cases} A\tilde{u}^a = f & \text{in } \Omega^\circ \\ \tilde{u}^a = 0 & \text{on } \Gamma^- \cup \Gamma^+ \end{cases} \quad \longrightarrow \quad A = -\left(k_1\Delta_1 + k_2\Delta_2\right)$$

The global continuum approximation

Linear mass-spring system with nearest neighbor interactions





The total continuum energy

Cauchy-Born rule: $u_i \approx \frac{1}{2}\left(u_{i+1} + u_{i-1}\right)$ ➡ $(u_{i+1} - u_{i-1})^2 \approx 2(u_{i+1} - u_i)^2 + 2(u_i - u_{i-1})^2$

$$E^c(u) = \sum_{i=0}^{N-1} \frac{k_c}{2}(u_{i+1} - u_i)^2 - \left(f, u\right)_{\ell^2(\Omega)}$$ ➡ $k_c = k_1 + 4k_2$

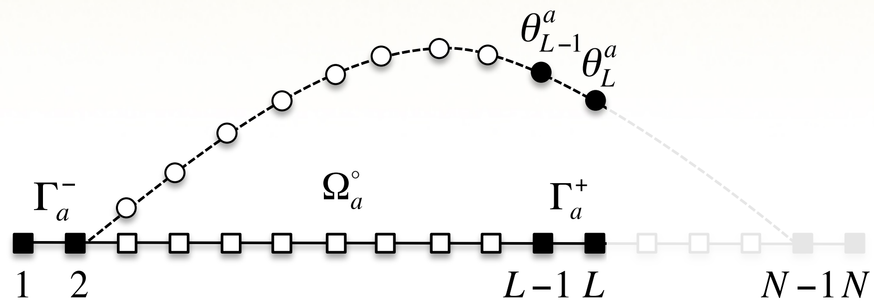
The continuum problem

$$\tilde{u}^c = \arg\min E^c(u) \quad \Rightarrow \quad \partial E^c(\tilde{u}^c) = 0 \quad \Rightarrow \quad \begin{cases} C\tilde{u}^c = f & \text{in } \Omega^\circ \\ \tilde{u}^c = 0 & \text{on } \Gamma^- \cup \Gamma^+ \end{cases}$$ ➡ $C = -\left(k_c \Delta_1\right)$

Optimization-based AtC. Step 1: splitting

The atomistic subdomain problem

$$\begin{cases} Au^a = f^a & \text{in } \Omega_a^\circ \\ u^a = \theta^a & \text{on } \Gamma_a^+ \\ u^a = 0 & \text{on } \Gamma_a^- \end{cases}$$

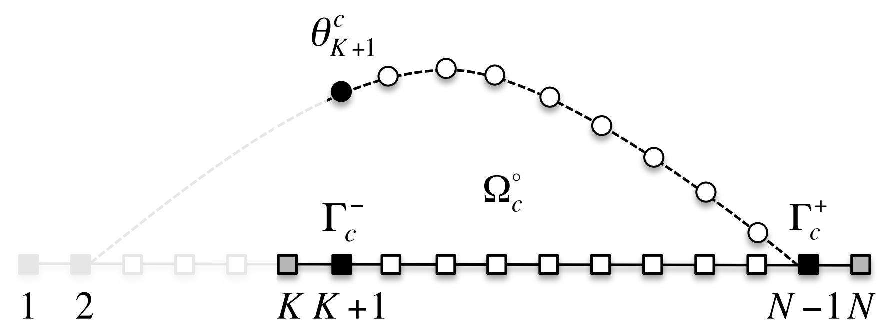


Γ_a^+ – an artificial atomistic domain boundary due to splitting

Θ^a – unknown boundary value on Γ_a^+

The continuum subdomain problem

$$\begin{cases} Cu^c = f^c & \text{in } \Omega_c^\circ \\ u^c = \theta^c & \text{on } \Gamma_c^- \\ u^c = 0 & \text{on } \Gamma_c^+ \end{cases}$$

