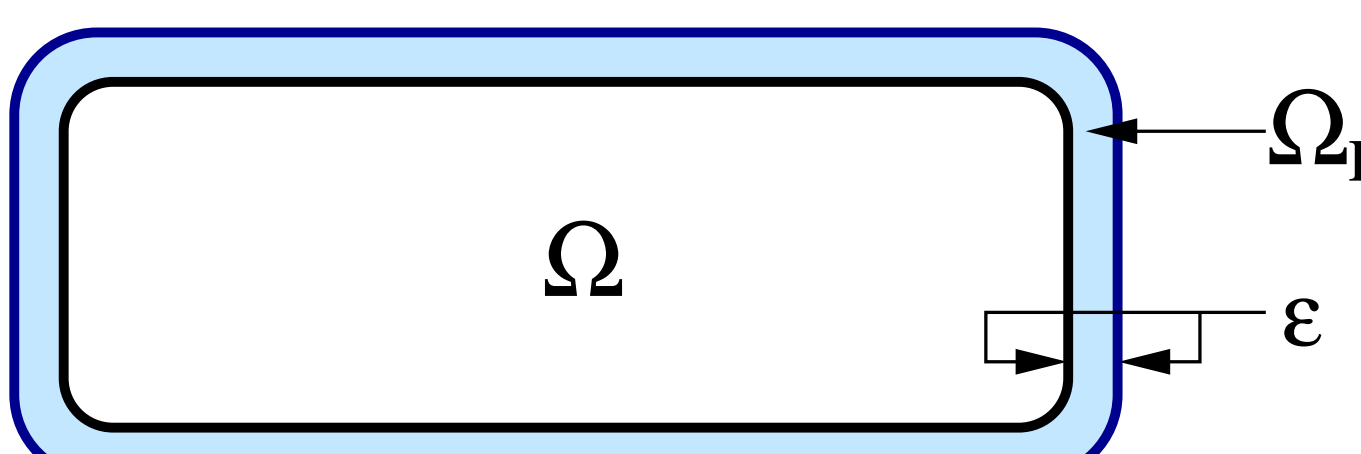


## Introduction

- Goal:**
  - Develop an accurate, efficient, and robust finite element method for the weak formulation of nonlocal mechanics problems.
- Quadrature challenges:**
  - High-dimension (integration over  $\mathbb{R}^{2d}$ )
  - Discontinuous integrand
  - Complicated shape of support of integrand
  - Singularities in some cases of interest

## Continuous problem

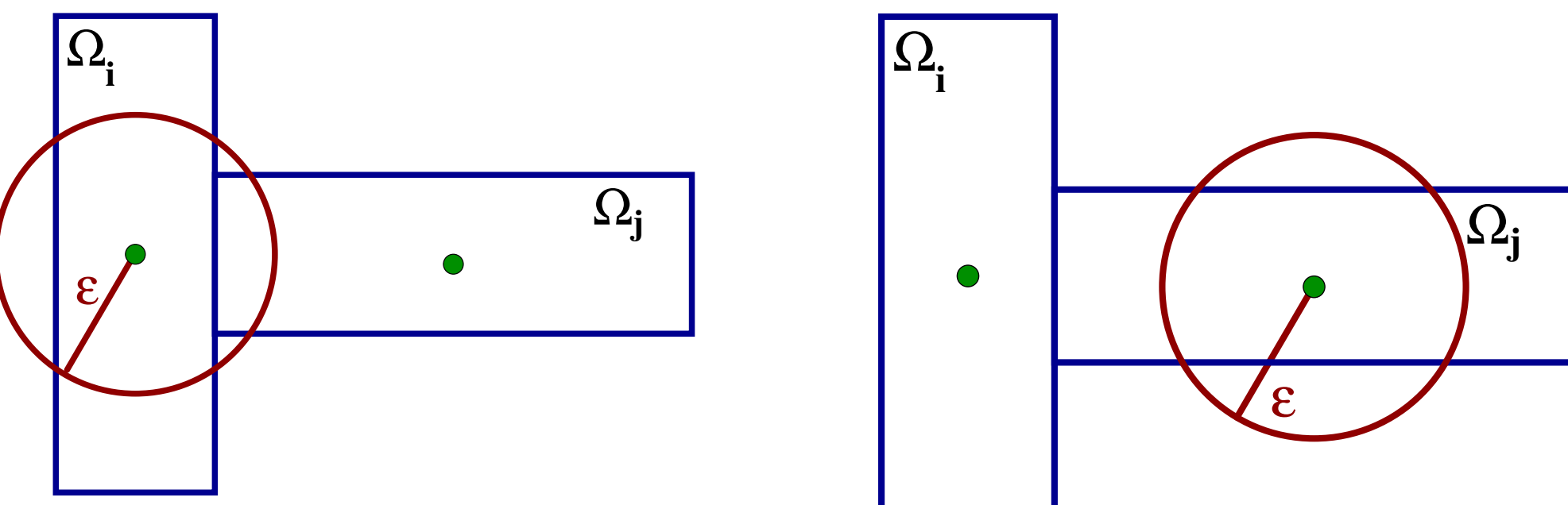
- Strong form:** Find  $u : \Omega \rightarrow \mathbb{R}$  such that
 
