High-Order Serendipity Finite Elements for Gkeyll

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Graduate Seminar Talk, 7 Jan 2013

Outline

Major Motivations

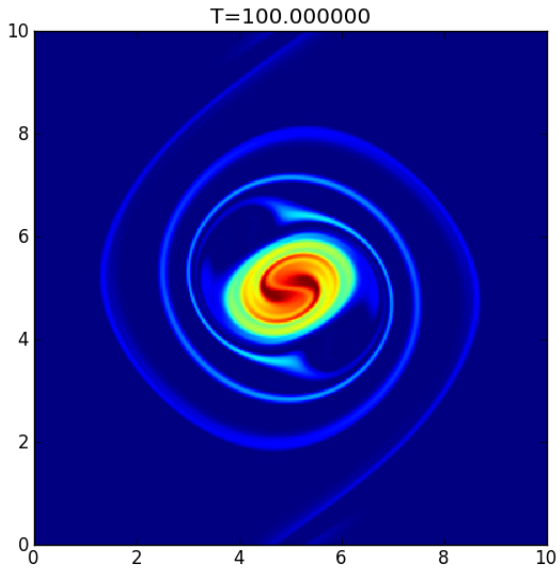
- Edge region is important, but complicated
- Tokamak edge physics relatively unexplored: no complete model of self-consistent cross-field transport in open-field line region, very little study of neutral transport, wall effects, etc.
- Large density/amplitude variations, large relative banana width, wide range of collisionalities

Major Motivations

- Need comprehensive simulations of edge turbulence because predicted fusion performance strongly dependent on edge temperature
  - ELM suppression/mitigation, spontaneous flow, Li walls
- Need new code or major extensions to existing codes to handle edge region
- Advanced algorithms can help with these additional challenges

Gkeyll Overview

- Prototype code to explore advanced algorithms for continuum edge gyrokinetic simulation (e.g. edge plasma turbulence)
  - Hybrid discontinuous/continuous Galerkin methods augmented with reconstruction techniques from finite volume schemes
- Main code is written in C++
- Lua scripts for simulations



Goal

A robust code capable of running very quickly at coarse velocity space resolution while preserving all conservation laws of gyro-fluid/fluid equations and giving fairly good results.

Objective

Explore basis functions that reduce computational effort, yet retain the formal high-order accuracy for 4-D/5-D gyrokinetic simulations

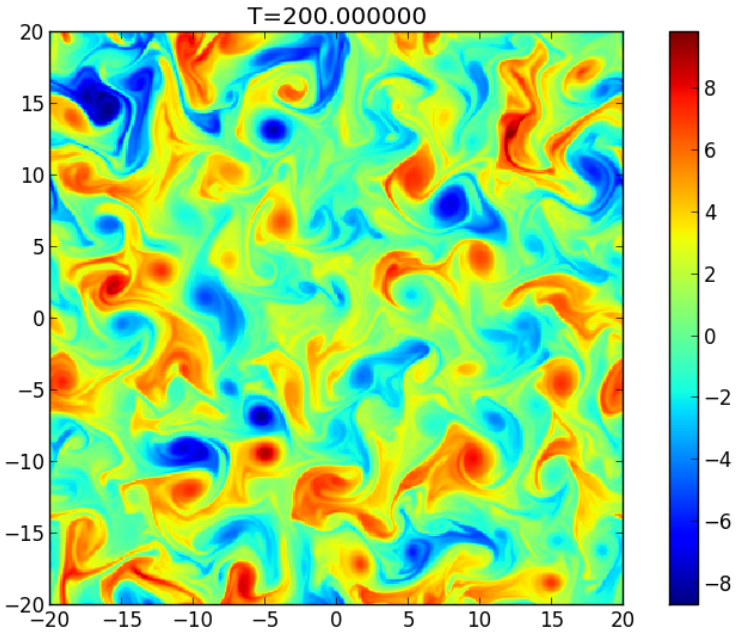
- 1024 unknowns per element using standard 3rd order element in 5-D
- Investigate serendipity basis functions

Hyperbolic PDEs

- Conservation laws

$$\frac{\partial Q}{\partial t} + \nabla \cdot \boldsymbol{F}(Q) = \psi(Q)$$

- Wave equations
- Euler equations
- Navier-Stokes equations
- Two-Fluid MHD
- Vlasov Equation
- Hasegawa-Wakatani equations
- Gyrokinetic equations



Finite Element Methods

- Technique for solving systems of PDEs
- Example: Consider a differential equation with the exact solution in blue
- Seek approximate solution (red) as a sum of piecewise linear functions

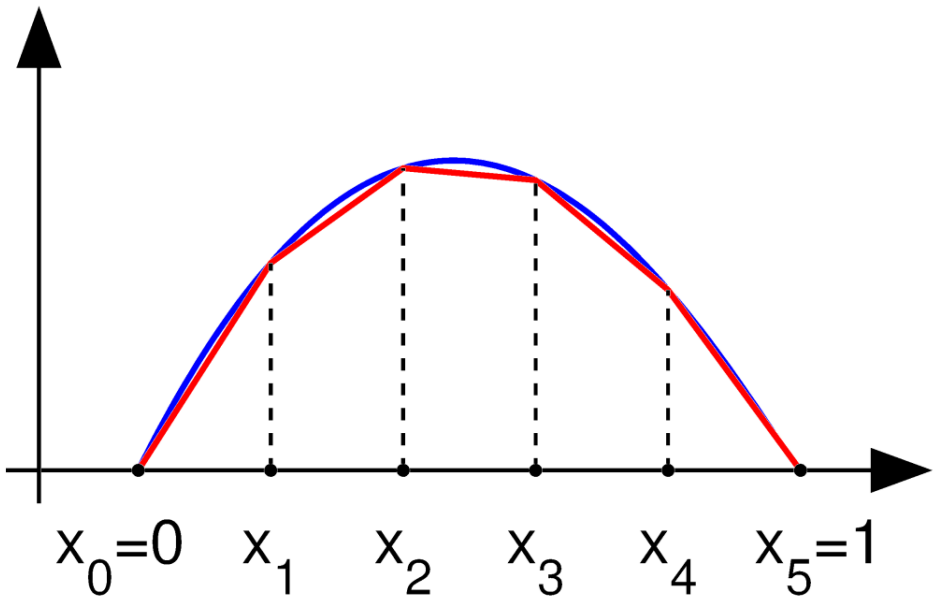


Image from Wikipedia

Finite Element Methods

- Partition solution domain into elements of simple geometrical shape (mesh)
  - Each element contains a number of nodes
- Use finite element analysis to find the 'optimal' linear combination of *basis functions* for approximate solution

$$u(x) \approx \tilde{u}(x) = \sum_{k=1}^{K} w_k N_k(x), \; N_k(x_j) = \delta_{kj}$$

