Simulations with adaptive modeling

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Introduction

- Engineering problems often involve models of different complexity, scales and accuracy
- Most accurate and validated model cannot be chosen because of computational costs
- Simpler models are computationally efficient but may only capture a few features of original problem

- Adaptive model simulation
  - Apply detailed model only where needed
  - Balance model and discretization errors
- Estimate modeling errors together with discretization errors
- Main tool: A posteriori error indicators of modeling and of discretization errors
  - Reliable (upper bound)
  - Efficient (lower bound)
  - Localized to mesh cells

Literature overview

- Computational solid and fluid mechanics
  - Fatone, Gervasio & Quarteroni '01 (NS/Oseen)
  - Perotto '04 (Shallow-water eqs.)
  - Amara, Capatina & Trujillo '04 (Free-surface NS 3D/2D/1D)
  - Oden & Vemaganti '00, Oden & Prudhomme '02 (elasticity)
- Hierarchical model dimension reduction
  - elliptic problems on thin plates
  - Vogelius & Babuška '81, Babuška & Schwab '96, Ainsworth '98
- Heterogeneous Multiscale Methods
  - E & Engquist '03

Outline

1. Adaptive modeling with invariant functional space
   - error estimates & computational results
   - coll. with M. Braack [Univ. Heidelberg] ’03
2. Micro-macro models of polymeric flows
   - no error estimates, promising computational results
   - coll. with T. Lelièvre [ENPC] & M. Braack
3. Hierarchical model dimension reduction
   - adaptive modeling with functional space conformity
   - error estimates, implementation in progress
   - coll. with S. Perotto & A. Veneziani [MOX]

Adaptive modeling with invariant functional space

- A posteriori error estimates
  - linear model error
  - nonlinear model error
  - nonlinear model and discretization errors
- An adaptive model-mesh algorithm
  - selecting and evaluating the error indicators
  - example on a toy problem
  - application: adaptive diffusion modeling in flames

Linear model error

- Exact solution

$$u \in V : \quad \underbrace{a(u,\phi)}_{\text{simple model}} + \underbrace{d(u,\phi)}_{\text{complexities}} = \underbrace{(f,\phi)}_{\text{data}} \quad \forall \phi \in V$$

- Approximate solution (same functional space)

$$u_m \in V : \quad a(u_m,\phi) = (f,\phi) \quad \forall \phi \in V$$

- Both problems are assumed to be well–posed
- Given linear output functional j, estimate modeling error

$$j(e_u) = j(u - u_m) = j(u) - j(u_m)$$

- Main tool: Duality-based a posteriori error estimates
  - discretization error estimates [Johnson '95, Becker & Rannacher, '96]
- Dual problem

$$\begin{cases} z \in V : \quad a(\phi, z) + d(\phi, z) = j(\phi) \quad \forall \phi \in V \\ j(e_u) = -d(u_m, z) \end{cases}$$

- Reduced dual problem

$$\begin{cases} z_m \in V : \quad a(\phi, z_m) = j(\phi) \quad \forall \phi \in V \\ j(e_u) = -d(u_m, z_m) + R \end{cases}$$

where

$$R = -\tfrac{1}{2}[(d(u_m, e_z) + d(e_u, z_m)]$$

is a h.o.t. in modeling errors $e_u := u - u_m$ and $e_z := z - z_m$

Nonlinear model error

- Semilinear forms $a(u;\phi)$ and $d(u;\phi)$
- Nonlinear output functional $j(u)$
- Directional (Gateaux)-derivative

$$a'(u;v,\phi) = \lim_{\epsilon\longrightarrow 0} \frac{1}{\epsilon}\Big(a(u+\epsilon v;\phi) - a(u;\phi)\Big)$$

- Full and reduced models

$$\begin{aligned} u \in V : \quad & a(u;\phi) + d(u;\phi) = (f,\phi) \quad \forall \phi \in V \\ u_m \in V : \quad & a(u_m;\phi) = (f,\phi) \quad \forall \phi \in V \end{aligned}$$

