Computational Multiscale Modeling: Adaptive Methods and FETK with Applications in Biophysics

Fast high-fidelity numerical methods inside APBS, SMOL, and related efforts

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Outline

Partial Differential Equations (PDE): Notation, etc

Let $x, y \in \mathbb{R}^d$, $u(x) \in C^\infty(\mathbb{R}^d)$.

- Summation convention: $x_i y_i \equiv \sum_{i=1}^d x_i y_i$
- Multi-index notation: $\alpha = (\alpha_1, \ldots, \alpha_d)$, $0 \leq \alpha_i \in \mathbb{Z}$:
  - Order relation: $\alpha \geq \beta$ iff $\alpha_i \geq \beta_i \ \forall i$
  - Magnitude: $|\alpha| \equiv \alpha_1 + \cdots + \alpha_d$.
  - Exponentiation: $x^\alpha \equiv x_1^{\alpha_1} \cdots + x_d^{\alpha_d}$.

  Used to denote partial differentiation of $u(x) \in C^\infty(\mathbb{R}^d)$:

$$D^\alpha u = \frac{\partial^{|\alpha|} u}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}}$$

  E.g., if $\alpha = (1, 2)$, then

$$D^\alpha u = \frac{\partial^3 u}{\partial x_1 \partial x_2^2}.$$

Differential operators in strong form

Using multi-indices, a compact expression for a $2m$-th-order linear differential operator L in d-space is:

$$Lu = \sum_{|\alpha| \leq 2m} a_\alpha(x) D^\alpha u(x)$$

Some of the most common operators arising in mathematical physics occur in *divergence* form:

$$Lu = \sum_{|\beta| \leq m} \sum_{|\alpha| \leq m} (-1)^{|\beta|} D^\beta (a_{\alpha\beta}(x) D^\alpha u(x))$$

The *principle part* of the operator consists of:

$$L_{\text{princ}} u = \sum_{|\beta| = m} \sum_{|\alpha| = m} (-1)^{|\beta|} D^\beta (a_{\alpha\beta}(x) D^\alpha u(x))$$

The properties of the matrix $[a_{ij}] = [a_{\alpha\beta}]$ formed by the d^2 coefficient functions in the principle part of a 2nd-order operator are key to understanding the properties of the particular PDE.

(The mapping here is $a_{ij} \equiv a_{(0,\ldots,0,1,0,\ldots,0)(0,\ldots,0,1,0,\ldots,0)}$.)

Classification of PDE into types

A differential operator is classified according to the properties of this matrix a_{ij}:

- *Elliptic* (at x): All eigenvalues of $[a_{\alpha\beta}(x)]$ have same (nonzero) sign.
- *Hyperbolic* (at x): All eigenvalues of $[a_{\alpha\beta}(x)]$ are nonzero; one has opposite sign of remaining $d-1$.
- *Parabolic* (at x): All eigenvalues of $[a_{\alpha\beta}(x)]$ have same nonzero sign, except for one zero eigenvalue.

Note that the type could change with x.

Elliptic operators can be further classified according to:

Strongly or *strictly* elliptic (at x): $a_{ij}(x)x_i x_j \geq \lambda |x|^2, \quad \forall\ 0 \neq x \in \mathbb{R}^d$.
Self-adjoint (principle part, at x): $a_{ij}(x) = a_{ji}(x)$.

Some key ideas from the theory of elliptic differential operators:

- Distributions
- Green functions
- Maximum principles

Examples

- *Elliptic*: Poisson equation:

$$\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} = f(x,y), \quad (x,y) \in \Omega = (0,1) \times (0,1).$$

- *Hyperbolic*: Wave equation (y=t):

$$\frac{\partial^2 u(x,y)}{\partial x^2} - \frac{\partial^2 u(x,y)}{\partial y^2} = 0, \quad (x,t) \in \Omega = (0,1) \times (0,T).$$

- *Parabolic*: Heat equation (y=t):

$$\frac{\partial u(x,y)}{\partial y} - \frac{\partial^2 u(x,y)}{\partial x^2} = 0, \quad (x,t) \in \Omega = (0,1) \times (0,T).$$

- A general linear elliptic operator in divergence form ($\Omega \subset \mathbb{R}^2$):

$$-\nabla \cdot (a \nabla u) + bu = -\frac{\partial}{\partial x}(a_{11}\frac{\partial}{\partial x}u) - \frac{\partial}{\partial y}(a_{22}\frac{\partial}{\partial y}u) + bu = f.$$

Side (boundary/initial) conditions for well-posedness

In order to determine the function which satisfies the differential equation, side conditions must be provided.

Specifying $u = g$ on $\partial\Omega$ is an *essential* or *Dirichlet* condition. Specifying $\nabla u \cdot n = g$ is a *natural* or *Neumann* condition. Specifying $\nabla u \cdot n + cu = g$ is a *mixed* or *Robin* condition.

There are obvious nonlinear generalizations; the requirement is compatibility with the PDE and *well-posedness* of the problem:

1. There exists a solution to the problem
2. The solution is unique.
3. The solution depends continuously on the "problem data".

Only certain domain/operator/boundary condition combinations lead to well-posed problems:

B.C.	Domain	Hyperbolic	Elliptic	Parabolic
D, N, or R	open	Under det.	Under det.	Well-posed
D, N, or R	closed	Not unique	Well-posed	Over det.
I.V.	open	Well-posed	Unstable	Over det.
I.V.	closed	Over det.	Over det.	Over det.

Weak PDE formulations (for analysis and numerics)

Consider the following simple problem:

$$-u_{xx} = f \quad \text{in } \Omega = (0,1), \tag{1}$$

$$u = 0 \quad \text{on } \Gamma = \partial\Omega = \{0,1\}.$$

Let $v \in C_0^2(\Omega)$ be arbitrary, where

$$C_0^k(\Omega) = \{v : v \in C^k(\Omega),\ D^\alpha v(x) = 0\ \forall x \in \partial\Omega,\ |\alpha| < k\}$$

is simply the vector space of real-valued functions defined over Ω which have two continuous derivatives and vanish on the boundary $\partial\Omega$ of Ω.

Multiply (1) by v, and integrate over the domain:

$$\int_\Omega [-u_{xx} v] dx = \int_\Omega f v dx.$$

Using integration by parts, we can shift some of the differentiability requirements on u over to v:

$$-u_x v\big|_0^1 + \int_0^1 u_x v_x dx = \int_0^1 f v dx.$$

Producing a weak formulation

Since v vanishes on the boundaries, we are left with:

$$\int_\Omega u_x v_x dx = \int_\Omega f v dx. \tag{2}$$

We can reverse the integration by parts, so that a function satisfying (2) clearly also satisfies (1).

Since v was arbitrary, the equation (2) holds for all $v \in C_0^2(\Omega)$.

Note that (2) only requires that the u, v have one derivative, so that we can *define* a *weak* form of the problem:

$$\text{Find } u \in C_0^1(\Omega) \text{ s.t. } \int_\Omega u_x v_x dx = \int_\Omega f v dx, \quad \forall v \in C_0^1(\Omega). \tag{3}$$

Key question: What are sufficient conditions for (3) to be well-defined?

In other words, what assumptions on u, v, f, and Ω are necessary to ensure that all terms in (3) are always finite?

(We will worry about well-posedness shortly...)

Functions and the vector spaces they live in

One answer is given by the Cauchy-Schwarz inequality:

$$\left|\int_\Omega u_x v_x dx\right| \leq \left(\int_\Omega |u_x|^2\right)^{1/2} \left(\int_\Omega |v_x|^2\right)^{1/2},$$

$$\left|\int_\Omega f v dx\right| \leq \left(\int_\Omega |f|^2\right)^{1/2} \left(\int_\Omega |v|^2\right)^{1/2}.$$

We don't really need to require $u, v \in C_0^1(\Omega)$; all we need is for the RHS of the above inequalities to be finite.

This leads us to define the function space (again, simply a vector space):

$$L^2(\Omega) = \{u : \|u\|_{L^2} < \infty\},$$

with norm and inner-product (making L^2 a normed as well as an inner-product space) defined as:

$$\|u\|_{L^2} = (u,u)_{L^2}^{1/2}, \quad (u,v)_{L^2} = \int_\Omega uv dx.$$

Note that $L^2(\Omega)$ is actually a well-defined (Hilbert, or complete inner-product) space for any (reasonable) open set $\Omega \subseteq \mathbb{R}^d$, for $d \geq 1$, not just $d = 1$.

The function space H^1

Note that if all we need at this point is to ensure both sides of the equation are finite using the the Cauchy-Schwarz inequality, then in fact the following "weak form" of the problem is all we really need:

$$\text{Find } u \in H_0^1(\Omega) \text{ s.t. } \int_\Omega u_x v_x dx = \int_\Omega f v dx, \quad \forall v \in H_0^1(\Omega). \tag{4}$$

Since all that is necessary is for these integrals to be finite, the weak form leads us naturally to define a *Sobolev* space:

$$H^1(\Omega) = \{u \in L^2(\Omega) : \|u\|_{H^1(\Omega)} < \infty\},$$

where again $\Omega \subseteq \mathbb{R}^d$, $d \geq 1$. The corresponding inner-product, semi-norm, and norm are:

$$(u, v)_{H^1} = \int_\Omega (\nabla u \cdot \nabla v + uv) dx, \quad |u|_{H^1} = \|\nabla u\|_{L^2},$$

$$\|u\|_{H^1} = (|u|_{H^1}^2 + \|u\|_{L^2}^2)^{1/2}.$$

We can then also define the subspace which vanishes on the boundary:

$$H_0^1(\Omega) = \{u \in H^1(\Omega) : u = 0 \text{ on } \partial\Omega\}.$$

Weak formulation of more general problems with $d \geq 1$

Consider now $\Omega \subset \mathbb{R}^d$, $d \geq 1$, with boundary $\Gamma = \Gamma_D \cup \Gamma_N$, where $\Gamma_D \cap \Gamma_N = \emptyset$.
Second order linear elliptic equations in divergence form can be written as:

$$-\nabla \cdot (\bar{\mathbf{a}} \nabla \hat{u}) + b\hat{u} = f \text{ in } \Omega, \tag{5}$$

$$\hat{u} = g_D \text{ on } \Gamma_D, \tag{6}$$

$$(\bar{\mathbf{a}} \nabla \hat{u}) \cdot \mathbf{n} + c\hat{u} = g_N \text{ on } \Gamma_N, \tag{7}$$

where
$b(\mathbf{x}) : \Omega \mapsto \mathbb{R}$, $f(\mathbf{x}) : \Omega \mapsto \mathbb{R}$, $g_D(\mathbf{x}) : \Gamma_D \mapsto \mathbb{R}$, $g_N(\mathbf{x}) : \Gamma_N \mapsto \mathbb{R}$,
$c(\mathbf{x}) : \Gamma_N \mapsto \mathbb{R}$, $\hat{u}(\mathbf{x}) : \Omega \mapsto \mathbb{R}$, $\bar{\mathbf{a}}(\mathbf{x}) : \Omega \mapsto \mathbf{L}(\mathbb{R}^d, \mathbb{R}^d)$.

Since we have a Dirichlet condition over part of the boundary, define:

$$H^1_{0,D}(\Omega) = \{u \in H^1(\Omega) : u = 0 \text{ on } \Gamma_D\}.$$

We will look for a solution in the form:

$$\hat{u} = u + w, \qquad u \in H^1_{0,D}(\Omega), \qquad w \in H^1(\Omega),$$

where w is an arbitrary (but known and fixed) function satisfying: $w|_{\Gamma_D} = g_D$.

Properties of the bilinear and linear weak forms

All of the steps we took in the one-dimensional case can be repeated using now the divergence theorem, giving the multi-dimensional weak formulation:

$$\text{Find } u \in H^1_{0,D}(\Omega) \text{ such that } A(u,v) = F(v)\ \forall v \in H^1_{0,D}(\Omega), \tag{8}$$

where the *bilinear form* $A(u,v)$ is defined as:

$$A(u,v) = \int_\Omega \bar{\mathbf{a}} \nabla u \cdot \nabla v + buv\ d\mathbf{x} + \int_{\Gamma_N} cuv\ ds, \tag{9}$$

and the *linear functional* $F(v)$ is defined as:

$$F(v) = \int_\Omega fv\ d\mathbf{x} + \int_{\Gamma_N} g_N v\ ds - A(w,v). \tag{10}$$

Note that if the strong form operator was *self-adjoint*, then the bilinear form is *symmetric*, $A(u,v) = A(v,u),\ \forall u, v \in H^1_{0,D}(\Omega)$.

Strongly ellipticity (and additional conditions) imply *coercivity* of the bilinear form, $A(u,u) \geq m\|u\|^2_{H^1},\ \forall u \in H^1_{0,D}(\Omega)$.

Boundedness is: $|A(u,v)| \leq M\|u\|_{H^1}\|v\|_{H^1},\ \ |F(v)| \leq L\|v\|_{H^1},\ \ \forall u, v \in H^1_{0,D}(\Omega)$.

These conditions are actually sufficient for well-posedness.

PDE with variational structure

Let $J : X \mapsto \mathbb{R}$, where X is a Banach space (complete normed vector space). $J(u)$ is called stationary at $u \in X$ if:

$$\langle J'(u), v \rangle = 0, \ \forall v \in X. \tag{11}$$

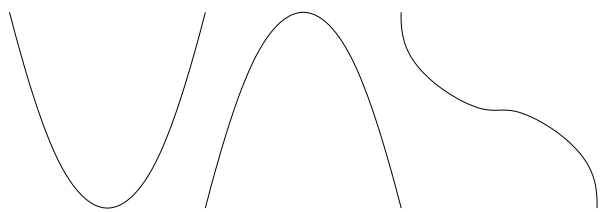
J' is the (Gateaux, or G-)derivative of J at u in the direction v,

$$\langle J'(u), v \rangle = \left. \frac{d}{d\epsilon} J(u + \epsilon v) \right|_{\epsilon=0}.$$

At each point $u \in X$, $J'(u) \in X^*$ (space of bounded linear functionals on X). Stationarity (11) is e.g. a necessary condition for u to be a solution to:

$$\text{Find } u \in X \text{ such that } J(u) \leq J(v), \ \forall v \in X. \tag{12}$$

However, the condition of stationarity is more general, since the functional $J(u)$ may have only saddle points; (11) then includes the principle of stationary action in dynamics.



Variational Problems: A Nonlinear Elliptic Example

Let $X = W_0^{1,p}(\Omega)$, with $\Omega \subset \mathbb{R}^d$ a "smooth" bounded domain. Define:

$$J(u) = \int_\Omega [\frac{1}{2}\nabla u \cdot \nabla u - g(u)]\ dx, \quad \text{with } g(u) \in L^1(\Omega) \text{ when } u \in W^{1,p}(\Omega).$$

The notation here is $(1 \leq p < \infty)$:

$$\|u\|_{W^{1,p}(\Omega)} = \left(\int_\Omega |u|^p + |\nabla u|^p\ dx \right)^{1/p},$$

$$W^{1,p}(\Omega) = \{ u \in L^p(\Omega) : \|u\|_{W^{1,p}(\Omega)} < \infty \},$$

$$W_0^{1,p}(\Omega) = \{ u \in W^{1,p}(\Omega) : \text{ trace } u = 0 \text{ on } \partial\Omega \}.$$

The condition for stationarity of $J(u)$ is:

$$\text{Find } u \in W_0^{1,p}(\Omega) \text{ s.t. } \langle J'(u), v \rangle = \int_\Omega [\nabla u \cdot \nabla v - g'(u)v]\ dx = 0,\ \forall v \in W_0^{1,p}(\Omega).$$

If a classical solution exists, this is equivalent to determining u from:

$$\begin{aligned} -\nabla^2 u &= g'(u) \text{ in } \Omega, \\ u &= 0 \text{ on } \partial\Omega. \end{aligned}$$

Solving General Nonlinear Variational Problems

Let X, Y be Banach spaces (possibly $X = Y$), and $F : X \mapsto Y^*$. Consider now:

$$\text{Find } u \in X \text{ such that } F(u) = 0 \in Y^*.$$

As a linear functional on Y, we can consider the general "variational" problem:

$$\text{Find } u \in X \text{ such that } \langle F(u), v \rangle = 0, \ \forall v \in Y. \tag{13}$$

If the nonlinear problem (13) is well-posed, one typically solves for u using a Newton iteration based on linearization with the G-derivative of $\langle F(u), v \rangle$:

$$\langle F'(u)w, v \rangle = \frac{d}{d\epsilon} \langle F(u + \epsilon w), v \rangle \Big|_{\epsilon=0}.$$

Given an initial approximation $u^0 \approx u$, a (global, inexact) Newton iteration is:

(a) Find $w \in X$ such that: $\langle F'(u^k)w, v \rangle = -\langle F(u^k), v \rangle + r, \quad \forall v \in Y$
(b) Set: $u^{k+1} = u^k + \lambda w$

One discretizes (a)-(b) at the "last moment", producing a matrix equation. Required Newton steps independent of "h" [e.g., Allgower et. al, 1986].

Our Nonlinear Potential Equation Example

From our earlier example, if

$$J(u) = \int_\Omega [\frac{1}{2}\nabla u \cdot \nabla u - g(u)]\ dx,$$

the condition for stationarity of $J(u)$ is:

$$\text{Find } u \in W_0^{1,p}(\Omega) \text{ such that } \langle F(u), v\rangle = 0,\ \forall v \in W_0^{1,p}(\Omega),$$

where

$$\langle F(u), v\rangle = \langle J'(u), v\rangle = \int_\Omega [\nabla u \cdot \nabla v - g'(u)v]\ dx.$$

To build a Newton iteration, we only need the additional derivative:

$$\langle F'(u)w, v\rangle = \frac{d}{d\epsilon}\langle F(u+\epsilon w), v\rangle\Big|_{\epsilon=0} = \int_\Omega [\nabla w \cdot \nabla v - g''(u)wv]\ dx.$$

Well-posedness of the linearized problem in a Newton iteration:

$$\text{Find } w \in W^{1,p}(\Omega) \text{ such that } \langle F'(u)w, v\rangle = -\langle F(u), v\rangle,\quad \forall v \in W^{1,p}(\Omega),$$

assured by e.g. establishing coercivity and boundedness properties on F' and F.

The Resulting Linear Problems when $X \neq Y$

Solving the nonlinear problem (13) requires repeatedly solving a linear problem:

$$\text{Find } u \in X \text{ such that } a(u,v) = f(v), \quad \forall v \in Y, \tag{14}$$

where for fixed $\bar{u} \in X$,

$$a(u,v) = \langle F'(\bar{u})u, v\rangle, \qquad f(v) = -\langle F(\bar{u}), v\rangle.$$

Assume the bilinear form $a(\cdot,\cdot)$ and linear functional $f(\cdot)$ satisfy four conditions:

$$\inf_{u\in X}\sup_{v\in Y}\frac{a(u,v)}{\|u\|_X\|v\|_Y} \geq m > 0, \qquad a(u,v) \leq M\|u\|_X\|v\|_Y, \qquad f(v) \leq L\|v\|_Y, \tag{15}$$

$$\text{For each } 0 \neq v \in Y, \text{ there exists } u \in X \text{ s.t. } a(u,v) \neq 0. \tag{16}$$

It follows [Babuska-Aziz, 1972] that (14) is well-posed, and *a priori* estimate:

$$\|u\|_X \leq \frac{L}{m}$$

follows from

$$m\|u\|_X \leq \sup_{v\in Y}\frac{a(u,v)}{\|v\|_Y} = \sup_{v\in Y}\frac{f(v)}{\|v\|_Y} \leq L.$$

If some of the properties (15)–(16) are lost, or if the problem is nonlinear as in (13) itself, other *a priori* estimates may still be possible (case-by-case basis).

The Resulting Linear Problems when $X = Y$

Consider again the linear problem, but now in special case of $X = Y$:

$$\text{Find } u \in X \text{ such that } a(u, v) = f(v), \quad \forall v \in X, \tag{17}$$

The following three conditions (with $m > 0$) are trivially equivalent to the three conditions (15) when $X = Y$ (condition (16) is no longer needed):

$$a(u, u) \geq m\|u\|_X^2, \qquad a(u, v) \leq M\|u\|_X\|v\|_X, \qquad f(v) \leq L\|v\|_X. \tag{18}$$

It follows [Lax-Milgram, 1957] that (17) is well-posed, and the *a priori* estimate:

$$\|u\|_X \leq \frac{L}{m}$$

follows now simply from

$$m\|u\|_X^2 \leq a(u, u) = f(u) \leq L\|u\|_X.$$

Again, If some of the properties (18) are lost, or if the problem is nonlinear as in (13) itself, other *a priori* estimates may still be possible (case-by-case basis).

Well-posedness, *A priori* Estimates, Related Questions

Given a nonlinear elliptic PDE (or other type of PDE):

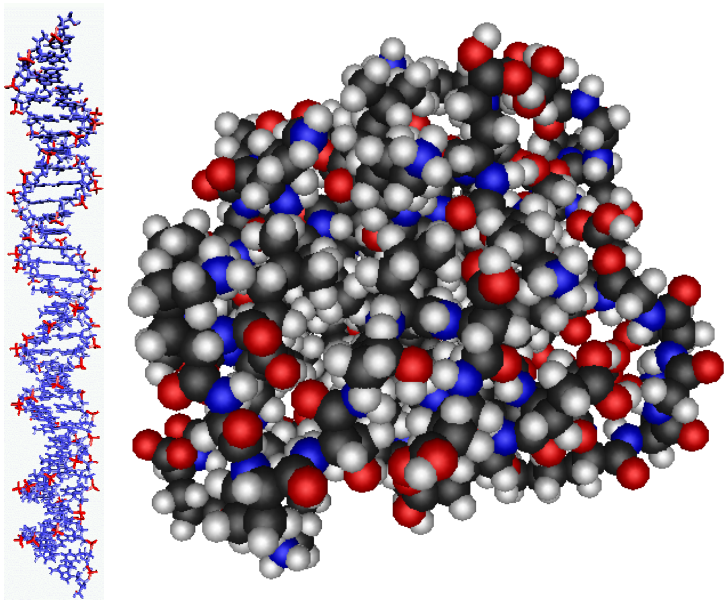
$$\text{Find } u \in \bar{u} + X \text{ such that } \langle F(u), v \rangle = 0 \quad \forall v \in Y, \qquad (*)$$

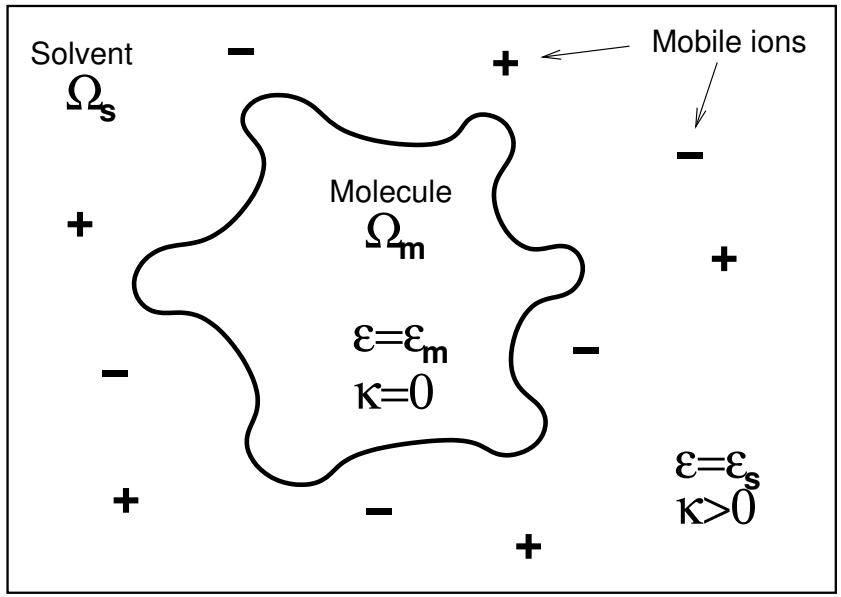
the following mathematical questions are of fundamental importance:

1. What function spaces X and Y produce a well-defined problem?
   (i.e., all terms in the equations are everywhere finite)
2. What function spaces X and Y give well-posedness?
   (i.e., existence, uniqueness, continuous dependence on the data)
3. How "smooth" are the functions in X?
   (i.e., is $X = C_0^\infty$, $X = L^p(\mathcal{M})$, $X = W^{k,p}(\mathcal{M})$, ...)
4. How well can we approximate a solution to (*) using standard methods?
   (i.e., for some approximation $u_h \approx u$, how large is: $\|u - u_h\|_X$)
5. Can we produce such approximations using algorithms that have optimal (linear) or near-optimal space and time complexity?

These questions are related, since standard discretizations, as well as techniques for solving the discrete system, depend on smoothness.

PDE example: The nonlinear Poisson-Boltzmann equation





The potential ϕ_k satisfies Gauss' law (and $\phi_3(\infty) = 0$)

$$\nabla^2 \phi_k(\mathbf{x}) = \frac{-4\pi\rho_k(\mathbf{x})}{\epsilon_k}, \qquad k = 1, 2, 3.$$

Below, $\epsilon_k, e_c, k_B, N_A, T$ will denote physical constants & temperature.