- The N_k(x) (blue) are basis functions, x_k are nodes

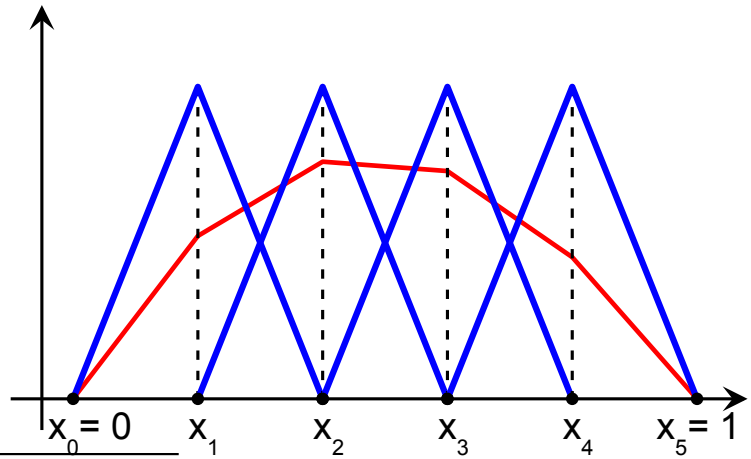


Image from Wikipedia

Finite Element Methods

- Due to basis function properties, approximate solution can be expressed in terms of the *function values* at the nodes

$$u(x) \approx \tilde{u}(x) = \sum_{k=1}^{K} \tilde{u}(x_k) N_k(x), \; N_k(x_j) = \delta_{kj}$$

- Solve K algebraic equations to find unknown weights $w_k = \tilde{u}(x_k, t)$

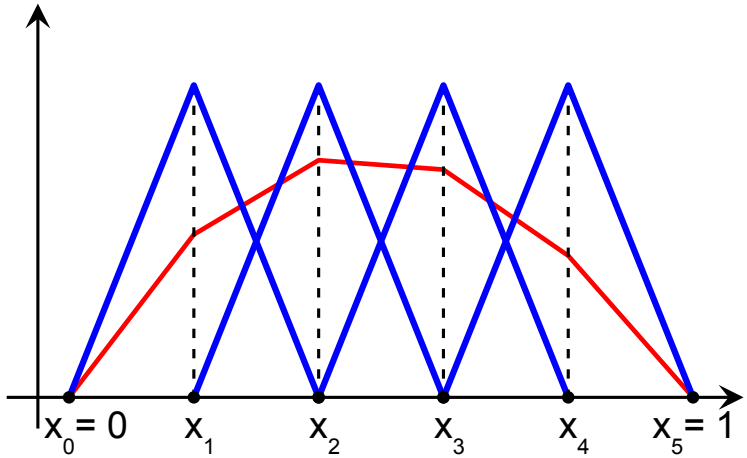


Image from Wikipedia

Finite Element Methods

- *Nodal* basis functions $N_k(x)$ evaluate to 1 at node x_k and 0 at every $x_{j \neq k}$
- There is flexibility in choosing basis functions–don't need to use tent functions
- Two strategies for increasing accuracy:
  - Use smaller elements (more elements to discretize domain)
  - Use basis functions composed of higher degree polynomials
- Cost of using higher-degree basis functions is more degrees of freedom (unknowns) per element
  - Use higher-degree basis functions with larger elements?

Polynomial Completeness

- If basis functions span a complete Nth degree polynomial and finite elements have length h, error behaves as

$$\|u - \tilde{u}\| \leq Ch^{N+1}$$

- Useful to recall Pascal triangle:

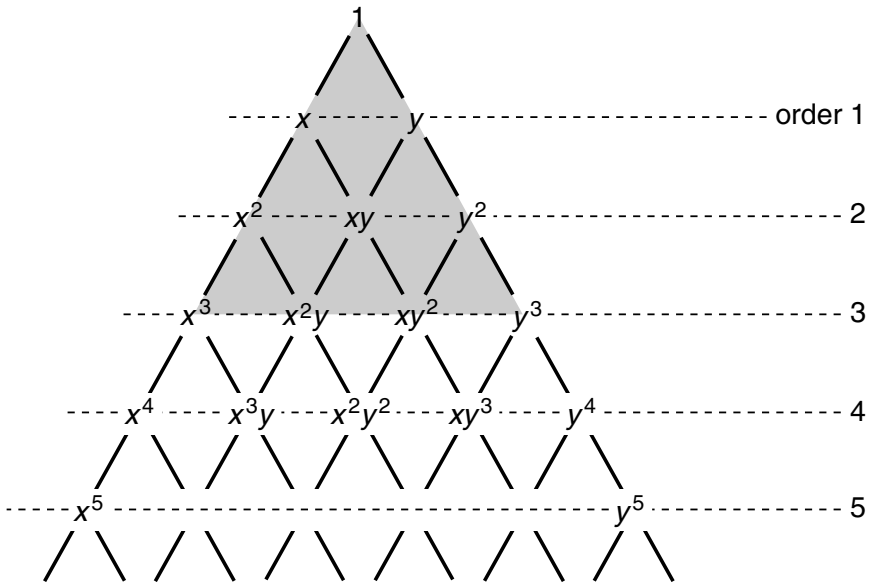


Fig. 4.5 The Pascal triangle. (Cubic expansion shaded – 10 terms.)

Image from *The Finite Element Method: Its Basis and Fundamentals*

Degrees of Freedom (DOF)

- In the FEM, solution is expressed in terms of a finite number of DOF + basis functions
- DOF are the unknown basis function weights, e.g.

$$u(x,t) \approx \tilde{u}(x,t) = \sum_{k=1}^{K} \tilde{u}(x_k,t) N_k(x)$$

- When using *nodal* elements, the DOF are characterized by the value(s) of a function at the nodes of each element
  - # unknowns = # DOF
  - Function can be $\tilde{u}$ and/or $\tilde{u}'$

Finite Elements in Higher Dimensions

- 1-D: elements of finite interval
- 2-D: elements of finite area (e.g. rectangles, triangles, curvilinear polygons)
- 3-D: elements of finite volumes (e.g. cubes, tetrahedra)
- All finite elements are transformations of reference elements (e.g. square, triangle, cube)

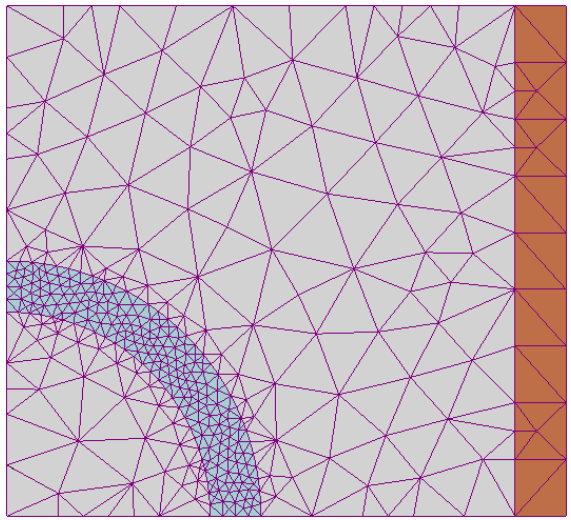


Figure: Example 2-D FEM mesh using triangles

Discontinuous Galerkin Background

- State-of-art for solution of hyperbolic partial differential equations
- First introduced by Reed and Hill for steady-state 2-D neutron transport in 1973
- Runge-Kutta DG for time-dependent problems by Cockburn and Shu (1998)
  - Finite element space discretization, Runge-Kutta time discretization
- Widely used in computational fluid dynamics, finding use in more applications (e.g. atmospheric modeling, MHD)

Discontinuous Galerkin Solutions

Discontinuous Galerkin schemes use function spaces that allow *discontinuities* across cell boundaries.

