Dimension Independent FEM

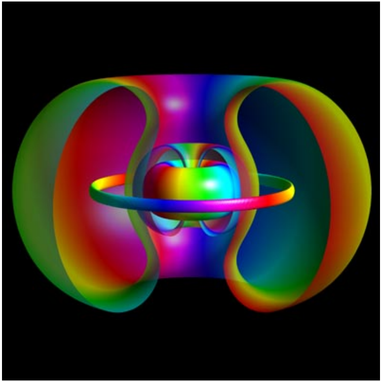
Peter Brune and Ridgway Scott

Department of Computer Science
University of Chicago

FEniCS '09
Simula Research Laboratory
June 11-12 2009, Fornebu, Norway

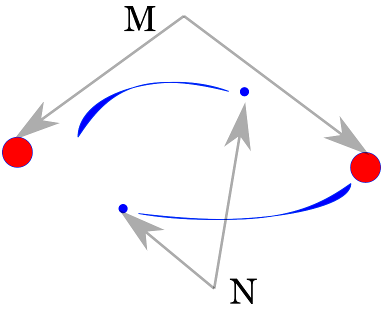
High Dimensional Problems

- Space-Time Meshing
- Finance
- Position + Momentum
- **Quantum Physics**



The Schrödinger Equation

- $< E\psi, \phi > = < \frac{1}{2}\nabla\phi, \nabla\psi > + < V * \phi, \psi >$
- $V = -\sum_j^M \sum_i^N \frac{Z_j}{R_{i,j}} + \sum_j^N \sum_i^N \frac{1}{r_{i,j}}$
- $\phi, \psi \in V_s$
- $V_s \subset L_2 : \psi(\vec{x_i}, .., \vec{x_j}) = \pm\psi(\vec{x_j}, ..., \vec{x_i})$ dependent on **Spin**



Problem Requirements

Numerical Methods for the Schrödinger equation need to:

- Account for **Exponential Decay**
- Avoid The **Coloumb Surfaces**
- Account for **Spin**

Previous Approaches

Sparse Grids

- Limit the total order of tensor product interval rules
- $Q_l^{(d)} f = ((\sum_{i=0}^{l} Q_i^{(1)} - Q_{i-1}^{(1)}) \otimes Q_{l-i}^{(d-1)}) f$
- $N^d \longrightarrow 2^d$
- Easy Antisymmetrization
- Limited support for non-hypercube geometries

Proposed Improvements

- More Interesting Domains than I^d
- Easier High-Order Adaptivity
- Meshes Conforming to **Spin** and **Potential**
- **Needed**: High Dimensional Finite Elements

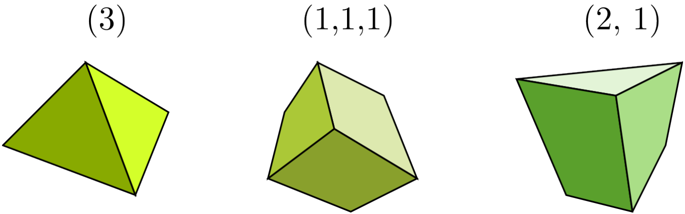
Required Components

Optimally-sparse:

- **Meshes** in n-D
- **Function Spaces** in n-D
- **Quadrature** in n-D

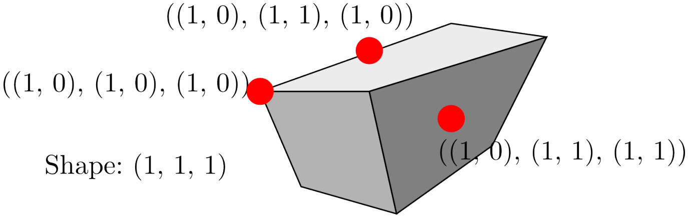
Cell Formulation

- $\Delta_1 \otimes \ldots \otimes \Delta_n$ for n simplicial subspaces
- includes **simplices**, **quads/hexes**, and **prisms**



