Finite Element Particle Transport using Wachspress Rational Basis Functions

Greg Davidson[1] Todd S. Palmer[2]

[1]Department of Nuclear Engineering and Radiological Sciences
University of Michigan

[2]Department of Nuclear Engineering and Radiation Health Physics
Oregon State University

CSGF Annual Conference
June 20

Outline

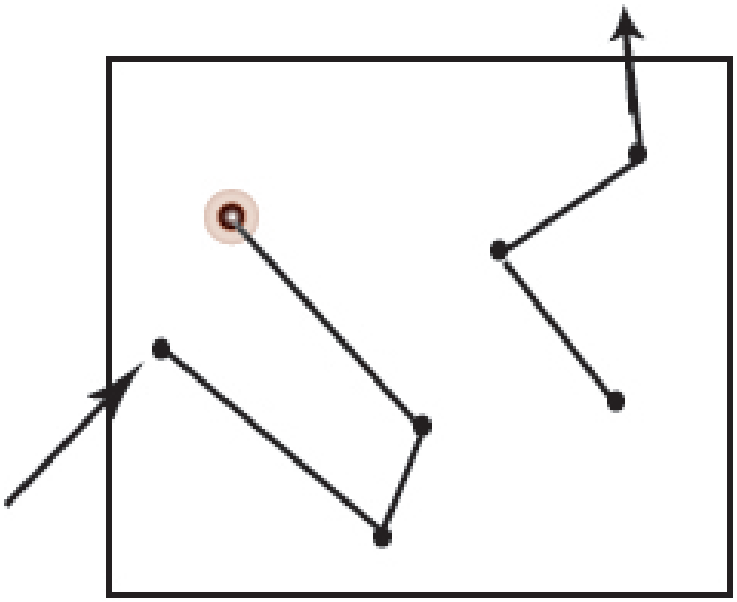
Outline

Introduction to Particle Transport

- Particle transport is concerned with describing how radiation flows through materials
- We are only concerned with time-independent and energy-independent two-dimensional particle transport.

Introduction to Particle Transport

- Particle transport is concerned with describing how radiation flows through materials
- We are only concerned with time-independent and energy-independent two-dimensional particle transport.



Introduction to Particle Transport

Particle transport is described by the linear Boltzmann transport equation:

$$\Omega \cdot \nabla \psi(\mathbf{x}, \Omega) + \Sigma_t \psi(\mathbf{x}, \Omega) = \frac{\Sigma_s}{2\pi} \int_{2\pi} \psi(\mathbf{x}, \Omega') \, \mathrm{d}\Omega' + \frac{Q}{2\pi} \quad (1)$$

Introduction to Particle Transport

Particle transport is described by the linear Boltzmann transport equation:

$$\Omega \cdot \nabla \psi(\mathbf{x}, \Omega) + \Sigma_t \psi(\mathbf{x}, \Omega) = \frac{\Sigma_s}{2\pi} \int_{2\pi} \psi(\mathbf{x}, \Omega') \, \mathrm{d}\Omega' + \frac{Q}{2\pi} \quad (1)$$

Streaming Term: Rate that particles at position $\mathbf{x}$ and angle Ω stream through the background media

Introduction to Particle Transport

Particle transport is described by the linear Boltzmann transport equation:

$$\Omega \cdot \nabla \psi(\mathbf{x}, \Omega) + \Sigma_t \psi(\mathbf{x}, \Omega) = \frac{\Sigma_s}{2\pi} \int_{2\pi} \psi(\mathbf{x}, \Omega') \, \mathrm{d}\Omega' + \frac{Q}{2\pi} \quad (1)$$

Collision Term: Rate that particles in $(\mathbf{x}, \Omega)$ collide with nuclei

Introduction to Particle Transport

Particle transport is described by the linear Boltzmann transport equation:

$$\Omega \cdot \nabla \psi(\mathbf{x}, \Omega) + \Sigma_t \psi(\mathbf{x}, \Omega) = \frac{\Sigma_s}{2\pi} \int_{2\pi} \psi(\mathbf{x}, \Omega') \, \mathrm{d}\Omega' + \frac{Q}{2\pi} \quad (1)$$

Scattering Term: Rate that particles at $\mathbf{x}$ scatter into angle Ω

Introduction to Particle Transport

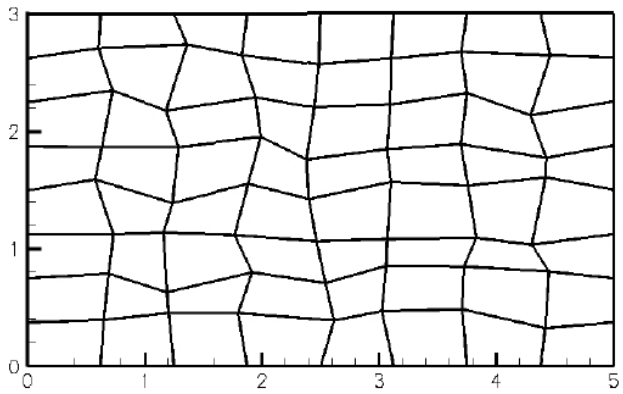
Particle transport is described by the linear Boltzmann transport equation:

$$\Omega \cdot \nabla \psi(\mathbf{x}, \Omega) + \Sigma_t \psi(\mathbf{x}, \Omega) = \frac{\Sigma_s}{2\pi} \int_{2\pi} \psi(\mathbf{x}, \Omega') \, \mathrm{d}\Omega' + \frac{Q}{2\pi} \quad (1)$$

Source Term: Rate that particles are created at position $\mathbf{x}$ and angle Ω

Introduction to the Finite Element Method

- Break the spatial domain into zones:

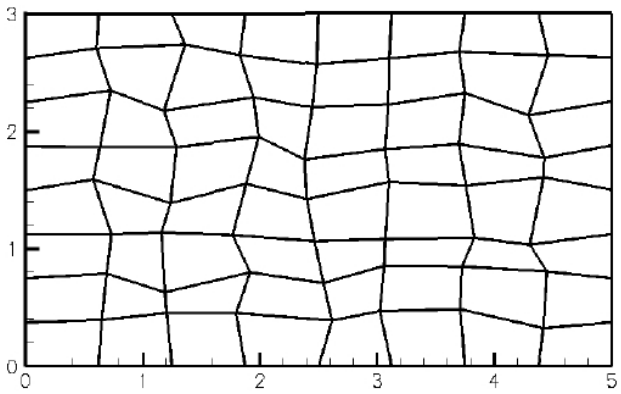


- Main idea: Represent $\psi(\mathbf{x}, \Omega)$ as an expansion in basis functions:

$$\psi(\mathbf{x}, \Omega) = \sum_{i=1}^{4} \psi_i(\Omega) b_i(\mathbf{x}) \tag{2}$$