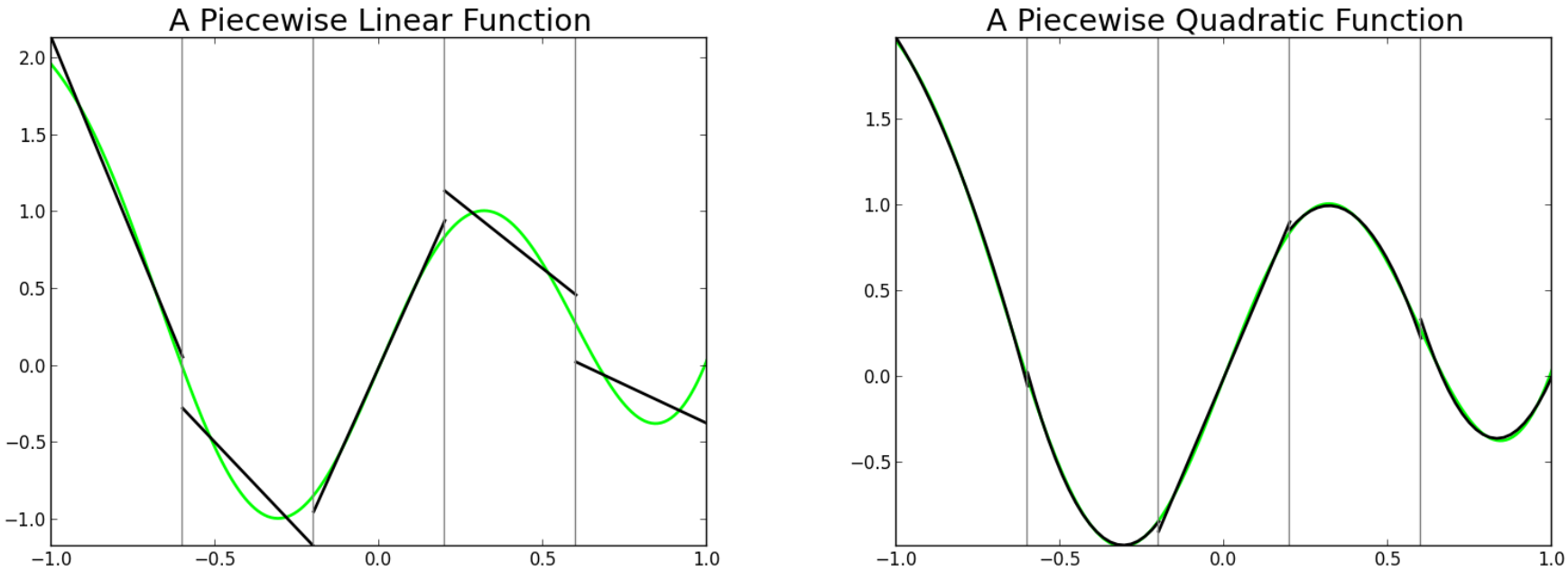


Figure: The best L^2 fit of $x^4 + \sin(5x)$ (green) with piecewise linear (left) and quadratic (right) basis functions.

Discontinuous Galerkin Features

- Numerical solution is discontinuous between elements
- Hybrid approach: exploit merits of classical finite element and finite volume methods
  - FV: slope limiters to control spurious oscillations, locality
  - FE: high-order accuracy, complex geometries
- Information only needs to be shared between neighboring elements–adapts well to massively parallel architectures

DG combined with FV schemes can lead to best-in-class explicit algorithms for *hyperbolic PDEs*.

Finite Elements in DG

- Finite elements are non-overlapping
- Basis functions are zero outside the element
- Solution within an element defined only in terms of that element's basis functions and DOF

$$u(x,t) \approx \tilde{u}(x,t) = \sum_{k=1}^{K} \tilde{u}(x_k,t) N_k(x)$$

Finite Element Spaces

- Set of all functions that can be written as linear combinations of the basis functions
- Specified for each degree and dimension by:
  1. Element shape (e.g. triangle, quadrilateral, hexahedron, etc.)
  2. Set of basis functions that span the function space
     - # basis functions per element = # DOF per element
     - (Nodal only): DOF on each face of dimension d (vertex, edge, interior)
- Example finite element spaces:
  - Lagrange (C^0)
  - Serendipity (C^0)
  - Hermite Cubic (C^1)

Lagrange Family

- Basis functions are tensor products of Lagrange polynomials

$$\ell_k^n(x) = \prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{x - x_i}{x_k - x_i}, \; N_a(x, y) \equiv l_a^n(x) l_a^m(y)$$

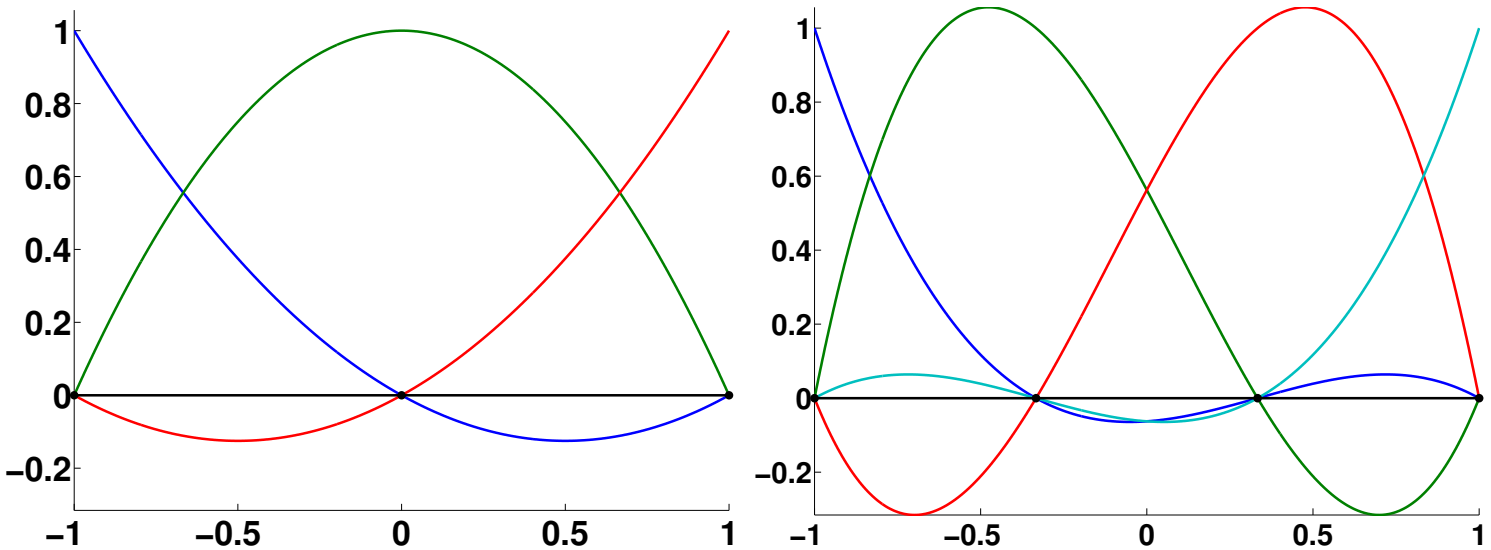


Figure: Basis functions for 2nd (right) and 3rd (left) order elements.

