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

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Outline

- Motivation
- The abstract framework
- The advection-diffusion model problem
- Projection and localization

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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, $\langle\cdot,\cdot\rangle_{V^*\times V}$ duality pairing, $\mathcal{L} : V \to V^*$ linear isomorphism.

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

$$\mathcal{L}u = f \tag{1}$$

VF: find $u \in V$ such that

$$\langle \mathcal{L}u, v\rangle_{V^*\times V} = \langle f, v\rangle_{V^*\times V} \quad \forall\, v \in V \tag{2}$$

Solution of (1) $u = \mathcal{G}f$, $\mathcal{G} : V^* \to V$, where $\mathcal{G} := \mathcal{L}^{-1}$

The variational multiscale formulation

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

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

$$V = \bar{V} \bigoplus V^{'} \tag{3}$$

$\Longrightarrow \forall\, v \in V,\ \ v = \bar{v} + v^{'}$ 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 $\bar{u} = \mathcal{P}u$

The variational multiscale formulation, contd.

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); $\mathcal{G}^{'} : V^* \to V$, which yields $u^{'} = \mathcal{G}^{'}(f - \mathcal{L}\bar{u})$

Having $\mathcal{G}^{'}$, eliminate $u^{'}$ from (4) $\Longrightarrow$ VMS for $\bar{u}$

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

admits a unique solution $\bar{u} = \mathcal{P}u$

The fine-scale Green's operator

$\mathcal{P}^T : \bar{V}^* \to V^*$ 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

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

$$\mathcal{G}^{'}\mathcal{P}^T = 0, \quad \textit{and} \quad \mathcal{P}\mathcal{G}^{'} = 0 \tag{8}$$

The fine-scale Green's operator, contd.

If $\dim(\bar{V}) = N$, we can find a set of functionals $\mu : V \to \mathbb{R}, \quad \{\mu_i\}_{i=1,\cdots,N}$ such that, for all $v \in V$

$$\langle \mu_i, v \rangle_{V^* \times V} = 0 \quad \forall \; i = 1, \cdots, N \quad \Longleftrightarrow \quad \mathcal{P} v = 0 \tag{9}$$

In this case, (8) is equivalent to:

$$\mathcal{G}^{'} \mu_i = 0 \quad \forall \, i = 1, \cdots, N \tag{10}$$

and

$$\langle \mu_i, \mathcal{G}^{'} \nu \rangle_{V^* \times V} = 0 \quad \forall \, \nu \in V^* \;\; \forall \, i = 1, \cdots, N \tag{11}$$

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

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

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

$$\mathcal{G}^{'} = \mathcal{G} - \mathcal{G}\boldsymbol{\mu}^T (\boldsymbol{\mu}\mathcal{G}\boldsymbol{\mu}^T)^{-1} \boldsymbol{\mu}\mathcal{G} \tag{12}$$

since $\{\mu_i\}_{i=1,\cdots,N}$ is a basis for the image of $\mathcal{P}^T$

Orthogonal projectors and optimization

Given scalar product $(\cdot,\cdot)$ defined on $V \times V$, the related **orthogonal projector** $\mathcal{P}$ is defined by

$$(\mathcal{P}w, \bar{v}) = (w, \bar{v}) \quad \forall\, w \in V, \;\; \bar{v} \in \bar{V}$$

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:

$$\mathcal{L}u = -\kappa\Delta u + \beta \cdot \nabla u = f \quad \text{in} \quad \Omega \quad u|_{\partial\Omega} = 0 \tag{13}$$

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

VF: $V = H_0^1 \equiv H_0^1(\Omega), \quad V^* = H^{-1}$

Representation: Green's operator $\mathcal{G}$ through the Green's function $g : \Omega \times \Omega \to \mathbb{R}$ such that:

$$u(y) = \int_\Omega g(x, y) f(x) dx \quad \text{a.e} \quad y \in \Omega$$

The advection-diffusion model problem, contd.

Similar representation: fine-scale Green's operator $\mathcal{G}^{'}$ through the fine-scale Green's function $g^{'} : \Omega \times \Omega \rightarrow \mathbb{R}$ gives the fine scale component $u^{'}$ of u from $r = f - \mathcal{L}\bar{u}$:

$$u^{'}(y) = \int_{\Omega} g^{'}(x, y) r(x) dx \tag{14}$$

where the space $V^{'}$ and function $g^{'}$ depends on the underlying projector $\mathcal{P}$

The advection-diffusion model problem, contd.