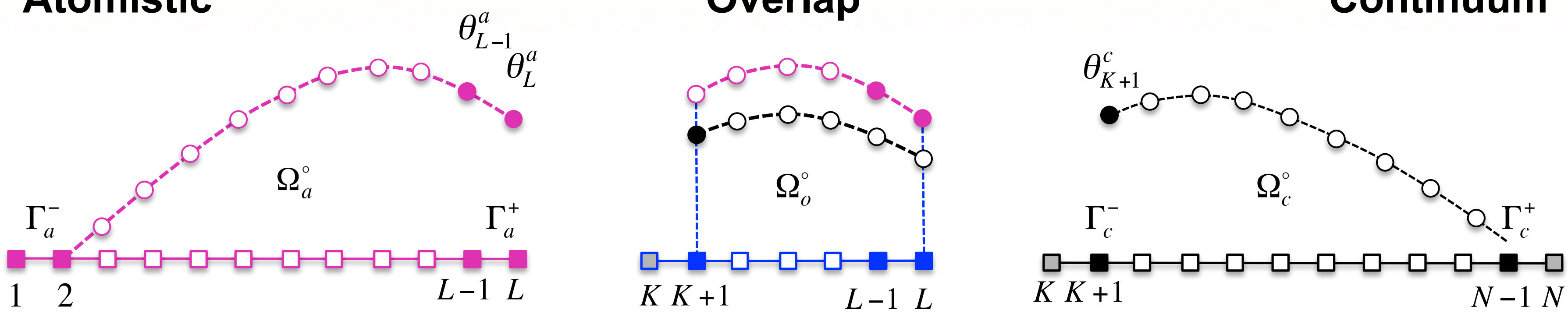


Γ_c^- – an artificial atomistic domain boundary due to splitting

Θ^c – unknown boundary value on Γ_c^-

Optimization-based AtC. Step 2: reconnection

Atomistic **Overlap** **Continuum**



$$\begin{cases} Au^a = f^a & \text{in } \Omega_a^\circ \\ u^a = \theta^a & \text{on } \Gamma_a^+ \\ u^a = 0 & \text{on } \Gamma_a^- \end{cases}$$

$$\underbrace{\left\|\theta^c - u^a\right\|^2_{\Gamma_c^-} + \left\|u^a - u^c\right\|^2_{\Omega_o^\circ} + \left\|\theta^a - u^c\right\|^2_{\Gamma_a^+}}_{\left\|u^a - u^c\right\|^2_{\Omega_o}}$$

$$\begin{cases} Cu^c = f^c & \text{in } \Omega_c^\circ \\ u^c = \theta^c & \text{on } \Gamma_c^- \\ u^c = 0 & \text{on } \Gamma_c^+ \end{cases}$$

– Atomistic and continuum problems are **separated** rather than blended

– Their solutions communicate through the **artificial boundary conditions**

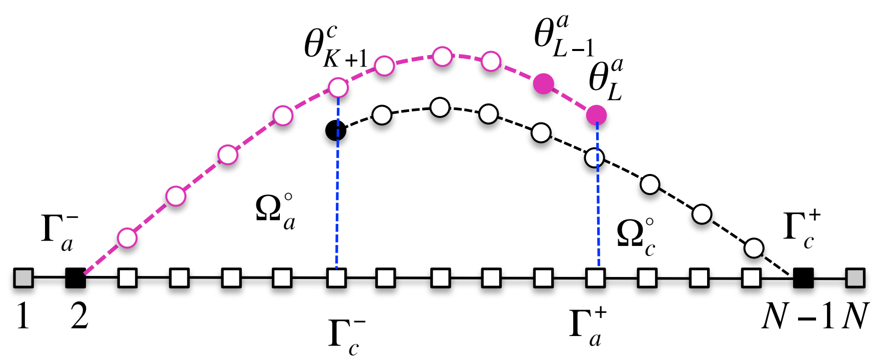
– The overlap terms measure an **artificial “mismatch” energy**

Optimization-based AtC formulation (OB-AtC)

$$\text{minimize} \quad \frac{1}{2}\left(\left\| u^a - u^c \right\|^2_{\Omega_o} + \left\| \theta^a - u^c \right\|^2_{\Gamma_a^+} + \left\| \theta^c - u^a \right\|^2_{\Gamma_c^-} \right)$$

$$\text{subject to} \begin{cases} Au^a = f^a & \text{in } \Omega_a^\circ \\ u^a = \theta^a & \text{on } \Gamma_a^+ \\ u^a = 0 & \text{on } \Gamma_a^- \end{cases} \text{ and } \begin{cases} Cu^c = f^c & \text{in } \Omega_c^\circ \\ u^c = \theta^c & \text{on } \Gamma_c^- \\ u^c = 0 & \text{on } \Gamma_c^+ \end{cases}$$

Minimize the artificial mismatch energy subject to the atomistic and continuum force balance equation



