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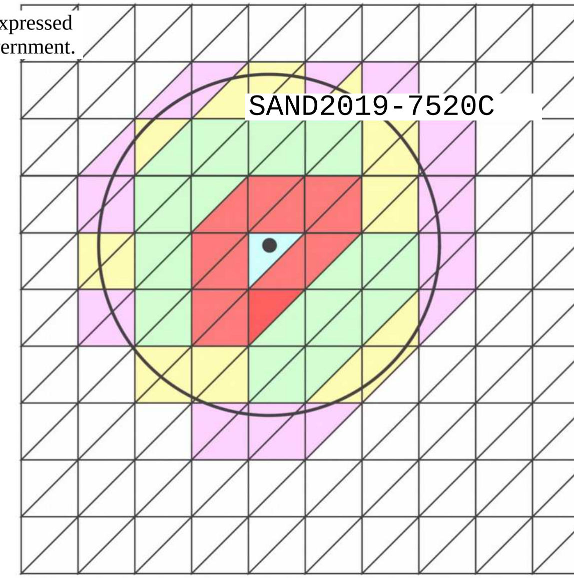

NONLOCAL MODELS with APPROXIMATE NONLOCAL NEIGHBORHOODS: towards fast FEM

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M. Gunzburger, *Florida State University, FL*

C. Vollman, *University of Trier, Germany*

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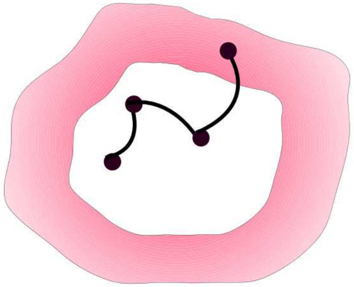
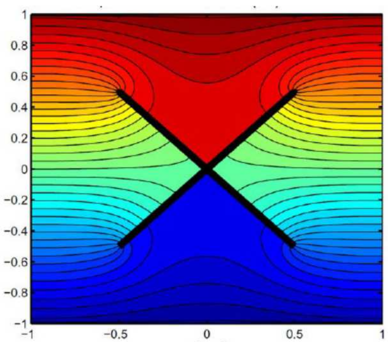
NONLOCAL MODELS AND RELATED CHALLENGES

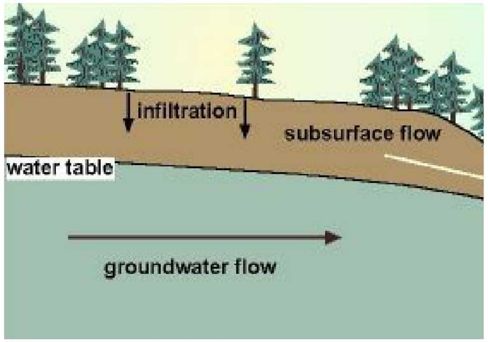
APPLICATIONS

- nonlocal models for continuum mechanics
- stochastic jump processes
- nonlocal heat conduction
- subsurface flow/porous media
- image processing





Bobaru, 2012

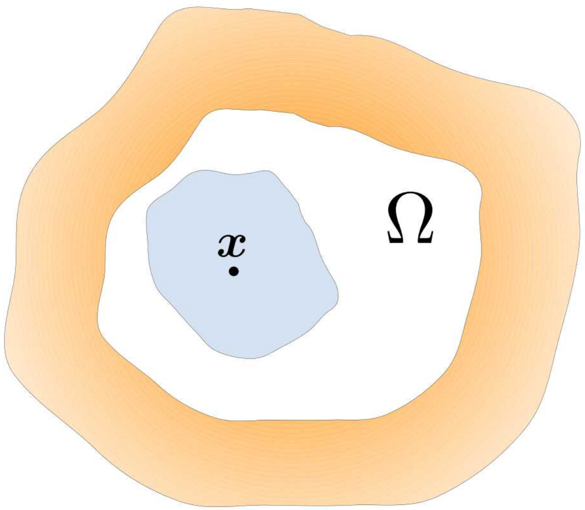


Buades, 2010

NONLOCAL DIFFUSION OPERATORS

how do they look?

$$\mathcal{L}u(\boldsymbol{x}) = \int_{\mathbb{R}^n} \big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\, \gamma(\boldsymbol{x}, \boldsymbol{y})\, d\boldsymbol{y}$$



what do we want to solve?