Having $\{\mu_i\}_{i,\cdots N}$ such that:

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

Then, $g^{'}$ is obtained by (12) as:

$$\begin{aligned} g'(x,y) \quad = \quad & g(x,y) - \left[\int_\Omega g(\tilde{x},y)\mu_1(\tilde{x})d\tilde{x} \quad \cdots \quad \int_\Omega g(\tilde{x},y)\mu_N(\tilde{x})d\tilde{x} \right] \\ & \times \begin{bmatrix} \int_\Omega g(\tilde{x},\tilde{y})\mu_1(\tilde{x})\mu_1(\tilde{y})d\tilde{x}d\tilde{y} & \dots & \int_\Omega g(\tilde{x},\tilde{y})\mu_N(\tilde{x})\mu_1(\tilde{y})d\tilde{x}d\tilde{y} \\ \vdots & \ddots & \vdots \\ \int_\Omega g(\tilde{x},\tilde{y})\mu_1(\tilde{x})\mu_N(\tilde{y})d\tilde{x}d\tilde{y} & \dots & \int_\Omega g(\tilde{x},\tilde{y})\mu_N(\tilde{x})\mu_N(\tilde{y})d\tilde{x}d\tilde{y} \end{bmatrix}^{-1} \\ & \times \begin{bmatrix} \int_\Omega g(x,\tilde{y})\mu_1(\tilde{y})d\tilde{y} \\ \vdots \\ \int_\Omega g(x,\tilde{y})\mu_N(\tilde{y})d\tilde{y} \end{bmatrix} \end{aligned} \tag{15}$$

VMS for advection-diffusion model problem

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

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

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

$$\begin{aligned}\int_\Omega (\kappa\nabla\bar{u}(x) - \beta\bar{u}) \cdot \nabla\bar{v}(x)dx - \int_\Omega\int_\Omega \mathcal{L}\bar{u}(x)g^{'}(x, y)\mathcal{L}^*\bar{v}(y)dxdy \\ = \int_\Omega f(x)\bar{v}dx - \int_\Omega\int_\Omega f(x)g^{'}(x, y)\mathcal{L}^*\bar{v}(y)dxdy \\ \forall\ \bar{v} \in \bar{V}\end{aligned}$$

Linear elements and H_0^1-optimality in 1D

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), $i =, \cdots, n_{el}$

For the H_0^1-projector $\mathcal{P} = \mathcal{P}_{H_0^1}$ the VMS provides a nodally exact approximation $\bar{u}$ of the exact solution u.

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

$$g^{'}(x, x_i) = g^{'}(x_i, y) = 0 \quad \forall\, i = 1, \cdots, N, \quad 0 \leq x, y \leq L; \tag{17}$$

i.e., $g^{'}$ vanishes if one of its two arguments is a node of the grid.

Linear elements and H_0^1-optimality in 1D, contd.

As a result, the expression (16) for the fine-scale Green's function in this case becomes:

$$
\begin{aligned}
g'(x,y) \quad = \quad & g(x,y) - \begin{bmatrix} g(x_1,y) & \cdots & g(x_N,y) \end{bmatrix} \\
& \times \begin{bmatrix} g(x_1,x_1) & \dots & g(x_N,x_1) \\ \vdots & \ddots & \vdots \\ g(x_1,x_N) & \dots & g(x_N,x_N) \end{bmatrix}^{-1} \\
& \times \begin{bmatrix} g(x,x_1) \\ \vdots \\ g(x,x_N) \end{bmatrix}
\end{aligned}
$$

Linear elements and H_0^1-optimality in 1D, contd.

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*:

$$V^{'} = \bigoplus_{i=1,\cdots,n_{el}} H_0^1(x_{i-1}, x_i),$$

Linear elements and H_0^1-optimality in 1D, contd.

If we assume piecewise-constant coefficients κ, β and source term f, the fine-scale VE:

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

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

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

$$\tau_1 \equiv \tau_{1,(x_{i-1},x_i)} = \frac{\int_{x_{i-1}}^{x_i} \int_{x_{i-1}}^{x_i} g'(x,y) dxdy}{x_i - x_{i-1}} = \frac{h}{2\beta}\Big(\coth(\alpha) - \frac{1}{\alpha}\Big)$$

where $\alpha = \frac{\beta h}{2\kappa}$ is the mesh Péclet number, $h = x_i - x_{i-1}$ is the local mesh-size

Higher order elements and H_0^1-optimality in 1D

Consider higher-order piecewise-polynomial coarse: $0 = x_0 < x_1 < \cdots < x_{n_{el}-1} = L$ and set

$$\bar{V} = \{\bar{v} \in H_0^1(0, L) \text{ such that } \bar{v}_{|(x_{i-1}, x_i)} \in \mathbb{P}_k,\ 1 \leq i \leq n_{el}\}$$

$V^{'}$ is a strict subset of *bubbles*:

$$V^{'} \subset_{\neq} \bigoplus_{i=1,\cdots,n_{el}} H_0^1(x_{i-1}, x_i), \tag{18}$$

Higher order elements and H_0^1-optimality in 1D, contd.

