Natural Neighbors and Voronoi Tessellations in Computational Mechanics

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Jigsaw Tessellations Workshop

Lorentz Center, Leiden

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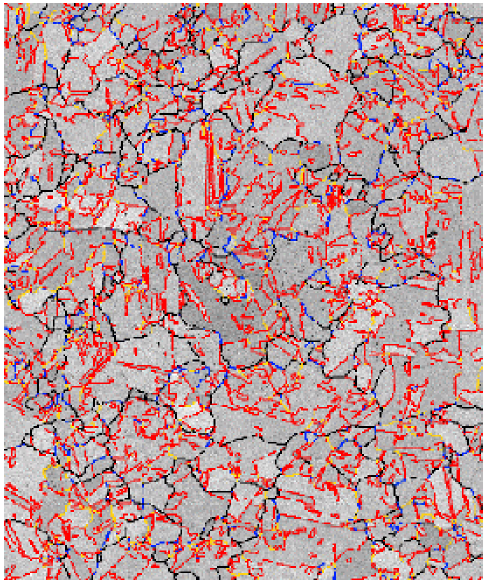
Collaborators and Contributors

- Numerical simulations using natural element method are courtesy of Professor Elias Cueto (Universidad de Zaragoza, Spain) and Dr. Mike Puso (LLNL)
- Fracture on Voronoi networks (with Professor John Bolander, UC Davis)
- Polygonal finite elements and adaptive computations on quadtrees (with Alireza Tabarraei, UC Davis)

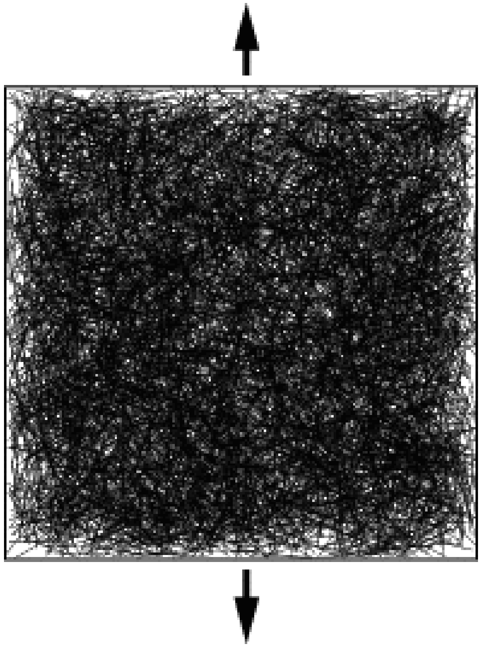
Voronoi Tesellations in Materials and Mechanics

Polycrystalline alloy



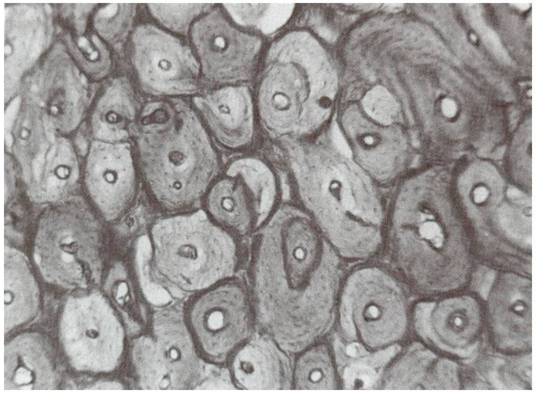
(Courtesy of Kumar, LLNL)

Fiber-matrix composite



(Bolander and S, PRB, 2004)

Osteonal bone

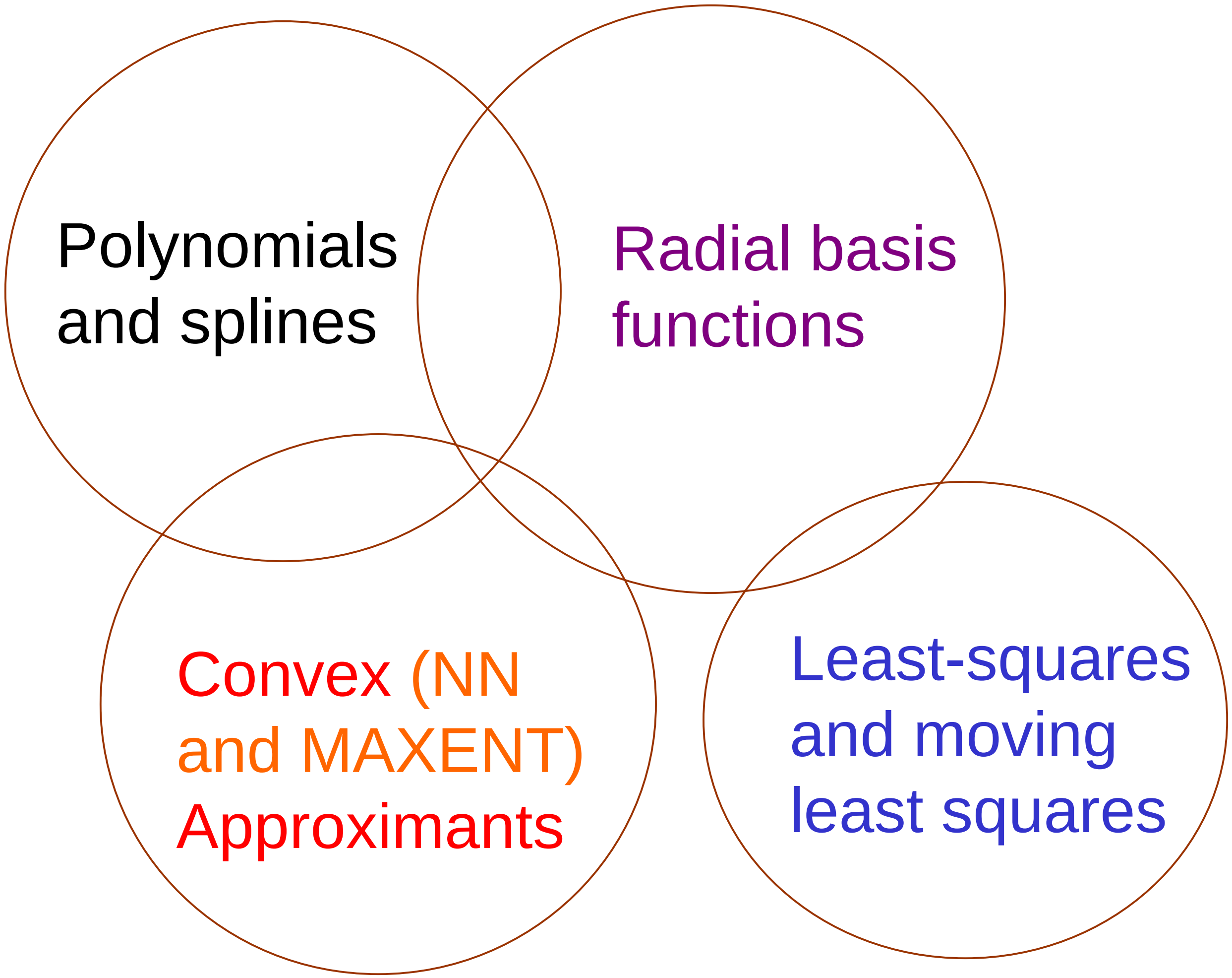


(Martin and Burr, 1989)

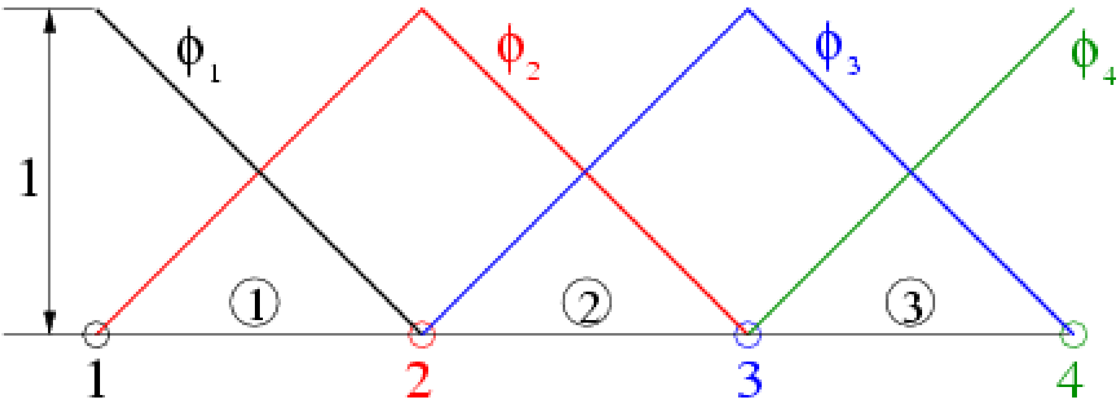
Outline

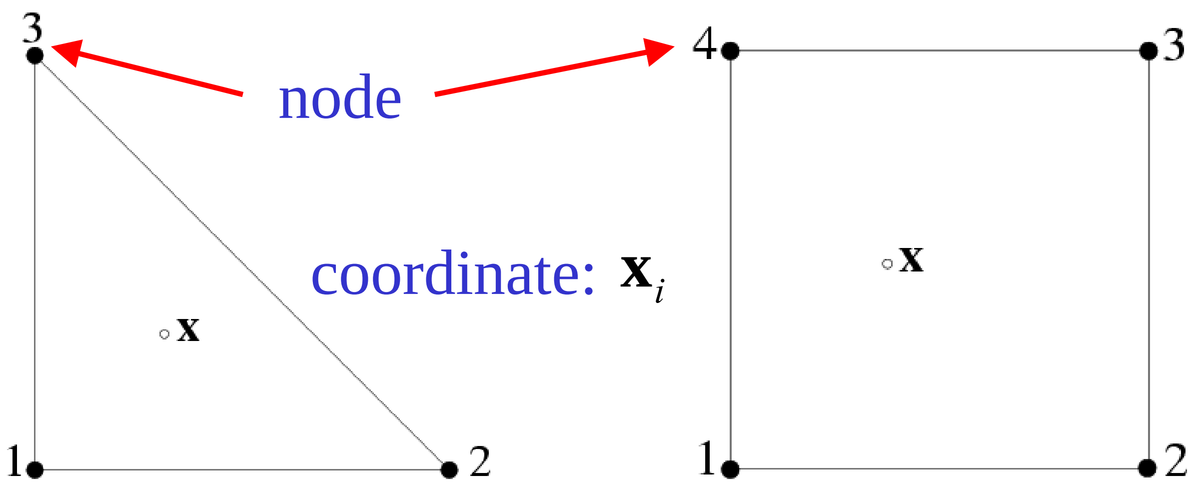
- Meshfree/Gridless Approximation Schemes
- Natural Neighbor (NN) Interpolants
- Fracture on Voronoi Networks
- Polygonal Finite Element Methods
- Closure and Outlook

Meshfree Approximation Schemes

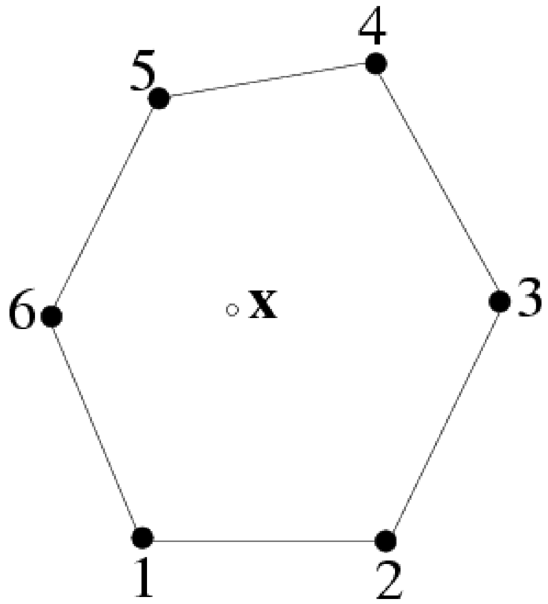


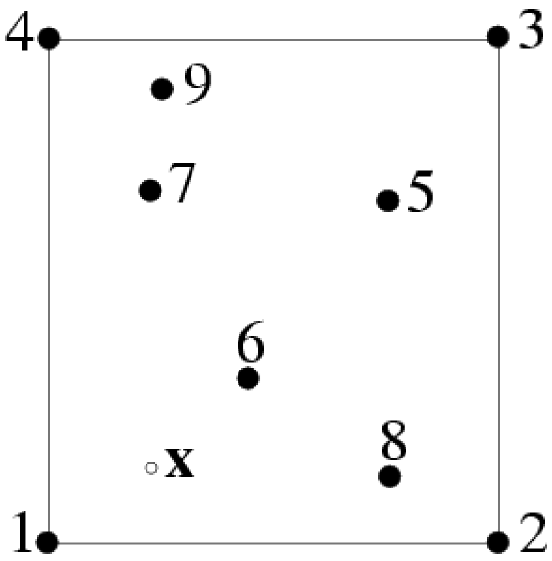
Polynomials and Finite Elements in 1D and 2D





