Stable Mesh Decimation

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1. Research Goals

There are three types of errors that accrue in solving PDEs numerically:

1. **Model error:** Formulation of the (weak) PDE problem to be solved.
2. **Discretization error:** Reduction of the smooth formulation to a discrete problem.
3. **Solver error:** Numerical solution of the linear system.

Solving PDEs on large meshes requires mesh decimation as a pre-processing step. Decimation is guided by a **real-valued cost function on mesh edges** as follows: edge values are computed, the lowest cost edge is collapsed, and the process is iterated as needed. **Current methods** select cost functions independent of the PDE to be solved:

select cost function→decimate input → define PDE problem → select solver → solve

A **stable mesh decimation pipeline** must select a cost function that minimizes both discretization error and numerical error for the specific PDE problem in question:

define PDE problem → select solver → select cost function→decimate input → solve

2. Methodology and Background

Large disparities in edge lengths (i.e. larger relative h values) cause worse stability estimates and thus greater discretization error. Large entries in the matrix of a linear system cause poor condition numbers and thus greater solver error. A stable decimation cost function should provide for **both small h values and small entries in the system matrix**.

The **Galerkin Finite Element Method** discretizes the solution space of the PDE:

$Lu = f$ on Ω (PDE problem) → $a(u,v) = (f,v)_{L^2}$, $\forall v \in V$ (Weak form of PDE) → $a(u,v) = (f,v)_{L^2}$, $\forall v \in V_h$ (Discretization) → **Ax = b** (Linear System)

Here, the entries of matrix **A** are a functional $a(\cdot,\cdot)$ on the basis functions of V_h. Hence, **decimation must also be guided by the geometry-sensitive components of the linear functional** $a(\cdot,\cdot)$.

Discrete Exterior Calculus methods discretize the operators of the PDE:

$Lu = f$ on Ω (PDE problem) → $\Delta \Rightarrow \delta d + d\delta$, etc. (Smooth operator form) → $d \Rightarrow \mathbb{D}$, etc. (Discretization) → **Ax = b** (Linear System)

In this case, the entries of matrix **A** depend heavily on the geometry-sensitive operators such as $*$ and δ and less on the topology sensitive operators such as d. Hence, **decimation must also be guided by the definition of the discrete operators**.

Poisson-Boltzmann Electrostatics

The linear Poisson-Boltzmann (PB) equations for electrostatics are:

$$\nabla^2\phi^{\text{int}}(r_p) = -\frac{1}{\epsilon_{\text{int}}}\sum_{k=1}^{N} q_k\delta(r_p - r_k), \quad p \in \Omega, \tag{1}$$

$$\nabla^2\phi^{\text{ext}}(r_p) = \kappa^2\phi^{\text{ext}}(r_p), \quad p \in \Omega, \tag{2}$$

A **mixed Galerkin finite element method** by Lu, Zhang, and McCammon [3] solves for surface potential $f = \phi^{\text{int}} = \phi^{\text{ext}}$ and the normal derivative $h = \partial\phi^{\text{ext}}/\partial n$:

$$\begin{pmatrix} \mathbb{B} & \mathbb{A} \\ \mathbb{D} & \mathbb{C} \end{pmatrix}\begin{pmatrix} f \\ h \end{pmatrix} = \begin{pmatrix} Q \\ 0 \end{pmatrix}$$

The four sub matrices $\mathbb{A}$, $\mathbb{B}$, $\mathbb{C}$ and $\mathbb{D}$ have entries of the form

$$\sum_t \int_{\text{mesh facet } t} \mathcal{I}\,dA \quad \text{where} \quad \mathcal{I} \in \left\{ G(x_i,x_j), \frac{\partial G(x_i,x_j)}{\partial n}, u(x_i,x_j), \frac{\partial u(x_i,x_j)}{\partial n} \right\}$$

The functions G and u are the Green functions for (1) and (2), respectively:

$$G(x_i,x_j) = \frac{1}{4\pi r_{ij}} \quad \text{and} \quad u(x_i,x_j) = \frac{\exp(-\kappa r_{ij})}{4\pi r_{ij}} \quad \text{where } r_{ij} = |x_i - x_j|$$

Hence, the **terms of the stiffness matrix decay like** $1/r_{ij}$ at worst. We **use the cost function** f_{pb} to avoid small r_{ij} values, i.e. to keep Gaussian quadrature points evenly spaced.