Introduction to the Finite Element Method

- Break the spatial domain into zones:



- Main idea: Represent $\psi(\mathbf{x}, \Omega)$ as an expansion in basis functions:

$$\psi(\mathbf{x}, \Omega) = \sum_{i=1}^{4} \psi_i(\Omega) b_i(\mathbf{x}) \tag{2}$$

Introduction to the Finite Element Method

- Multiply by a weight function and integrate over the zones
- Apply the divergence theorem to the streaming term
- Substitute the expansion into the transport equation
- When we're all done we end up with, in each zone:

$$\underline{\underline{A}}\,\underline{\psi}(\Omega) = \underline{\underline{B}} \int_{2\pi} \underline{\psi}(\Omega)\,\mathrm{d}\Omega + \frac{1}{2\pi}\underline{Q} \tag{3}$$

- The matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ involve integrals of the (known) basis and weight functions

Introduction to the Finite Element Method

- Multiply by a weight function and integrate over the zones
- Apply the divergence theorem to the streaming term
- Substitute the expansion into the transport equation
- When we're all done we end up with, in each zone:

$$\underline{\underline{A}}\,\underline{\psi}(\Omega) = \underline{\underline{B}} \int_{2\pi} \underline{\psi}(\Omega)\,\mathrm{d}\Omega + \frac{1}{2\pi}\underline{Q} \tag{3}$$

- The matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ involve integrals of the (known) basis and weight functions

Introduction to the Finite Element Method

- Multiply by a weight function and integrate over the zones
- Apply the divergence theorem to the streaming term
- Substitute the expansion into the transport equation
- When we're all done we end up with, in each zone:

$$\underline{\underline{A}}\,\underline{\psi}(\Omega) = \underline{\underline{B}} \int_{2\pi} \underline{\psi}(\Omega)\,\mathrm{d}\Omega + \frac{1}{2\pi}\underline{Q} \tag{3}$$

- The matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ involve integrals of the (known) basis and weight functions

Introduction to the Finite Element Method

- Multiply by a weight function and integrate over the zones
- Apply the divergence theorem to the streaming term
- Substitute the expansion into the transport equation
- When we're all done we end up with, in each zone:

$$\underline{\underline{A}}\,\underline{\psi}(\Omega) = \underline{\underline{B}} \int_{2\pi} \underline{\psi}(\Omega)\,\mathrm{d}\Omega + \frac{1}{2\pi}\underline{Q} \tag{3}$$

- The matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ involve integrals of the (known) basis and weight functions

Introduction to the Finite Element Method

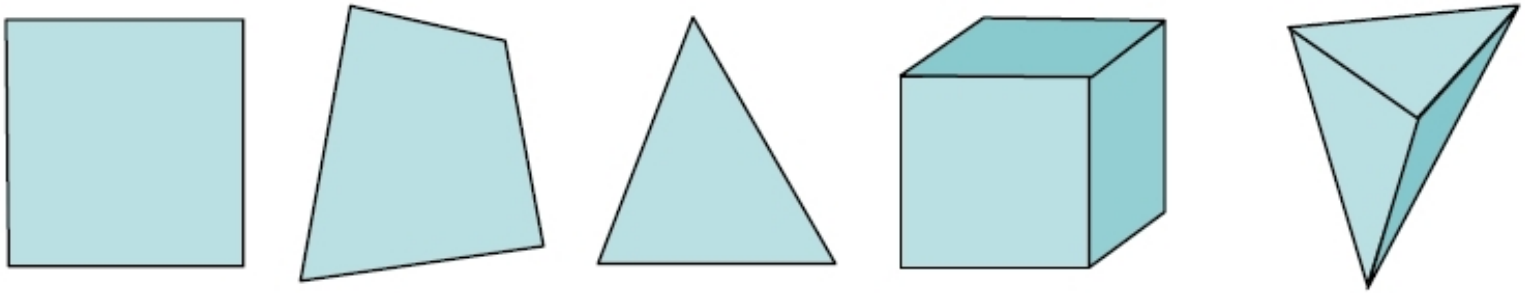
- Multiply by a weight function and integrate over the zones
- Apply the divergence theorem to the streaming term
- Substitute the expansion into the transport equation
- When we're all done we end up with, in each zone:

$$\underline{\underline{A}}\,\underline{\psi}(\Omega) = \underline{\underline{B}} \int_{2\pi} \underline{\psi}(\Omega)\,\mathrm{d}\Omega + \frac{1}{2\pi}\underline{Q} \tag{3}$$

- The matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ involve integrals of the (known) basis and weight functions

Motivation of Research

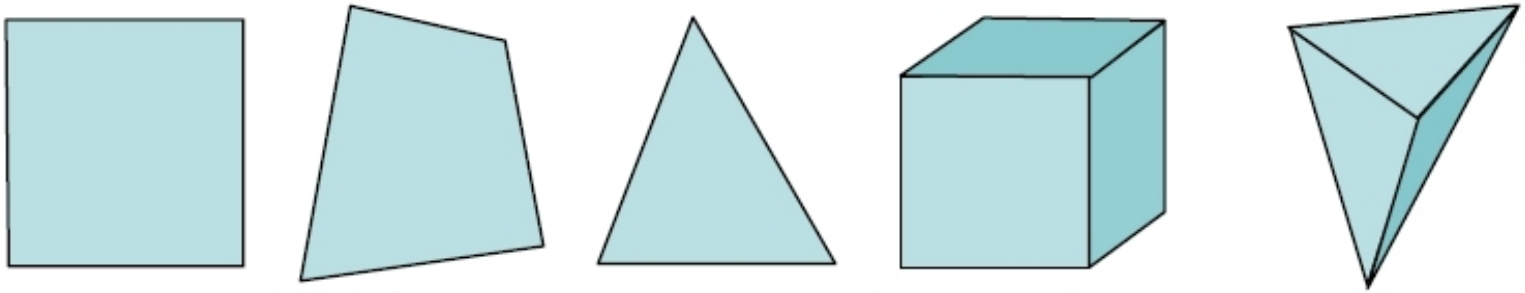
- Traditionally, finite element methods are restricted to the finite element zoo:



- Wachspress rational functions are shape functions (or interpolation functions, or basis functions) that can be built on a variety of zone shapes
- Some discretizations give unphysical solutions in the thick diffusive limit, but Adams (2001) predicted that Wachspress rational functions will have *full resolution* in the thick diffusive limit

