What’s relevant in molecular modeling?

Cross-Section of an Animal Cell

(bottom image: David Goodsell)
What's relevant in neuronal modeling?

(right image: Chandrajit Bajaj)
What’s relevant in diffusion modeling?
Mathematics helps answer distinguish relevant and irrelevant features of a model:

- Does the PDE have a unique solution, bounded in some norm?
- Does the domain discretization affect the quality of the approximate solution?
- Is the solution method optimally efficient? (e.g. Why isn’t my code working?)

Focus of my research in these areas: the **Finite Element Method**
1. Introduction to the Finite Element Method
2. Tensor product finite element methods
3. The minimal approximation question
4. Serendipity finite element methods
5. RTG Project Ideas
Outline

1. Introduction to the Finite Element Method
2. Tensor product finite element methods
3. The minimal approximation question
4. Serendipity finite element methods
5. RTG Project Ideas
The finite element method is a way to numerically approximate the solution to PDEs.

(Example worked out on board)

**Ex:** The 1D Laplace equation: find $u(x) \in U \ (\dim U = \infty)$ s.t.

$$
\begin{cases}
-u''(x) = f(x) & \text{on } [a, b] \\
u(a) = 0, \\
u(b) = 0
\end{cases}
$$

Weak form: find $u(x) \in U \ (\dim U = \infty)$ s.t.

$$
\int_a^b u'(x)v'(x) \, dx = \int_a^b f(x)v(x) \, dx, \quad \forall v \in V \ (\dim V = \infty)
$$

Discrete form: find $u_h(x) \in U_h \ (\dim U_h < \infty)$ s.t.

$$
\int_a^b u'_h(x)v'_h(x) \, dx = \int_a^b f(x)v_h(x) \, dx, \quad \forall v_h \in V_h \ (\dim V_h < \infty)
$$
The Finite Element Method: 1D

(Example worked out on board)

Suppose $u_h(x)$ can be written as linear combination of $V_h$ elements:

$$u_h(x) = \sum_{v_i \in V_h} u_i v_i(x)$$

The discrete form becomes: find coefficients $u_i \in \mathbb{R}$ such that

$$\sum_i \int_a^b u_i v_i'(x) v_j'(x) \, dx = \int_a^b f(x) v_j(x) \, dx, \quad \forall v_h \in V_h \quad (\text{dim } V_h < \infty)$$

Written as a linear system:

$$[A]_{ji} [u]_i = [f]_j, \quad \forall v_j \in V_h$$

With some functional analysis we can prove: $\exists C > 0$, independent of $h$, s.t.

$$\|u - u_h\|_{H^1(\Omega)} \leq C h |u|_{H^2(\Omega)}, \quad \forall u \in H^2(\Omega)$$

holds for any $u$ with bounded 2nd derivs.

where $h =$ maximum width of elements use in discretization.
Outline

1. Introduction to the Finite Element Method
2. Tensor product finite element methods
3. The minimal approximation question
4. Serendipity finite element methods
5. RTG Project Ideas
**Goal:** Efficient, accurate approximation of the solution to a PDE over $\Omega \subset \mathbb{R}^n$ for arbitrary dimension $n$ and arbitrary rate of convergence $r$.

Standard $O(h^r)$ tensor product finite element method in $\mathbb{R}^n$:

- Mesh $\Omega$ by $n$-dimensional cubes of side length $h$.
- Set up a linear system involving $(r + 1)^n$ degrees of freedom (DoFs) per cube.
- For unknown continuous solution $u$ and computed discrete approximation $u_h$:

\[
\|u - u_h\|_{H^1(\Omega)} \leq Ch^r |u|_{H^{r+1}(\Omega)}, \quad \forall u \in H^{r+1}(\Omega).
\]

Approximation error \(\|u - u_h\|_{H^1(\Omega)}\) \(\leq\) Optimal error bound \(|u|_{H^{r+1}(\Omega)}\) for all $u \in H^{r+1}(\Omega)$.

