Variational Multiscale Analysis:
The fine-scale Green’s function, projection, optimization, and localization

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14th November 2011
Motivation
- The abstract framework
- The advection-diffusion model problem
- Projection and localization
Outline

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Motivation

- Introduced as a framework for incorporating missing fine-scale effects into numerical problems governing coarse-scale behaviour.

- Provided a rationale for stabilized methods and for development of robust methods.

- Direct application of Galerkin’s methods with standard bases (such as FE) in the presence of multiscale phenomena leads to wrong solution.

- Multiscale phenomena is ubiquitous in science and engineering applications.
The abstract framework

The abstract problem

Let $V$ Hilbert space, $\| \cdot \|_V$ norm, $(\cdot, \cdot)_V$ scalar product, $V^*$ dual of $V$, $(\cdot, \cdot)_{V^* \times V}$ duality pairing, $L : V \to V^*$ linear isomorphism.

Given $f \in V^*$, find $u \in V$ such that

$$Lu = f$$

(1)

VF: find $u \in V$ such that

$$(Lu, v)_{V^* \times V} = (f, v)_{V^* \times V} \quad \forall \ v \in V$$

(2)

Solution of (1) $u = Gf$, $G : V^* \to V$, where $G := L^{-1}$
The variational multiscale formulation

Let $\bar{V}$ closed subspace of $V$, $P : V \to \bar{V}$ linear projection

$\mathcal{R}(P) = \bar{V}$, define $\text{Ker}(P) = V'$ and let $P$ continuous in $V$

$$V = \bar{V} \bigoplus V'$$

$\Rightarrow \forall v \in V$, $v = \bar{v} + v'$ where $\bar{v} \in \bar{V}$, $v' \in V'$

also, $u = \bar{u} + u'$

$\bar{V} \equiv$ space of computable coarse scale, $V' \equiv$ space of unresolved fine scale

Aim of VMS: Find $\bar{u} = Pu$
Procedure: VF (2) splits;

\[
\langle \mathcal{L} \bar{u}, \bar{v} \rangle_{V^* \times V} + \langle \mathcal{L} u', \bar{v} \rangle_{V^* \times V} = \langle f, \bar{v} \rangle_{V^* \times V} \quad \forall \bar{v} \in \bar{V} \tag{4}
\]

\[
\langle \mathcal{L} \bar{u}, v' \rangle_{V^* \times V} + \langle \mathcal{L} u', v' \rangle_{V^* \times V} = \langle f, v' \rangle_{V^* \times V} \quad \forall v' \in V' \tag{5}
\]

Assume (4) and (5) are well posed for \( \bar{u} \) and \( u' \) respectively.

Associate with (5); \( G' : V^* \rightarrow V \), which yields \( u' = G'(f - \mathcal{L} \bar{u}) \)

Having \( G' \), eliminate \( u' \) from (4) \( \implies \) VMS for \( \bar{u} \)

\[
\langle \mathcal{L} \bar{u}, \bar{v} \rangle_{V^* \times V} - \langle \mathcal{L} G' \mathcal{L} \bar{u}, \bar{v} \rangle_{V^* \times V} = \langle f, \bar{v} \rangle_{V^* \times V} \langle \mathcal{L} G' f, \bar{v} \rangle_{V^* \times V} \quad \forall \bar{v} \in \bar{V} \tag{6}
\]

admits a unique solution \( \bar{u} = \mathcal{P} u \)
The fine-scale Green's operator

\( \mathcal{P}^T : \bar{V}^* \rightarrow V^* \) adjoint of \( \mathcal{P} \), i.e

\[
\langle \mathcal{P}^T \bar{\mu}, v \rangle_{V^* \times V} = \langle \bar{\mu}, \mathcal{P} v \rangle_{V^* \times V} \quad \forall \bar{\mu} \in \bar{V}^*
\]