Motivation of Research

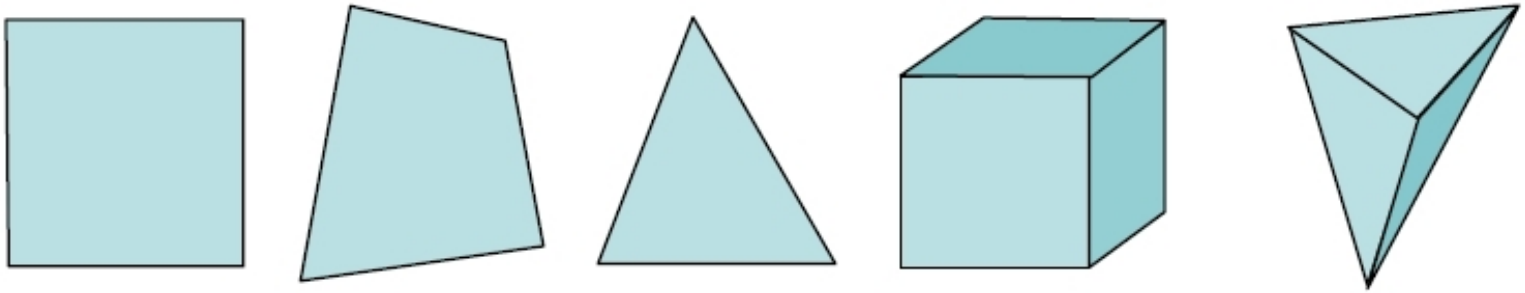
- Traditionally, finite element methods are restricted to the finite element zoo:



- Wachspress rational functions are shape functions (or interpolation functions, or basis functions) that can be built on a variety of zone shapes
- Some discretizations give unphysical solutions in the thick diffusive limit, but Adams (2001) predicted that Wachspress rational functions will have *full resolution* in the thick diffusive limit

Motivation of Research

- Traditionally, finite element methods are restricted to the finite element zoo:



- Wachspress rational functions are shape functions (or interpolation functions, or basis functions) that can be built on a variety of zone shapes
- Some discretizations give unphysical solutions in the thick diffusive limit, but Adams (2001) predicted that Wachspress rational functions will have *full resolution* in the thick diffusive limit

Outline

Properties of basis functions

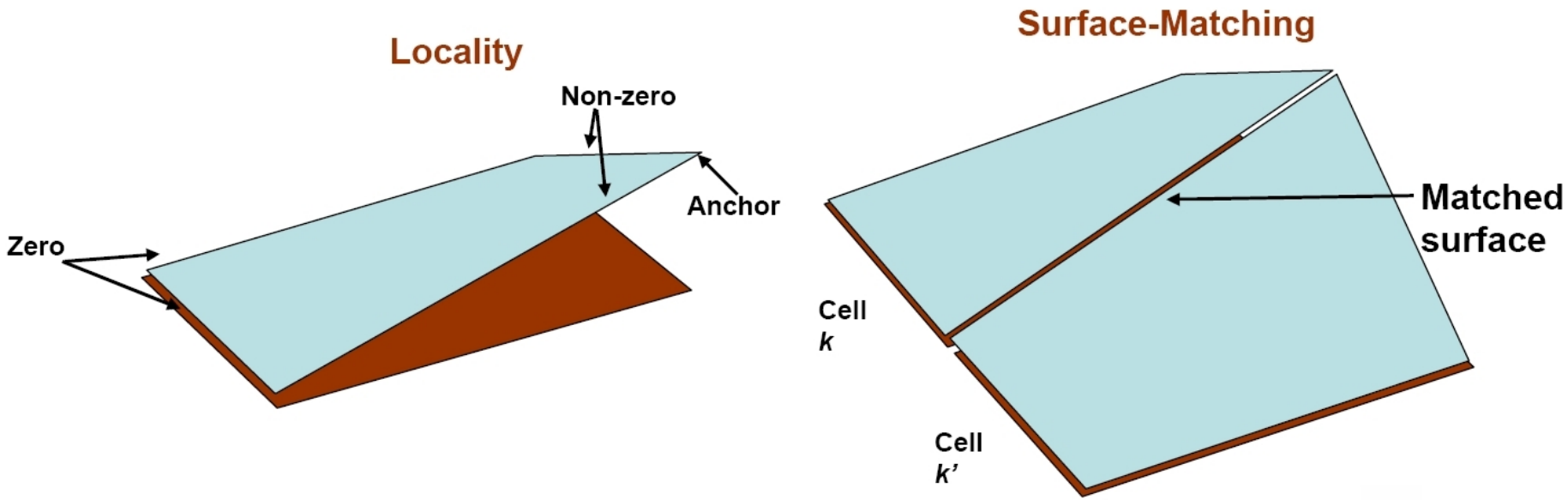
- Wachspress asserted four requirements for a “proper” basis function:
  - Continuous over the zone
  - Normalized to unity at its anchor vertex
  - Linear on the two sides adjacent to the anchor
  - Equal to zero on the sides opposite the anchor
- Two new bases are being investigated for extending the finite element method: Wachspress rational functions and piecewise-linear functions

Properties of basis functions

- Wachspress asserted four requirements for a “proper” basis function:
  - Continuous over the zone
  - Normalized to unity at its anchor vertex
  - Linear on the two sides adjacent to the anchor
  - Equal to zero on the sides opposite the anchor
- Two new bases are being investigated for extending the finite element method: Wachspress rational functions and piecewise-linear functions

