Research Problems in Finite Element Theory: Analysis, Geometry, and Application

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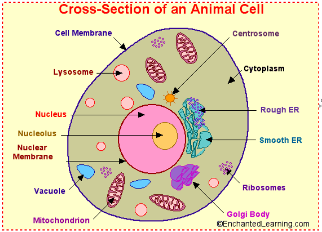
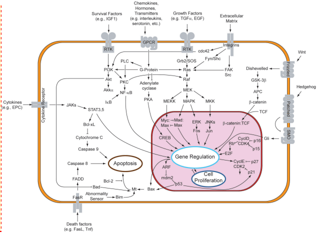
Research Tutorial Group Presentation

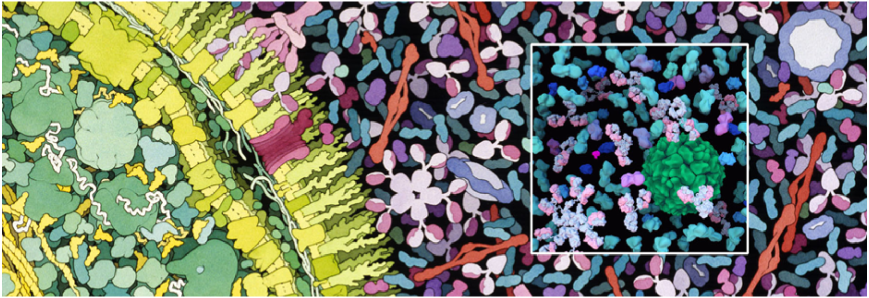
Slides and more info at:

http://math.arizona.edu/∼agillette/

What’s relevant in molecular modeling?

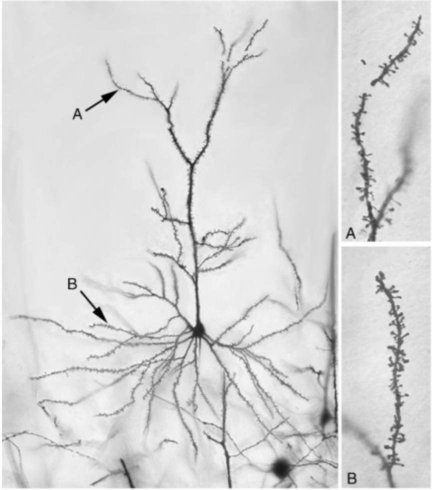


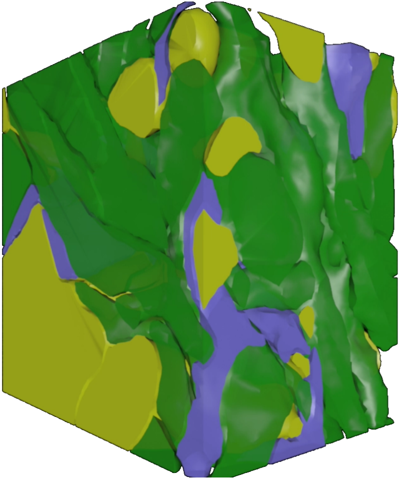




(bottom image: David Goodsell)

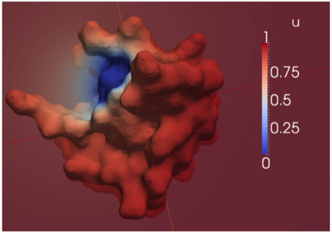
What’s relevant in neuronal modeling?

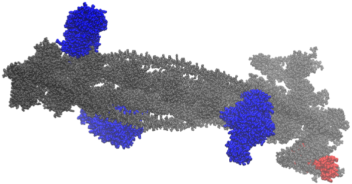


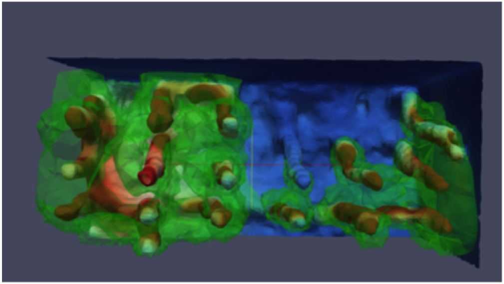


(right image: Chandrajit Bajaj)

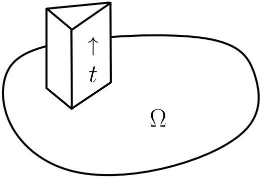
What's relevant in diffusion modeling?