$$2 \int_{\Omega \cup \Omega_I} (u(x) - u(x')) \gamma_\varepsilon(x, x') dx' = f(x), \quad \forall x \in \Omega,$$
 subject to the Dirichlet volume–constraint
 
$$u(x) = g(x), \quad \forall x \in \Omega_d \subseteq \Omega_I,$$
 and Neumann volume–constraint
 
$$2 \int_{\Omega \cup \Omega_I} (u(x) - u(x')) \gamma_\varepsilon(x, x') dx' = h(x), \quad \text{for } x \in \Omega_n \subseteq \Omega_I.$$

- Weak form:** Find  $u \in U$  such that
 
$$\langle u, v \rangle_\gamma = \int_\Omega v(x) f(x) dx + \int_{\Omega_n} v(x) h(x) dx,$$
 for all  $v \in V$ , subject to the Dirichlet volume–constraint.
- Bilinear form:**

$$\langle u, v \rangle_\gamma = \int_{\Omega \cup \Omega_I} \int_{\Omega \cup \Omega_I} (u(x) - u(x')) (v(x) - v(x')) \gamma_\varepsilon(x, x') dx' dx$$
- Energy:**

$$E(u) = \frac{1}{2} \langle u, u \rangle_\gamma - \int_\Omega v(x) f(x) dx - \int_{\Omega_n} v(x) h(x) dx$$
- Flux:**

$$\text{flux}_{j \rightarrow i} = \langle \mathbb{1}_{(\Omega_i)}, u \mathbb{1}_{(\Omega_j)} \rangle_\gamma - \langle \mathbb{1}_{(\Omega_j)}, u \mathbb{1}_{(\Omega_i)} \rangle_\gamma$$

## Strong vs. Weak form



- Does  $\Omega_i$  interact with  $\Omega_j$ ?
- Strong Form:** Points interact with volumes (asymmetric)
  - “Saved” by low-order quadrature?
- Weak Form:** Volumes interact with volumes (symmetric)
  - Requires more advanced quadrature!

## Nonlocal kernel

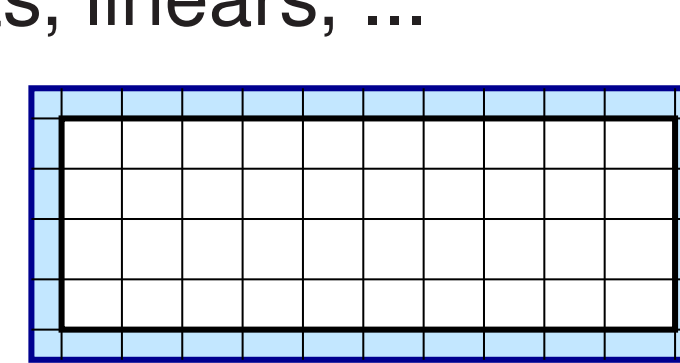
$$\gamma_\varepsilon(x, x') = \frac{1}{\varepsilon^2 \text{Vol}(P_{N,\varepsilon})} \begin{cases} \psi(\|x - x'\|), & \|x - x'\| \leq \varepsilon, \\ 0, & \text{otherwise} \end{cases}$$