Implementation requires a clear characterization of the isomorphisms:

\[
\begin{align*}
\{ x^r y^s \mid 0 \leq r, s \leq 3 \} & \longleftrightarrow \{ \psi_i(x) \psi_j(y) \mid 1 \leq i, j \leq 4 \} & \longleftrightarrow \{ \text{monomials} \} & \longleftrightarrow \{ \text{basis functions} \} & \longleftrightarrow \{ \text{domain points} \}
\end{align*}
\]
Cubic Hermite Geometric Decomposition (1D, \( r=3 \))

\[
\{1, x, x^2, x^3\} \quad \longleftrightarrow \quad \{\psi_1, \psi_2, \psi_3, \psi_4\} \quad \longleftrightarrow \quad \text{domain points}
\]

\[
\begin{bmatrix}
\psi_1 \\
\psi_2 \\
\psi_3 \\
\psi_4
\end{bmatrix} :=
\begin{bmatrix}
1 - 3x^2 + 2x^3 \\
x - 2x^2 + x^3 \\
x^2 - x^3 \\
3x^2 - 2x^3
\end{bmatrix}
\]

**Cubic Hermite Basis on \([0, 1]\)**

Approximation: \( x^r = \sum_{i=1}^{4} \varepsilon_{r,i} \psi_i \), for \( r = 0, 1, 2, 3 \), where \( [\varepsilon_{r,i}] = \begin{pmatrix}
1 & 0 & 0 & 1 \\
0 & 1 & -1 & 1 \\
0 & 0 & -2 & 1 \\
0 & 0 & -3 & 1
\end{pmatrix} \)

Geometry: If \( a(x) \) is a cubic polynomial then:

\[
a(x) = a(0) \psi_1 + a'(0) \psi_2 - a'(1) \psi_3 + a(1) \psi_4
\]
We can use our 1D Hermite functions to make 2D Hermite functions:

\[ \psi_1(x) \times \psi_1(y) = \psi_{11}(x, y) \]

\[ \psi_1(x) \times \psi_2(y) = \psi_{12}(x, y) \]
Cubic Hermite Geometric Decomposition (2D, \( r = 3 \))

\[
\begin{align*}
\{ & x^r y^s \\
\text{0} \leq r, s \leq 3 \} & \iff & \{ & \psi_i(x) \psi_j(y) \\
\text{1} \leq i, j \leq 4 \} & \iff & \text{domain points}
\end{align*}
\]

\text{monomials} \iff \text{basis functions} \iff \text{domain points}

**Approximation:**
\[
x^r y^s = \sum_{i=1}^{4} \sum_{j=1}^{4} \varepsilon_{r,i} \varepsilon_{s,j} \psi_{ij}, \text{ for } 0 \leq r, s \leq 3, \varepsilon_{r,i} \text{ as in 1D.}
\]

**Geometry:**

\[
a(x, y) = a\big|_{(0,0)} \psi_{11} + \partial_x a\big|_{(0,0)} \psi_{21} + \partial_y a\big|_{(0,0)} \psi_{12} + \partial_x \partial_y a\big|_{(0,0)} \psi_{22} + \cdots
\]

Andrew Gillette - U. Arizona

Finite Element Research Problems

RTG Talk - Jan 2014
Cubic Hermite Geometric Decomposition (3D, $r=3$)

\[
\begin{aligned}
\{ x^r y^s z^t & \quad 0 \leq r, s, t \leq 3 \} & \quad \leftrightarrow & \quad \psi_i(x)\psi_j(y)\psi_k(z) & \quad 1 \leq i, j, k \leq 4 \\
\end{aligned}
\]

monomials $\leftrightarrow$ basis functions $\leftrightarrow$ domain points

**Approximation:**
\[
x^r y^s z^t = \sum_{i=1}^{4} \sum_{j=1}^{4} \sum_{k=1}^{4} \varepsilon_{r,i}\varepsilon_{s,j}\varepsilon_{t,k} \psi_{ijk}, \quad \text{for } 0 \leq r, s, t \leq 3, \quad \varepsilon_{r,i} \text{ as in 1D.}
\]

**Geometry:** Contours of level sets of the basis functions:

\[
\begin{align*}
\psi_{111} & \quad \psi_{112} & \quad \psi_{212} & \quad \psi_{222}
\end{align*}
\]
### Tensor Product FEM Summary