Example: The Poisson-Boltzmann equation

- $I_s = 1000M/N_A$ moles/liter, $M =$ solvent ions/cm^3
- $q_i = z_i e_c =$ charge at point r_i, $z_i \in [-1, 1]$, $i = 1, \ldots, N_m$.
- $u(\mathbf{x}) = \frac{e_c \phi(\mathbf{x})}{k_B T}, \quad \kappa = \left(\frac{8\pi N_A e_c^2}{1000 e_3 k_B T} \right)^{1/2} I_s^{1/2}$
- $\bar{\kappa}(\mathbf{x}) = \begin{cases} 0, & \mathbf{x} \in \mathbf{\Omega}_1, \mathbf{\Omega}_2 \\ \epsilon_3^{1/2}\kappa, & \mathbf{x} \in \mathbf{\Omega}_3 \end{cases}, \quad \epsilon(\mathbf{x}) = \begin{cases} \epsilon_1, & \mathbf{x} \in \mathbf{\Omega}_1 \\ \epsilon_2 (= \epsilon_3), & \mathbf{x} \in \mathbf{\Omega}_2, \mathbf{\Omega}_3 \end{cases}$

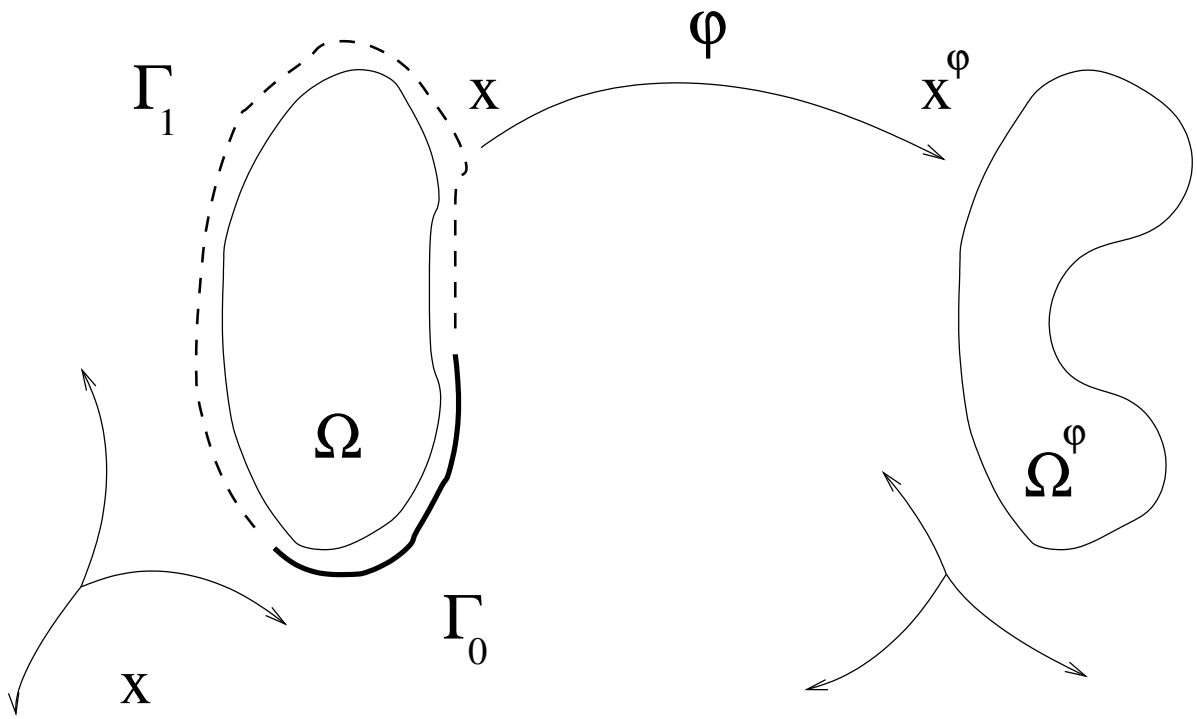
A Boltzmann assumption on the ion concentration ratio gives rise to the nonlinear Poisson-Boltzmann equation:

$$-\nabla \cdot (\epsilon(\mathbf{x}) \nabla u(\mathbf{x})) + \bar{\kappa}^2 \sinh(u(\mathbf{x})) = \left(\frac{4\pi e_c^2}{k_B T} \right) \sum_{i=1}^{N_m} z_i \delta(\mathbf{x} - \mathbf{x}_i).$$

Computing the formal variational (or Gateaux) derivative of the nonlinear PBE operator gives the *linearized* PBE:

$$-\nabla \cdot (\epsilon(\mathbf{x}) \nabla u(\mathbf{x})) + \bar{\kappa}^2 u(\mathbf{x}) = \left(\frac{4\pi e_c^2}{k_B T} \right) \sum_{i=1}^{N_m} z_i \delta(\mathbf{x} - \mathbf{x}_i).$$

More Complexity: Elasticity models of biological structures



Notation:

- $\varphi(\mathbf{x}) = id + u(\mathbf{x}) : \overline{\Omega} \mapsto \mathbb{R}^3$; deformation & displacement
- $\nabla\varphi(\mathbf{x}), \quad \nabla u(\mathbf{x}) : \overline{\Omega} \mapsto \mathbb{M}^3$; def. & disp. gradients
- $C = \nabla\varphi^T \nabla\varphi, \quad E = \frac{1}{2}(C - I) : \overline{\Omega} \mapsto \mathbb{S}^3$; RCG & GSV strains

Stress and strain, and Cauchy's equations

$$\Sigma(\mathbf{x}) = \hat{\Sigma}(\mathbf{x}, \nabla\varphi(\mathbf{x})). \quad (\text{E.g., } \check{\Sigma}(E) = \lambda(\mathrm{tr}E)I + 2\mu E.)$$

Cauchy equations (via Piola-transformation) for $(\varphi_1, \varphi_2, \varphi_3)$:

$$\begin{aligned} -\nabla \cdot (\nabla\varphi(\mathbf{x})\Sigma(\mathbf{x})) &= f(\mathbf{x}) \quad \text{in } \Omega, \\ n(\mathbf{x}) \cdot (\nabla\varphi(\mathbf{x})\Sigma(\mathbf{x})) &= g(\mathbf{x}) \quad \text{on } \Gamma_1, \\ \varphi(\mathbf{x}) &= \varphi_0(\mathbf{x}) \quad \text{on } \Gamma_0 = \Gamma - \Gamma_1 \end{aligned}$$

An immersed nonlinear elastic dielectric can be described by

$$\begin{aligned} -\nabla \cdot \left\{ (I + \nabla u(\mathbf{x}))\, \check{\Sigma}(E(u)) \right\} &= f(\mathbf{x}) \text{ in } \Omega \\ -\nabla(\epsilon(\mathbf{x})\nabla\phi(\mathbf{x})) + \bar{\kappa}^2(\mathbf{x}) \sinh(\phi(\mathbf{x})) &= \rho(\mathbf{x}) \text{ in } \mathbb{R}^3 \\ n(\mathbf{x}) \cdot (I + \nabla u(\mathbf{x}))\, \check{\Sigma}(E(u)) &= g(\mathbf{x}) \text{ on } \Gamma_1, \\ u(\mathbf{x}) &= 0 \text{ on } \Gamma_0 = \Gamma - \Gamma_1, \\ \phi(\infty) &= 0. \end{aligned}$$

Dealing with various difficulties in the PBE

The PBE has several interesting (read "hard") features:

- Domain $\Omega \subseteq \mathbb{R}^d$, $d = 3$;
- Coefficients $\epsilon(x)$ and $\bar{\kappa}(x)$ are discontinuous at interfaces in Ω;
- Supercritical nonlinearity $\sinh(u)$: stronger than u^p, $p = (d+2)/(d-1)$, $d > 1$.
- Source term contains delta functions: these are not bounded linear functionals on the natural function space $H^1(\Omega)$ for $d > 1$.

We have tried to address these difficulties over the last several years:

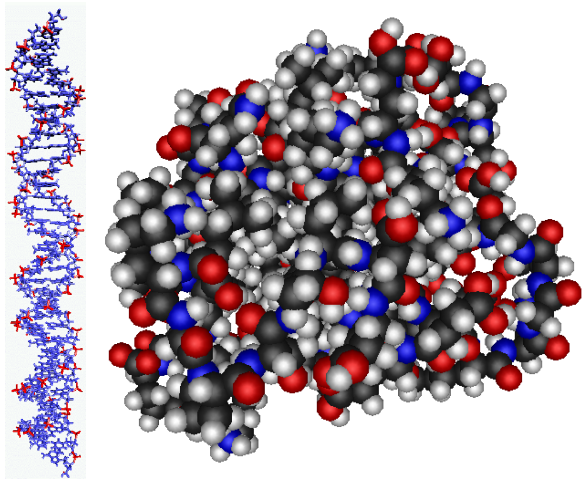
1. Properties the PBE and *a priori* estimates of the solution. [CHX2,YHM,HYZ]
2. Approximation theory (general and specific methods). [CHX2,H1]
3. Properties of discrete approximations of the PBE. [CHX2,YHM,HYZ]

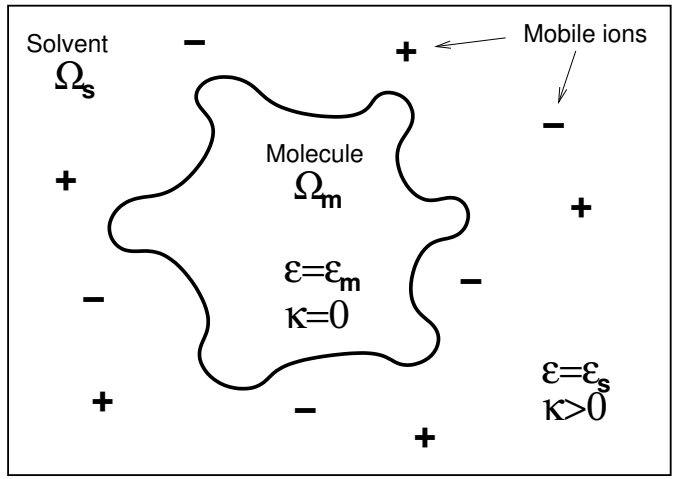
These results have been used to develop high-resolution numerical methods for PBE:

1. Design of iterative methods for the discrete eqns. [AH,ABH]
2. Design of adaptive algorithms for nonlinear approx. [H1,CHX1,CHX2]
3. Convergence of such adaptive algorithms. [CHX1,CHX2]
4. Adaptive algorithms for parallel computers. [BH,H1,H2,EHL]

We will outline the developments that have been implemented in FETK below.

Regularized forms of the PBE





Problem: Charge source term produces non-smooth PBE solutions $\tilde{u}$:

$$-\nabla\cdot(\epsilon\nabla\tilde{u})+\bar{\kappa}^2\sinh(\tilde{u})=\sum_{i=1}^{N_m}q_i\delta_i,\qquad \tilde{u}(\infty)=0.$$

Solution: Exploit a two-scale expansion usually reserved for linear problems:

$$\tilde{u}=u+G,\quad \text{where } G=\sum_{i=1}^{N_m}G_i,\qquad G_i=\frac{q_i}{\epsilon_m}\frac{1}{|x-x_i|}.$$

Gives the *Regularized PBE (RPBE)* for the smooth remainder u:

$$\begin{aligned}-\nabla\cdot(\epsilon\nabla u)+\bar{\kappa}^2\sinh(u+G) &= \nabla\cdot((\epsilon-\epsilon_m)\nabla G)\quad \text{in } \Omega\subseteq\mathbb{R}^3,\\ u &= g-G,\quad \text{on } \partial\Omega.\end{aligned}$$

This idea goes back to at least 1996 (Z. Zhou et al).

Finite difference and spectral discretizations

We very quickly review the four primary discretization techniques that are used to generate discrete (linear and nonlinear algebraic) equations as approximations to ordinary and partial differential equations.

Finite difference methods: Very simple approach: $\frac{du}{dx} \approx \frac{u(x+h)-u(x)}{h}$, where h is sufficiently small for "good" approximation.

One ends up with an algebraic equation $Au = f$ for a set of approximate solution values $u_i = u(x_i)$ at a finite "mesh" of points.

The matrix A tend to be very large and sparse due to the local natural of the difference expression, and hence iterative methods must be used.

Spectral methods: $u(x) \approx \sum_{J=1}^{N} \alpha_j \phi_j(x)$, where N is sufficiently large for "good" approximation, and where $\phi_j(x)$ are "spectral" basis functions, e.g. trigonometric or other functions defined globally over the domain.

One ends up with an algebraic equation $Au = f$ for the spectral coefficients α_j; thus, the spectral solution is globally defined (not just at mesh points).

The spectral basis functions generally have global support, hence matrix A tends to be dense and expensive to invert directly or iteratively.

Finite volume (box) discretization methods

Box methods: Consider the following domain partition of $\Omega \subset \mathbb{R}^3$:

- $\Omega \equiv \bigcup_{j=1}^{l} \tau^j$, the *elements* τ^j are rectangles or triangles (or perhaps hexahedra or tetrahedra in 3D).
- Associated with the l elements τ^j are the n *nodes* x_i.
- $\{\tau^{j;i}\} \equiv \{\tau^j : x_i \in \tau^j\}, \qquad \tau^{(i)} \equiv \bigcup_j \tau^{j;i} \equiv \{\bigcup_j \tau^j : x_i \in \tau^j\}.$
- Mesh parameter h, $\Omega_h = \{x^1, \ldots, x^n\}$, $\mathcal{T}_h = \{\tau^1, \ldots, \tau^l\}$.
- Assume $u(x)$ and $a\nabla u \cdot n$ are continuous.

Begin by integrating the strong form over an arbitrary $\tau^{(i)}$:

$$-\sum_j \int_{\tau^{j;i}} \nabla \cdot (a\nabla u)\ dx + \sum_j \int_{\tau^{j;i}} bu\ dx = \sum_j \int_{\tau^{j;i}} f\ dx.$$

Box discretization methods (continued)

Employing the divergence theorem:

$$-\sum_j \int_{\partial\tau^{j;i}} (a\nabla u)\cdot n \; ds + \sum_j \int_{\tau^{j;i}} bu \; dx = \sum_j \int_{\tau^{j;i}} f \; dx,$$

Interior surface integrals vanish ($a\nabla u \cdot n$ is continuous):

$$-\int_{\partial\tau^{(i)}} (a\nabla u)\cdot n \; ds + \sum_j \int_{\tau^{j;i}} bu \; dx = \sum_j \int_{\tau^{j;i}} f \; dx,$$

The relationship is exact in each $e^{(i)}$.

Integrals are then approximated with quadrature, yielding a linear algebraic system for an approximate u at the nodes x_i:

$$Au = f.$$

Box method error estimation: through Taylor expansion as in finite differences; a more powerful modern approach employs finite element approximation theory.

Box methods: A one-dimensional example

Consider the following simple problem:

$$-\frac{d}{dx}\left(a(x)\frac{d}{dx}u(x)\right) + b(x)u(x) = f(x) \text{ in } (c,d), \quad u(c) = u(d) = 0.$$

Define a discrete mesh $c = x_0 < x_1 < \cdots < x_{n+1} = d$, with $x_{i+1} = x_i + h_i$, $h_i > 0$. We define the *boxes* around x_i to be

$$[x_i - \frac{h_{i-1}}{2}, x_i + \frac{h_i}{2}]$$

The continuity assumptions at x_i are:

$$\lim_{x \to x_i^-} u(x) = \lim_{x \to x_i^+} u(x), \qquad \lim_{x \to x_i^-} a(x)\frac{du(x)}{dx} = \lim_{x \to x_i^+} a(x)\frac{du(x)}{dx}.$$

Some notation: $x_{i-1/2} \equiv x_i - h_{i-1}/2, \quad x_{i+1/2} \equiv x_i + h_i/2.$

One-dimensional example continued

Integration by parts over a particular box, employing the continuity conditions, produces (still exact):

$$\left(a(x_{i-1/2})\frac{d}{dx}u(x_{i-1/2})\right) - \left(a(x_{i+1/2})\frac{d}{dx}u(x_{i+1/2})\right)$$

$$+\int_{x_{i-1/2}}^{x_{i+1/2}} b(x)u(x)dx = \int_{x_{i-1/2}}^{x_{i+1/2}} f(x)dx.$$

Employing now some quadrature rules and centered differences ($O(h^2)$ for $h_i = h$), gives the approximation:

$$a(x_{i-1/2})\left(\frac{u_h(x_i) - u_h(x_{i-1})}{h_{i-1}}\right) - a(x_{i+1/2})\left(\frac{u_h(x_{i+1}) - u_h(x_i)}{h_i}\right)$$

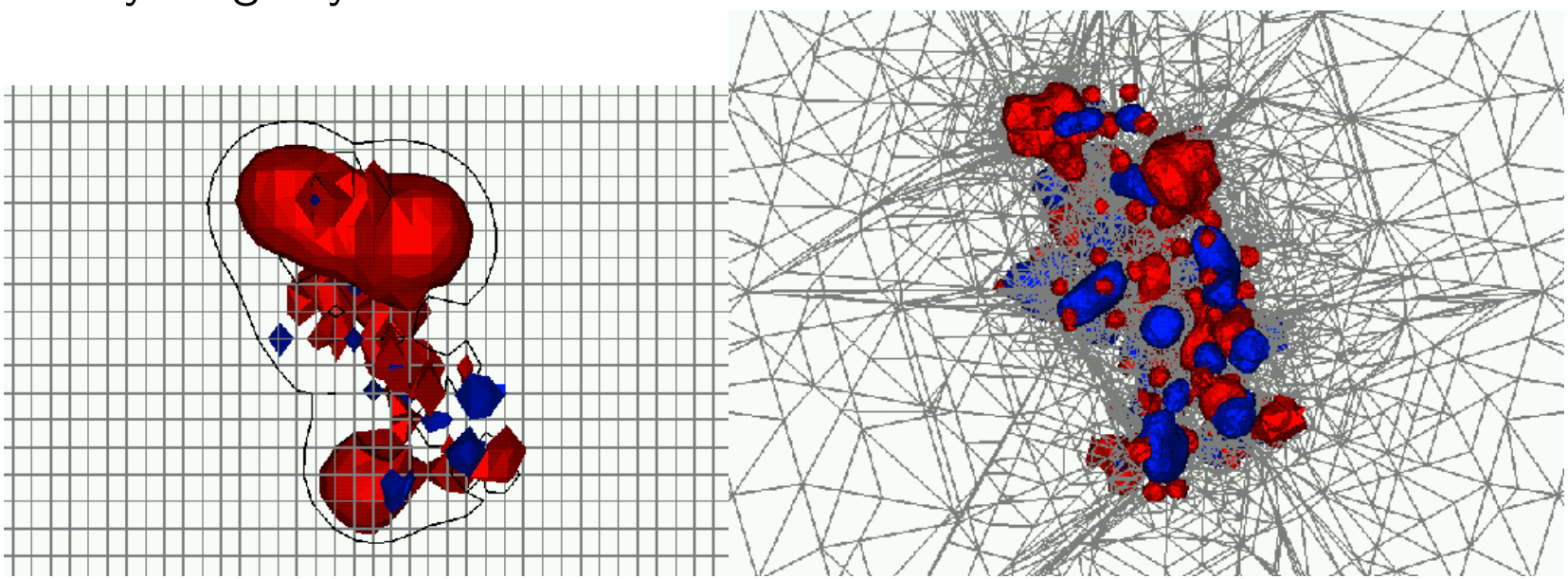
$$+u_h(x_i)\left(\frac{h_{i-1}b(x_i^-) + h_i b(x_i^+)}{2}\right) = \left(\frac{h_{i-1}f(x_i^-) + h_i f(x_i^+)}{2}\right).$$

APBS: Discretization with the Box Method and PMG

APBS based on PMG (Parallel algebraic MultiGrid), which has:

- Box method discretization of PBE on a tensor-product mesh of unit cube.
- Fast multigrid solution of the resulting linear and nonlinear algebraic system.
- Provably and (emperically demonstratable) optimal (linear) computational and storage complexity.

Why do anything beyond this? Consider:



Left: Approx 500K degrees of freedom; Right: Approx 50K degrees of freedom.

Alternative Discretization with Adaptive FEM

Among the host of possible numerical discretization techniques available for this class of problems, we focus primarily on finite element methods, due to:

1. Representation of complex domain shapes and boundaries.
2. Discretization of general nonlinearities and bndry conds.
3. Well-suited for general coupled nonlinear elliptic systems.
4. General nonlinear (adaptive) approximation theory framework.
5. Ideal setting for building optimal multilevel solvers.

Key play: Finite Element Methods (FEM) provide a powerful discretization and numerical solver framework to improve on box method-type discretization of the PBE and similar problems in the following ways:

- More accurate/realistic representation of biomolecular structures with geometric complexity (mesh generation);
- Minimization of degrees of freedom in the discrete problem through use of Adaptive FEM (AFEM; *posteriori* estimates, mesh refinement);
- Preservation of the linear computational and storage complexity of the resulting numerical methods (fast multilevel solvers for AFEM).

Discretizing Nonlinear Variational Problems

A *Petrov-Galerkin (PG) method* looks for an approximation $u_h \approx u$ satisfying the variational problem (13) in subspaces:

$$\text{Find } u_h \in X_h \subseteq X \text{ such that } \langle F(u_h), v_h \rangle = 0, \ \forall v_h \in Y_h \subseteq Y.$$

A *Galerkin method* is the special case of $Y = X$ and $Y_h = X_h$.

Consider now the case $\dim(X_h) = \dim(Y_h) = n < \infty$.

If $\text{span}\{\phi_1, \ldots, \phi_n\} = X_h \subseteq X$ and $\text{span}\{\psi_1, \ldots, \psi_n\} = Y_h \subseteq Y$ for bases $\{\phi_j\}$, $\{\psi_j\}$, the problem is then to determine the appropriate coefficients in the expansion:

$$u_h = \sum_{j=1}^{n} \alpha_j \phi_j.$$

The variational problem gives n (nonlinear) equations for the n coefficients:

$$\text{Find } u_h = \sum_{j=1}^{n} \alpha_j \phi_j \text{ such that } \langle F(u_h), \psi_i \rangle = 0, \ i = 1, \ldots, n.$$

Finite Element Methods

For a PG approximation $u_h = \sum_{j=1}^{n} \alpha_j \phi_j$, an $n \times n$ matrix equation is produced at each Newton iteration for the Newton correction $w_h = \sum_{j=1}^{n} \gamma_j \phi_j$:

$$AX = B,$$

where

$$A_{ij} = \langle F'(u_h)\phi_j, \psi_i) \rangle, \qquad X_i = \gamma_i, \qquad B_i = -\langle F(u_h), \psi_i \rangle.$$

Regarding this linear system, for practical reasons one hopes that:

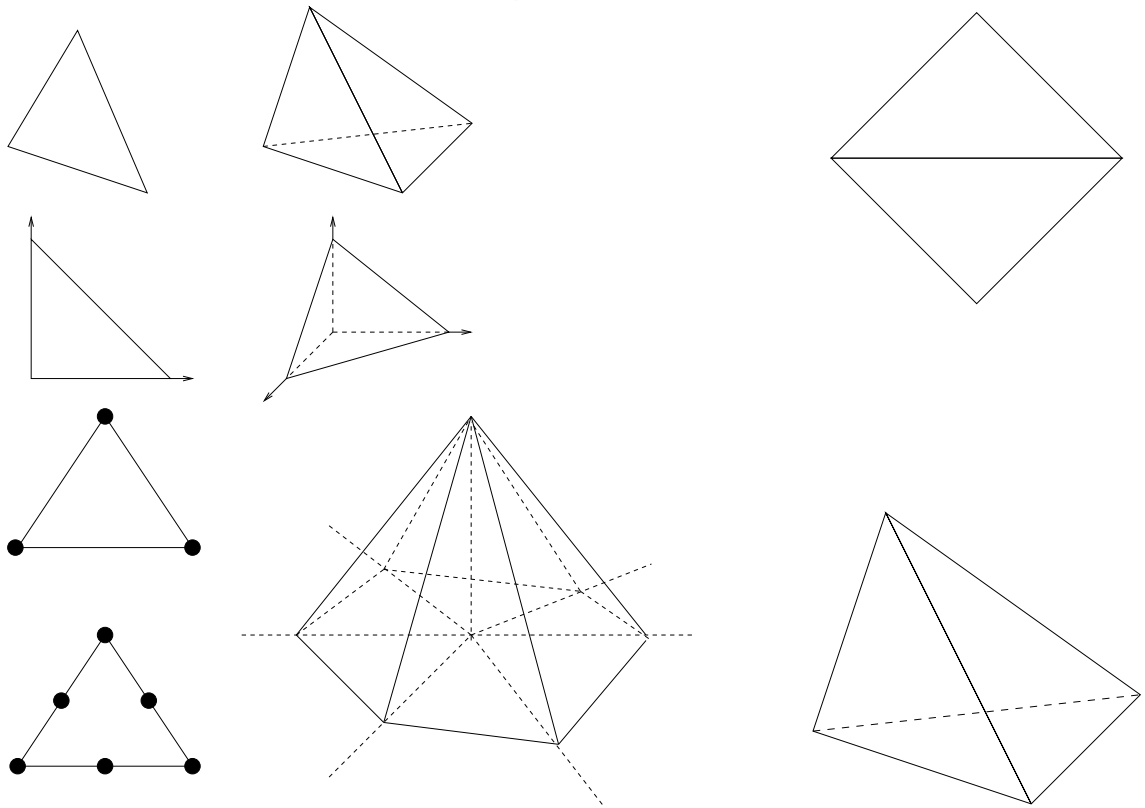
- The cost of storing the matrix A is as close to optimal $O(n)$ as possible;
- The cost of inverting the matrix A is as close to optimal $O(n)$ as possible.

Roughly speaking, finite element (FE) methods are computational techniques that allow management of two issues related to PG approximation:

1. Control of the approximation error: $E(u - u_h) = \|u - u_h\|_X$,
2. Space/time complexity of storing and solving the n equations: $AX = B$.

Locally Supported FE Bases and Simplex Subdivision

FE methods use piecewise polynomial spaces (controls $E(u - u_h)$) with local support (generates sparse matrices A), defined on *elements* such as simplices.



Error-estimate-driven adaptive finite element methods often based on simplex subdivision. (Above: 2/4/8-section and conformity.)