- Full and reduced dual problems

$$\begin{aligned} z \in V : \quad & a'(u;\phi,z) + d'(u;\phi,z) = j'(u;\phi) \quad \forall \phi \in V \\ z_m \in V : \quad & a'(u_m;\phi,z_m) = j'(u_m;\phi) \quad \forall \phi \in V \end{aligned}$$

- Dual problems are linear

Error representation

$$
\begin{aligned}
j(u) - j(u_m) = & - d(u_m; z_m) && \text{(order 0)} \\
& - \tfrac{1}{2}[d(u_m; e_z) + d'(u_m; e_u, z_m)] && \text{(order 1)} \\
& - R && \text{(order 3)}
\end{aligned}
$$

with $e_u := u - u_m$ and $e_z := z - z_m$

Nonlinear model and discretization error

- Discretization subspace $V_h \subset V$
- Residuals

$$\rho(u_{hm})(\phi) := (f,\phi) - a(u_{hm};\phi)$$
$$\rho^*(u_{hm},z_{hm})(\phi) := j'(u_{hm};\phi) - a'(u_{hm};\phi,z_{hm})$$

- Discrete reduced problems

$$u_{hm} \in V_h : \quad \rho(u_{hm})(\phi) = 0 \qquad \forall \phi \in V_h$$
$$z_{hm} \in V_h : \quad \rho^*(u_{hm},z_{hm})(\phi) = 0 \quad \forall \phi \in V_h$$

Error representation

$$
\begin{aligned}
j(u) - j(u_{hm}) = &- d(u_{hm}; z_{hm}) && \text{(order 0)}\\
&- \tfrac{1}{2}[\rho(u_{hm})(z - i_h z) + \rho^*(u_{hm}, z_{hm})(u - i_h u)] && \text{(order 0)}\\
&- \tfrac{1}{2}[d(u_{hm}; e_z) + d'(u_{hm}; e_u, z_{hm})] && \text{(order 1)}\\
&- R && \text{(order 3)}
\end{aligned}
$$

for arbitrary interpolation operator $i_h : V \to V_h$

An adaptive model-mesh algorithm

Recall: $$j(u) - j(u_{hm}) = -d(u_{hm}; z_{hm}) - \tfrac{1}{2}[\rho(u_{hm})(z - i_h z) + \rho^*(u_{hm}, z_{hm})(u - i_h u)] - \tfrac{1}{2}[d(u_{hm}; e_z) + d'(u_{hm}; e_u, z_{hm})] - R$$

- Model error indicator

$$\eta_m = -d(u_{hm}; z_{hm})$$

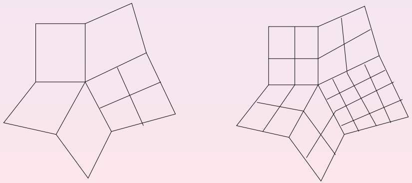
- Mesh error indicator

$$\eta_h = -\tfrac{1}{2}[\rho(u_{hm})(z - i_h z) + \rho^*(u_{hm}, z_{hm})(u - i_h u)]$$

- Neglect higher-order terms
  - some can be estimated by solving local problems

Evaluating the error indicators

- $\eta_m = -d(u_{hm}; z_{hm})$ can be readily evaluated
- Many techniques available to evaluate η_h
  - V_h: pcw. linears on locally refined, tensor-product meshes
  - $V_{2h}^{(2)}$: pcw. quadratics on coarser mesh
  - interpolation operator $i_{2h}^{(2)} : V_h \to V_{2h}^{(2)}$



- Approximate

$$u - i_h u \approx i_{2h}^{(2)} u_{hm} - u_{hm}$$

$$z - i_h z \approx i_{2h}^{(2)} z_{hm} - z_{hm}$$

- Mesh error indicator

$$\eta_h = \frac{1}{2}[\rho(u_{hm})(i_{2h}^{(2)} z_{hm}) + \rho^*(u_{hm}, z_{hm})(i_{2h}^{(2)} u_{hm})]$$