Properties of basis functions

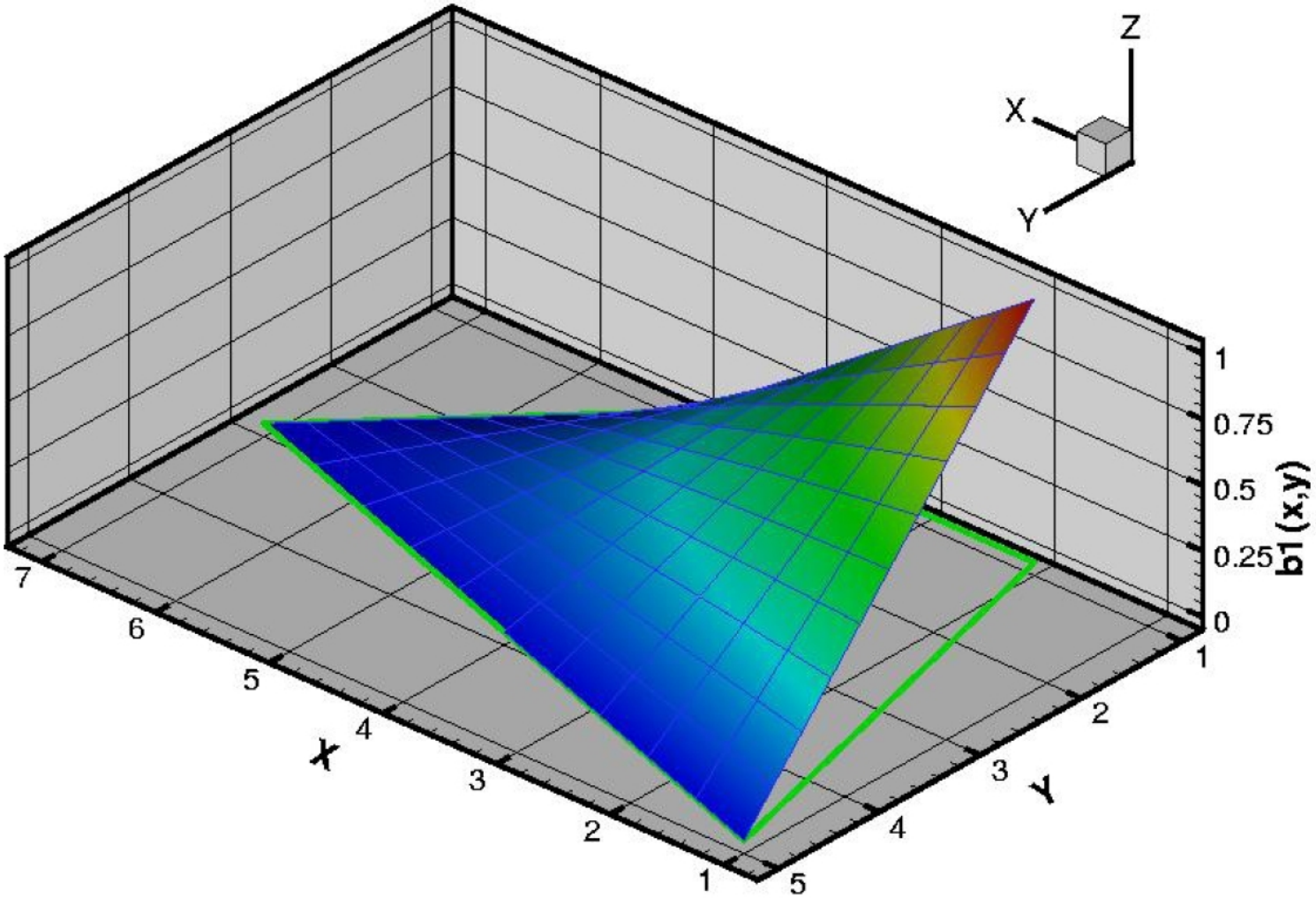
- Adams (2001) found that for full-resolution, weight functions must have locality and surface-matching



Comparison between PWL and WRF

Property	PWL	WRF
Polygons and Polyhedra	Yes	Yes
Polycons and Polypols	No	Yes
Full-resolution	Yes	Yes
Continuous in zone	Yes	Yes
Smooth in zone	No	Yes
Easily integrated	Yes	No