Case 1:  $\psi(r) = C$  (no smoothing)

Case 2:  $\psi(r) = \frac{C}{r^{d+2s}}$  (smoothing;  $0 < s < 1$ )

## Discrete problem

- Approximation:** Discontinuous constants, linears, ...

$$u_h = \sum_{i=1}^N \alpha_i \phi_i(x), \quad \overline{\Omega \cup \Omega_I} = \bigcup_{i=1}^N \overline{\Omega_i}$$


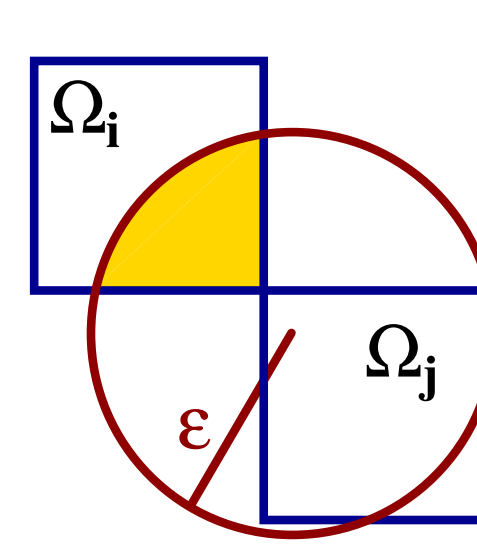
- System of equations**

$$\begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} \vec{\alpha} \\ \vec{\beta} \end{bmatrix} = \begin{bmatrix} \vec{b} \\ \vec{c} \end{bmatrix}, \quad \beta_k = \text{Lagrange multipliers}$$

$$A_{i,j} = \langle \phi_i, \phi_j \rangle_\gamma, \quad B_{i,k} = \int_{\Omega_d} \phi_i(x) \phi_{j(k)}(x) dx,$$

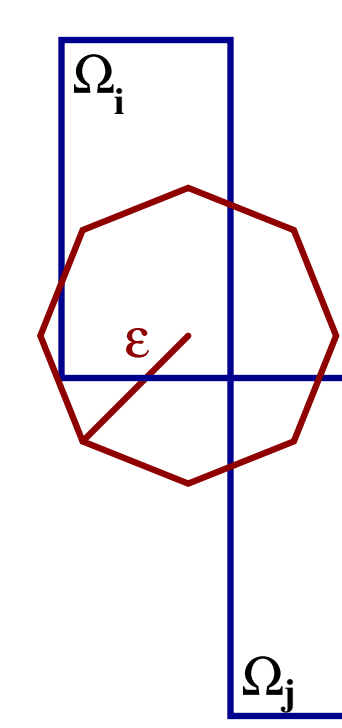
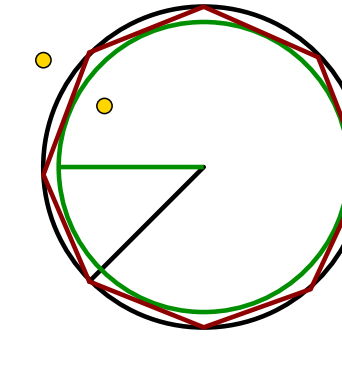
$$b_i = \int_\Omega \phi_i(x) f(x) dx + \int_{\Omega_n} \phi_i(x) h(x) dx, \quad c_k = \int_{\Omega_d} \phi_{j(k)}(x) g(x) dx$$

## Assembly

- Task:** Compute
 
$$A_{i,j} = \int_{\Omega \cup \Omega_I} \int_{\Omega \cup \Omega_I} (\phi_i(x) - \phi_i(x')) (\phi_j(x) - \phi_j(x')) \gamma_\varepsilon(x, x') dx' dx$$
- Difficulty:** Support of integrand is complicated
 
$$((\Omega_i \times \Omega_i) \cap B_\varepsilon(\Omega_i, \Omega_j)) \cup ((\Omega_j \times \Omega_i) \cap B_\varepsilon(\Omega_i, \Omega_j)),$$
 where
 
$$B_\varepsilon(\Omega_i, \Omega_j) := \{(x, x') \in \Omega_i \times \Omega_j \mid \|x - x'\| \leq \varepsilon\}$$