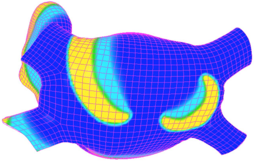






Mathematics used in biological models





$$\mathbb{A}\,\vec{\mathbf{x}} = \vec{\mathbf{b}}$$

Analysis

PDEs

Geometry

Topology

Combinatorics

Linear algebra

Numerical analysis

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**

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Outline

1. Introduction to the Finite Element Method
2. Tensor product finite element methods
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4. Serendipity finite element methods
5. RTG Project Ideas

The Finite Element Method: 1D

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.

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

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

$$\int_a^b u_h'(x)v_h'(x)\,dx = \int_a^b f(x)v_h(x)\,dx, \quad \forall v_h \in V_h \quad (\dim V_h < \infty)$$

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

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

Written as a linear system:

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

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

$$\underbrace{||u - u_h||_{H^1(\Omega)}}_{\substack{\text{error between cnts} \\ \text{and discrete solution}}} \quad \leq \quad \underbrace{C\, h\, |u|_{H^2(\Omega)}}_{\substack{\text{bound in terms of} \\ \text{2nd order osc. of } u}} \quad , \quad \underbrace{\forall u \in H^2(\Omega)}_{\substack{\text{holds for any } u \text{ with} \\ \text{bounded 2nd derivs.}}} \quad .$$

where h = maximum width of elements use in discretization.

Outline

Generalizing the 1st order, 1D method

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 $\mathbb{R}^n$:

$\rightarrow$ Mesh Ω by n-dimensional cubes of side length h.

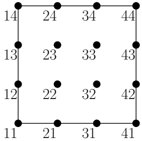
$\rightarrow$ Set up a linear system involving $(r+1)^n$ degrees of freedom (DoFs) per cube.

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

$$\underbrace{||u - u_h||_{H^1(\Omega)}}_{\text{approximation error}} \leq \underbrace{C\, h^r\, |u|_{H^{r+1}(\Omega)}}_{\text{optimal error bound}}, \qquad \forall u \in H^{r+1}(\Omega).$$

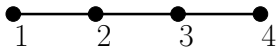
Implementation requires a clear characterization of the isomorphisms:

$$\left\{ \begin{array}{c} x^r y^s \\ 0 \leq r, s \leq 3 \end{array} \right\} \longleftrightarrow \left\{ \begin{array}{c} \psi_i(x)\psi_j(y) \\ 1 \leq i, j \leq 4 \end{array} \right\} \longleftrightarrow$$



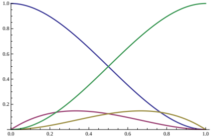
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

Cubic Hermite Geometric Decomposition (1D, r=3)

monomials	approxim.	basis functions	geometry	domain points
$\{1, x, x^2, x^3\}$	$\longleftrightarrow$	$\{\psi_1, \psi_2, \psi_3, \psi_4\}$	$\longleftrightarrow$	

Cubic Hermite Basis on $[0, 1]$

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



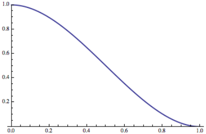
Approximation: $x^r = \sum_{i=1}^{4} \varepsilon_{r,i}\psi_i$, for $r = 0, 1, 2, 3$, where $[\varepsilon_{r,i}] = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 1 \\ 0 & 0 & -2 & 1 \\ 0 & 0 & -3 & 1 \end{pmatrix}$