$\mathcal{L}u = f$

$+$ volume contraints

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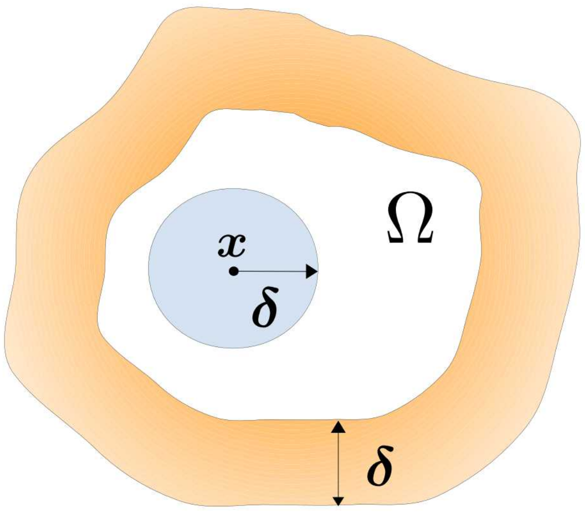
"standard" model



CHALLENGES

Modeling:
- prescription of volume constraints
- choice of kernel functions
- modeling of nonlocal interfaces

Computations:
- numerical solution can be prohibitively expensive
- implementation is troublesome

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- design of efficient nonlocal solvers
- design of efficient quadrature rules/approximations

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FEM FOR NONLOCAL MODELS

Meshfree methods: popular means for discretizing nonlocal equations

Variational methods:

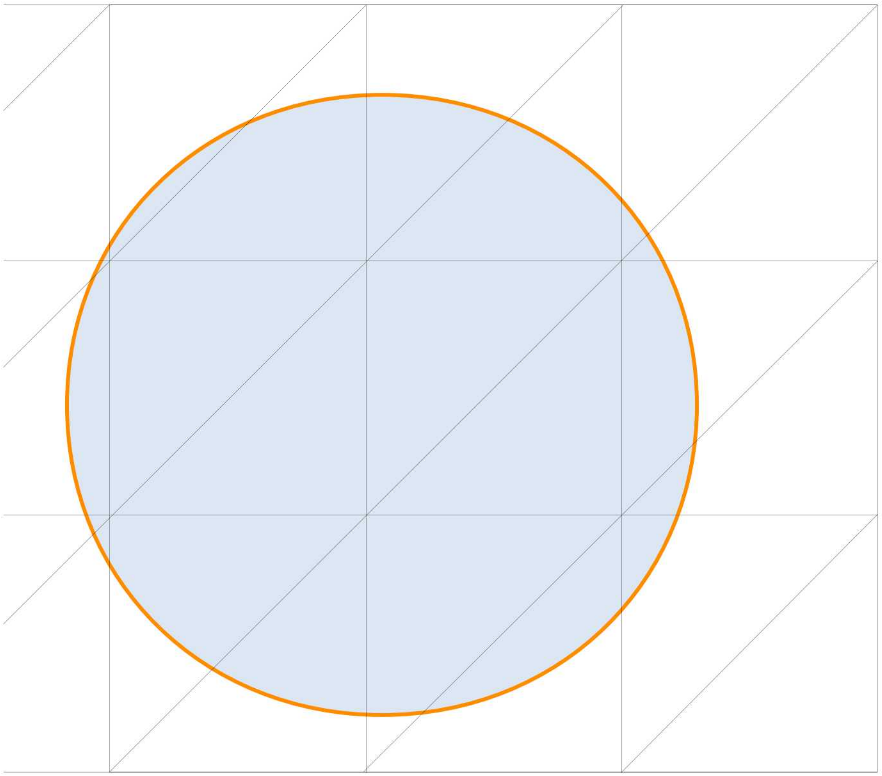
- ease in dealing with complicated domains
- higher-order convergence rates
- adaptive meshing methods (for the treatment of, e.g., discontinuities)
- rigorous mathematical treatment of operator and solution properties (convergence, stability, ...)