Curved boundaries in  $\mathbb{R}^4$  (for 2D) or  $\mathbb{R}^6$  (for 3D)

## Quadrature

- Approach:** Subdivide (or approx. subdivide) the region of integration into polygonal subregions and apply Gauss quadrature in each subregion.
 
- Method:**
  - Use polyhedral approx. of spherical horizon
  - Describe convex region,  $\tilde{B}_\varepsilon(\Omega_i, \Omega_j)$ , with linear inequality constraints
  - Delaunay “triangulate” region with `Qhull`
  - Apply standard/Gauss quadrature rules on each high-dimensional simplex
- Cost reduction:**
  - Use symmetric polyhedral approx. of spherical horizon
  - Combine simplicial quadrature rules to form a simple low-complexity rule for each pair of elements
  - Bound polyhedral regions with spheres for identification of completely interacting/noninteracting elements

## Quadrature accuracy

$$\left| \int_{\Omega_i} \int_{\Omega_j} F(x, x') (S_\varepsilon(x - x') - P_{N,\varepsilon}(x - x')) dx' dx \right| \leq \|F\|_\infty C(N, \varepsilon)$$

where

$$C(N, \varepsilon) \propto \varepsilon^d \frac{1}{N^k} \quad \text{with } k = 2, 1 \text{ for } d = 2, 3$$

## Quadrature derivation complexity

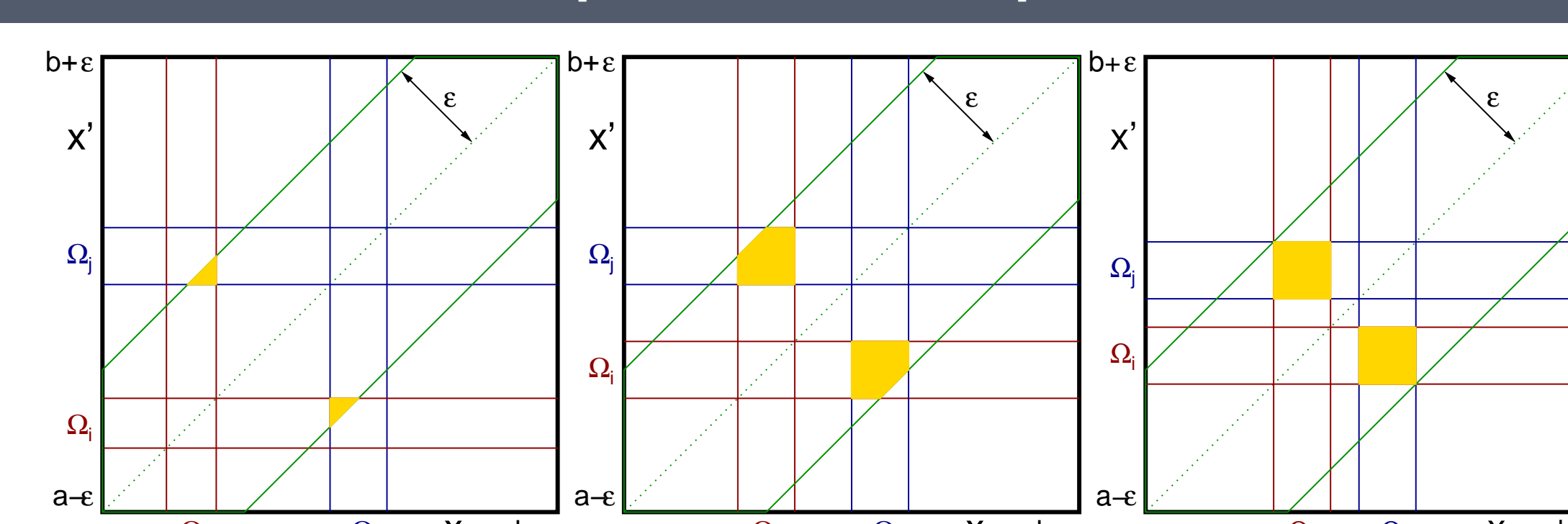
- Number of linear inequality constraints
  - Element distance bounded bounding spheres
 