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

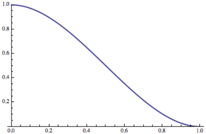
$$a(x) = \underbrace{a(0)}_{\text{value}}\psi_1 + \underbrace{a'(0)}_{\text{derivative}}\psi_2 - \underbrace{a'(1)}_{\text{derivative}}\psi_3 + \underbrace{a(1)}_{\text{value}}\psi_4$$

Tensor Product Polynomials

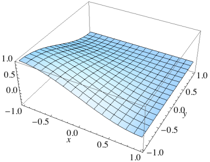
We can use our 1D Hermite functions to make 2D Hermite functions:



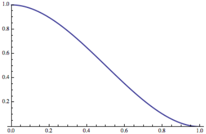
$\times$



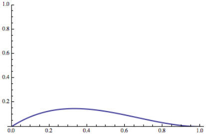
$=$



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



$\times$



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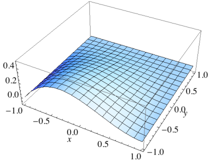
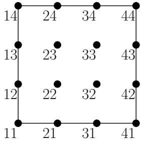


$$\psi_1(x) \times \psi_2(y) = \psi_{12}(x, y)$$

Cubic Hermite Geometric Decomposition (2D, r=3)

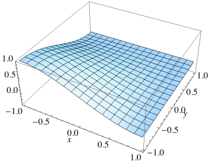
$$\left\{ \begin{array}{c} x^r y^s \\ 0 \le r, s \le 3 \end{array} \right\} \quad \longleftrightarrow \quad \left\{ \begin{array}{c} \psi_i(x)\psi_j(y) \\ 1 \le i, j \le 4 \end{array} \right\} \quad \longleftrightarrow$$



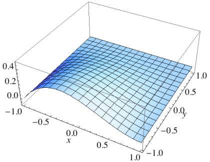
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

Approximation: $x^r y^s = \displaystyle\sum_{i=1}^{4} \sum_{j=1}^{4} \varepsilon_{r,i}\varepsilon_{s,j}\psi_{ij}$, for $0 \le r, s \le 3$, $\varepsilon_{r,i}$ as in 1D.

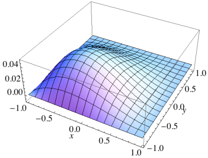
Geometry:



ψ_{11}



ψ_{21}

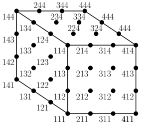


ψ_{22}

$$a(x,y) = \underbrace{a|_{(0,0)}}_{\text{value}} \psi_{11} + \underbrace{\partial_x a|_{(0,0)}}_{\text{1st deriv.}} \psi_{21} + \underbrace{\partial_y a|_{(0,0)}}_{\text{1st deriv.}} \psi_{12} + \underbrace{\partial_x \partial_y a|_{(0,0)}}_{\text{2nd deriv.}} \psi_{22} + \cdots$$

Cubic Hermite Geometric Decomposition (3D, r=3)

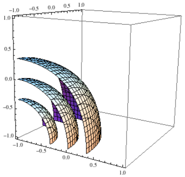
$$\left\{ \begin{array}{c} x^r y^s z^t \\ 0 \le r, s, t \le 3 \end{array} \right\} \longleftrightarrow \begin{array}{c} \psi_i(x)\psi_j(y)\psi_k(z) \\ 1 \le i, j, k \le 4 \end{array} \longleftrightarrow$$



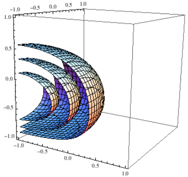
monomials $\longleftrightarrow$ **basis functions** $\longleftrightarrow$ **domain points**

Approximation: $x^r y^s z^t = \sum_{i=1}^{4} \sum_{j=1}^{4} \sum_{k=1}^{4} \varepsilon_{r,i}\varepsilon_{s,j}\varepsilon_{t,k}\psi_{ijk}$, for $0 \le r, s, t \le 3$, $\varepsilon_{r,i}$ as in 1D.