Generalized Born Electrostatics

The Generalized Born (GB) model of electrostatic solvation defines electrostatic solvation energy in terms of the pairwise interaction between atoms i and j:

$$G_{\text{pol}} = -\frac{\tau}{2}\sum_{i,j}\frac{q_i q_j}{[r_{ij}^2 + R_i R_j \exp(-r_{ij}^2/4R_iR_j)]^{1/2}} \quad \text{where} \quad \tau = \frac{1}{\epsilon_p} - \frac{1}{\epsilon_w}$$

ϵ_p, ϵ_w = solute and solvent dielectric constants, respectively
q_i, R_i = charge and effective Born radius of atom i, respectively
r_{ij} = distance between atom i and atom j

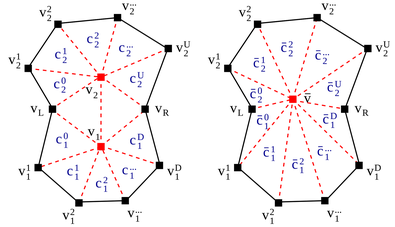
The success of a GB method hinges upon efficient and accurate approximation of the effective Born radii R_i. Bajaj and Zhao [2] use a surface integration technique to approximate

$$R_i^{-1} \approx \frac{1}{4\pi}\sum_{k=1}^{N} w_k \frac{(\mathbf{r}_k - \mathbf{x}_i)\cdot\mathbf{n}(\mathbf{r}_k)}{|\mathbf{r}_k - \mathbf{x}_i|^4} dS, \quad i = 1,\ldots,M$$

$\mathbf{r}_k$ = Gaussian quadrature nodes with weights w_k on a triangular mesh of surface Γ

Hence, the computation of R_i^{-1} is **sensitive to changes in** $|\mathbf{r} - \mathbf{x}_i|$, i.e. changes in the position of Gauss points relative to the nearest atomic centers. We **use the cost function** f_{gb} to minimize the cumulative change in $|\mathbf{r} - \mathbf{x}_i|$ values.

3. Problem-Specific Cost Functions



Notation for collapse of edge $(\mathbf{v}_1, \mathbf{v}_2)$ to $\bar{\mathbf{v}}$. Black vertices and edges are unchanged in the collapse while red vertices and dashed edges may change. The c_i denote circumcenters:

$$c_2^u := \frac{1}{3}\left(\mathbf{v}_2 + \mathbf{v}_2^u + \mathbf{v}_2^{u+1}\right), \quad u = 0,1,\ldots,U$$

$$c_1^d := \frac{1}{3}\left(\mathbf{v}_1 + \mathbf{v}_1^d + \mathbf{v}_1^{d+1}\right), \quad d = 0,1,\ldots,D$$

Cost Function for PB: $f_{pb}(\mathbf{v}_1,\mathbf{v}_2;\bar{\mathbf{v}}) := \sum_i q(T_{\bar{c}_i}) - q(T_{c_i})$

- f_{pb} is larger for edge collapses which bring Gaussian quadrature points closer together.
- $q(T)$ = quality(triangle T) := $\frac{\text{longest side of } T}{\text{shortest side of } T} + \frac{\text{maximum angle of } T}{\text{minimum angle of } T}$

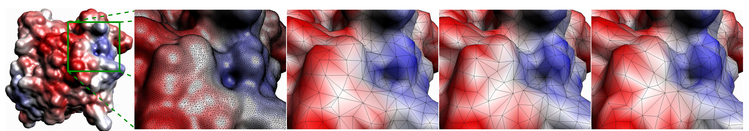
smaller discr. error [1] larger numerical error

larger discr. error smaller numerical error

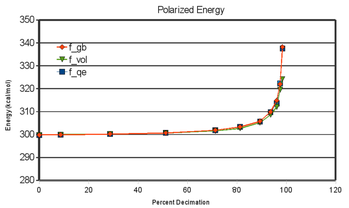
Cost Function for GB: $f_{gb}(\mathbf{v}_1,\mathbf{v}_2;\bar{\mathbf{v}}) := f_{geom}(\mathbf{v}_1,\mathbf{v}_2;\bar{\mathbf{v}}) + \lambda\left|\sum_{i,j}|c_i - x_j|^2 - |\bar{c}_i - x_j|^2\right|$

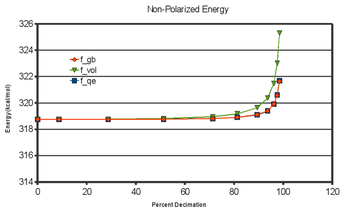
- f_{gb} is larger for edge collapses with a larger cumulative change in $|c_i - x_j|$ values.
- f_{geom} is any geometric error measure, such as $|\mathbf{v}_1 - \mathbf{v}_2|$ or a quadratic error measure.
- $\{x_j\}$ is the set of atomic centers lying within a fixed distance ρ (usually 2 - 5 Å) of $\mathbf{v}_1$ or $\mathbf{v}_2$.

4. Experimental Results



mAChE molecule | before decimation | 98.45% f_{qe} decimation | 98.45% f_{vol} decimation | 98.45% f_{gb} decimation





References

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