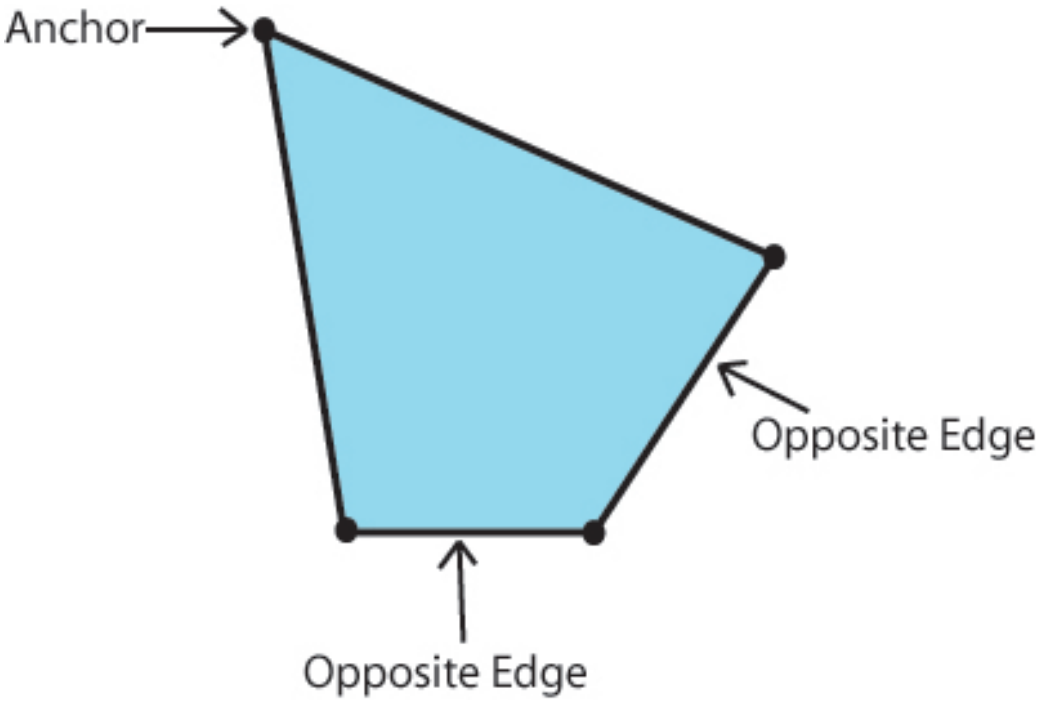
A Wachspress Rational Function



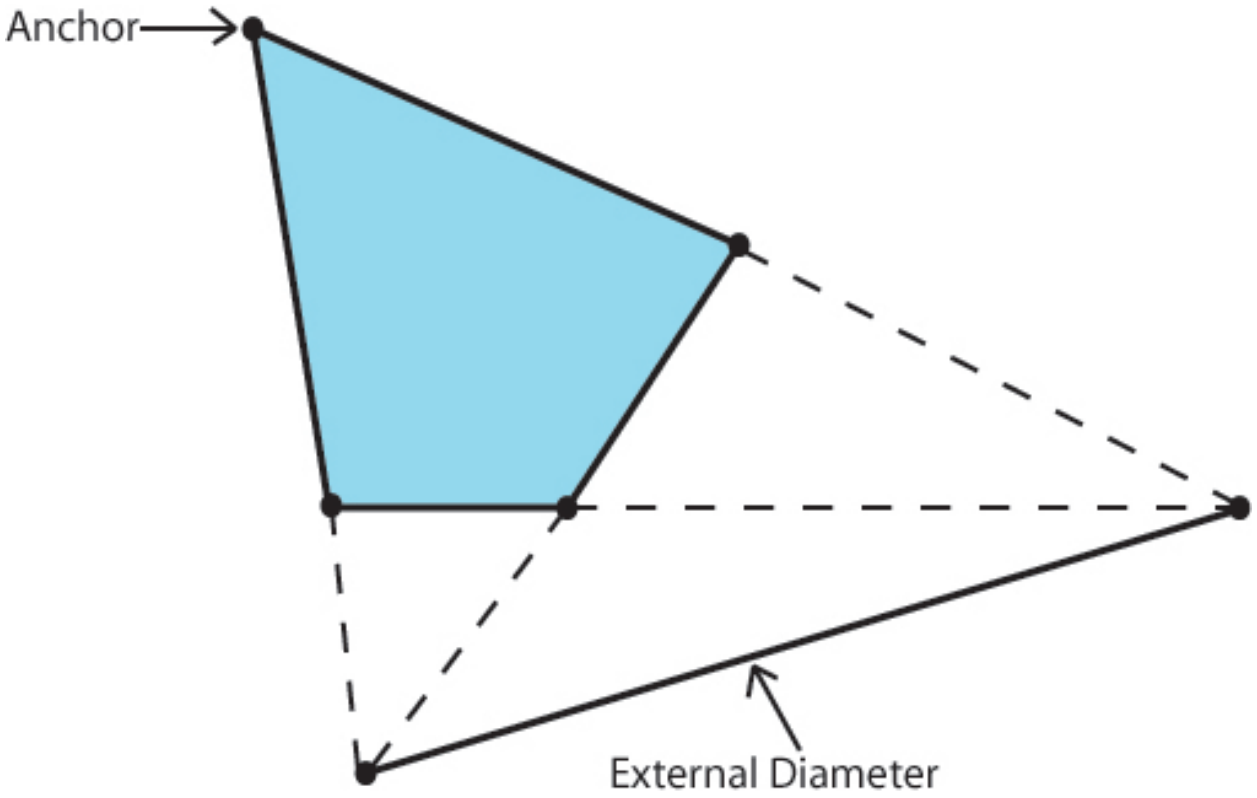
Outline

Construction of Wachspress Rational Functions

$$b_i(x,y) = k_i \frac{l_{opp1}(x,y) l_{opp2}(x,y)}{l_{ext}(x,y)} \tag{4}$$

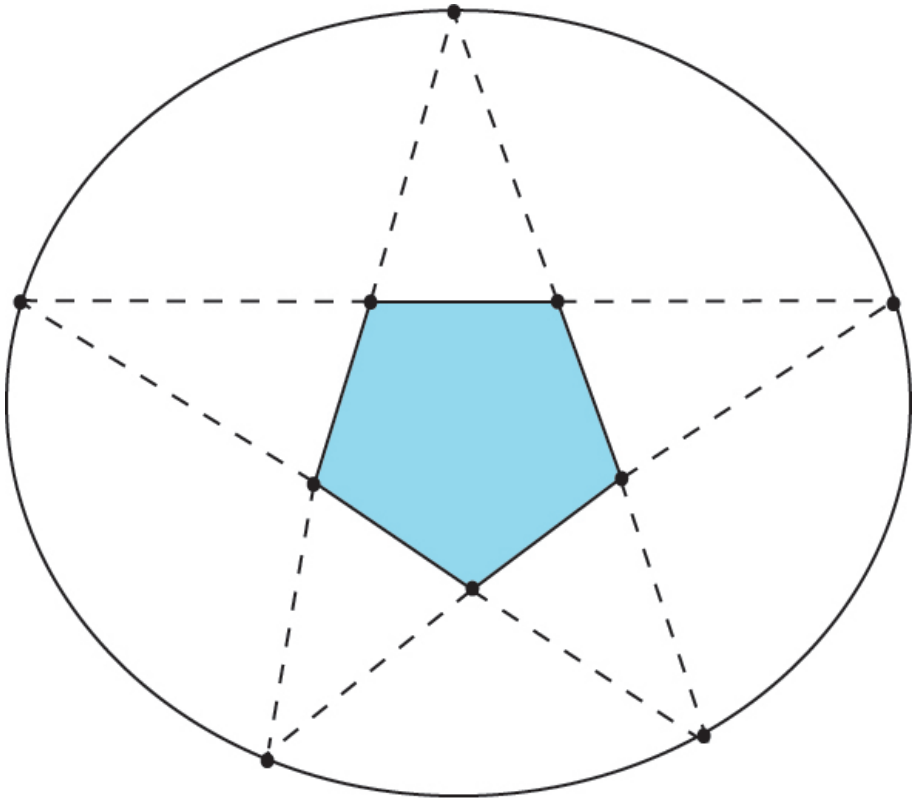


Construction of Wachspress Rational Functions



- Normalize k_i such that $b_i(x, y) = 1$ at the anchor node

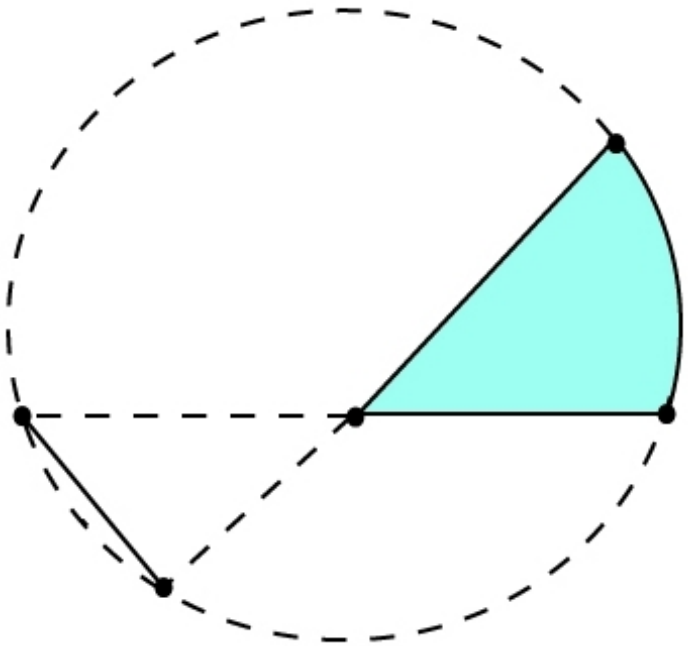
Construction of Wachspress Rational Functions