Objective: measures the mismatch energy

States: atomistic and continuum solutions

Controls: artificial boundary conditions

Atomistic and continuum problems are patch test consistent individually

⇒ OB-AtC passes patch test by construction

OB-AtC is well-posed

Reduced space problem

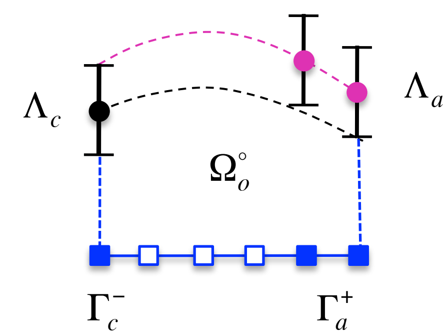
We switch to an equivalent **reduced space problem** in terms of the virtual controls only

$$\begin{cases} Au^a = f^a & \text{in } \Omega_a^\circ \\ u^a = \theta^a & \text{on } \Gamma_a^+ \\ u^a = 0 & \text{on } \Gamma_a^- \end{cases} \quad \rightarrow \quad u^a = u^a(\theta^a)$$

$$\begin{cases} Cu^c = f^c & \text{in } \Omega_c^\circ \\ u^c = \theta^c & \text{on } \Gamma_c^- \\ u^c = 0 & \text{on } \Gamma_c^+ \end{cases} \quad \rightarrow \quad u^c = u^c(\theta^c)$$

$$\underset{\Lambda_a \times \Lambda_c}{\text{minimize}} \ \frac{1}{2}\left\| u^a(\theta^a) - u^c(\theta^c) \right\|_{\Omega_o}^2$$

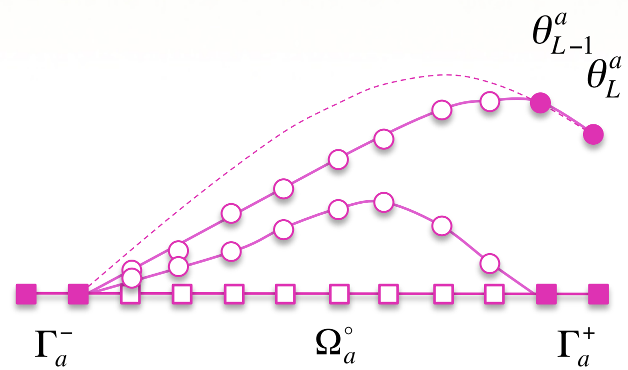
Unconstrained minimization problem over the atomistic and continuum trace spaces Λ_a and Λ_c



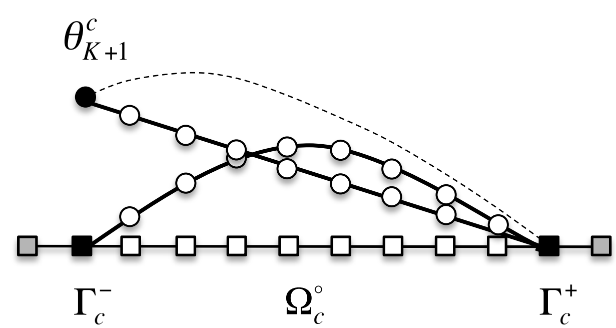
Existence and uniqueness of optimal solutions

Decomposition of the states

$$u^a(\theta^a) = v^a(\theta^a) + u^{a,0} \quad \rightarrow \quad \begin{cases} Av^a = 0 & \text{in } \Omega_a^\circ \\ v^a = \theta^a & \text{on } \Gamma_a^+ \end{cases} \qquad \begin{cases} Au^{a,0} = f^a & \text{in } \Omega_a^\circ \\ u^{a,0} = 0 & \text{on } \Gamma_a \end{cases} \quad \rightarrow$$



$$u^c(\theta^c) = v^c(\theta^c) + u^{c,0} \quad \rightarrow \quad \begin{cases} Cv^c = 0 & \text{in } \Omega_c^\circ \\ v^c = \theta^c & \text{on } \Gamma_c^- \end{cases} \qquad \begin{cases} Cu^{c,0} = f^c & \text{in } \Omega_c^\circ \\ u^{c,0} = 0 & \text{on } \Gamma_c \end{cases} \quad \rightarrow$$



This decomposition follows the idea of Gervasio et al., Num. Math. 2001

The dual inner product and norm

Theorem. The following form defines an inner product on the trace space $\Lambda_a \times \Lambda_c$.

$$\left\langle \left\{\theta^a, \theta^c\right\}, \left\{\mu^a, \mu^c\right\} \right\rangle := \left(v^a(\theta^a) - v^c(\theta^c), v^a(\mu^a) - v^c(\mu^c) \right)_{\ell^2(\Omega_o)}$$

Reduced space problem in terms of the dual norm

$$\underset{\Lambda_a \times \Lambda_c}{\text{minimize}} \ \frac{1}{2} \left\| \left\{\theta^a, \theta^c\right\} \right\|_{\ell^*}^2 + \left(v^a(\theta^a) - v^c(\theta^c), u^{a,0} - u^{c,0} \right)_{\ell^2(\Omega_o)} + \frac{1}{2} \left\| u^{a,0} - u^{c,0} \right\|_{\ell^2(\Omega_o)}$$