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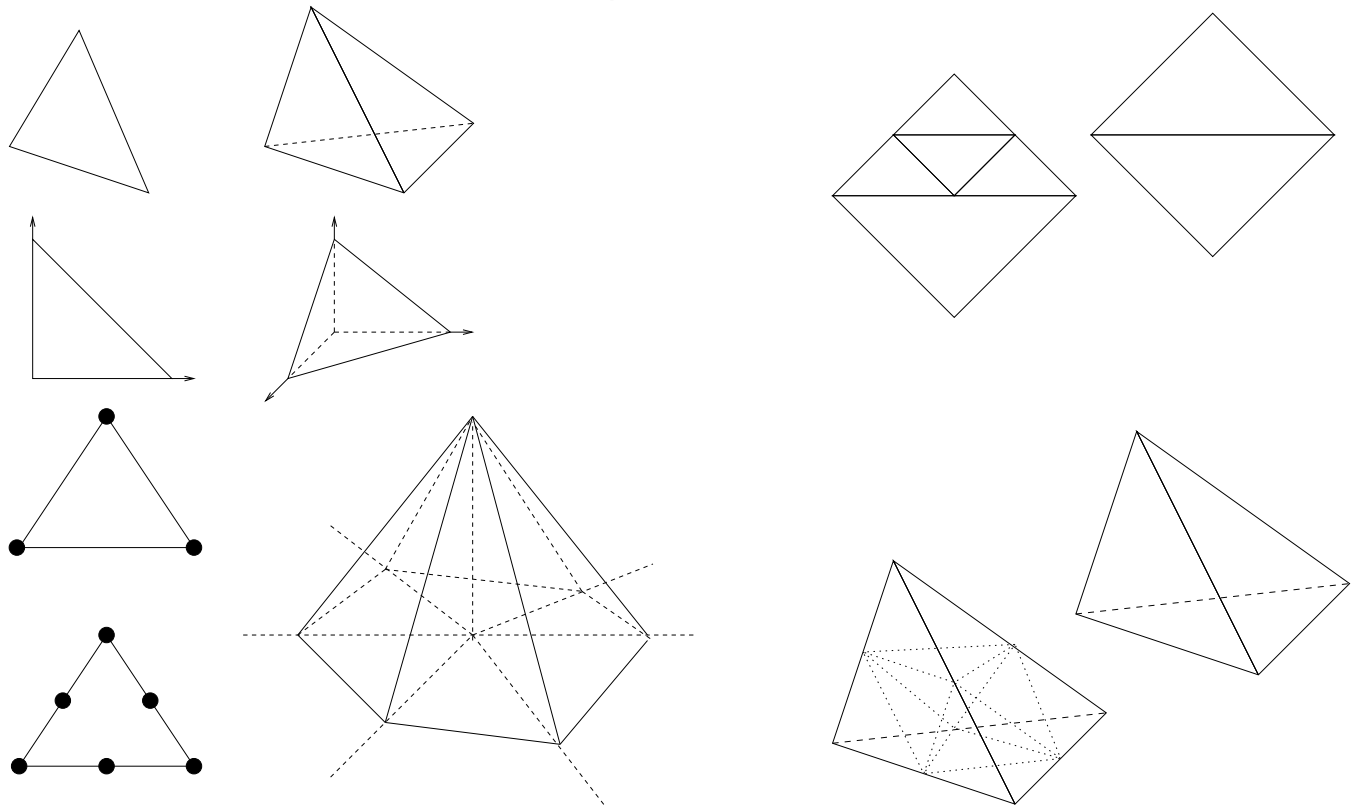

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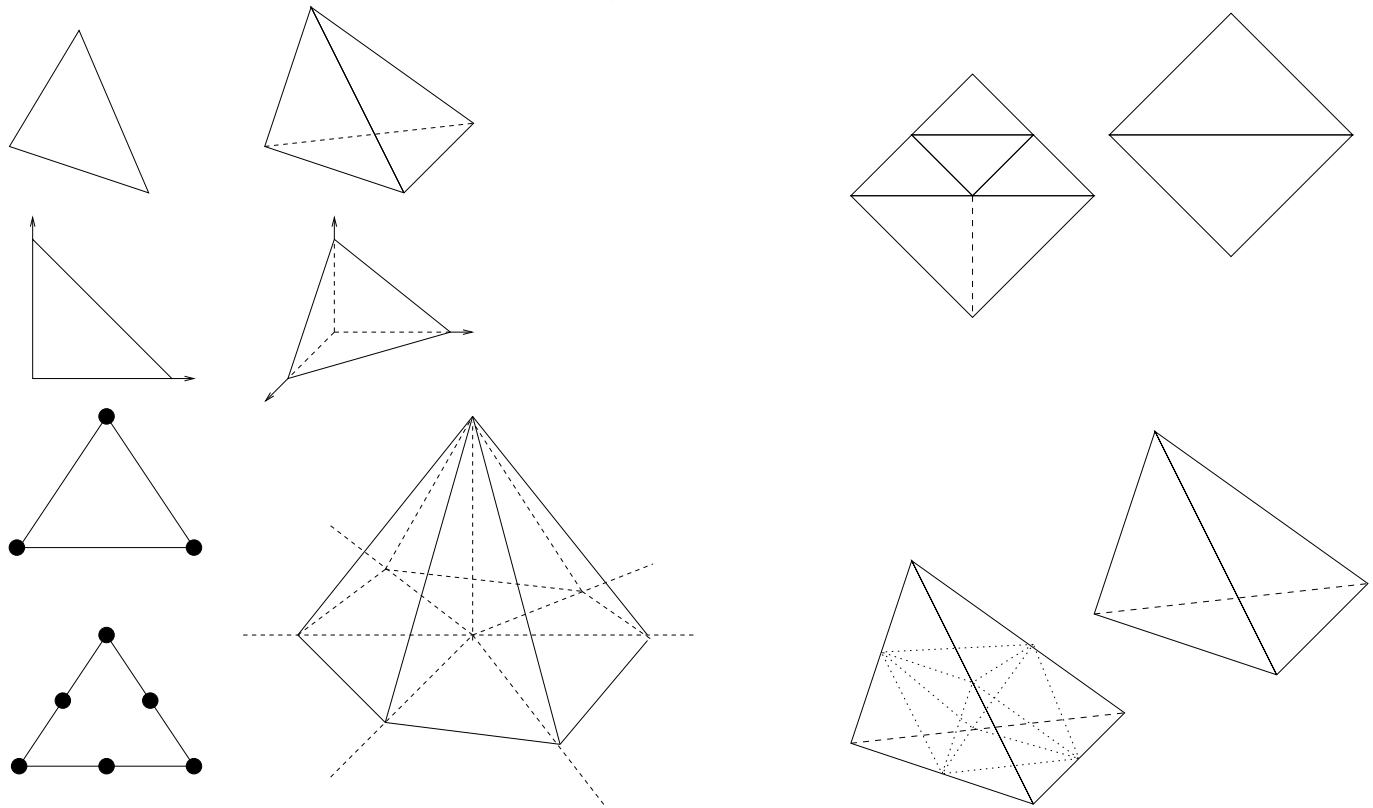

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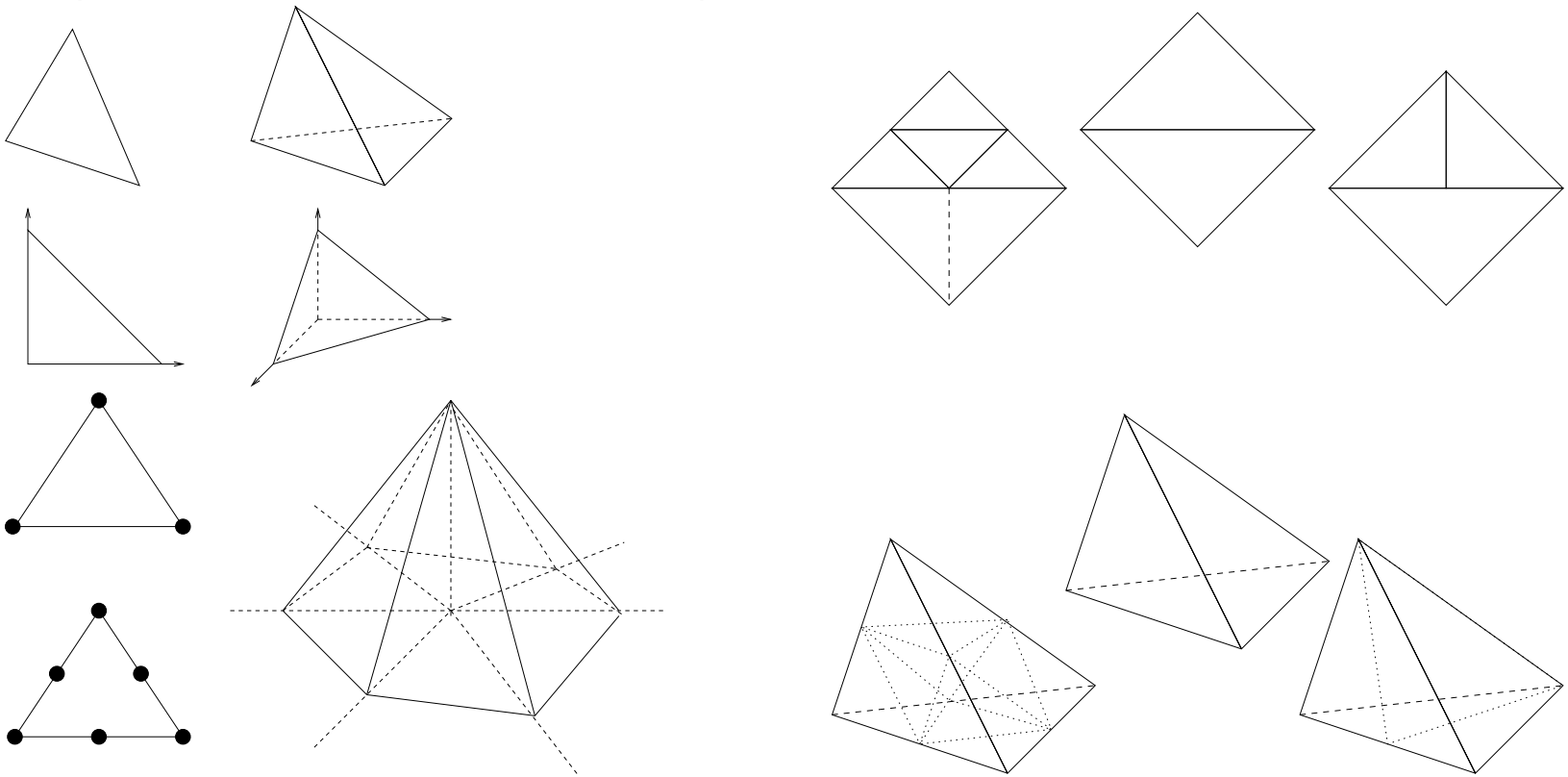

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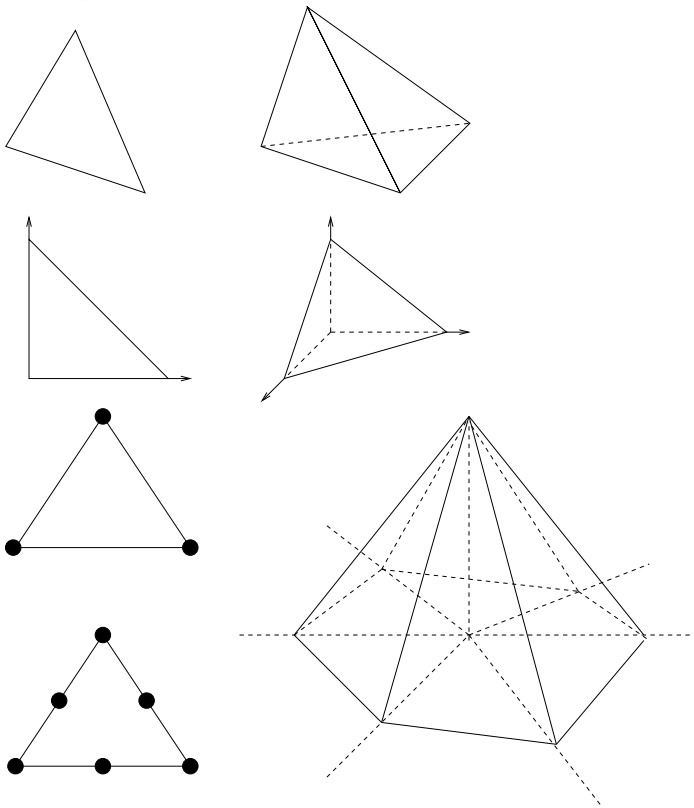
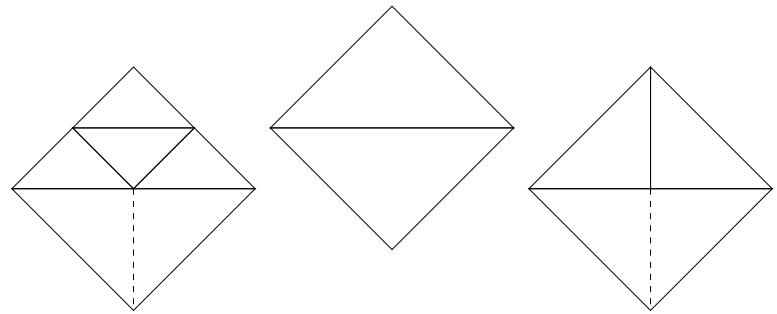
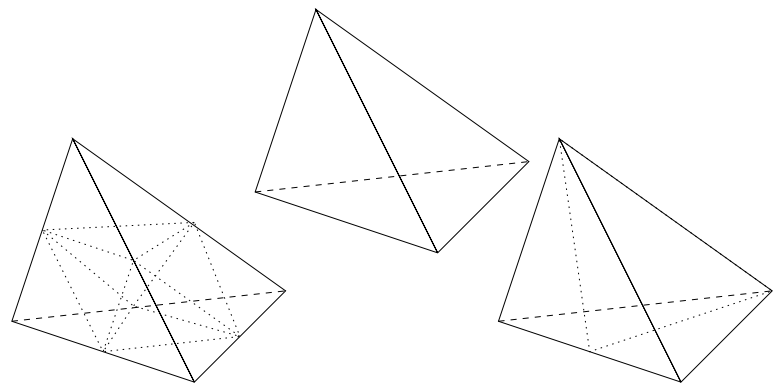






Error-estimate-driven adaptive finite element methods often based on simplex subdivision. (Above: 2/4/8-section and conformity.)

Assembling FE Systems Using An Atlas of Charts

Interesting aspect of FE techniques: coordinate transformations.

For example, if our variational problem $a(u, v) = f(v)$ involves

$$a(u, v) = \int_\Omega [\nabla u \cdot \nabla v + cuv] \, dx, \qquad f(v) = \int_\Omega fv \, dx,$$

and if the domain $\Omega \subset \mathbb{R}^d$ is disjointly covered by conforming elements T_k,

$$\bar{\Omega} = \bigcup_{k=1}^{m} T_k, \qquad \emptyset = \bigcap_{k=1}^{m} \mathrm{int}(T_k),$$

then

$$A_{ij} = a(\phi_j, \psi_i) = \int_\Omega [\nabla \phi_j \cdot \nabla \psi_i + c\phi_j \psi_i] \, dx = \sum_{k=1}^{m} \int_{T_k} [\nabla \phi_j \cdot \nabla \psi_i + c\phi_j \psi_i] \, dx,$$

$$B_i = f(\psi_i) = \int_\Omega f\psi_i \, dx = \sum_{k=1}^{m} \int_{T_k} f\psi_i \, dx.$$

Implementation involves integration on each element T_k via coordinate transformation to a model of $\mathbb{R}^d$ (*reference element*), doing the integral there using transformation jacobians, and then mapping the result back to T_k.

Linear Petrov-Galerkin Approximation Error ($X \neq Y$)

To analyze the error, consider a linear problem and its PG approximation:

$$\text{Find } u \in X \text{ s.t. } a(u,v) = f(v), \quad \forall v \in Y, \tag{19}$$

$$\text{Find } u_h \in X_h \subseteq X \text{ s.t. } a(u_h,v_h) = f(v_h), \quad \forall v_h \in Y_h \subseteq Y, \tag{20}$$

where the following are assumed to hold for $[X, Y]$ (AND ALSO $[X_h, Y_h]$!):

$$\inf_{u\in X}\sup_{v\in Y}\frac{a(u,v)}{\|u\|_X\|v\|_Y} \geq m > 0, \qquad a(u,v) \leq M\|u\|_X\|v\|_Y, \qquad f(v) \leq L\|v\|_Y. \tag{21}$$

The following *a priori* error estimate [Babuska;Brezzi] for PG approx holds:

$$\|u - u_h\|_X \leq \left(1 + \frac{M}{m}\right) \inf_{w_h\in X_h} \|u - w_h\|_X. \tag{22}$$

To see this, first let P_h denote the projection of u onto the unique PG approx $u_h = P_h u$, and let $\|P_h\|$ denote the subordinate operator norm on X.

Linear Petrov-Galerkin Approximation Error ($X \neq Y$)

Then,

$$\|u-u_h\|_X = \|(I-P_h)(u-w_h)\|_X \leq \|I-P_h\|\ \|u-w_h\|_X \leq (1+\|P_h\|)\ \|u-w_h\|_X. \tag{23}$$

Using the fact that $a(u_h, v_h) = a(u, v_h),\ \forall v_h \in Y_h$, one notes:

$$m\|P_h u\|_X = m\|u_h\|_X \leq \sup_{v_h \in Y_h} \frac{a(u_h, v_h)}{\|v_h\|_Y} = \sup_{v_h \in Y_h} \frac{a(u, v_h)}{\|v_h\|_Y} \leq M\|u\|_X,$$

giving $\|P_h\| = M/m$. Employing this in (23) gives then (22).

It is interesting to note that the "1" in the constant can be removed using a result on projectors.

Improving the Constant in P-G Approximation

Consider the following result on non-trivial idempotent linear operators.

Lemma: *[Kato,Xu-Zikatanov] Let H be a Hilbert space. If $P \in L(H,H)$ satisfies $0 \neq P^2 = P \neq I$, and if $\|\cdot\|$ denotes the subordinate operator on H, then*

$$\|P\| = \|I - P\|.$$

As pointed out by [Xu-Zikatanov], this result can be used to remove the leading "1" in the PG constant. As before, let P_h denote the projection of u onto the unique PG approximation $u_h = P_h u$. The result on idempotent linear operators gives now:

$$\|u-u_h\|_X = \|(I-P_h)(u-w_h)\|_X \leq \|I-P_h\|\,\|u-w_h\|_X = \|P_h\|\,\|u-w_h\|_X. \quad (24)$$

As before, using the fact that $a(u_h, v_h) = a(u, v_h),\ \forall v_h \in Y_h$, one notes:

$$m\|P_h u\|_X = m\|u_h\|_X \leq \sup_{v_h \in Y_h} \frac{a(u_h, v_h)}{\|v_h\|_Y} = \sup_{v_h \in Y_h} \frac{a(u, v_h)}{\|v_h\|_Y} \leq M\|u\|_X,$$

giving $\|P_h\| = M/m$. Employing this in (24) gives now an improved constant:

$$\|u - u_h\|_X \leq \left(\frac{M}{m}\right) \|u - w_h\|_X.$$

Linear Galerkin Approximation Error ($X = Y$)

To analyze the error, consider a linear problem and its Galerkin approximation:

$$\text{Find } u \in X \text{ s.t. } a(u, v) = f(v), \quad \forall v \in X, \tag{25}$$

$$\text{Find } u_h \in X_h \subseteq X \text{ s.t. } a(u_h, v_h) = f(v_h), \quad \forall v_h \in X_h \subseteq X, \tag{26}$$

where

$$a(u, u) \geq m\|u\|_X^2, \qquad a(u, v) \leq M\|u\|_X\|v\|_X, \qquad f(v) \leq L\|v\|_X. \tag{27}$$

The following *a priori* error estimate [Cea's Lemma] for the Galerkin approx:

$$\|u - u_h\|_X \leq \left(\frac{M}{m}\right) \inf_{w_h \in X_h} \|u - w_h\|_X,$$

follows from $a(u - u_h, v_h) = 0$, $\forall v_h \in X_h$, and from

$$m\|u - u_h\|_X^2 \leq a(u - u_h, u - u_h) = a(u - u_h, u - w_h) \leq \|u - u_h\|_X\|u - w_h\|_X.$$

If some of the properties (27) are lost, or if the problem is nonlinear, *a priori* estimates for Galerkin methods may still be possible (case-by-case basis).

Nonlinear Petrov-Galerkin Approx. Error ($X \neq Y$)

To analyze the error, consider a nonlinear problem and its PG approximation:

$$\text{Find } u \in X \text{ s.t. } a(u,v) + \langle b(u), v\rangle = f(v), \quad \forall v \in Y, \tag{28}$$

$$\text{Find } u_h \in X_h \subseteq X \text{ s.t. } a(u_h,v_h) + \langle b(u_h), v_h\rangle = f(v_h), \quad \forall v_h \in Y_h \subseteq Y, \tag{29}$$

where the following are assumed to hold for $[X, Y]$ (AND ALSO $[X_h, Y_h]$!):

$$\inf_{u\in X}\sup_{v\in Y}\frac{a(u,v)}{\|u\|_X\|v\|_Y} \geq m > 0, \quad a(u,v) \leq M\|u\|_X\|v\|_Y, \quad f(v) \leq L\|v\|_Y, \tag{30}$$

as well as the following conditions on the nonlinearity:

$$\begin{aligned}\sup_{v_h\in Y_h}\langle b(u_h) - b(w_h), v_h\rangle &\geq 0,\\ \langle b(u) - b(w_h), v_h\rangle &\leq K\|u - w_h\|_X\|v_h\|_Y, \quad \forall w_h \in X_h, \quad v_h \in Y_h.\end{aligned}$$

The following *a priori* error estimate holds for nonlinear PG approximation:

$$\|u - u_h\|_X \leq \left(1 + \frac{M+K}{m}\right)\inf_{w_h\in X_h}\|u - w_h\|_X.$$

To see this, first note that the Petrov-Galerkin solution u_h satisfies:

$$a(u - u_h, v_h) + \langle B(u) - B(u_h), v_h\rangle = 0, \quad \forall v_h \in Y_h.$$

Nonlinear Petrov-Galerkin Approx. Error ($X \neq Y$)

This implies $\forall v_h \in Y_h$ that:

$$\begin{aligned} a(u - w_h, v_h) + \langle B(u) - B(w_h), v_h \rangle &= a(u_h - w_h, v_h) + \langle B(u_h) - B(w_h), v_h \rangle \\ &+ a(u - u_h, v_h) + \langle B(u) - B(u_h), v_h \rangle \\ &= a(u_h - w_h, v_h) + \langle B(u_h) - B(w_h), v_h \rangle. \end{aligned}$$

Then

$$\begin{aligned} m\|u_h - w_h\|_X &\leq \sup_{v_h \in Y_h} \frac{a(u_h - w_h, v_h)}{\|v_h\|_Y} \\ &\leq \sup_{v_h \in Y_h} \left\{ \frac{a(u_h - w_h, v_h) + b(u_h - w_h, v_h)}{\|v_h\|_Y} \right\} \\ &= \sup_{v_h \in Y_h} \left\{ \frac{a(u - w_h, v_h) + b(u - w_h, v_h)}{\|v_h\|_Y} \right\} \\ &\leq (M + K)\|u - w_h\|_X. \end{aligned}$$

From the triangle inequality we have then

$$\|u - u_h\|_X \leq \|u - w_h\|_X + \|u_h - w_h\|_X \leq \left(1 + \frac{M + K}{m}\right) \|u - w_h\|_X.$$

Unlike the linear case, the leading "1" cannot be easily removed.

Nonlinear Galerkin Approximation Error ($X = Y$)

To analyze the error, consider a linear problem and its Galerkin approximation:

$$\begin{aligned} \text{Find } u \in X \text{ s.t. } a(u,v) + \langle b(u), v\rangle &= f(v), \quad \forall v \in X, && (31)\\ \text{Find } u_h \in X_h \subseteq X \text{ s.t. } a(u_h,v_h) + \langle b(u_h), v_h\rangle &= f(v_h), \quad \forall v_h \in X_h \subseteq X && (32) \end{aligned}$$

where the following are assumed to hold for $[X, Y]$:

$$a(u,u) \geq m\|u\|_X^2, \qquad a(u,v) \leq M\|u\|_X\|v\|_X, \qquad f(v) \leq L\|v\|_X.$$

as well as the following conditions on the nonlinearity at the solutions u and u_h:

$$\begin{aligned} \langle b(u) - b(u_h), u - u_h\rangle &\geq 0,\\ \langle b(u) - b(u_h), u - w_h\rangle &\leq K\|u - u_h\|_X\|u - w_h\|_Y, \quad \forall w_h \in X_h. \end{aligned}$$

The following *a priori* error estimate **[H1]** holds for the nonlinear Galerkin approximation:

$$\|u - u_h\|_X \leq \left(\frac{M+K}{m}\right) \inf_{w_h \in X_h} \|u - w_h\|_X.$$

Nonlinear Galerkin Approximation Error ($X = Y$)

To see this, note that the Petrov-Galerkin solution u_h satisfies:

$$a(u - u_h, v_h) + \langle b(u) - b(u_h), v_h \rangle = 0, \quad \forall v_h \in X_h,$$

and the result then follows now from:

$$\begin{aligned} m\|u - u_h\|_X^2 &\leq a(u - u_h, u - u_h) \\ &\leq a(u - u_h, u - u_h) + \langle b(u) - b(u_h), u - u_h \rangle \\ &= a(u - u_h, u - w_h) + \langle b(u) - b(u_h), u - w_h \rangle \\ &\leq (M + K)\|u - u_h\|_X \|u - w_h\|_X . \end{aligned}$$

Provably Convergent Discretization of the PBE

The discrete PBE problem is to determine the expansion coefficients:

$$\text{Find } u_h = \sum_{j=1}^{n} \alpha_j \phi_j \text{ such that } \langle F(u_h), \psi_i \rangle = 0, \ i = 1, \ldots, n,$$

using Newton methods by (repeatedly) solving for the correction $w_h = \sum_{j=1}^{n} \gamma_j \phi_j$:

$$\begin{array}{rcl} AW & = & G, \\ U & = & U + W, \end{array} \quad \text{where} \left\{ \begin{array}{rclrcl} A_{ij} & = & \langle F'(u_h)\phi_j, \psi_i \rangle, & U_i & = & \alpha_i, \\ G_i & = & -\langle F(u_h), \psi_i \rangle, & W_i & = & \gamma_i. \end{array} \right\}$$

Again, FE methods allow management of two critical PG approximation issues:

1. Control of the approximation error: $E(u - u_h) = \|u - u_h\|_X$,
2. Space/time complexity of storing and solving the n equations: $AW = G$.

Problem: Standard discretizations in use for the PBE do not converge.
Solution: Convergent discretization method build from RPBE two-scale splitting:

Theorem: [CHX2] *Let u and u_h be the RPBE solution and the finite element approximation, respectively. When u_h is uniformly bounded, we have*

$$\|u - u_h\|_X \lesssim \inf_{v_h \in X_h} \|u - v_h\|_X.$$

Nonlinear Approximation using Adaptive Methods in FETK

Adaptive FEM (AFEM): build approximation spaces adaptively, meeting target quality using spaces having minimal dimension. This is *nonlinear approximation*.