Arbitrary Nodal Discretization





$$u^h(\mathbf{x}) = \sum_{i=1}^{n} \phi_i(\mathbf{x})\, u_i$$

shape (basis) function

Desirable Properties of Shape Functions

- Affine Combination: $\sum_i \phi_i(\mathbf{x}) = 1, \quad \sum_i \phi_i \mathbf{x}_i = \mathbf{x}$

  ensures convergence

- Convex combination: $\phi_i \geq 0$

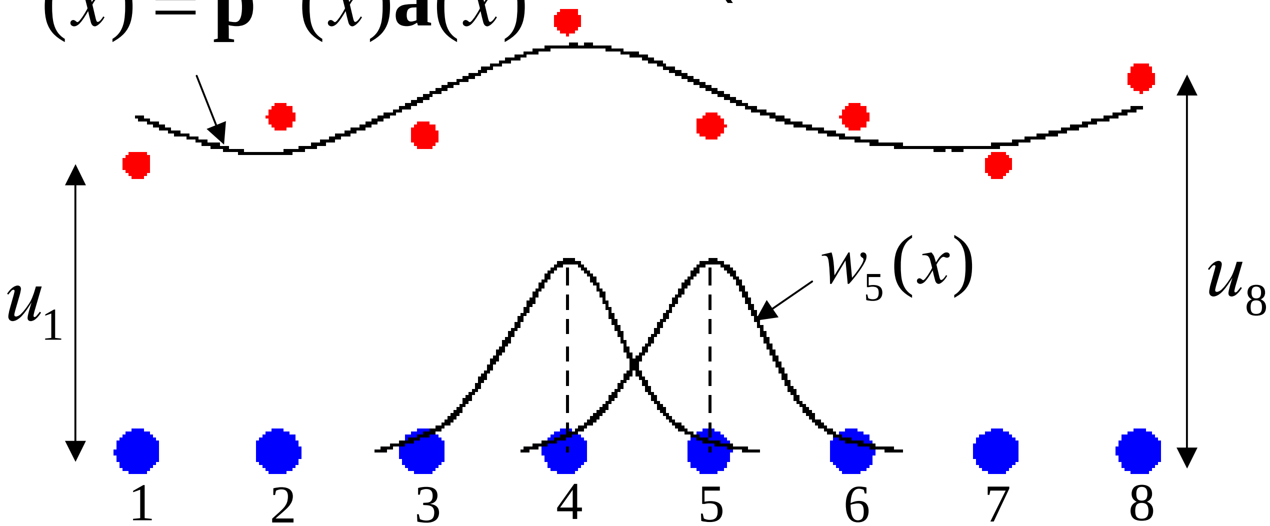
- Regularity: $\phi_i \in C^\infty(\Omega)$

- Piece-wise linear on the boundary: C^0 conformity and for imposing essential boundary conditions

Moving Least Squares (MLS) Approximant

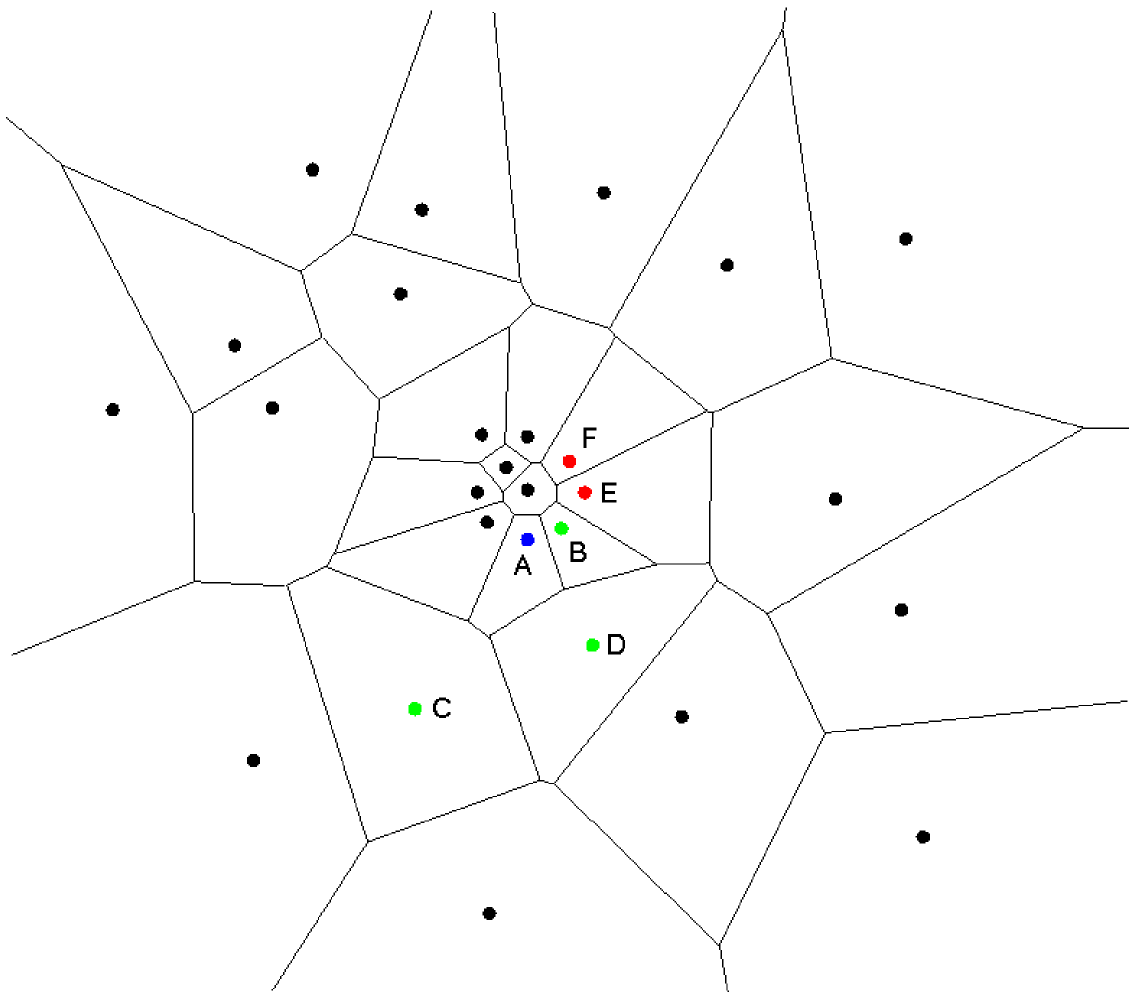
(Lancaster & Salkauskas, 1982)

$$u^h(x) = \mathbf{p}^T(x)\mathbf{a}(x)$$

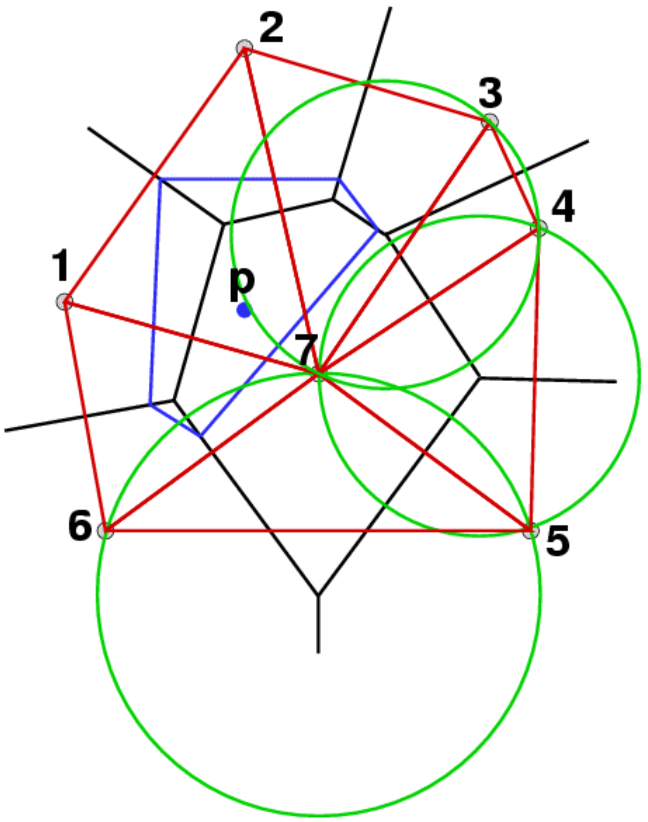


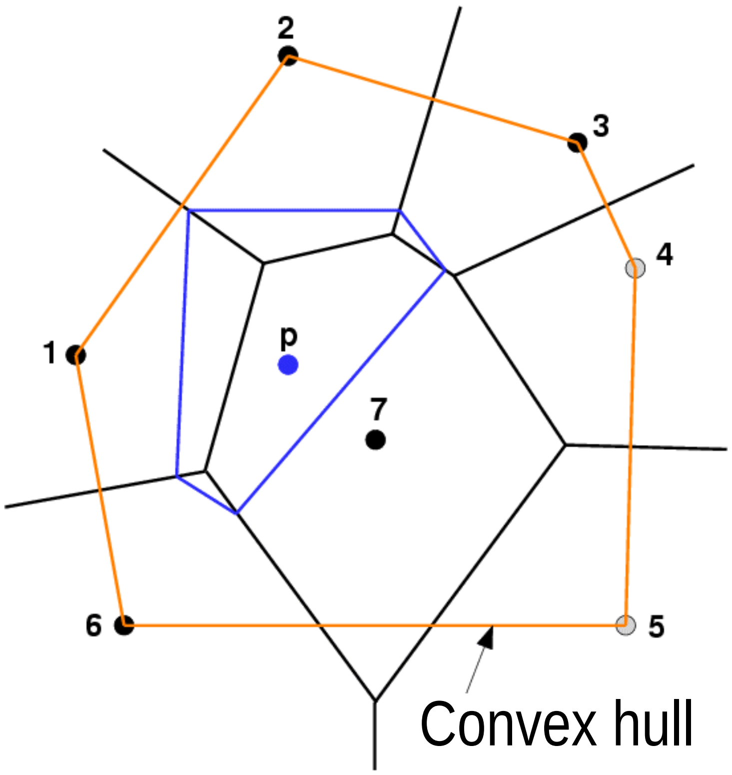
$$\min_{\mathbf{a}} \begin{pmatrix} J[\mathbf{a}] = \sum_{i=1}^{n} w_i(x)[\mathbf{p}^T(x_i)\mathbf{a}(x) - u_i]^2 \\ = \left\| \mathbf{W}^{1/2}(\mathbf{P}^T\mathbf{a} - \mathbf{u}) \right\|_2^2 \end{pmatrix}, \quad \mathbf{p} = [1, x, \ldots, x^m]^T$$

Voronoi Neighbors



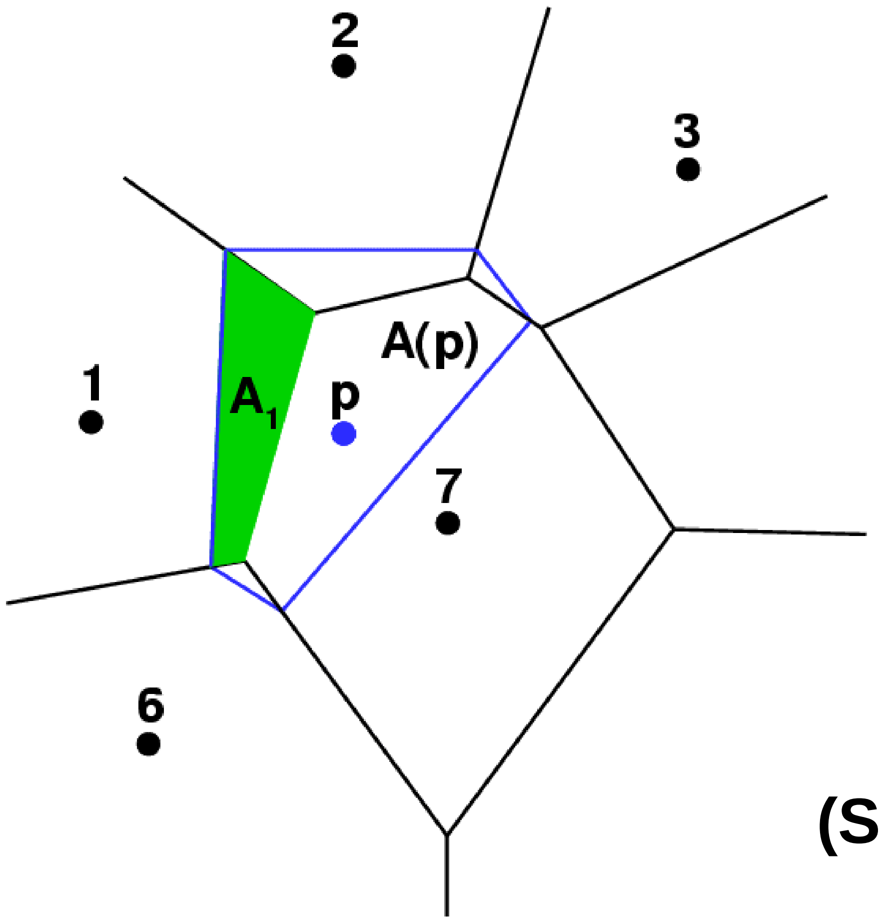
Natural Neighbors and NN-Interpolants





p lies outside the circumcircles in green

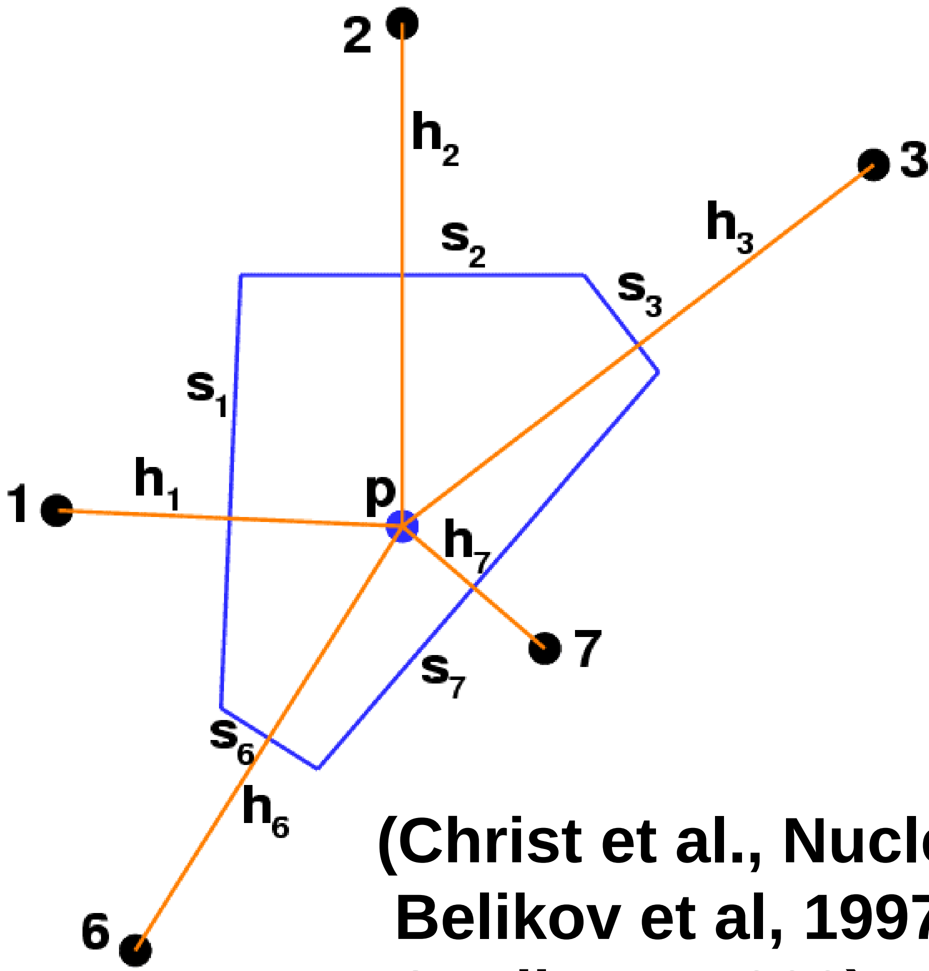
Sibson Interpolant



$$\phi_i(p) = \frac{A_i(p)}{A(p)}$$

(Sibson, 1980)