however... additional challenges

BALLS AND MESHES

Challenge: matrix assembling using FEM in 2D and 3D simulations

- determining intersections
- computing integrals of round domains
- find appropriate quadrature rules



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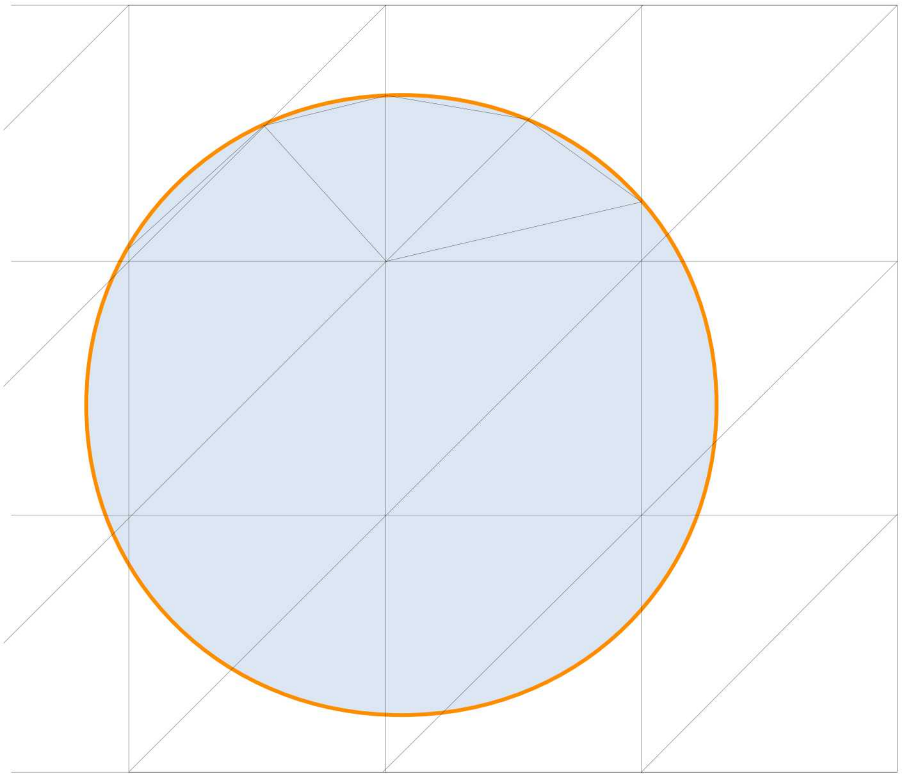