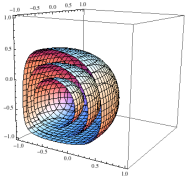
Geometry: Contours of level sets of the basis functions:



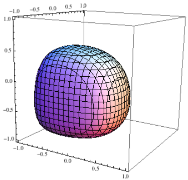
ψ_{111}



ψ_{112}

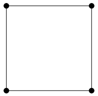
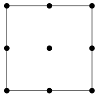
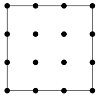
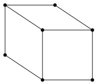
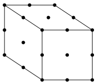
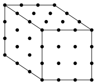


ψ_{212}



ψ_{222}

Tensor Product FEM Summary

$O(h)$	$O(h^2)$	$O(h^3)$	$O(h^r)$
$\left\{ \begin{array}{c} x^r y^s \\ r, s \leq 1 \end{array} \right\}$	$\left\{ \begin{array}{c} x^r y^s \\ r, s \leq 2 \end{array} \right\}$	$\left\{ \begin{array}{c} x^r y^s \\ r, s \leq 3 \end{array} \right\}$	$\left\{ \begin{array}{c} x^r y^s \\ r, s \leq r \end{array} \right\}$
			
4	9	16	$(r+1)^2$
$\left\{ \begin{array}{c} x^r y^s z^t \\ r, s, t \leq 1 \end{array} \right\}$	$\left\{ \begin{array}{c} x^r y^s z^t \\ r, s, t \leq 2 \end{array} \right\}$	$\left\{ \begin{array}{c} x^r y^s z^t \\ r, s, t \leq 3 \end{array} \right\}$	$\left\{ \begin{array}{c} x^r y^s z^t \\ r, s, t \leq r \end{array} \right\}$
			
8	27	64	$(r+1)^3$ $\leftarrow$ a lot!

Outline

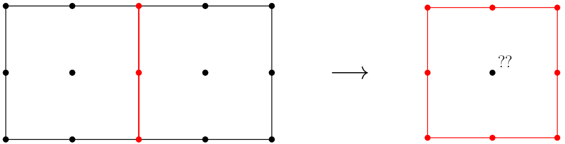
How many functions are *minimally* needed?

For unknown continuous solution u and computed discrete approximation u_h:

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

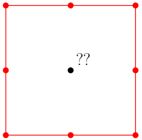
The proof of the above estimate relies on two properties of finite elements:

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



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

$$\underbrace{\{1, x, y, x^2, y^2, xy\}}_{\substack{\text{required for} \\ O(h^2)\text{ approximation}}} \longrightarrow$$



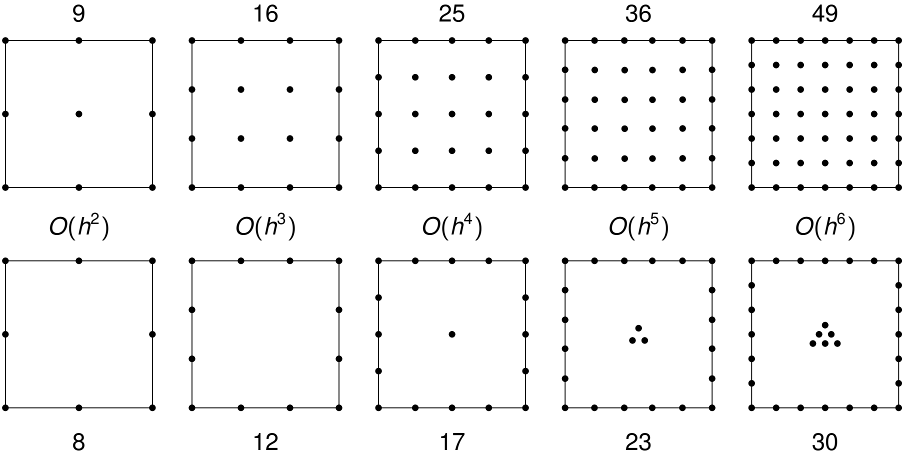
$$\longleftrightarrow \underbrace{\{1, x, y, x^2, y^2, xy, x^2y, xy^2, x^2y^2\}}_{\substack{\text{standard polynomials in} \\ O(h^2)\text{ tensor product method}}}$$