Laplace Interpolant



$$\alpha_i(p) = \frac{s_i(p)}{h_i(p)}$$

$$\phi_i(p) = \frac{\alpha_i(p)}{\sum_j \alpha_j(p)}$$

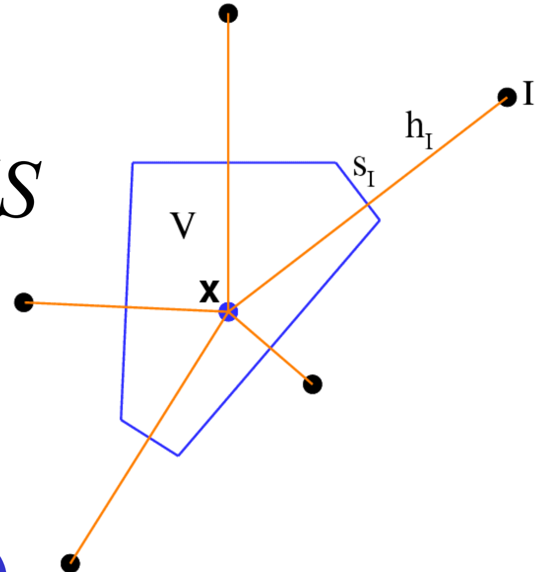
(Christ et al., Nuclear Physics B, 1982; Belikov et al, 1997; Hiyoshi and Sugihara, 1999)

Properties

- Non-negative and PU: $0 \le \phi_i \le 1, \sum_i \phi_i(\mathbf{x}) = 1$
- Interpolate data: $\phi_i(\mathbf{x}_j) = \delta_{ij}$
- Linear precision: $\sum_i \phi_i \mathbf{x}_i = \mathbf{x}$
- Smoothness: $\phi_i^{\mathrm{LAP}} \in C^0(\Omega),\ \phi_i^{\mathrm{S}} \in C^1(\Omega \setminus \mathbf{x}_j)$
- Linear essential boundary conditions can be exactly imposed

Linear Precision (Laplace Interpolant)

Gauss's theorem: $$\int_V \nabla f \, dV = \int_S f \mathbf{n} \, dS$$



Let $f = 1$: $$\int_S \mathbf{n} \, dS = \mathbf{0}$$

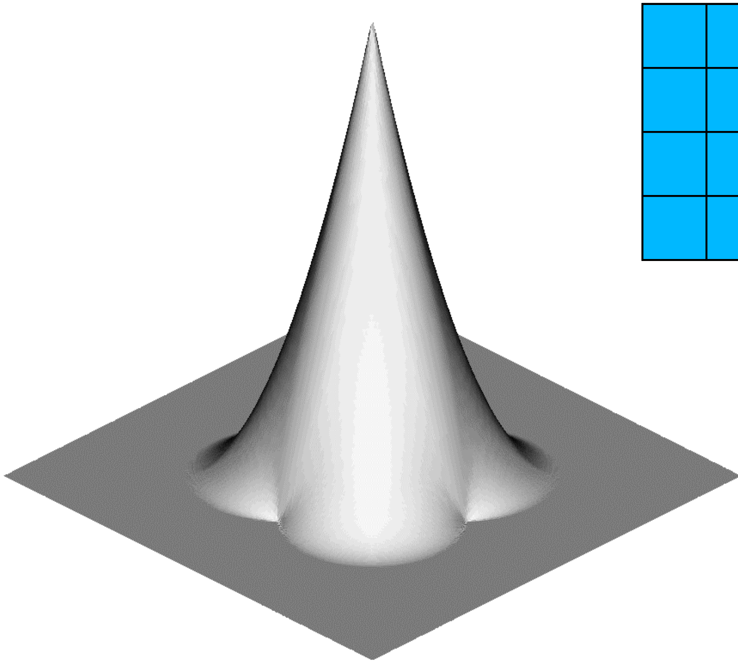
(Minkowski theorem)

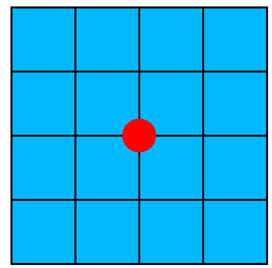
$$\therefore \sum_i \frac{\mathbf{x}_i - \mathbf{x}}{\| \mathbf{x}_i - \mathbf{x} \|} s_i(\mathbf{x}) = \mathbf{0} \quad \Rightarrow \quad \sum_i \frac{\mathbf{x}_i - \mathbf{x}}{h_i(\mathbf{x})} s_i(\mathbf{x}) = \mathbf{0}$$

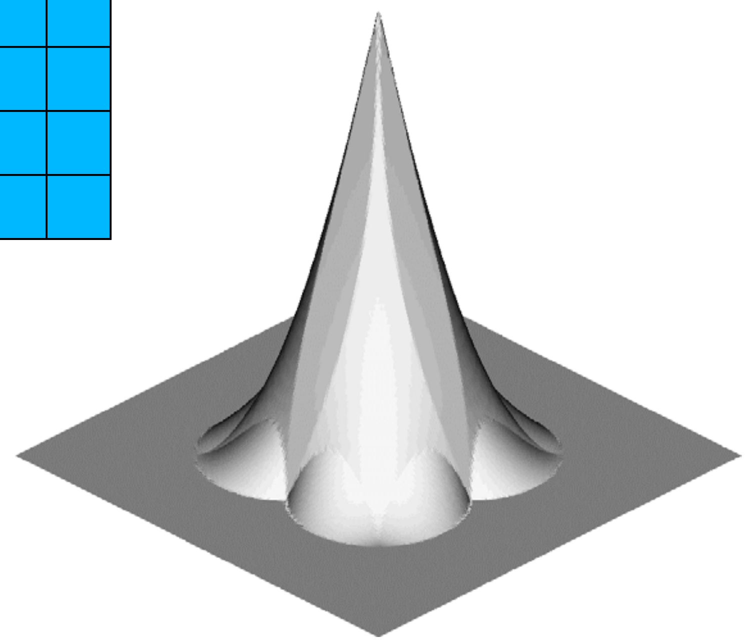
$$\Rightarrow \boxed{\sum_i \phi_i(\mathbf{x}) \mathbf{x}_i = \mathbf{x}}$$

(Christ et al., 1982)

Basis Function Plots







Sibson

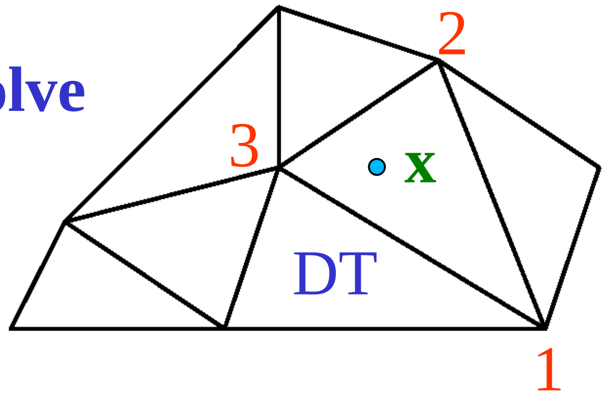
Laplace

Meshfree Approximations in CG/Graphics

- Surface Reconstruction: Boissonnat (France)
- Polygonal Graphics Models: Warren (Rice University), Floater (Norway), Schroeder and Desbrun (Caltech)
- Fracture and Failure Animations: Turk (Georgia Tech.) O’Brien (UC Berkeley), Mark Pauly (Stanford), etc.
- Surface and Volume Visualization at UC Davis: Faculty (Graduate Student) are Bernd Hamann (Sung Park), Ken Joy (Chris Co), and Nina Amenta (Yong Kil)

Galerkin Finite Element and Meshfree Methods

FEM: Function-based method to solve partial differential equations



steady-state heat conduction

Strong Form: $-\nabla^2 u = f \text{ in } \Omega, \; u = \bar{u} \text{ on } \partial\Omega$

Variational (Weak) Form:

$$u^* = \arg\min_{u} \left[\pi[u] = \int_{\Omega} \left(\nabla u \bullet \nabla u - 2fu \right) d\Omega \right]$$

Galerkin Methods (Cont'd)

Variational Form

$$\delta \pi[u] = \delta \int_{\Omega} \left(\nabla u \bullet \nabla u - 2 f u \right) d\Omega = 0$$

$$\int_{\Omega} \nabla \delta u \bullet \nabla u \, d\Omega - \int_{\Omega} f \, \delta u \, d\Omega = 0 \quad \forall \, \delta u \in H_0^1(\Omega)$$

Finite-dimensional approximations for trial function and admissible variations

$$u^h(\mathbf{x}) = \sum_j \phi_j(\mathbf{x}) u_j, \;\; \delta u^h = \phi_i(\mathbf{x})$$

Galerkin Methods (Cont'd)

Discrete Weak Form and Linear System of Equations

$$\int_{\Omega} \nabla \delta u^h \bullet \nabla u^h \, d\Omega = \int_{\Omega} f \, \delta u^h \, d\Omega$$

$$\sum_{j=1}^{M} \left(\int_{\Omega} \nabla \phi_i \bullet \nabla \phi_j \, d\Omega \right) u_j = \int_{\Omega} f \phi_i \, d\Omega$$

$$\mathbf{K}\mathbf{u} = \mathbf{f}$$

$$K_{ij} = \int_{\Omega} \nabla \phi_i \bullet \nabla \phi_j \, d\Omega, \quad f_i = \int_{\Omega} f \phi_i \, d\Omega$$

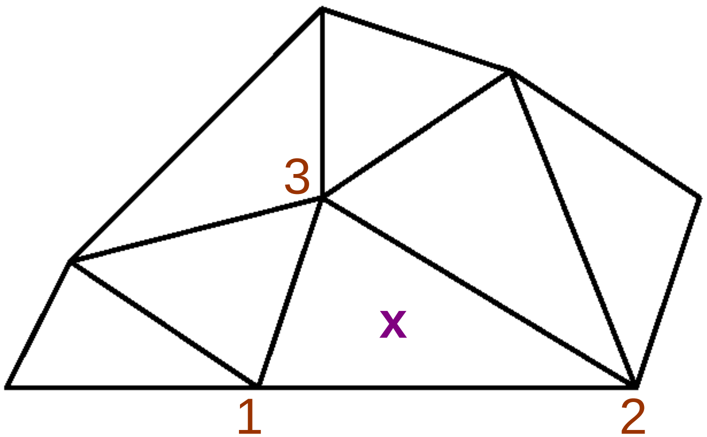
Finite Element Method

$$u^h(\xi,\eta) = \sum_{j=1}^{M} N_j(\xi,\eta) u_j$$

shape function

$$\delta u^h(\xi,\eta) = N_i(\xi,\eta),$$

$$i = 1, 2, \ldots, M$$

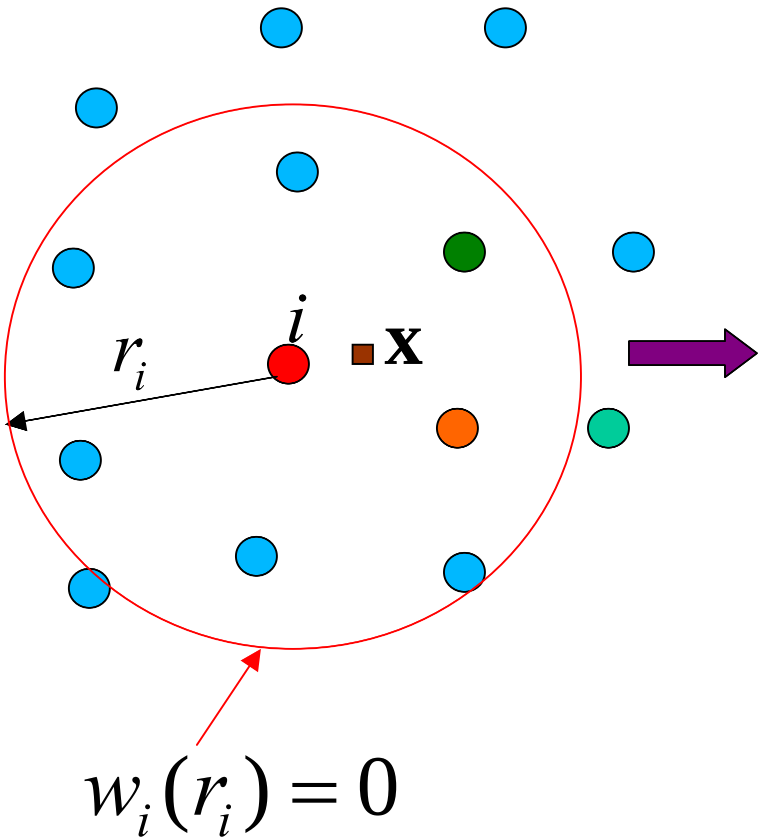


- Facilitates modeling complex-geometries
- Local interpolant (polynomials in ξ-space)
- ``Exact'' numerical integration
- Accuracy, robustness, and convergence