**Theorem**

*Under the assumption of the abstract problem and VMS formulation, we have*

\[
\mathcal{G}' = \mathcal{G} - \mathcal{G} \mathcal{P}^T (\mathcal{P} \mathcal{G} \mathcal{P}^T)^{-1} \mathcal{P} \mathcal{G} \quad \tag{7}
\]

\[
\mathcal{G}' \mathcal{P}^T = 0, \quad \text{and} \quad \mathcal{P} \mathcal{G}' = 0 \quad \tag{8}
\]
If \( \text{dim}(\bar{V}) = N \), we can find a set of functionals \( \mu : V \to \mathbb{R}, \ \{\mu_i\}_{i=1,...,N} \) such that, for all \( v \in V \)

\[
\langle \mu_i, v \rangle_{V^* \times V} = 0 \quad \forall \ i = 1, \ldots, N \quad \iff \quad \mathcal{P}v = 0
\]  

(9)

In this case, (8) is equivalent to:

\[
\mathcal{G}'\mu_i = 0 \quad \forall \ i = 1, \ldots, N
\]  

(10)

and

\[
\langle \mu_i, \mathcal{G}'\nu \rangle_{V^* \times V} = 0 \quad \forall \nu \in V^* \quad \forall \ i = 1, \ldots, N
\]  

(11)

Introduce \( \mu \in (V^*)^N, \ \mathcal{G}\mu^T \in V^N, \)

\[
\mu\mathcal{G}\mu^T = \begin{bmatrix}
\langle \mu_1, \mathcal{G}\mu_1 \rangle_{V^* \times V} & \cdots & \langle \mu_1, \mathcal{G}\mu_N \rangle_{V^* \times V} \\
\vdots & \ddots & \vdots \\
\langle \mu_N, \mathcal{G}\mu_1 \rangle_{V^* \times V} & \cdots & \langle \mu_N, \mathcal{G}\mu_N \rangle_{V^* \times V}
\end{bmatrix} \in \mathbb{R}^{R \times R} \quad \forall \nu \in V^*
\]

and vector of functionals; i.e \( \mu\mathcal{G} : (V^*) \to \mathbb{R}^N \), then (7) is equivalent to:

\[
\mathcal{G}' = \mathcal{G} - \mathcal{G}\mu^T(\mu\mathcal{G}\mu^T)^{-1}\mu\mathcal{G}
\]  

(12)

since \( \{\mu_i\}_{i=1,...,N} \) is a basis for the image of \( \mathcal{P}^T \)
Given scalar product \((\cdot, \cdot)\) defined on \(V \times V\), the related **orthogonal projector** \(P\) is defined by

\[
(Pw, \bar{v}) = (w, \bar{v}) \quad \forall \ w \in V, \ \bar{v} \in \bar{V}
\]

In this case, \(V'\) and \(\bar{V}\) are orthogonal complements with respect to \((\cdot, \cdot)\), and the VMS formulation thus provide **optimal approximation** \(\bar{u} \in \bar{V}\) of \(u\), with respect to the \(\| \cdot \|\) induced by the scalar product \((\cdot, \cdot)\).
The advection-diffusion model problem

Model problem:

\[ \mathcal{L} u = -\kappa \Delta u + \beta \cdot \nabla u = f \quad \text{in} \quad \Omega \quad u|_{\partial\Omega} = 0 \]  \hspace{1cm} (13)

- \( \kappa > 0 \) (scalar diffusivity)
- \( \beta : \Omega \to \mathbb{R}^d, \ \text{div}(\beta) = 0 \)
- \( \Omega \subset \mathbb{R}^d \) \((d = 1, 2)\); regular domain
- \( f \in L^2(\Omega) \)

VF: \( V = H^1_0 \equiv H^1_0(\Omega), \ V^* = H^{-1} \)

Representation: Green’s operator \( G \) through the Green’s function \( g : \Omega \times \Omega \to \mathbb{R} \)
such that:

\[ u(y) = \int_{\Omega} g(x, y)f(x)dx \quad \text{a.e} \quad y \in \Omega \]
Similar representation: fine-scale Green’s operator $G'$ through the fine-scale Green’s function $g' : \Omega \times \Omega \to \mathbb{R}$ gives the fine scale component $u'$ of $u$ from

\[
r = f - \mathcal{L}\bar{u} :
\]

\[
u'(y) = \int_{\Omega} g'(x, y)r(x)dx
\]