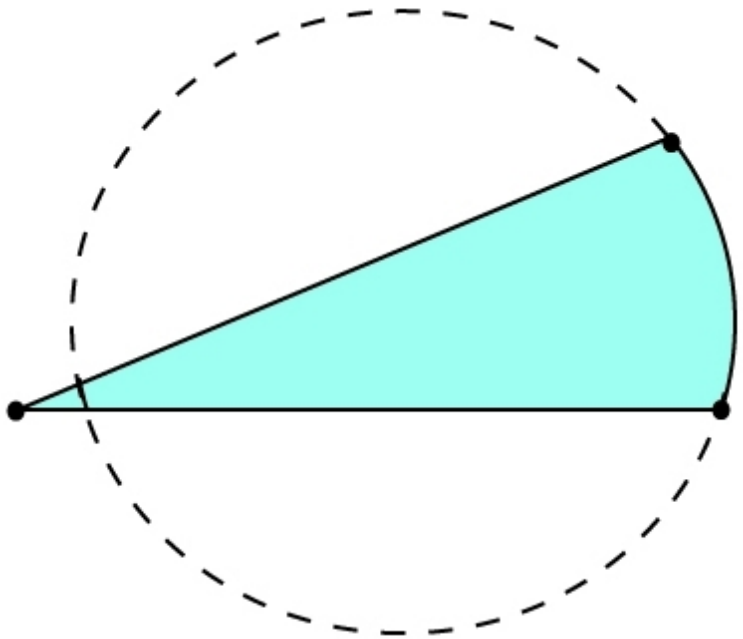
- More complex polygons can be constructed using Dasgupta's (2003) method

Construction of Wachspress Rational Functions

This works:



This doesn't:



Outline

Integration of Wachspress Rational Functions

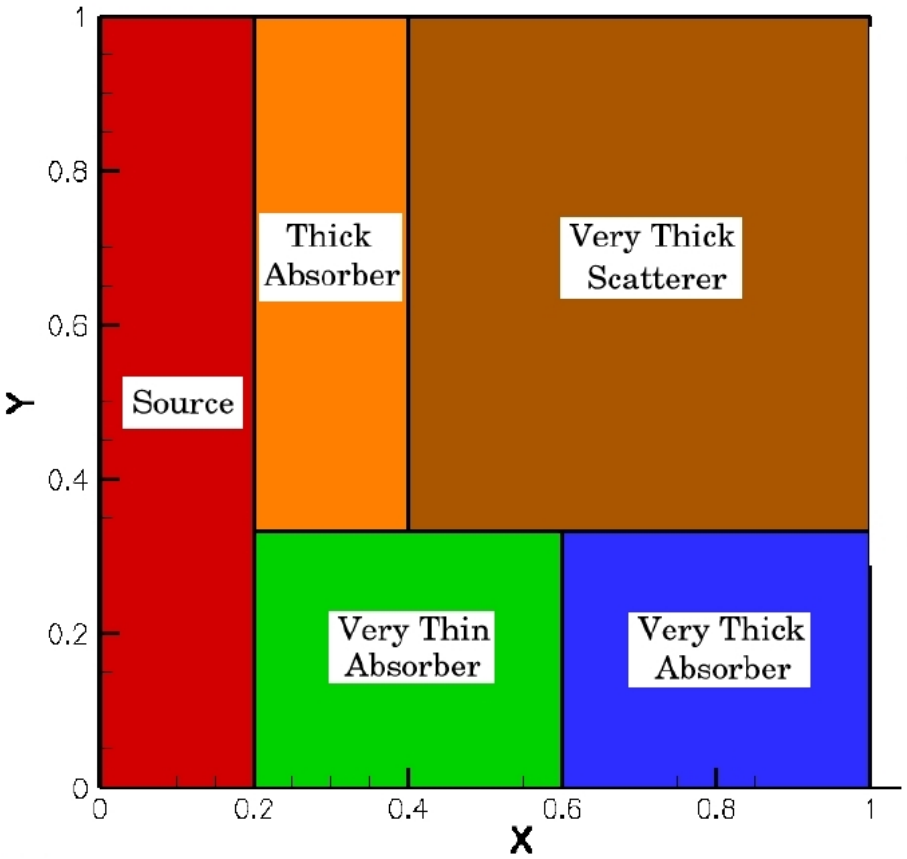
- Isoparametric Mapping
  - Maps the quadrilateral onto an isoparametric square
  - Integral done numerically in isoparametric space
  - Only for quadrilaterals!
- Dasgupta Integration (2003)
  - Repeatedly apply Divergence Theorem
  - End up with integrals around zone edges
  - Integrand becomes very complex
  - Requires a computer algebra system!

Integration of Wachspress Rational Functions

- Isoparametric Mapping
  - Maps the quadrilateral onto an isoparametric square
  - Integral done numerically in isoparametric space
  - Only for quadrilaterals!
- Dasgupta Integration (2003)
  - Repeatedly apply Divergence Theorem
  - End up with integrals around zone edges
  - Integrand becomes very complex
  - Requires a computer algebra system!