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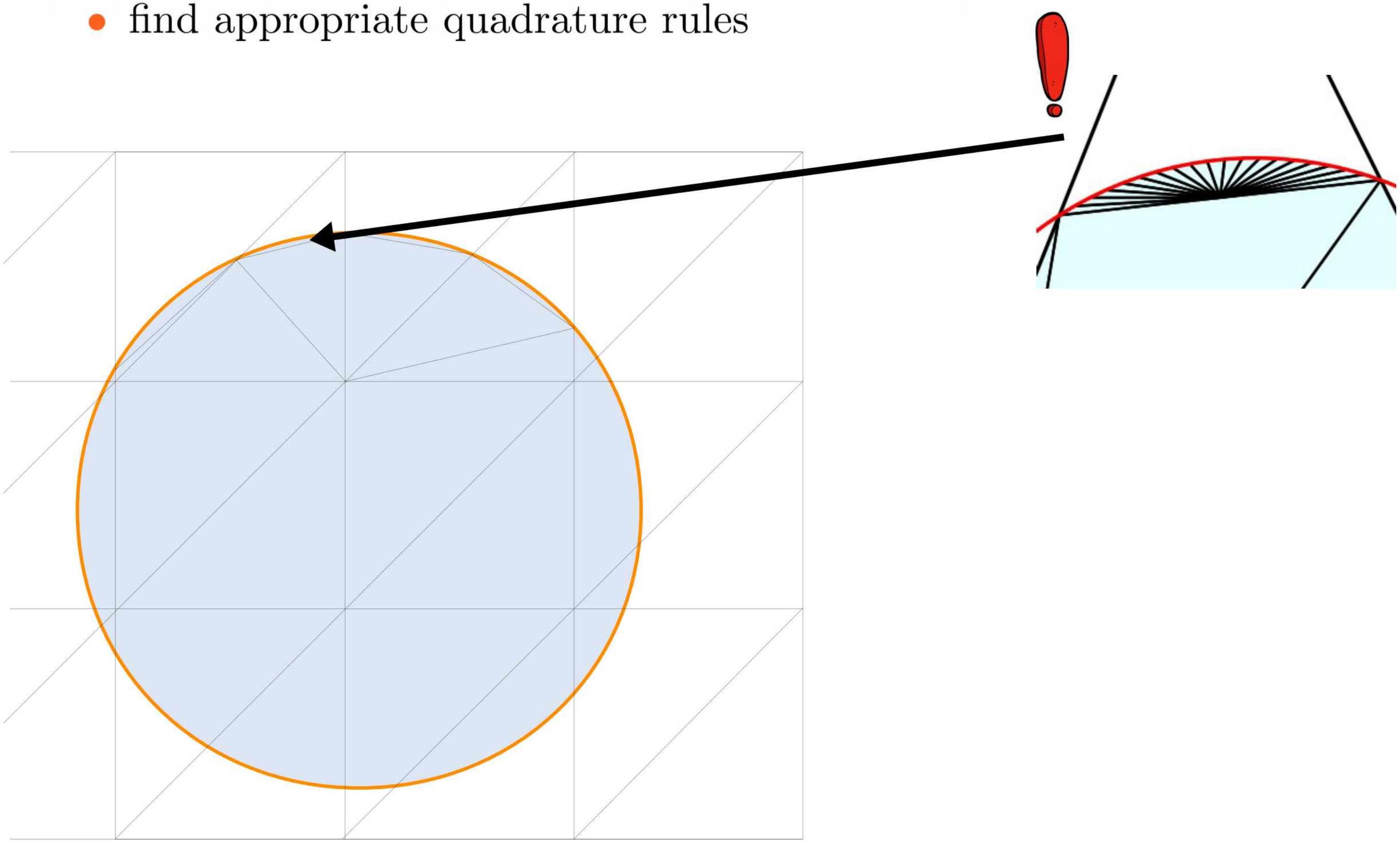
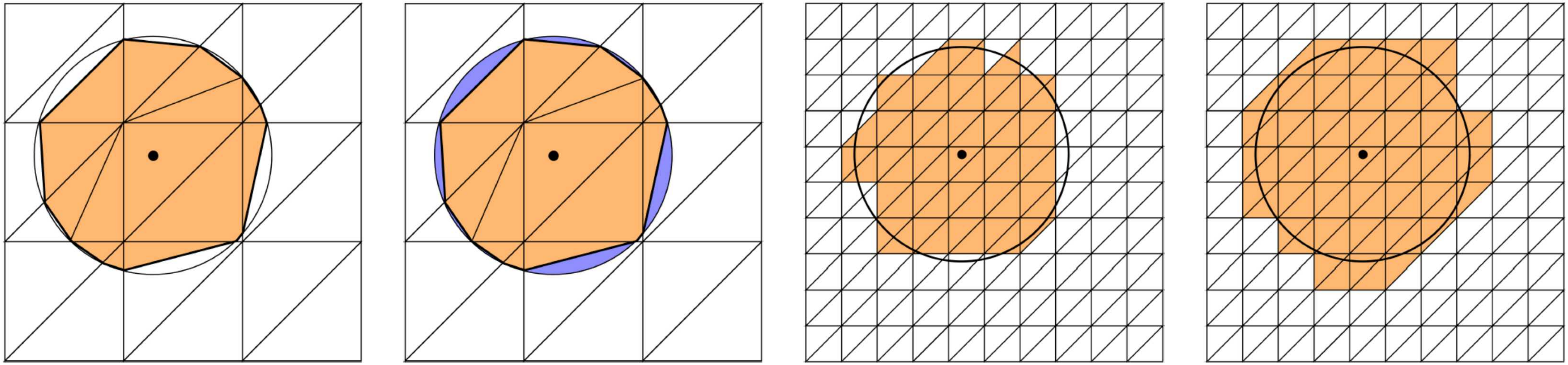