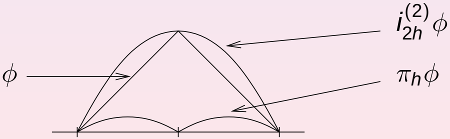
- Localize error indicators η_m and η_h
  - no theoretical justification
- Nodal localization of model error indicator
  - Lagrangian nodal basis $\{\phi_i\} \subset V_h$
  - U, Z: nodal components of u_{hm} and z_{hm}
  - nodal model error estimator $\eta_{m,i} = Z_i d(u_{hm}; \phi_i)$

- Nodal localization of mesh error indicator
  - quadratic basis functions $\phi_i^{(2)} = i_{2h}^{(2)}\phi_i$
  - residual contributions

$$\Psi_i = \rho(u_{hm})(\phi_i^{(2)}) \qquad \Psi_i^* = \rho^*(u_{hm}, z_{hm})(\phi_i^{(2)})$$

  - nodal mesh error estimator $\eta_h = \frac{1}{2}\sum_i(\Psi_i Z_i + \Psi_i^* U_i)$

- Filter to remove node to node oscillation of residual
  - filter operator $\pi_h\phi = \phi - i_{2h}^h\phi$
  - filtered estimator $\eta_h = \frac{1}{2}\sum_i(\Psi_i^\pi Z_i + \Psi_i^{*\pi} U_i)$



Adapting the model and the mesh

- Adaptive step i
- Discrete subspace V_i depends on i because of mesh refinement
- Semilinear form a_i depends on i because of model modification
- Solve

$$\begin{aligned} u_i \in V_i : \quad & a_i(u_i;\phi) &= (f,\phi) \quad & \forall \phi \in V_i \\ z_i \in V_i : \quad & a_i'(u_i;\phi,z_i) &= j'(u_i;\phi) \quad & \forall \phi \in V_i \end{aligned}$$

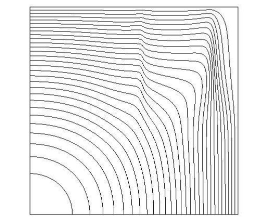
- Transfer nodal error indicators to mesh cells
- Error balancing to select cells where modifications occur

$$\eta_i > \alpha\overline{\eta} \qquad \alpha \in (0,1)$$

- Either the model or the mesh is modified locally
  - check locally which error indicator is larger

Example on toy problem

- Model problem: $-\nabla \cdot (\mu \nabla u) = f$ on $\Omega = (0,1)^2$
- Adaptivly choosing between
  - detailed model: μ oscillates on upper right quadrant
  - simplified model: $\mu \equiv 1$ everywhere



- Very fine mesh is used (no discretization error)

$$j(u) = \int_{(0.8,1)\times(0.4,0.6)} u \, dx$$

iter	% exact m.	η_m	$j(e)$	I_{eff}
1	0	2.78e-04	3.95e-04	0.70
2	32.25	-8.88e-05	-5.07e-05	1.75
3	42.88	-6.39e-05	-3.92e-05	1.63
4	50.49	-2.84e-05	-1.73e-05	1.64
5	67.09	-4.65e-07	-2.93e-07	1.59
6	78.53	-6.99e-08	-6.81e-08	1.03

- Areas with exact model (light) and crude model (dark)

2 iterations

4 iterations

Application: adaptive diffusion models in flames

- Systems of nonlinear coupled PDE's
- Ozone flame (6 PDE's)
  - moderate impact of detailed model
- Hydrogen flame (12 PDE's)
  - sizeable impact of detailed model

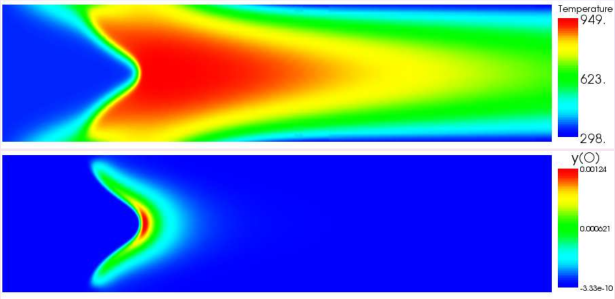
Ozone flame

- Ozone flame: $2O_3 + O_2 \to 4O_2$
- Three chemical species participating in 6 elementary reactions with Arrhenius type rates