The Euler-Lagrange equation

$$\left\langle \left\{\theta^a, \theta^c\right\}, \left\{\mu^a, \mu^c\right\} \right\rangle := -\left(u^{a,0} - u^{c,0}, v^a(\mu^a) - v^c(\mu^c) \right)_{\ell^2(\Omega_o)} \quad \forall \left\{\mu^a, \mu^c\right\} \in \Lambda_a \times \Lambda_c$$

Corollary. The reduced space problem has a unique solution $\left\{\theta^a, \theta^c\right\} \in \Lambda_a \times \Lambda_c$.

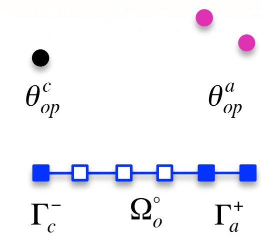
The OB-AtC approximation

Solution procedure

1. Solve the reduced space problem:

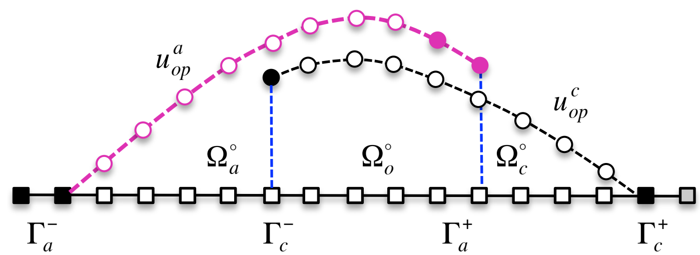
$$\left\{\theta_{op}^{a}, \theta_{op}^{c}\right\} \in \Lambda_a \times \Lambda_c$$

approximate solution traces →



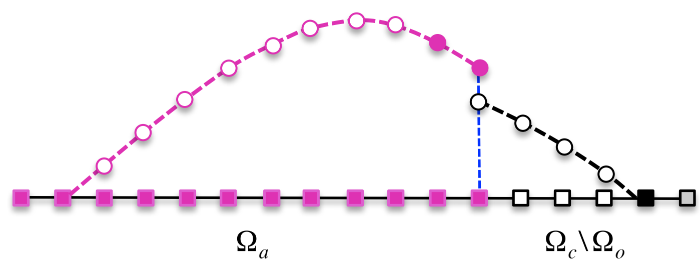
2. Recover the optimal states

$$u_{op}^{a} = u^{a,0} + v^{a}(\theta_{op}^{a}) \quad \text{and} \quad u_{op}^{c} = u^{c,0} + v^{c}(\theta_{op}^{c})$$



3. Define the AtC approximation

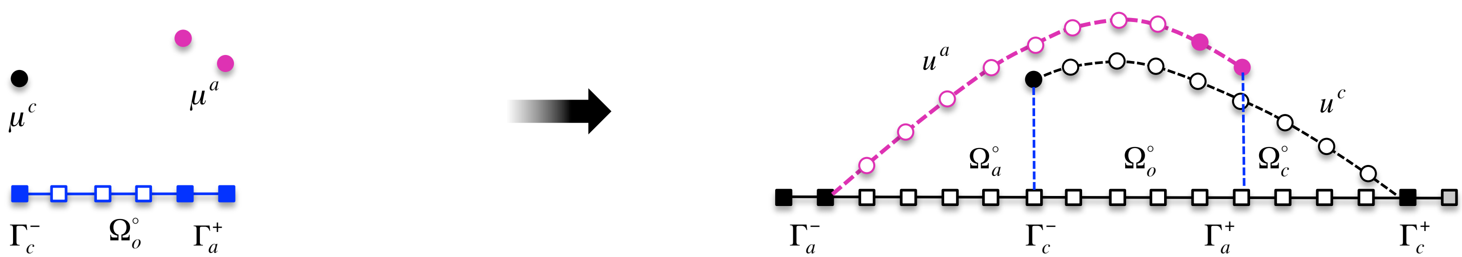
$$u^{atc} = \begin{cases} u_{op}^{a} & \text{in } \Omega_a \\ u_{op}^{c} & \text{in } \Omega_c \backslash \Omega_o \end{cases}$$



The AtC approximation error

Define the trace lifting operator

$$P\left(\left\{\mu^a,\mu^a\right\}\right) = U_0 + Q\left(\left\{\mu^a,\mu^a\right\}\right) \quad \text{where} \quad U_0 = \begin{pmatrix} u^{a,0} \\ u^{c,0} \end{pmatrix} \quad \text{and} \quad Q\left(\left\{\mu^a,\mu^a\right\}\right) = \begin{cases} v^a(\mu^a) & \text{in } \Omega_a \\ v^c(\mu^c) & \text{in } \Omega_c \setminus \Omega_o \end{cases}$$