Lagrange Family

- Pros: Easy to implement, generalizes to arbitrary dimension and order
- Cons: Large number of DOF in higher dimension and order
  - In 5-D, need $(3 + 1)^5 = \mathbf{1024}$ DOF per element for 3rd order
- Large number of terms above those needed for complete expansion present!

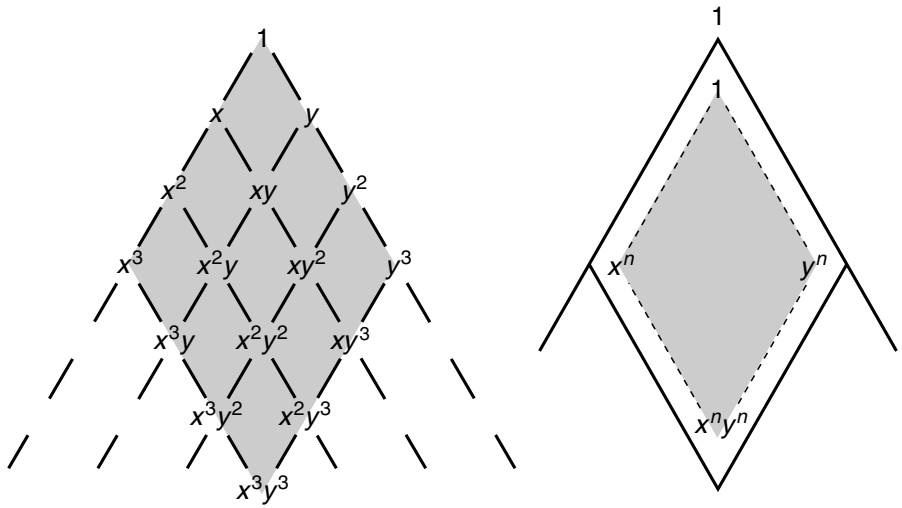


Fig. 4.8 Terms generated by a lagrangian expansion of order 3 × 3 (or $m \times n$). Complete polynomials of order 3 (or n).

Image from *The Finite Element Method: Its Basis and Fundamentals*

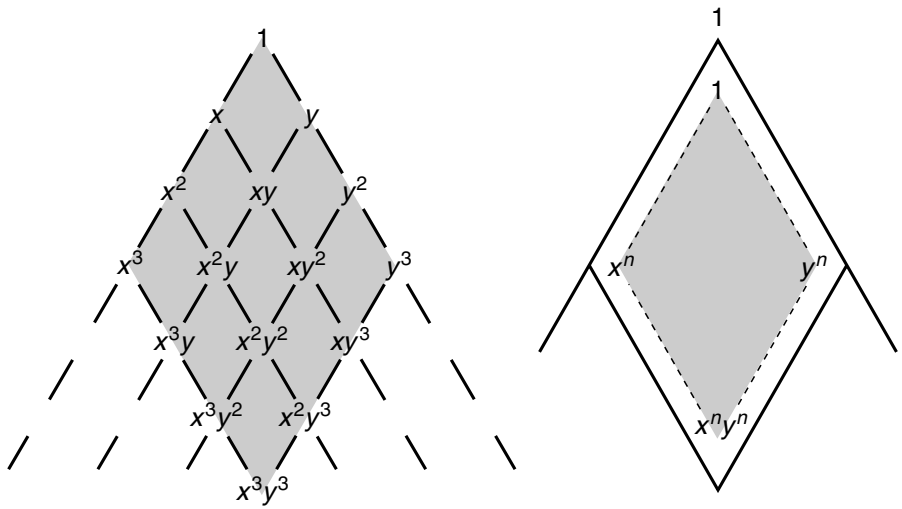
Serendipity Family

- Basis functions originally derived by inspection ('serendipity')
- Fewer interior nodes compared to Lagrange element of same order
  - Fewer DOF per element
  - Smaller dimension function space
- Expect lower accuracy, but faster than Lagrange elements of the same order

Key Question

Can serendipity elements deliver the same error at a lower computational cost (by choice of element size and order)?

Lagrange and Serendipity Compared in 2-D



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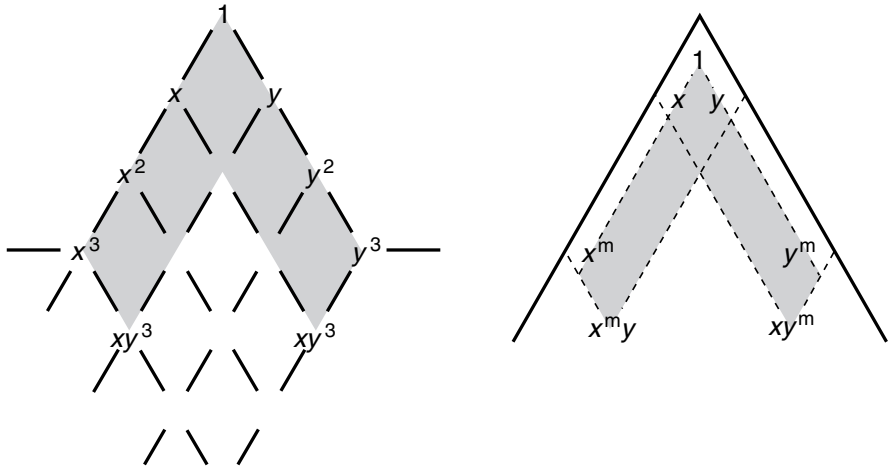


Fig. 4.12 Terms generated by edge shape functions in serendipity-type elements (3 × 3 and $m \times m$).

Image from *The Finite Element Method: Its Basis and Fundamentals*

Lagrange and Serendipity Compared in 2-D

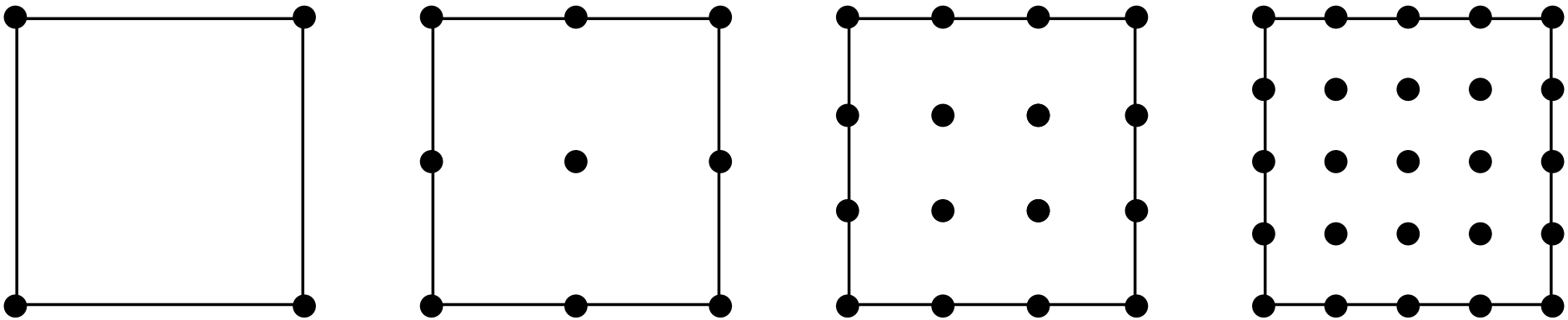


Figure: Node placement of 1st to 4th order Lagrange elements.