O_3, O_2 and O

Reaction			A	β	E_a
O+O+M	$\to$	O_2+M	2.900×10^{17}	-1	0
O_2+M	$\to$	O+O+M	6.772×10^{18}	-1	496
O_2+O+M	$\to$	O_3+M	3.426×10^{13}	0	-4.234
O_3+M	$\to$	O_2+O+M	9.500×10^{14}	0	95.03
O+O_3	$\to$	O_2+O_2	5.200×10^{12}	0	17.38
O_2+O_2	$\to$	O+O_3	4.381×10^{12}	0	414.39

- 2D premixed flame in a slot with heated lateral walls
- Temperature and O-radical profiles



- Governing equations
  - compressible NS equations for 2D flow velocities
  - energy balance for temperature
  - 3 mass balance equations for chemical species
  - 6 coupled, strongly nonlinear PDE's
- Species balance equations

$$v(y) \cdot \nabla y + \nabla \cdot \mathcal{F}(y) = f(y)$$

$y = (y_{\mathrm{O}_3}, y_{\mathrm{O}_2}, y_{\mathrm{O}})^T$: species mass fractions

$\mathcal{F} = (\mathcal{F}_{\mathrm{O}_3}, \mathcal{F}_{\mathrm{O}_2}, \mathcal{F}_{\mathrm{O}})^T$: species diffusion fluxes

- Simplified model
  - Fick type diffusion

$$\mathcal{F}_i = -D_i \nabla y_i$$

- Detailed model
  - multicomponent diffusion and thermal diffusion (Soret effect)

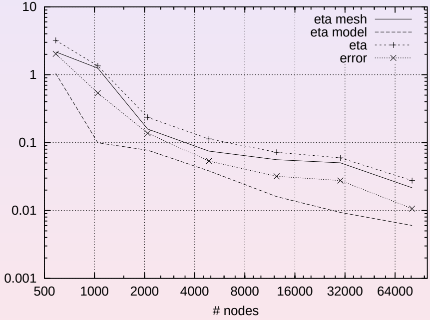
$$\mathcal{F}_i = -\sum_j D_{ij}(y)\nabla y_j - \theta_i(y)\nabla T$$

  - D_{ij} and θ_i can be evaluated from the kinetic theory of gas mixtures
  - need to solve constrained linear systems of size the number of species at each mesh node
  - use transport algorithms of Ern & Giovangigli '94

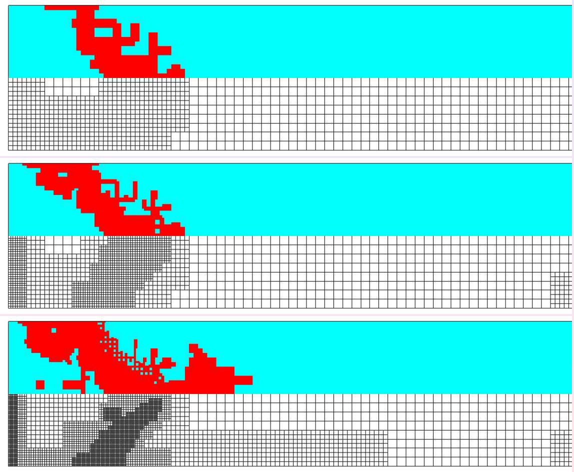
- Output functional $j(u) = c \int_\Omega y_{\mathrm{O}}$
- Reference solution with detailed model on very fine mesh
- Impact of detailed model is moderate

#nodes	% of multi.	η_h	η_m	η	$j(u-u_{hm})$	I_{eff}
585	0	2.168	1.043	3.210	2.031	1.58
1 047	21.1	1.250	9.953e-2	1.350	5.385e-1	2.51
2 085	37.4	1.584e-1	7.729e-2	2.356e-1	1.378e-1	1.71
4 871	48.9	7.488e-2	3.830e-2	1.132e-1	5.351e-2	2.12
12 421	52.4	5.605e-2	1.602e-2	7.206e-2	3.186e-2	2.26
30 013	66.3	5.029e-2	9.372e-3	5.966e-2	2.757e-2	2.16
81 021	79.4	2.160e-2	6.017e-3	2.761e-2	1.065e-2	2.59