<table>
<thead>
<tr>
<th>$O(h)$</th>
<th>$O(h^2)$</th>
<th>$O(h^3)$</th>
<th>$O(h^r)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>${ x^r y^s }$ ( r, s \leq 1 )</td>
<td>${ x^r y^s }$ ( r, s \leq 2 )</td>
<td>${ x^r y^s }$ ( r, s \leq 3 )</td>
<td>${ x^r y^s }$ ( r, s \leq r )</td>
</tr>
<tr>
<td>![Square]</td>
<td>![Square]</td>
<td>![Square]</td>
<td>![Square]</td>
</tr>
<tr>
<td>4</td>
<td>9</td>
<td>16</td>
<td>((r + 1)^2)</td>
</tr>
</tbody>
</table>

| $\{ x^r y^s z^t \}$ \( r, s, t \leq 1 \) | $\{ x^r y^s z^t \}$ \( r, s, t \leq 2 \) | $\{ x^r y^s z^t \}$ \( r, s, t \leq 3 \) | $\{ x^r y^s z^t \}$ \( r, s, t \leq r \) |
| ![Cube] | ![Cube] | ![Cube] | ![Cube] |
| 8        | 27         | 64         | \((r + 1)^3\) | ← a lot!
Outline

1. Introduction to the Finite Element Method
2. Tensor product finite element methods
3. The minimal approximation question
4. Serendipity finite element methods
5. RTG Project Ideas
How many functions are minimally needed?

For unknown continuous solution $u$ and computed discrete approximation $u_h$:

$$\|u - u_h\|_{H^1(\Omega)} \leq C h^r |u|_{H^{r+1}(\Omega)}, \quad \forall u \in H^{r+1}(\Omega).$$

The proof of the above estimate relies on two properties of finite elements:

**Continuity:** Adjacent elements agree on order $r$ polynomials their shared face

**Approximation:** Basis functions on each element span all degree $r$ monomials

\[ \{1, x, y, x^2, y^2, xy\} \quad \rightarrow \quad \{1, x, y, x^2, y^2, xy, x^2y, xy^2, x^2y^2\} \]

required for $O(h^2)$ approximation

standard polynomials in $O(h^2)$ tensor product method
Next time...

- Characterization of the ‘minimal’ approximation question for any order
- Intriguing mathematical difficulties and recent ‘serendipitous’ solutions
- Benefits of serendipity solutions to biological modeling
- Open research problems for an RTG study
Outline

1. Introduction to the Finite Element Method
2. Tensor product finite element methods
3. The minimal approximation question
4. Serendipity finite element methods
5. RTG Project Ideas
For $r \geq 4$ on squares:

$O(h^r)$ tensor product method: $r^2 + 2r + 1$ dots

$O(h^r)$ serendipity method: $\frac{1}{2}(r^2 + 3r + 6)$ dots

$$\|u - u_h\|_{H^1(\Omega)} \leq C h^r |u|_{H^{r+1}(\Omega)}, \quad \forall u \in H^{r+1}(\Omega).$$
Why $r + 1$ dots per edge?
Ensures continuity between adjacent elements.

Why interior dots only for $r \geq 4$?
Consider, e.g. $p(x, y) := (1 + x)(1 - x)(1 - y)(1 + y)$
Observe $p$ is a degree 4 polynomial but $p \equiv 0$ on $\partial([-1, 1]^2)$.

How can we recover tensor product-like structure . . .

. . . without a tensor product structure?
Mathematical Challenges More Precisely

Goal: Construct basis functions for serendipity elements satisfying the following:

- **Symmetry:** Accommodate interior degrees of freedom that grow according to triangular numbers on square-shaped elements.

- **Tensor product structure:** Write as linear combinations of standard tensor product functions.

- **Hierarchical:** Generalize to methods on $n$-cubes for any $n \geq 2$, allowing restrictions to lower-dimensional faces.
Which monomials do we need?

\( O(h^3) \) serendipity element:

- total degree at most cubic (req. for \( O(h^3) \) approximation)
- at most cubic in each variable (used in \( O(h^3) \) tensor product methods)

\[ \{1, x, y, x^2, y^2, xy, x^3, y^3, x^2y, xy^2, x^3y, xy^3, x^2y^2, x^3y^2, x^2y^3, x^3y^3\} \]

We need an intermediate set of 12 monomials!

The superlinear degree of a polynomial ignores linearly-appearing variables.