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

Serendipity Elements

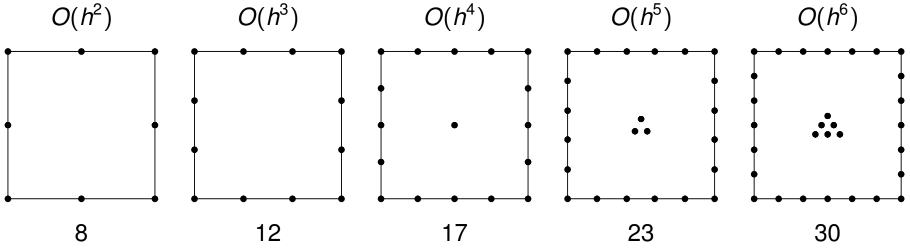


For $r \geq 4$ on squares:

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

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

Serendipity Elements

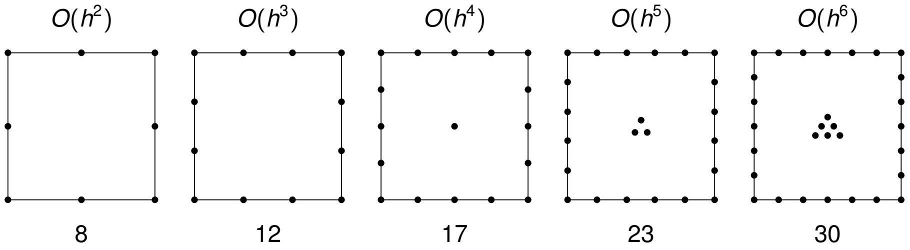


$\rightarrow$ Why $r + 1$ dots per edge?
Ensures continuity between adjacent elements.

$\rightarrow$ 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 $\partial([-1, 1]^2)$.

$\rightarrow$ How can we recover tensor product-like structure...
...without a tensor product structure?

Mathematical Challenges More Precisely

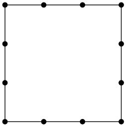


Goal: Construct basis functions for serendipity elements satisfying the following:

- **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:



$$\Big\{ \overbrace{1, x, y, x^2, y^2, xy, x^3, y^3, x^2y, xy^2}^{\substack{\text{total degree at most cubic} \\ \text{(req. for } O(h^3) \text{ approximation)}}}, x^3y, xy^3, x^2y^2, x^3y^2, x^2y^3, x^3y^3 \Big\}$$

$$\underbrace{\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad}_{\substack{\text{at most cubic in each variable} \\ \text{(used in } O(h^3) \text{ tensor product methods)}}}$$

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 $\deg(xy^3) = 4$

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

$$\Big\{ \underbrace{1, x, y, x^2, y^2, xy, x^3, y^3, x^2y, xy^2, x^3y, xy^3}_{\text{superlinear degree at most 3 (dim=12)}}, x^2y^2, x^3y^2, x^2y^3, x^3y^3 \Big\}$$

ARNOLD, AWANOU *The serendipity family of finite elements*, Found. Comp. Math, 2011.

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 α 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 $\boxed{\alpha \in S_r,\ \mu \leq \alpha \implies \mu \in S_r}$

We can thus apply the following recent result.

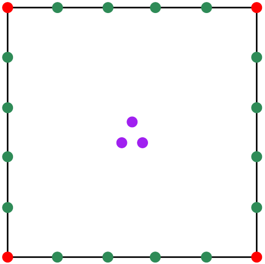
Theorem (Dyn and Floater, 2013)

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 $p \in \operatorname{span}\{x^\alpha : \alpha \in L\}$ that interpolates f at the points z_α, with partial derivative interpolation for repeated z_α values.

