Numerical Methods: Adaptive Methods for nonlinear PDE with Application to the Poisson-Boltzmann Eqn

IPAM Workshop: Bridging Time and Length Scales in Materials Science and Bio-Physics

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- Partial differential equations (PDE); types, side conditions, etc.
- Various discretization techniques for PDE.
- Nonlinear variational problems, finite element methods, and adaptivity.
- Low complexity methods for solving linear and nonlinear equations.
- Some new parallel adaptive algorithms for cluster computers.
- Application: Analysis and numerical solution of the Poisson-Boltzmann eqn
- Some examples with the Finite Element ToolKit (FEtk).

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:

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

The *principle part* of the operator consists of:

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

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}:

- *Eliptic* (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): $a_{ij}(x)x_ix_j \geq \lambda|x|^2, \quad \forall\ 0 \neq x \in \mathbb{R}^d$.

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.

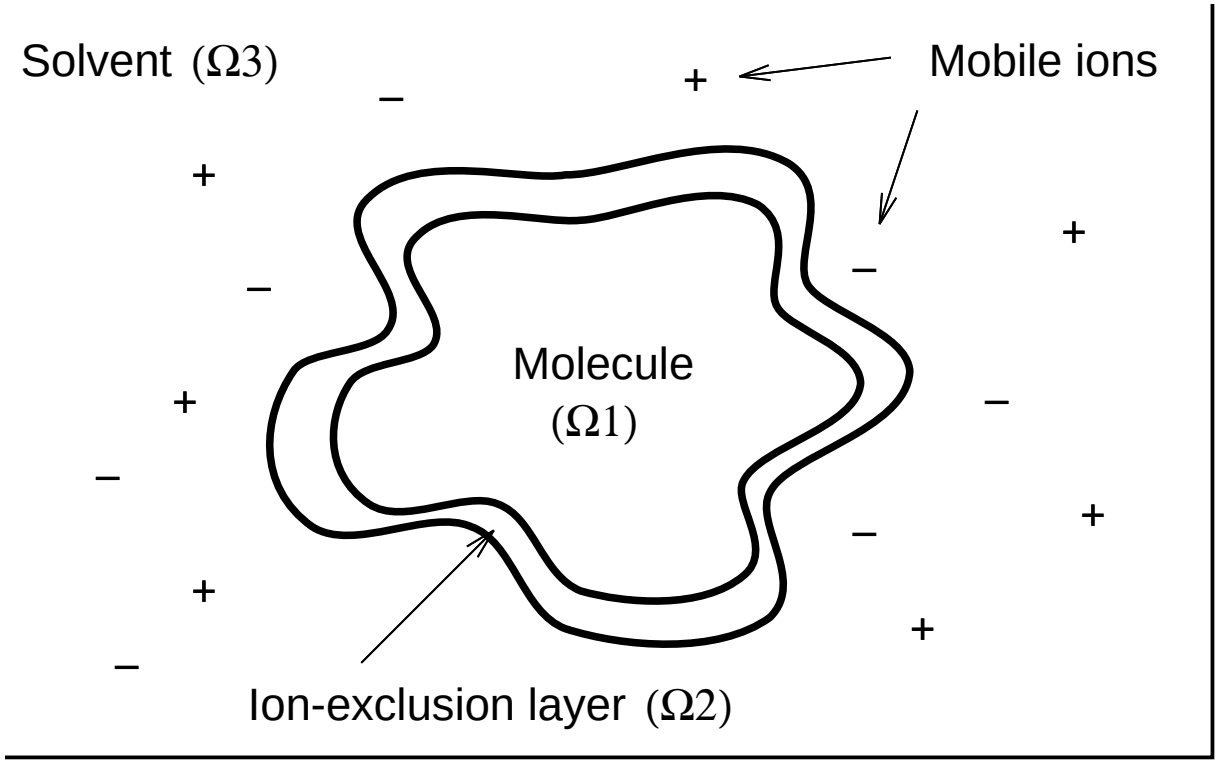
Specifying $u = g$ on $\partial\Omega$ is an *essential* or *Dirichlet* condition. Specifying $\nabla u \cdot n = g$ is a *natural* or *Neumann* condition. Specifying $\nabla u \cdot n + cu = g$ is a *mixed* or *Robin* condition.

There are obvious nonlinear generalizations; the requirement is compatibility with the PDE and *well-posedness* (to be defined shortly).

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.

Example 1: Poisson-Boltzmann equation.



The potential ψ_k satisfies Gauss' law (and $\psi_3(\infty) = 0$)

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

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

Nonlinear and linearized 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, $z_i \in [-1, 1]$, $i = 1, \ldots, N_m$.
- $\phi(\mathbf{x}) = \frac{e_c \psi(\mathbf{x})}{k_B T}$, $\quad \kappa = \left(\frac{8\pi N_A e_c^2}{1000 e_3 k_B T} \right)^{1/2} I_s^{1/2}$
- $\bar{\kappa}(\mathbf{x}) = \begin{cases} 0, & \mathbf{x} \in \mathbf{\Omega}_1, \mathbf{\Omega}_2 \\ \epsilon_3^{1/2} \kappa, & \mathbf{x} \in \mathbf{\Omega}_3 \end{cases}$, $\epsilon(\mathbf{x}) = \begin{cases} \epsilon_1, & \mathbf{x} \in \mathbf{\Omega}_1 \\ \epsilon_2 (= \epsilon_3), & \mathbf{x} \in \mathbf{\Omega}_2, \mathbf{\Omega}_3 \end{cases}$

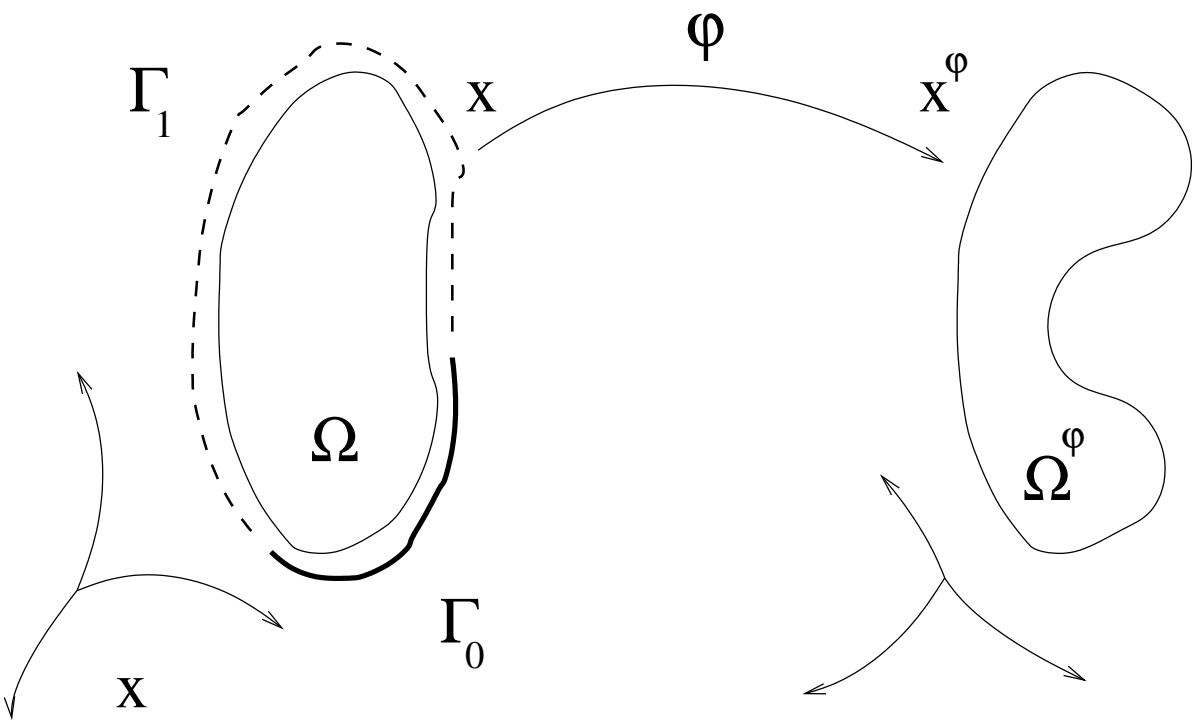
A Boltzmann assumption on the ion concentration ratio gives rise to the nonlinear Poisson-Boltzmann equation:

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

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

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

Example 2: 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.

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

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

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

How do we solve these types of complicated equations?

As is typically the case, there are analytical solutions only in very special (unrealistic) situations. We must employ *approximation*.

Before using approximation, we should first establish if the problem is *well-posed*:

- There exists a solution
- This solution is unique
- This solution depends continuously on the problem data

Although "well-posedness" seems to have nothing to do with numerical methods and computers, in fact it is quite important to understand this completely before doing anything with approximation methods.

Moreover, we often have to establish some or all of these properties for discretized equations.

While general results often apply to linear problems such as the linearized PBE to establish well-posedness, nonlinear problems must usually be analyzed on a case-by-case basis.

Research questions for e.g. the PBE.

An applied mathematician would want to resolve the following:

1. Well-posedness of the PBE.
2. General approximation theory (how close can we get).

A computational mathematician would also want to resolve the following:

1. Well-posedness of discrete versions of the PBE.
2. Approximation theory again (for specific numerical methods).
3. Complexity of algorithms for solving the discrete equations.
4. Implementation of the methods on (parallel) computers.

Regarding well-posedness of the PBE, one can establish e.g. the following:

Theorem 1. *(***[HL,HX]***) Then there exists a unique solution* $u(x)$ *to the nonlinear and linearized PBE equations. The solution* $u(x)$ *satisfies* a priori *bounds (*a.e.*) in* Ω*.*

The "a priori" bounds guarantee that ϕ lies between upper and lower bounds pointwise (in a certain sense). It turns out to be important to establish this for approximation theory purposes.

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" bsais 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

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 $\tau^{(i)}$:

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

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

A one-dimensional example (cont.)

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:

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

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

Weak formulations (for e.g. finite element methods)

Consider the following simple problem:

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

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

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

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

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 $v \in C_0^2(\Omega)$.

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?

Functions and the vector spaces they live in.

One answer is given by the Schwarz inequality:

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

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

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 (simply a vector space):

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

where an inner-product and norm are defined as:

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

The function space H^1

We are also led to define the *Sobolev* space:

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

where an inner-product, semi-norm, and norm are:

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

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

We can then define:

$$H^1_0(\Omega) = \{u \in H^1(\Omega) : u = 0 \text{ on } \partial\Omega\}.$$

We now have a weaker formulation of the original problem:

$$\text{Find } u \in H^1_0(\Omega) \text{ s.t. } \int_\Omega u_x v_x dx = \int_\Omega f v dx, \quad \forall v \in H^1_0(\Omega). \tag{4}$$

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

Consider a bounded open set $\Omega \subset \mathbb{R}^d$ with boundary $\Gamma = \Gamma_D \cup \Gamma_N$, where $\Gamma_D \cap \Gamma_N = \emptyset$.

Our concern is general second order linear elliptic equations, which can be written in the strong, divergence form 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:

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

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*, $A(u,v) = A(v,u), \ \forall u, v.$

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

Boundedness is: $|A(u,v)| \leq M\|u\|_{H^1}\|v\|_{H^1}, \qquad |F(v)| \leq L\|v\|_{H^1}.$

Nonlinear Variational Problems.

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,

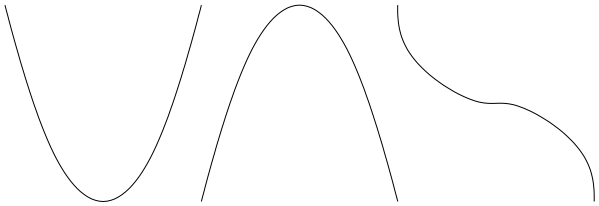
$$\langle J'(u), v \rangle = \left. \frac{d}{d\epsilon} J(u + \epsilon v) \right|_{\epsilon=0}.$$

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:

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

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

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

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

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

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

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

which (if a classical solution exists) 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

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

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).

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:

$$AX = B,$$

where

$$A_{ij} = a(\phi_j, \psi_i), \qquad X_i = \alpha_i, \qquad B_i = f(\psi_i).$$

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

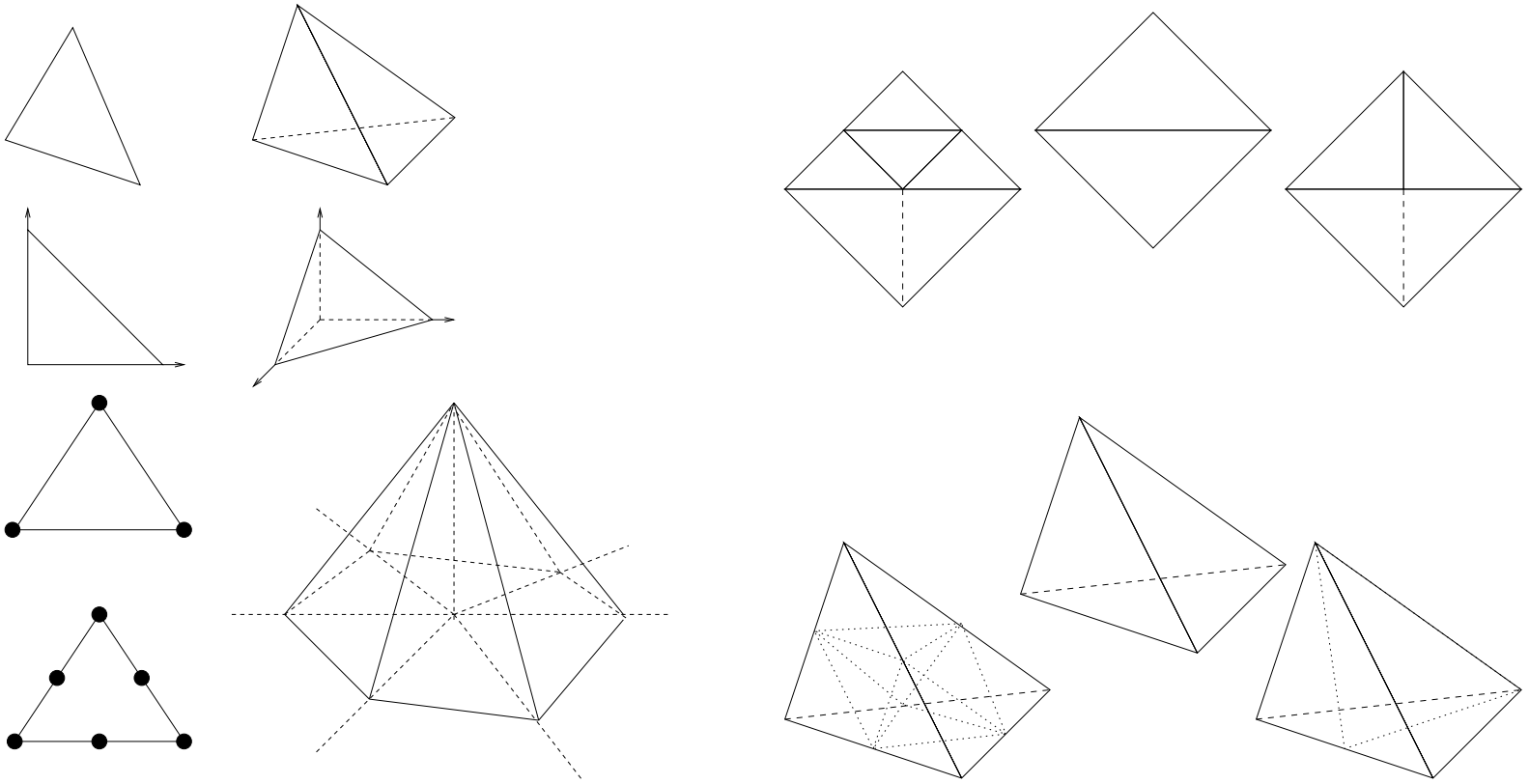
- The cost of storing the matrix A is as close to optimal $O(n)$ as possible;
- The cost of inverting the matrix A is as close to optimal $O(n)$ as possible.