Meshfree Methods

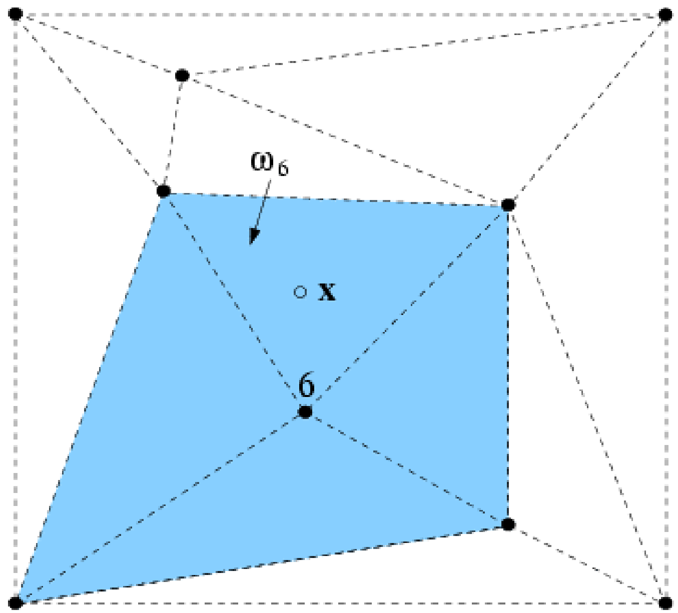
(Reviews: Belytschko et al., 1996; Li and Liu, 2002)

(Atluri and Shen, 2002; Liu, 2003; Li and Liu, 2004)

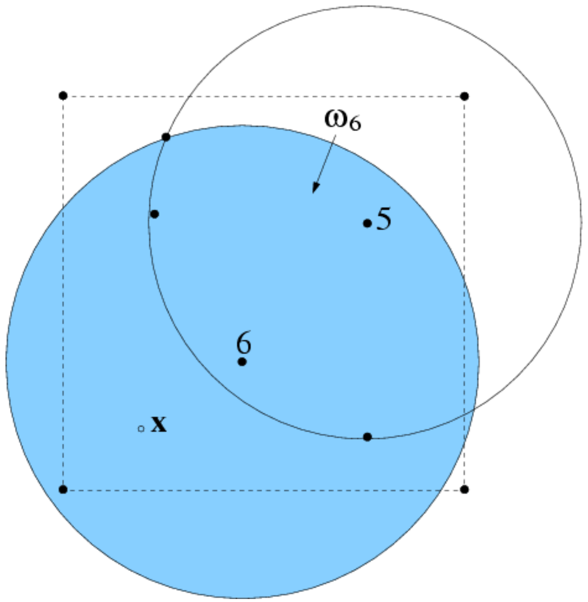


- SPH, RBFs, and MLS
- Natural neighbors (NEM)
  (Braun and Sambridge, 1995)
- *Maximum entropy approxi-mants*
  (S, 2004/2005; Arroyo and Ortiz, 2006)

Nodal Shape Function Support



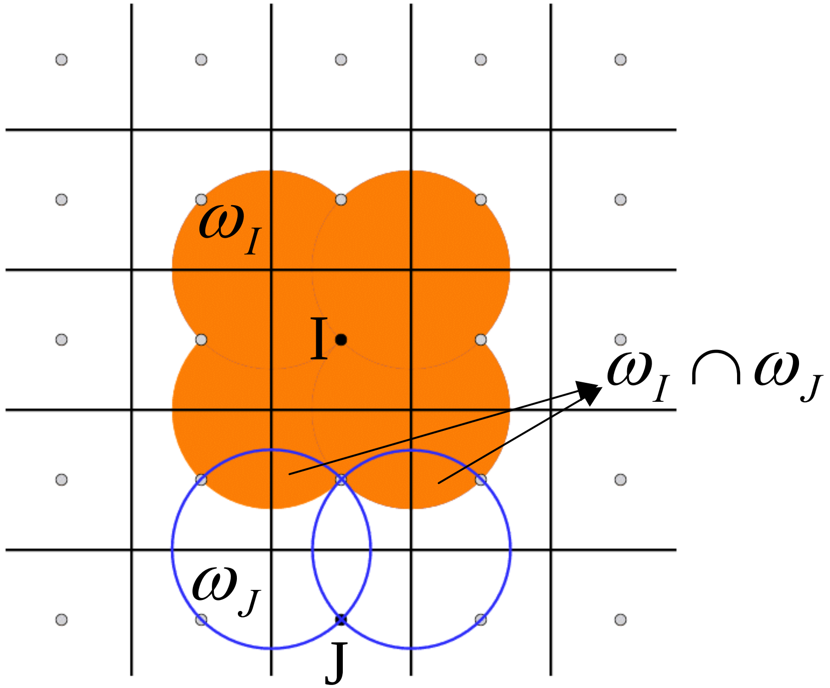
FEM



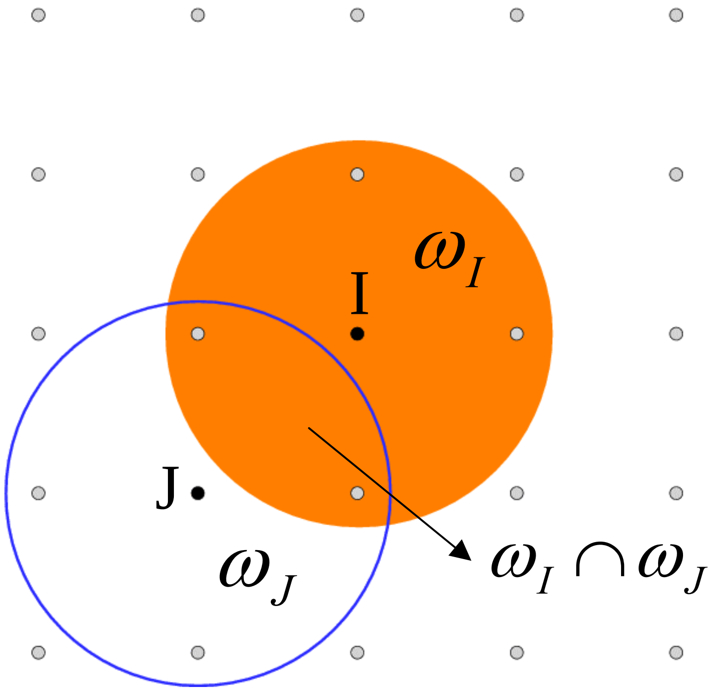
MLS

- Compact support
- Boundary behavior

Support (Cont'd)



Natural Neighbor



MLS

Important and Unresolved Issues

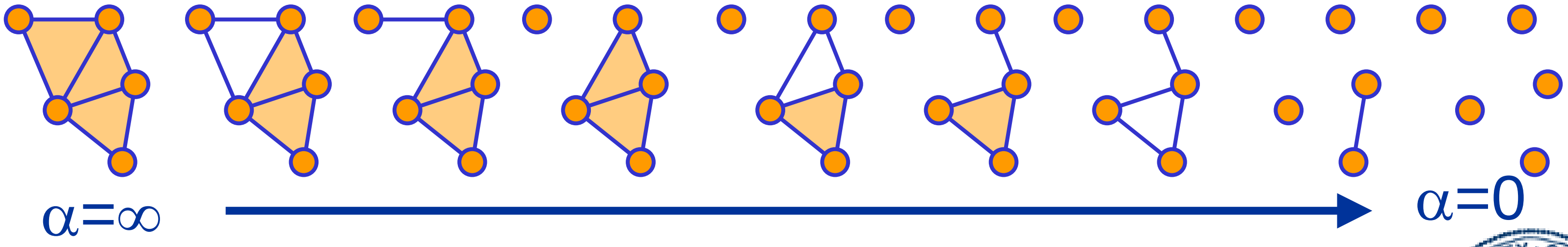
- Imposing essential boundary conditions
- Numerical integration of the Galerkin weak form
- Handling non-convex boundaries (especially pertinent in large deformations)
- Stability and robustness of the method

NEM and α-Shapes

- Shape constructors are geometric structures that transform finite point sets into continuous shapes

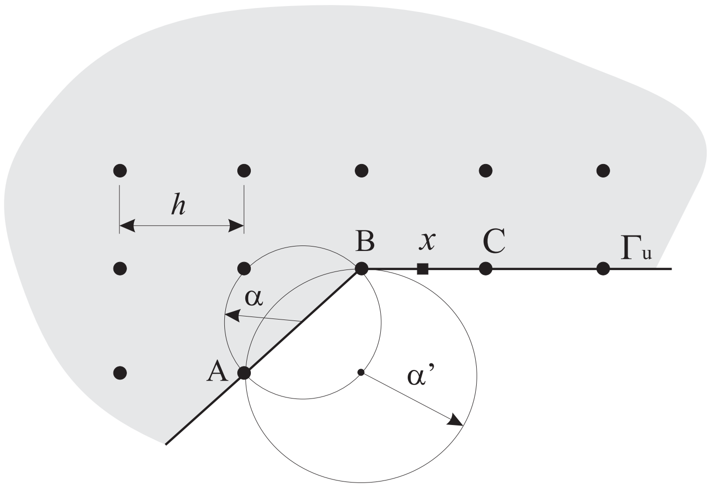
- Use α-shapes **(Edelsbrunner and Mucke, *ACT*, 1994)**

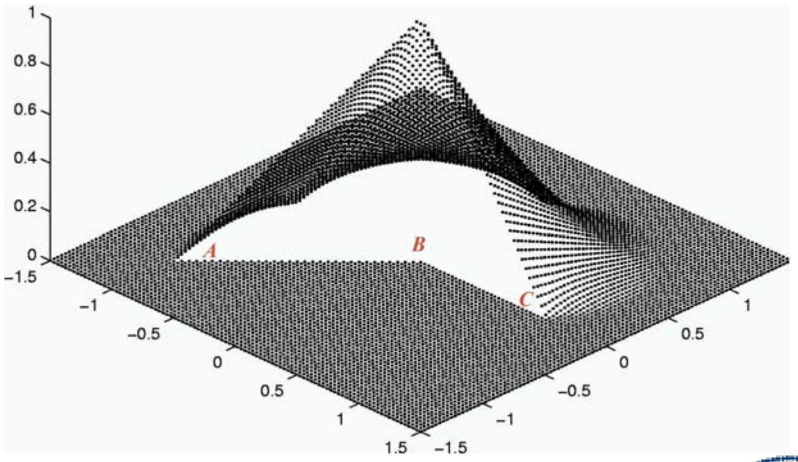
- Each cloud of points defines a finite family of shapes ranging from coarse to finer level of detail



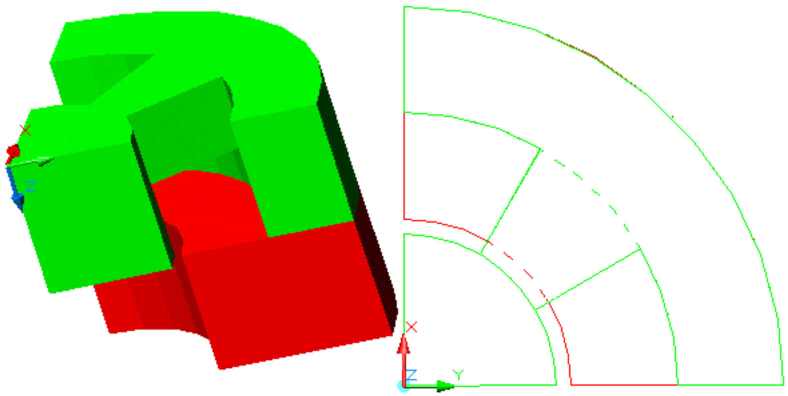
Shape Function Construction

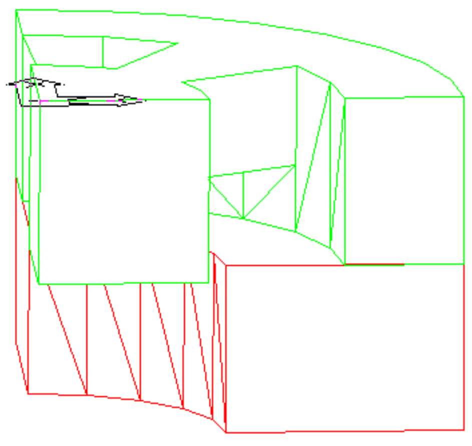
Construction of natural neighbor interpolants over an appropriate α-shape leads to interpolation along the essential boundary **(Cueto *et al.*, IJNME, 2000)**