CURRENT STRATEGIES

triangles:
- triangulation of caps (Xu, Google Inc., Stoyanov, ORNL)
- approximation of the ball with a polygon (Bond, SNL)
- inclusion of partial triangles based on barycenters (Borthagaray, U. Maryland)



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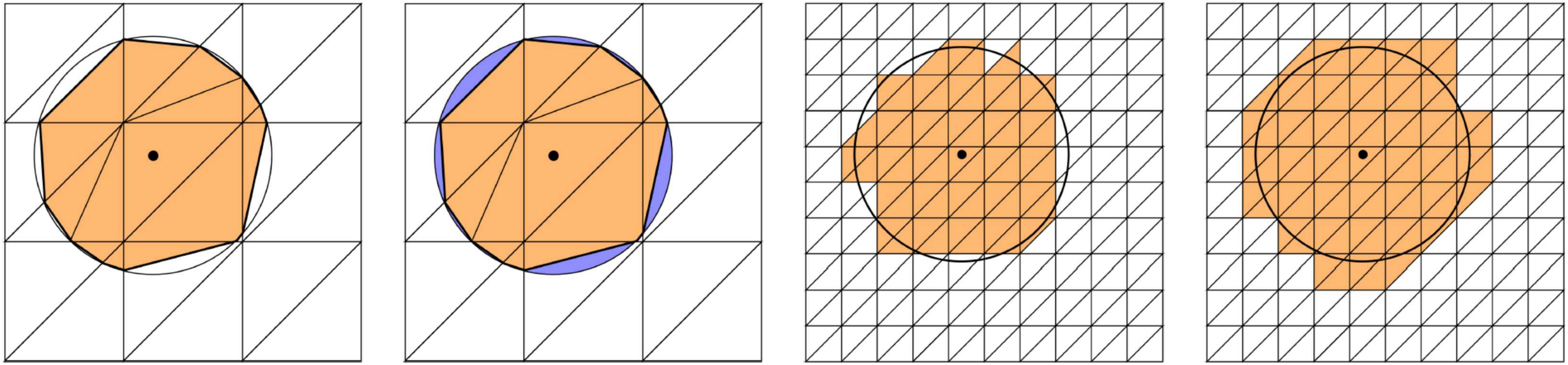
these may be unnecessary, inaccurate or inefficient!



CONTRIBUTIONS OF THIS WORK

- introduce **approximate neighborhoods** that facilitate the assembly procedure and mitigate the computational effort
- quantify the **approximation error** and its contribution to the overall accuracy
- provide guidance on the choice of quadrature rules
- introduce a **cheap and easy-to-implement** approximation that
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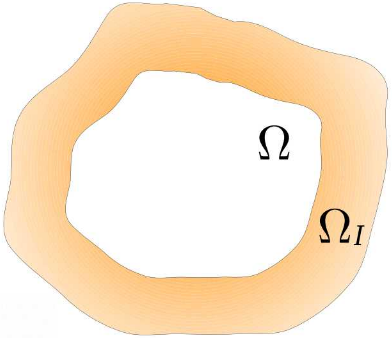
! **making variational methods a preferable alternative?**