$$|\text{Facets } \Omega_i| + |\text{Facets } \Omega_j|$$
  - Bounding sphere test fails
 
$$|\text{Facets } \Omega_i| + |\text{Facets } \Omega_j| + |\text{Facets } P_{N,\varepsilon}|$$
- Overall complexity
 
$$O(\text{vert}_{\text{in}} \text{facet}_{\text{out}} / \text{vert}_{\text{out}})$$

## Simplicial quadrature in $\mathbb{R}^d$

Degree	Quadrature Pts.	$ \mathbb{P}_k(\mathbb{R}^d) $
$k = 1$	1	$n + 1$
$k = 2$	$n + 1$	$(n + 2)(n + 1)/2$
$k = 3$	$n + 2$	$(n + 3)(n + 2)(n + 1)/6$
$k$	?	$(n + k)! / (n! k!)$

See: N. J. Walkington, 2000

## One-dimensional quadrature example

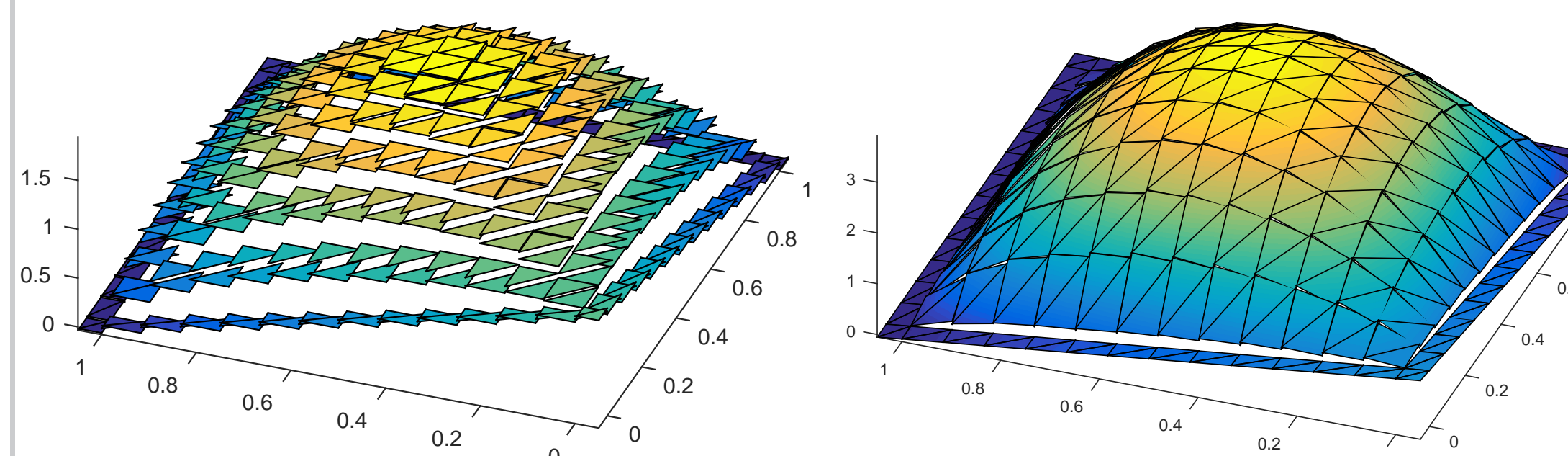


- Support is not a simple Cartesian product
- Can precompute weight,  $w_c$ , and centroid,  $(x_c, x'_c)$ .
 