The AtC approximation error

$$u^{atc} = P\left(\left\{\theta_{op}^a,\theta_{op}^c\right\}\right) \quad \Rightarrow \quad \left\|\tilde{u}^a - u^{atc}\right\|_{\ell^2(\Omega)} = \left\|\tilde{u}^a - P\left(\left\{\theta_{op}^a,\theta_{op}^c\right\}\right)\right\|_{\ell^2(\Omega)}$$

Where $\tilde{u}^a$ is the global atomistic solution.

The AtC error estimate

Define the trace operator $r(u)=\left\{\begin{pmatrix}u_{L-1}\\ u_L\end{pmatrix};(u_K)\right\}=\left\{r(u^a),r(u^a)\right\}$

Error splitting

$$\left\|\tilde{u}^a-u^{atc}\right\|_{\ell^2(\Omega)}=\left\|\tilde{u}^a-P\left(\left\{\theta^a_{op},\theta^c_{op}\right\}\right)\right\|_{\ell^2(\Omega)}=\left\|\tilde{u}^a-P\left(r(\tilde{u}^a)\right)+P\left(r(\tilde{u}^a)\right)-P\left(\left\{\theta^a_{op},\theta^c_{op}\right\}\right)\right\|_{\ell^2(\Omega)}$$

$$=\left\|\tilde{u}^a-P\left(r(\tilde{u}^a)\right)\right\|_{\ell^2(\Omega)}+\left\|Q\left(r(\tilde{u}^a)\right)-Q\left(\left\{\theta^a_{op},\theta^c_{op}\right\}\right)\right\|_{\ell^2(\Omega)}$$

$$\leq\left\|\tilde{u}^a-P\left(r(\tilde{u}^a)\right)\right\|_{\ell^2(\Omega)}+\left\|Q\right\|\cdot\left\|r(\tilde{u}^a)-\left\{\theta^a_{op},\theta^c_{op}\right\}\right\|_{\ell^*}$$

The error components

$$\left\|\tilde{u}^a-P\left(r(\tilde{u}^a)\right)\right\|_{\ell^2(\Omega)}$$

Consistency error

$$\left\|r(\tilde{u}^a)-\left\{\theta^a_{op},\theta^c_{op}\right\}\right\|_{\ell^*}$$

Approximation error

$$\left\|Q\right\|=\sup_{\{\mu^a,\mu^c\}}\frac{\left\|Q\{\mu^a,\mu^c\}\right\|_{\ell^2(\Omega)}}{\left\|\{\mu^a,\mu^c\}\right\|_{\ell*}}$$

Lifting operator norm

Estimate of the consistency error

Assumptions

$|\Omega_a| \leq |\Omega|^{1/p}$ for some $0 < p$ ← The atomistic domain Ω_a is **small** compared to Ω

$|\Omega_o| = (1-\gamma)|\Omega_a|$ for some $0 < \gamma < 1$ ← The overlap domain Ω_o remains **proportional** to Ω_a

Lemma. Let $\tilde{u}^a$ be the exact atomistic solution and u^c-the continuum lifting of its trace

$$\left\| \tilde{u}^a - P\left(r(\tilde{u}^a)\right) \right\|_{\ell^2(\Omega)} \leq \left\| \tilde{u}^a - u^c \right\|_{\ell^2(\Omega_c \setminus \Omega_o)}$$

Proof.

$$P\left(r(\tilde{u}^a)\right) = P\left(\left\{ r^a(\tilde{u}^a), r^c(\tilde{u}^a) \right\}\right) = \begin{cases} \tilde{u}^a & \text{in } \Omega_a \\ u^c & \text{in } \Omega_c \setminus \Omega_o \end{cases}$$

← Recovers the exact atomistic solution in Ω_a

← Continuum lifting of the exact atomistic trace

$$\left\| \tilde{u}^a - P\left(r(\tilde{u}^a)\right) \right\|_{\ell^2(\Omega)} \leq \left\| \tilde{u}^a - \tilde{u}^a \right\|_{\ell^2(\Omega_a)} + \left\| \tilde{u}^a - u^c \right\|_{\ell^2(\Omega_c \setminus \Omega_o)} = \left\| \tilde{u}^a - u^c \right\|_{\ell^2(\Omega_c \setminus \Omega_o)}$$

Consistency error is confined to the pure continuum region

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Estimate of the approximation error