Barycentric coordinates on tensor-product simplices

- Expressed as $d+1$ coordinates for each Δ_d

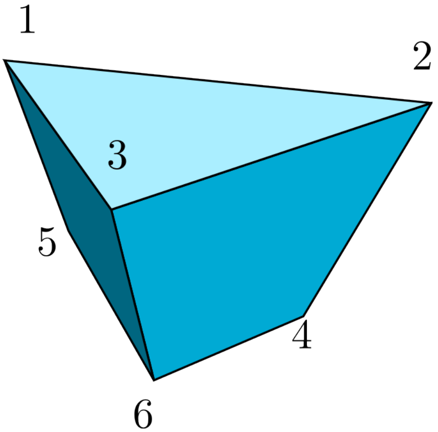


Cell Representation

- **Shape**: Tuple of Simplex Dimensions
- **Tensor**: Integer Corner Names

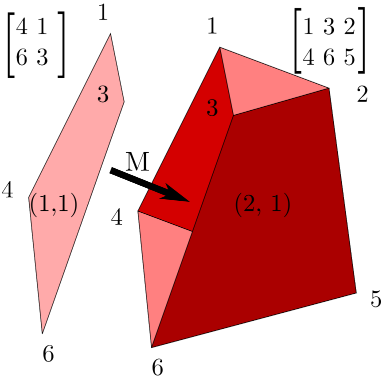
Shape: (2, 1)

$$T_{ij} = \begin{bmatrix} 1 & 2 & 3 \\ 5 & 6 & 4 \end{bmatrix}$$



Cell Connectivity

- Shared facets contain some intersection of the vertices
- have a **shape** like cells.
- connectivity a *mapping* between facet and cell coordinates

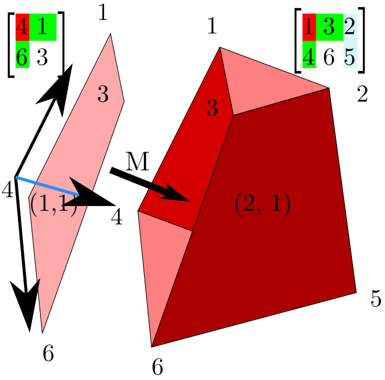


$$F = ((a, b), (c, d))$$

$$M = ((c, d, 0), (b, a))$$

Orientation

- Each facet has a *base point* in V
- defined as $x \in \Delta_{0,0}, \ldots, \Delta_{n,0}$
- compute orientation of cotangent spaces vs. base point



$$F = ((a, b), (c, d))$$

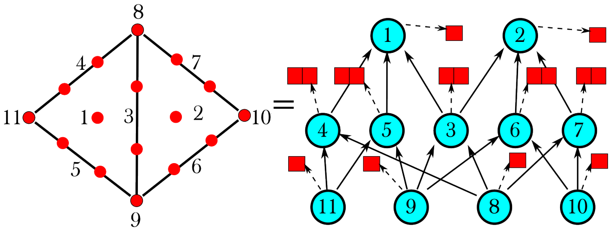
$$M = ((c, d, 0), (b, a))$$

Cell Complexity

- **Simplicial**: $2^{d+1} - 1$ facets
- **Hypercube**: 3^d facets
- Only ever represent *DoF-Containing Facets*

Sieve Representation

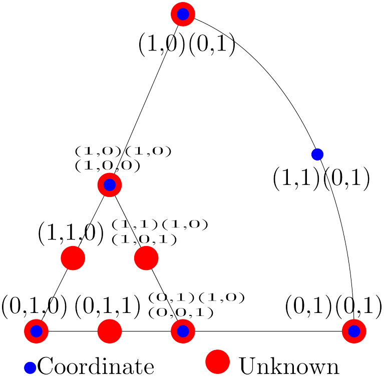
- Want to compute cell connectivity **ONCE**
- Store orientation/ordering on arrows of a *sieve*
- Allows for fast assembly
- Ties into parallelized codes for **cell complices**