WEAK FORM AND ITS DISCRETIZATION

FEM FOR NONLOCAL MODELS



Weak form: for $u = 0$ in Ω_I

$$0 = \int_{\Omega} (-\mathcal{L}u - f)\, v \, d\boldsymbol{x} = \int_{\Omega\cup\Omega_I} \int_{\Omega\cup\Omega_I} \big(u(\boldsymbol{y}) - u(\boldsymbol{x})\big)\big(v(\boldsymbol{y}) - v(\boldsymbol{x})\big)\gamma(\boldsymbol{x},\boldsymbol{y})\, d\boldsymbol{y}\, d\boldsymbol{x} - \int_{\Omega} f v \, d\boldsymbol{x}$$

$$A(u,v) = F(v), \quad \forall\, v \in V_c(\Omega\cup\Omega_I)$$

nonlocal Green's identity [Du et al., 2012]

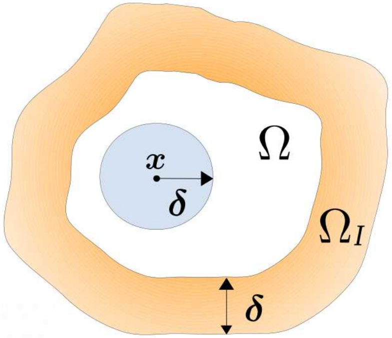
Energy norm and spaces:

– "energy norm": $|||w||| = \sqrt{A(w,w)}$ (norm on $V_c(\Omega\cup\Omega_I)$)

– energy space: $V(\Omega\cup\Omega_I) = \{w \in L^2(\Omega\cup\Omega_I) \; : \; |||w||| < \infty\}$

– constrained energy space: $V_c(\Omega\cup\Omega_I) = \{w \in V \; : \; w = 0 \text{ on } \Omega_I\}$

FEM FOR NONLOCAL MODELS



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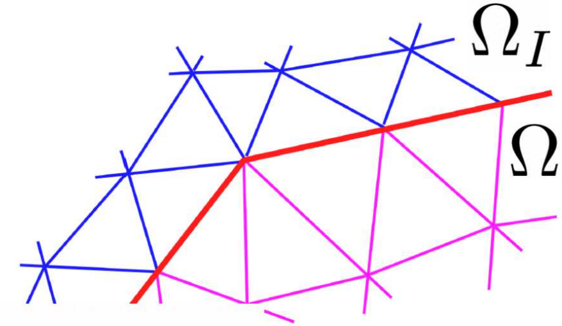
Kernels: $\gamma(\boldsymbol{x}, \boldsymbol{y}) = \psi(\boldsymbol{x}, \boldsymbol{y}) \mathcal{X}_{B_\delta(\boldsymbol{x})(\boldsymbol{y})}$

FEM FOR NONLOCAL MODELS



FEM nodes and basis

– $\{\widetilde{\boldsymbol{x}}_j\}_{j=1}^J$: set of nodes, with $\{\widetilde{\boldsymbol{x}}_j\}_{j=1}^{J_\Omega} \subset \Omega$ and $\{\widetilde{\boldsymbol{x}}_j\}_{j=J_\Omega+1}^{J} \subset \overline{\Omega}_I$

– $\{\phi_j(\boldsymbol{x})\}_{j=1}^J$: piecewise-polynomial functions such that $\phi_j(\widetilde{\boldsymbol{x}}_{j'}) = \delta_{jj'}$ for $j' = 1, \ldots, J$

– FEM spaces: $V^h = \text{span}\{\phi_j(\boldsymbol{x})\}_{j=1}^J \subset V(\Omega \cup \Omega_I)$ of dimension J

$$V_c^h = \text{span}\{\phi_j(\boldsymbol{x})\}_{j=1}^{J_\Omega} \subset V_c(\Omega \cup \Omega_I) \text{ of dimension } J_\Omega$$

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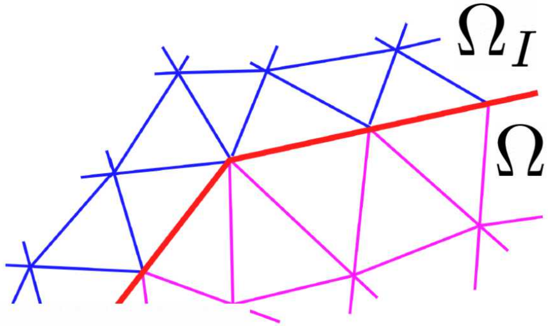

