Applications of the Hodge Decomposition to Biological Structure and Function Modeling

Preliminary Report

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joint work with

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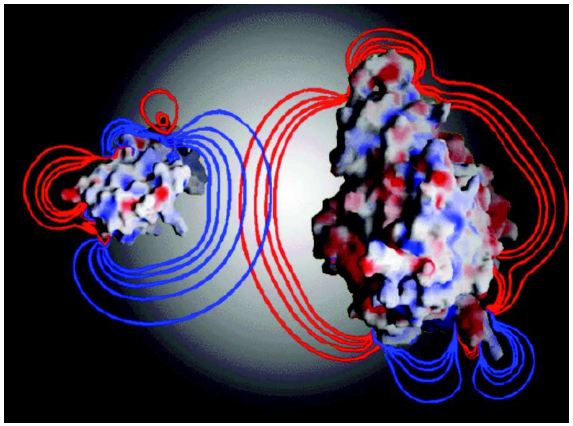
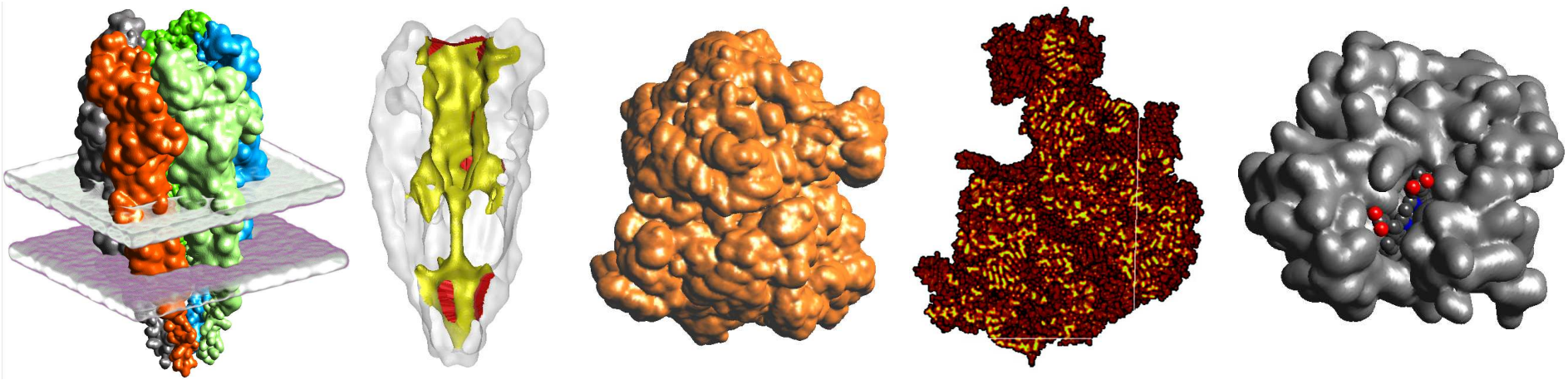
Introduction



- Molecular dynamics are governed by electrostatic forces of attraction and repulsion.
- These forces are described as the solutions of a PDE over the molecular surfaces.
- Molecular surfaces may have complicated topological features affecting the solution.



The Hodge Decomposition relates topological properties of the surface to solution spaces of PDEs over the surface.

The Hodge Decomposition for Vector Fields

Given a sufficiently smooth vector field $\eta : \mathbb{R}^3 \rightarrow \mathbb{R} \times \mathbb{R} \times \mathbb{R}$, there exists

- a unique scalar potential field $u : \mathbb{R}^3 \rightarrow \mathbb{R}$
- a unique vector potential field $v : \mathbb{R}^3 \rightarrow \mathbb{R} \times \mathbb{R} \times \mathbb{R}$
- a unique harmonic vector field $h : \mathbb{R}^3 \rightarrow \mathbb{R} \times \mathbb{R} \times \mathbb{R}$

such that:

$$\eta = \nabla u + \nabla \times v + h.$$

That is, η decomposes into a curl-free component ∇u, a divergence-free component $\nabla \times v$ and a harmonic component h which satisfies $\Delta h = 0$.