(14)

where the space $V'$ and function $g'$ depends on the underlying projector $\mathcal{P}$
Having \( \{ \mu_i \}_{i=1}^N \) such that:

\[
\int_{\Omega} \mu_i(x) v(x) dx = 0 \quad \forall \ i, \ldots, N \quad \iff \quad \mathcal{P} v = 0
\]

Then, \( g' \) is obtained by (12) as:

\[
g'(x, y) = g(x, y) - \left[ \int_{\Omega} g(\tilde{x}, y) \mu_1(\tilde{x}) d\tilde{x} \quad \cdots \quad \int_{\Omega} g(\tilde{x}, y) \mu_N(\tilde{x}) d\tilde{x} \right]^{-1} \times \\
\times \left[ \begin{array}{c}
\int_{\Omega} g(\tilde{x}, \tilde{y}) \mu_1(\tilde{x}) \mu_1(\tilde{y}) d\tilde{x} d\tilde{y} \\
\vdots \\
\int_{\Omega} g(\tilde{x}, \tilde{y}) \mu_N(\tilde{x}) \mu_N(\tilde{y}) d\tilde{x} d\tilde{y} \\
\int_{\Omega} g(x, \tilde{y}) \mu_1(\tilde{y}) d\tilde{y} \\
\vdots \\
\int_{\Omega} g(x, \tilde{y}) \mu_N(\tilde{y}) d\tilde{y}
\end{array} \right]
\]

(15)
The property \((10)\) and \((11)\) \(\implies\) for all \(x, y \in \Omega\) and for all \(i = 1, \cdots, N\)

\[
\int_{\Omega} g'(\tilde{x}, y) \mu_i(\tilde{x}) d\tilde{x} = 0 \quad \text{and} \quad \int_{\Omega} g'(x, \tilde{y}) \mu_i(\tilde{y}) d\tilde{y} = 0
\] (16)

In this context, the VMS formulation \((6)\) reads: Find \(\bar{u} \in \bar{V}\) such that

\[
\int_{\Omega} (\kappa \nabla \bar{u}(x) - \beta \bar{u}) \cdot \nabla \bar{v}(x) dx - \int_{\Omega} \int_{\Omega} \mathcal{L}\bar{u}(x) g'(x, y) \mathcal{L}^* \bar{v}(y) dx dy = \int_{\Omega} f(x) \bar{v} dx - \int_{\Omega} \int_{\Omega} f(x) g'(x, y) \mathcal{L}^* \bar{v}(y) dx dy
\]

\[\forall \ \bar{v} \in \bar{V}\]
Take: $d = 1$, $\Omega = (0, L)$, and consider: $0 = x_0 < x_1 < \cdots < x_{el-1} < x_{el} = L$

Subdivision: $(0, L)$ into $n_{el}$ elements $(x_{i-1}, x_i)$, $i = 1, \cdots, n_{el}$

For the $H^1_0$-projector $P = P_{H^1_0}$ the VMS provides a nodally exact approximation $\tilde{u}$ of the exact solution $u$.

In this case, $\mu_i = \delta(x - x_i)$ and the property (16) in the theorem is equivalent to:

$$g'(x, x_i) = g'(x_i, y) = 0 \quad \forall \ i = 1, \cdots, N, \ 0 \leq x, y \leq L;$$

(17)

i.e., $g'$ vanishes if one of its two arguments is a node of the grid.
As a result, the expression (16) for the fine-scale Green's function in this case becomes:

\[
g'(x, y) = g(x, y) - \begin{bmatrix} g(x_1, y) & \cdots & g(x_N, y) \end{bmatrix} \begin{bmatrix} g(x_1, x_1) & \cdots & g(x_N, x_1) \\ \vdots & \ddots & \vdots \\ g(x_1, x_N) & \cdots & g(x_N, x_N) \end{bmatrix}^{-1} \begin{bmatrix} g(x_1) \\ \vdots \\ g(x_N) \end{bmatrix}
\]
Since \( g(x, y)' \neq 0 \) only when \( x \) and \( y \) belong to the same element, (14) can be localized within each element:

\[
    u'(y) = \int_{x_{i-1}}^{x_i} g'(x, y) r(x) \, dx \quad y \in (x_{i-1}, x_i)
\]