Function Spaces

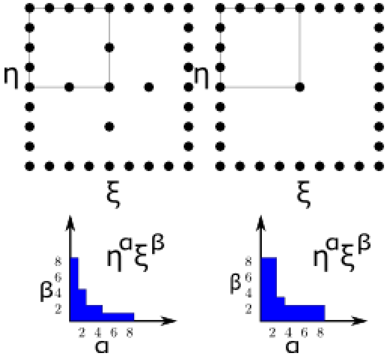
Easily phrased in terms of **BCCs**:

- **Nodal Locations** or **Polynomial Order**
- both easily expressed as **addresses** in this setting
- Function spaces can be built on the fly



Sparse basis functions

- Limit the mixed order of the basis functions
- Relates both to **Sparse Grids** and **Serendipity**
- Limit the dimension of the *support* of a DoF

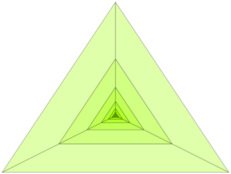


Meshing

- Standard 2D/3D Mesh $\otimes$ Extra Dimensions
- Mesh in line with the features of our problem

Example Mesh

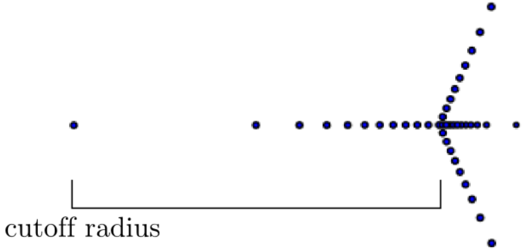
- Tesselation of $S^{d-1} \otimes I$
- **Nested Simplices**
- Extends to n-dimensions simply with O(n) cells



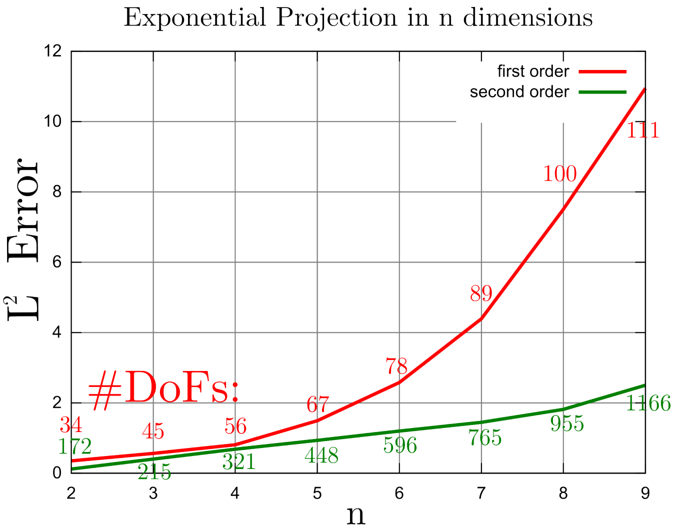
Optimal Mesh for functions tending to e^{-r}

Difference equation for optimal spacing:

- $\frac{x_{i+1}-x_i}{h} = \sqrt{2}e^{-r_c/2}$



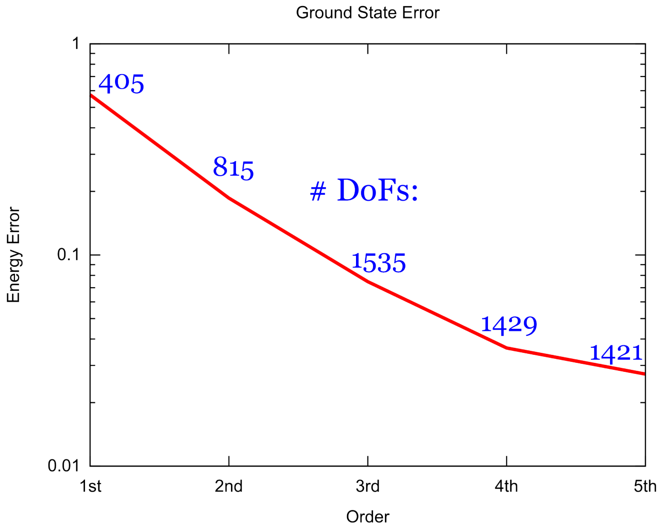
Error in Representing e^{-r}



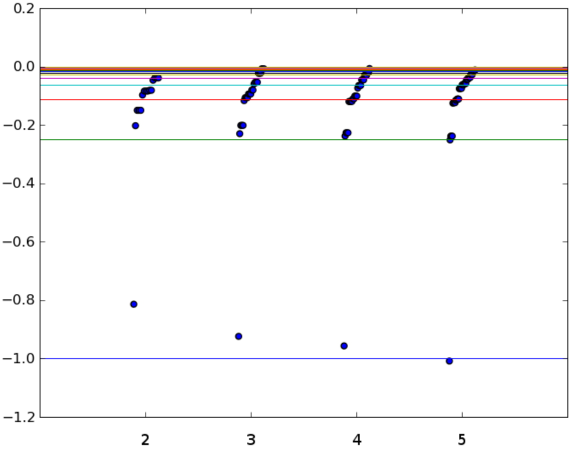
The Hydrogen Atom

- $-\frac{1}{2}\nabla\Psi - \frac{1}{|\vec{x}|}\Psi = E\Psi$
- $\vec{x} \in \mathbb{R}^3$
- $E_n = \frac{Z^2}{2n^n}$
- $\Psi_n = e^{\frac{-Zr}{n}}(\frac{2Zr}{n})^l L_{n+l-1}^{2l+1}(\frac{2Zr}{n})Y(\theta,\phi)$

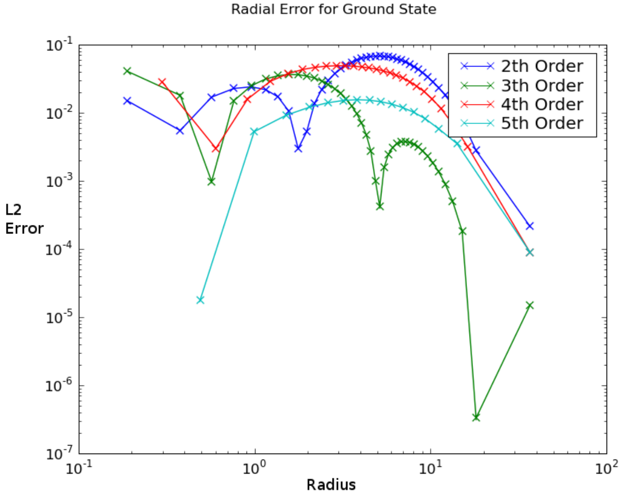
Energy Error for Hydrogen



Spectrum Recovery



Radial Error for Hydrogen



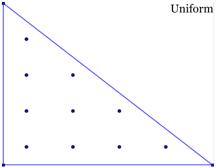
Missing Pieces

- Adaptivity
- High-Dimensional Quadrature
- Meshing for N-Electrons

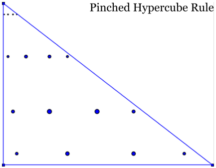
Adaptivity Options

- Mesh Refinement is **OUT** in 3N-Dim
- HAVE: anisotropic *a priori* radial refinement
- WANT: notion of *a priori* angular p-refinement given *aspect ratios*
- IMPLEMENT: *a posteriori* anisotropic estimation and p-refinement