Associated Problems for Molecular Electromagnetics

- Determine if the electric or magnetic forces are more dominant in the interaction forces between solvated molecules.
- For a particular model of molecular interaction, characterize individual terms as curl-free, divergence-free, harmonic, or a combination.
- Provide stable vector finite elements (both linear and higher order) appropriate for these calculations.

Outline

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Selected Prior Work 1

POLTHIER AND PREUSS *Identifying vector fields singularities using a discrete hodge decomposition* Proc. of Vis. Math. III, 2003
TONG, LOMBEYDA, HIRANI AND M. DESBRUN *Discrete multiscale vector field decomposition* ACM Trans. Graph., 22(3), 2003.

- Detect and classify singularities of 2D (former) and 3D (latter) vector fields by minimizing certain functionals.
- For 2D, the potential u of the curl-free component minimizes

$$F(u) := \int_{M_h} \left(|\nabla u|^2 - 2 < \nabla u, \xi > \right)$$

while the potential v of the div-free component minimizes

$$G(v) := \int_{M_h} (|\delta(v\omega)|^2 - 2 < \delta(v\omega), \xi >)$$

where M_h is a simplicial surface. The harmonic component is the remainder

$$v := \xi - \nabla u - J\nabla v$$

where J is an operator which rotates each vector by $\pi/2$ on M_h.

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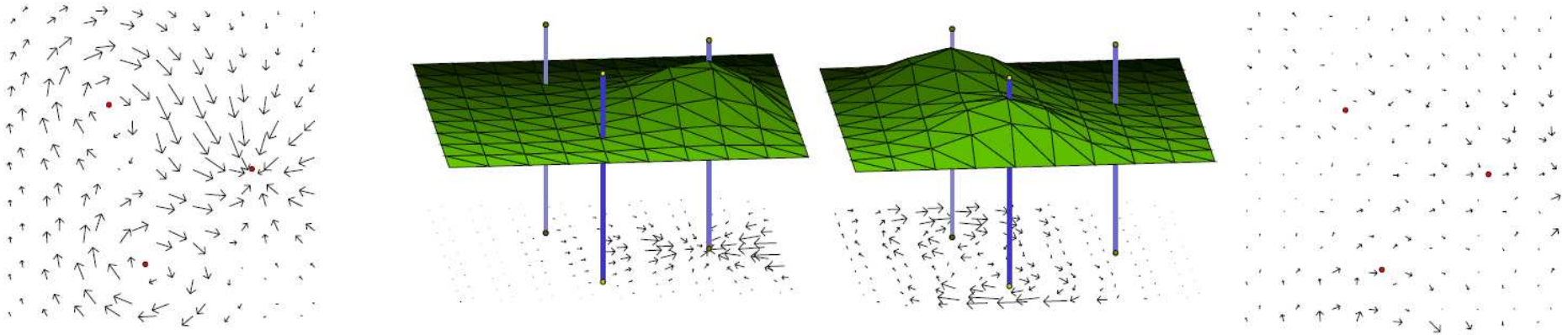
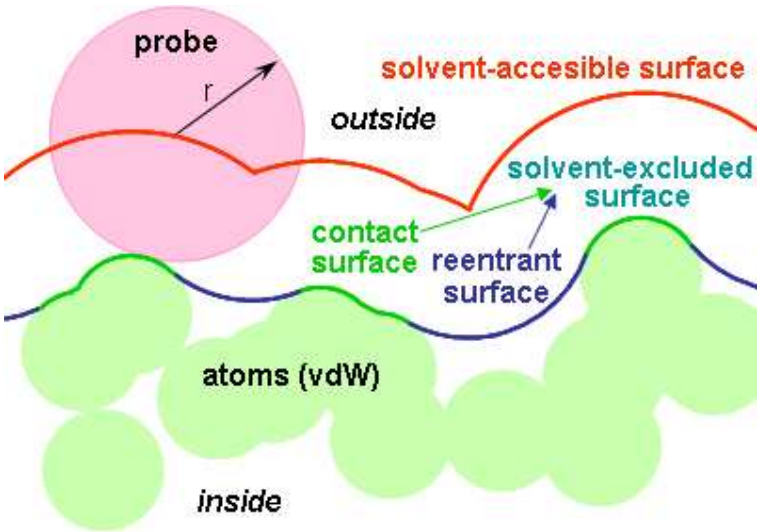


- Arguably more robust than Jacobian-based methods of singularity detection since there is no need to approximate partial derivatives.
- Requires solving a global linear system which may be unfeasible for the large data sets encountered in the biological domain.