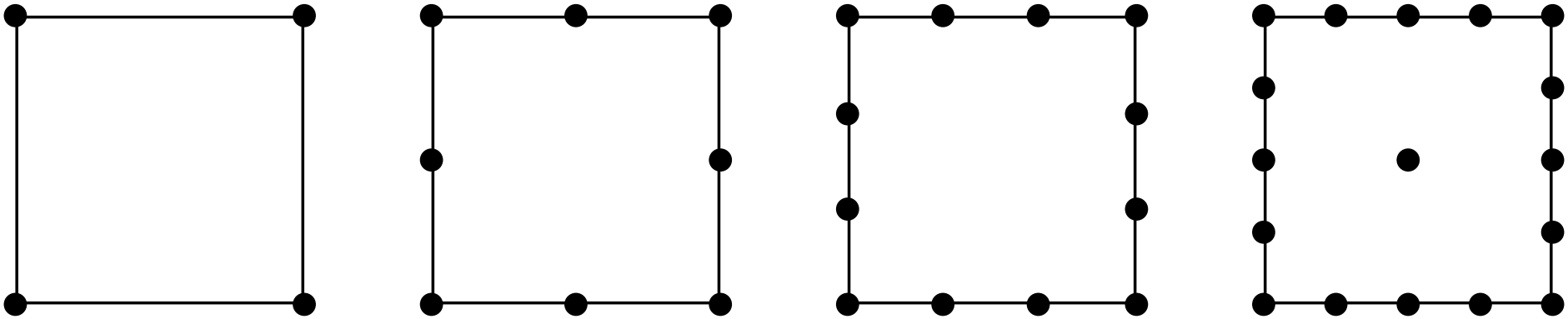


Figure: Node placement of 1st to 4th order Serendipity elements.

Larger savings in higher dimensions and order

Three Dimensions

Order	Lagrange	Serendipity
1	8	8
2	27	20
3	64	32
4	125	50

Five Dimensions

Order	Lagrange	Serendipity
1	32	32
2	243	112
3	1024	192
4	3125	352

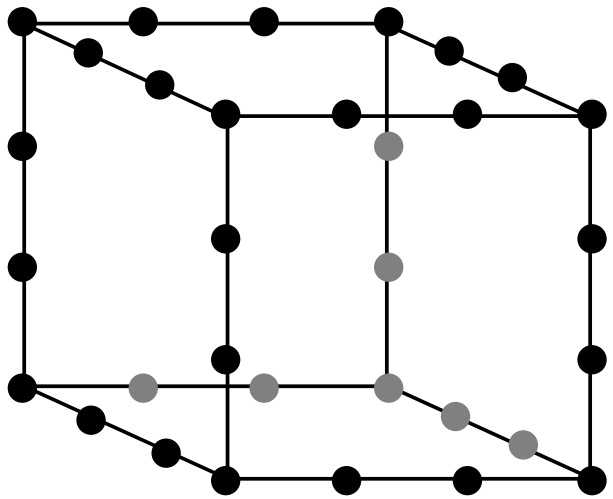


Figure: 3rd order Serendipity element in 3-D

Serendipity Family Definition

- Typically used with low order (r<3) in 2-D and to a lesser extent in 3-D
- Pattern for progression to higher orders, higher dimensions not evident ('serendipity')
- Simple and new dimension-independent definition given by Arnold[1] for serendipity elements

Definition

The serendipity space $\mathcal{S}_r(I^n)$ is the space of all polynomials in n variables with superlinear degree (total degree with respect to variables entering at least quadratically) at most r.

[1] **serendipity**.

Example: Degree 3 Polynomial Spaces (2-D)

$\mathcal{P}_r(I^n)$:=span{monomials in n variables with degree $\leq r$}
$\mathcal{S}_r(I^n)$:=span{monomials in n variables with superlinear degree $\leq r$}
$\mathcal{Q}_r(I^n)$:=span{monomials in n variables with each variable degree $\leq r$}

$$\mathcal{P}_3(I^2) = \text{span}\{1, x, y, x^2, y^2, xy, x^3, y^3, x^2y, xy^2\}$$
$$\mathcal{S}_3(I^2) = \mathcal{P}_3(I^2) \cup \text{span}\{x^3y, xy^3\}$$
$$\mathcal{Q}_3(I^2) = \mathcal{S}_3(I^2) \cup \text{span}\{x^2y^2, x^3y^2, x^2y^3, x^3y^3\}$$

- Note that $\mathcal{P}_r(I^n) \subset \mathcal{S}_r(I^n) \subset \mathcal{Q}_r(I^n)$

Example: $\mathcal{S}_2(I^2)$ Basis Functions

$$\begin{pmatrix} N_0 \\ N_1 \\ N_2 \\ N_3 \\ N_4 \\ N_5 \\ N_6 \\ N_7 \end{pmatrix} = \begin{pmatrix} -\frac{(x-1)(y-1)(x+y+1)}{4} \\ \frac{(x^2-1)(y-1)}{2} \\ \frac{(x+1)(y-1)(y-x+1)}{4} \\ -\frac{(y^2-1)(x+1)}{2} \\ \frac{(x+1)(y+1)(x+y-1)}{4} \\ -\frac{(x^2-1)(y+1)}{2} \\ \frac{(x-1)(y+1)(x-y+1)}{4} \\ \frac{(y^2-1)(x-1)}{2} \end{pmatrix}$$

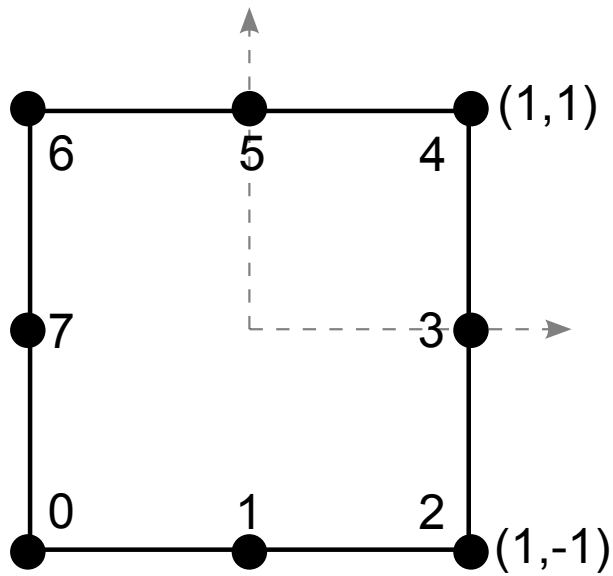


Figure: $\mathcal{S}_2(I^2)$ element centered at origin

Generating Serendipity Basis Functions

1. Given an order and dimension, determine the monomials v_k that span the serendipity space
2. Determine location of nodes $\mathbf{x_k}$ on reference element
3. Set up matrix equation for basis functions

$$N_j(\mathbf{x}) = \sum_k c_j^{(k)} v_k(\mathbf{x})$$

$$N_j(\mathbf{x_k}) = \delta_{kj}$$

4. Solve system for weights $c_j^{(k)}$ by a matrix inversion
5. Map reference space basis functions to physical space

3-D Gaussian Pulse Advection

- Advection at constant speed in 3-D

$$\frac{\partial f}{\partial t} + \nabla \cdot (f\mathbf{u}) = 0$$

- Solution is given by

$$f(\mathbf{x}, t) = f_0(\mathbf{x} - \mathbf{u}t)$$

- Periodic boundary conditions
- Design simulation to end when pulse has completed one period of its motion
- Compute error *per node* by summing over all nodes in domain:

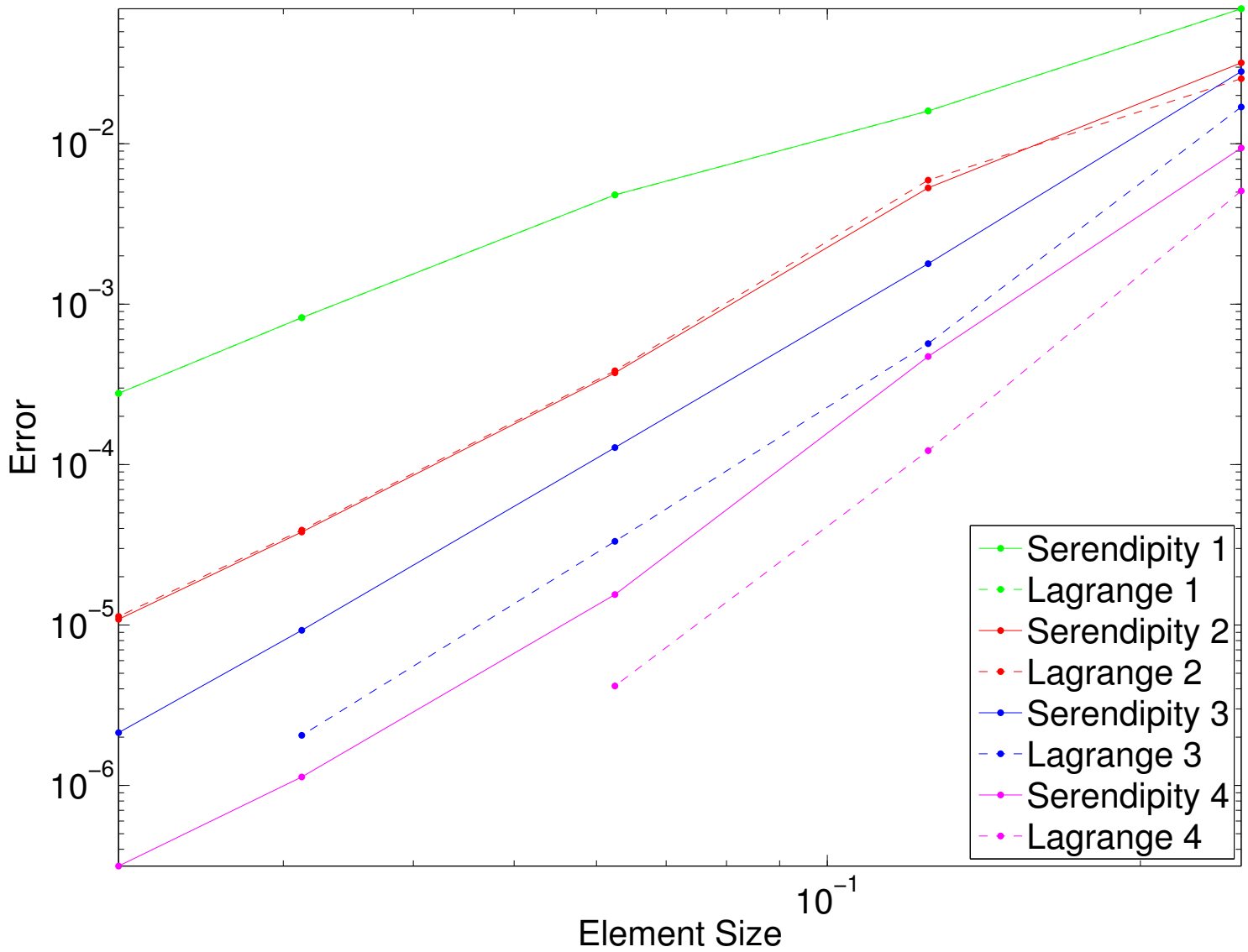
$$E = \sum_{k}^{N_{nodes}} \frac{|u(t_f, \vec{x_k}) - u(t_0, \vec{x_k})|}{N_{nodes}}$$

Convergence Study

- Order of serendipity element and total number of elements varied ($n \times n \times n$ for $n = 4, 8, 16, 32$)
- Since error E scales as $O(h^c)$ with element size h, plot $\log E$ vs. $\log h$ and find slope of best-fit line

Order of Element	Order of Scheme (S)	Order of Scheme (L)
1	2.09	2.09
2	3.30	3.20
3	3.85	4.31
4	4.40	5.13

Error vs. Element Size



Computation Time

- Execution time results for a $32 \times 32 \times 32$ element grid:

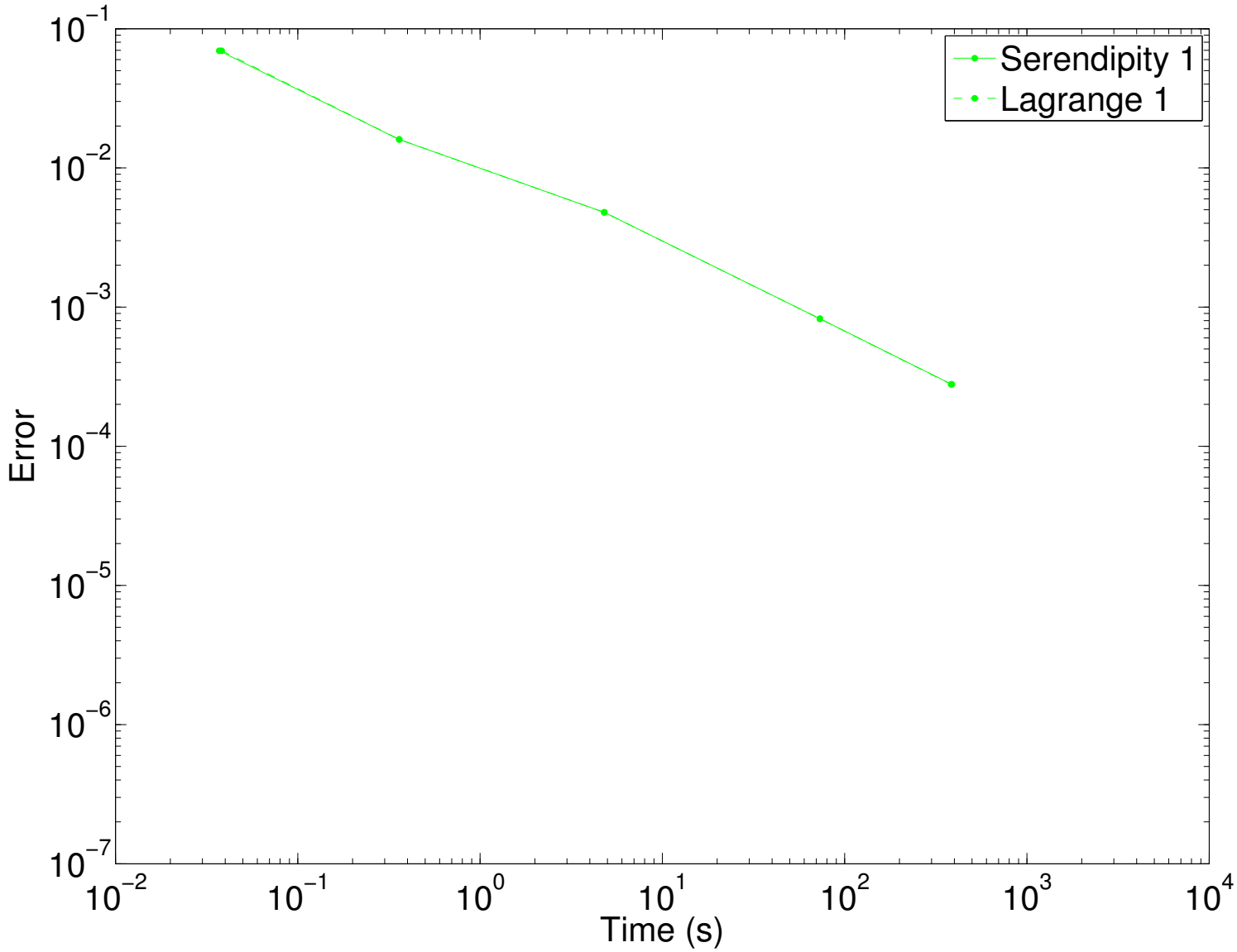
Order of Element	Serendipity	Lagrange	Ratio
1	73.2 s	73.2 s	1.00
2	220 s	663 s	0.331
3	654 s	5350 s	0.122