Iterative SOLVE-ESTIMATE-MARK-REFINE algorithms try to equi-distribute error over simplices using subdivision driven by *a posteriori* error estimates:

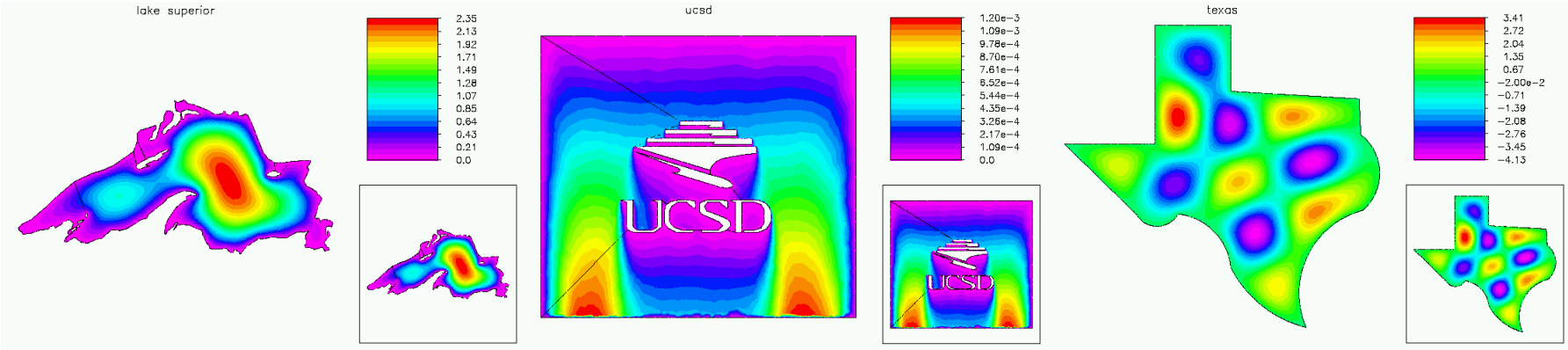
1. Construct problem (build mesh, define PDE coefficients, etc)
2. While ($e(u - u_h)$ is "large") do:
   1. SOLVE: Find $u_h \in X_h$ such that $\langle F(u_h), v_h \rangle = 0, \forall v_h \in Y_h$
   2. ESTIMATE: Estimate $e(u - u_h)$ over each element, set $Q1 = Q2 = \phi$.
   3. MARK: Mark subset of elements for refinement, place in $Q1$.
   4. REFINE:
      1. (R) Place simplices with large error in "refinement" $Q1$
      2. Bisect simplices in $Q1$; place nonconforming simplices in $Q2$.
      3. $Q1$ is now empty; set $Q1 = Q2$, $Q2 = \phi$.
      4. If $Q1$ is not empty, goto (R).
3. end while

Problem: Very few convergence results on adaptive methods for nonlinear problems.
Solution: Convergence proof of an AFEM algorithm for the RPBE [CHX2]:

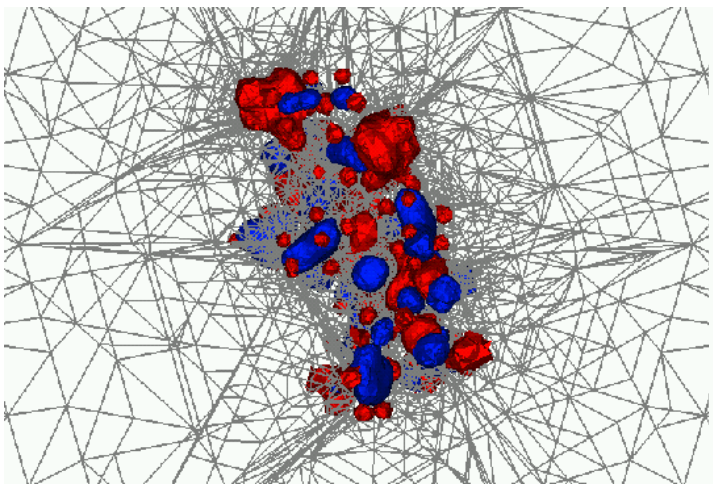
Theorem: [CHX2] *There exists* $0 \leq \gamma < 1$ *such that*

$$\|u - u_{k+1}\|_X \leq \gamma \|u - u_k\|_X, \quad \text{so that} \quad \lim_{k \to \infty} \|u - u_k\|_X = 0,$$

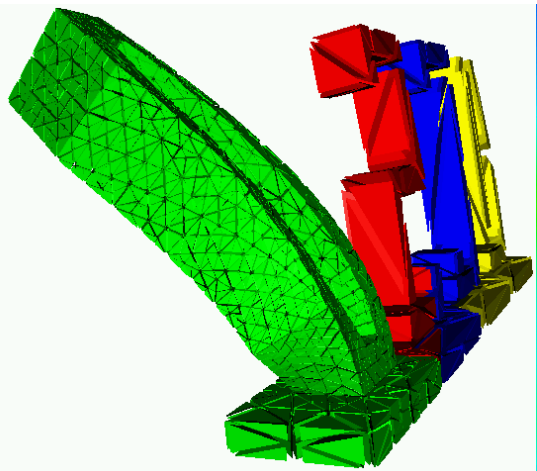
Examples with adaptive FE codes PLTMG and FETK



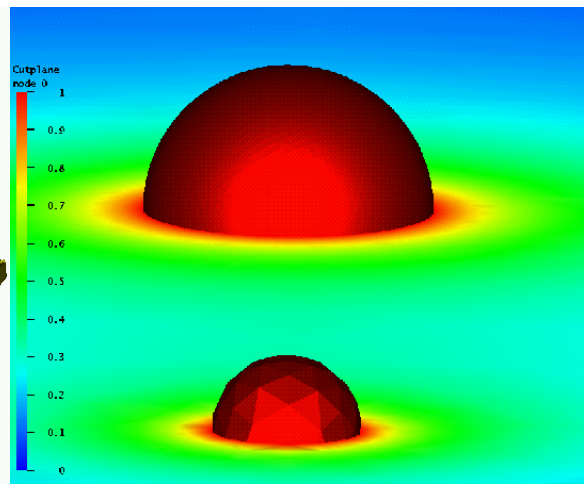
$-\Delta u = 1$ $\quad -\nabla \cdot (\nabla u + \beta u) = 1$ $\quad -\Delta u - 2u = 1$



$-\nabla \cdot (\epsilon \nabla u) + \bar{\kappa}^2 \sinh(u) = f$



$-\nabla \cdot \{(I + \nabla u)\, \check{\Sigma}(E(u))\} = f$



$\hat{\gamma}^{ab} \hat{D}_a \hat{D}_b \phi = P(\phi, W^{ab})$

$\hat{D}_b (\hat{l} W)^{ab} = \frac{2}{3} \phi^6 \hat{D}^a \mathrm{tr} K + 8\pi \hat{j}^a$

A posteriori error estimation for driving *h*-adaptivity

Idea: estimate $E(u - u_h)$ and use information to improve u_h. Some standard options with a well-developed literature:

1. Nonlinear (strong) residual error estimation [Babuska,Verfurth,...].
2. Linearized global dual problem error estimation [Johnson,Estep,...].

Residual estimation: given Banach spaces X, Y, and $X_h \subset X$, $Y_h \subset Y$, consider

$$F(u) = 0, \quad F \in C^1(X, Y^*), \qquad F_h(u_h) = 0, \quad F_h \in C^0(X_h, Y_h^*).$$

The nonlinear residual $F(u_h)$ can be used to estimate $\|u - u_h\|_X$:

$$\left[\frac{1}{2}\|DF(u)\|^{-1}_{\mathcal{L}(X,Y^*)}\right] \cdot \|F(u_h)\|_{Y^*} \leq \|u - u_h\|_X \leq \left[2\|DF(u)^{-1}\|_{\mathcal{L}(Y^*,X)}\right] \cdot \|F(u_h)\|_{Y^*}.$$

Theorem: (E.g., [H1]) *(Residual-based) The galerkin solution u_h satisfies*

$$E(u - u_h) = \|u - u_h\|_X \leq C \left(\sum_{s \in \mathcal{S}} \eta_s^p \right)^{1/p}, \quad (p \text{ depends on choice of } X \text{ and } Y)$$

where η_s is a computable element-wise error "indicator" and C is a "constant".

Proof Outline: *A few inequalities and a quasi-interpolation argument.* □

A general residual *a posteriori* error estimate

In our setting of second order nonlinear PDE, what is needed is a bound on the dual norm with the index q determined by the weak formulation:

$$\|F(u)\|_{W^{-1,q}(\mathcal{M})} = \sup_{0 \neq v \in W^{1,q}(\mathcal{M})} \frac{|\langle F(u), v \rangle|}{\|v\|_{W^{1,q}(\mathcal{M})}}.$$

We derive such a bound for the following class of elliptic problems:

$$\begin{aligned} -A^{ia}(x^b, u^j, u^k_{;c})_{;a} + B^i(x^j, u^k, u^k_{;c}) &= 0 \ \text{ in } \mathcal{M}, \\ A^{iq}(x^b, u^j, u^k_{;c}) n_a + C^i(x^j, u^k) &= 0 \ \text{ on } \partial_1\mathcal{M}, \\ u^i(x^b) &= E(x^b) \ \text{ on } \partial_0\mathcal{M}, \end{aligned}$$

which includes all the nonlinear elliptic problems above, where:

$$1 \leq a, b, c \leq d, \qquad 1 \leq i, j, k \leq n,$$

$$A : \mathcal{M} \times \mathbb{R}^n \times \mathbb{R}^{nd} \mapsto \mathbb{R}^{nd}, \qquad B : \mathcal{M} \times \mathbb{R}^n \times \mathbb{R}^{nd} \mapsto \mathbb{R}^n, \qquad C : \partial_1\mathcal{M} \times \mathbb{R}^n \mapsto \mathbb{R}^n,$$

$$E : \partial_0\mathcal{M} \mapsto \mathbb{R}^n, \qquad \partial_0\mathcal{M} \cup \partial_1\mathcal{M} = \partial\mathcal{M}, \qquad \partial_0\mathcal{M} \cap \partial_1\mathcal{M} = \emptyset.$$

We are using tensor notation here, with $X_{;c} = \frac{\partial X}{\partial x^c}$ representing partial differentiation, and with summation convention in play.

Residual *a posteriori* error estimate (cont)

Under growth restrictions on A^{ia}, B^i, C^i, there exists $1 < p_k, q_k, r_k < \infty$ such that the weak formulation is well-defined:

$$\text{Find } u^i \in \bar{u}^i + \mathcal{B}_1 \text{ s.t. } \langle F(u^i), v^j \rangle = 0, \quad \forall v^j \in \mathcal{B}_2,$$

where $E^i = \text{tr } \bar{u}^i$ via a covariant Trace Theorem, and where

$$\mathcal{B}_1 = W^{1,r_1}_{0,D}(\mathcal{M}) \times \cdots \times W^{1,r_k}_{0,D}(\mathcal{M}), \qquad \mathcal{B}_2 = W^{1,q_1}_{0,D}(\mathcal{M}) \times \cdots \times W^{1,q_k}_{0,D}(\mathcal{M}),$$

with $1/p_k + 1/q_k = 1$, and $r_k \geq \min\{p_k, q_k\}$.

The form is produced by (covariant) integration-by-parts:

$$\langle F(u), v \rangle = \int_{\mathcal{M}} \mathcal{G}_{ij}(A^{ia} v^j{}_{;a} + B^i v^j) \, dx + \int_{\partial_1 \mathcal{M}} \mathcal{G}_{ij} C^i v^j \, ds = 0,$$

for suitable product metric $\mathcal{G}_{ij}$.

Residual *a posteriori* error estimate (cont)

Some additional notation:

$$[v]_f(x) = \lim_{\epsilon \longrightarrow 0^+} v(x + \epsilon n_f) - \lim_{\epsilon \longrightarrow 0^-} v(x - \epsilon n_f).$$

$$\begin{array}{lcl}
\mathcal{S} & = & \text{Set of shape-regular simplices forming } \mathcal{M} \\
\mathcal{N}(s) & = & \text{The union of faces in } s \text{ lying on } \partial_1 \mathcal{M} \\
\mathcal{I}(s) & = & \text{The union of faces in } s \text{ not in } \mathcal{N}(s) \\
\mathcal{F}(s) & = & \mathcal{N}(s) \cup \mathcal{I}(s) \\
\omega_s & = & \bigcup \{ \tilde{s} \in \mathcal{S} \mid s \bigcap \tilde{s} \neq \emptyset, \text{ where } s \in \mathcal{S} \} \\
\omega_f & = & \bigcup \{ \tilde{s} \in \mathcal{S} \mid f \bigcap \tilde{s} \neq \emptyset, \text{ where } f \in \mathcal{F} \} \\
h_s & = & \text{The diameter of the simplex } s \\
h_f & = & \text{The diameter of the face } f.
\end{array}$$

Residual *a posteriori* error estimate (cont)

Theorem: [H1] *The galerkin solution u_h satisfies*

$$\|u - u_h\|_{W^{1,r}(\mathcal{M})} \leq C \left(\sum_{s \in \mathcal{S}} \eta_s^p \right)^{1/p}, \qquad 1/p + 1/q = 1, \quad r \geq \min\{p, q\},$$

where C and the element-wise residual error indicator η_s are:

$$C = 2 \cdot \max\{C_s, C_f\} \cdot \max\{D_s^{1/q}, D_f^{1/q}\} \cdot \|DF(u)^{-1}\|_{\mathcal{L}(W^{-1,q}, W^{1,p})},$$

$$\eta_s = \left(h_s^p \| B^i - A^{ia}{}_{;a} \|_{L^p(s)}^p + \frac{1}{2} \sum_{f \in \mathcal{I}(s)} h_f \| \left[A^{ia} n_a \right]_f \|_{L^p(f)}^p + \sum_{f \in \mathcal{N}(s)} h_f \| C^i + A^{ia} n_a \|_{L^p(f)}^p \right)^{1/p}.$$

Proof: *A few inequalities (continuous and discrete Hölder) and $W^{k,p}$-quasi-interpolation (Clément or Scott-Zhang) argument.* □

Duality-based *a posteriori* error estimation

Assume $F : X \mapsto Y$, X and Y Banach spaces, and $F \in C^1$, s.t.

$$F(u+h) = F(u) + \left\{ \int_0^1 DF(u+\xi h) d\xi \right\} h.$$

Taking $h = u_h - u$, $F(u) = 0$, and u_h a Galerkin approximation to u, gives

$$F(u_h) = F(u+h) = F(u+[u_h-u]) = F(u) + \mathcal{A}(u_h - u) = -\mathcal{A}(u - u_h),$$

where

$$\mathcal{A} = \int_0^1 DF(u+\xi h) d\xi.$$

We wish to estimate linear functionals $E(u-u_h) = \langle u - u_h, \psi \rangle$ of the error $u - u_h$.

Theorem: (E.g., [H1]) *(Duality-based) If ϕ_h is a Galerkin approximation to the solution of the dual problem: $\mathcal{A}^T \phi = \psi$, then*

$$E(u-u_h) = -\langle F(u_h), \phi - \phi_h \rangle.$$

Proof Outline:

$$E(u-u_h) = \langle u-u_h, \psi \rangle = \langle u-u_h, \mathcal{A}^T \phi \rangle = \langle \mathcal{A}(u-u_h), \phi - \phi_h \rangle = -\langle F(u_h), \phi - \phi_h \rangle.$$

□

Solving the resulting nonlinear discrete equations

Each iteration of these types of adaptive algorithm requires:

1. Solve discrete nonlinear problem (e.g. via Global Inexact Newton).
2. Estimate the error in each simplex.
3. Locally adapt the mesh; go back to 1.

Solution of Newton linearization systems completely dominate space and time complexity of overall adaptive algorithm (everything else has linear complexity).

Fundamental Problems:

- Algorithms must have (nearly) linear space and (sequential) time complexity.
- Algorithms must scale (nearly) linearly with P on a parallel computer.
- MG *does not* have linear space OR time complexity on adapted meshes.

Our Solutions: Fast linear elliptic solvers based on:

- BPX [Bramble-Pasciak-Xu] & stabilized HB [Bank;Vassilevski-Wang]. **[AH]**
- De-coupling algorithms for scalability on parallel computers. **[BH]**

Iterative methods for solving discretized *linear* PDE

We wish to solve the operator equation $Au = f$.
Given a *preconditioner* $B \approx A^{-1}$, consider *preconditioned system* $BAu = Bf$, and a resulting linear iterative method:

$$u^{n+1} = u^n + B(f - Au^n) = (I - BA)u^n + Bf. \tag{33}$$

The identity $u = u - BAu + Bf$ yields an error equation for $e^n = u - u^n$:

$$e^{n+1} = (I - BA)e^n = (I - BA)^2 e^{n-1} = \cdots = (I - BA)^{n+1} e^0. \tag{34}$$

The convergence of Algorithm 33 is determined by the spectral radius of the error propagator $E = I - BA$.

Theorem: *The condition* $\rho(I - BA) < 1$ *is necessary and sufficient for convergence of Algorithm 33.*

Note that any symmetric positive definite (SPD) $n \times n$ matrix M can be used to define an alternative norm on $\mathbb{R}^n$ as follows:

$$\|u\|_A = (Au, u), \qquad (u, v) = \sum_{i=1}^{n} u_i v_i.$$

Iterative methods for solving linear equations

Since $|\lambda|\|u\| = \|\lambda u\| = \|Mu\| \leq \|M\| \ \|u\|$ for any norm $\|\cdot\|$, it follows that $\rho(M) \leq \|M\|$ for all norms $\|\cdot\|$.
Thus, $\|I - BA\| < 1$ and $\|I - BA\|_A < 1$ are both sufficient conditions for convergence of Algorithm 33.
In fact, it is the norm of the error propagation operator which will bound the reduction of the error at each iteration, which follows from (34):

$$\|e^{n+1}\|_A \leq \|I - BA\|_A \|e^n\|_A \leq \|I - BA\|_A^{n+1} \|e^0\|_A. \tag{35}$$

The spectral radius $\rho(E)$ of the error propagator E is called the *convergence factor* for Algorithm 33, whereas the norm of the error propagator $\|E\|$ is referred to as the *contraction number* (with respect to the particular choice of norm $\|\cdot\|$).
Define the *A-condition number* of an invertible operator M by extending the standard notion to the A-inner-product:

$$\kappa_A(M) = \|M\|_A \|M^{-1}\|_A.$$

It can be shown that if M is A-self-adjoint, then:

$$\kappa_A(M) = \frac{\lambda_{\max}(M)}{\lambda_{\min}(M)}.$$

Complexity of linear methods

To reduce the initial error $\|e^0\|_A$ by the factor ϵ, then equation (35) implies this is guaranteed if

$$\|E\|_A^{n+1} \leq \epsilon.$$

Taking logarithms of both sides and solving for n, the maximum number of iterations required to reach the desired tolerance is

$$n \geq \frac{|\ln \epsilon|}{|\ln \|E\|_A|}. \tag{36}$$

If the bound on the norm is of the form in Lemma 59, then to achieve a tolerance of ϵ after n iterations will require:

$$n \geq \frac{|\ln \epsilon|}{\left|\ln\left(1 - \frac{2}{1+\kappa_A(BA)}\right)\right|} = \frac{|\ln \epsilon|}{\left|\ln\left(\frac{\kappa_A(BA)-1}{\kappa_A(BA)+1}\right)\right|}. \tag{37}$$

Using the approximation:

$$\ln\left(\frac{a-1}{a+1}\right) = \ln\left(\frac{1+(-1/a)}{1-(-1/a)}\right) = 2\left[\left(\frac{-1}{a}\right) + \frac{1}{3}\left(\frac{-1}{a}\right)^3 + \frac{1}{5}\left(\frac{-1}{a}\right)^5 + \cdots\right] <$$

Iterative methods for solving linear equations

we have $|\ln[(\kappa_A(BA)-1)/(\kappa_A(BA)+1)]| > 2/\kappa_A(BA)$, so:

$$n \geq \frac{1}{2}\kappa_A(BA)|\ln\epsilon| + 1.$$

The maximum number of iterations required ϵ is then

$$n = O\left(\kappa_A(BA)|\ln\epsilon|\right).$$

If a single iteration of the method costs $O(N)$ operations, the complexity to solve the problem is $O(\kappa_A(BA)N|\ln\epsilon|)$.
If $\|E\|_A$ or $\kappa_A(BA)$ independent of N, complexity is near optimal $O(N|\ln\epsilon|)$.
We have made use of the following classical result:

Lemma: *If A and B are SPD, then*

$$\rho(I-\alpha BA) = \|I-\alpha BA\|_A < 1.$$

if and only if $\alpha \in (0, 2/\rho(BA))$. Convergence is optimal when $\alpha = 2/[\lambda_{\min}(BA)+\lambda_{\max}(BA)]$, giving

$$\rho(I-\alpha BA) = \|I-\alpha BA\|_A = 1 - \frac{2}{1+\kappa_A(BA)} < 1.$$

Preconditioned conjugate gradient methods

Given some (method for applying) $B \approx A^{-1}$, we can either formulate a linear method or employ a CG method.

(A preconditioned CG method)

Let $u^0 \in \mathcal{H}$ be given, $\quad r^0 = f - Au^0, \quad s^0 = Br^0, \quad p^0 = s^0.$

Do $i = 0, 1, \ldots$ until convergence:

$\alpha_i = (r^i, s^i)/(Ap^i, p^i)$

$u^{i+1} = u^i + \alpha_i p^i$

$r^{i+1} = r^i - \alpha_i A p^i$

$s^{i+1} = Br^{i+1}$

$\beta_{i+1} = (r^{i+1}, s^{i+1})/(r^i, s^i)$

$p^{i+1} = s^{i+1} + \beta_{i+1} p^i$

End do.

The error at each CG iteration be written as a polynomial in BA times the initial error:

$$e^{i+1} = [I - BAp_i(BA)]e^0,$$

where $p_i \in \mathcal{P}_i$, the space of polynomials of degree i.

Preconditioned conjugate gradient methods

At each step the energy norm $\|e^{i+1}\|_A = \|u - u^{i+1}\|_A$ is minimized over the Krylov subspace:

$$V_{i+1}(BA, Br^0) = \text{span}\,\{Br^0, (BA)Br^0, (BA)^2Br^0, \ldots, (BA)^i Br^0\}.$$

Thus,

$$\|e^{i+1}\|_A = \min_{p_i \in \mathcal{P}_i} \|[I - BAp_i(BA)]e^0\|_A.$$

Using some simple well-known properties of the scaled and shifted Chebyshev polynomials, the following contraction bound is easily derived:

$$\|e^{i+1}\|_A \leq 2 \left(\frac{\sqrt{\frac{\lambda_{\max}(BA)}{\lambda_{\min}(BA)}} - 1}{\sqrt{\frac{\lambda_{\max}(BA)}{\lambda_{\min}(BA)}} + 1} \right)^{i+1} \|e^0\|_A = 2\ \delta_{\text{cg}}^{i+1}\ \|e^0\|_A, \tag{38}$$

$$\delta_{\text{cg}} = \frac{\sqrt{\kappa_A(BA)} - 1}{\sqrt{\kappa_A(BA)} + 1} = 1 - \frac{2}{1 + \sqrt{\kappa_A(BA)}}.$$

Theorem: *If A and B are SPD, and $\|I - BA\|_A \leq \delta < 1$, then $\delta_{\text{cg}} < \delta$.*

Preconditioned conjugate gradient methods

Proof is by noting $\kappa_A(BA) > 1$, so $\delta_{\mathrm{cg}} < \delta_{\mathrm{opt}} \leq \delta$ follows from:

$$\delta_{\mathrm{opt}} = 1 - \frac{2}{1 + \kappa_A(BA)}, \qquad \delta_{\mathrm{cg}} = 1 - \frac{2}{1 + \sqrt{\kappa_A(BA)}}.$$

Complexity of CG methods

The cost to reduce the energy norm of the error below a tolerance ϵ can be determined using δ_{cg} and (38).
To achieve a tolerance of ϵ after n iterations will require:

$$2\ \delta_{\mathrm{cg}}^{n+1} = 2\ \left(\frac{\sqrt{\kappa_A(BA)}-1}{\sqrt{\kappa_A(BA)}+1}\right)^{n+1} < \epsilon.$$

Dividing by 2 and taking natural logarithms yields:

$$n \geq \left|\ln\frac{\epsilon}{2}\right| \cdot \left|\ln\left(\frac{\sqrt{\kappa_A(BA)}-1}{\sqrt{\kappa_A(BA)}+1}\right)\right|^{-1}.$$

Using the approximation:

$$\ln\left(\frac{a-1}{a+1}\right) = 2\left[\left(\frac{-1}{a}\right) + \frac{1}{3}\left(\frac{-1}{a}\right)^3 + \frac{1}{5}\left(\frac{-1}{a}\right)^5 + \cdots\right] < \frac{-2}{a},$$

we have $|\ln[(\kappa_A^{1/2}(BA)-1)/(\kappa_A^{1/2}(BA)+1)]| > 2/\kappa_A^{1/2}(BA)$, and:

$$n \geq \frac{1}{2}\kappa_A^{1/2}(BA)\left|\ln\frac{\epsilon}{2}\right| + 1.$$

Complexity of CG methods

We then have that the maximum number of iterations required to reach an error on the order of the tolerance ϵ is:

$$n = O\left(\kappa_A^{1/2}(BA)\left|\ln\frac{\epsilon}{2}\right|\right).$$

If the cost of each iteration is $O(N)$, which holds in the case of sparse matrices generated by FEM, the complexity to solve the problem is $O(\kappa_A^{1/2}(BA)N|\ln[\epsilon/2]|)$. If $\kappa_A^{1/2}(BA)$ can be bounded independently of the problem size N, then the complexity becomes (near) optimal order $O(N|\ln[\epsilon/2]|)$.

Complexities of various methods: to force $||u - u^n|| < \epsilon$ for model problems:

Method	2D	3D
Gaussian elimination (GE)	$O(N^3)$	$O(N^3)$
Banded GE	$O(N^2)$	$O(N^{2.33})$
Sparse GE	$O(N^{1.5})$	$O(N^2)$
Jacobi/Gauss-Seidel iteration	$O(N^2 \ln N)$	$O(N^{1.67} \ln N)$
SOR	$O(N^{1.5} \ln N)$	$O(N^{1.33} \ln N)$
Conjugate gradients (CG)	$O(N^{1.5}) \ln N)$	$O(N^{1.33} \ln N)$
Preconditioned CG	$O(N^{1.25} \ln N)$	$O(N^{1.17} \ln N)$
Multilevel methods	$O(N \ln N)$	$O(N \ln N)$
Nested multilevel methods	$O(N)$	$O(N)$

Nonlinear approximation: BPX and HB methods

Problem: Local refinement driven by *a posteriori* error estimation forces ML methods to be sub-optimal, due to slow dimension growth in space hierarchy:

- Worse than linear storage requirements.
- Worse than linear computational complexity for a *single* iteration.

Solution: Change multilevel algorithm to work only at new DOF in each space; result is HB-Method [Bank-Dupont-Yserentant, 1986]. Regains linear space and time complexity, *per iteration*.
New Problem: $\kappa_A(BA)$ grows like $O(N \log N)$ in 2D, much worse in $3D$.
Potential Solutions:

- BPX Preconditioner: Optimality shown by Oswald, Xu, others in quasi-uniform case; 2D local refinement optimal due to Dahmen-Kunoth.
- Stabilized HB: Optimality shown by Vassilevski-Wang in 2D/3D quasi-uniform case.

Dahmen-Kunoth BPX result extended to 3D/n-D local refinement in **[AH]**.

Vassilevski-Wang result extended to 2D/3D/n-D local refinement in **[AH]**.

We will discuss briefly the 3D BPX results in **[AH]**.

Linear complexity methods for nonlinear approximation

Given an SPD $A \in \mathbf{L}(X, X)$, where $\{X, (\cdot,\cdot), \|\cdot\| = (\cdot,\cdot)^{1/2}\}$ is a Hilbert space, we wish to solve the operator equation for u:

$$Au = f.$$

The SPD operator A defines a second inner-product $(\cdot,\cdot)_A = (A\cdot,\cdot)$ on X, inducing a second norm $\|\cdot\|_A = (\cdot,\cdot)_A^{1/2}$.
Some (method for applying) $B \approx A^{-1}$ to $v \in \mathcal{H}$, we can either:

1. Use a linear method: $u^{n+1} = u^n - \alpha BAu^n + \alpha Bf = (I - \alpha BA)u^n + \alpha Bf$.
2. Use CG on preconditioned $BAu = Bf$.