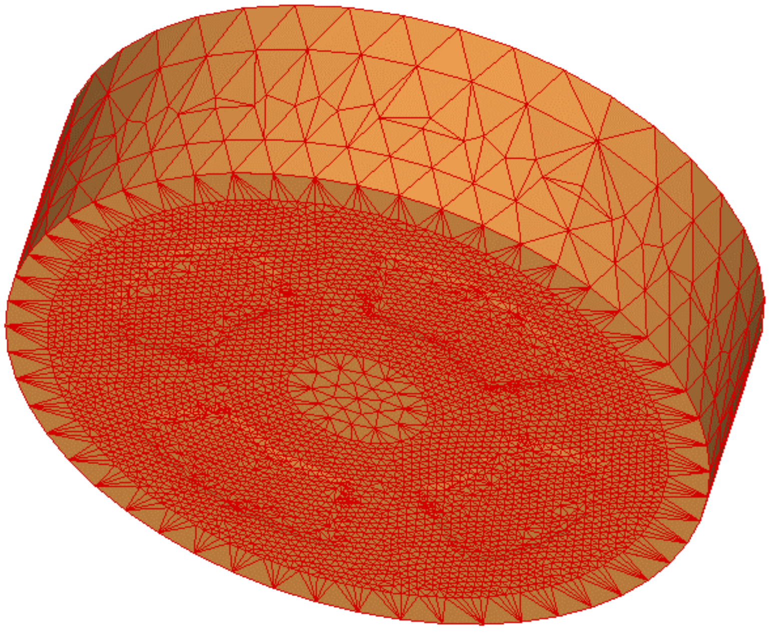




Extrusion of Hollow Profiles

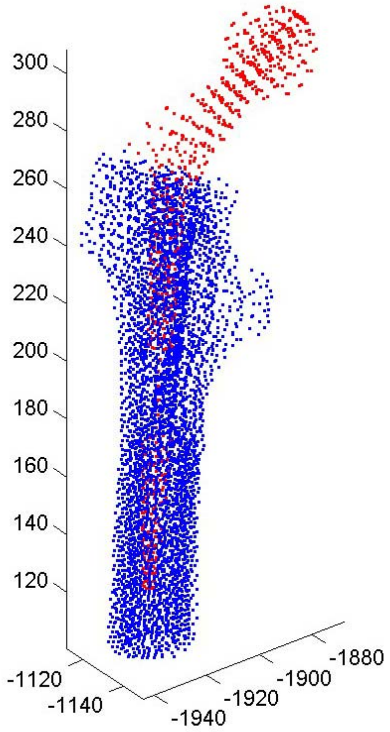




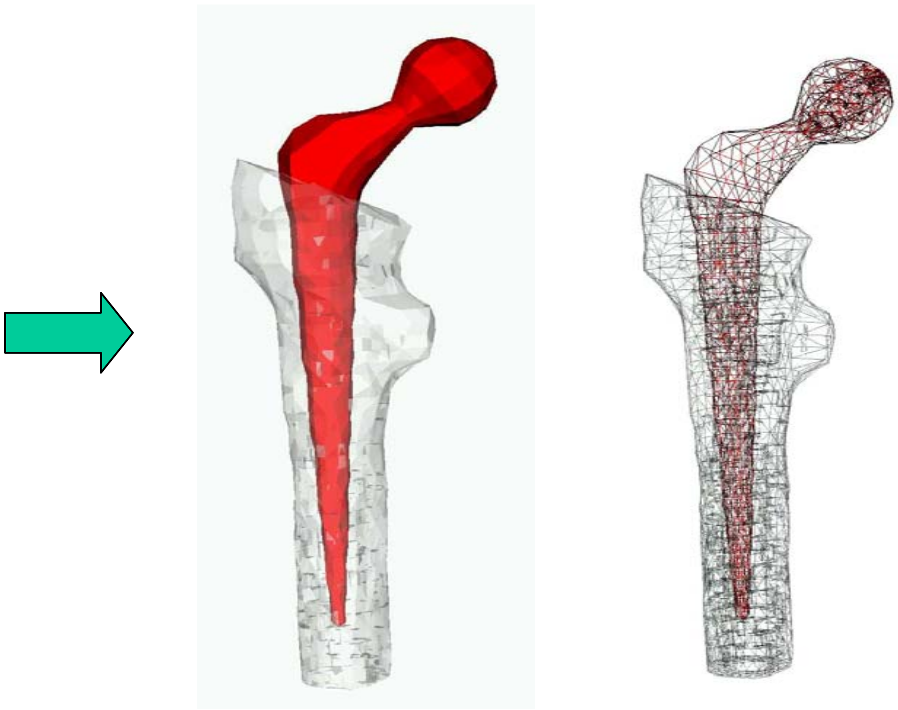


(Alfaro et al., CMAME, in press, 2006)

Biomechanics



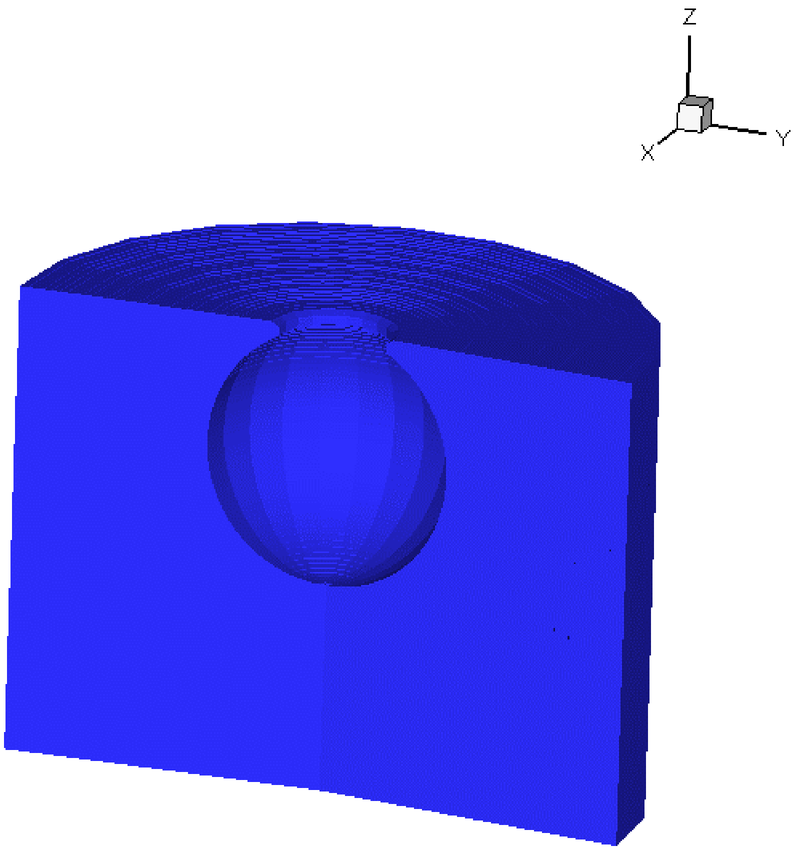
Cloud of points



α-NEM model

(Doblare et al., CMAME, 2005)

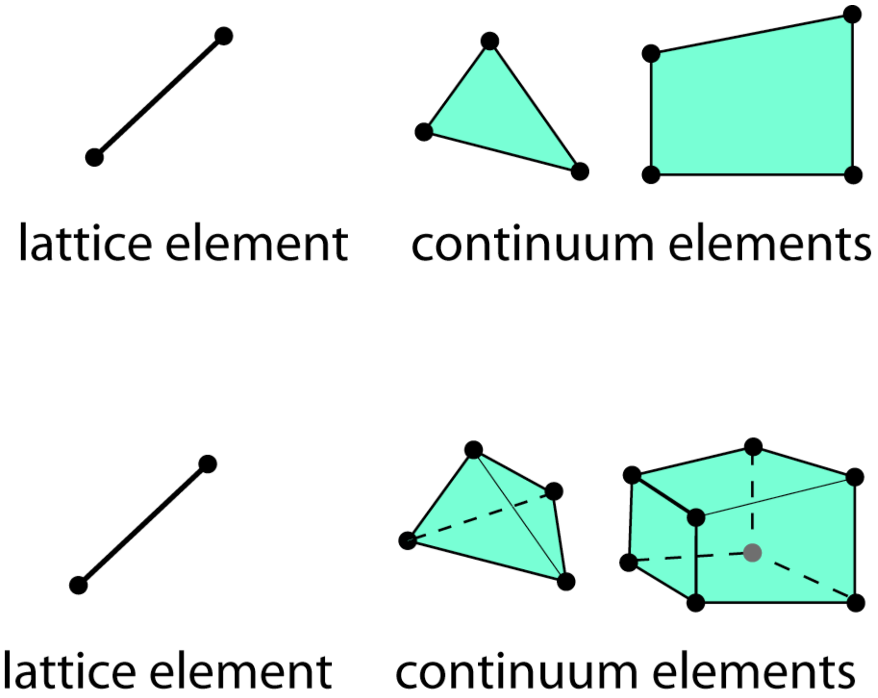
Bubble Bursting at Free Surface (Buoyancy Only)



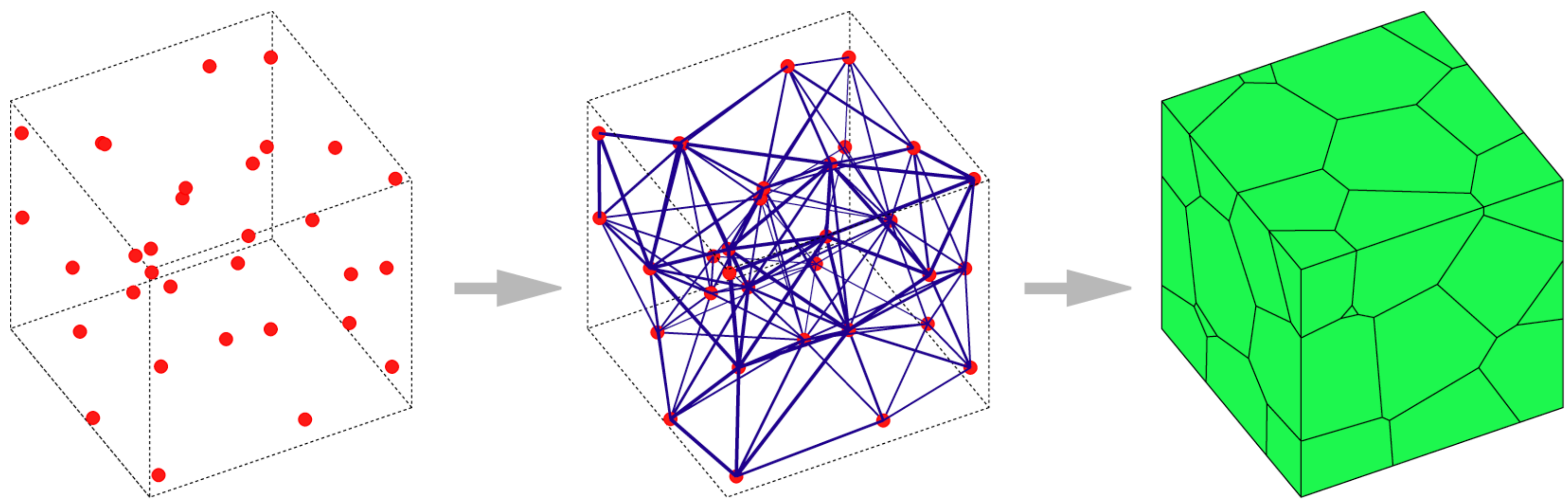
(Gonzalez **et al., in review, 2006)**

Irregular Lattice Model

Dimensional reduction using two-node elements

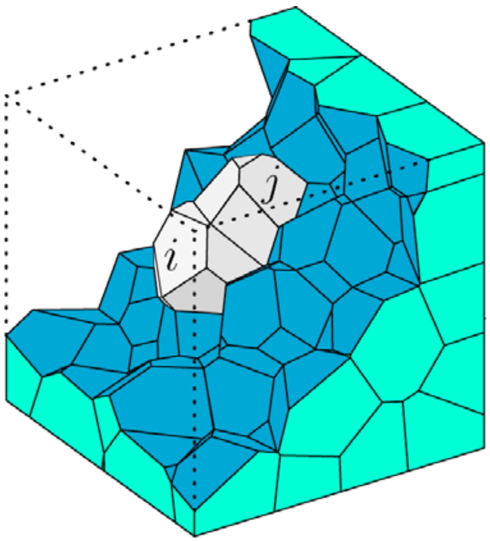


Domain Discretization

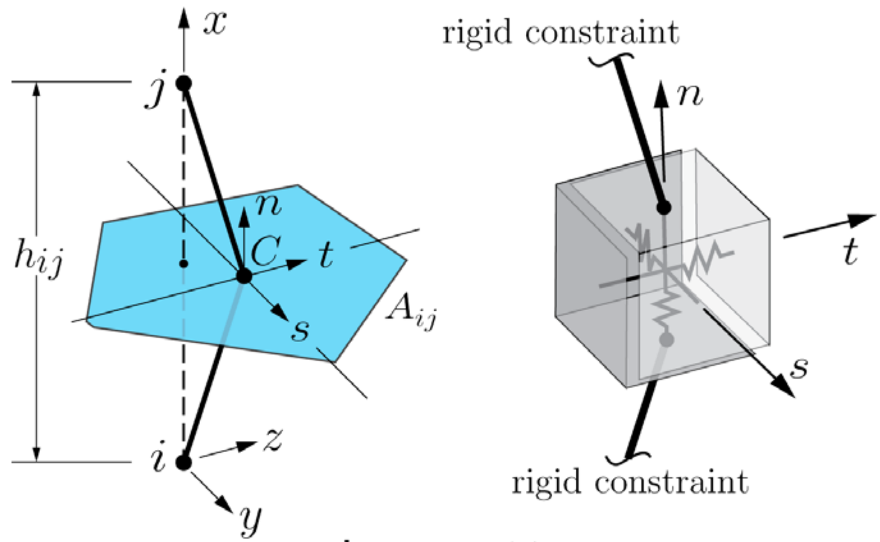


irregular point set   Delaunay tessellation   Voronoi tessellation

Rigid-Body Spring Network (RBSN)



element ij within mesh



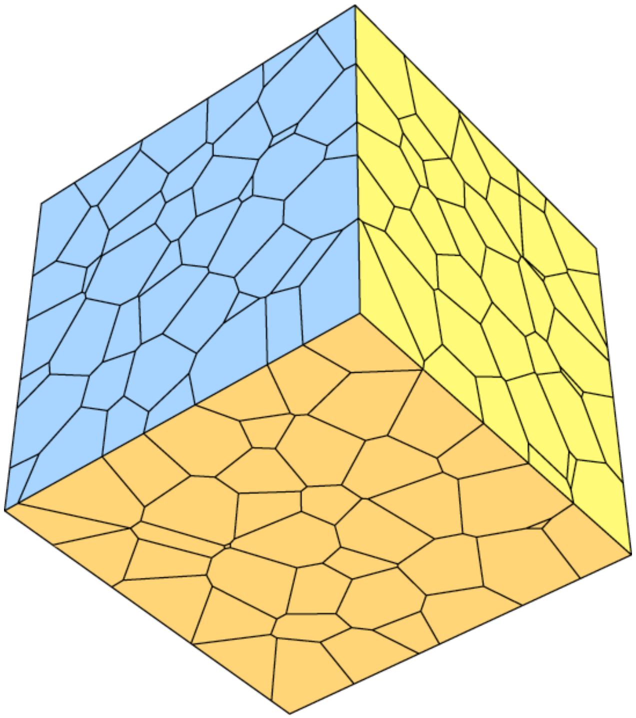
element ij

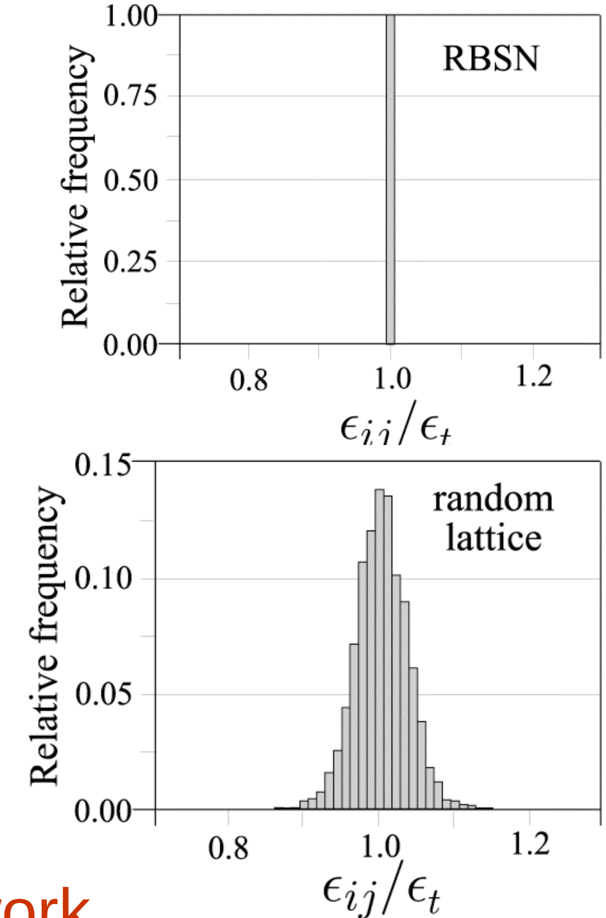
local stiffness terms

$$k_x = k_y = k_z = E\frac{A_{ij}}{h_{ij}}$$

$$k_{\phi x} = E\frac{J_p}{h_{ij}}, \qquad k_{\phi y} = E\frac{I_{22}}{h_{ij}}, \qquad k_{\phi z} = E\frac{I_{11}}{h_{ij}}$$