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FEM solution and projection

$$u_h(\boldsymbol{x}) = \sum_{j=1}^{J} U_j \phi_j(\boldsymbol{x})$$

discrete weak formulation: projection of the weak form onto V^h, i.e.

find $u_h(\boldsymbol{x}) \in V^h$ such that $\quad A(u_h, \phi_j) = F(\phi_j) \;\; \forall\, j = 1, \ldots J_\Omega$

FEM FOR NONLOCAL MODELS

Elements, balls and quadrature rules

$\sum_{j=1}^{J} A(\phi_{j'}, \phi_j) U_j = F(\phi_{j'}) \quad \text{for } j' = 1, \ldots, J,$

$$A(\phi_{j'}, \phi_j) = \sum_{k=1}^{K} \int_{\mathcal{E}_k} \int_{\overline{\Omega} \cap B_\delta(\boldsymbol{x})} \big(\phi_j(\boldsymbol{x}) - \phi_j(\boldsymbol{y})\big)\big(\phi_{j'}(\boldsymbol{x}) - \phi_{j'}(\boldsymbol{y})\big)\psi(\boldsymbol{x}, \boldsymbol{y}) d\boldsymbol{y} \qquad j = 1, \ldots, J, j' = 1, \ldots, J_\Omega$$

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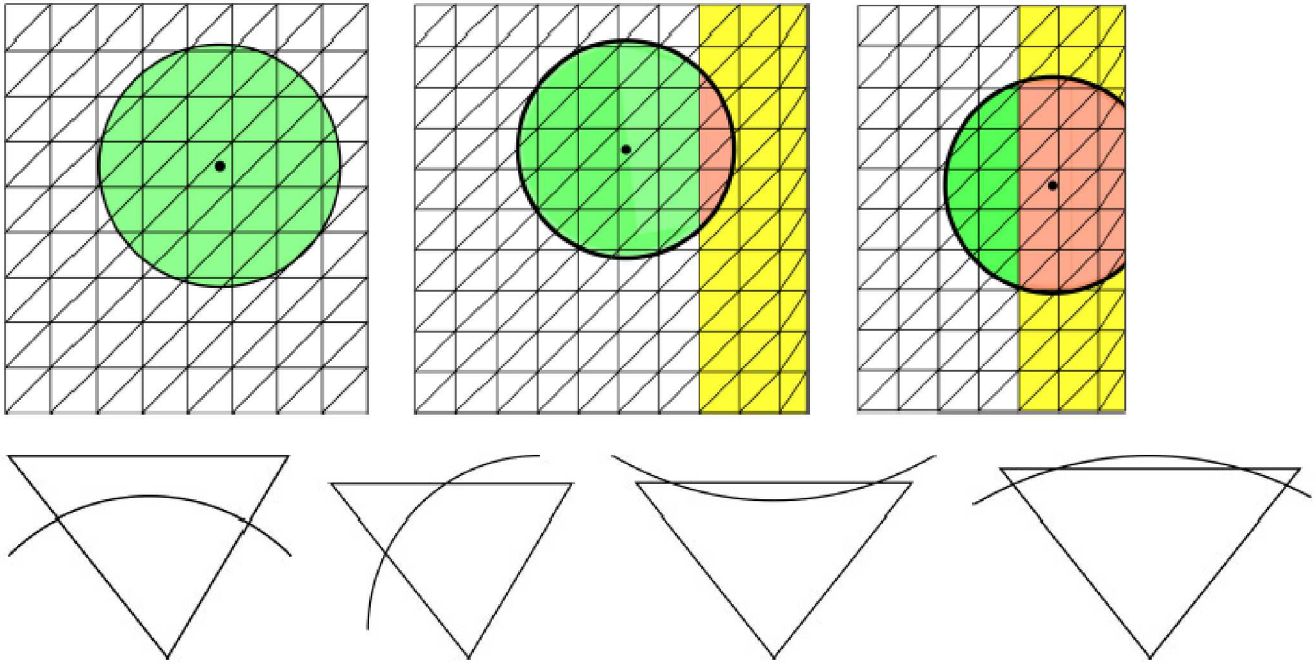