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.)

Assembling FE Systems Using An Atlas of Charts.

An interesting feature of FE methods is that one typically uses coordinate transformations to assemble the matrix problem $AX = B$.

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 performing the integral on each element T_k by first doing a coordinate transformation to a model of $\mathbb{R}^d$ (the *reference element*), doing the integral there using transformation jacobians, and then mapping the result back to the element T_k using coordinate transformations again.

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 on $[X,Y]$ (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, 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. 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).

Improving the Constant in P-G Approximation.

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

Lemma 1 (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 on $[X,Y]$ (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:

$$\sup_{v_h\in Y_h}\langle b(u_h) - b(w_h), v_h\rangle \geq 0,$$

$$\langle b(u) - b(w_h), v_h\rangle \leq K\|u - w_h\|_X\|v_h\|_Y, \qquad \forall w_h \in X_h, \quad v_h \in Y_h.$$

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

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

follows by the following argument.

The Petrov-Galerkin solution u_h satisfies:

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

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

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

This then gives

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

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 nonlinear problem and its Galerkin approximation:

$$\text{Find } u \in X \text{ s.t. } a(u,v) + \langle b(u), v\rangle = f(v), \quad \forall v \in X, \tag{31}$$

$$\text{Find } u_h \in X_h \subseteq X \text{ s.t. } a(u_h,v_h) + \langle b(u_h), v_h\rangle = f(v_h), \quad \forall v_h \in X_h \subseteq X, \tag{32}$$

where the following are assumed to hold on X:

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

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

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

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

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

follows by the following argument.

The 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:

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

Nonlinear Approximation using Adaptive Methods.

Adaptive FE alorithms: build approximation spaces adaptively, meeting target quality using spaces having minimal dimension. This is *nonlinear approximation*.

A priori estimates (generally non-computable) establish convergence; these *asymptotic* statements not useful for driving adaptivity.

A posteriori error estimates (by definition computable) are critical for driving adaptivity in nonlinear approximation schemes.

FE codes such as PLTMG (2D) and FEtk (3D; descibed below) 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. Find $u_h \in X_h$ such that $\langle F(u_h), v_h \rangle = 0, \forall v_h \in Y_h$
    2. Estimate $E(u - u_h)$ over each element, set $Q1 = Q2 = \phi$.
    3. Place simplices with large error in "refinement" $Q1$
    4. Bisect simplices in $Q1$ (removing from $Q1$), placing nonconforming simplices created in temporary $Q2$.
    5. $Q1$ is now empty; set $Q1 = Q2$, $Q2 = \phi$.
    6. If $Q1$ is not empty, goto (d).
7. end while

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 2. (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".

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

A general residual *a posteriori* error estimate.

What is needed is a bound on the dual norm:

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

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

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

which includes all the nonlinear elliptic problems above, where:

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

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

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

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:

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

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

Residual *a posteriori* error estimate (cont).

Theorem 3. [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:*

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

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

Outline of 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 4. (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*

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

Outline of Proof:

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

□

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:

- Our algorithms need to have (nearly) linear space and time complexity on a sequential computer. (Linear in number of discrete degrees of freedom.)
- Our algorithms need to scale (nearly) linearly with the number of processors on a parallel computer.
- MG *does not* have linear space or time complexity on locally adapted meshes.

Our Solutions: Fast linear elliptic solvers based on:

- BPX-type [Bramble-Pasciak-Xu] and stabilized HB [Bank;Vassilevski-Wang] methods for locally adapted FE spaces **[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:

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

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

$$e^{n+1} = (I - BA)e^n = (I - BA)^2 e^{n-1} = \cdots = (I - BA)^{n+1} e^0. \tag{33}$$

The convergence of Algorithm 1 is determined by the spectral radius of the error propagator $E = I - BA$.

Theorem 5. *The condition $\rho(I - BA) < 1$ is necessary and sufficient for convergence of Algorithm 1.*

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:

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

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 1.

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 (33):

$$\|e^{n+1}\|_A \leq \|I - BA\|_A \|e^n\|_A \leq \|I - BA\|_A^{n+1} \|e^0\|_A. \tag{34}$$

The spectral radius $\rho(E)$ of the error propagator E is called the *convergence factor* for Algorithm 1, 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 (34) 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

$$n \geq \frac{|\ln \epsilon|}{|\ln \|E\|_A|}. \tag{35}$$

If the bound on the norm is of the form in Lemma 2, then to achieve a tolerance of ϵ after n iterations will require:

$$n \geq \frac{|\ln \epsilon|}{\left|\ln\left(1 - \frac{2}{1+\kappa_A(BA)}\right)\right|} = \frac{|\ln \epsilon|}{\left|\ln\left(\frac{\kappa_A(BA)-1}{\kappa_A(BA)+1}\right)\right|}. \tag{36}$$

Using the approximation:

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

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 2. *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.

Algorithm 2. *(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:*

$$\alpha_i = (r^i, s^i)/(Ap^i, p^i)$$
$$u^{i+1} = u^i + \alpha_i p^i$$
$$r^{i+1} = r^i - \alpha_i A p^i$$
$$s^{i+1} = B r^{i+1}$$
$$\beta_{i+1} = (r^{i+1}, s^{i+1})/(r^i, s^i)$$
$$p^{i+1} = s^{i+1} + \beta_{i+1} p^i$$

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.

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

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

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:

$$\|e^{i+1}\|_A \leq 2 \left(\frac{\sqrt{\frac{\lambda_{\max}(BA)}{\lambda_{\min}(BA)}} - 1}{\sqrt{\frac{\lambda_{\max}(BA)}{\lambda_{\min}(BA)}} + 1} \right)^{i+1} \|e^0\|_A = 2 \ \delta_{\text{cg}}^{i+1} \ \|e^0\|_A, \tag{37}$$

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

Theorem 6. *If A and B are SPD, and $\|I - BA\|_A \leq \delta < 1$, then $\delta_{\text{cg}} < \delta$.*

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

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

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 (37).

To achieve a tolerance of ϵ after n iterations will require:

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

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:

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

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):

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

CG iterations to reach ϵ:

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

Apparently we need to estimate condition numbers.

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

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

then by simple spectral theory arguments one has

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

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

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

Spaces from approximation theory that will arise.

Besov and approximation spaces arise naturally in modern approximation theory:

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

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:

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

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:

$$\lambda_j^{-1} \|v\| \eqsim (\tilde{R}_j v, v), \quad v \in \tilde{\mathcal{S}}_j. \tag{38}$$

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

$$\lambda_{j+1} \eqsim \beta \lambda_j, \quad j = 0, \ldots, J-1. \qquad (\lambda_j \eqsim h_j^{-2}, \; \lambda_j = 2^j, \; \text{etc.}) \tag{39}$$

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

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

Outline of Proof: Orthogonality of $\tilde{Q}_k$ and assumptions (38) and (39). □

Proof. (More detailed version of the proof.)

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

$$
(\bar{B}u,u) = \sum_{j=0}^{J}\lambda_j^{-1}(\tilde{Q}_j u,\tilde{Q}_j u)\eqsim\sum_{j=0}^{J}(\tilde{R}_j\tilde{Q}_j u,\tilde{Q}_j u)=\sum_{j=0}^{J}(\tilde{R}_j\tilde{Q}_j u,u)=(Bu,u).
$$

□

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:

$$\|u\|_{A^1_{2,2}(\Omega)} \eqsim \|u\|_{H^1(\Omega)}, \tag{40}$$

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 (40)?

Jackson and Bernstein inequalities.

If one can estalish a Bernstein inequality of the form:

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

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:

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

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:

$$\frac{c_1}{\tilde{v}_J^{(2)}} \|u\|_{A^s_{p,q}(\Omega)} \leq \|u\|_{B^s_{p,q}(\Omega)} \leq c_2 \|u\|_{A^s_{p,q}(\Omega)}, \quad u \in \mathcal{S}_J, \tag{41}$$

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

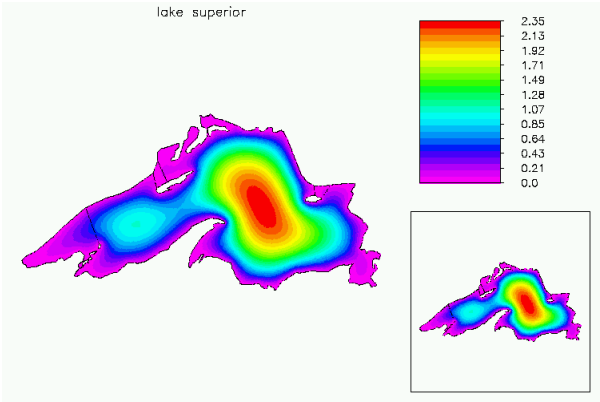
$$\|u\|_{A^1_{2,2}(\Omega)} \eqsim \|u\|_{H^1(\Omega)}.$$

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

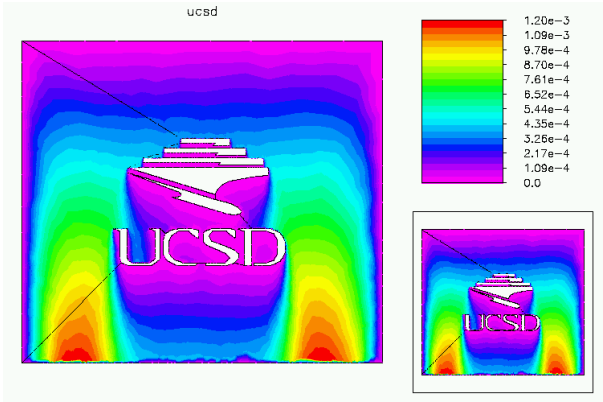
In particular, we establish (41) for finite element hierarchies built from practical octa-section and bisection-based 3D local refinement algorithms.

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.

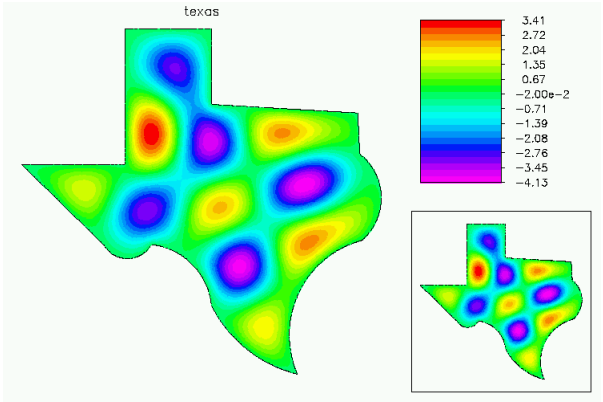
Putting it all togeter in the codes PLTMG and FEtk.



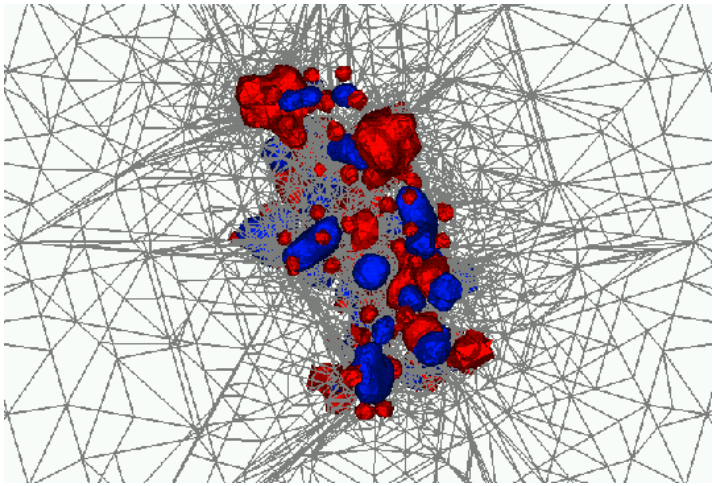
$$-\Delta u = 1$$



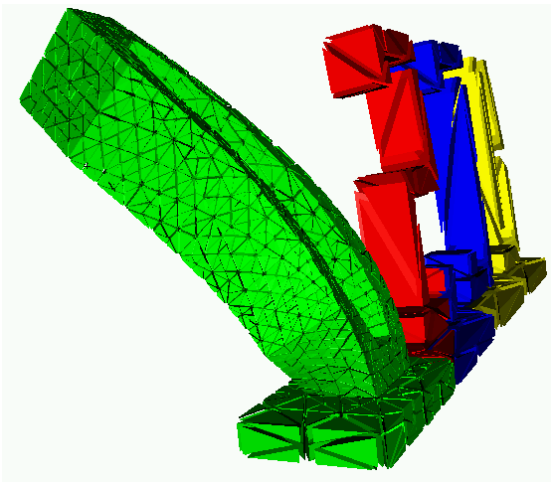
$$-\nabla \cdot (\nabla u + \beta u) = 1$$



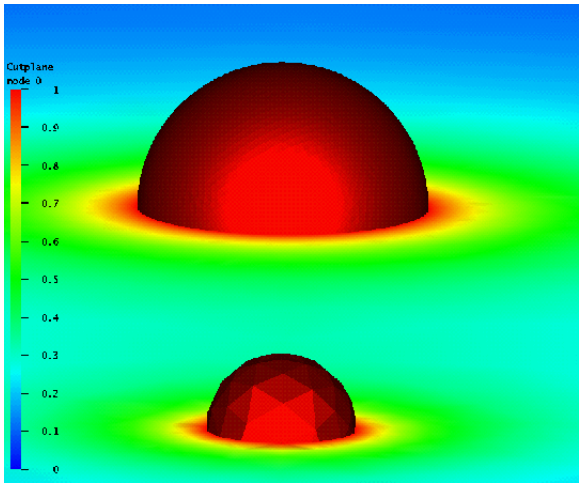
$$-\Delta u - 2u = 1$$



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



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



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

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 PDE problems:

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.

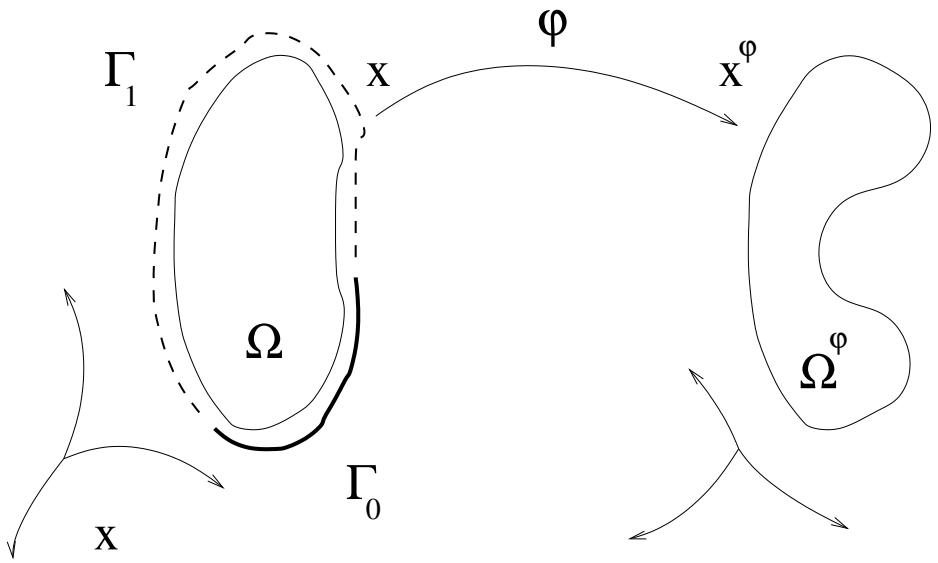
Observations:

- 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 emperical 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.