Selected Prior Work 2

GILSON ET AL. *Computation of Electrostatic Forces on Solvated Molecules Using the P-B Equation* J. Phys. Chem. 97, 3591-3600, 1993.
LU, CHENG, HOU, MCCAMMON *Calculation of the Maxwell Stress Tensor and the P-B Force one a Solvated Molecular Surface Using Hypersingular Boundary Integrals* J. Chem. Phys. 123, 1-8, 2005.

- Describe three terms constituting the net force on a molecule:



1. Force due to free charge within the electrical field
2. Force due to dielectric jump at the molecular boundary
3. Force due to ion-exclusion at solvent accessible surface.

Selected Prior Work 2

GILSON ET AL. *Computation of Electrostatic Forces on Solvated Molecules Using the P-B Equation* J. Phys. Chem. 97, 3591-3600, 1993.
LU, CHENG, HOU, MCCAMMON *Calculation of the Maxwell Stress Tensor and the P-B Force one a Solvated Molecular Surface Using Hypersingular Boundary Integrals* J. Chem. Phys. 123, 1-8, 2005. Approach:

- The electric potential is computed at a finite collection of points on the molecular surface.
- These points are meshed with triangles so that the potential or normal derivative of the potential (force) can be linearly interpolated.
- Due to a jump in the dielectric coefficient across a molecular boundary, computing the normal derivative at a point p requires resolving an integral over the triangle with a singularity at point p.
- The final force calculations by this method depend on whether the point p is taken to be in the interior of the associated triangle or at one of its nodes.

Conclusion: The type of interpolation (in this case linear) and choice of finite element (Lagrange, Hermite, or other) affects the force fields computed by this method.

Relation to the Hodge Decomposition

How does the type of interpolation relate to the Hodge Decomposition?

To answer this question, we examine the Hodge Decomposition in the context of differential forms and the ability of discrete methods to replicate the result.

Outline

Smooth Differential Forms

Let Ω denote a smooth n-manifold and $T_x(\Omega)$ the tangent space of Ω at x. A **k-form** ω is a mapping from Ω to the space of alternating k-tensors on the tangent space of Ω at the input point:

$$\omega : \Omega \rightarrow \Lambda^k[T_x(\Omega)^*], \qquad \omega(x) : \bigoplus_{i=1}^{k} T_x(\Omega) \rightarrow \mathbb{R},$$

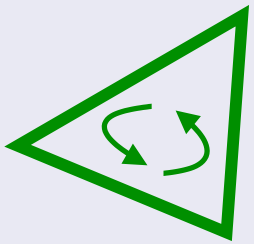
where $\omega(x)$ is an alternating k-tensor. The space of k-forms is denoted $\Lambda^k(\Omega)$.

Alternate Characterization of k-forms

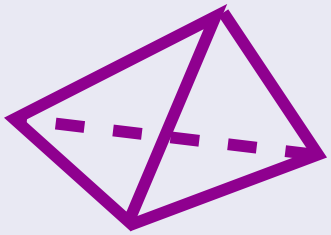
A k-form represents an intrinsically k-dimensional phenomena and can be integrated over a k-dimensional region.