- Convergence history as a function of number of nodes



- Local model and mesh adaption after 2, 3 and 4 iterations



Hydrogen flame

- 9 chemical species, 19 elementary reactions
- Underventilated diffusion flame flown from a slot in periodic setting
- Simplified model: Fick type diffusion
- Detailed model: Multicomponent diffusion with Soret effect
- Sizeable impact of detailed model

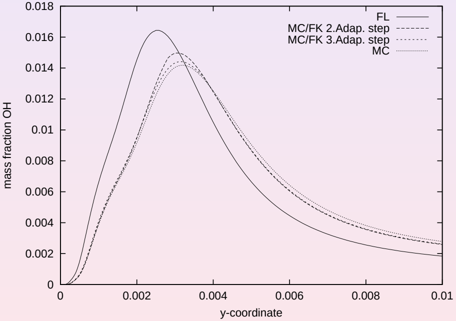
simplified

detailed

- Output functional $j(u) = \int_\Gamma y_{\mathrm{OH}}$ along a line Γ cutting the flame

#nodes	% of multi.	$j(u_h)$	η_h	η_m	η
8 481	0	1.1920	-4.705e-02	-3.211e-01	-3.681e-01
8 901	15.5	0.8286	9.177e-03	-3.754e-03	5.423e-03
13 285	45.8	0.8312	6.341e-03	-8.836e-03	-2.496e-03
25 767	71.8	0.8251	-2.083e-03	-5.040e-03	-7.123e-03
48 575	84.4	0.8171	-1.267e-03	-9.894e-04	-2.256e-03

- Comparison of OH mass fraction along a line
- Profile well captured after only 2/3 adaptive steps



Micro-macro models of polymeric fbws

- Dilute polymeric fluids
  - non-interacting polymer chains
  - diluted in a Newtonian solvent
- Rheology of the fluid influenced by polymer chains: Non-Newtonian behavior
- Stress tensor depends in a complicated manner on the history of the deformation of the fluid

- Micro-macro models
  - microscopic description of the dynamics of polymer chains
  - stochastic PDE modeling solvent-polymer interactions
  - coupled to macroscopic description of solvent through stress tensor
  - compare favorably with experiments
  - computationally intensive
  - CONNFFESSIT approach (Monte Carlo+FE) [Laso & Öttinger '93; Hulsen et al. '97; Bonvin & Picasso '99, Keunings '00]
- Macro models
  - full macroscopic description
  - can be derived from micro-macro models *via* closure relations linking stress and strain (e.g. Oldroyd-B)
  - less favorable comparison with experiments
  - computationally cheaper than micro-macro models

Micro-macro model

- Dumbbell model
  - polymer chain modeled by two beads linked by a spring
  - end-to-end vector: random variable $\boldsymbol{X}_t$
  - Brownian configuration field: $\boldsymbol{X}_t$ depends on $\boldsymbol{x}$
- Governing equations

$$\mathrm{Re}\,(\partial_t \boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}) = (1-\epsilon)\Delta\boldsymbol{u} - \nabla p + \nabla\cdot\boldsymbol{\tau}$$

$$\nabla\cdot\boldsymbol{u} = 0$$

$$\boldsymbol{\tau} = \frac{\epsilon}{\mathrm{We}}\left(\mathbb{E}\,(\boldsymbol{X}_t \otimes \nabla\Pi(\boldsymbol{X}_t)) - \mathrm{Id}\right)$$

$$d\boldsymbol{X}_t + \boldsymbol{u}\cdot\nabla_{\boldsymbol{x}}\boldsymbol{X}_t\,dt = \left(\nabla_{\boldsymbol{x}}\boldsymbol{u}\boldsymbol{X}_t - \frac{1}{2\mathrm{We}}\nabla\Pi(\boldsymbol{X}_t)\right)dt + \frac{1}{\sqrt{\mathrm{We}}}d\boldsymbol{W}_t$$