Linear method iterations to reach ϵ (with optimal α):

$$k \geq \frac{1}{2}\kappa_A(BA)|\ln\epsilon| + 1, \qquad \text{so that :} \quad k = O\left(\kappa_A(BA)|\ln\epsilon|\right). \quad \text{(or worse!)}$$

CG iterations to reach ϵ:

$$k \geq \frac{1}{2}\kappa_A^{1/2}(BA)|\ln\frac{\epsilon}{2}| + 1. \qquad \text{so that :} \quad k = O\left(\kappa_A^{1/2}(BA)|\ln\frac{\epsilon}{2}|\right). \quad \text{(or better!)}$$

Apparently we need to estimate condition numbers

If any of the following (equivalent) norm equivalences hold,

$$\begin{aligned}
c_1(Au,u) &\le (ABAu,u) \le c_2(Au,u),\\
c_1(Bu,u) &\le (BABu,u) \le c_2(Bu,u),\\
c_1(A^{-1}u,u) &\le (Bu,u) \le c_2(A^{-1}u,u),\\
c_1(B^{-1}u,u) &\le (Au,u) \le c_2(B^{-1}u,u),\\
c_2^{-1}(Au,u) &\le (B^{-1}u,u) \le c_1^{-1}(Au,u),\\
c_2^{-1}(Bu,u) &\le (A^{-1}u,u) \le c_1^{-1}(Bu,u),
\end{aligned}$$

then by simple spectral theory arguments one has

$$\kappa_A(BA) \le c_1^{-1}c_2.$$

The following notation is useful, where $x, y \in \mathbb{R}$ and $c \in \mathbb{R}$ a universal constant:

$$\begin{aligned}
x \lesssim y \quad &\text{if} \quad x \le cy,\\
x \gtrsim y \quad &\text{if} \quad y \le cx,\\
x \eqsim y \quad &\text{if} \quad \frac{1}{c}y \le x \le cy \quad (\text{i.e., } x \lesssim y \text{ and } x \gtrsim y).
\end{aligned}$$

Spaces from approximation theory that will arise

Besov and approximation spaces arise naturally in modern approximation theory:

$$B^s_{p,q}(\mathcal{M}) = \left\{ u \ : \ \|u\|_{B^s_{p,q}(\mathcal{M})} < \infty \right\}, \quad A^s_{p,q}(\mathcal{M}) = \left\{ u \ : \ \|u\|_{A^s_{p,q}(\mathcal{M})} < \infty \right\},$$

where

$$\begin{aligned} \|u\|_{B^s_{p,q}(\mathcal{M})} &= \|u\|_{L^p(\mathcal{M})} + |u|_{B^s_{p,q}(\mathcal{M})}, \\ |u|_{B^s_{p,q}(\mathcal{M})} &= \|\{2^{sj}\omega_k(f, 2^{-j}, \mathcal{M})_p\}_{j\in\mathbb{N}_0}\|_{l^q}, \\ \|u\|_{A^s_{p,q}(\mathcal{M})} &= \|\{2^{sj}\|(Q_j - Q_{j-1})u\|_{L^p(\mathcal{M})}\}_{j\in\mathbb{N}_0}\|_{l^q}, \quad Q_{-1} = 0, \ Q_\infty = I. \end{aligned}$$

with

$$\begin{aligned} \omega_k(f, t, \mathcal{M})_p &= \sum_{|h|\le t} \|\Delta^k_h f\|_{L^p(\mathcal{M}_{h,k})}, \\ (\Delta^k_h f)(x) &= \sum_{r=0}^{k} \binom{k}{r} (-1)^{k-r} f(x + rh), \quad x, h \in \mathbb{R}^d, \\ \mathcal{M}_{h,k} &= \{x \in \mathbb{R}^d \ : \ [x, x + kh] \subset \mathcal{M}\}. \end{aligned}$$

Connection to Sobolev spaces:

$$\begin{aligned} W^{s,p}(\mathcal{M}) &= B^s_{p,p}(\mathcal{M}), \ \ p \ge 1, \ s > 0, \ \ \text{when } s \text{ is not an integer}, \\ H^s(\mathcal{M}) &= B^s_{2,2}(\mathcal{M}), \ \ \forall s > 0. \end{aligned}$$

The BPX preconditioner

Let the Hilbert space X contain a multilevel hierarchy of Hilbert spaces:

$$\mathcal{S}_0 \subseteq \mathcal{S}_1 \subseteq \ldots \subseteq \mathcal{S}_J = X \subset H^k(\Omega), \quad \dim(X) < \infty,$$

with $\mathcal{S}_k$ inheriting Hilbert space structure from X. Subspaces $\tilde{\mathcal{S}}_j$ arise naturally:

$$\mathcal{S}_j \setminus \mathcal{S}_{j-1} \subseteq \tilde{\mathcal{S}}_j \subseteq \mathcal{S}_j.$$

Let $\tilde{Q}_j$ be set of local projection (orthogonal and idempotent) operators:

$$\tilde{Q}_j : L^2(\Omega) \mapsto \tilde{\mathcal{S}}_j, \quad j = 0, \ldots, J, \qquad \tilde{Q}_{-1} = 0, \ \tilde{Q}_J = I.$$

The BPX preconditioner can be defined as e.g.:

$$\bar{B}u = \sum_{j=0}^{J} \lambda_j^{-1} \tilde{Q}_j u, \qquad Bu = \sum_{j=0}^{J} \tilde{R}_j \tilde{Q}_j u. \qquad \left(\text{Note} : \bar{B}^{-1} u = \sum_{j=0}^{J} \lambda_j \tilde{Q}_j u \right)$$

Here, $\tilde{R}_j : \tilde{\mathcal{S}}_j \mapsto \tilde{\mathcal{S}}_j$ is a local smoothing operator satisfying:

$$\lambda_j^{-1} \|v\| \eqsim (\tilde{R}_j v, v), \quad v \in \tilde{\mathcal{S}}_j. \tag{39}$$

Natural assumption on λ_j: There exists $\beta > 1$ such that

$$\lambda_{j+1} \eqsim \beta \lambda_j, \quad j = 0, \ldots, J-1. \qquad (\lambda_j \eqsim h_j^{-2}, \ \lambda_j = 2^j, \ \text{etc.}) \tag{40}$$

Multilevel splittings and the *slice norm*

In classical approximation theory one considers multilevel splittings of the form:

$$u = \sum_{j=0}^{J} (\tilde{Q}_j - \tilde{Q}_{j-1})u.$$

The *approximation* or *slice* operator has the form (with e.g. $\lambda_j = 2^j$):

$$Cu = \sum_{j=0}^{J} \lambda_j (\tilde{Q}_j - \tilde{Q}_{j-1})u, \qquad C^{-1}u = \sum_{j=0}^{J} \lambda_j^{-1} (\tilde{Q}_j - \tilde{Q}_{j-1})u.$$

The approximation (or *slice*) norm can then be written as:

$$(Cu, u) = \|u\|_C^2 = \|u\|_{A^1_{2,2}(\Omega)}^2.$$

Theorem: [Classical; see e.g. AH] *The slice norm and BPX preconditioners are spectrally equivalent:*

$$(C^{-1}u, u) \eqsim (\bar{B}u, u) \eqsim (Bu, u).$$

Proof: *Orthogonality of $\tilde{Q}_k$ and assumptions (39) and (40).* $\square$

(More detailed version of the proof.)

$$
\begin{aligned}
(C^{-1}u,u) &= \sum_{j=0}^{J}\lambda_j^{-1}((\tilde{Q}_j-\tilde{Q}_{j-1})u,u)\\
&= \sum_{j=0}^{J}\lambda_j^{-1}(\tilde{Q}_j u,u)-\sum_{j=0}^{J-1}\lambda_{j+1}^{-1}(\tilde{Q}_j u,u)\\
&\simeq \sum_{j=0}^{J}\lambda_j^{-1}(\tilde{Q}_j u,u)-\sum_{j=0}^{J-1}\frac{1}{\beta}\lambda_j^{-1}(\tilde{Q}_j u,u)\\
&= \lambda_J^{-1}(\tilde{Q}_J u,u)+\sum_{j=0}^{J-1}(1-\frac{1}{\beta})\lambda_j^{-1}(\tilde{Q}_j u,u)\\
&\simeq \lambda_J^{-1}(\tilde{Q}_J u,u)+\sum_{j=0}^{J-1}\lambda_j^{-1}(\tilde{Q}_j u,u)\\
&= \sum_{j=0}^{J}\lambda_j^{-1}(\tilde{Q}_j u,u)=(\bar{B}u,u).
\end{aligned}
$$

$$
(\bar{B}u,u) = \sum^{J}\lambda_i^{-1}(\tilde{Q}_i u,\tilde{Q}_i u)\simeq\sum^{J}(\tilde{R}_i\tilde{Q}_i u,\tilde{Q}_i u)=\sum^{J}(\tilde{R}_i\tilde{Q}_i u,u)=(Bu,u)
$$

Fundamental norm equivalence in multilevel theory

If one can establish that $\|u\|_{A^1_{2,2}(\Omega)} \eqsim \|u\|_{H^1(\Omega)}$, then one has:

$$(Cu, u) = \|u\|^2_{A^1_{2,2}(\Omega)} \eqsim \|u\|^2_{H^1(\Omega)} \eqsim (Au, u),$$

where e.g. $(Au, v) = \int_\Omega a_{ij}\partial_i u \partial_j v + buv \; dx$. This in turn gives the chain:

$$(A^{-1}u, u) \;\eqsim\; (C^{-1}u, u) \;\eqsim\; (\bar{B}u, u) \;\eqsim\; (Bu, u).$$

By earlier remarks, this gives exactly what we want:

$$\kappa_A(BA) = O(1).$$

Therefore, fundamental to multilevel approximation theory is the equivalence:

$$\|u\|_{A^1_{2,2}(\Omega)} \eqsim \|u\|_{H^1(\Omega)}, \tag{41}$$

for given projection operators $\tilde{Q}_j$ and resulting approximation space norm:

$$\|u\|^2_{A^1_{2,2}(\Omega)} = (Cu, u) = (\sum_{j=0}^{J} 2^j(\tilde{Q}_j - \tilde{Q}_{j-1})u, u)_{L^2(\Omega)}.$$

How does one establish (41)?

Jackson and Bernstein inequalities

If one can establish a Bernstein inequality of the form:

$$\omega_2(u,t,\Omega)_p \leq c(\min\{1,t2^J\})^\beta \|u\|_{L^p(\Omega)}, \quad \forall u \in \mathcal{S}_J,$$

then one can show $A^s_{p,q} \hookrightarrow B^s_{p,q}$, $0 < s < \beta$, which implies

$$\|u\|_{B^s_{p,q}(\Omega)} \lesssim \|u\|_{A^s_{p,q}(\Omega)}.$$

Similarly, if one can establish a Jackson inequality of the form:

$$E_{\mathcal{S}_J}(f)_p = \inf_{g\in\mathcal{S}_J} \|f-g\|_{L^p(\Omega)} \leq c\omega_2(f,2^{-J},\Omega)_p, \quad f \in L^p(\Omega),$$

then one can show $B^s_{p,q} \hookrightarrow A^s_{p,q}$, $0 < s < 2$, which implies

$$\|u\|_{A^s_{p,q}(\Omega)} \lesssim \|u\|_{B^s_{p,q}(\Omega)}.$$

Together this gives

$$\|u\|_{A^s_{p,q}(\Omega)} \lesssim \|u\|_{B^s_{p,q}(\Omega)} \lesssim \|u\|_{A^s_{p,q}(\Omega)}.$$

Using the fact that $H^s = B^s_{2,2}$, $\forall s > 0$, we finally have:

$$\|u\|_{A^1_{2,2}(\Omega)} \eqsim \|u\|_{H^1(\Omega)}.$$

Jackson and Bernstein on locally adapted 3D meshes

It is not difficult to see that Jackson cannot hold on locally adapted meshes (although Bernstein continues to hold).

Dahmen and Kunoth (1992) showed for special types of 2D local refinement:

$$\frac{c_1}{\tilde{v}_J^{(2)}}\|u\|_{A^s_{p,q}(\Omega)} \le \|u\|_{B^s_{p,q}(\Omega)} \le c_2\|u\|_{A^s_{p,q}(\Omega)}, \quad u \in \mathcal{S}_J, \tag{42}$$

with $\tilde{v}_J^{(2)} = O(1)$ as $J \to \infty$. With $H^s = B^s_{2,2}$, $\forall s > 0$, this yields again

$$\|u\|_{A^1_{2,2}(\Omega)} \eqsim \|u\|_{H^1(\Omega)}.$$

In **[AH]**, we extend the Dahmen-Kunoth analysis framework to cover several 3D local mesh refinement algorithms.

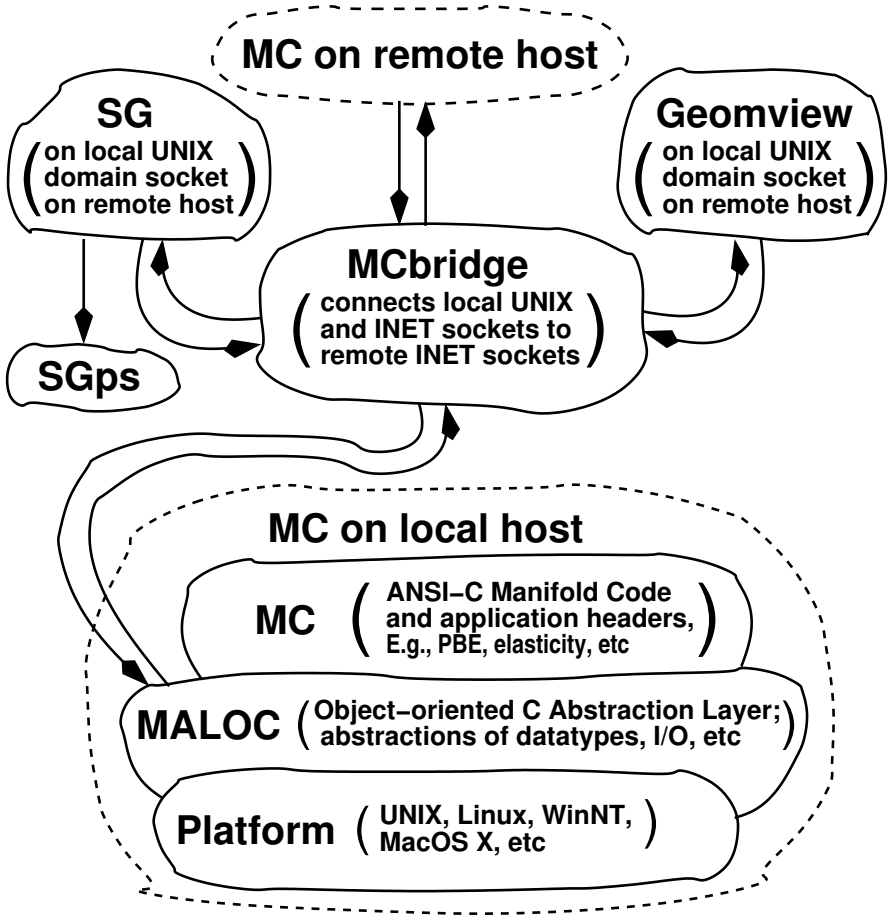
In particular, we establish (42) for finite element hierarchies built from practical octa-section and bisection-based 3D local refinement algorithms.

Key technical hurdle is the construction of a stable scaled Riesz basis for the resulting locally adapted 3D finite element spaces; requires proving a number of geometrical properties of the local refinement schemes.

Some examples using FETK (Finite Element ToolKit)

FETK (MALOC + MC + SG) is a general FE ToolKit for geometric PDE.

Developed collaboratively over a number of years, it has the following structure:



Application-specific codes such as APBS and GPDE are built on top of FETK.

The MALOC, PUNC, and SG components of FETK

FETK is released under the LGPL, and can be found at: `www.FETK.org`.

FETK is written almost entirely in Clean-C (the intersection of ISO-C and ISO-C++), with some pieces in C++, Java, and FORTRAN.

The FETK build environment is GNU autoconf.

MALOC: Minimal Abstraction Layer for Object-Oriented C.

MALOC is essentially a portability layer that FETK (and all downstream applications) use to obtain platform-independent access to ISO-C/C++, signals, sockets (UNIX and INET), OpenGL. It also has some additional class libraries that provide low-level datastructures and algorithms that are commonly needed for implementing numerical methods generally, and finite element methods in particular. (E.g., a logged replacement for malloc/free, dynamic sets/arrays, etc.)

PUNC: Portable Understructure for Numerical Computing.

PUNC is collection of commonly needed standard low-level numerical libraries such as BLAS, LAPACK, ARPACK, and SUPERLU. It also contains a few less-standard libraries such as CgCode and PMG, as well as the f2c linkage headers. The autoconf installation procedure looks for installed versions of these libraries, and only builds them if installed versions cannot be found.

SG: Socket Graphics.

SG is very light-weight polygon display tool for looking at finite element meshes and functions on such meshes. It can take various types of input (OFF, BH, OpenInventor, PDB, BREP, and other inputs), from various sources (file, pipe, UNIX or INET sockets). It can generate high-quality postscript images from any displayed scene, using the feedback buffer in OpenGL together with a simple linear programming algorithm which finds a feasible point in the sense of scene paintable using the Painter's algorithm.

The MC component of FETK

MC, the finite element kernel of FETK, allows for the adaptive treatment of nonlinear elliptic systems of tensor equations on 2- and 3-manifolds.

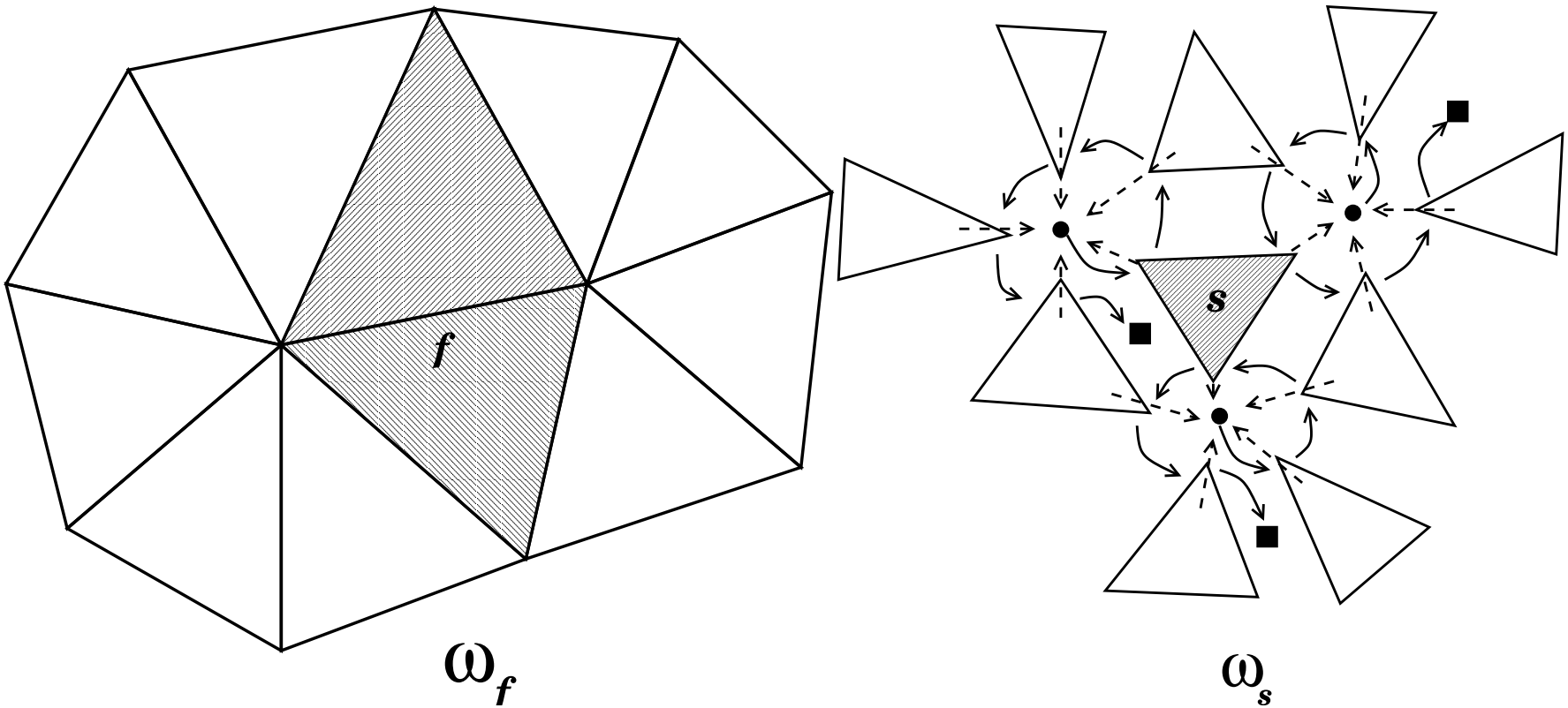
MC has the following features:

- *Abstraction of the elliptic system*: PDE defined only through the nonlinear weak form $\langle F(u), v \rangle$ over the domain manifold, along with the associated bilinear linearization form $\langle DF(u)w, v \rangle$.
- *Abstraction of the domain manifold*: Domain specified via polyhedral representation of topology, with set of user-interpreted coordinate labels (possibly consisting of multiple charts).
- *Dimension-independence*: The same code paths are taken for both 2D and 3D problems, by employing the simplex as the fundamental topological object.

These abstractions are inherited by application codes built on top of FETK.

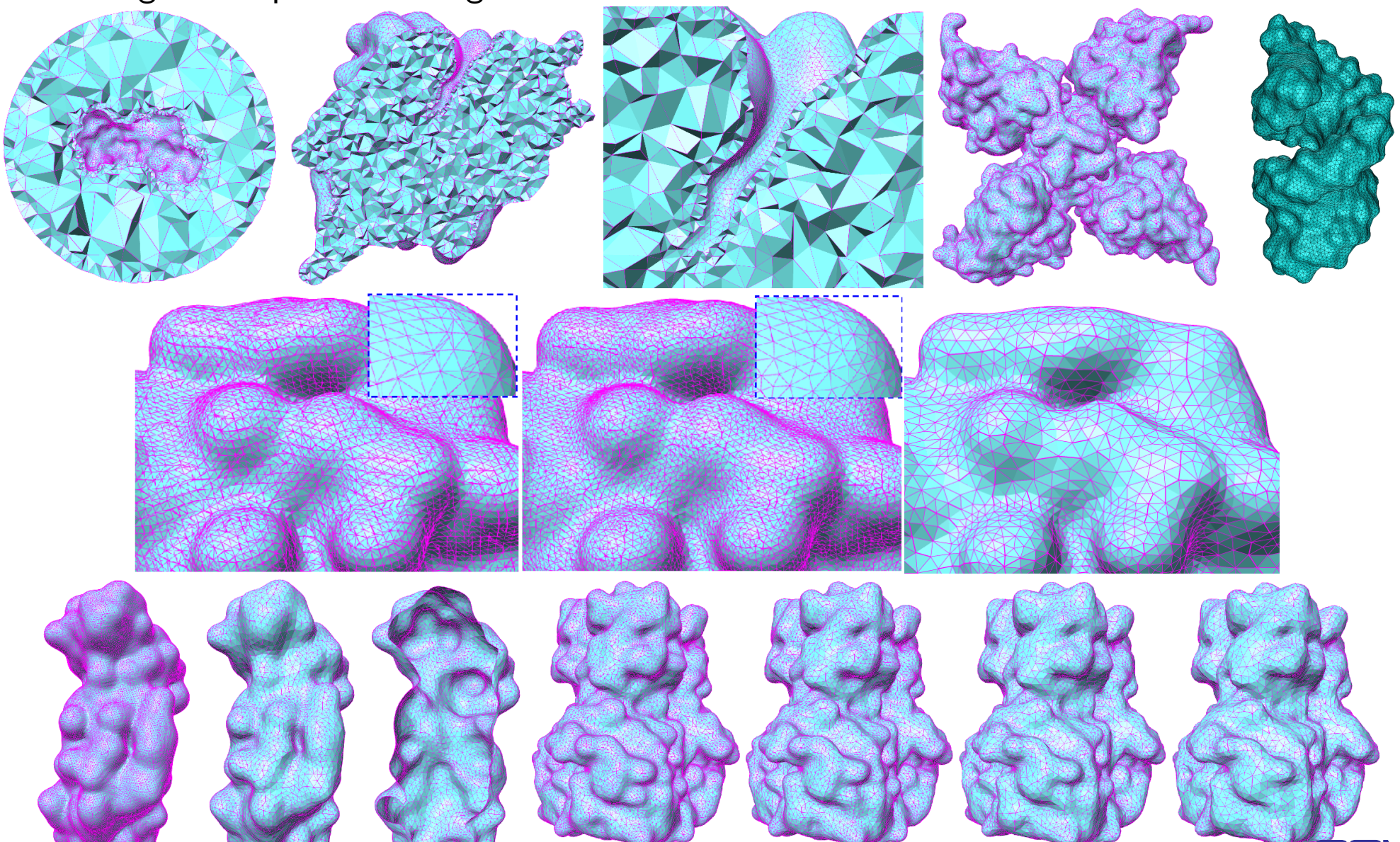
The RInged VERtex datastructure in MC

The topology datastructure in MC is the RIVER (RInged VERtex):

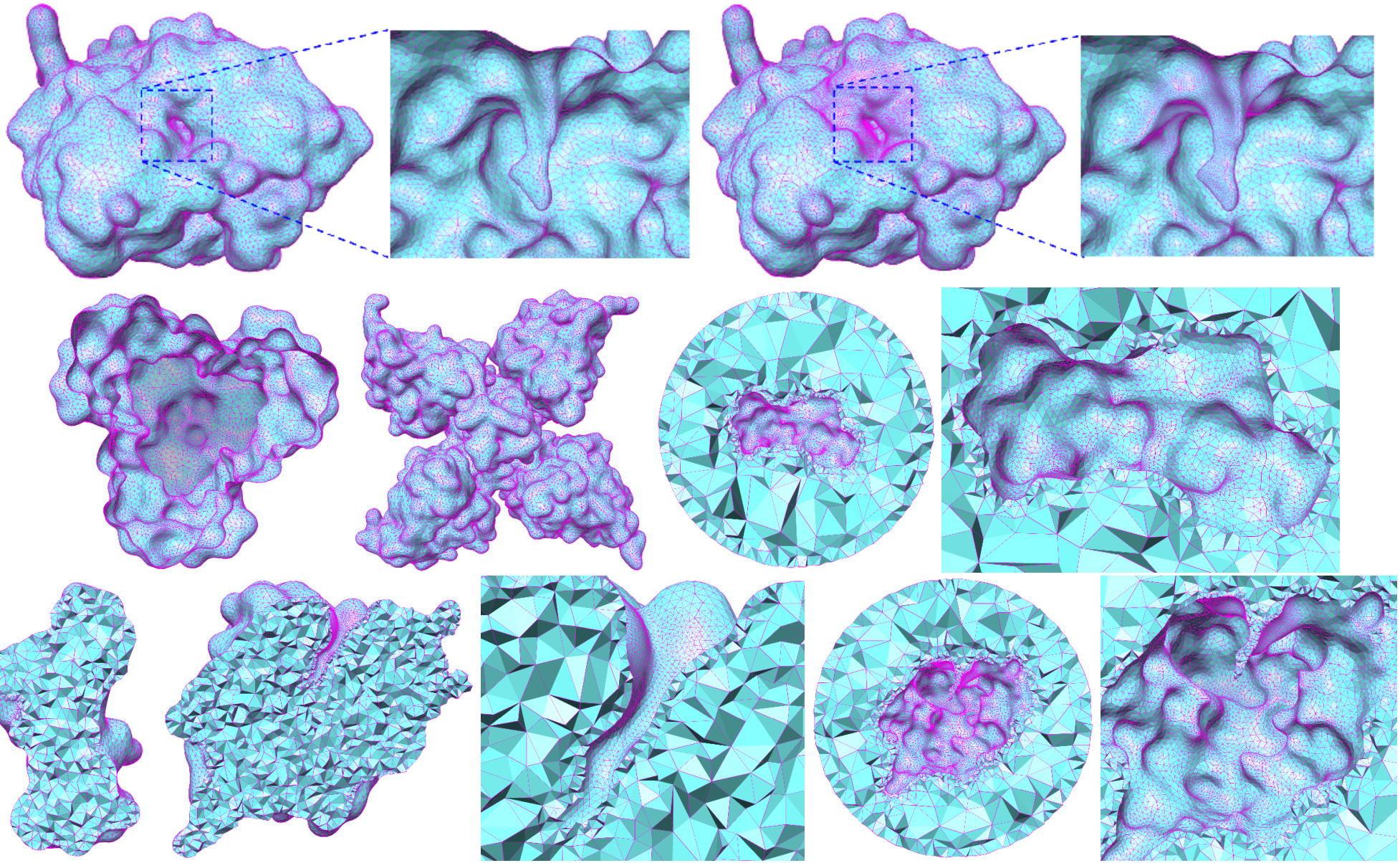


The GAMer component of FETK

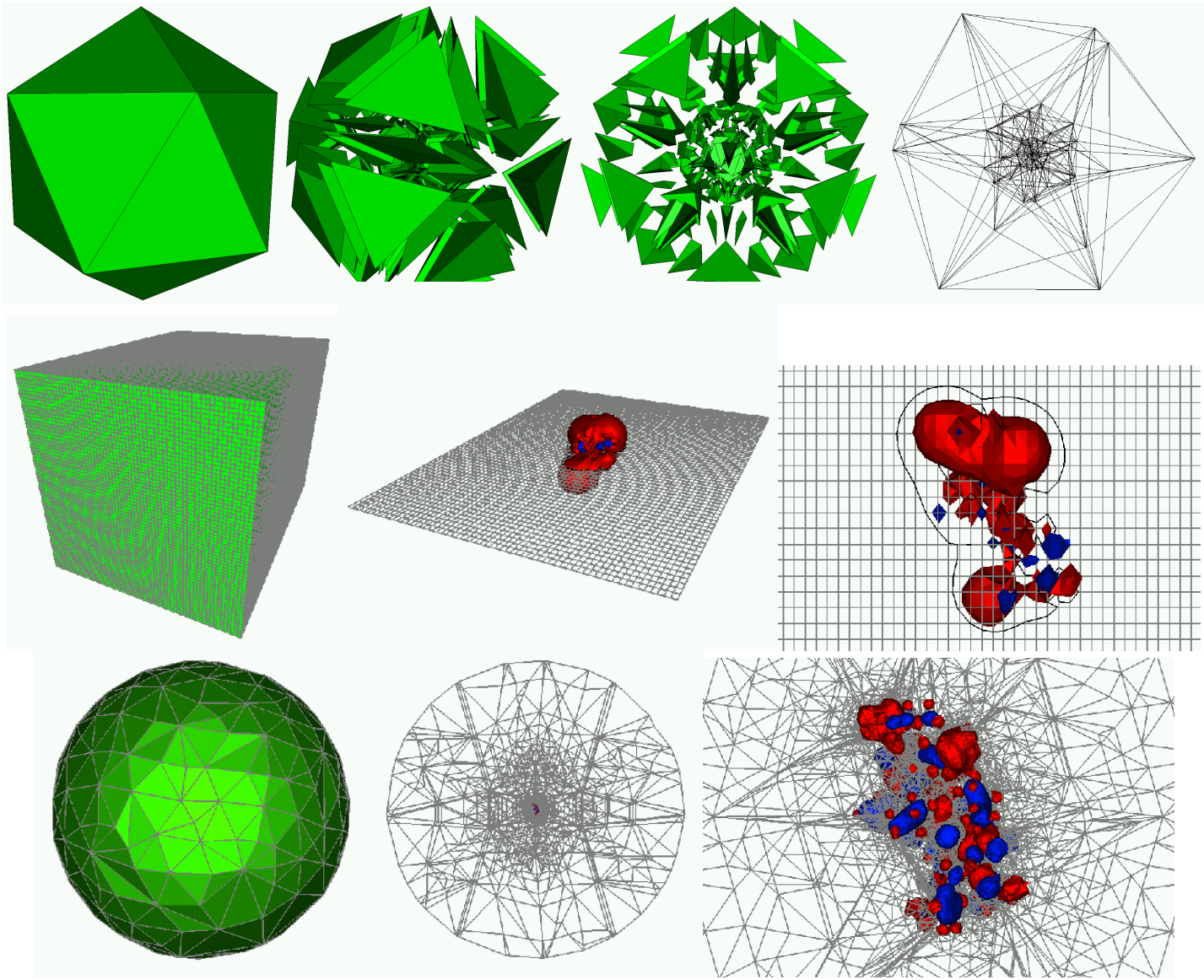
The GAMer component of FETK is essentially a toolchain that combines some surface meshing and improvement algorithms with TRIANGLE and TETGEN.