- DOF per element comparison:

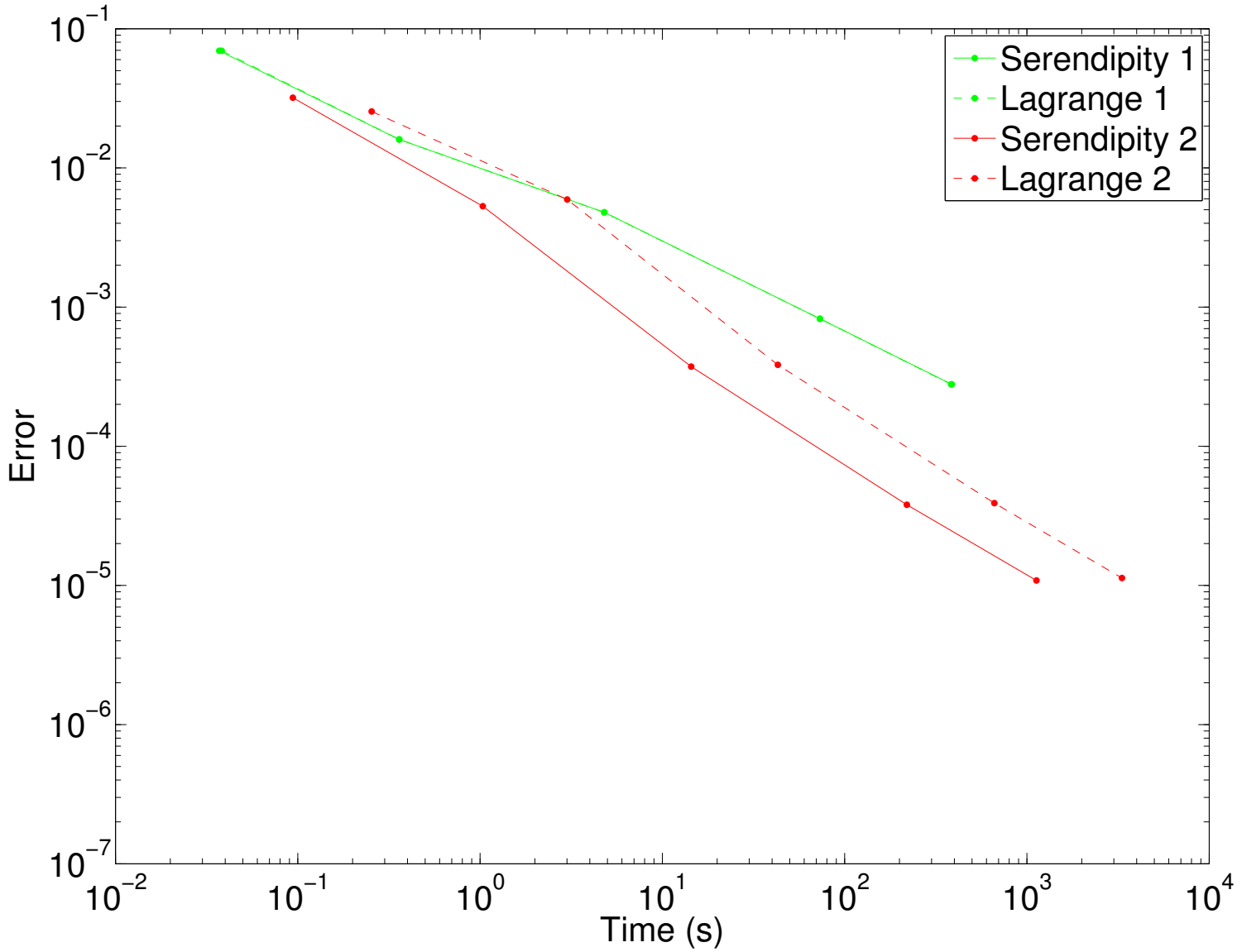
Order of Element	Serendipity	Lagrange	Ratio
1	8	8	1.00
2	20	27	0.741
3	32	64	0.500