Outline

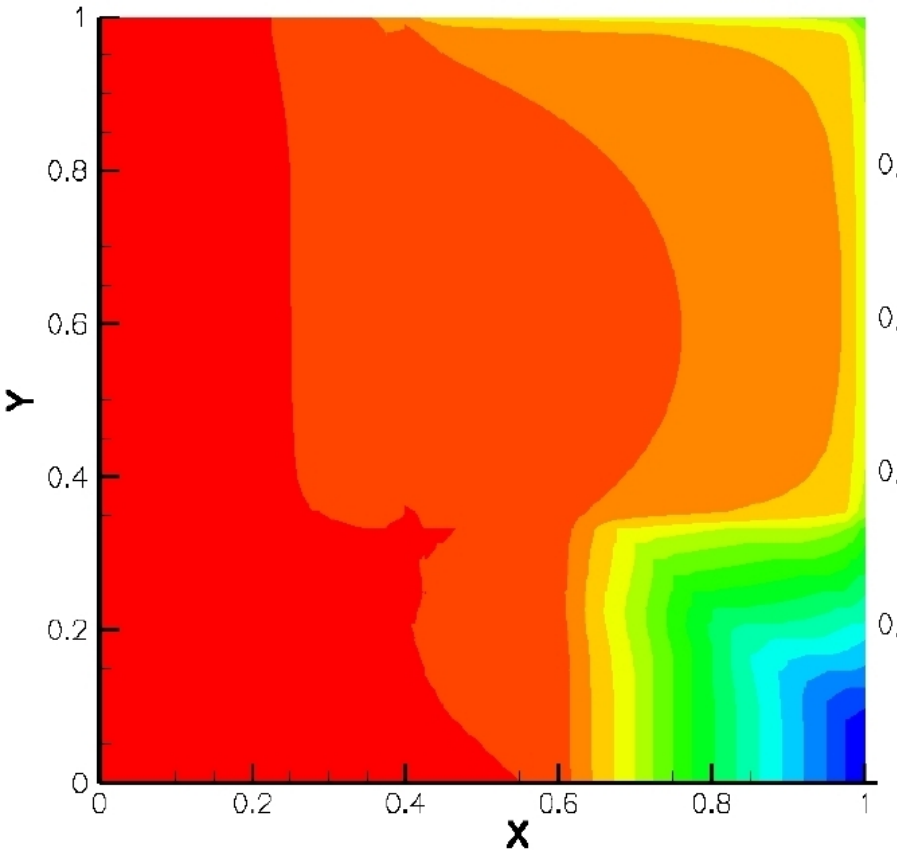
Strongly Heterogeneous Problem, Adams, (1991)



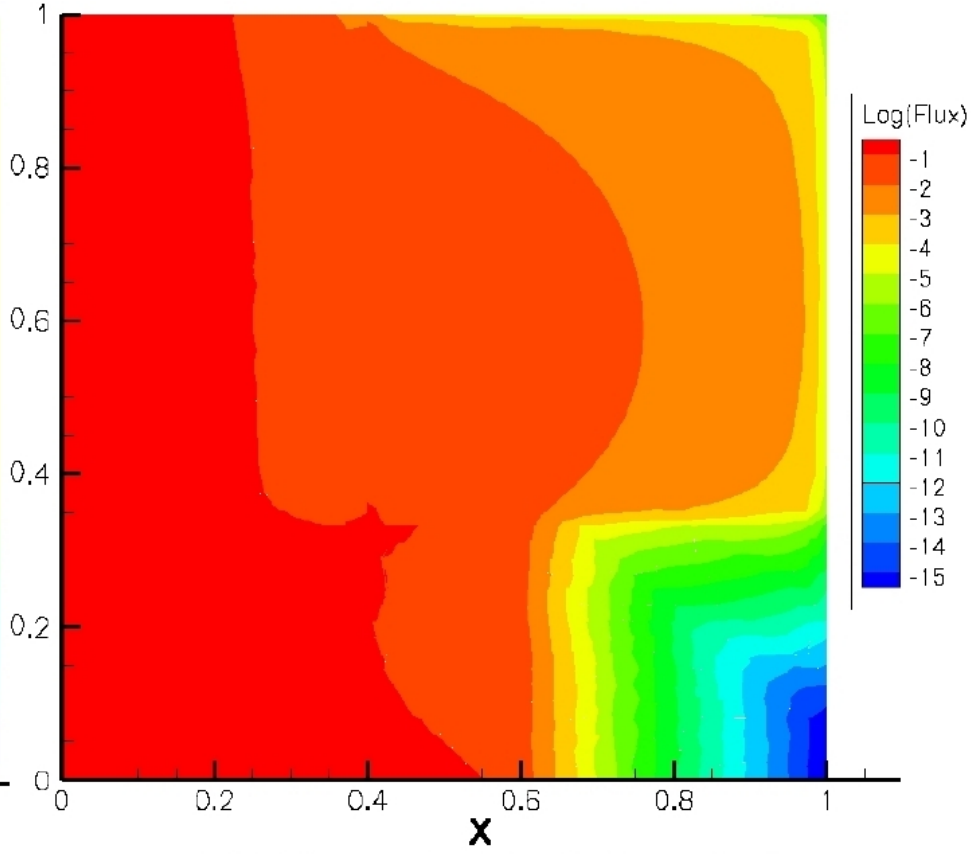
Material Region	σ_t [cm^{-1}]	σ_s [cm^{-1}]
Source	1.0	1.0
Very Thin Absorber	0.0001	0.0
Thick Absorber	10.0	0.0
Very Thick Absorber	100.0	0.0
Very Thick Scatterer	1000.0	1000.0

Problem was accelerated using Asymptotic-P1 DSA

Strongly Heterogeneous Problem, Adams, (1991)