electric potential is point−valued

electric fields are valued based on a linear current flow



magnetic fields are are dual to electric fields and valued on planes



charge density is valued over a volume

Discrete Differential Forms

- *k-forms are meant to be integrated over k dimensional regions*

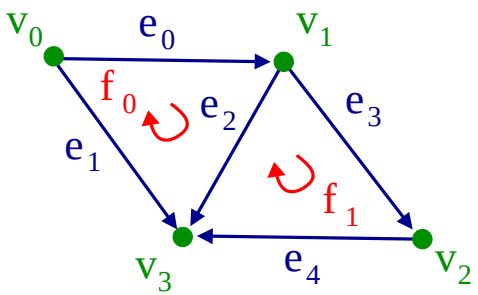
Let $\mathfrak{T}$ be a triangulation of a smooth compact n-manifold Ω. Let $\mathfrak{T}_k$ denote the k-simplicies of $\mathfrak{T}$. A k-**chain** c is a linear combination of the elements of $\mathfrak{T}_k$:

$$c = \sum_{\tau \in \mathfrak{T}_k} c_\tau \tau, \quad c_\tau \in \mathbb{R}$$

The set of all such chains form the **vector space of** k**-chains** is denoted $\mathcal{C}_k$.
A k-**cochain** ω is a linear map

$$\omega : \mathcal{C}_k \to \mathbb{R}$$

The vector space of k-cochains is denoted $\mathcal{C}^k$.



Cochains are the discrete analogues of differential forms.

The Exterior Derivative Operator

The **exterior derivative** is an operator on smooth forms which *increases* form degree:

$$d : \Lambda^k(\Omega) \to \Lambda^{k+1}(\Omega)$$

It generalizes the familiar operators grad, curl, and div for $\Omega = \mathbb{R}^3$:

$$0 \longrightarrow \Lambda^0(\Omega) \xrightarrow[\text{grad}]{d} \Lambda^1(\Omega) \xrightarrow[\text{curl}]{d} \Lambda^2(\Omega) \xrightarrow[\text{div}]{d} \Lambda^3(\Omega) \longrightarrow 0$$

Example: Given $f \in \Lambda^0(\mathbb{R}^3)$, we have $f : \mathbb{R}^3 \to \mathbb{R}$. Accordingly:

$$\text{grad } f := \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right) = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz =: df$$

Stokes' Theorem

Given a compact, oriented n-dimensional manifold Ω with boundary $\partial\Omega$ and a smooth $(n-1)$ form ω on Ω, the following equality holds:

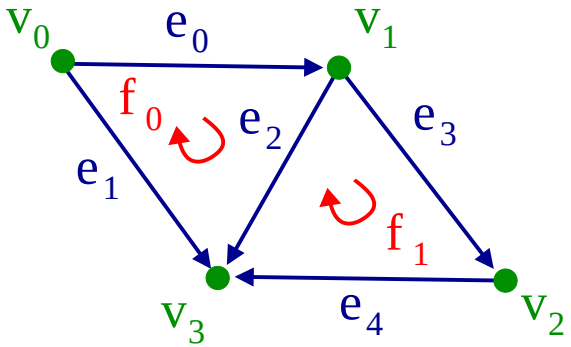
$$\int_{\partial\Omega} \omega = \int_{\Omega} d\omega$$

Discrete Exterior Derivative

- $d : \Lambda^k \rightarrow \Lambda^{k+1}$ *is characterized by Stokes' theorem*

The k**th discrete exterior derivative** is the transpose of the $(k+1)$st boundary operator: $\mathbb{D}_k = \partial_{k+1}^T$

Example: Let ω be the 1-cochain $\omega(e_i) := i$.

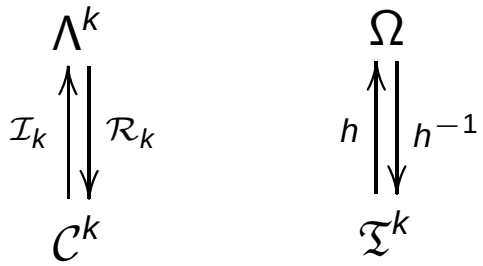


$$\mathbb{D}_1\omega = \begin{bmatrix} 1 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 1 \\ 5 \end{bmatrix}$$

$$\int_{e_0-e_1+e_3+e_4} \omega = \begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}^T \begin{bmatrix} 1 \\ -1 \\ 0 \\ 1 \\ 1 \end{bmatrix} = -1+3+4 = 1+5 = \begin{bmatrix} 1 \\ 5 \end{bmatrix}^T \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \int_{f_0+f_1} \mathbb{D}_1\omega$$