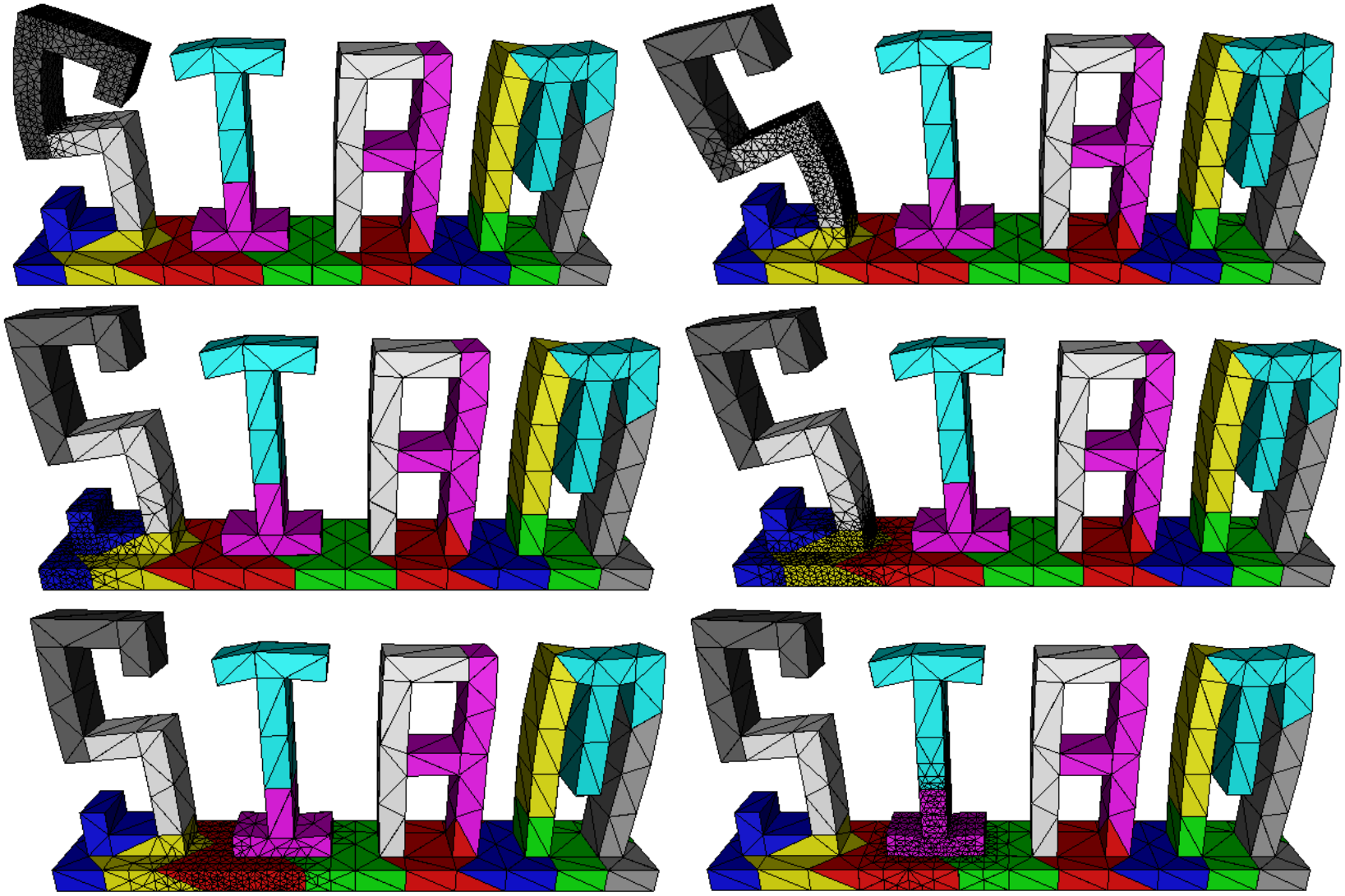
- $\varphi(\mathbf{x}) : \overline{\Omega} \mapsto \mathbb{R}^3$, $\nabla\varphi(\mathbf{x}) : \overline{\Omega} \mapsto \mathbb{M}^3$; deformation & deformation gradient
- $C = \nabla\varphi^T \nabla\varphi, \quad E = \frac{1}{2}(C - I) : \overline{\Omega} \mapsto \mathbb{S}^3$; RCG & GSV strains
-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

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

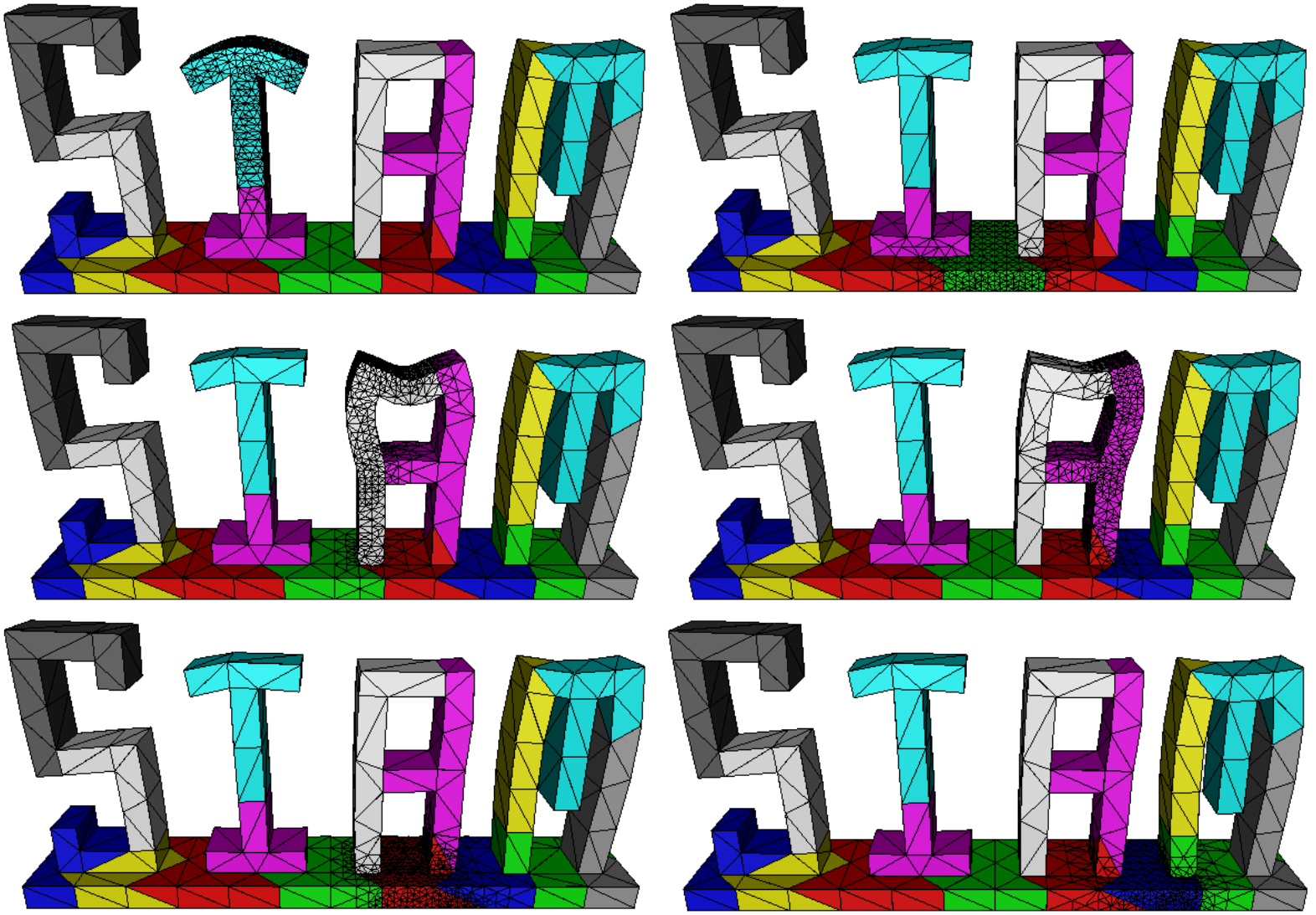
$$\begin{aligned} -\nabla \cdot (\nabla\varphi(\mathbf{x})\Sigma(\mathbf{x})) &= f(\mathbf{x}) \quad \text{in } \Omega, \\ n(\mathbf{x}) \cdot (\nabla\varphi(\mathbf{x})\Sigma(\mathbf{x})) &= g(\mathbf{x}) \quad \text{on } \Gamma_1, \\ \varphi(\mathbf{x}) &= \varphi_0(\mathbf{x}) \quad \text{on } \Gamma_0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

Tetrahedralized solid and its spectral bisection.

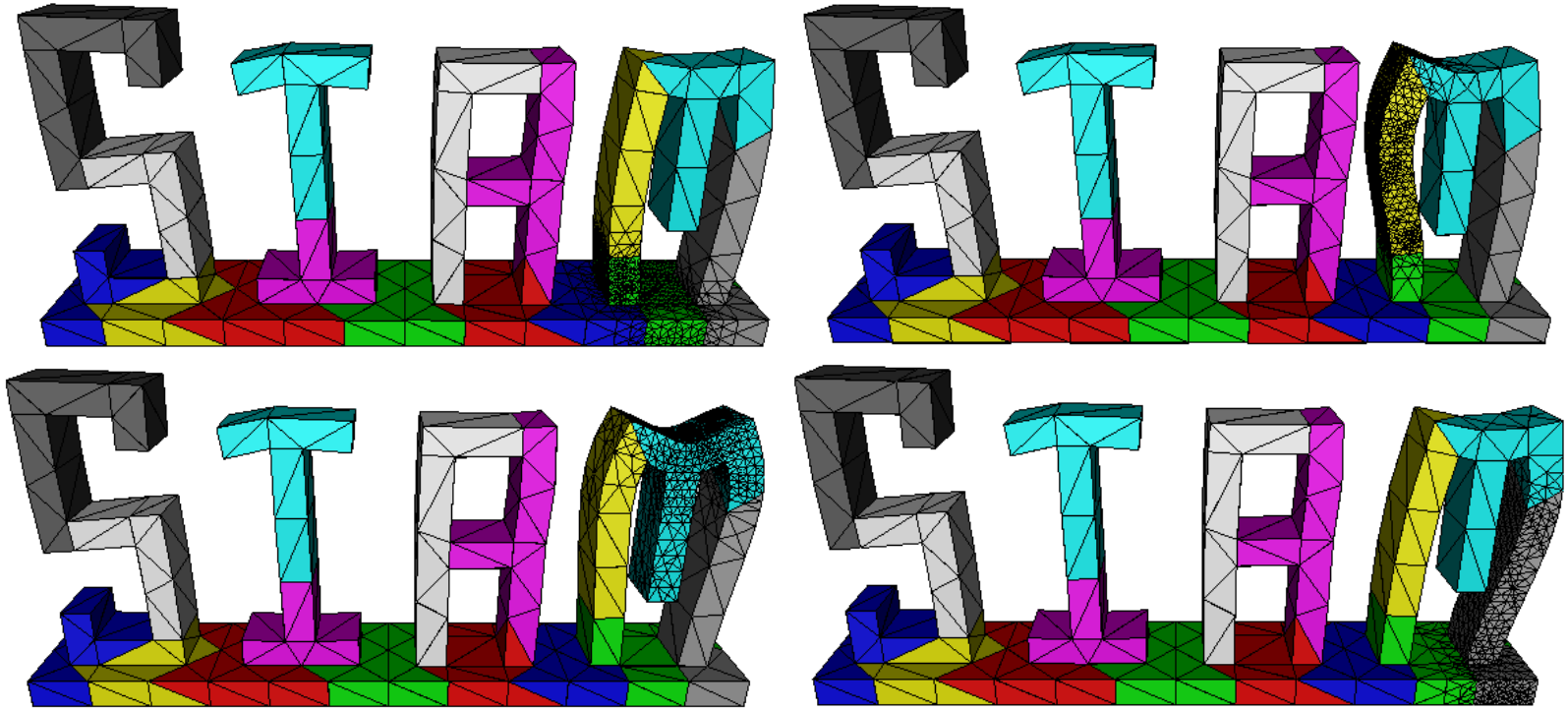
Local subdomain adaptivity: domains 1 through 6.



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 3. *Let* $w, w_i \in H^1(\Omega)$ *with* $\text{supp } w_i \subseteq \overline{\Omega \cap \Omega_i}$. *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 8. [Babuška and Melenk 1997] *If the local spaces* V_i *have the following approximation properties:*

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

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

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

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

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

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

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

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 9. [H1] *If* $\operatorname{diam}(\Omega_i) \geq 1/Q > 0 \quad \forall i$, *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:*

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

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

Duality-based Decomposition: Approximation Theory.

Theorem 10. [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:

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

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

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

Approximation Theory for Duality-based Approach.