Lemma. Let $\tilde{u}^a$ be the exact atomistic solution and u^c-the continuum lifting of its trace

$$\left\| r(\tilde{u}^a) - \left\{\theta^a_{op}, \theta^c_{op}\right\} \right\|_{\ell^*} \le \left\| \tilde{u}^a - u^c \right\|_{\ell^2(\Omega_o)}$$

Proof. Using that $\left\{\theta^a_{op}, \theta^c_{op}\right\}$ solves the Euler-Lagrange equation of the reduced problem

$$\left\| r(\tilde{u}^a) - \left\{\theta^a_{op}, \theta^c_{op}\right\} \right\|_{\ell^*} = \sup_{\{\mu^a, \mu^c\}} \frac{\left\langle r(\tilde{u}^a), \left\{\mu^a, \mu^c\right\} \right\rangle + \left(u^{a,0} - u^{c,0}, v^a(\mu^a) - v^a(\mu^a) \right)_{\ell^2(\Omega_o)}}{\left\| \left\{\mu^a, \mu^c\right\} \right\|_{\ell^*}}$$

$$\left\langle r(\tilde{u}^a), \left\{\mu^a, \mu^c\right\} \right\rangle + \left(u^{a,0} - u^{c,0}, v^a(\mu^a) - v^a(\mu^a) \right)_{\ell^2(\Omega_o)}$$

Using definition of the dual inner product

$$= \left(\tilde{u}^a - u^c, v^a(\mu^a) - v^a(\mu^a) \right)_{\ell^2(\Omega_o)}$$

$$\le \left\| \tilde{u}^a - u^c \right\|_{\ell^2(\Omega_o)} \left\| v^a(\mu^a) - v^a(\mu^a) \right\|_{\ell^2(\Omega_o)} \le \left\| \tilde{u}^a - u^c \right\|_{\ell^2(\Omega_o)} \left\| \left\{\mu^a, \mu^c\right\} \right\|_{\ell^*}$$

Approximation error is confined to the overlap region

Estimate of the operator norm

Lemma. The norm of *Q* is inversely proportional to the size of the overlap domain:

$$\|Q\| \le \frac{C}{1-\gamma} \cdot \left(\frac{|\Omega|}{|\Omega_o|} \right)^{1/2}$$

Proof. Definition of the operator norm implies that the statement is equivalent to

$$\left\| Q\{\mu^a, \mu^c\} \right\|_{\ell^2(\Omega)} \le \frac{C}{1-\gamma} \cdot \left(\frac{|\Omega|}{|\Omega_o|} \right)^{1/2} \left\| \{\mu^a, \mu^c\} \right\|_{\ell *} \qquad \forall \{\mu^a, \mu^c\} \in \Lambda_a \times \Lambda_c$$

Which in turn is equivalent to

$$\left\| v^a(\mu^a) \right\|^2_{\ell^2(\Omega_a)} + \left\| v^c(\mu^c) \right\|^2_{\ell^2(\Omega_c \setminus \Omega_o)} \le \frac{C}{1-\gamma} \cdot \left(\frac{|\Omega|}{|\Omega_o|} \right)^{1/2} \left\| v^a(\mu^a) - v^c(\mu^c) \right\|^2_{\ell^2(\Omega_o)} \quad \forall \{\mu^a, \mu^c\} \in \Lambda_a \times \Lambda_c$$

We use the structure of the atomistic and continuum solutions to prove this bound.
Equivalent to the existence of a **strong Cauchy-Schwartz** inequality for $\left(v^a(\mu^a), v^c(\mu^c) \right)$.

The AtC error estimate

Lemma. Let $\tilde{u}^a$ be the exact atomistic solution and u^c-the continuum lifting of its trace

$$\left\|\tilde{u}^a - u^{atc}\right\|_{\ell^2(\Omega)} \leq C\left(1 + \frac{1}{1-\gamma}\right) \cdot \left(\frac{|\Omega|}{|\Omega_o|}\right)^{1/2} \left\|\tilde{u}^a - u^c\right\|_{\ell^2(\Omega_c)}$$

AtC accuracy is determined by 2 independent factors:

Continuum modeling error $\left\|\tilde{u}^a - u^c\right\|_{\ell^2(\Omega_c)}$

- Small if solution is smooth in Ω_c i.e., there are no defects (basic premise of AtC)
- Independent of the choice of coupling mechanism

Optimization based coupling $\left(1 + \frac{1}{1-\gamma}\right) \cdot \left(\frac{|\Omega|}{|\Omega_o|}\right)^{1/2}$

- Inversely proportional to Ω_c i.e., better for larger overlap regions
- Independent of the continuum modeling error