Maps Between Smooth and Discrete Forms

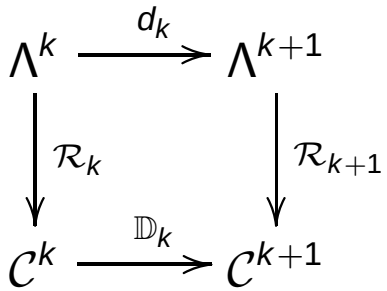
To pass our theory between smooth and discrete settings, we will need maps:



The k**th deRham map** $\mathcal{R}_k : \Lambda^k \to \mathcal{C}^k$ is defined as follows. Let $\mathfrak{T}$ be a triangulation of Ω with $h : \mathfrak{T} \to \Omega$ a homeomorphism. Given $\omega \in \Lambda^k$ and $c \in \mathcal{C}_k$ a chain, define

$$(\mathcal{R}_k \omega)(c) := \int_{h(c)} \omega$$

The map $\mathcal{R}$ satisfies $\mathcal{R}d = \mathbb{D}\mathcal{R}$, i.e. the following is a commutative diagram:



Maps Between Smooth and Discrete Forms

The map $\mathcal{I}_k : \mathcal{C}^k \to \Lambda^k$ is called an interpolation map and has no canonical choice since $\mathcal{R}$ is not invertible. We can require, however, that $\mathcal{I}_k$ be chosen such that:

- $\mathcal{R}\mathcal{I} = \mathrm{id}$ (consistency)
- $\mathcal{I}\mathcal{R} = \mathrm{id} + O(h^s)$ (approximation)

where $h \in \mathbb{R}_{>0}$ is the partition size of the mesh and $s \in \mathbb{R}_{>0}$ is the approximation order ($s = 1$ for linear, $s = 2$ for quadratic, etc.).

This approximation error can be incorporated into the discretization of forms in distinct ways, based on whether one defines the discrete inner product or discrete Hodge star first.

Outline

Force Expressions - PBE

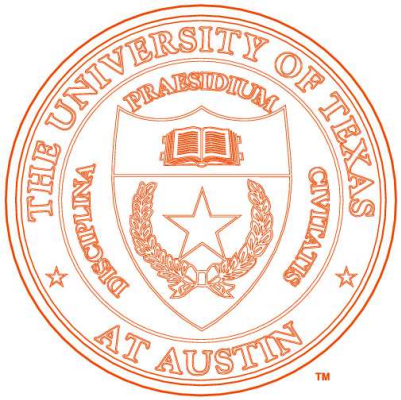
The force density f for the Poisson-Boltzmann equation is

$$\underbrace{\rho^f E}_{1} - \underbrace{\frac{1}{2}E^2\nabla\epsilon}_{2} - \underbrace{kT\sum_{i}^{N}[(\exp(-q_i\phi/kT)-1)c_i]\nabla\lambda}_{3}$$

1. Interaction forces of fixed changes with electric field.
2. Forces acting at boundaries between different electric media. These forces are always normal to the molecular boundary.
3. Forces acting at the ion-exclusion boundary, the region where mobile solvent ions cannot penetrate. These forces are always normal to the ion-exclusion boundary.

ρ^f	$=$	fixed charge density	N	$=$	number of ionic species
E	$=$	electrostatic field vector	q_i	$=$	charge of ith ionic species
ϵ	$=$	permittivity w.r.t. position	c_i	$=$	concentration of ith ionic species
k	$=$	Boltzmann's constant	ϕ	$=$	electrostatic potential w.r.t. position
T	$=$	absolute temperature	λ	$=$	0 inside ion boundary, 1 otherwise

Acknowledgements



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- This talk was presented at the 2009 AMS-MAA Joint Mathematics Meetings in Washington DC.

- A copy of these slides is available at

http : //www.math.utexas.edu/users/agillette/