Outline of Proof: 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:

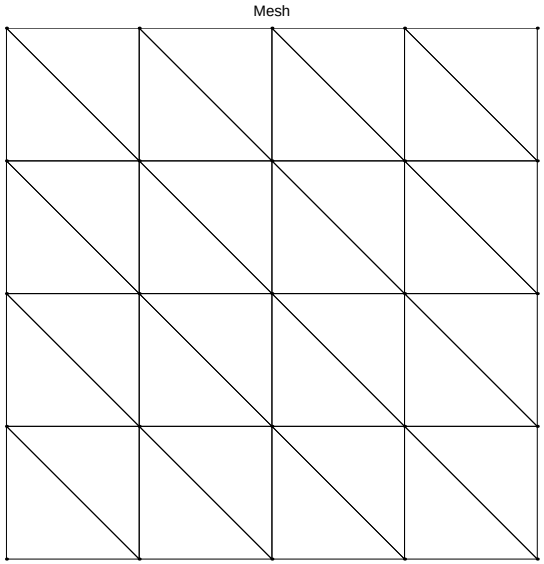
$$\begin{aligned} (\phi_i (u - u_i^g), \psi)_{L^2(\Omega \cap \Omega_i)} &= (u - u_i^g, \phi_i \psi)_{L^2(\Omega \cap \Omega_i)} \\ &= (u - u_i^g, \mathcal{A}^T \omega_i)_{L^2(\Omega)} \\ &= (\mathcal{A}(u - u_i^g), \omega_i)_{L^2(\Omega)} \\ &= -(F(u_i^g), \omega_i)_{L^2(\Omega)}. \end{aligned}$$

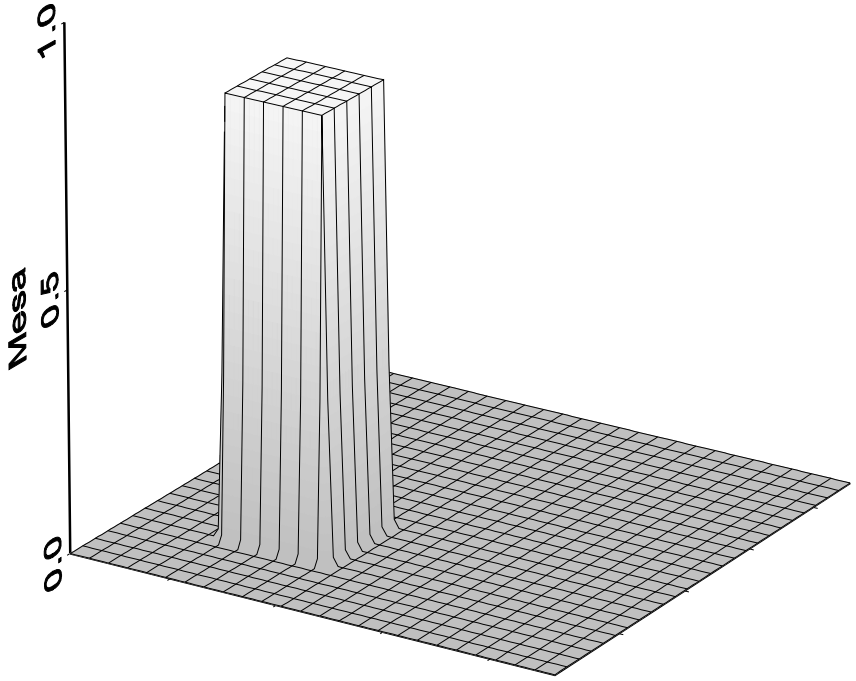
This gives then

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

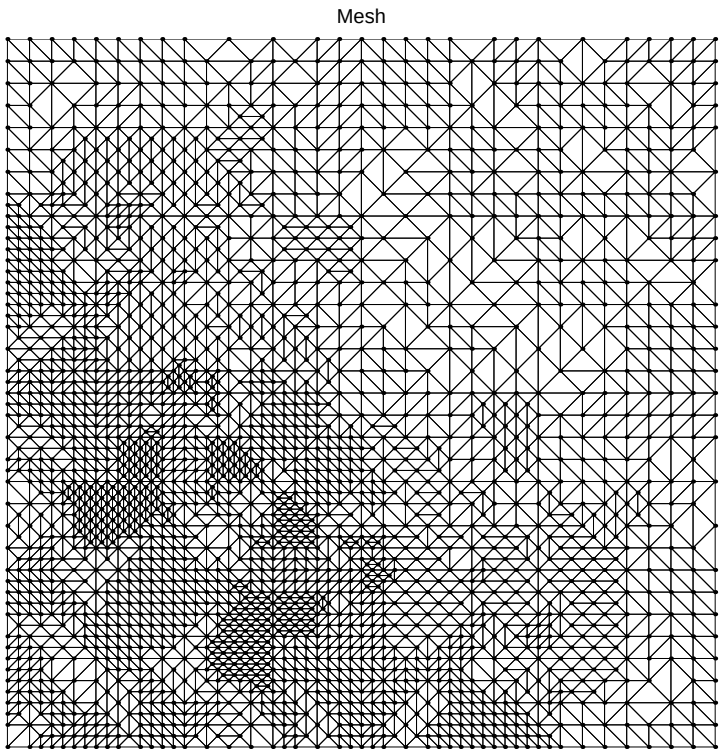
□

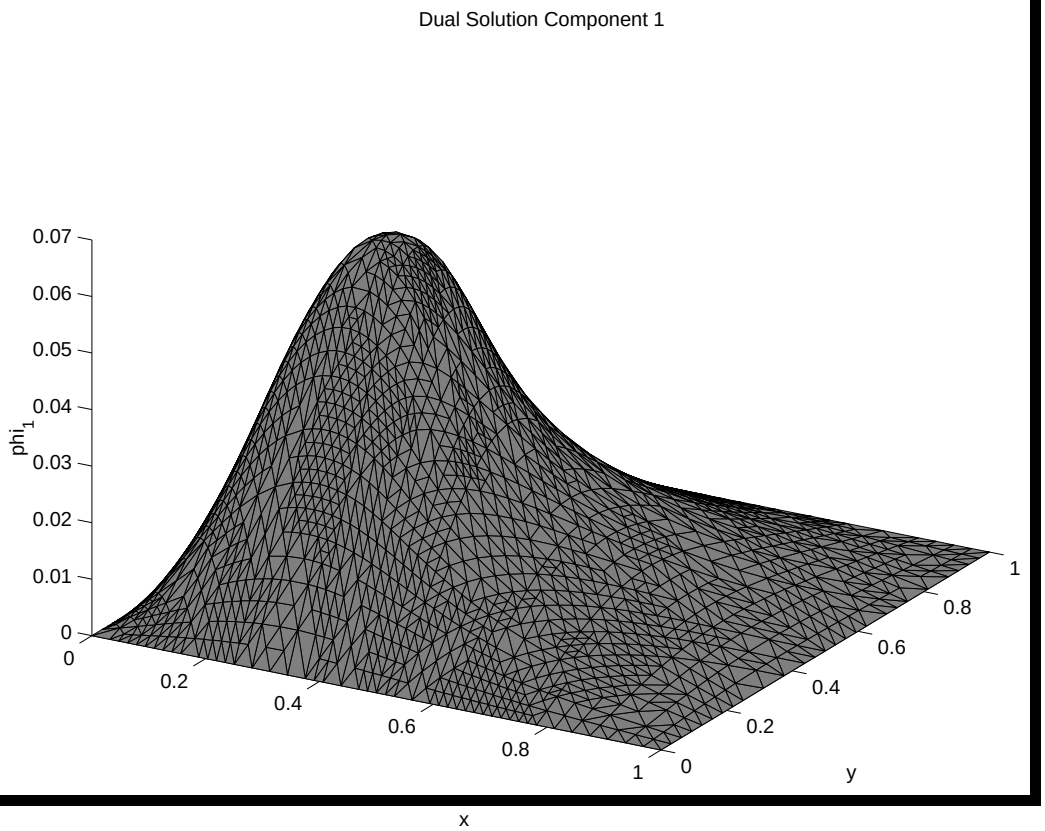
Example: initial mesh and a partition function.



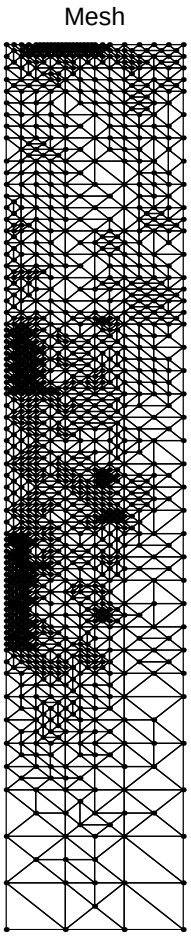


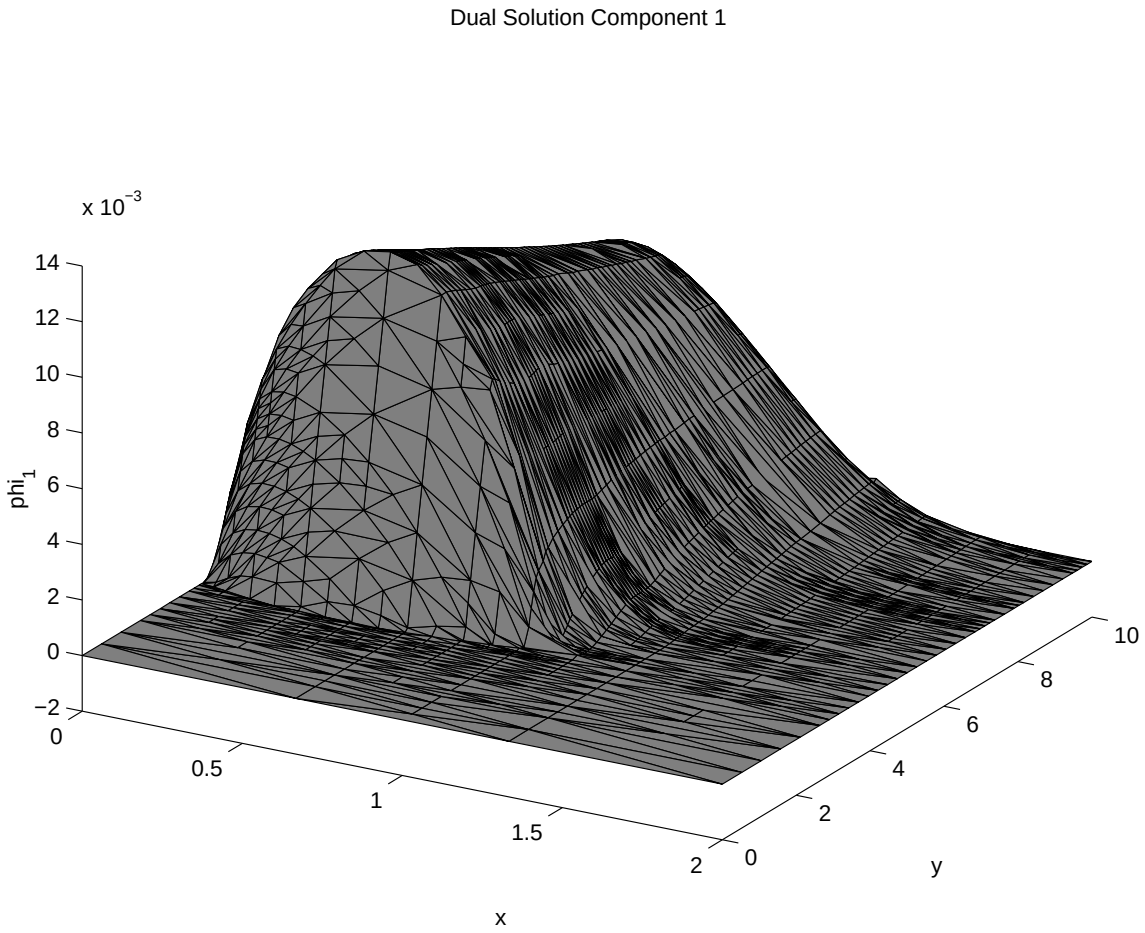
The dual solution on an adapted mesh.





Another dual solution and adapted mesh.





Properties of Duality-based PPUM Algorithms.

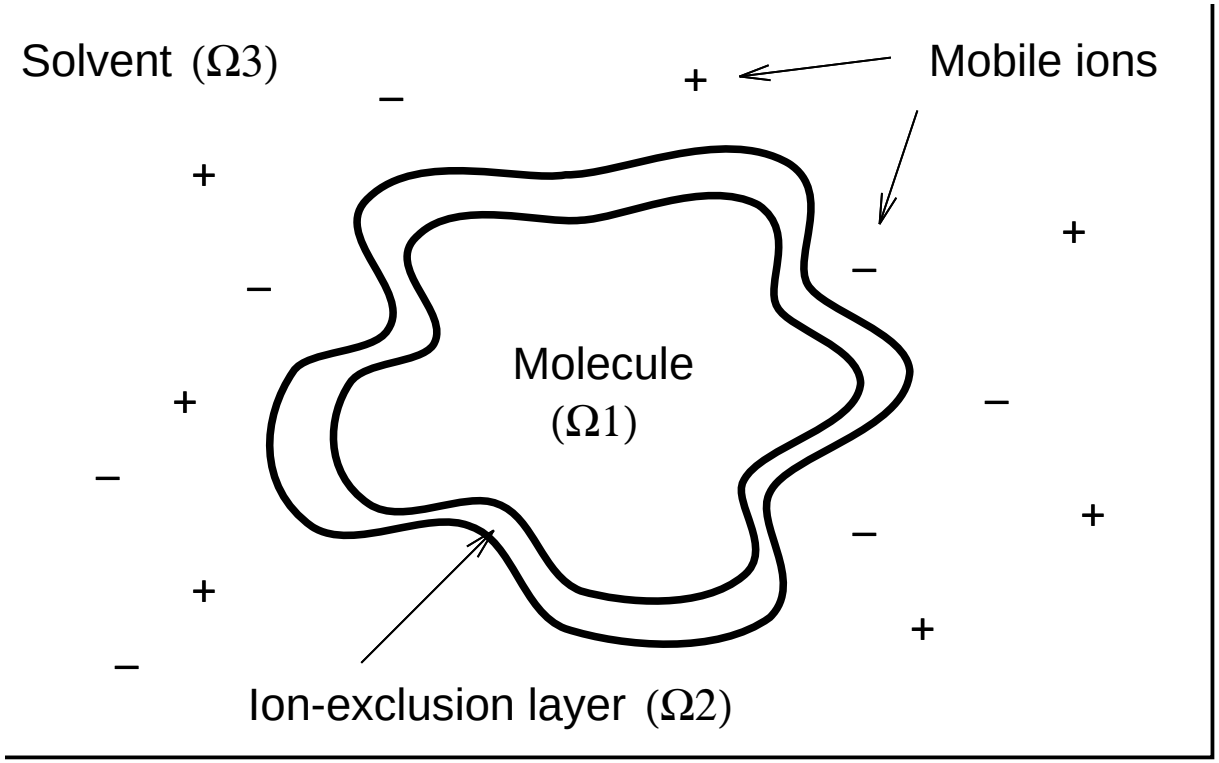
Typical duality-based PPUM Algorithm (cf. [H2]):

- 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.

Application: The Poisson-Boltzmann equation.



The potential ψ_k satisfies Gauss' law (and $\psi_3(\infty) = 0$)

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

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

Nonlinear and linearized 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, $z_i \in [-1, 1]$, $i = 1, \ldots, N_m$.
- $\phi(\mathbf{x}) = \frac{e_c \psi(\mathbf{x})}{k_B T}$, $\quad \kappa = \left(\frac{8\pi N_A e_c^2}{1000 e_3 k_B T} \right)^{1/2} I_s^{1/2}$
- $\bar{\kappa}(\mathbf{x}) = \begin{cases} 0, & \mathbf{x} \in \mathbf{\Omega}_1, \mathbf{\Omega}_2 \\ \epsilon_3^{1/2} \kappa, & \mathbf{x} \in \mathbf{\Omega}_3 \end{cases}$, $\epsilon(\mathbf{x}) = \begin{cases} \epsilon_1, & \mathbf{x} \in \mathbf{\Omega}_1 \\ \epsilon_2 (= \epsilon_3), & \mathbf{x} \in \mathbf{\Omega}_2, \mathbf{\Omega}_3 \end{cases}$

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

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

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

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

How do we solve these types of complicated equations?

As is typically the case, there are analytical solutions only in very special (unrealistic) situations. We must employ *approximation*.

Before using approximation, we should first establish if the problem is *well-posed*:

- There exists a solution
- This solution is unique
- This solution depends continuously on the problem data

Although "well-posedness" seems to have nothing to do with numerical methods and computers, in fact it is quite important to understand this completely before doing anything with approximation methods.

Moreover, we often have to establish some or all of these properties for discretized equations.

While general results often apply to linear problems such as the linearized PBE to establish well-posedness, nonlinear problems must usually be analyzed on a case-by-case basis.

Questions about the PBE.

An applied mathematician would want to resolve the following:

1. Well-posedness of the PBE.
2. General approximation theory (how close can we get).

A computational mathematician would also want to resolve the following:

1. Well-posedness of discrete versions of the PBE.
2. Approximation theory again (for specific numerical methods).
3. Complexity of algorithms for solving the discrete equations.
4. Implementation of the methods on (parallel) computers.