$$w_c = \int_{\Omega_i} \int_{\Omega_j} \gamma(x, x'),$$

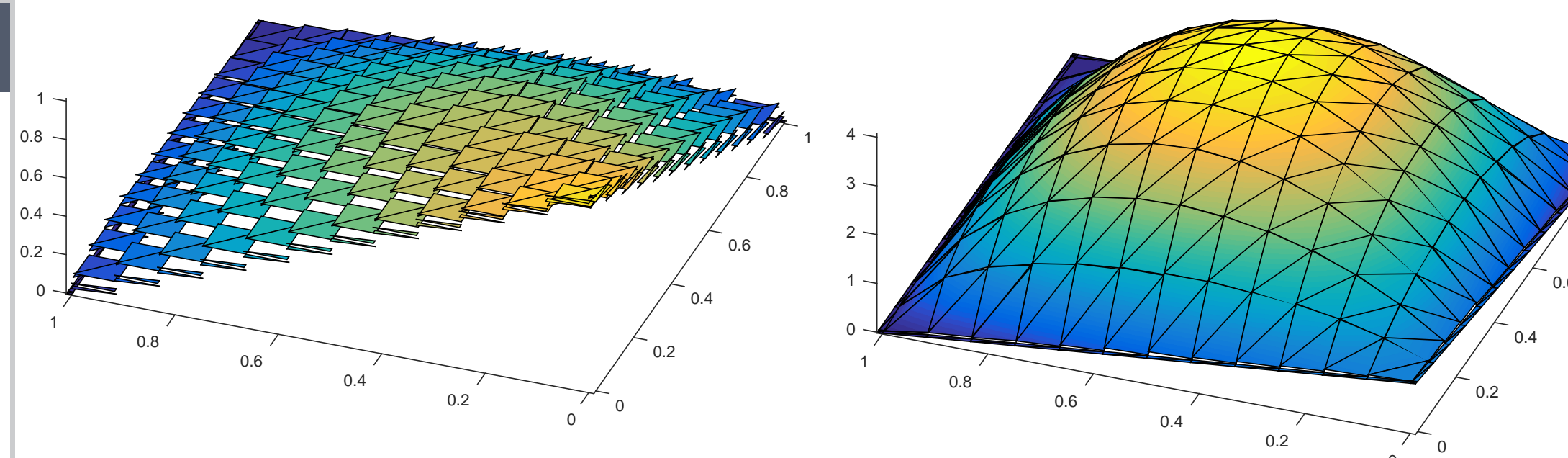
$$w_c x_c = \int_{\Omega_i} \int_{\Omega_j} x \gamma(x, x') dx dx', \quad w_c x'_c = \int_{\Omega_i} \int_{\Omega_j} x' \gamma(x, x') dx dx',$$
 for each pair  $\Omega_i$  and  $\Omega_j$ .
- One-point is sufficient for discontinuous linears ( $i \neq j$ )
- Higher-order and  $i = j$  requires more points

## Numerical results

- The nonlocal kernel,  $\gamma_\varepsilon$ , is piecewise constant
- $h = \frac{1}{12}, \quad f = 75, \quad C = \frac{9}{4}$



Piecewise Constant,  $\varepsilon = \frac{1}{20}$       Piecewise Linear,  $\varepsilon = \frac{1}{20}$