$d\boldsymbol{W}_t$: d-dimensional standard Brownian motion
$\boldsymbol{F}(\boldsymbol{X}_t) := \nabla\Pi(\boldsymbol{X}_t)$ models the force between the two beads

- Non-dimensional numbers
  - Re : Reynolds number
  - We : Weissenberg number (polymer chain time to fluid time ratio)
  - $\epsilon \in (0,1)$: polymer chain viscosity to total viscosity ratio
- Finite extensible nonlinear elastic (FENE) dumbbells [Warner '72]

$$\Pi(\boldsymbol{X}) = -\frac{b}{2}\ln\left(1 - \frac{|\boldsymbol{X}|^2}{b}\right) \qquad \boldsymbol{F}(\boldsymbol{X}) = \frac{\boldsymbol{X}}{1 - |\boldsymbol{X}|^2/b}$$

Polymer contribution to stresses

$$\boldsymbol{\tau} = \frac{\epsilon}{\mathrm{We}}\left(\mathbb{E}\left(\frac{\boldsymbol{X}_t \otimes \boldsymbol{X}_t}{1 - |\boldsymbol{X}_t|^2/b}\right) - \mathrm{Id}\right)$$

Macro model

- FENE-P model [Peterlin '66; Bird et al. '81]

$$\boldsymbol{F}(\boldsymbol{X}_t) = \frac{\boldsymbol{X}_t}{1 - \mathbb{E}(|\boldsymbol{X}_t|^2)/b}$$

- Covariance tensor obtained from nonlinear macroscopic PDE

$$\frac{d\boldsymbol{A}}{dt} + \boldsymbol{u}\cdot\nabla\boldsymbol{A} - \nabla\boldsymbol{u}\boldsymbol{A} + \boldsymbol{A}\nabla\boldsymbol{u}^T = -\frac{1}{\mathrm{We}}\frac{\boldsymbol{A}}{1-\mathrm{tr}(\boldsymbol{A})/b} + \frac{1}{\mathrm{We}}\mathrm{Id}$$

and recover

$$\boldsymbol{\tau} = \frac{\epsilon}{\mathrm{We}}\left(\frac{\boldsymbol{A}}{1-\mathrm{tr}(\boldsymbol{A})/b} - \mathrm{Id}\right)$$

- FENE-P model can be simulated by deterministic methods

Adaptive micro-macro approach

- Use elementwise either detailed (FENE, micro-macro) or simplified (FENE-P, macro) models
- Solvers
  - FENE: CONNFFESSIT method plus VR
  - FENE-P: P_1(velocity)/P_0(stresses) FE

Adaptive algorithm

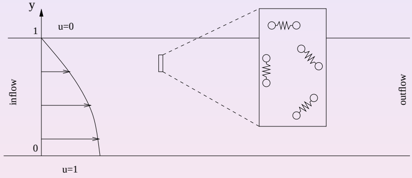
For each time step, at each mesh cell,

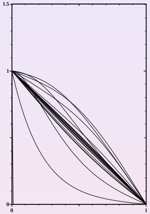
1. compute stress tensor and velocity
2. estimate alternative stress tensor and velocity (which would have been obtained with the other model)
3. based on these estimates, possibly switch model

- If detailed (FENE, micro-macro) model is used in a cell,
  - Monte Carlo method to solve stochastic PDE for M dumbbells
  - switching to simplified model simply involves ensemble averages
- If simplified (FENE-P, macro) model is used in a cell,
  - evolve $\frac{1}{\delta}M$, $\delta \gg 1$, dumbbells to compute estimates
  - switch to detailed model by replicating the ensemble of $\frac{1}{\delta}M$ dumbbells δ times

Results

- Start-up of shear flow (1D problem)