The PBE has several features which make both analysis and the development of provably good numerical methods difficult:

- Domain $\Omega \subseteq \mathbb{R}^d$, $d = 3$;
- Coefficients $\epsilon(x)$ and $\bar{\kappa}(x)$ are discontinuous at interfaces in Ω;
- Supercritical nonlinearity $\sinh(u)$: faster growth than u^p ($p = 5$ when $d = 3$);
- Source term contains delta functions: these are not bounded linear functionals on $H^1(\Omega)$ for $d > 1$.

Solution theory for the PBE.

In [HL,HX], we seek a solution to the PBE in the form $\phi = u + w$.

It is not difficult to show that there exists a fixed computable w such that the remainder function u satisfies the following *regularized* PBE: Find $u \in H^1(\Omega)$ such that

$$\int_\Omega \left[\varepsilon(x)\nabla u \cdot \nabla v + \kappa(x)^2 \sinh(u+w)\, v\right] dx = [\varepsilon] \int_\gamma v \frac{\partial w}{\partial n} dS, \qquad \forall v \in H_0^1(\Omega). \quad (42)$$

In [HL], we show that this regularized formulation is well-posed: there exists a unique solution u that depends continuously on the data. We also estalish *a priori* L^∞-bounds for u:

$$\alpha \leq u(x) \leq \beta, \quad \text{a.e. in } \Omega.$$

In [HX], we establish the following *a priori* error estimate for Galerkin approximations to the PBE, leading to a provably convergent numerical method for the PBE.

Approximation Error for the Regularized PBE.

To analyze the error, consider the nonlinear PBE and its Galerkin approximation:

$$\text{Find } u \in X \text{ s.t. } a(u,v) + \langle b(u), v\rangle = f(v), \quad \forall v \in X, \tag{43}$$

$$\text{Find } u_h \in X_h \subseteq X \text{ s.t. } a(u_h,v_h) + \langle b(u_h), v_h\rangle = f(v_h), \quad \forall v_h \in X_h \subseteq X, \tag{44}$$

where the following are assumed to hold on X:

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

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

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

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

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

follows by the following argument.

The 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:

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

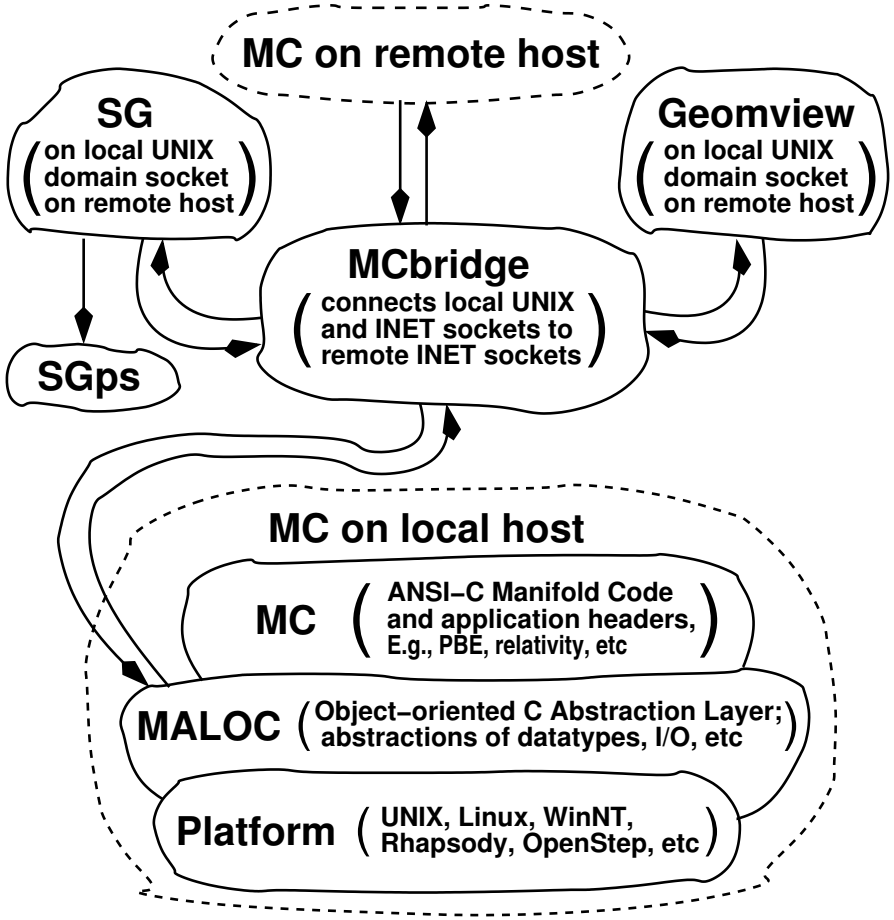
Establishing the Lipshitz continuity assumption on $b(u)$ is the only technical hurdle; it follows from *a priori* L^∞-bounds on u and on u_h.

We also establish some *a posteriori* error estimates for the PBE in [HX].

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.

Unusual features of MC (Manifold Code).

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

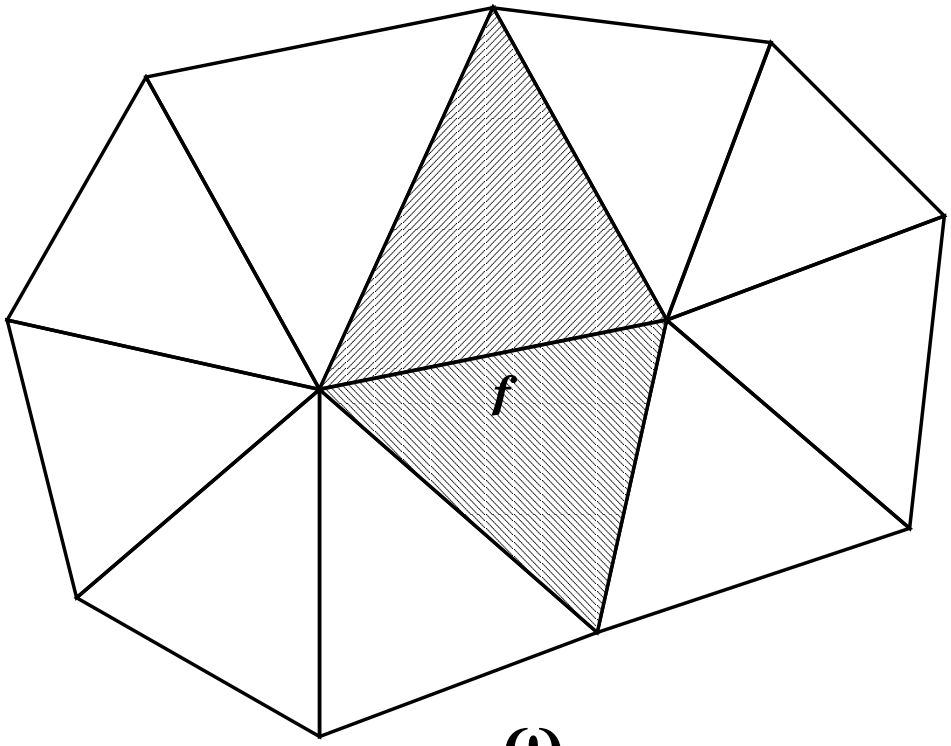
MC implements a variant of the solve-estimate-refine iteration described earlier, and has the following features:

- *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.

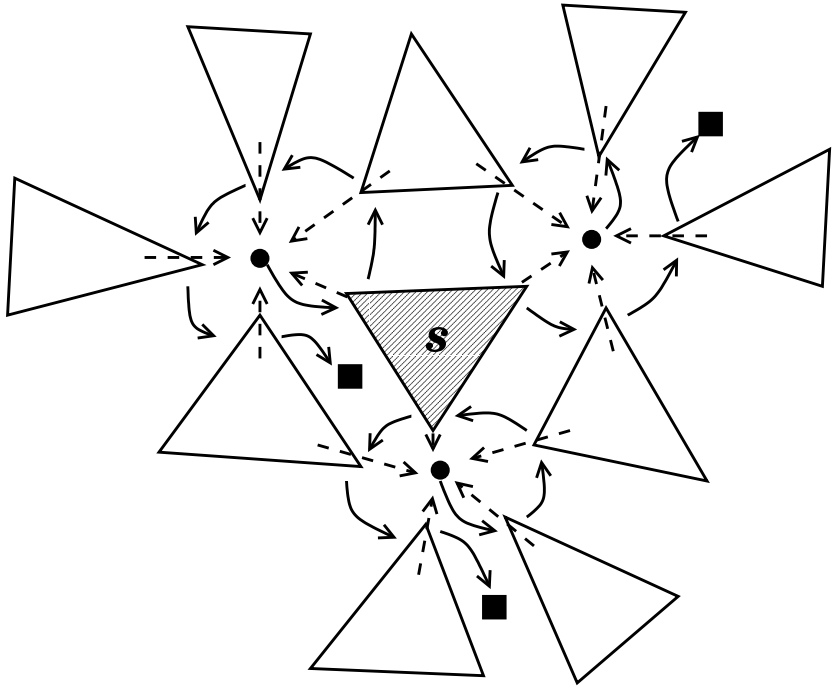
These abstractions are inherited by application codes built on top of FEtk.

The RInged VERtex datastructure in MC.

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

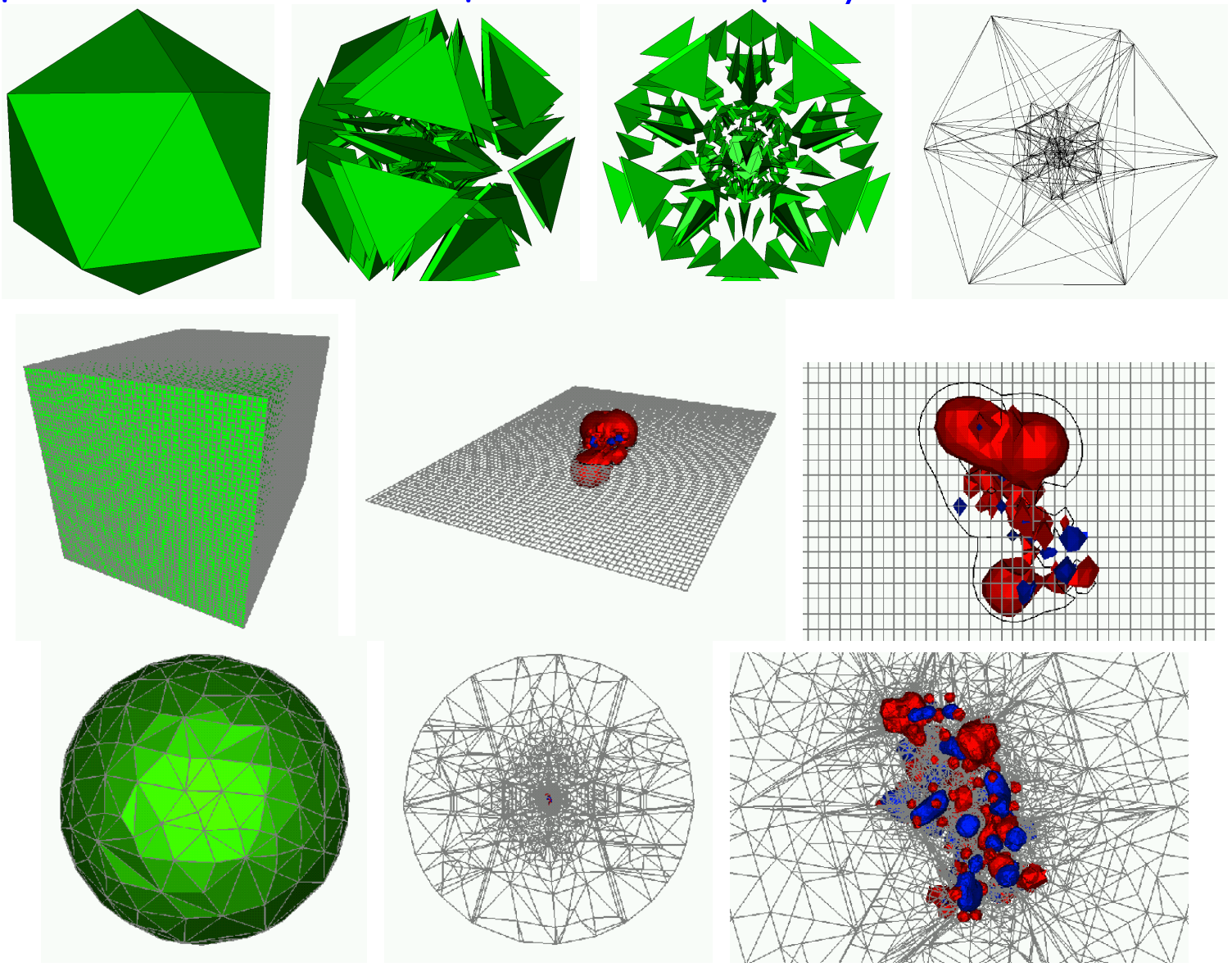


ω_f

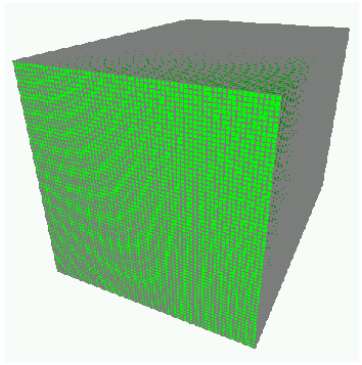


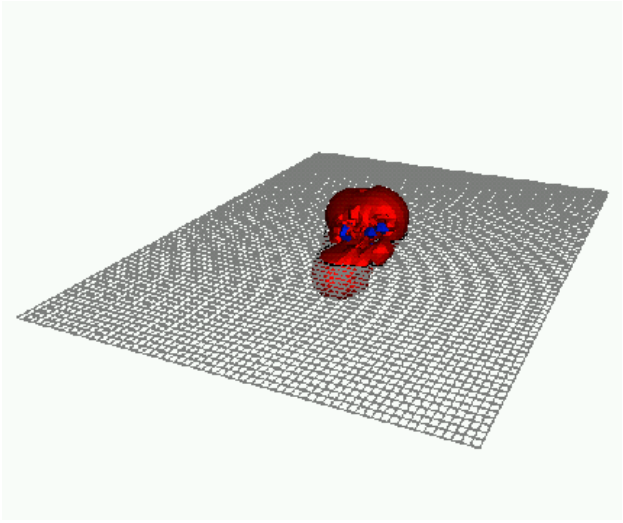
ω_s

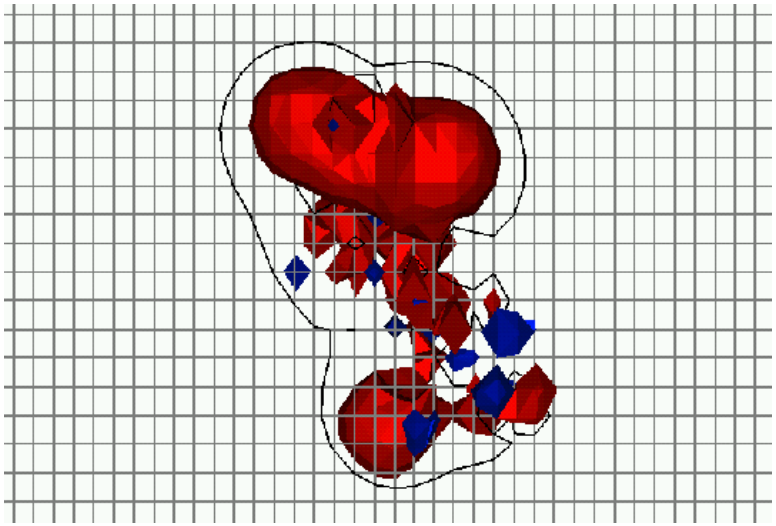
Adaptive vs. non-adaptive: cheaper/more accurate