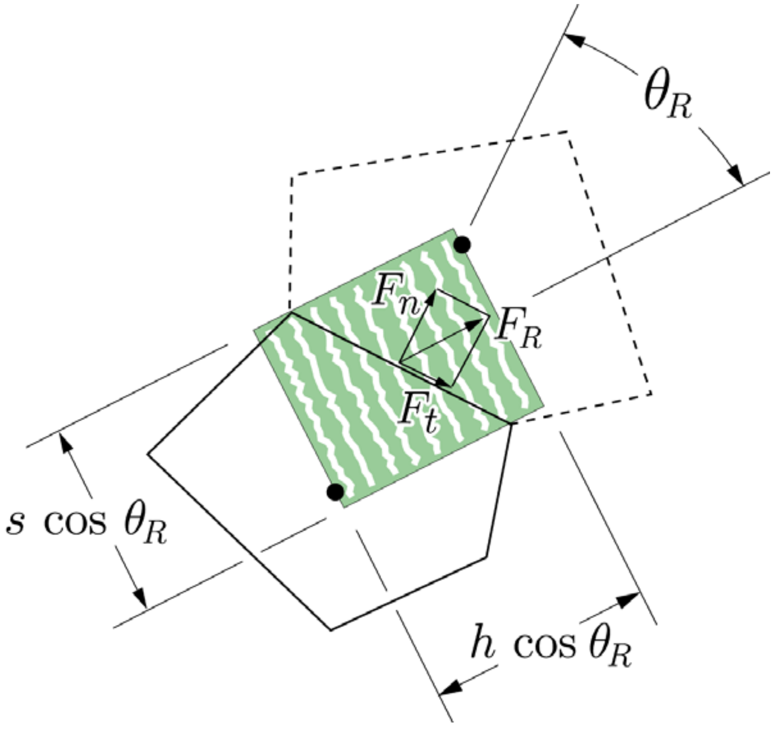
Elastic Uniformity





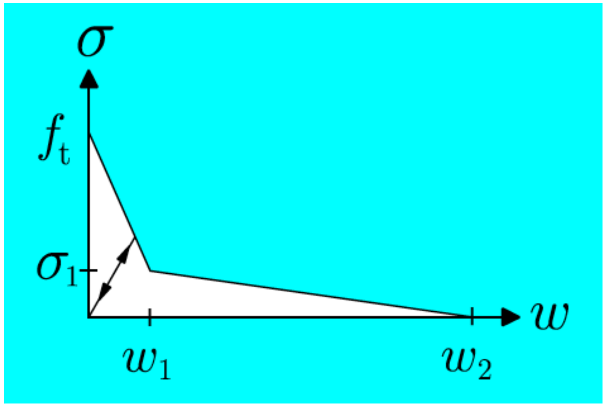
Strain production in 3D network subjected to uniform thermal loading

Crack Initiation and Propagation



$$\sigma_R = \frac{F_R}{s \cos \theta_R}$$

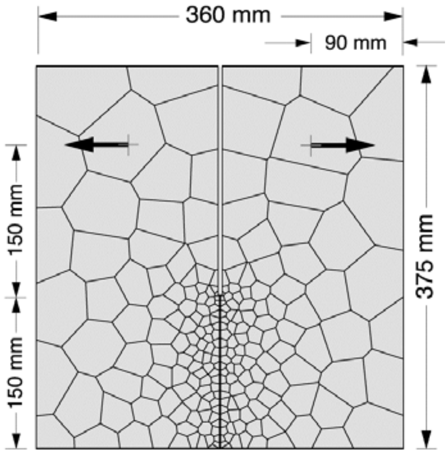
$$\varepsilon^{cr} = \frac{w}{h \cos \theta_R}$$



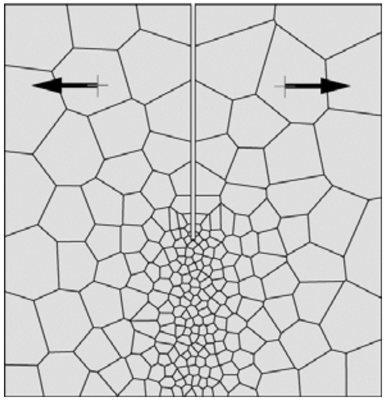
Crack band (Bazant, 1984)

Softening Relation

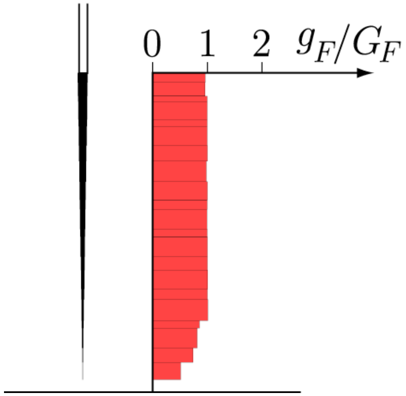
Crack Propagation

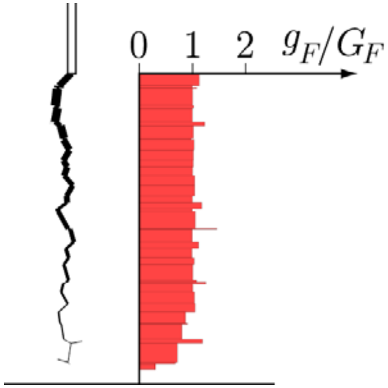


straight line discretization



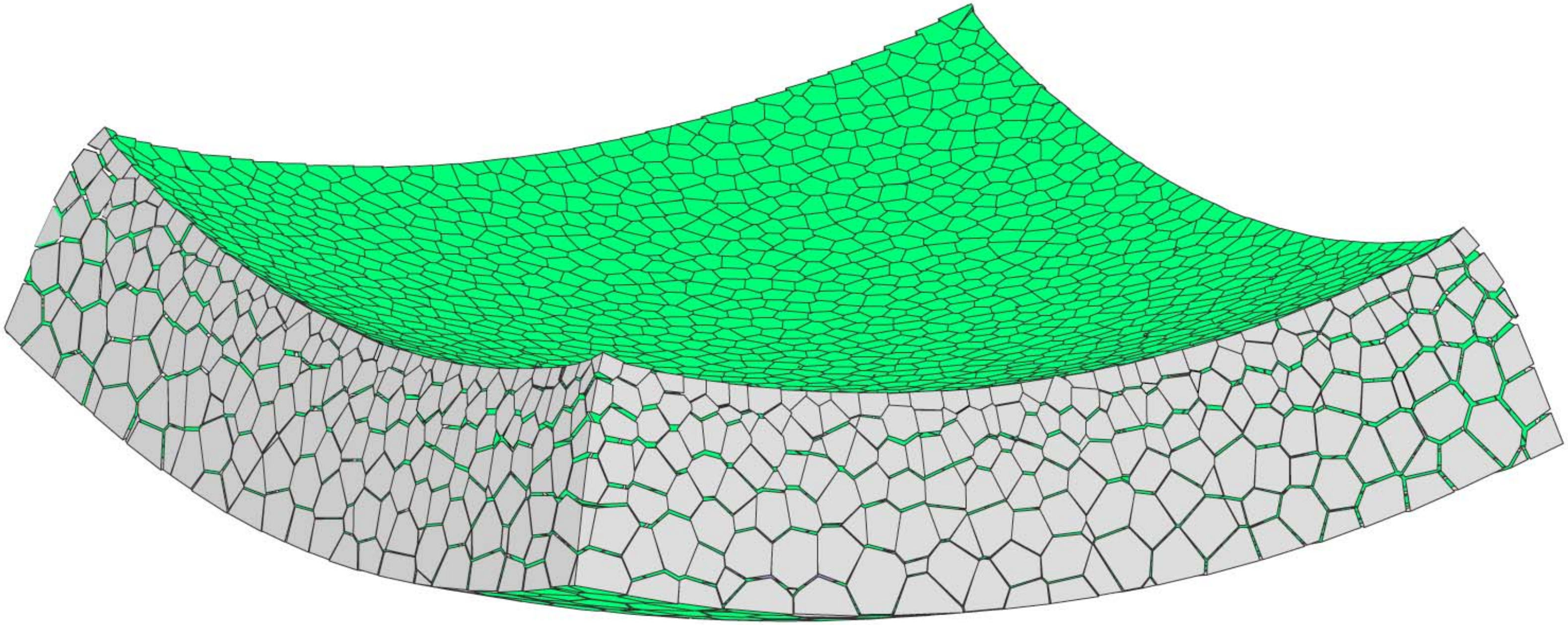
random discretization



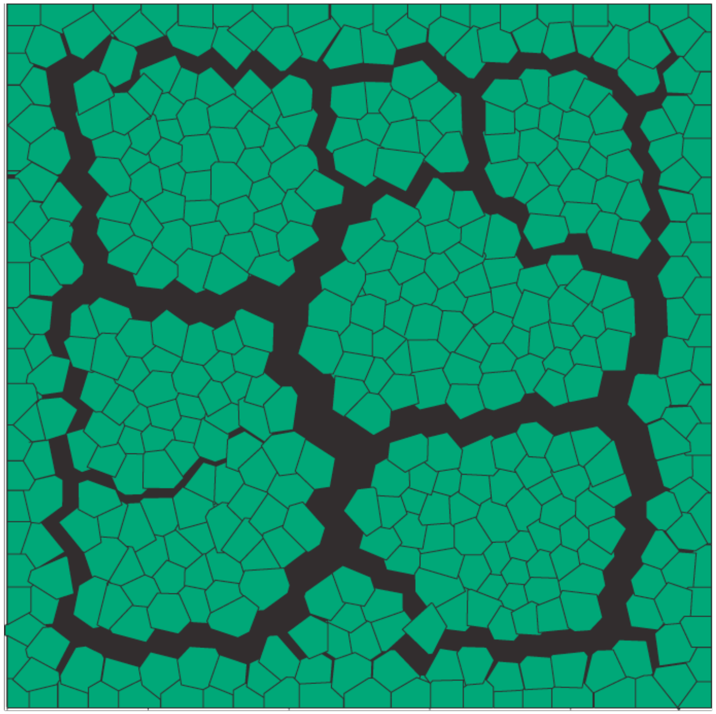


Energy consumption along ligament length

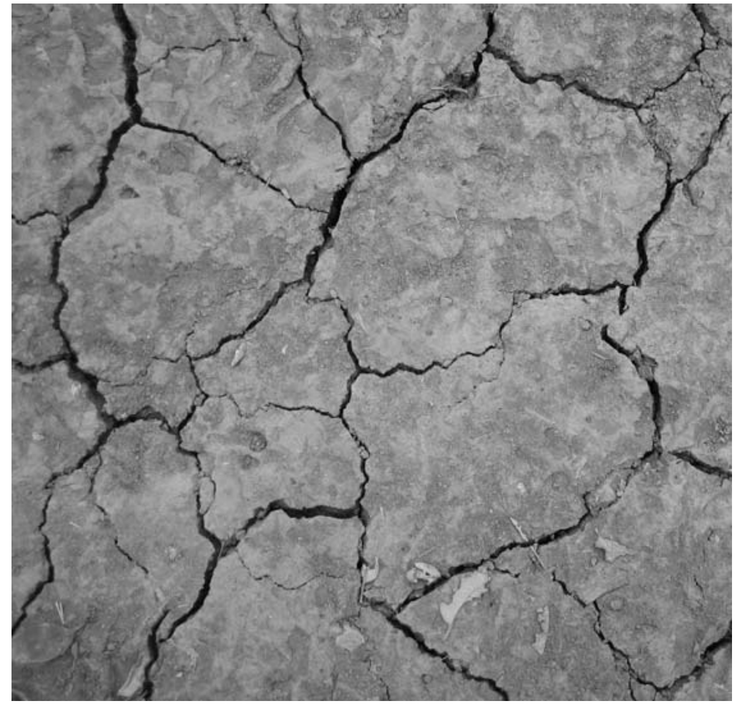
Plate Structure Drying From Top Surface



Shrinkage Cracking



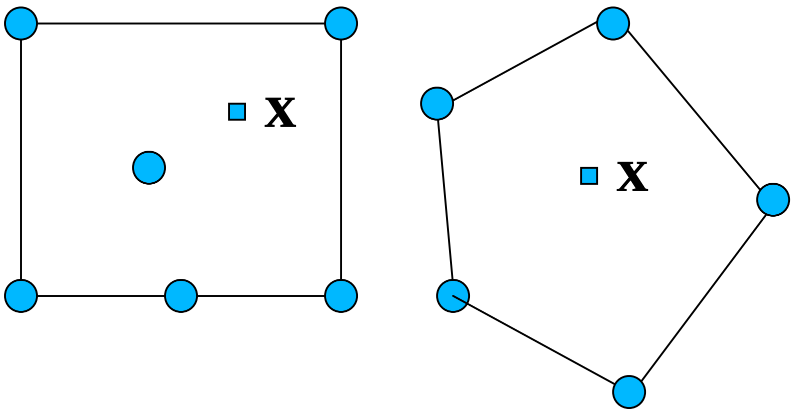
Animation (plan view)