\( V' \) is the space of bubbles:

\[
    V' = \bigoplus_{i=1}^{n_{el}} H^1_0(x_{i-1}, x_i),
\]
If we assume piecewise-constant coefficients $\kappa, \beta$ and source term $f$, the fine-scale VE:

$$\int_0^L \int_0^L \mathcal{L}^* \bar{v}(y) g'(x, y) r(x) dx dy = \sum_{i=1}^{n_{el}} \int_{x_{i-1}}^{x_i} \int_{x_{i-1}}^{x_i} \mathcal{L}^* \bar{v}(y) g'(x, y) r(x) dx dy$$

$$= \sum_{i=1}^{n_{el}} \int_{x_{i-1}}^{x_i} \int_{x_{i-1}}^{x_i} \frac{g'(x, y) dx dy}{x_i - x_{i-1}} \int_{x_{i-1}}^{x_i} r(x) \mathcal{L}^* \bar{v}(x) dx,$$

which is recognized as a classical stabilization term depending on the parameter

$$\tau_1 \equiv \tau_1, (x_{i-1}, x_i) = \frac{\int_{x_{i-1}}^{x_i} \int_{x_{i-1}}^{x_i} g'(x, y) dx dy}{x_i - x_{i-1}} = \frac{h}{2\beta} \left( \coth(\alpha) - \frac{1}{\alpha} \right)$$

where $\alpha = \frac{\beta h}{2k}$ is the mesh Péclet number, $h = x_i - x_{i-1}$ is the local mesh-size.
Consider higher-order piecewise-polynomial coarse: \( 0 = x_0 < x_1 < \cdots < x_{n_{el} - 1} = L \)

and set

\[
V = \{ \bar{v} \in H^1_0(0, L) \text{ such that } \bar{v}|_{(x_{i-1}, x_i)} \in \mathbb{P}_k, \ 1 \leq i \leq n_{el} \}
\]

\( V' \) is a strict subset of \textit{bubbles}:

\[
V' \subsetneq \bigoplus_{i=1, \cdots, n_{el}} H^1_0(x_{i-1}, x_i), \quad (18)
\]
Consider: \( V'_i = V'_{(x_{i-1}, x_i)} \); as fine-scale of bubbles,

\[
\bar{V}_i = \bar{V}_{(x_{i-1}, x_i)} \cap H^1_0(x_{i-1}, x_i) \text{ space of bubbles of coarse-scale}
\]

\[
\tilde{V}_i = H^1_0(x_{i-1}, x_i) = \bar{V}_i \bigoplus V'_i \text{ space of unconstrained bubbles}
\]

In this case, the Green’s function of the unconstrained bubble is the element Green’s function \( g^{el} \). From (12), we get \( g' \) in terms of \( g^{el} \): on \((0, h) \times (0, h)\)

\[
g'(x, y) = g^{el}(x, y) - \left[ \int_0^h g^{el}(\bar{x}, y) d\bar{x} \ldots \int_0^h \bar{x}^{k-2} g^{el}(\bar{x}, y) d\bar{x} \right]^{-1} \\
\times \begin{bmatrix}
\int_0^h \int_0^h g^{el}(\bar{x}, \bar{y}) d\bar{x} d\bar{y} & \ldots & \int_0^h \int_0^h \bar{x}^{k-2} g^{el}(\bar{x}, \bar{y}) d\bar{x} d\bar{y} \\
\vdots & \ddots & \vdots \\
\int_0^h \int_0^h \bar{y}^{k-2} g^{el}(\bar{x}, \bar{y}) d\bar{x} d\bar{y} & \ldots & \int_0^h \int_0^h \bar{x}^{k-2} \bar{y}^{k-2} g^{el}(\bar{x}, \bar{y}) d\bar{x} d\bar{y} \\
\int_0^h g^{el}(x, \bar{y}) d\bar{y} & \ddots & \vdots \\
\vdots & \ddots & \ddots \\
\int_0^h \bar{y}^{k-2} g^{el}(x, \bar{y}) d\bar{y} & \int_0^h \bar{x}^{k-2} \bar{y}^{k-2} g^{el}(\bar{x}, \bar{y}) d\bar{x} d\bar{y}
\end{bmatrix}
\]