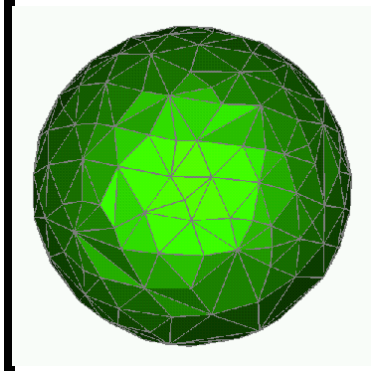


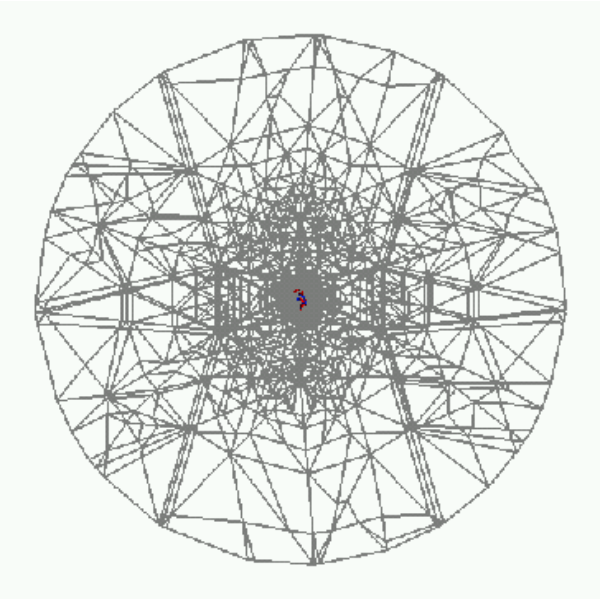
Adaptive vs. non-adaptive: cheaper/more accurate

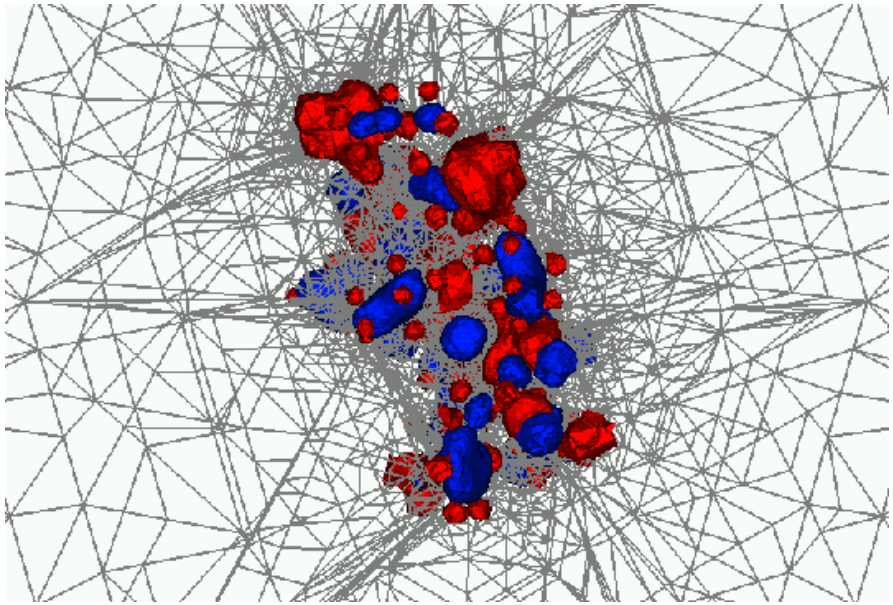






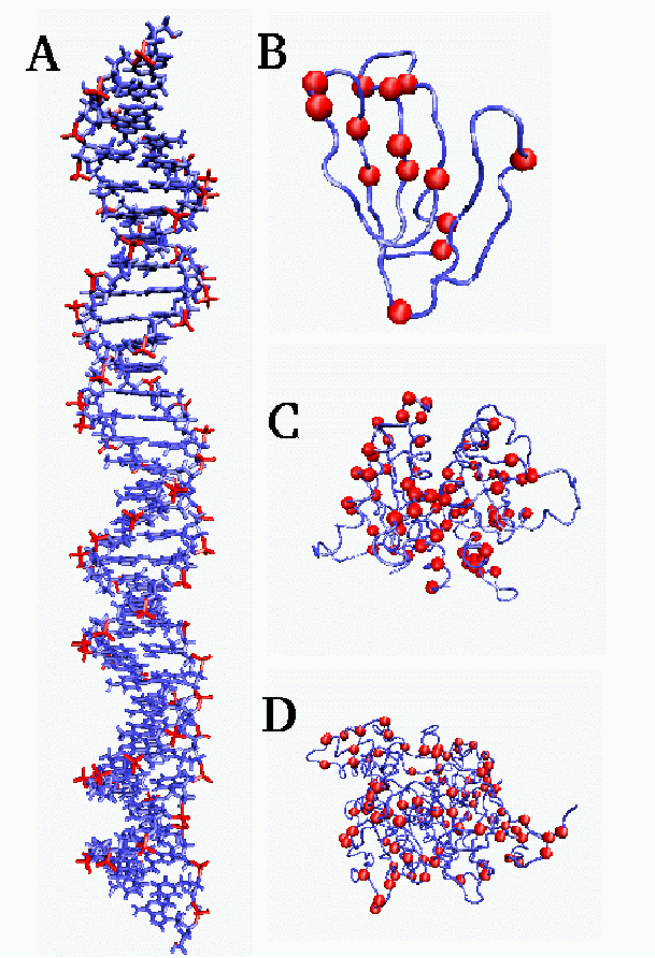






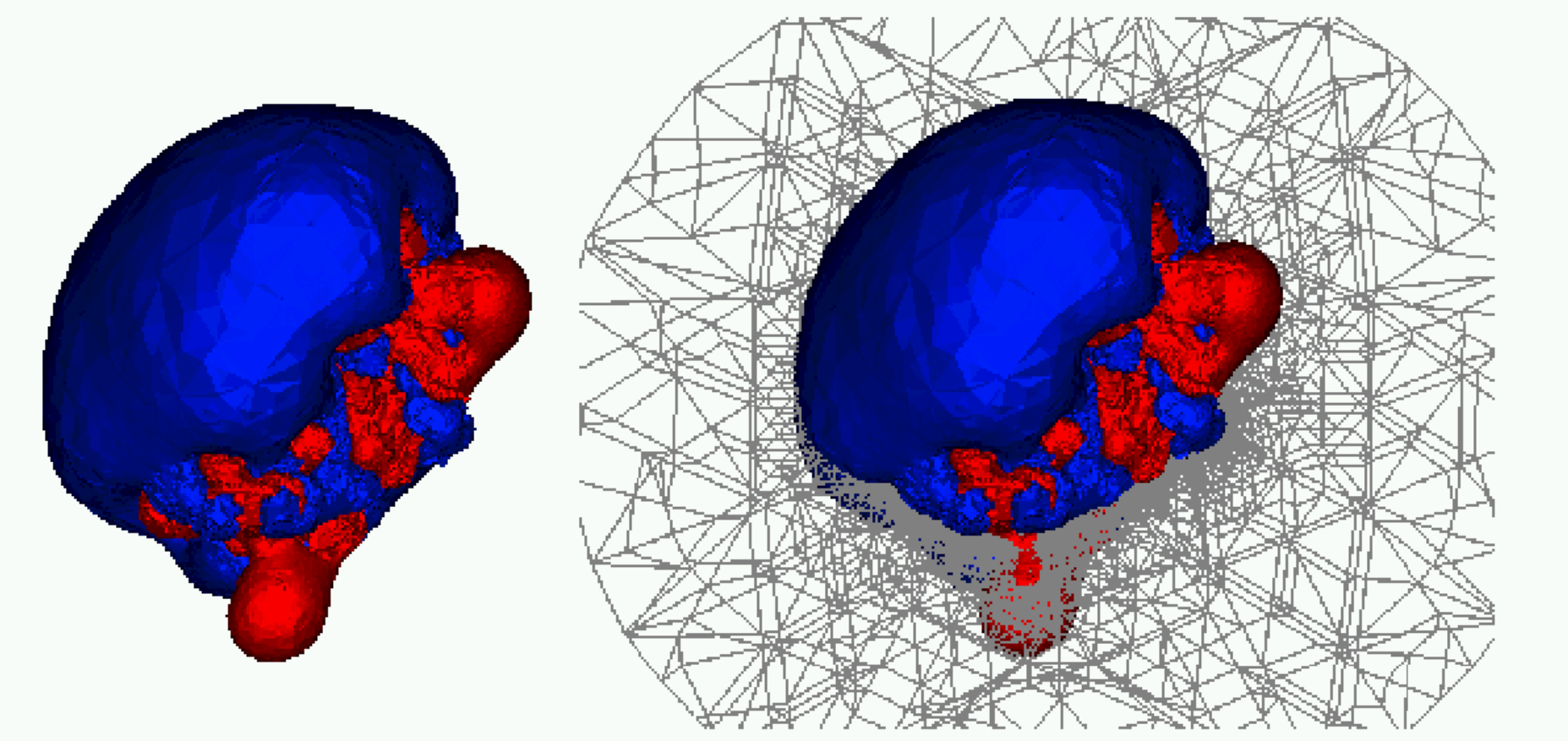
Collaborations with McCammon Group in Chemistry

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



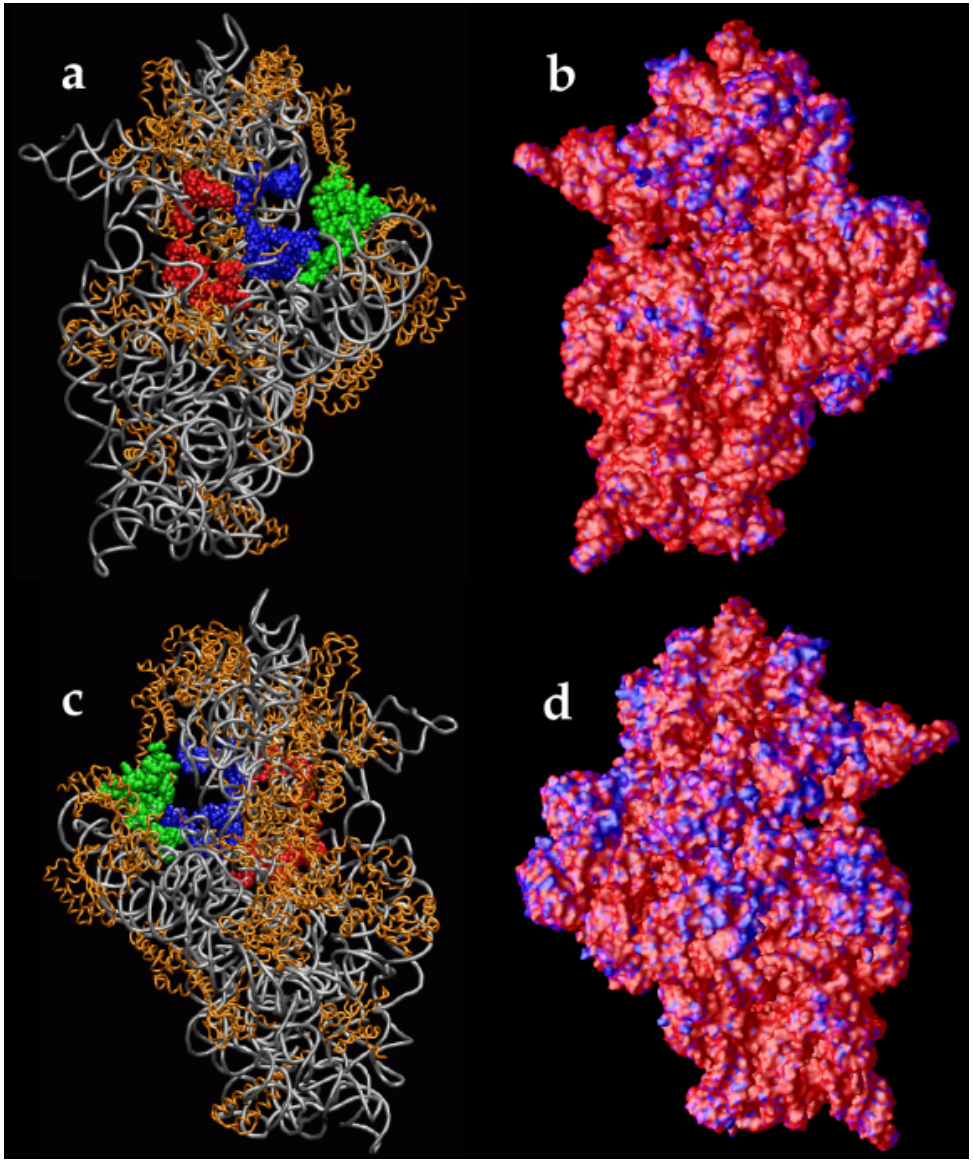
Charged groups are displayed as red spheres, other atoms as blue lines or by a protein backbone tube.
A=DNA 36-mer, B=fasciculin-2, C=HIV integrase, D=AChE. Figure courtesy of N. Baker.