Expt (clay-rich mud)

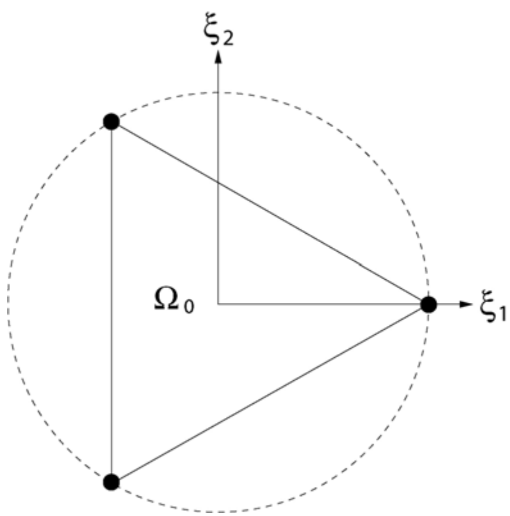
Construction of Polygonal Interpolants

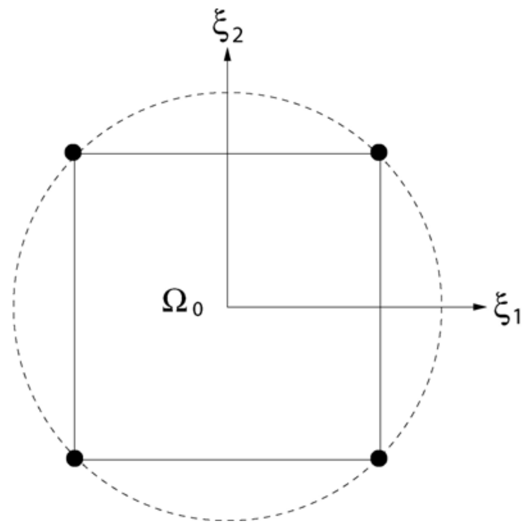
- Wachspress basis functions **(Wachspress, 1975; Meyer et al, 2002; Hormann, 2004)**
- Mean value coordinates **(Floater, 2003)**



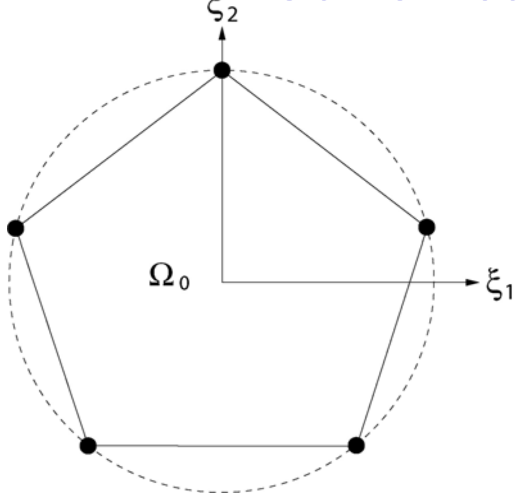
- Laplace shape functions **(S et al., 2004, 2005)**
- Maximum entropy (MAXENT) shape functions **(S, 2004)**

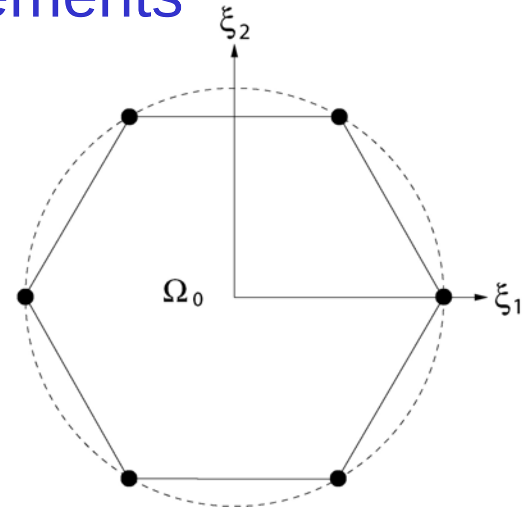
Laplace Shape Functions





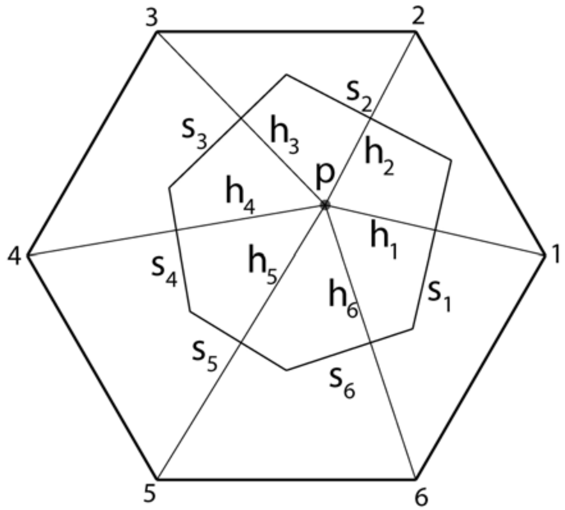
Canonical Elements

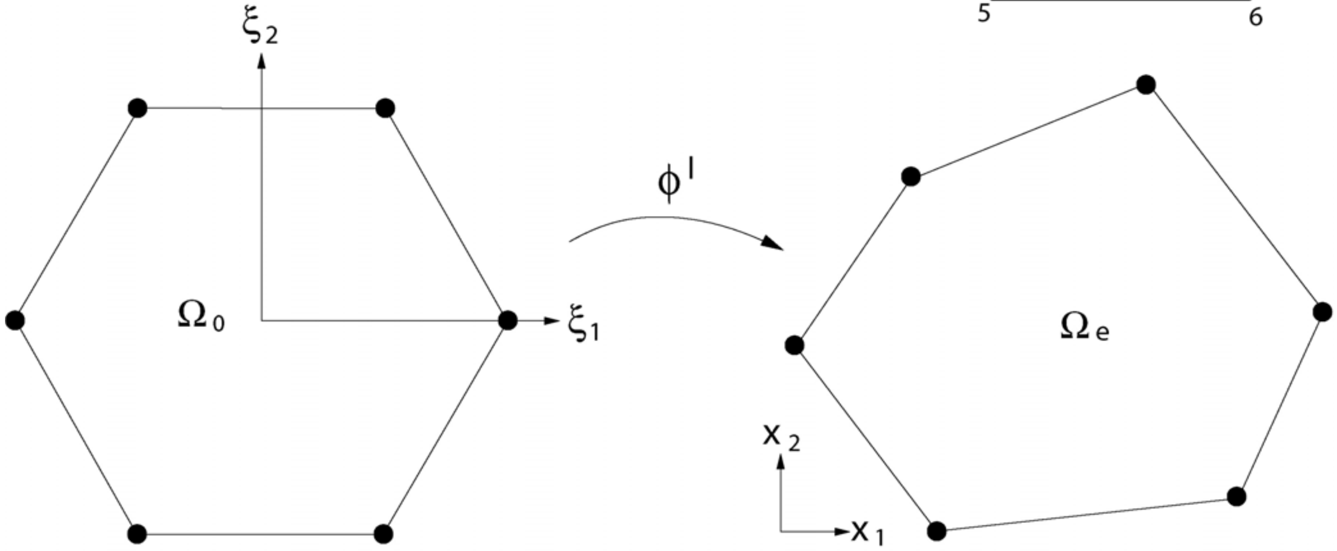




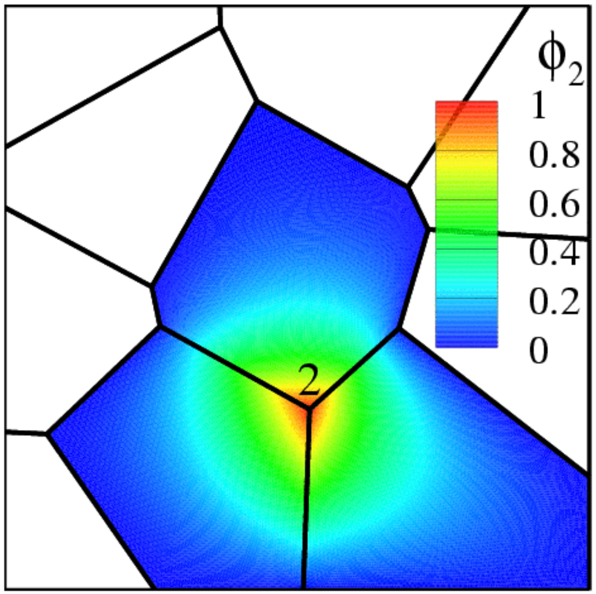
Polygonal Interpolant Using Isoparametric Mapping

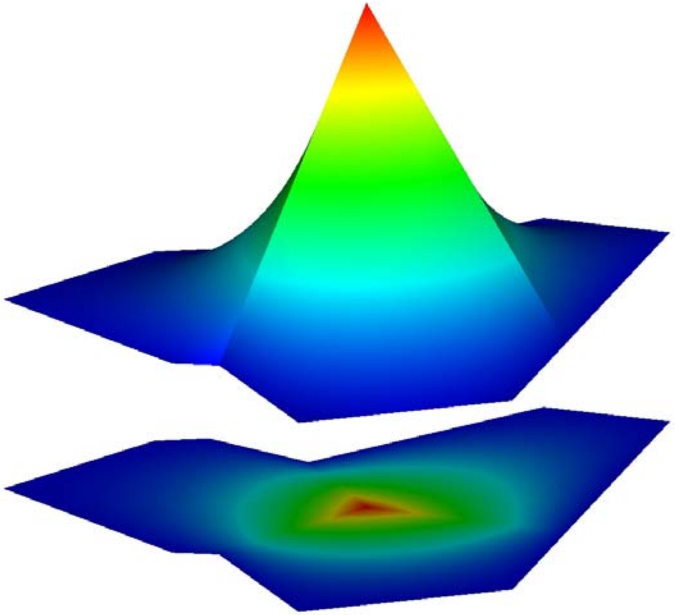
Laplace Shape Function



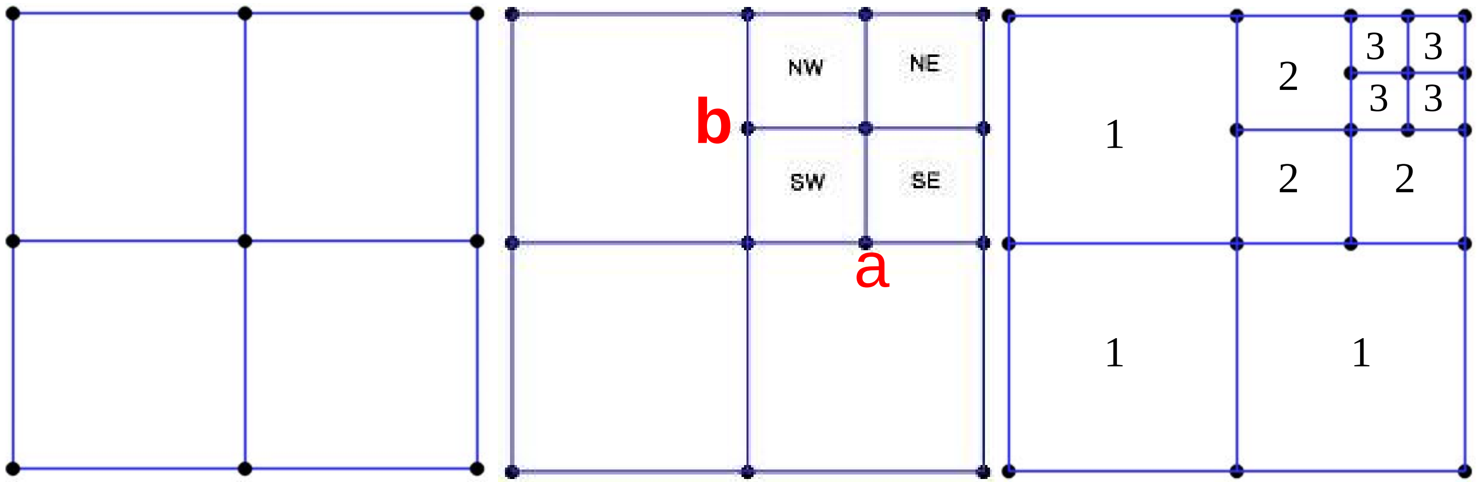


Polygonal Basis Function



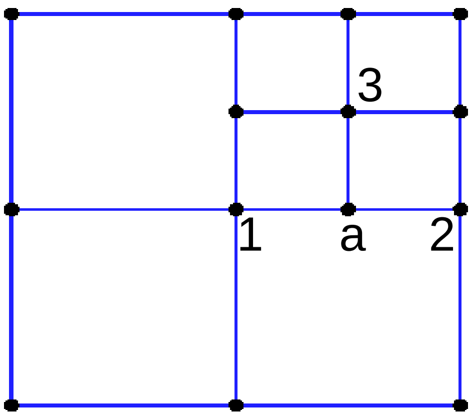


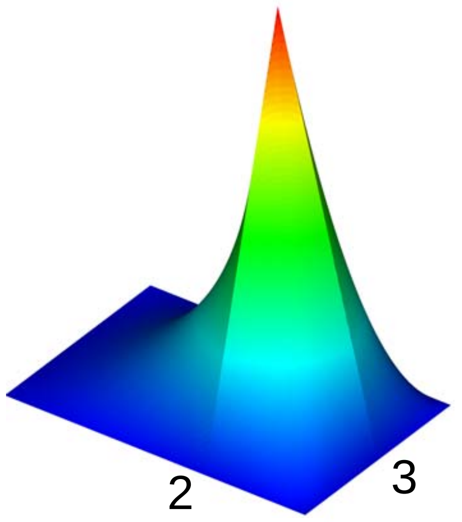
Quadtree Data Structure

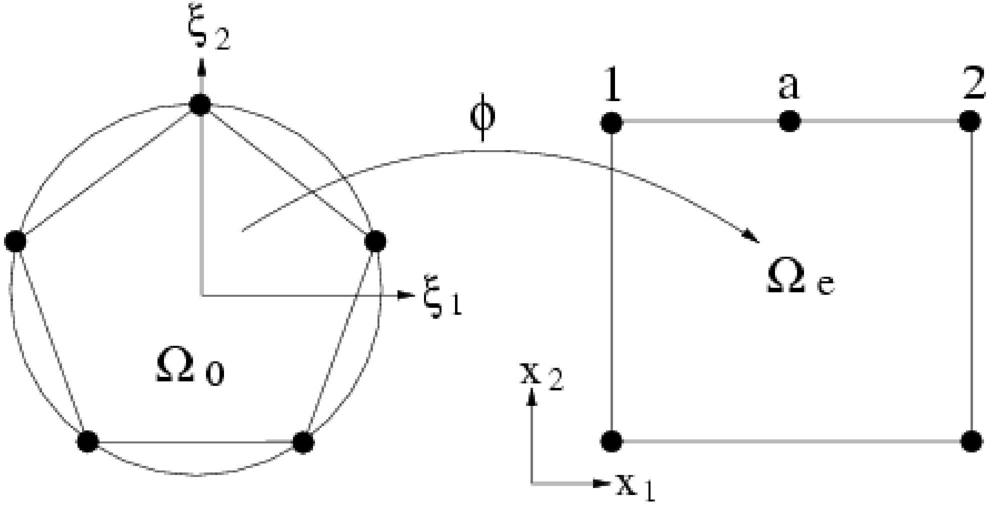


Quadtree is a hierarchical data structure based on the principle of recursive decomposition