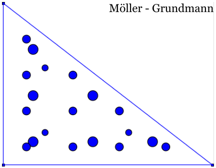
Quadrature



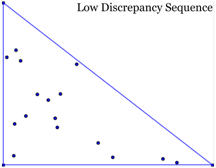
(a) $|P| = \binom{n+s+1}{n}$



(b) $|P| = s^n$



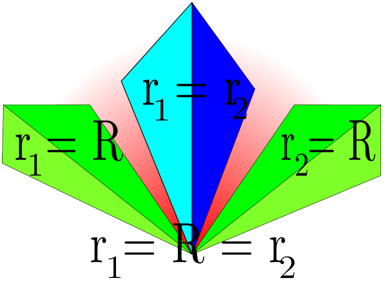
(c) $|P| = \binom{n+s+1}{s}$



(d) $|\epsilon| = O(\frac{log(|P|)}{|P|})$

Potential Function Cusps

- Coloumb interactions create *singular hypersurfaces*
- Easy in 1-Electron or 3D-approximation case
- Hard in the configuration space

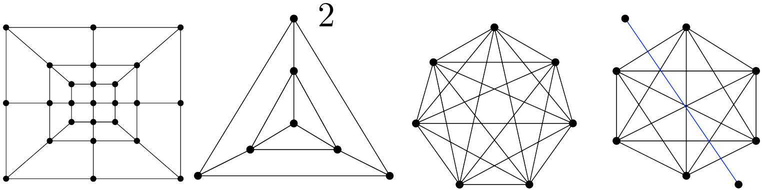


Helium

- $H = -\frac{1}{2}\sum_i^2 \Delta_i \Psi(r_1, r_2) - \sum_i^2 \frac{2}{r_i} + \frac{1}{r_{12}}$
- **Parahelium** – spin can be neglected
- Current discretizations – problematic
- Can rotate the unit 6-simplex to avoid cusps
- Truly seems to need **adaptivity**

Potential Meshes for Helium

- Expanding Cartesian
- Tensor Product Hydrogen
- $6D$ Simplicial Mesh
- Lens-Space Mesh



What have we learned?

- How to engineer a **general mesh framework**
- How to create function-spaces for n-dimensional systems
- Discretization of QM systems is still difficult
- We are looking for better apps for this technology

Extra Topics

- 3D Methods
- Antisymmetrization of the Space
- Lower-Dimensional Possibilities
- Lessons for FEniCS?

Approximation Methods in Quantum Chemistry

- (Post) Hartree-Fock and the Self-Consistent Field
- CI, CC, etc.
- DFT Methods
- Both are *nonlinear* eigenvalue problems
- Every approximation causes some **error**

Antisymmetry and Pauli Exclusion

- 1-particle wavefunctions antisymmetrized by **Slater Determinant**

$$\begin{vmatrix} \psi(\vec{x}_1)_1 & \dots & \psi(\vec{x}_s)_1 \\ \dots & & \dots \\ \psi(\vec{x}_1)_s & \dots & \psi(\vec{x}_s)_s \end{vmatrix}$$

- Antisymmetry as a **Condition on** V_s
- Keep each equal-spinned electron on the other "side" of a hyperplane from the previous

Advantages in “*Normal*” Settings

- Quick setup of a variety of geometries and function spaces
- Mixed orders, mixed geometries
- Isoparametry
- Should Try: H-P Methods

Complexity Caveats

- $J = \frac{\partial}{\partial \vec{\xi}_i} \vec{x}(\vec{\xi}_j)$ in $\int_{\Omega_c} \phi_i \psi_j |J| d\Omega_c$
- $d \times d$ matrix
- $O(D_c d^2)$ construction
- $O(d^3)$ determinant computation
- Nonlinear jacobian; reevaluate on quadrature points

FEniCS Tie-Ins

- **Human-Readible** *DoF* labels for UFL/UFC
- Quad and Hex Elements **or** mixed geometries
- *Elementless* Finite Elements?!?