Electrostatic Potential of Fasciculin-2

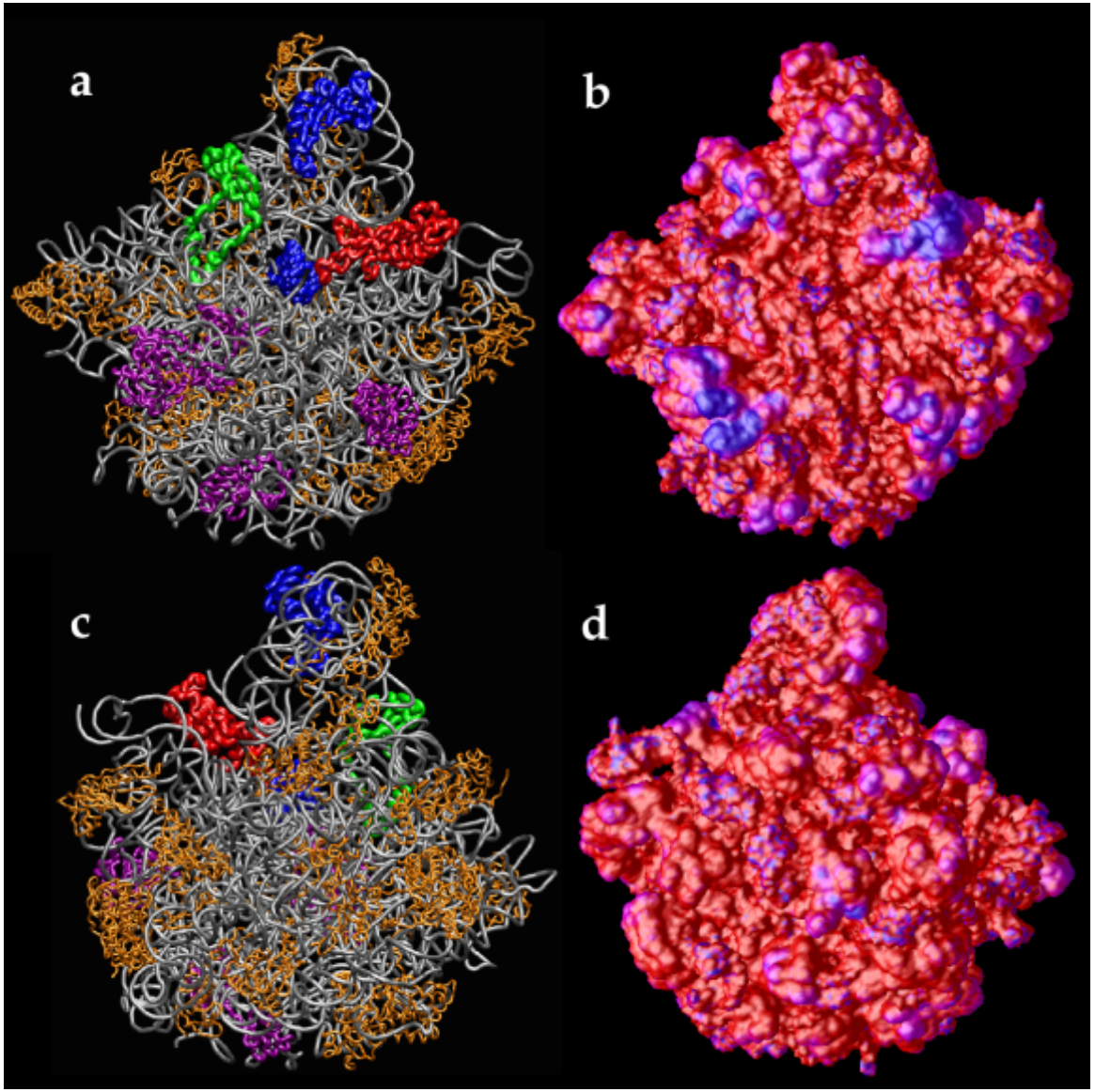


Potential contours from solution to linear PBE for FAS2 shown with a slice through the finite element mesh. Solution was computed using the adaptive finite element software MC.

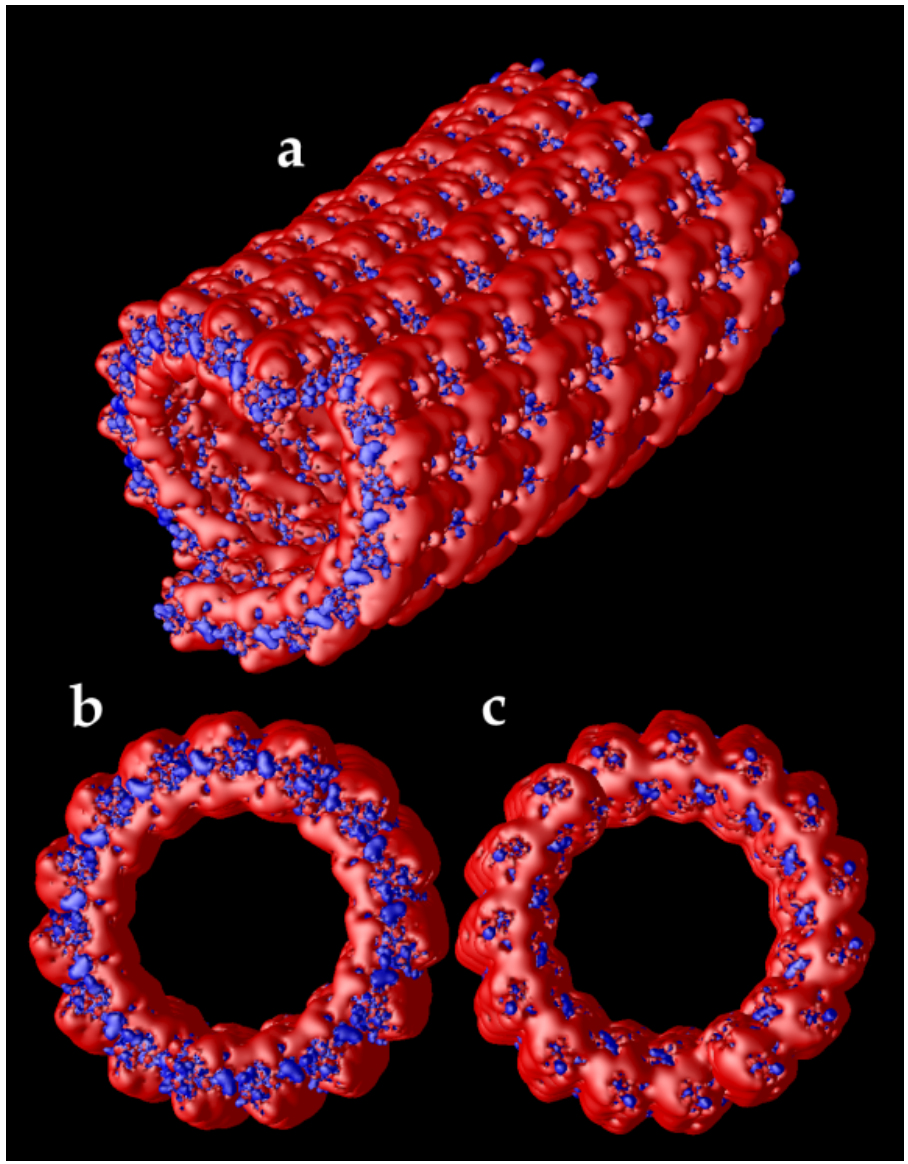
Rhibosome example (Ph.D. work of N. Baker)



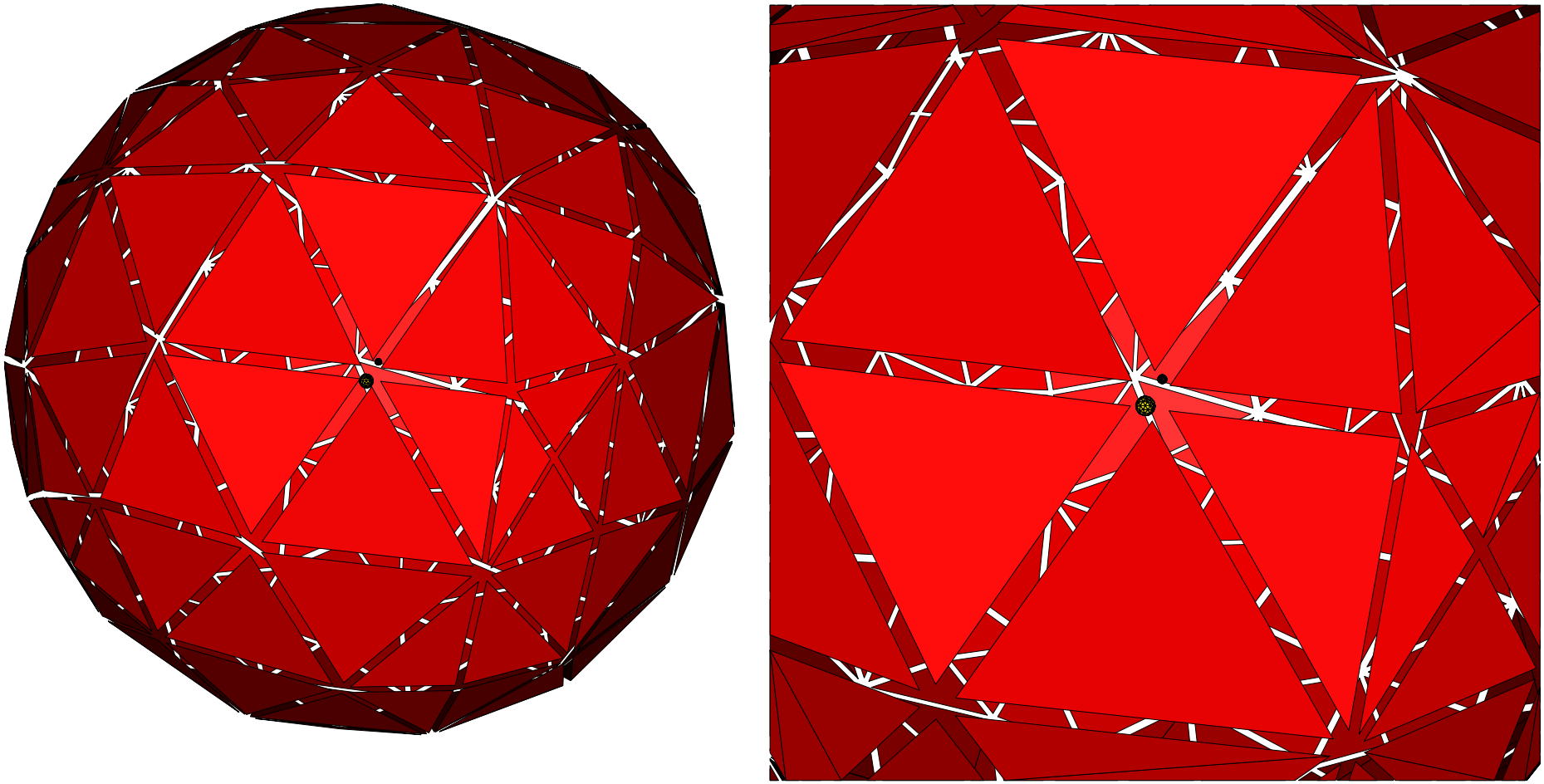
Rhibosome example (Ph.D. work of N. Baker)



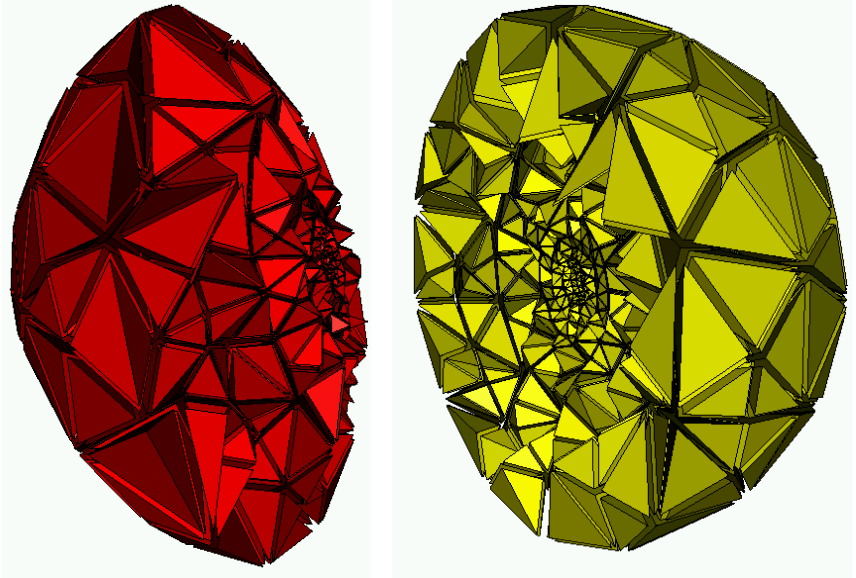
Microtubule example (Ph.D. work of N. Baker)



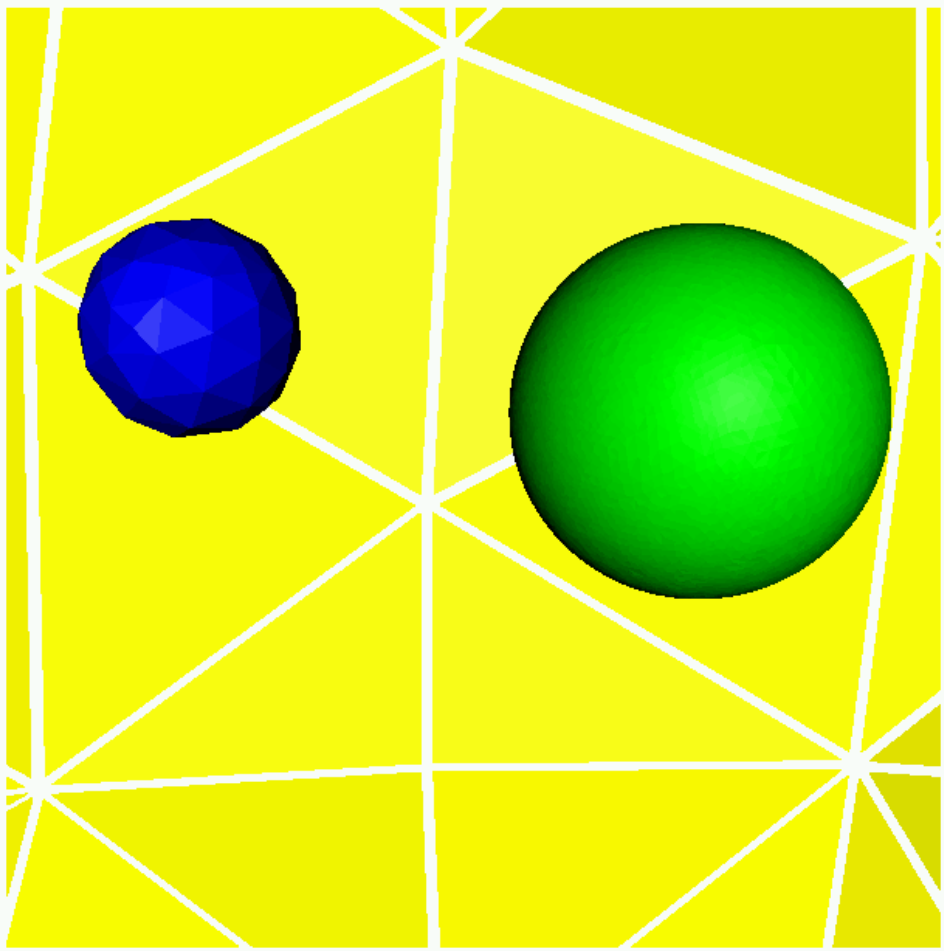
Parallel solution algorithm example.