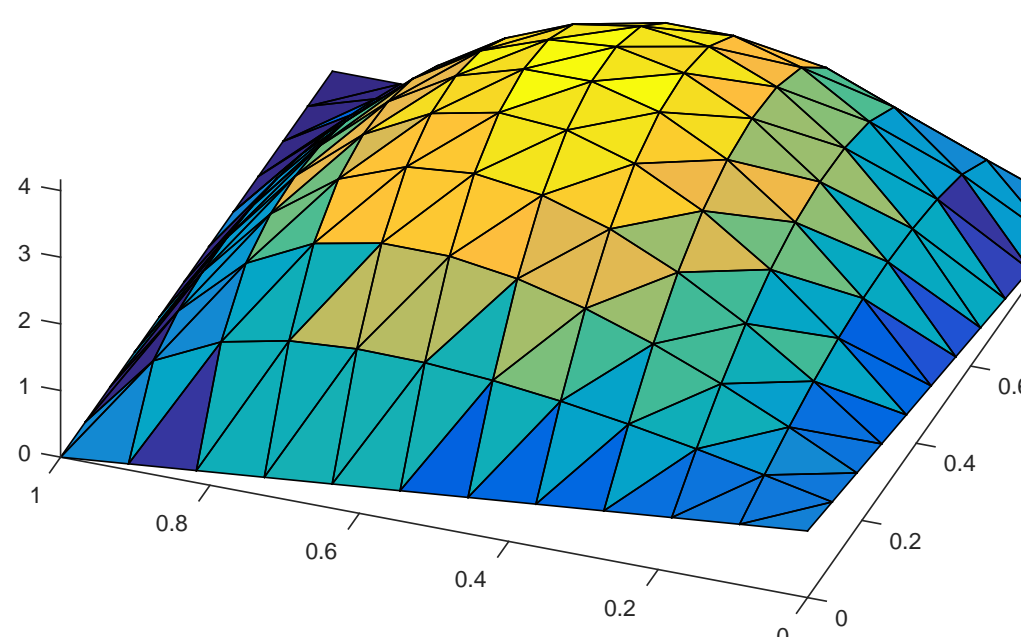
Piecewise Constant,  $\varepsilon = \frac{1}{100}$       Piecewise Linear,  $\varepsilon = \frac{1}{100}$

Convergence  $\varepsilon \rightarrow 0$

- Piecewise Constant = No
- Piecewise Linear = Yes

$L_2$  Convergence  $h \rightarrow 0$

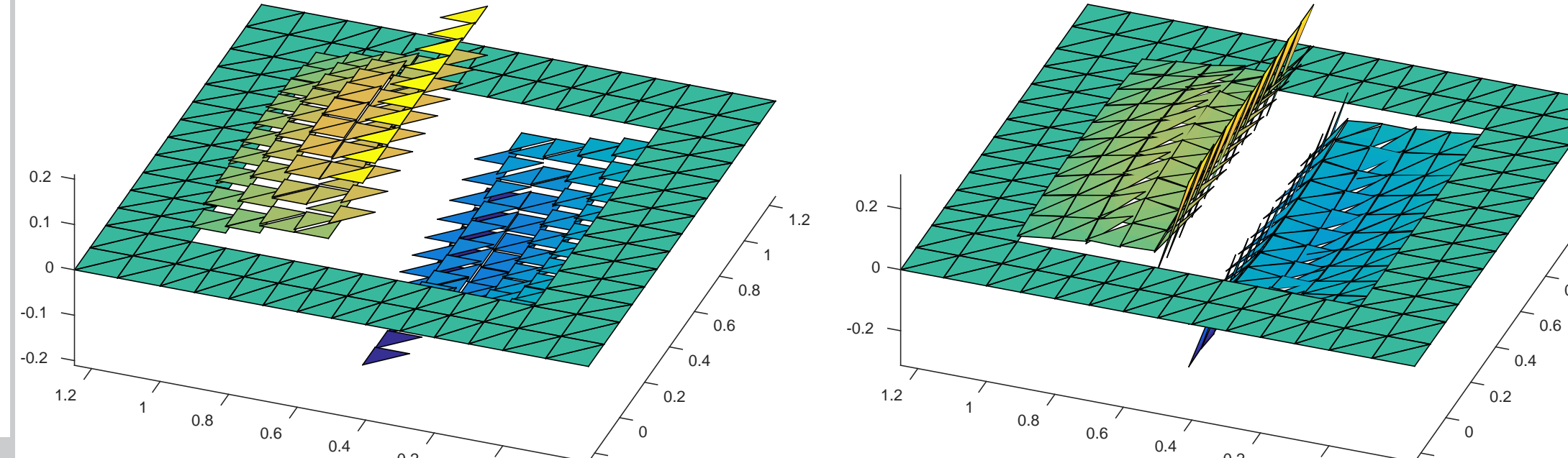
- Piecewise Constant =  $O(h)$
- Piecewise Linear =  $O(h^2)$