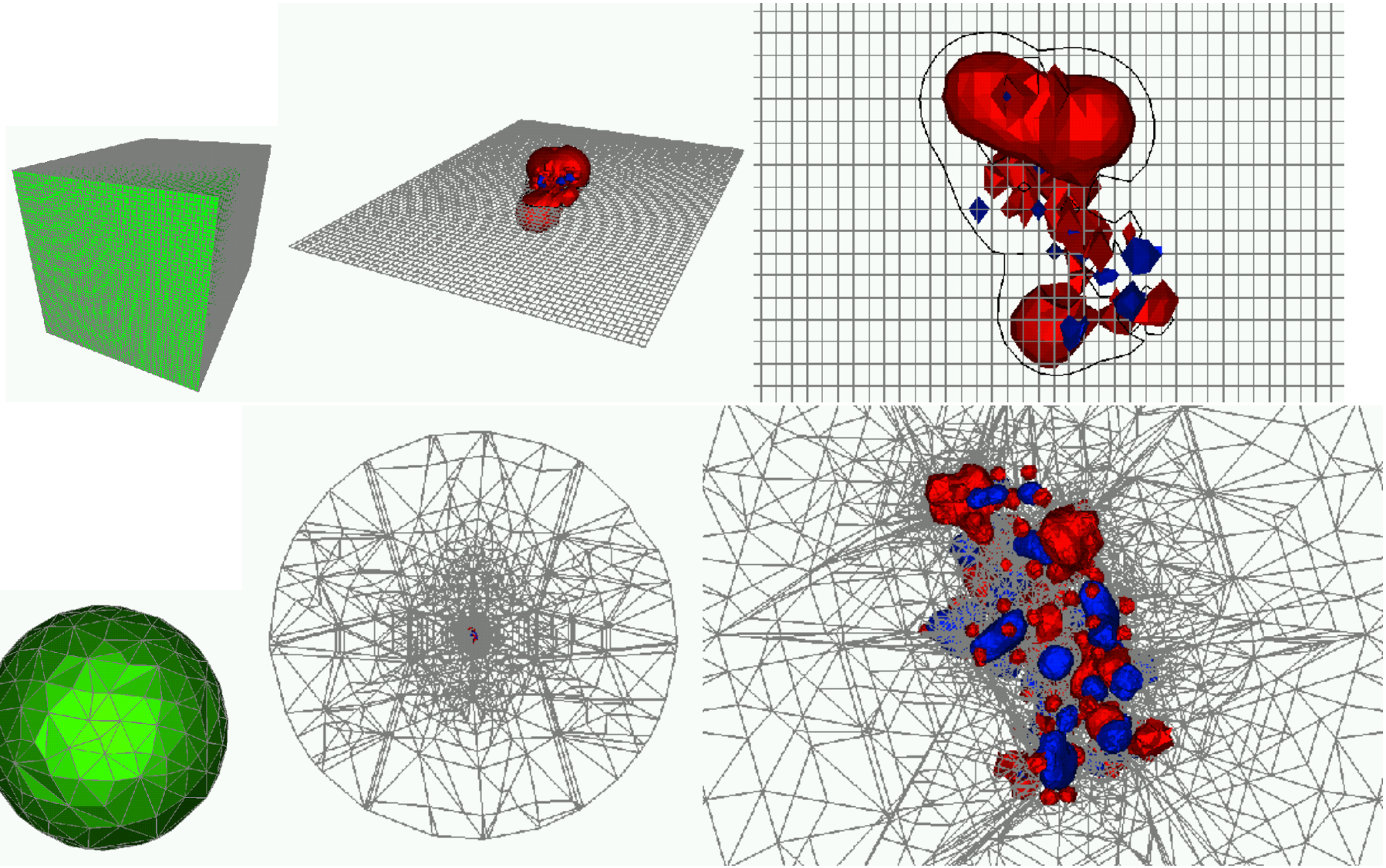
GAMer: Multiscale surface and volume meshing



Adaptive vs. non-adaptive: cheaper/more accurate

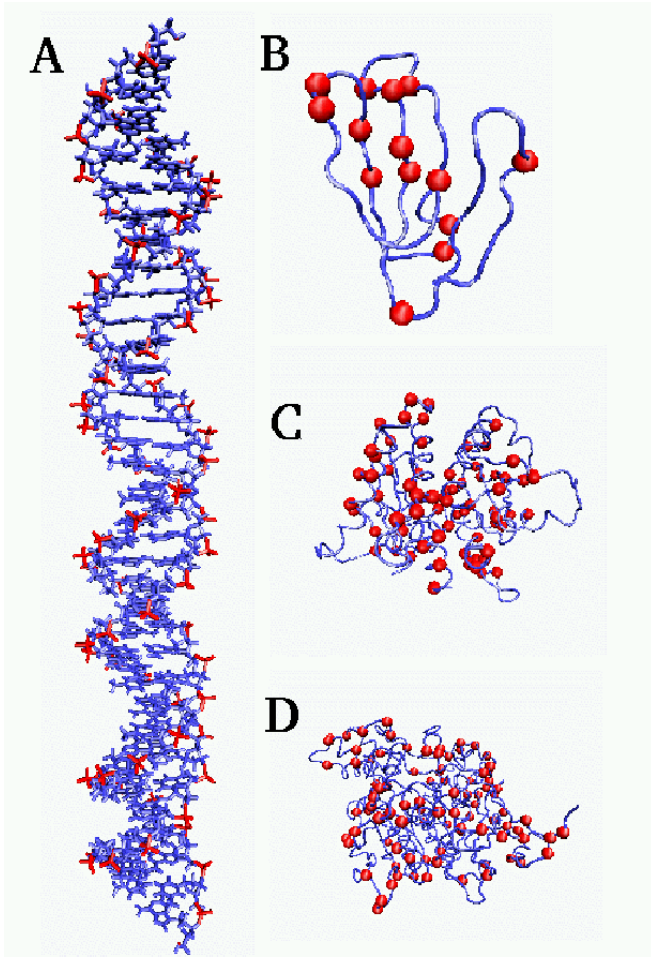


Adaptive vs. non-adaptive: cheaper/more accurate



Collaborations with McCammon Group in Chemistry

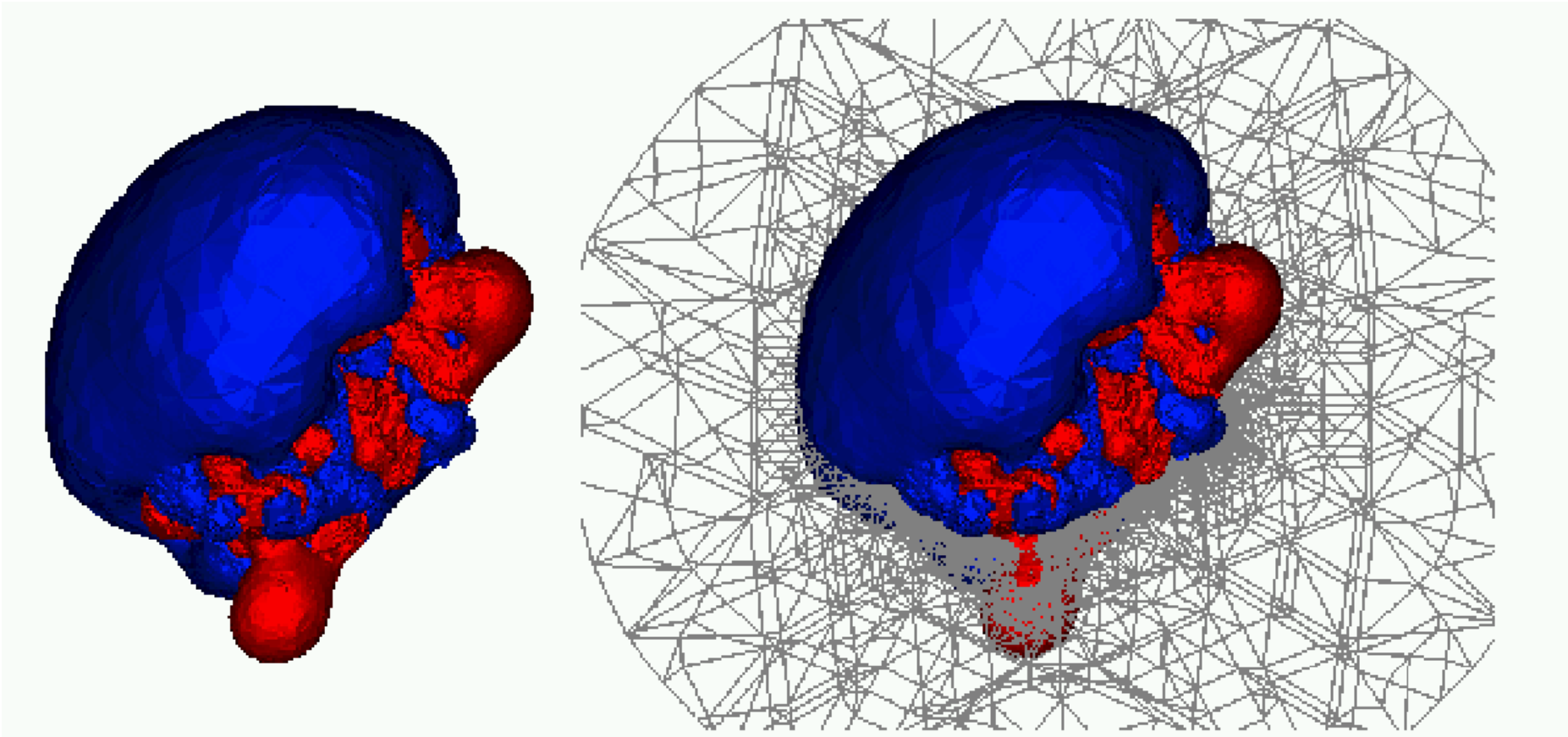
(Joint work with N. Baker, A. McCammon, and F. Wang)



Charged groups are displayed as red spheres, other atoms as blue lines or by a protein backbone tube.

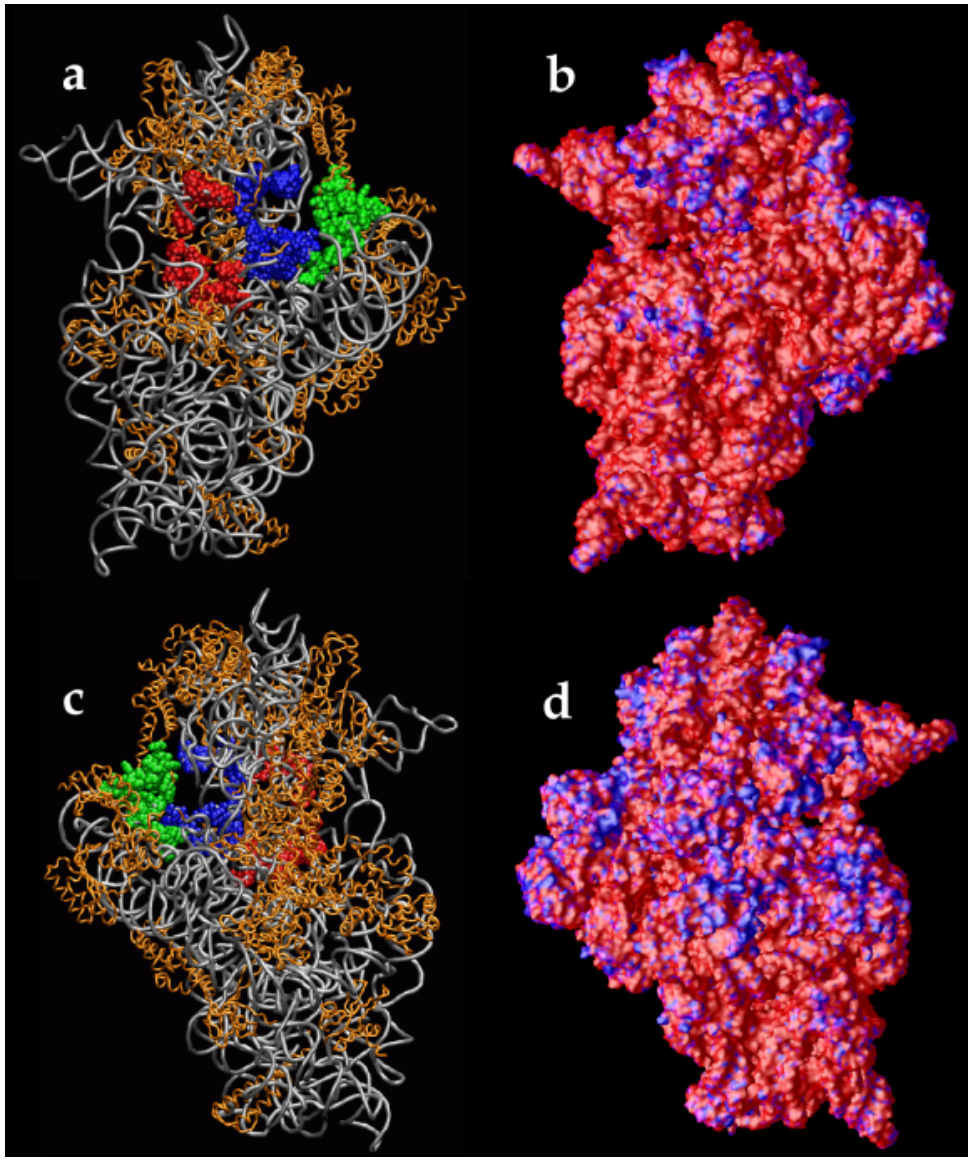
A=DNA 36-mer, B=fasciculin-2, C=HIV integrase, D=AChE. Figure courtesy of N. Baker.

Electrostatic Potential of Fasciculin-2

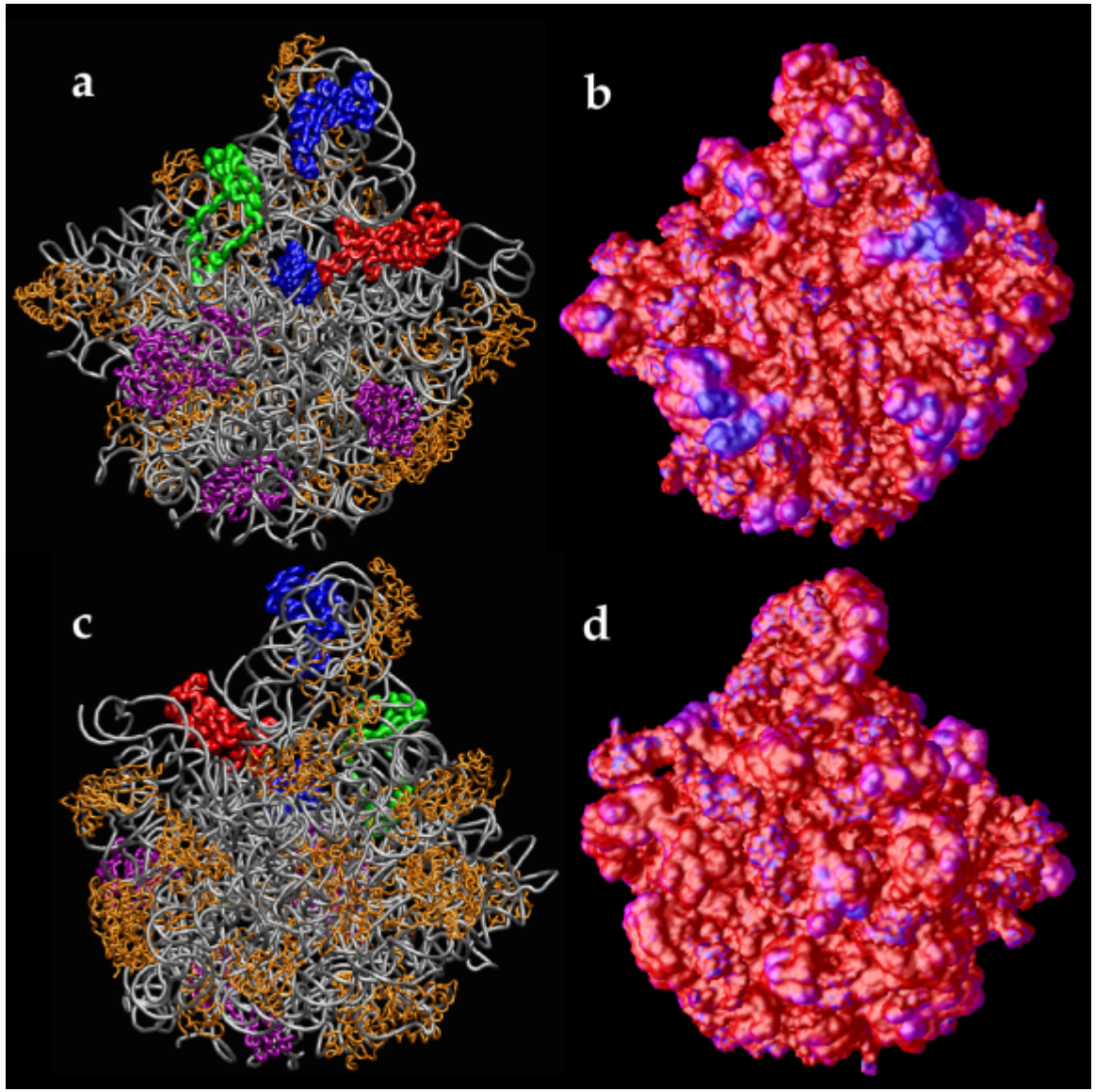


Potential contours from solution to linear PBE for FAS2 shown with a slice through the finite element mesh. Solution was computed using the adaptive finite element software MC.

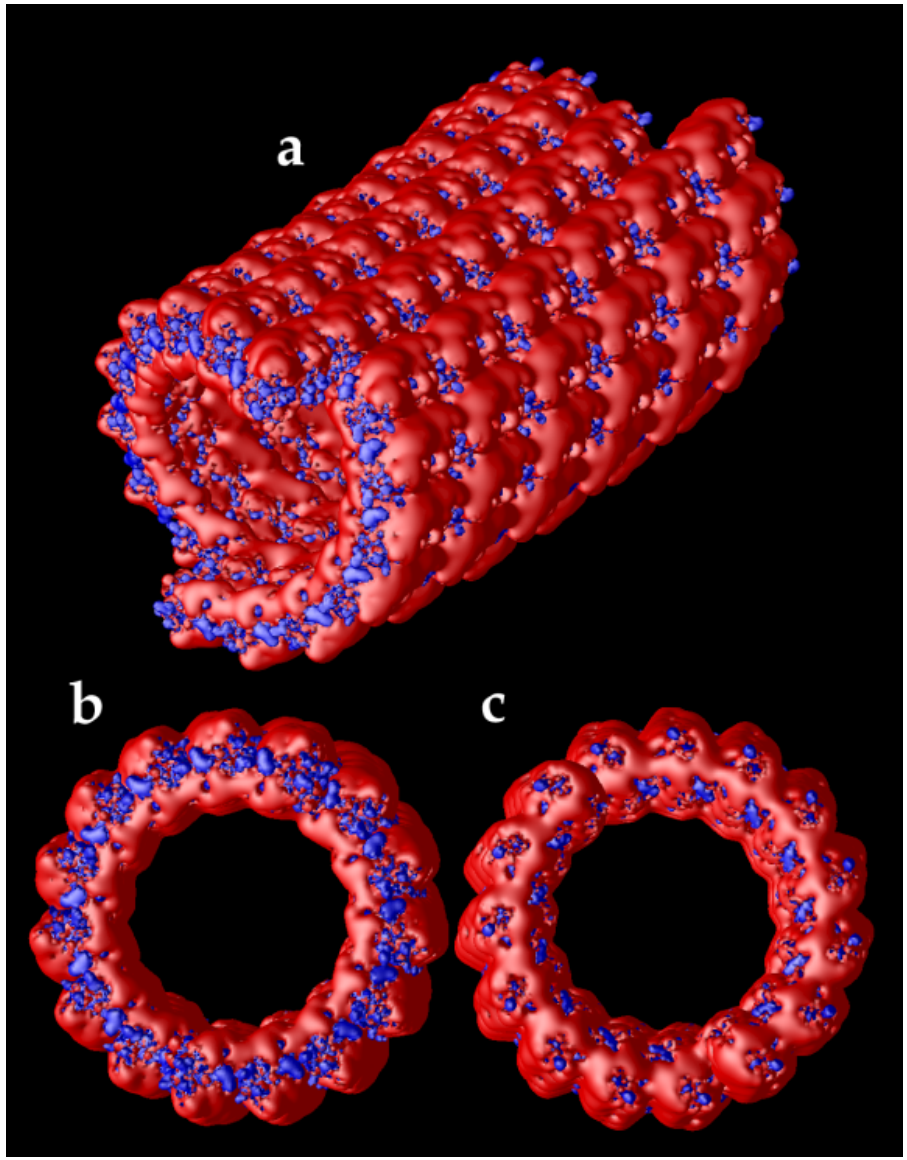
Rhibosome example (Ph.D. work of N. Baker)



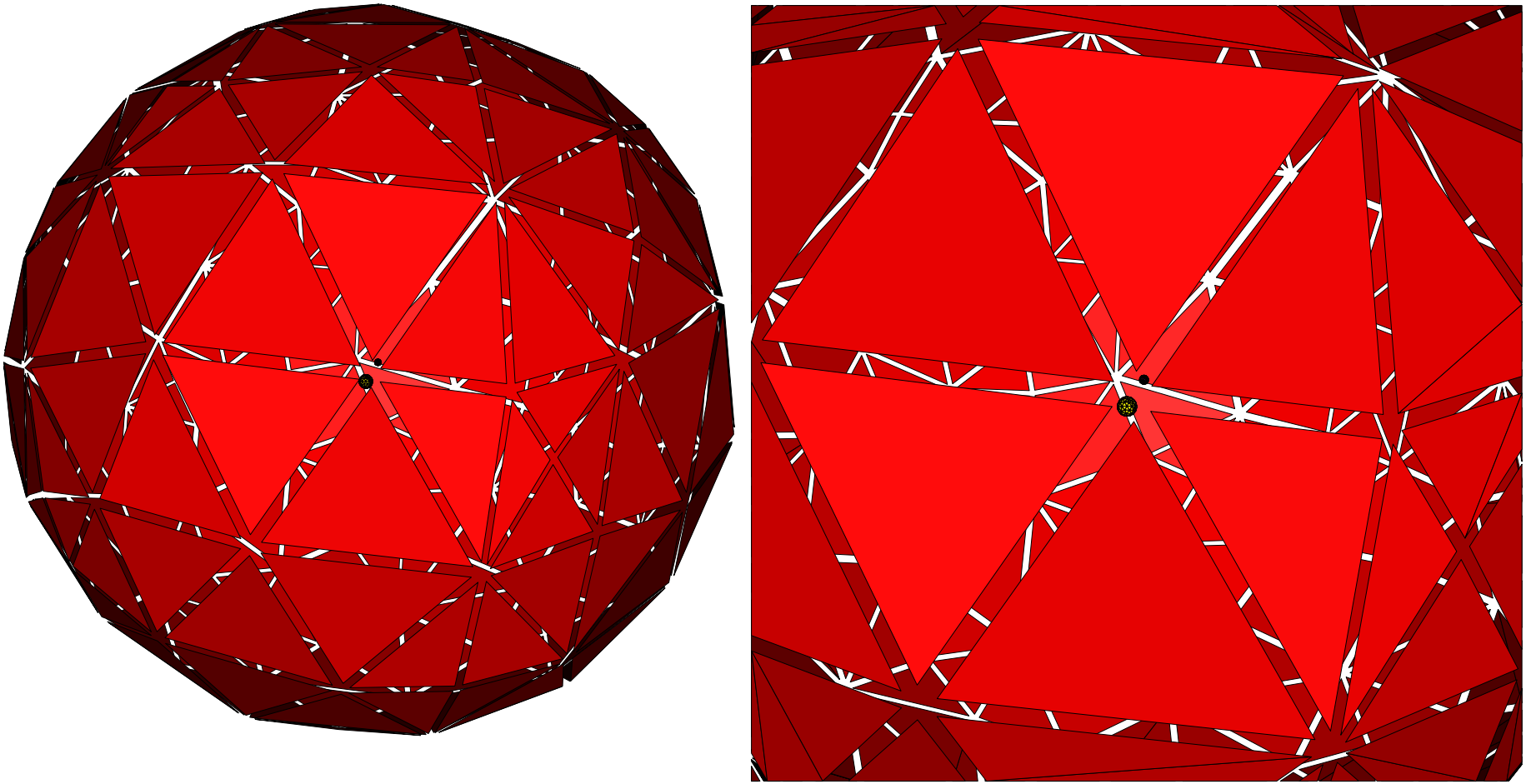
Rhibosome example (Ph.D. work of N. Baker)