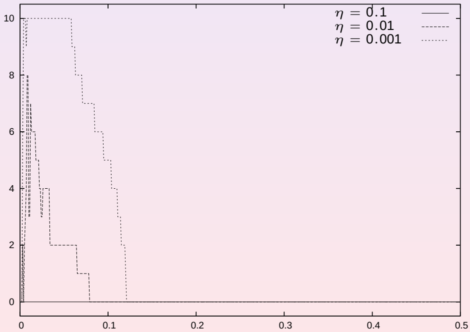
- Initially, flow is at rest and dumbbells at equilibrium
  - $\boldsymbol{X}_0$ follows the law $\frac{b+2}{2\pi b}(1 - |\boldsymbol{X}|^2/b)^{b/2} 1_{|\boldsymbol{X}|^2<b}\, d\boldsymbol{X}$
- Simplified model initially used in each cell
- Parameters: $\mathrm{Re} = 0.1$, $\mathrm{We} = 0.5$, $\epsilon = 0.9$, $b = 20$, $M = 10^4$, $\delta = 10^2$, $I = 10$ mesh cells, $N = 2000$ timesteps

- Speedups w.r. to execution time of fully detailed model

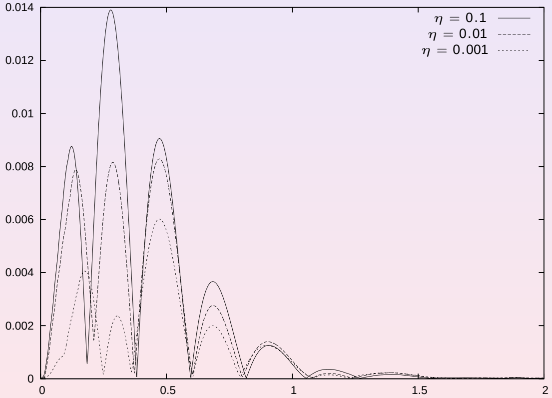
η	0.1	0.01	0.001
speedup	81	37	19

η: error control parameter

- Number of cells where detailed model is used



- Accuracy assessment: time evolution of relative velocity error

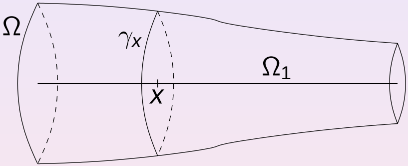


Hierarchical model dimension reduction

- Elliptic problems on thin plates [Babuška & Vogelius '81]
  - problem dimension reduced by 1 (3D→2D; 2D→1D)
  - reduced space spanned by modal basis functions
  - reduced solution: energy projection of exact solution onto reduced space
  - careful selection of modal basis for asymptotic optimality w.r. to plate thickness
- A posteriori error analysis
  - residual-type modeling error estimates [Babuška & Schwab '96]
  - modeling and discretization error estimates by solving local problems [Ainsworth '98]

The present setting

- Fibre domain $\Omega = \bigcup_{x\in\Omega_1} \gamma_x$ with 1D generatrix Ω_1 and fibers γ_x



- Geometric maps

$$\psi_x : \gamma_x \longrightarrow S_{d-1} \subset \mathbb{R}^{d-1}$$

C^1-diffeomorphisms with smooth dependence on x

- Model reduction: 3D→1D
- Targetted applications
  - haemodynamics (blood flows in vessels)
  - hydraulics (river flows in estuaries)
- Simpler setting: elliptic linear PDE with energy space V

$$u \in V \quad : \quad a(u,v) = f(v) \quad \forall v \in V$$

- Reduced energy space: Two ingredients
  - energy space for 1D problem on Ω_1: V^{1D}
  - modal basis functions $\{\varphi_k\}_{k\in\mathbb{N}}$, $\varphi_k : S_{d-1} \to \mathbb{R}$

$$V_m = \left\{ v(x,\mathbf{y}) = \sum_{k=1}^{m} v_k(x)\, \varphi_k(\psi_x(\mathbf{y})), \text{ with } v_k \in V^{\mathrm{1D}} \right\}$$