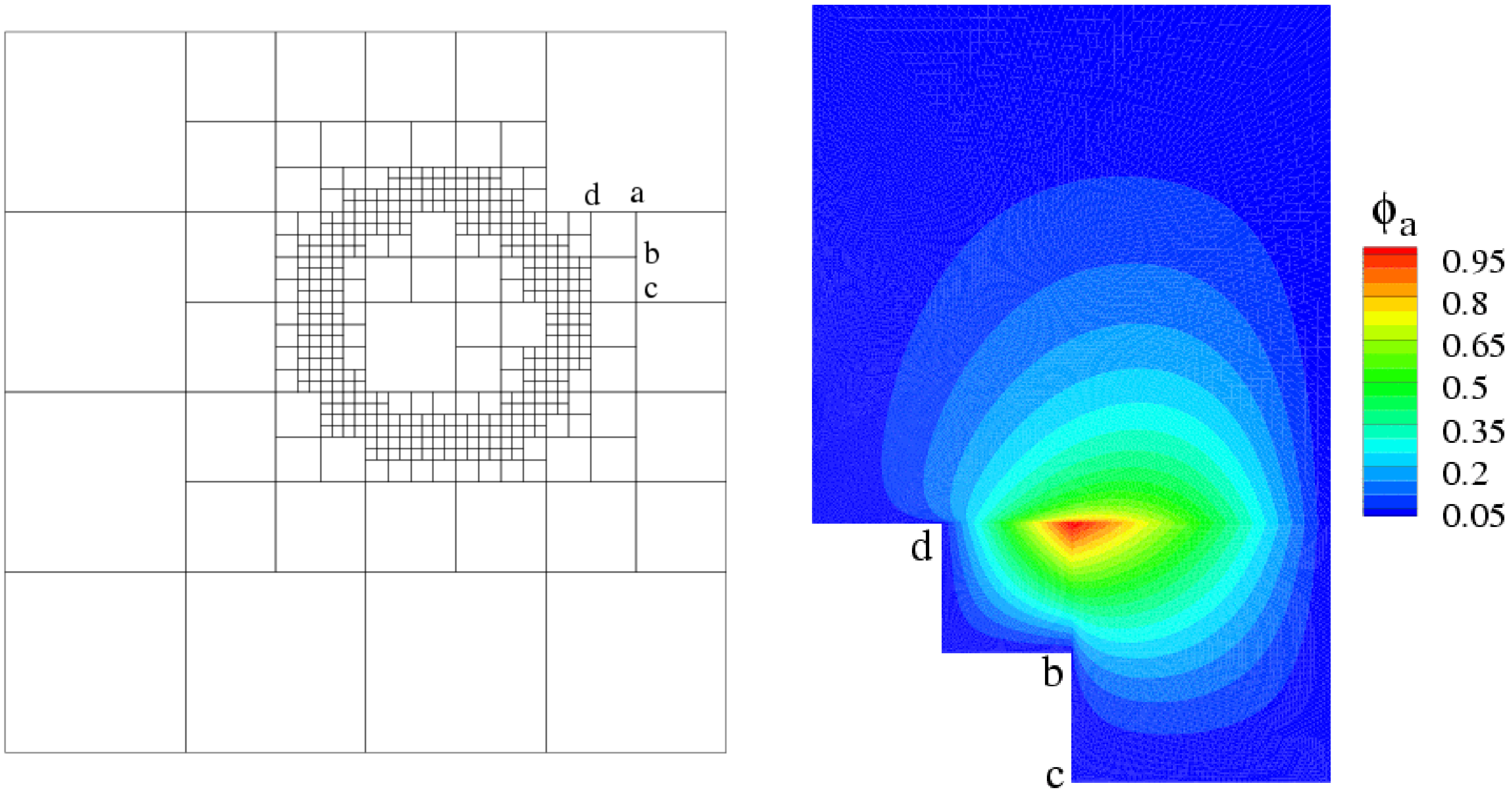
Handling Hanging Nodes







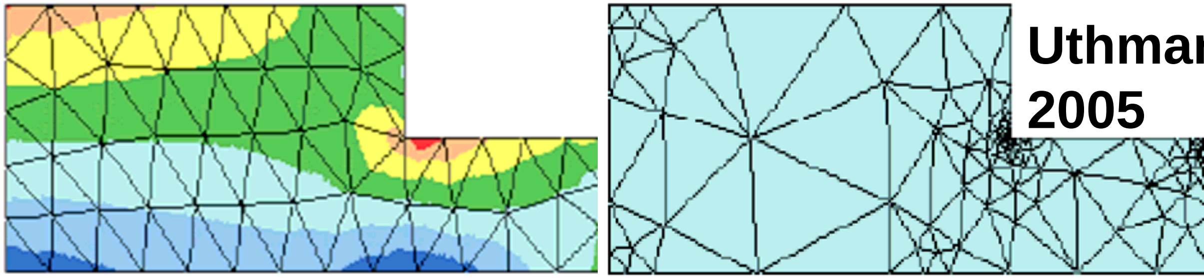
Shape Function (Hanging Node)



Support of basis function for node a

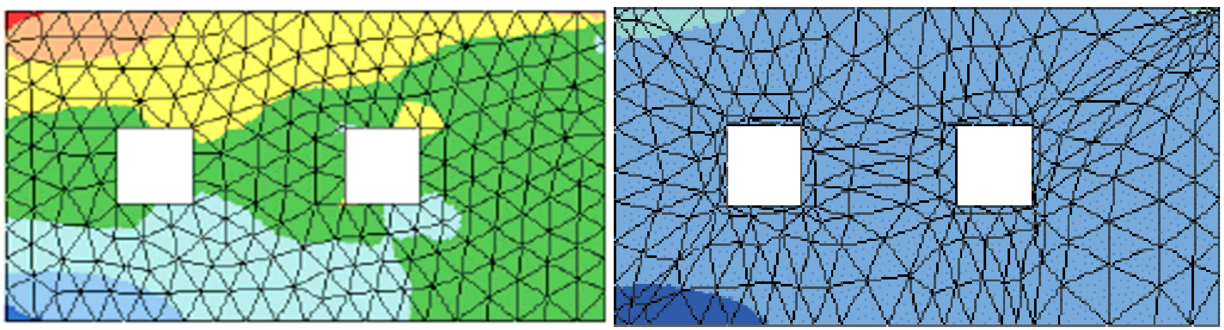
Mesh Adaptivity

- *h*-

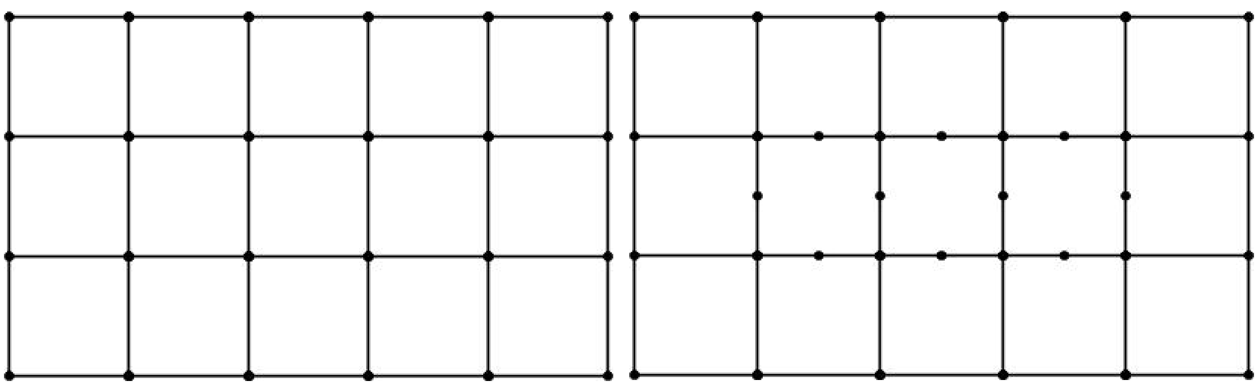


Uthman and Askes, 2005

- *r*-

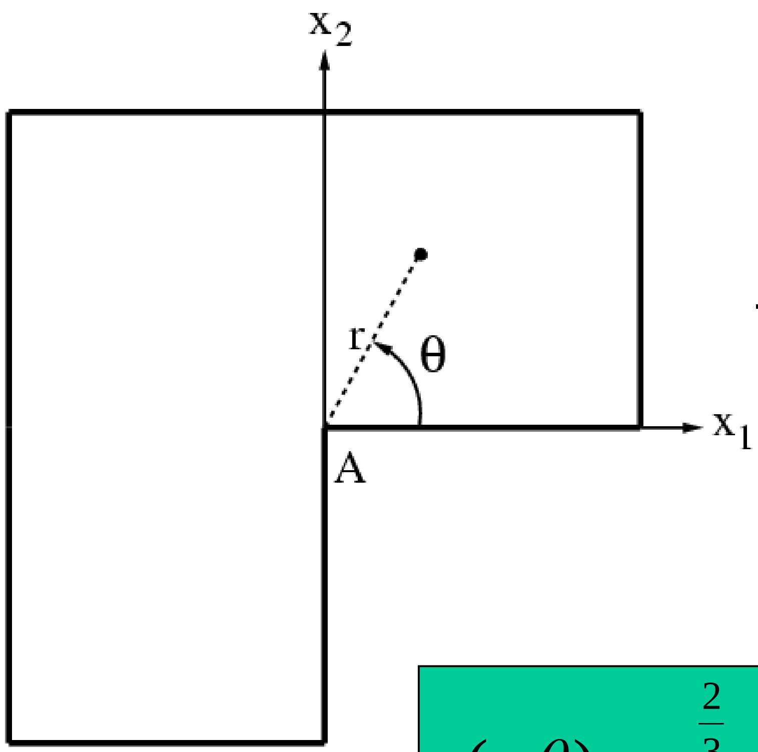


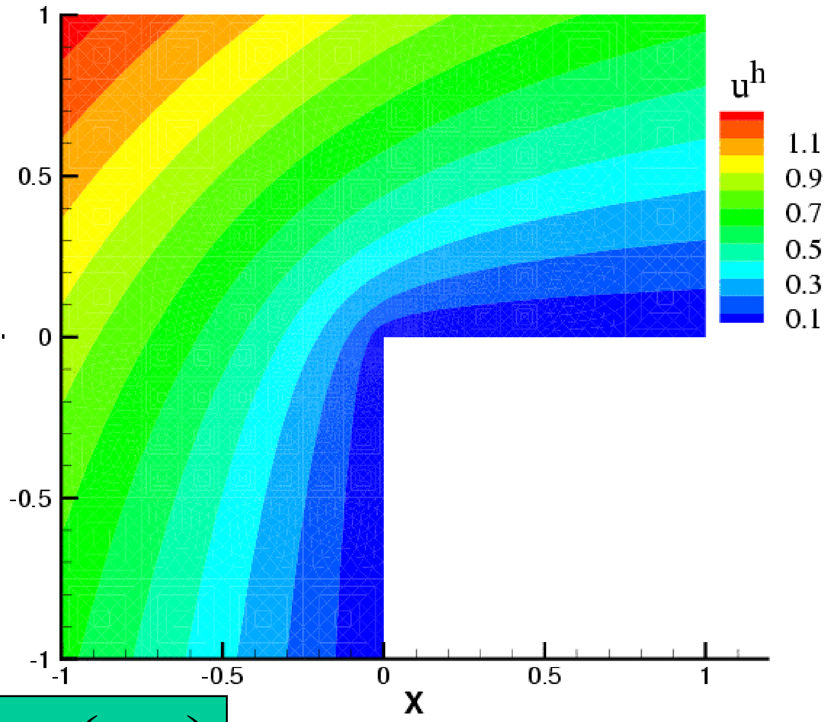
- *p*-



Numerical Example: Corner Singularity

Model Dirichlet Problem: $\nabla^2 u = 0 \quad \text{in} \quad \Omega$





$$u(r,\theta) = r^{\frac{2}{3}} \sin\left(\frac{2\theta}{3}\right)$$

Closure and Outlook

- An overview of meshfree approximation schemes was presented with particular emphasis on natural neighbor interpolants and NEM

- A natural neighbor-based scaling on Voronoi meshes was used to perform fracture simulations on irregular lattices and polygonal finite elements were proposed

- Development of meshfree methods that are suitable for evolving (non-convex) domains with stable nodal numerical integration schemes are needed