(19)
For \( k = 2 \), (21) yields:

\[
g'(x, y) = g_{el}(x, y) - \frac{\int_0^h g_{el}(\tilde{x}, y) d\tilde{x}}{\int_0^h \int_0^h g_{el}(\tilde{x}, \tilde{y}) d\tilde{x} d\tilde{y}} \int_0^h g_{el}(x, \tilde{y}) d\tilde{y}
\]

and for \( k = 3 \), (21) becomes:

\[
g'(x, y) = g_{el}(x, y) - \left[ \int_0^h g_{el}(\tilde{x}, y) d\tilde{x} \right] \left[ \int_0^h \tilde{x} g_{el}(\tilde{x}, y) d\tilde{x} \right]^{-1} \times \left[ \begin{array}{c} \int_0^h \int_0^h g_{el}(\tilde{x}, \tilde{y}) d\tilde{x} d\tilde{y} \\ \int_0^h \int_0^h \tilde{y} g_{el}(\tilde{x}, \tilde{y}) d\tilde{x} d\tilde{y} \\ \int_0^h \int_0^h \tilde{x} \tilde{y} g_{el}(\tilde{x}, \tilde{y}) d\tilde{x} d\tilde{y} \\ \int_0^h \int_0^h \tilde{x} \tilde{y}^2 g_{el}(\tilde{x}, \tilde{y}) d\tilde{x} d\tilde{y} \end{array} \right]
\]
Element Green’s function: \( g_{el}(x, y) \)

\[
\begin{align*}
\mathcal{L}^* g_{el}(x, y) &= \delta(x - y) \quad \forall \quad x \in \Omega \\
g_{el}(x, y) &= 0 \quad \forall \quad x \in \Gamma \\
\end{align*}
\]

where \( \mathcal{L}^* = -\kappa \Delta u - \beta \cdot \nabla \), and solution of (20) [T.J.R. Hughes, et al 1998]

\[
g_{el}(x, y) = \begin{cases} 
C_1(y)(1 - e^{-2\alpha x/h}) & x \leq y \\
C_2(y)(e^{-2\alpha x/h} - e^{-2\alpha}) & x \geq y 
\end{cases}
\]

where

\[
C_1 = \frac{1 - e^{-2\alpha (1-(y/h))}}{\beta(1 - e^{-2\alpha})}, \quad C_2 = \frac{e^{2\alpha (y/h)} - 1}{\beta(1 - e^{-2\alpha})}
\]

where \( \alpha = \frac{\beta h}{2\kappa} \) is the mesh Péclet number, \( h = x_i - x_{i-1} \) is the local mesh-size
In 1D, $\mathcal{P} = \mathcal{P}_{H_0}$, fine-scale Green’s function $g'$ is **fully localized** within each element $\Rightarrow$ convenient evaluation of the fine-scale effects in VMS formulation.

This feature is not guaranteed for other projectors, e.g. $\mathcal{P} = \mathcal{P}_{L^2}$

**Remark:**
Selection of the projection is crucial in the development of a multiscale method
In 2D:

- There is difficulty in getting an analytical expression for \( g \) and \( g' \) through (18).
  
  **Remedy:** Numerically compute \( g \) and \( g' \) on a fine mesh of 524,288 elements (by standard Galerkin method) which is able to resolve the fine-scale effects.

- In general (for finer mesh), \( g' \) when \( \mathcal{P} = \mathcal{P}_{H^1_0} \) is better than \( \mathcal{P} = \mathcal{P}_{L^2} \) because it's fully localized \( \implies \) coarse-scale approximation \( \bar{u} \) for \( \mathcal{P}_{H^1_0} \) is better than \( \mathcal{P}_{L^2} \).

- However, if coarse scales are piecewise-polynomials, then fine-scales are not localized within each element for any projector (including \( \mathcal{P}_{H^1_0} \)) \( \implies \) difficulty in evaluating the fine-scale effects in VMS formulation.
Thank You!