Additional savings due to larger permissible time step for serendipity elements

Error vs. Computation Time



Error vs. Computation Time



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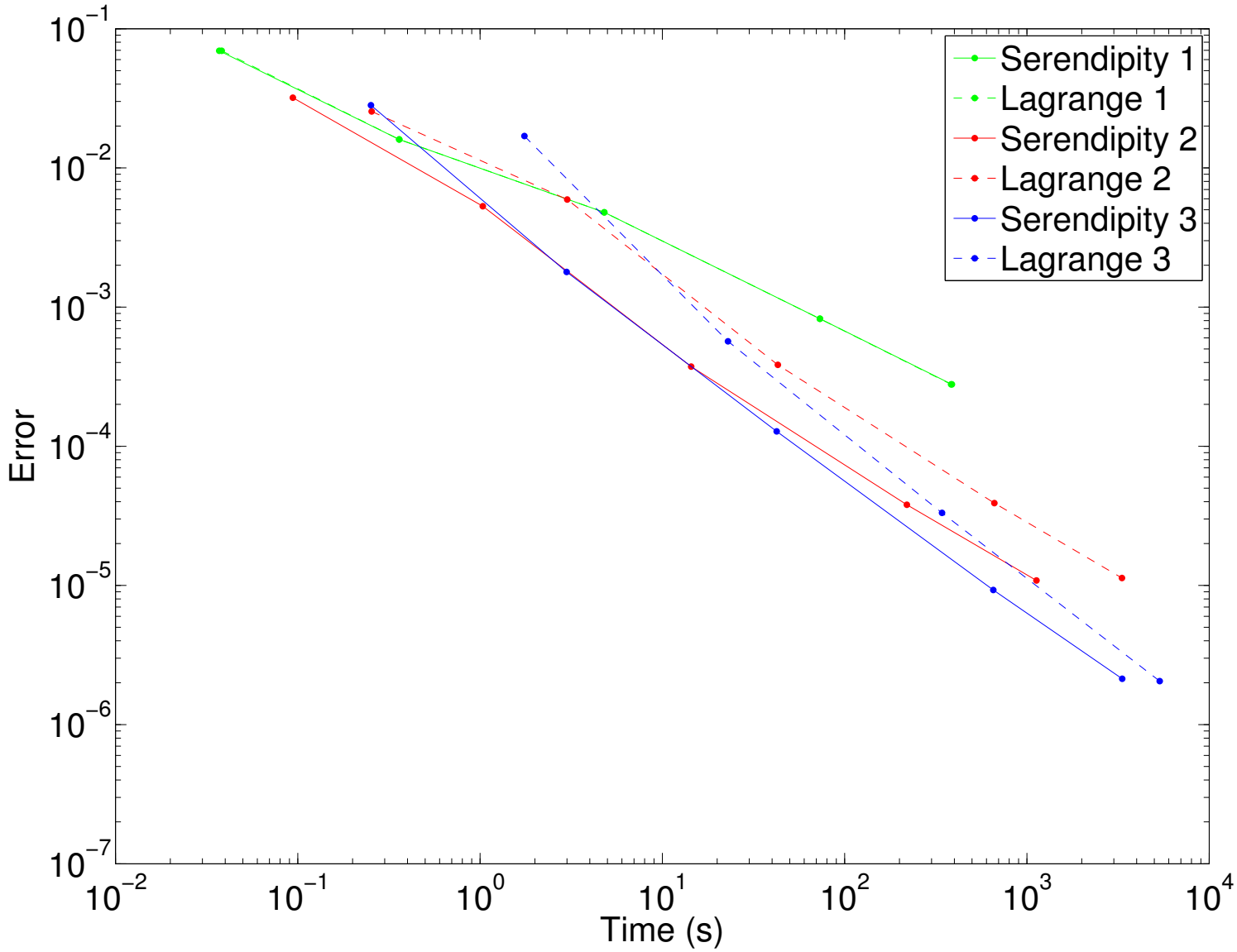

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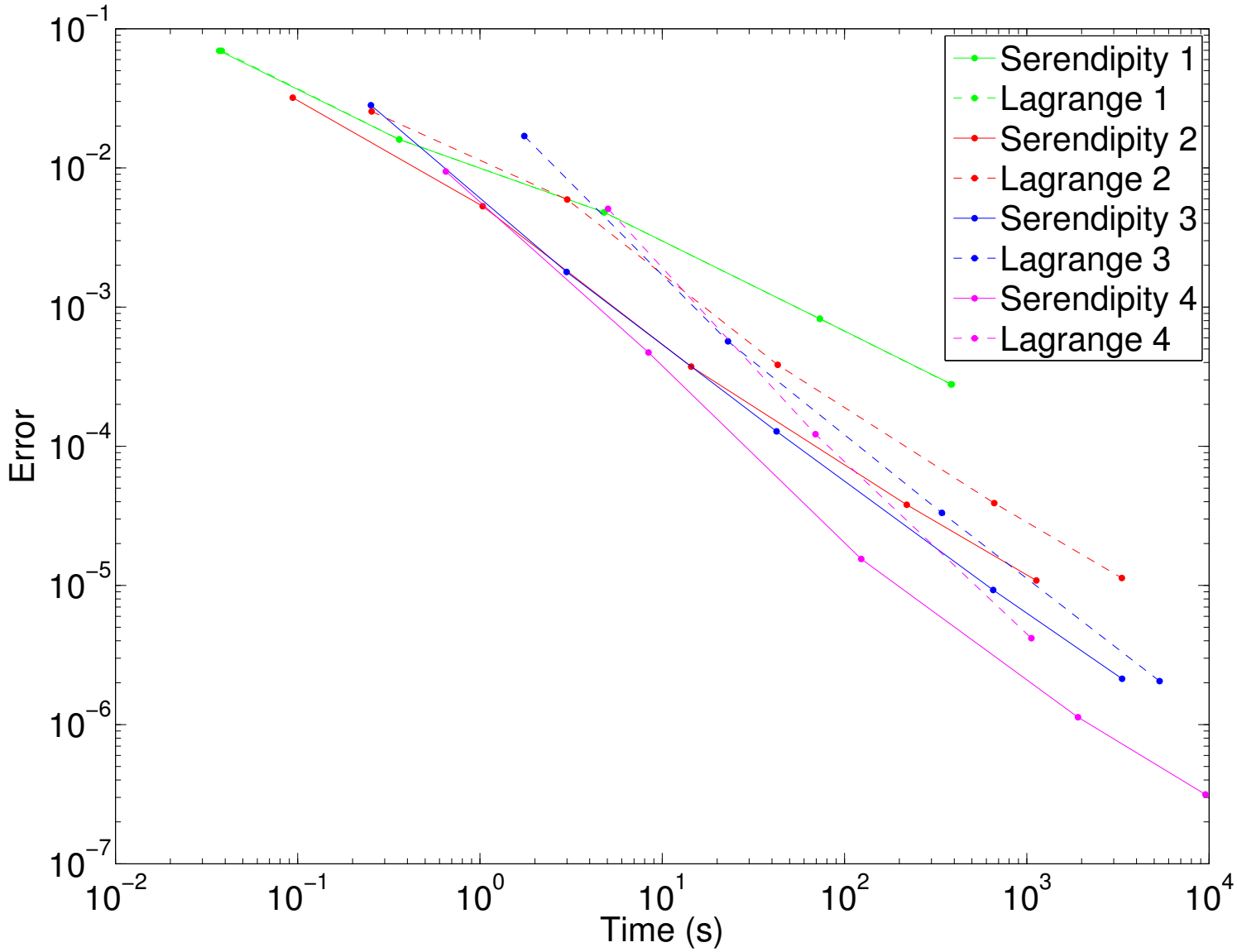


Conclusions

Initial results indicate that:

- Serendipity elements are more efficient than Lagrange elements for obtaining the same level of error
- Additional savings in computational time from larger maximum permissible time step for convergence (CFL condition)

Future Work

- Investigate performance of serendipity elements in multi-block structured grids
- Use serendipity elements in 1D2V simulations
  - Scrape-off layer model
- Add full Lenard-Bernstein collision operator
- Extend serendipity elements in Gkeyll to 4-D and 5-D
- Investigate Maxwellian-weighted basis functions for velocity space discretization

Acknowledgements

Thanks to:

- Jeffrey Parker
- Chang Liu

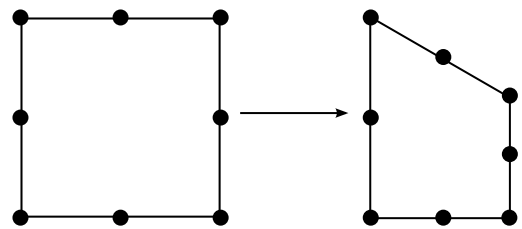
Alpha testing:

- Sam Cohen
- Allan Reiman

Caveats

- Reference element in results was mapped to the physical space by scaling each dimension by a constant
  - This is an example of an **affine** map

- Unfortunately, serendipity elements do not attain the same optimal rate of convergence on non-affine meshes



- Can avoid this problem by defining basis functions in physical space