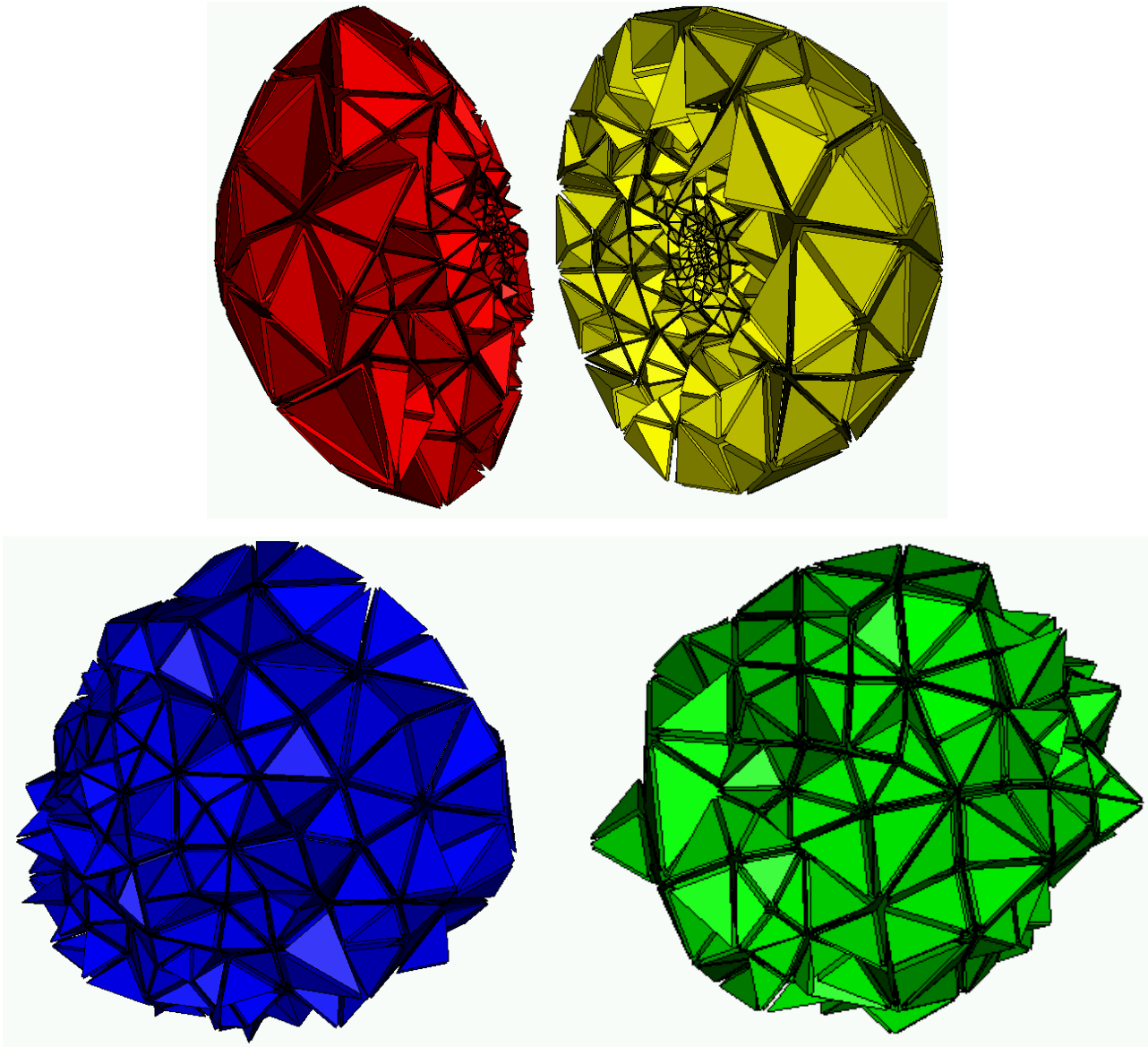
Microtubule example (Ph.D. work of N. Baker)



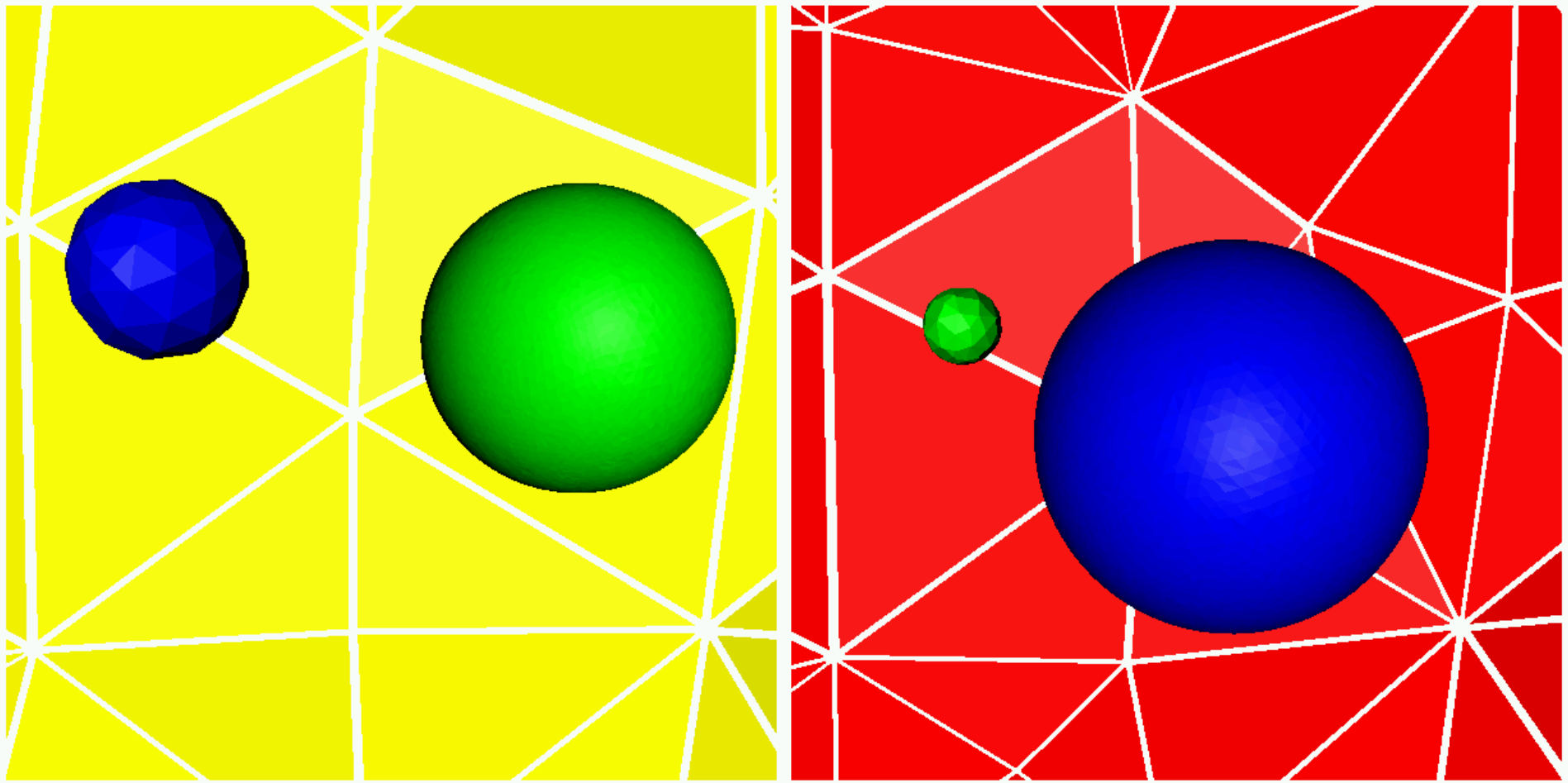
Parallel solution algorithm example



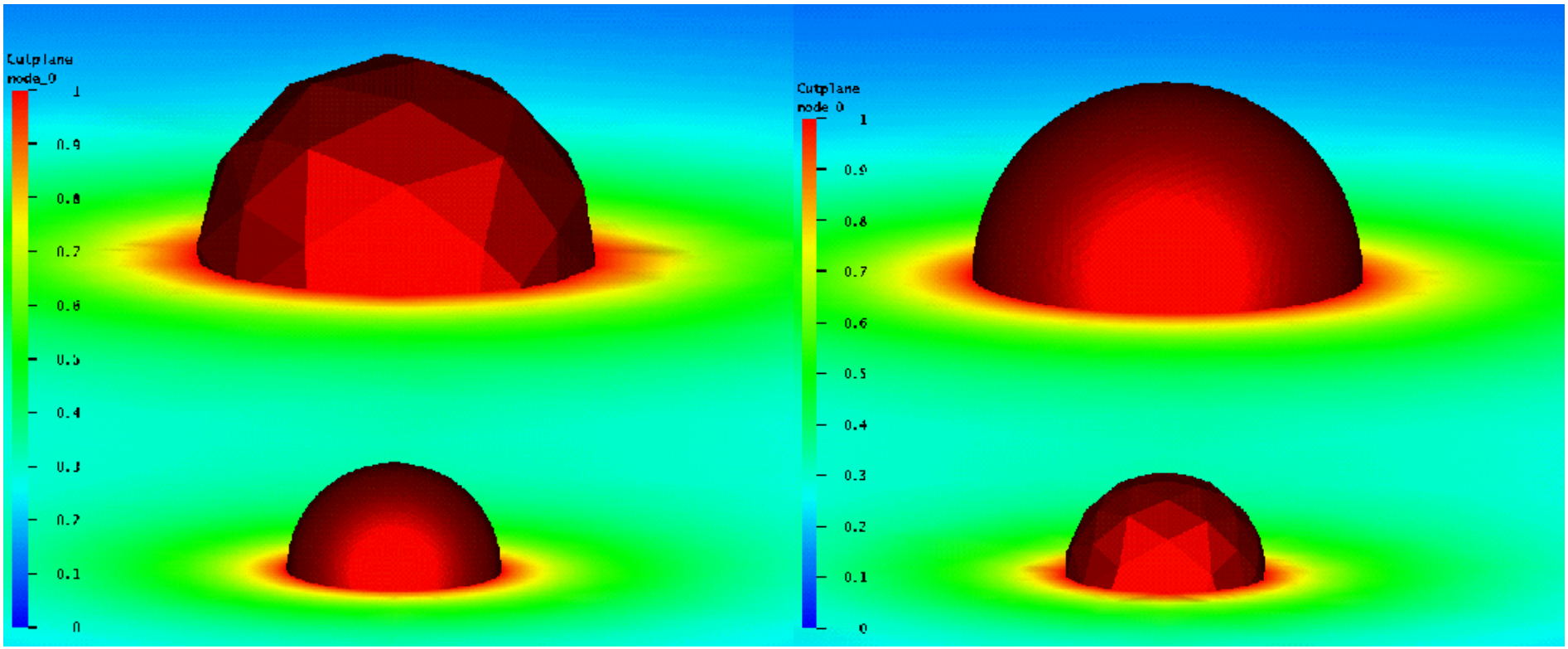
Spectrally partitioned coarse mesh



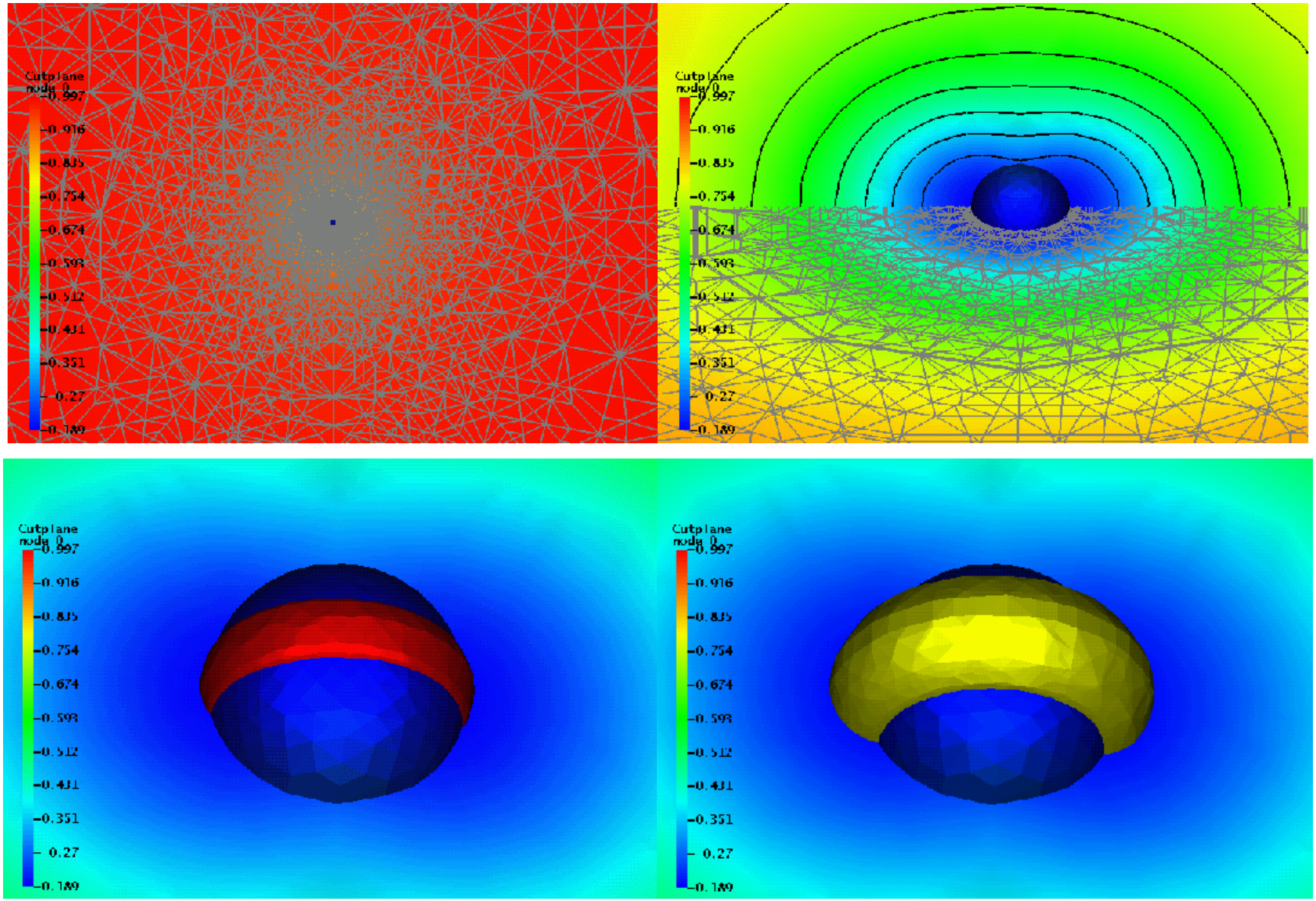
Subdomain adaptivity around the interior domain holes



The two subdomain solutions



A more complex example: some isosurfaces



Adaptive Methods + Parallel Computers = Big Mess

An ideal parallel adaptive algorithm:

- Allow use of *sequential* adaptive FE codes with parallel computers.
- Avoid "load balancing" problems inherent with adaptive methods.
- Scale "well" with # processors, with low (or no) communication costs.

Proposed Algorithm from **[BH]** to decouple geometric PDE on manifolds:

1. Solve entire problem on coarse mesh, compute *a posteriori* estimates.
2. Bisect (spectral/inertial) mesh to achieve *equal error* via estimates.
3. Give coarse solution and mesh to a number of computers.
4. Each computer solves entire problem adaptively AND independently, restricting refinement to "subdomain".
5. A final global solution is formed by (pick one):
   a. forming a global mesh and doing Schwarz iteration **[BH]**.
   b. using mortar elements [Bank and Lu].
   c. evaluating via partition of unity **[H1,H2]**.

Decoupling Algorithm: Observations &Claims

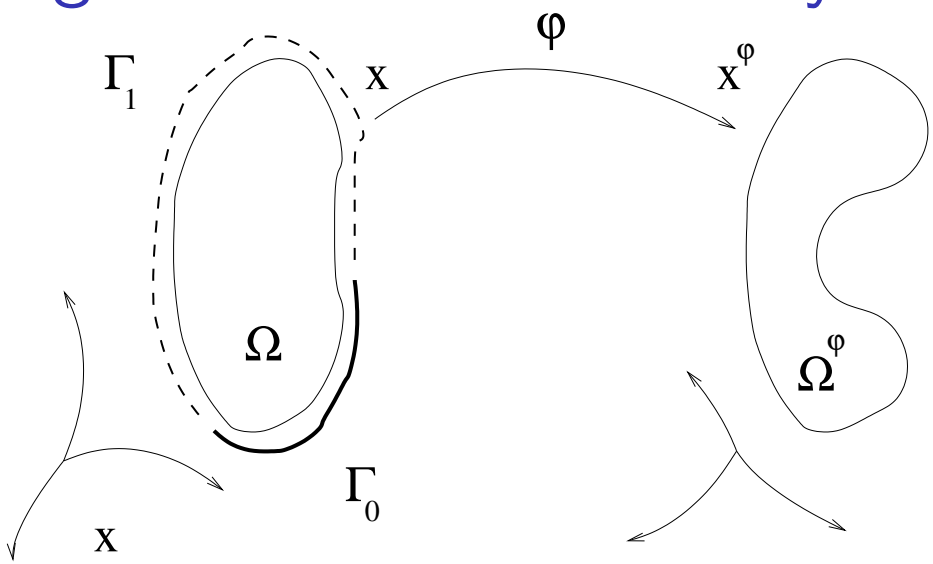
Observations:

- Steps 1 and 2 can be done on all processors, requiring only a sequential adaptive solver. This avoids the need for Step 3 (initial "broadcast" of coarse problem).
- Step 4 requires again only a sequential adaptive solver, where the error estimator is multiplied by a small constant outside a selected subdomain.
- Any choice of Step 5abc can be done in both 2D and 3D.
- The communication requirements are extremely low (except Step 5ab).

Claims:

1. The load balancing problem is approximately solved *a priori*.
   I.e., the final adapted mesh which is distributed over the processors is nearly load-balanced. (Good empirical evidence.)
2. Step 5c can produce a solution which is (asymptotically) as good in a certain sense as steps 5a and/or 5b, in some special situations (below...)

An Example: Large-deformation elasticity



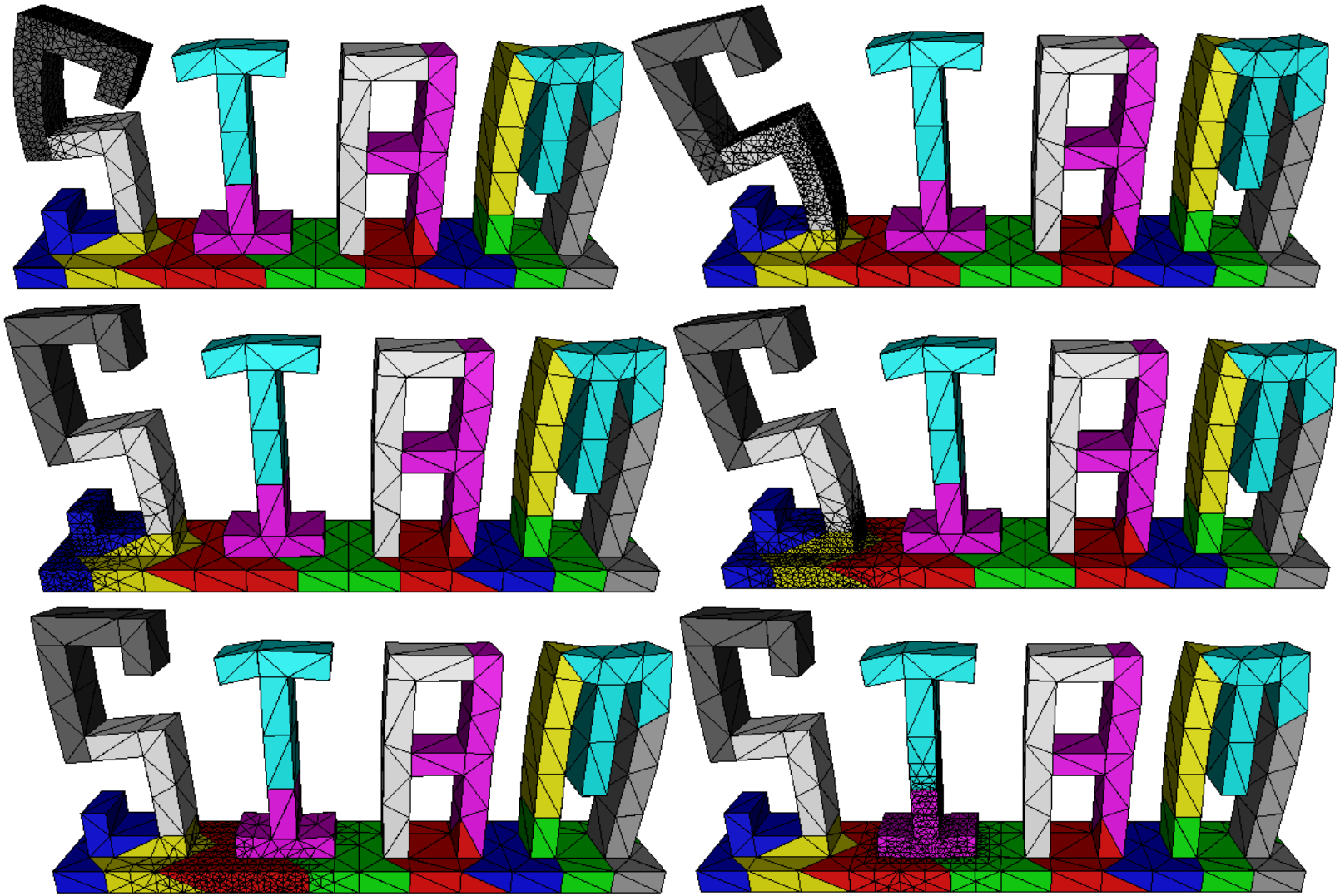
- $\varphi(\mathbf{x}) : \overline{\Omega} \mapsto \mathbb{R}^3$, $\nabla\varphi(\mathbf{x}) : \overline{\Omega} \mapsto \mathbb{M}^3$; deformation & deformation gradient
- $C = \nabla\varphi^T\nabla\varphi$, $E = \frac{1}{2}(C - I) : \overline{\Omega} \mapsto \mathbb{S}^3$; RCG & GSV strains
- $\Sigma(\mathbf{x}) = \hat{\Sigma}(\mathbf{x}, \nabla\varphi(\mathbf{x})) : \overline{\Omega} \mapsto \mathbb{S}^3$; Second Piola stress
  ($\check{\Sigma}(E) = \lambda(\mathrm{tr}E)I + 2\mu E$.)