Consider: $V_i^{'} = V^{'}_{|(x_{i-1},x_i)}$; as fine-scale of bubbles,

$\bar{V}_i = \bar{V}_{|(x_{i-1},x_i)} \cap H_0^1(x_{i-1}, x_i)$ space of bubbles of coarse-scale

$V_i = H_0^1(x_{i-1}, x_i) = \bar{V}_i \bigoplus V_i^{'}$ 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 $(0, h) \times (0, h)$

$$
\begin{aligned}
g'(x,y) \quad = \quad & g_{el}(x,y) - \left[\int_0^h g_{el}(\tilde{x},y)d\tilde{x} \quad \cdots \quad \int_0^h \tilde{x}^{k-2} g_{el}(\tilde{x},y)d\tilde{x} \right] \\
& \times \begin{bmatrix} \int_0^h \int_0^h g_{el}(\tilde{x},\tilde{y})d\tilde{x}d\tilde{y} & \cdots & \int_0^h \int_0^h \tilde{x}^{k-2} g_{el}(\tilde{x},\tilde{y})d\tilde{x}d\tilde{y} \\ \vdots & \ddots & \vdots \\ \int_0^h \int_0^h \tilde{y}^{k-2} g_{el}(\tilde{x},\tilde{y})d\tilde{x}d\tilde{y} & \cdots & \int_0^h \int_0^h \tilde{x}^{k-2}\tilde{y}^{k-2} g_{el}(\tilde{x},\tilde{y})d\tilde{x}d\tilde{y} \end{bmatrix}^{-1} \\
& \times \begin{bmatrix} \int_0^h g_{el}(x,\tilde{y})d\tilde{y} \\ \vdots \\ \int_0^h \tilde{y}^{k-2} g_{el}(x,\tilde{y})d\tilde{y} \end{bmatrix}
\end{aligned}
\tag{19}
$$

Higher order elements and H_0^1-optimality in 1D, contd.

For $k = 2$, (21) yields:

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

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

$$\begin{aligned} g'(x,y) &= g_{el}(x,y) - \begin{bmatrix} \int_0^h g_{el}(\tilde{x},y)d\tilde{x} & \int_0^h \tilde{x}g_{el}(\tilde{x},y)d\tilde{x} \end{bmatrix} \\ &\times \begin{bmatrix} \int_0^h \int_0^h g_{el}(\tilde{x},\tilde{y})d\tilde{x}d\tilde{y} & \int_0^h \int_0^h \tilde{x}g_{el}(\tilde{x},\tilde{y})d\tilde{x}d\tilde{y} \\ \int_0^h \int_0^h \tilde{y}g_{el}(\tilde{x},\tilde{y})d\tilde{x}d\tilde{y} & \int_0^h \int_0^h \tilde{x}\tilde{y}g_{el}(\tilde{x},\tilde{y})d\tilde{x}d\tilde{y} \end{bmatrix}^{-1} \\ &\times \begin{bmatrix} \int_0^h g_{el}(x,\tilde{y})d\tilde{y} \\ \int_0^h \tilde{y}^{k-2}g_{el}(x,\tilde{y})d\tilde{y} \end{bmatrix} \end{aligned}$$

Expression for element Green's function

Element Green's function : $g_{el}(x, y)$

$$\left.\begin{aligned} \mathcal{L}^* g_{el}(x,y) = \delta(x-y) \quad \forall \quad x \in \Omega \\ g_{el}(x,y) = 0 \quad \forall \quad x \in \Gamma \end{aligned}\right\} \quad e = 1, \cdots, n_{el} \tag{20}$$

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

L^2-optimality in 1D and localization of $g^{'}$

In 1D, $\mathcal{P} = \mathcal{P}_{H_0^1}$ fine-scale Green's function $g^{'}$ is **fully localized** within each element $\implies$ conveniet 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

Linear element in 2D

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 $\mathcal{P} = \mathcal{P}_{H_0^1}$ is better than $\mathcal{P} = \mathcal{P}_{L^2}$ because it's **fully localized** $\Longrightarrow$ coarse-scale approximation $\bar{u}$ for $\mathcal{P}_{H_0^1}$ 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 $\mathcal{P}_{H_0^1}$) $\Longrightarrow$ difficulty in evaluating the fine-scale effects in VMS formulation.

Thank You!