Example: \( \text{sldeg}(xy^3) = 3 \), even though \( \text{deg}(xy^3) = 4 \)

Definition: \( \text{sldeg}(x_1^{e_1} x_2^{e_2} \cdots x_n^{e_n}) := \left( \sum_{i=1}^{n} e_i \right) - \# \{ e_i : e_i = 1 \} \)

\[ \{1, x, y, x^2, y^2, xy, x^3, y^3, x^2y, xy^2, x^3y, xy^3, x^2y^2, x^3y^2, x^2y^3, x^3y^3\} \]

superlinear degree at most 3 \((\text{dim}=12)\)

**Superlinear polynomials form a lower set**

Given a monomial $x^\alpha := x_1^{\alpha_1} \cdots x_d^{\alpha_d}$, associate the multi-index of $d$ non-negative integers $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_d) \in \mathbb{N}_0^d$.

Define the superlinear norm of $\alpha$ as $|\alpha|_{sprlin} := \sum_{\substack{j=1 \\alpha_j \geq 2}}^{d} \alpha_j$, so that the superlinear multi indices are $S_r = \left\{ \alpha \in \mathbb{N}_0^d : |\alpha|_{sprlin} \leq r \right\}$.

Observe that $S_r$ has a partial ordering $\mu \leq \alpha$ means $\mu_i \leq \alpha_i$.

Thus $S_r$ is a lower set, meaning $\alpha \in S_r, \mu \leq \alpha \implies \mu \in S_r$.

We can thus apply the following recent result.

**Theorem (Dyn and Floater, 2013)**

Fix a lower set $L \subset \mathbb{N}_0^d$ and points $z_\alpha \in \mathbb{R}^d$ for all $\alpha \in L$. For any sufficiently smooth $d$-variate real function $f$, there is a unique polynomial $p \in \text{span}\{x^\alpha : \alpha \in L\}$ that interpolates $f$ at the points $z_\alpha$, with partial derivative interpolation for repeated $z_\alpha$ values.

By a judicious choice of the interpolation points $z_\alpha = (x_i, y_j)$, we recover the dimensionality associations of the degrees of freedom of serendipity elements.

The order 5 serendipity element, with degrees of freedom color-coded by dimensionality. The lower set $S_5$, with equivalent color coding. The lower set $S_5$, with domain points $z_\alpha$ reordered.
By collecting the re-ordered interpolation points \( z_\alpha = (x_i, y_j) \), at midpoints of the associated face, we recover the dimensionality associations of the degrees of freedom of serendipity elements.

The lower set \( S_5 \), with domain points \( z_\alpha \) reordered.

A symmetric reordering, with multiplicity. The associated interpolant recovers values at dots, three partial derivatives at edge midpoints, and two partial derivatives at the face midpoint.
**Symmetry:** Accommodate interior degrees of freedom that grow according to triangular numbers on square-shaped elements.
The Dyn-Floater interpolation scheme is expressed in terms of tensor product interpolation over ‘maximal blocks’ in the set using an inclusion-exclusion formula.

Put differently, the linear combination is the sum over all blocks within the lower set with coefficients determined as follows:

→ Place the coefficient calculator at the extremal block corner.
→ Add up all values appearing in the lower set.
→ The coefficient for the block is the value of the sum.

Hence: black dots → +1; white dots → -1; others → 0.
Thus, using our symmetric approach, each maximal block in the lower set becomes a standard tensor-product interpolant.
**Tensor product structure:** Write basis functions as linear combinations of standard tensor product functions.
**Hierarchical:** Generalize to methods on \( n \)-cubes for any \( n \geq 2 \), allowing restrictions to lower-dimensional faces.
3d coefficient computation

Lower sets for superlinear polynomials in 3 variables:

Decomposition into a linear combination of tensor product interpolants works the same as in 2D, using the 3D coefficient calculator at left. (Blue $\rightarrow +1$; Orange $\rightarrow -1$).

FLOATER, GILLETTE *Nodal basis functions for the serendipity family of finite elements*, in preparation.
What video game is shown on the right?
Outline

1. Introduction to the Finite Element Method
2. Tensor product finite element methods
3. The minimal approximation question
4. Serendipity finite element methods
5. RTG Project Ideas
Email me if you’d like a copy of the slides with the project ideas.