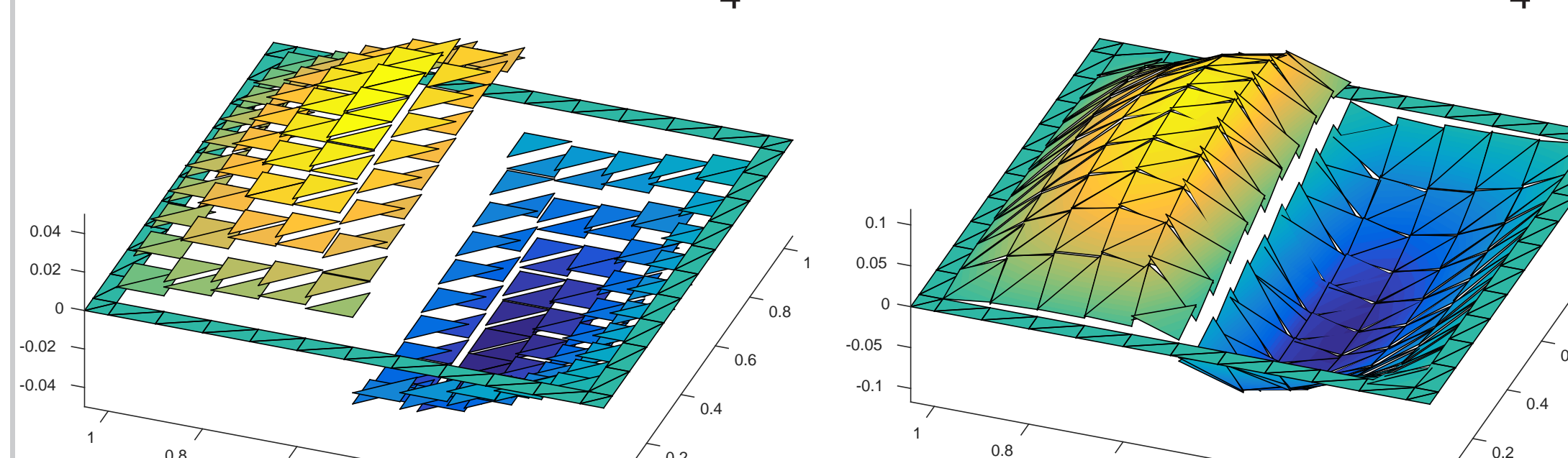
Finite Element Solution

## Numerical results

- The nonlocal kernel,  $\gamma_\varepsilon$ , is piecewise constant
- $h = \frac{1}{10}, \quad f = 1/(x_2 - 0.5), \quad C = \frac{9}{4}$
- Singularity aligned with element boundaries



Piecewise Constant,  $\varepsilon = \frac{1}{4}$       Piecewise Linear,  $\varepsilon = \frac{1}{4}$



Piecewise Constant,  $\varepsilon = \frac{1}{20}$       Piecewise Linear,  $\varepsilon = \frac{1}{20}$

## References

- S.D. Bond, R.B. Lehoucq, “Quadrature for nonlocal mechanics problems”, Sandia Technical Report (2012).
- S. A. Silling & E. Askari, *Computers & Structures* **83** (2005), 1526–1535.
- B. Kilic & E. Madenci, *International Journal of Non-Linear Mechanics* **44** (2009), 845–854.
- X. Chen & M. Gunzburger, *Computer Methods in Applied Mechanics and Engineering* **200** (2011), 1237–1250.
- K. Yu, X. J. Xin, & K. B. Lease, *Modelling and Simulation in Materials Science and Engineering* **19** (2011), 045003.
- B. Aksoylu & M. L. Parks, *Applied Mathematics and Computation* **217** (2011), 6498–6515.
- Q. Du, M. Gunzburger, R. B. Lehoucq, and K. Zhou, *SIAM Review* **54** (2012), 667–696.
- X. Tian & Q. Du, *SIAM J. Numer. Anal.*, **51** (2013) 3458–3482.
- Q. Du & X. Tian, *LNCSE*, **100** (2014) 97–113.
- N. J. Walkington, “Quadrature on Simplicies of Arbitrary Dimension”, CMU Tech Report (2000).

## Acknowledgment

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.