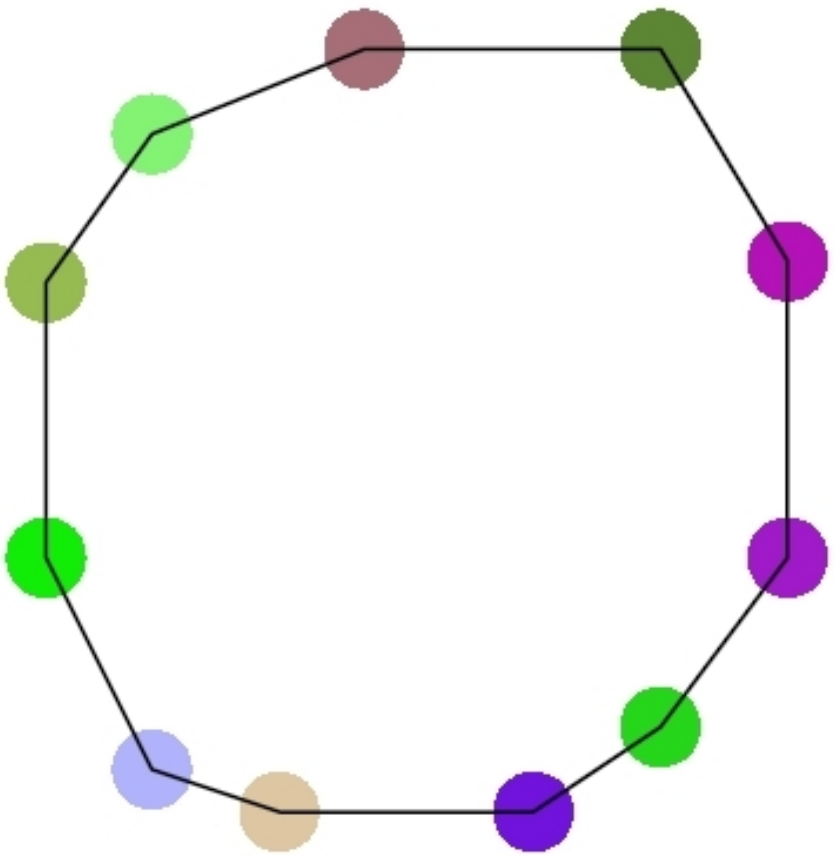


FL Orthogonal Mesh Results



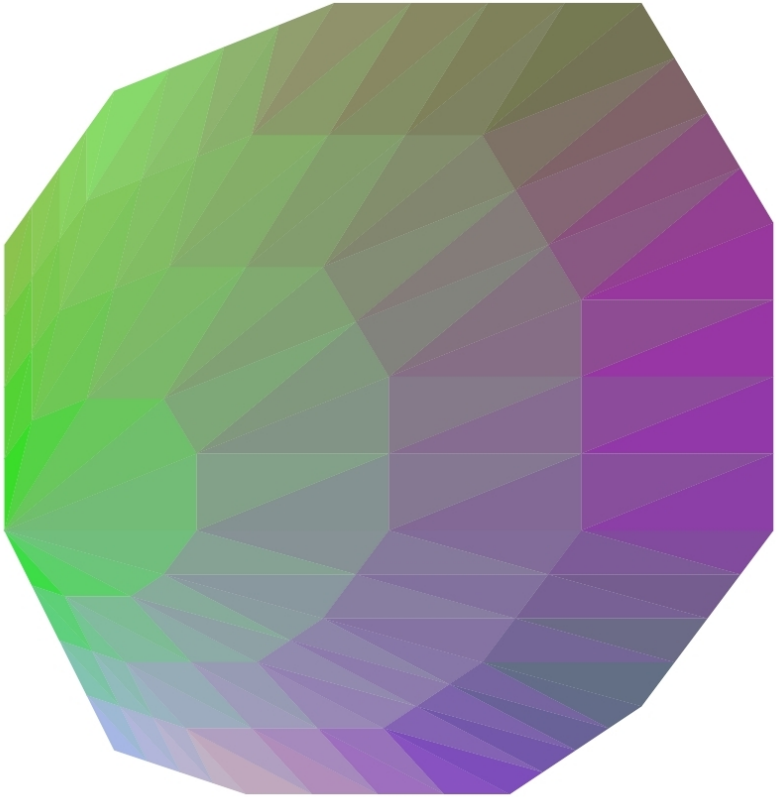
FL Skewed Mesh Results

Wachspress Rational Functions in Computer Graphics (Dasgupta, Malsch, 2001)



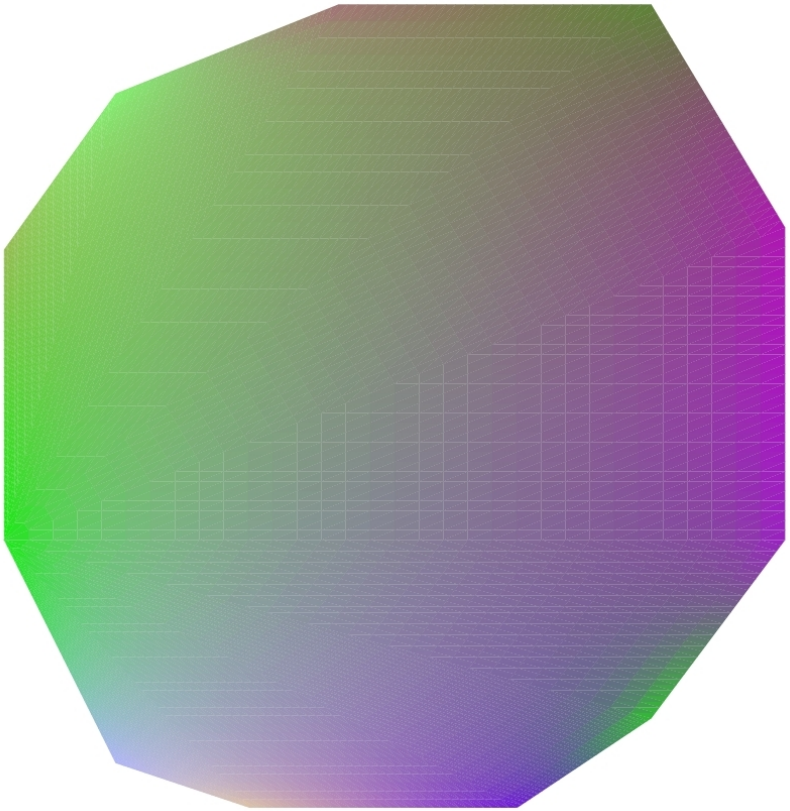
Wachspress Rational Functions in Computer Graphics (Dasgupta, Malsch, 2001)

Using triangular interpolation:



Wachspress Rational Functions in Computer Graphics (Dasgupta, Malsch, 2001)

Using Wachspress interpolation:



Conclusions

- Wachspress rational functions provide smooth interpolation over polygonal domains
- Wachspress rational functions can be integrated over quadrilateral domains numerically
- Wachspress rational functions provide a full-resolution discretization to the particle transport equation
- Wachspress rational functions can provide numerically robust solutions to the particle transport equation in the diffusive limit

Conclusions

- Wachspress rational functions provide smooth interpolation over polygonal domains
- Wachspress rational functions can be integrated over quadrilateral domains numerically
- Wachspress rational functions provide a full-resolution discretization to the particle transport equation
- Wachspress rational functions can provide numerically robust solutions to the particle transport equation in the diffusive limit

Conclusions

- Wachspress rational functions provide smooth interpolation over polygonal domains
- Wachspress rational functions can be integrated over quadrilateral domains numerically
- Wachspress rational functions provide a full-resolution discretization to the particle transport equation
- Wachspress rational functions can provide numerically robust solutions to the particle transport equation in the diffusive limit

Conclusions

- Wachspress rational functions provide smooth interpolation over polygonal domains
- Wachspress rational functions can be integrated over quadrilateral domains numerically
- Wachspress rational functions provide a full-resolution discretization to the particle transport equation
- Wachspress rational functions can provide numerically robust solutions to the particle transport equation in the diffusive limit

Future Work

- Investigate construction of Wachspress rational functions in 3-D
- Investigate behavior on concave zones
- Faster integration!

Future Work

- Investigate construction of Wachspress rational functions in 3-D
- Investigate behavior on concave zones
- Faster integration!

Future Work

- Investigate construction of Wachspress rational functions in 3-D
- Investigate behavior on concave zones
- Faster integration!

Acknowledgements

This research was funded by the DOE Computational Science Graduate Fellowship