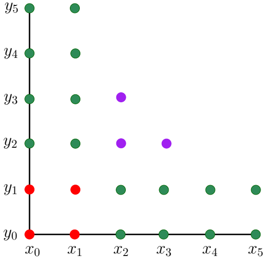
DYN AND FLOATER *Multivariate polynomial interpolation on lower sets*, J. Approx. Th., to appear.

Partitioning and reordering the multi-indices

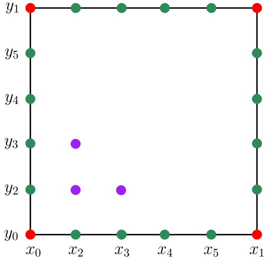
By a judicious choice of the interpolation points $z_\alpha = (x_i, y_j)$, we recover the dimensionality associations of the degrees of freedom of serendipity elements.



The order 5 serendipity element, with degrees of freedom color-coded by dimensionality.



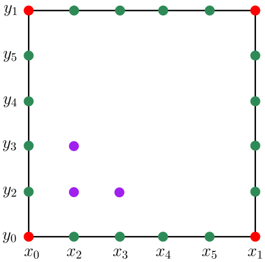
The lower set S_5, with equivalent color coding.



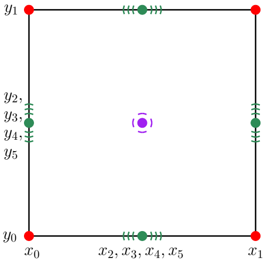
The lower set S_5, with domain points z_α reordered.

Symmetrizing the multi-indices

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.



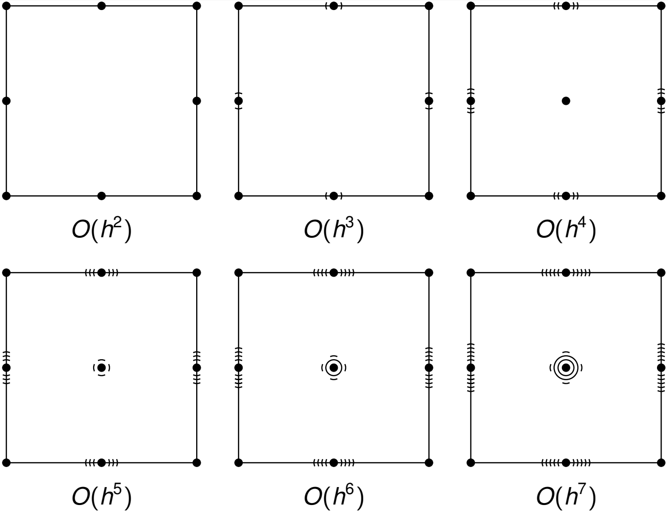
The lower set S_5, with domain points z_α reordered.



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.

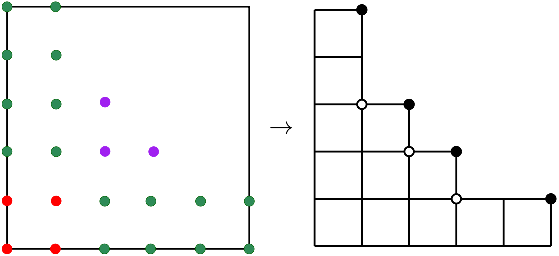
2D symmetric serendipity elements

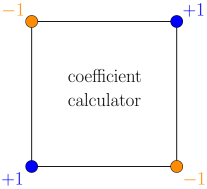
Symmetry: Accommodate interior degrees of freedom that grow according to triangular numbers on square-shaped elements.



Tensor product structure

The Dyn-Floater interpolation scheme is expressed in terms of tensor product interpolation over ‘maximal blocks’ in the set using an inclusion-exclusion formula.