Cauchy equations (via Piola-transformation) for $(\varphi_1, \varphi_2, \varphi_3)$:

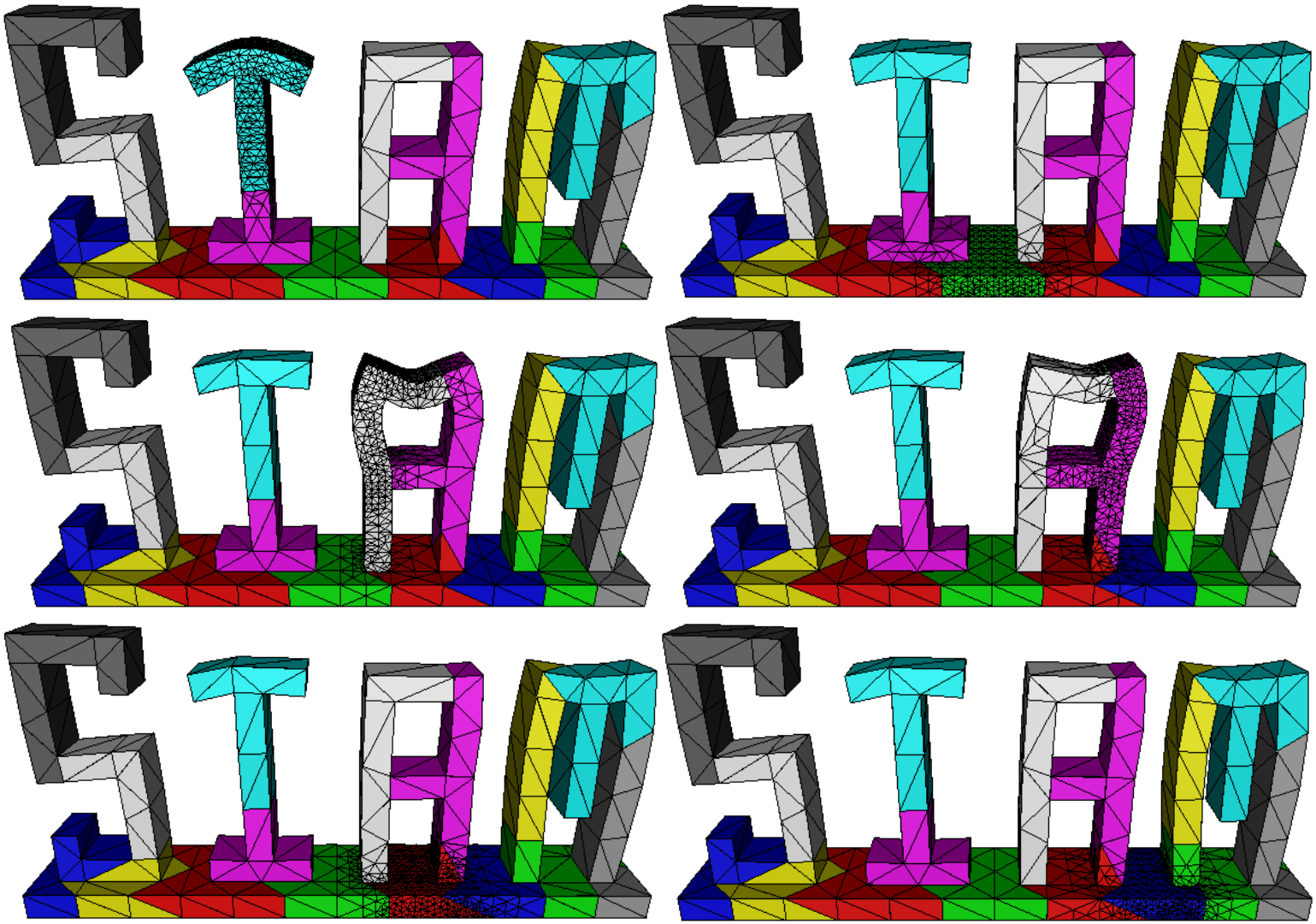
$$\begin{aligned} -\nabla \cdot (\nabla\varphi(\mathbf{x})\Sigma(\mathbf{x})) &= f(\mathbf{x}) \quad \text{in } \Omega, \\ n(\mathbf{x}) \cdot (\nabla\varphi(\mathbf{x})\Sigma(\mathbf{x})) &= g(\mathbf{x}) \quad \text{on } \Gamma_1, \\ \varphi(\mathbf{x}) &= \varphi_0(\mathbf{x}) \quad \text{on } \Gamma_0 = \Gamma - \Gamma_1 \end{aligned}$$

Tetrahedralized solid and its spectral bisection

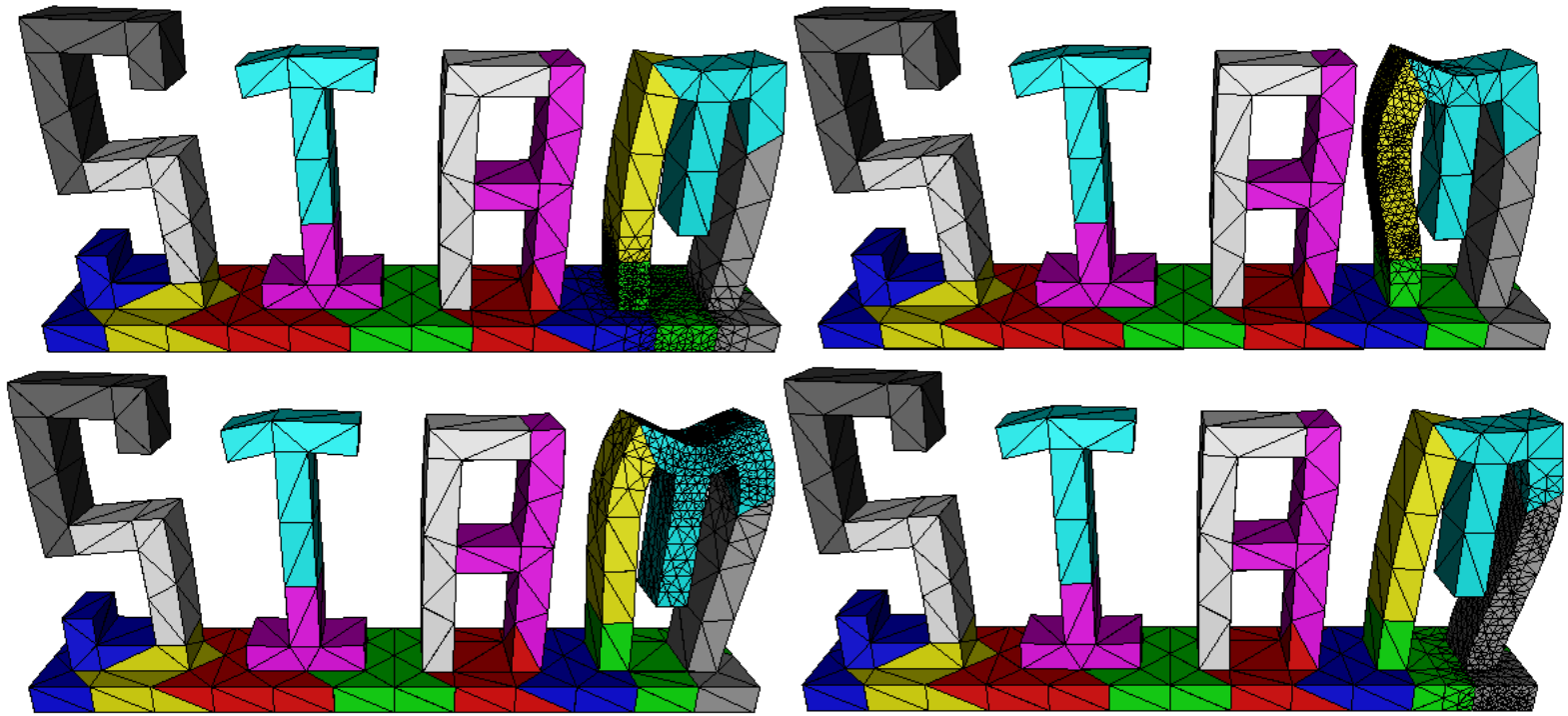
Local subdomain adaptivity: domains 1 through 6



Local subdomain adaptivity: domains 7 through 12



Local subdomain adaptivity: domains 13 through 16



Babuška & Melenk's Partition of Unity Method (PUM)

Let $\Omega \subset \mathbb{R}^d$ be an open set and let $\{\Omega_i\}$ be an open cover of Ω with a bounded local overlap property: For all $x \in \Omega$, there exists a constant M such that

$$\sup_i \{\ i \mid x \in \Omega_i\ \} \leq M.$$

A Lipschitz *partition of unity* $\{\phi_i\}$ subordinate to cover $\{\Omega_i\}$ satisfies:

$$\sum_i \phi_i(x) \equiv 1, \quad \forall x \in \Omega,$$

$$\phi_i \in C^k(\Omega) \quad \forall i, \quad (k \geq 0),$$

$$\text{supp } \phi_i \subset \overline{\Omega}_i, \quad \forall i,$$

$$\|\phi_i\|_{L^\infty(\Omega)} \leq C_\infty, \quad \forall i,$$

$$\|\nabla \phi_i\|_{L^\infty(\Omega)} \leq \frac{C_G}{\text{diam}(\Omega_i)}, \quad \forall i.$$

The *partition of unity method (PUM)* forms $u_{ap} = \sum_i \phi_i v_i \in V \subset H^1(\Omega)$ from the global PUM space $V = \sum_i \phi_i V_i$, where the V_i are local approximation spaces:

$$V_i \subset C^k(\Omega \cap \Omega_i) \subset H^1(\Omega \cap \Omega_i), \quad \forall i, \quad (k \geq 0).$$

Approximation properties of PUM

Lemma: *Let* $w, w_i \in H^1(\Omega)$ *with* $\operatorname{supp} w_i \subseteq \overline{\Omega \cap \Omega_i}$. *Then*

$$\sum_i \|w\|^2_{H^k(\Omega_i)} \leq M \|w\|^2_{H^k(\Omega)}, \qquad k = 0, 1$$

$$\|\sum_i w_i\|^2_{H^k(\Omega)} \leq M \sum_i \|w_i\|^2_{H^k(\Omega \cap \Omega_i)}, \qquad k = 0, 1$$

Theorem: [Babuška and Melenk 1997] *If the local spaces* V_i *have the following approximation properties:*

$$\|u - v_i\|_{L^2(\Omega \cap \Omega_i)} \leq \epsilon_0(i), \qquad \|\nabla(u - v_i)\|_{L^2(\Omega \cap \Omega_i)} \leq \epsilon_1(i), \quad \forall i,$$

then the following a priori *global error estimates hold:*

$$\|u - u_{ap}\|_{L^2(\Omega)} \leq \sqrt{M} C_\infty \left(\sum_i \epsilon_0^2(i) \right)^{1/2},$$

$$\|\nabla(u - u_{ap})\|_{L^2(\Omega)} \leq \sqrt{2M} \left(\sum_i \left(\frac{C_G}{\operatorname{diam}(\Omega_i)} \right)^2 \epsilon_1^2(i) + C_\infty^2 \epsilon_0^2(i) \right)^{1/2}.$$

Proof Outline: *Via Lemma with* $w_i = \phi_i(u - v_i)$ *and* $u - u_{ap} = \sum_i w_i$. $\square$

B-H + PUM = PPUM

The Parallel Partition of Unity Method (PPUM) builds a PUM approximation $u_{ap} = \sum_i \phi_i v_i$ where the v_i are taken from the local B-H spaces:

$$V_i = \mathcal{X}_i V_i^g \subset C^k(\Omega \cap \Omega_i) \subset H^1(\Omega \cap \Omega_i), \quad \forall i, \quad (k \geq 0),$$

where $\mathcal{X}_i$ is the characteristic function for Ω_i, and where

$$V_i^g \subset C^k(\Omega) \subset H^1(\Omega), \quad \forall i, \quad (k \geq 0).$$

The global spaces V_i^g are built from locally enriching an initial coarse global space V_0. The PUM space V is then

$$V = \left\{ v \mid v = \sum_i \phi_i v_i, \quad v_i \in V_i \right\}$$

$$= \left\{ v \mid v = \sum_i \phi_i \mathcal{X}_i v_i^g = \sum_i \phi_i v_i^g, \quad v_i^g \in V_i^g \right\} \subset H^1(\Omega).$$

Global error in the PPUM approximation

PUM solves a PDE via Galerkin in global PUM space (cf. Griebel/Schweitzer):

$$\text{Find } u_{ap} \in V \text{ such that } \langle F(u_{ap}), v\rangle = 0, \quad \forall v \in V.$$

PPUM instead builds $u_{ap} = \sum_i \phi_i u_i = \sum_i \phi_i u_i^g$, where u_i^g satisfies:

$$\text{Find } u_i^g \in V_i^g \text{ such that } \langle F(u_i^g), v_i^g\rangle = 0, \quad \forall v_i^g \in V_i^g.$$

Babuška/Melenk *a priori* PUM estimates require:

$$\|u - u_i\|_{L^2(\Omega\cap\Omega_i)} = \|u - u_i^g\|_{L^2(\Omega\cap\Omega_i)} \le \epsilon_0(i),$$
$$\|\nabla(u - u_i)\|_{L^2(\Omega\cap\Omega_i)} = \|\nabla(u - u_i^g)\|_{L^2(\Omega\cap\Omega_i)} \le \epsilon_1(i).$$

Such local estimates hold for general classes of nonlinear Poisson-like problems (Xu/Zhou 1998, Nitsche/Schatz 1974, Schatz/Wahlbin 1977,1995):

$$\|u - u_i^g\|_{H^1(\Omega_i\cap\Omega)} \le C\left(\inf_{v_i^0 \in V_i^0} \|u - v_i^0\|_{H^1(\Omega_i^0\cap\Omega)} + \|u - u_i^g\|_{L^2(\Omega)}\right)$$

where

$$V_i^0 \subset C^k(\Omega_i^0\cap\Omega) \subset H^1(\Omega_i\cap\Omega), \;\; \Omega_i \subset\subset \Omega_i^0, \;\; \Omega_{ij} = \Omega_i^0 \bigcap \Omega_i^0, \;\; |\Omega_{ij}| \approx |\Omega_i| \approx |\Omega_j|.$$

Global PPUM approximation error: Two-level case

If $u \in H^{1+\alpha}(\Omega)$, $\alpha > 0$, and quasi-uniform meshes of sizes h and $H > h$ used for Ω_i^0 and $\Omega \backslash \Omega_i^0$ (resp), then:

$$\|u - u_i^g\|_{H^1(\Omega_i \cap \Omega)} = \left(\|u - u_i^g\|^2_{L^2(\Omega_i \cap \Omega)} + \|\nabla(u - u_i^g)\|^2_{L^2(\Omega_i \cap \Omega)} \right)^{1/2} \leq C_1 h^\alpha + C_2 H^{1+\alpha}.$$

I.e., $\epsilon_0(i) = \epsilon_1(i) = C_1 h^\alpha + C_2 H^{1+\alpha}$.

Theorem: [H1] *If* $\operatorname{diam}(\Omega_i) \geq 1/Q > 0 \ \ \forall i$, *then the global solution* u_{bh} *produced by the PPUM Algorithm satisfies the following global bounds:*

$$\|u - u_{bh}\|_{L^2(\Omega)} \leq \sqrt{PM} C_\infty \left(C_1 h^\alpha + C_2 H^{1+\alpha} \right),$$

$$\|\nabla(u - u_{bh})\|_{L^2(\Omega)} \leq \sqrt{2PM(Q^2 C_G^2 + C_\infty^2)} \left(C_1 h^\alpha + C_2 H^{1+\alpha} \right),$$

where $P =$ *number of local spaces* V_i. *Further, if* $H \leq h^{\alpha/(1+\alpha)}$ *then:*

$$\|u - u_{bh}\|_{L^2(\Omega)} \leq \sqrt{PM} C_\infty \max\{C_1, C_2\} h^\alpha,$$

$$\|\nabla(u - u_{bh})\|_{L^2(\Omega)} \leq \sqrt{2PM(Q^2 C_G^2 + C_\infty^2)} \max\{C_1, C_2\} h^\alpha.$$

Proof Outline: *Tracing the constants through the PUM framework.* □

Duality-based Decomposition: Approximation Theory

Theorem: [H2] *Let $\{\phi_i\}$ be a partition of unity subordinate to a cover $\{\Omega_i\}$. If ψ is the Riesz-representer for a linear functional $l(u)$, then the functional of the error in the PPUM approximation u_{pp} satisfies*

$$l(u - u_{pp}) = -\sum_{k=1}^{p} \langle F(u_i^g), \omega_i \rangle,$$

where u_i^g are the solutions to the B-H subspace problems, and where the ω_i are the solutions to the following global dual problems *with localized data:*

$$\text{Find } \omega_i \in H_0^1(\Omega) \text{ such that } (A^T \omega_i, v)_{L^2(\Omega)} = (\phi_i \psi, v)_{L^2(\Omega)}, \quad \forall v \in H_0^1(\Omega).$$

Moreover, if the local residual $F(u_i^g)$, weighted by the localized dual solution ω_i, satisfies the following error tolerance in each subspace:

$$|\langle F(u_i^g), \omega_i \rangle| < \frac{\epsilon}{p}, \qquad i = 1, \ldots, p$$

then the linear functional of the global error $u - u_{pp}$ satisfies

$$|l(u - u_{pp})| < \epsilon.$$

Approximation Theory for Duality-based Approach

Proof Outline: *With* $l(u - u_{pp}) = (u - u_{pp}, \psi)_{L^2(\Omega)}$, *the localized representation comes from:*

$$(u - u_{pp}, \psi)_{L^2(\Omega)} = (\sum_{k=1}^{p} \phi_i u - \sum_{i=1}^{p} \phi_i u_i^g, \psi)_{L^2(\Omega)} = \sum_{k=1}^{p} (\phi_i (u - u_i^g), \psi)_{L^2(\Omega \cap \Omega_i)}.$$

Each term in the sum can be written in terms of the local nonlinear residual $F(u_i^g)$ *as follows:*

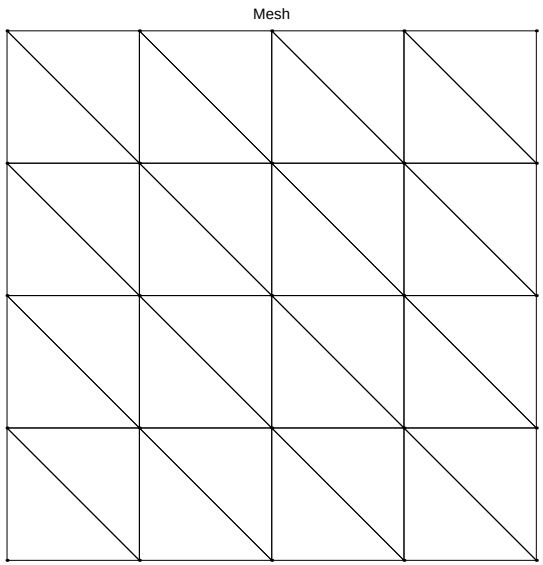
$$\begin{aligned} (\phi_i (u - u_i^g), \psi)_{L^2(\Omega \cap \Omega_i)} &= (u - u_i^g, \phi_i \psi)_{L^2(\Omega \cap \Omega_i)} \\ &= (u - u_i^g, \mathcal{A}^T \omega_i)_{L^2(\Omega)} \\ &= (\mathcal{A}(u - u_i^g), \omega_i)_{L^2(\Omega)} \\ &= -(F(u_i^g), \omega_i)_{L^2(\Omega)}. \end{aligned}$$

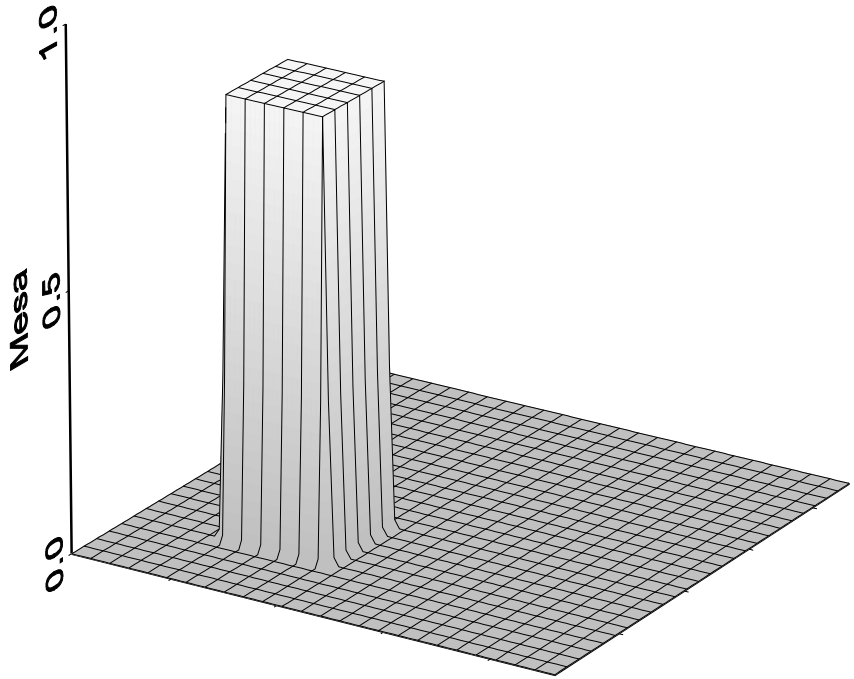
This gives then

$$|(u - u_{pp}, \psi)_{L^2(\Omega)}| \leq \sum_{k=1}^{p} |\langle F(u_i^g), \psi \rangle| < \sum_{k=1}^{p} \frac{\epsilon}{p} = \epsilon.$$

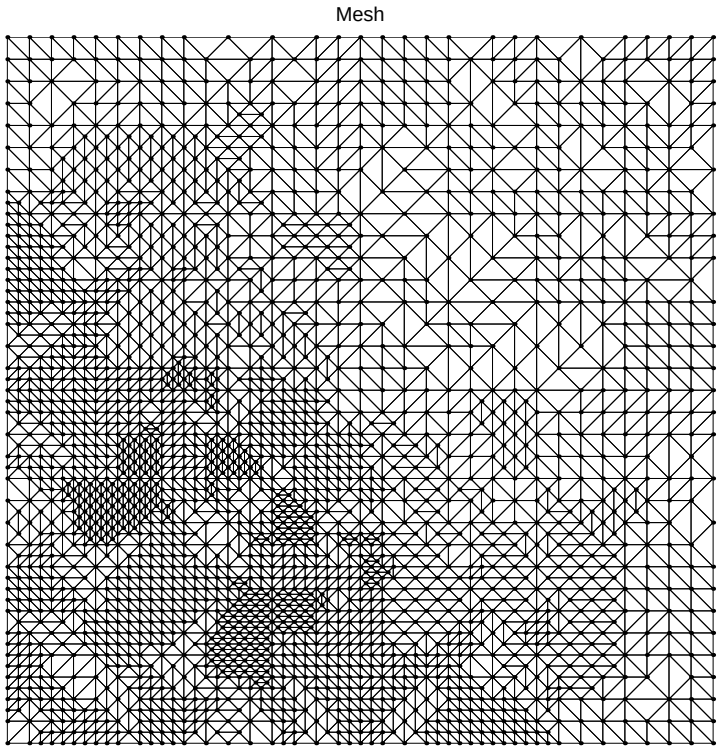
□

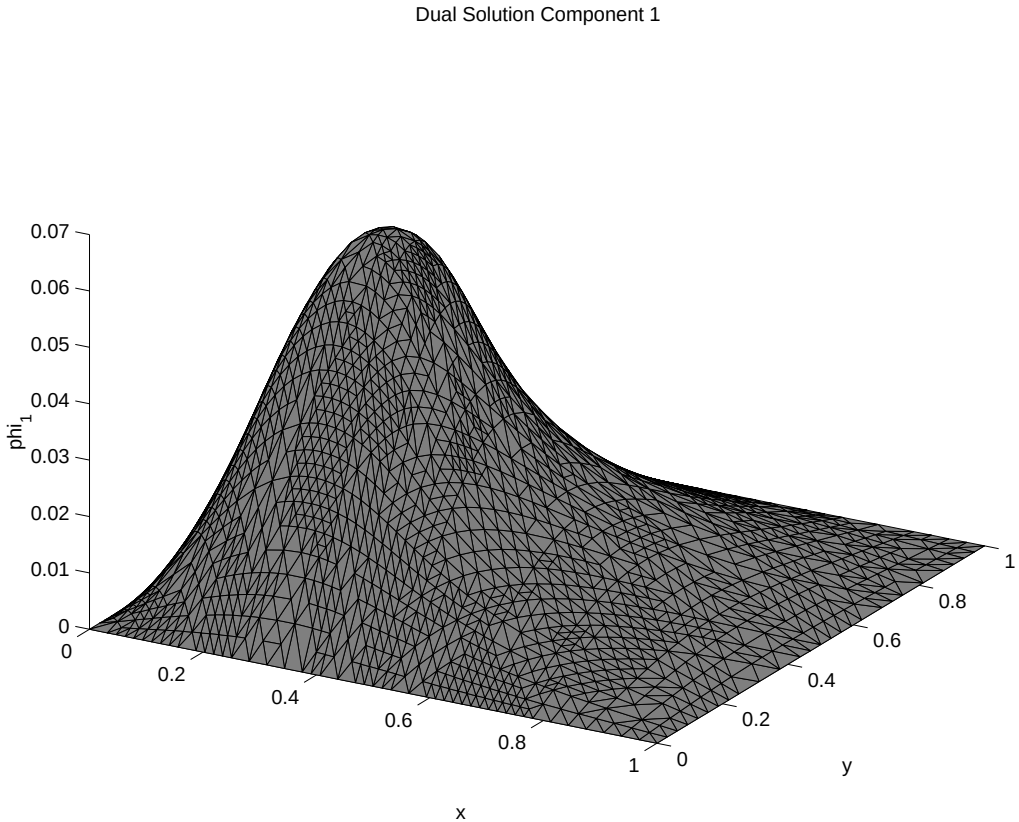
Example: initial mesh and a partition function



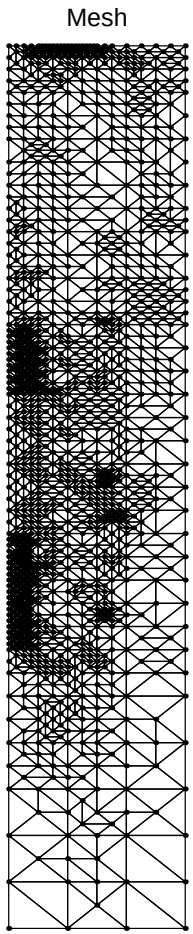


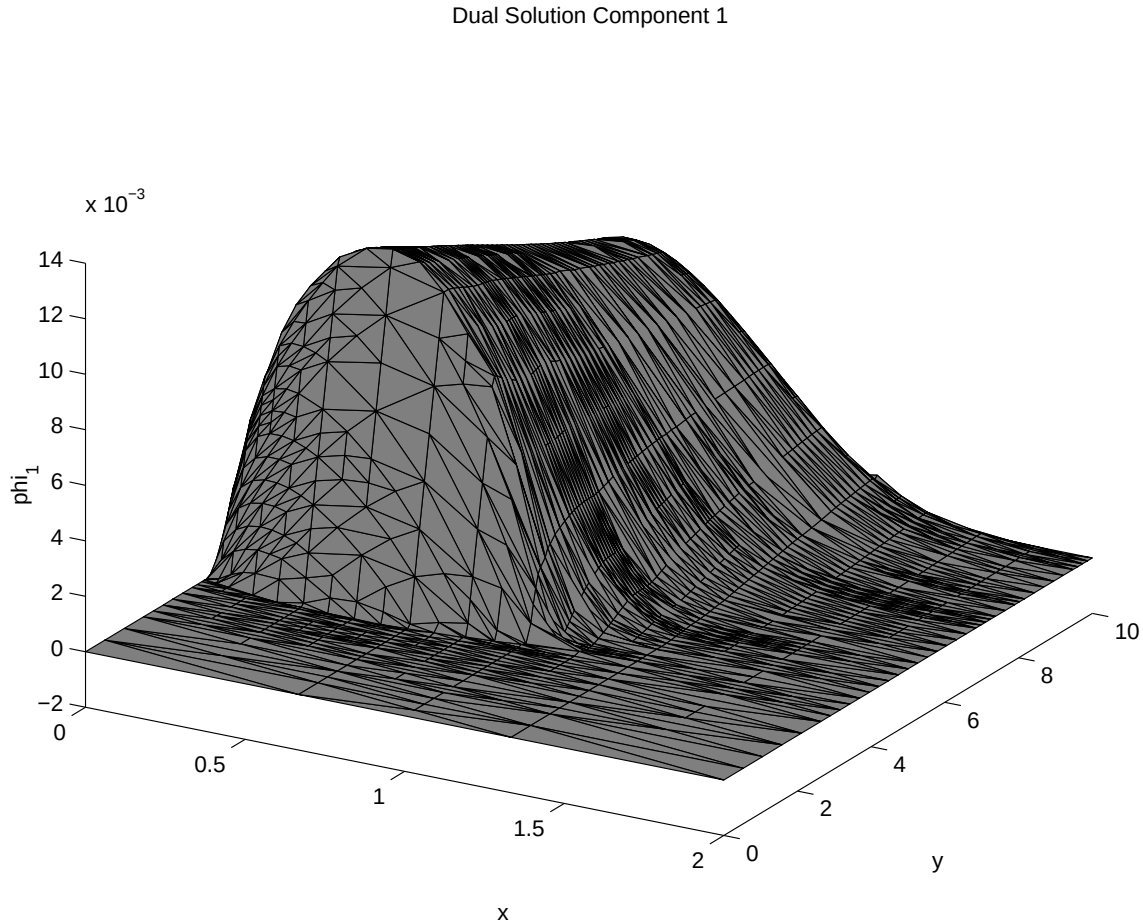
The dual solution on an adapted mesh





Another dual solution and adapted mesh





Properties of Duality-based PPUM Algorithms

Typical duality-based PPUM Algorithm (cf. **[H2]**):

- Solve entire problem on coarse mesh, compute *a posteriori* estimates.
- Bisect (spectral/inertial) mesh to achieve *equal error* via estimates.
- Give coarse solution and mesh to a number of computers.
- Each computer solves entire problem adaptively AND independently, solving localized dual problems with partition function data.
- A processor stops when local tolerance is achieved locally.
- Global solution built via partition of unity; global quality guaranteed.

Comments:

- The constants C_∞ and C_G do not impact the error estimates.
- No *a priori* large overlap assumptions of unknown size.
- No *a priori* local estimates needed.
- Not restricted to elliptic or to linear problems; general decomposition.

Pointers to People/Papers/Software (www.FETK.org)

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