The AtC error estimate

Theorem. Let $\tilde{u}^a$ be the exact atomistic solution and u^c -the continuum lifting of its trace

$$\left\|\tilde{u}^a - u^{atc}\right\|_{\ell^2(\Omega)} \le C\left(1+\frac{1}{1-\gamma}\right)\cdot\left(\frac{|\Omega|}{|\Omega_o|}\right)^{1/2}|\Omega_c|\cdot\left\|\Delta_1^2\tilde{u}^a\right\|_{\ell^2(\Omega_c)}$$

Proof. Follows from the upper bound on the modeling error

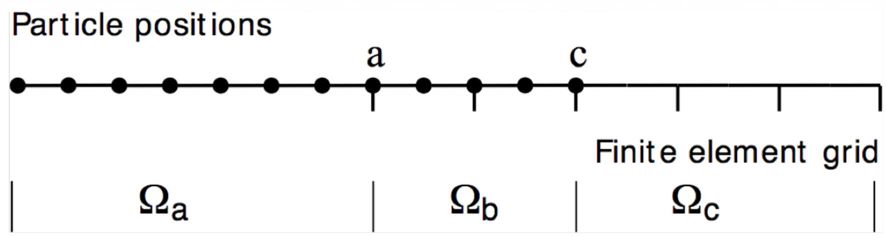
$$\left\|\tilde{u}^a - u^c\right\|_{\ell^2(\Omega_c)} \le |\Omega_c|\cdot\left\|\Delta_1^2\tilde{u}^a\right\|_{\ell^2(\Omega_c)}$$

Corollary. Set *ε=1/N* and rescale the lattice according to *i→εi*. The AtC error then is:

$$\left\|\tilde{u}^a - u^{atc}\right\|_{\ell^2(\Omega)\varepsilon} \le C\,\frac{\varepsilon^2}{|\Omega_o|^{1/2}}\cdot\left\|\Delta_1^2\tilde{u}^a\right\|_{\ell^2(\Omega_c)\varepsilon}$$

Numerical results

Model one-dimensional AtC problem (Curtin, Miller, 2003)



$\Omega_a = [0,74]$

$\Omega_c = [30,105]$

$\Omega_b = [30,74]$

A – mass spring network: next nearest neighbor interaction

$$Q_a = -k_1(u_{i-1} - 2u_i + u_{i+1}) - k_2(u_{i-2} - 2u_i + u_{i+2})$$

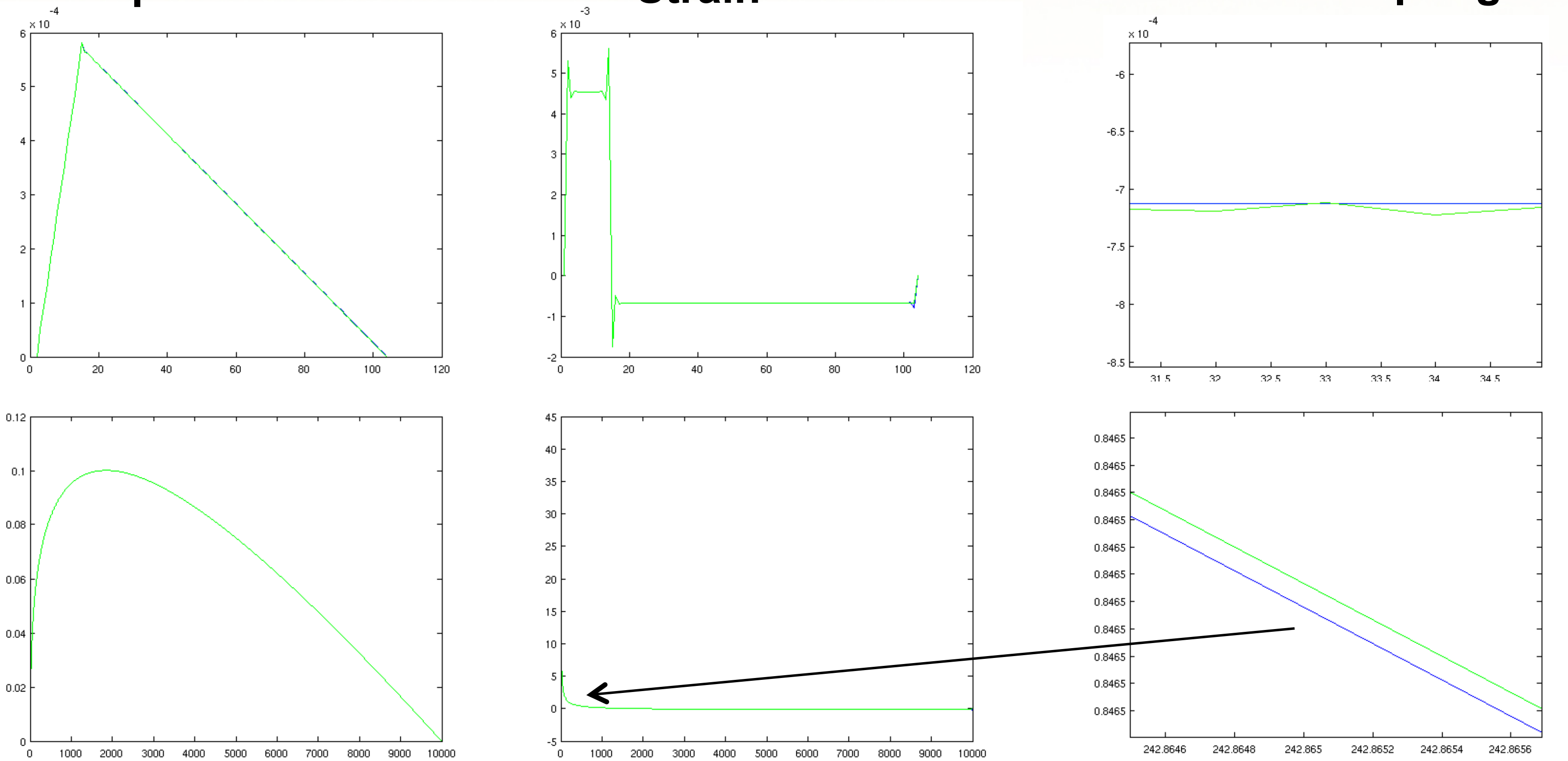
C – linear elasticity with averaged spring constant