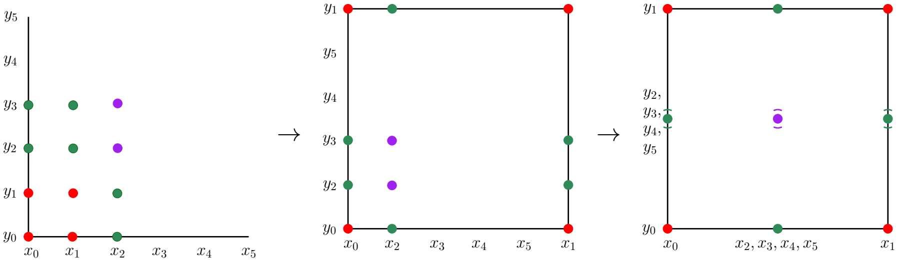
Put differently, the linear combination is the sum over *all* blocks within the lower set with coefficients determined as follows:

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

Hence: black dots $\rightarrow$ +1;   white dots $\rightarrow$ -1;   others $\rightarrow$ 0.

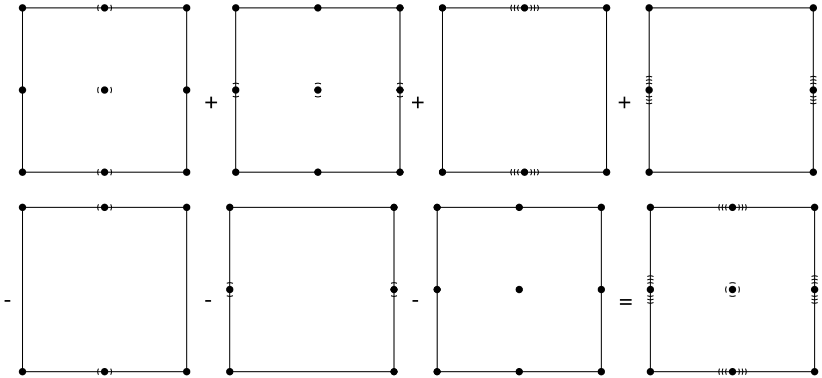
Tensor product structure

Thus, using our symmetric approach, each maximal block in the lower set becomes a standard tensor-product interpolant.



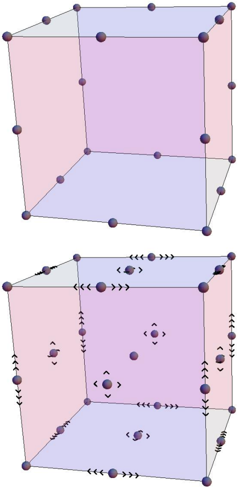
Linear combination of tensor products

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



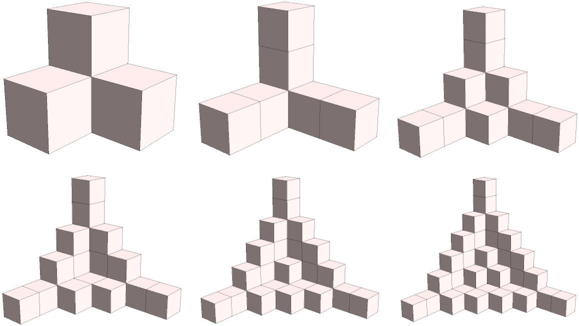
3D elements

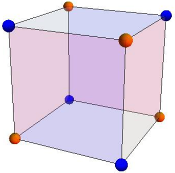
Hierarchical: Generalize to methods on n-cubes for any $n \geq 2$, allowing restrictions to lower-dimensional faces.



3d coefficient computation

Lower sets for superlinear polynomials in 3 variables:



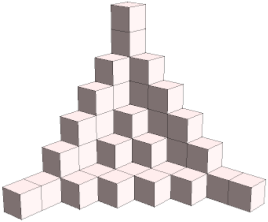


Decomposition into a linear combination of tensor product interpolants works the same as in 2D, using the 3D coefficient calculator at left. (Blue $\rightarrow$ +1;   Orange $\rightarrow$ -1).

FLOATER, GILLETTE *Nodal basis functions for the serendipity family of finite elements*, in preparation.

Brief aside: historical quiz

What video game is shown on the right?



Outline

RTG Project ideas

Email me if you'd like a copy of the slides with the project ideas.