- Conformity: $V_m \subset V$
- Spectral approximability

$$\forall v \in V, \qquad \lim_{m\to+\infty} \left(\inf_{v_m \in V_m} \|v - v_m\|_V \right) = 0$$

- Reduced problem: energy projection of exact solution onto V_m

$$u_m \in V_m \quad : \quad a(u_m, v_m) = f(v_m) \quad \forall v_m \in V_m$$

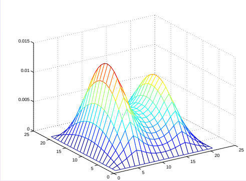
- Spectral optimality

$$\|u - u_m\|_V \lesssim \inf_{v_m \in V_m} \|u - v_m\|_V$$

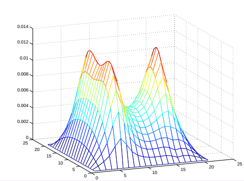
- Reduced problem amounts to solving m coupled 1D problems

Illustrations

- Transverse effects induced by source term

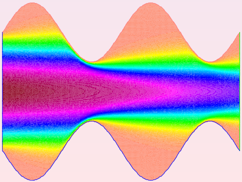


1 mode



3 modes

- Transverse effects induced by shape of domain



FE approximation of reduced problem

- FE approximation for 1D problem, mesh $\mathcal{T}_h$

$$V_h^{\mathrm{1D}} \subset V^{\mathrm{1D}}$$

- Spatially variable modal expansions $m := \{m_T\}_{T \in \mathcal{T}_h}$

$$V_{hm}^* = \left\{ \forall T \in \mathcal{T}_h,\ v|_T = \sum_{k=1}^{m_T} v_{kh}(x)\,\varphi_k(\psi_x(\mathbf{y})),\ \text{with } v_{kh} \in V_h^{\mathrm{1D}} \right\}$$

- Conforming subspace $V_{hm} = V_{hm}^* \cap V$

- Discrete reduced problem

$$u_{hm} \in V_{hm} \quad : \quad a(u_{hm}, v_{hm}) = f(v_{hm}) \quad \forall v_{hm} \in V_{hm}$$

- Practical implementation
  - discrete reduced problem posed on V^*_{hm}
  - matching conditions at interfaces between different modal expansions enforced by DN-type iterations

A posteriori error analysis

- Hierarchical setting
- Spectrally enriched space

$$V_{hm}^{+} = \left\{ \forall T \in \mathcal{T}_h,\ v|_T = \sum_{k=1}^{m_T^+} v_{kh}(x)\, \varphi_k(\psi_x(\mathbf{y})),\ \text{with } v_{kh} \in V_h^{\mathrm{1D}} \right\}$$

with $m_T^+ > m_T$ for all $T \in \mathcal{T}_h$

- Auxiliary problem to be solved

$$u_{hm}^+ \in V_{hm}^+ \quad : \quad a(u_{hm}^+, v_{hm}^+) = f(v_{hm}^+) \quad \forall v_{hm}^+ \in V_{hm}^+$$

- Output functional $J : V \to \mathbb{R}$
- Saturation assumption $|J(u - u_m^+)| \leq \beta |J(u - u_m)|$ $(\beta \in (0,1))$ yields

$$|J(u - u_{hm})| \lesssim \underbrace{|J(u_m^+ - u_{hm}^+)|}_{A} + \underbrace{|J(u_m - u_{hm})|}_{B} + \underbrace{|J(u_{hm}^+ - u_{hm})|}_{C}$$

$A + B$: discretization errors estimated by standard techniques
C: modeling error readily computable

- Global lower bounds can be established under additional assumptions
- Implementation in progress

Conclusions

- Adaptive model/mesh simulations driven by a posteriori error estimates are feasible
- Many interesting mathematical issues remain open, including
  - error analysis for coupled stochastic/determinsitic PDE's
  - well-posedness of dimensionally reduced problems beyond coercivity paradigm [Amara et al. '04]
- Is it computationally worthwhile?
  - moderate speedups in flame simulation: model and mesh refinement strongly correlated
  - significant speedups for polymeric fluid flow simulations
  - speedups must be weighted against implementing complex code

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