$$Q_c = -k_c(u_{i-1} - 2u_i + u_{i+1}) \quad k_c = k_1 + 4k_2$$

f_a – point force at lattice location #25

Numerical results

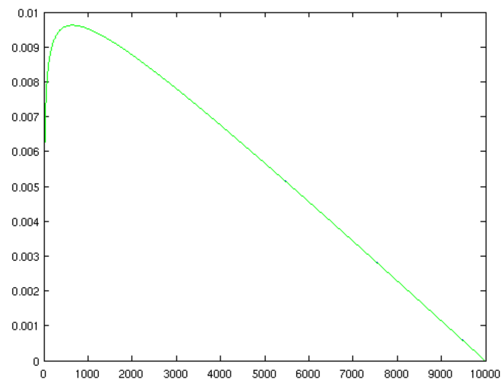
Displacement | **Strain** | **Strain in the overlap region**



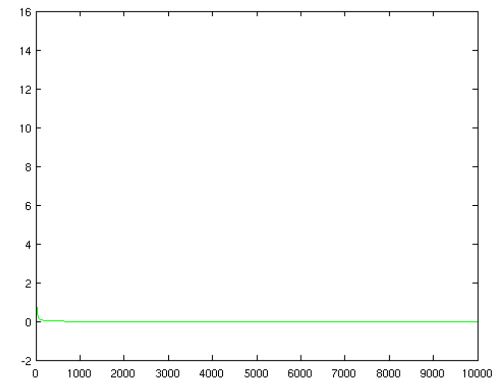
Blue = exact solution
Green = OBM solution

Numerical results

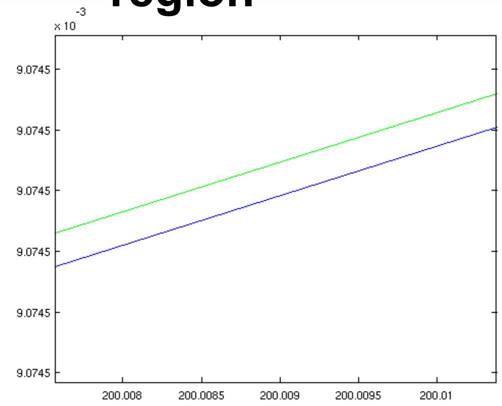
Displacement



Strain



Displacement in the overlap region



Blue = exact solution
Green = OBM solution

Summary

We use optimization and control ideas to automatically manage discretization tasks that are difficult to accomplish directly:

— Reconcile solutions from constituent components of multi-physics problems

— Reconcile different representations of the same field in physically consistent manner

— Automatically figure out the needed "ghost forces" to balance the interfaces

Advantages

— Increase concurrency by exposing constituent physics components

— Remove order limitations (reformulation yields **nearly equivalent** problems)

— Rigorous mathematical foundations inherited from rich optimization theory

— Restore physical constraints that were lost during discretization

— Reuse of software components through "synthesis" of solvers and discretizations