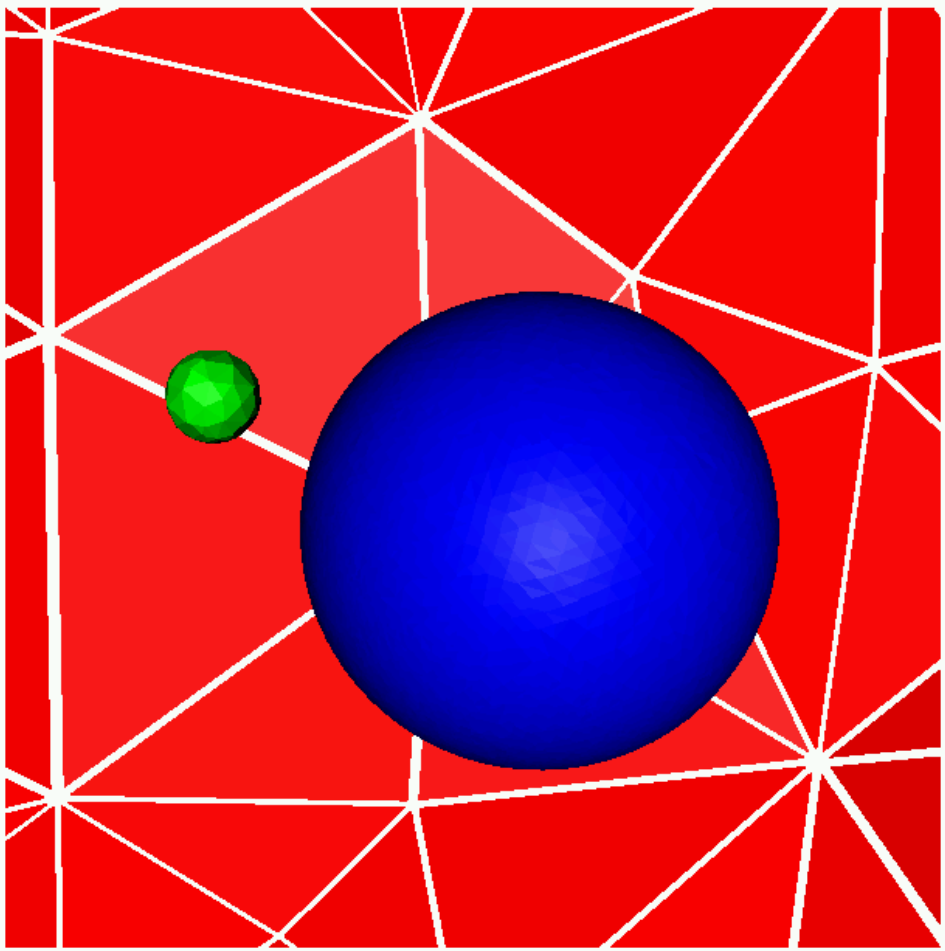


Spectrally partitioned coarse mesh.

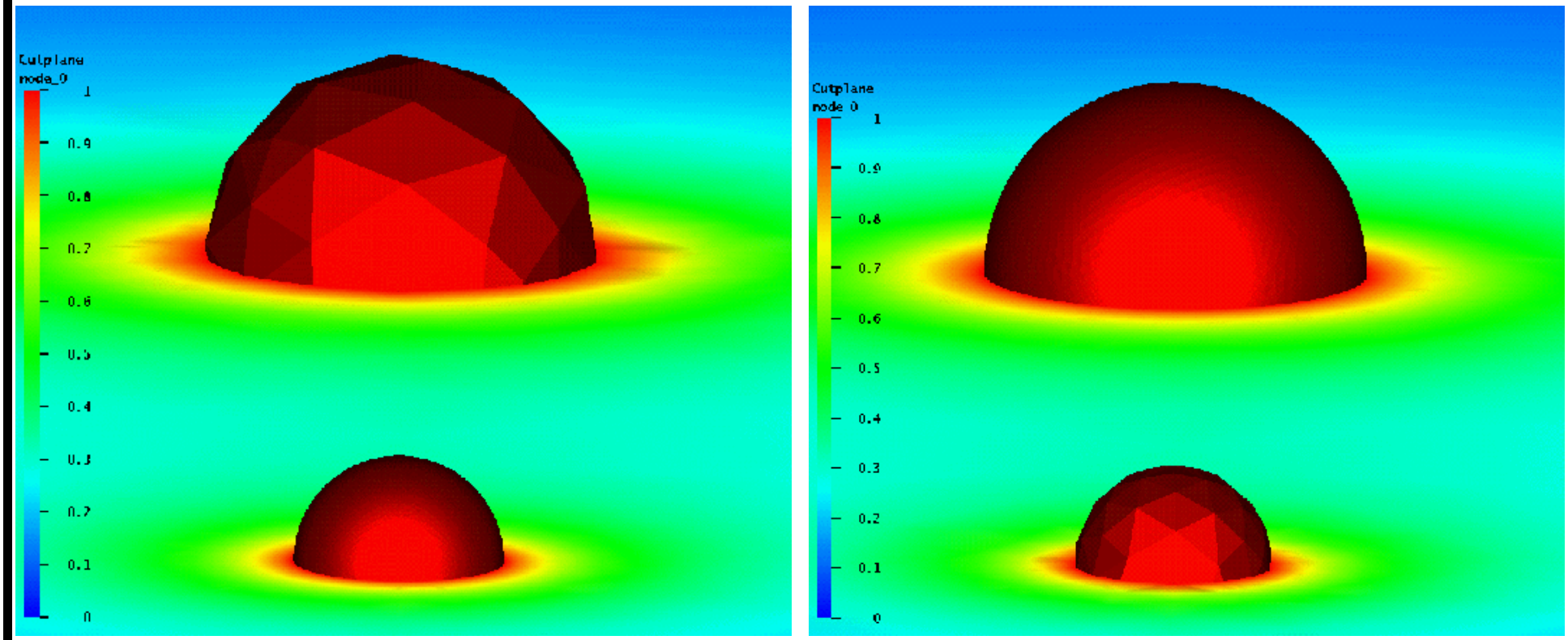


Subdomain adaptivity around the interior domain holes.

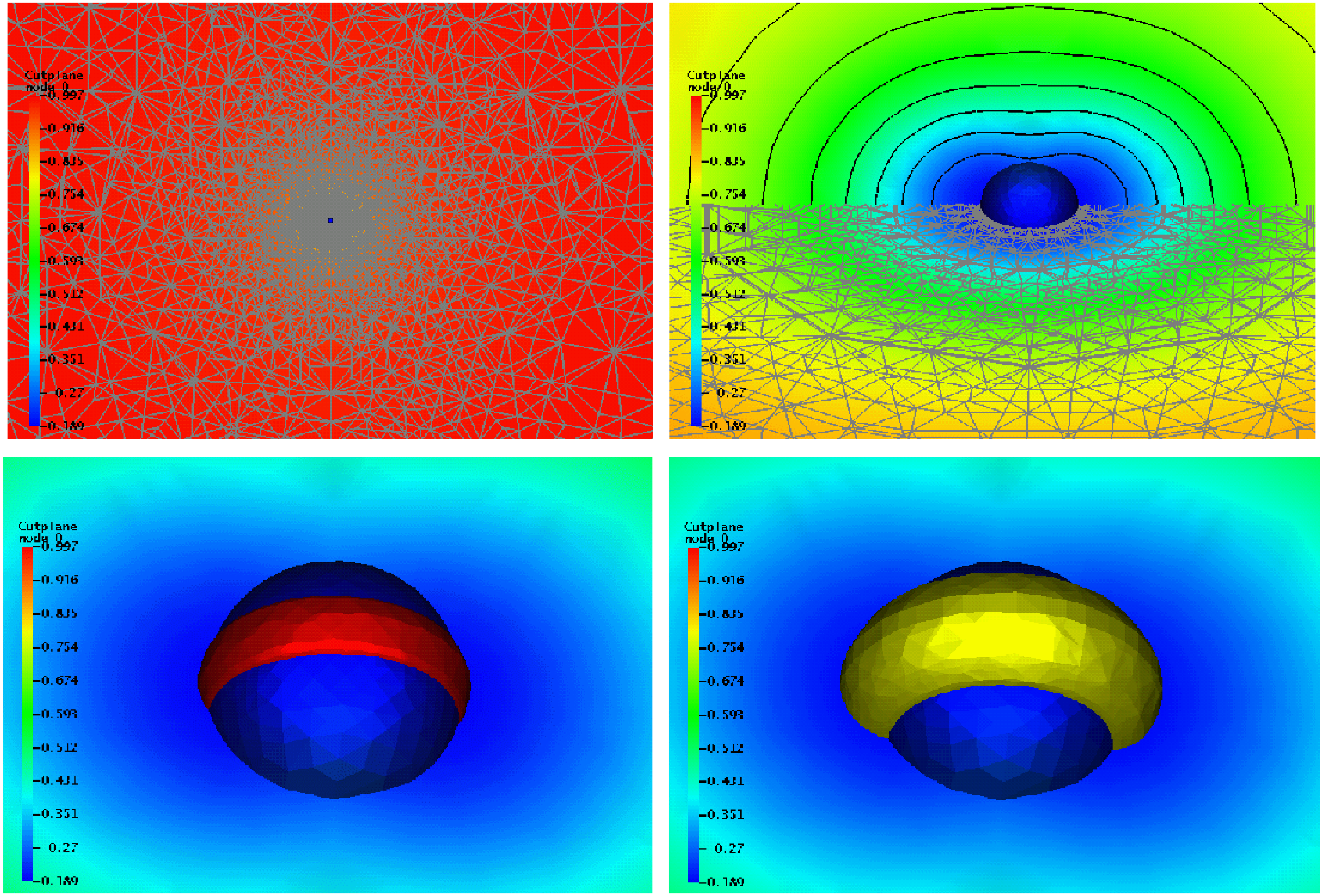




The two subdomain solutions.



A more complex example: some isosurfaces.



Relevant Manuscripts and Collaborators.

- Error estimates and adaptive methods for PDE.

[H1] MH, *Adaptive numerical treatment of elliptic systems on manifolds*. Advances in Computational Mathematics, 15 (2001), pp. 139–191.

[H2] MH, *Applications of domain decomposition and partition of unity methods in physics and geometry*. Plenary paper, Proc. of 14th Int. Conf. on Domain Decomp., January 2002, Mexico.

[BH] R. Bank and MH, *A new paradigm for parallel adaptive methods*. SIAM Review, 45 (2003), pp. 291-323.

[EHL] D. Estep, MH, and M. Larson, *Generalized Green's Functions and the Effective Domain of Influence*. SIAM J. Sci. Comput., Vol. 26, No. 4, 2005, pp. 1314-1339.

- Linear complexity methods for nonlinear approximation.

[AH] B. Aksoylu and MH, *Local refinement and multilevel preconditioning: Optimality of the BPX Preconditioner and Stabilizing hierarchical basis methods*. (Submitted to SIAM J. Numer. Anal.)

[ABH] B. Aksoylu, S. Bond, and MH, *Local refinement and multilevel preconditioning: Implementation and numerical experiments*. SIAM J. Sci. Comput., 25 (2003), pp. 478-498.

- Methods for PBE and other nonlinear PDE arising in biophysics.

[TB] K. Tai, S. Bond, H. MacMillan, N. Baker, M. Holst, and J. A. McCammon, *Finite element simulations of acetylcholine diffusion in neuromuscular junctions*, Biophys. J., 84 (2003), pp. 2234–2241.

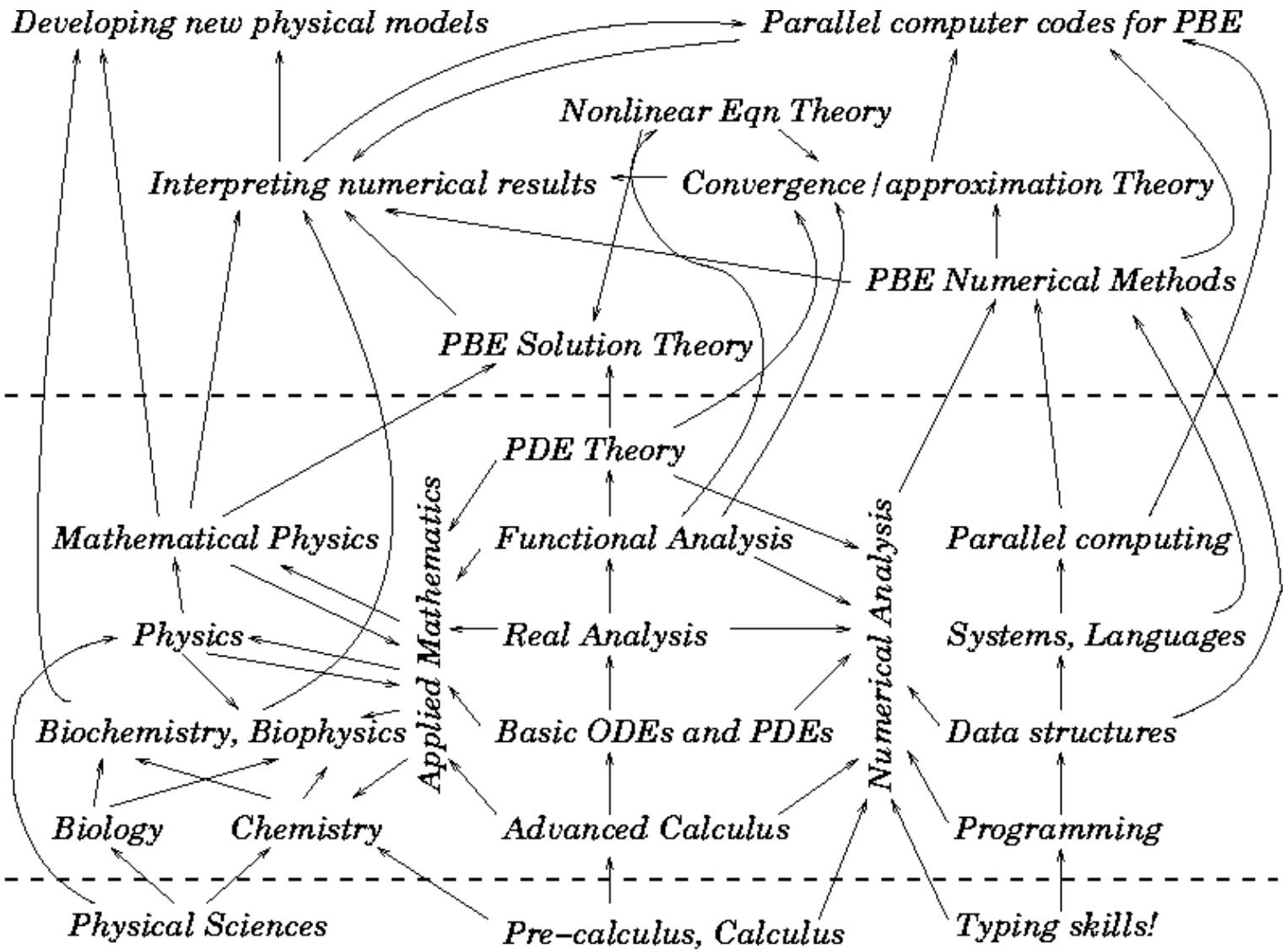
[BSJHM] N. Baker, D. Sept, S. Joseph, M. Holst, and J. A. McCammon, *Electrostatics of nanosystems: Application to microtubules and the ribosome*, Proc. Natl. Acad. Sci. USA, 98 (2001), pp. 10037–10041.

[HBW] M. Holst, N. Baker, and F. Wang, *Adaptive multilevel finite element solution of the Poisson-Boltzmann equation I: algorithms and examples*, J. Comput. Chem., 21 (2000), pp. 1319–1342.

[HX] M. Holst and J. Xu, *The Poisson-Boltzmann Equation: Approximation theory, regularization by singular functions, and adaptive techniques*. In preparation.

[HL] M. Holst and B. Li, *Boundary-value problems of the Poisson-Boltzmann equation*. In preparation.

The CAM path to working on biophysics problems.



Concluding remarks.

- Computational mathematics has become one of the most important tools available to researchers in biophysics.
- An amazingly broad array of interdisciplinary skills is necessary to work effectively with computational mathematics, including skills in classical and modern applied mathematics.
- Journal articles describing our research can be downloaded from:

  `http://scicomp.ucsd.edu/~mholst/pubs/publications`

- Our software package *FEtk* can be downloaded from:

  `http://www.FEtk.ORG`

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NSF CAREER Award 9875856
UCSD's Center for Theoretical Biological Physics (NSF ITR 0225630)
NSF Award 0411723 (Numerical geometric PDE)
DOE Award DE-FG02-05ER25707 (Multiscale methods)
Caltech Physics and Caltech ACM