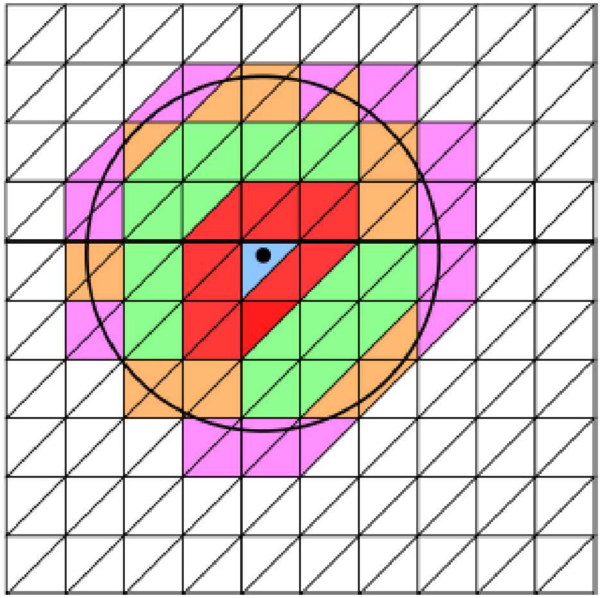

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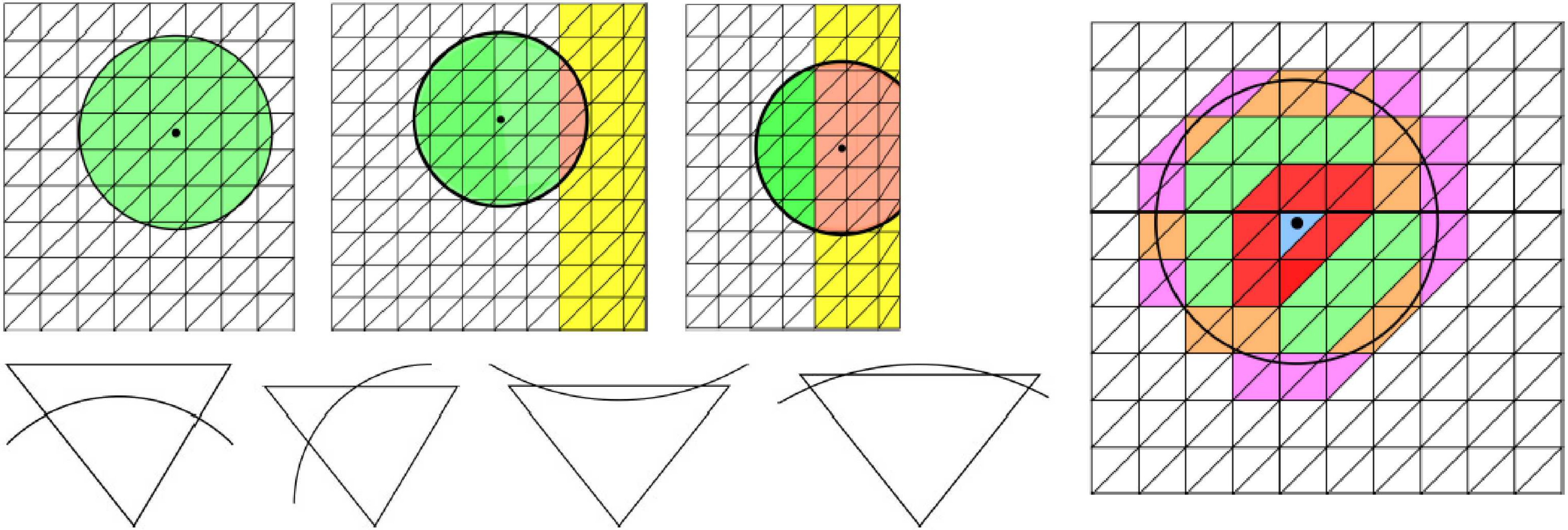

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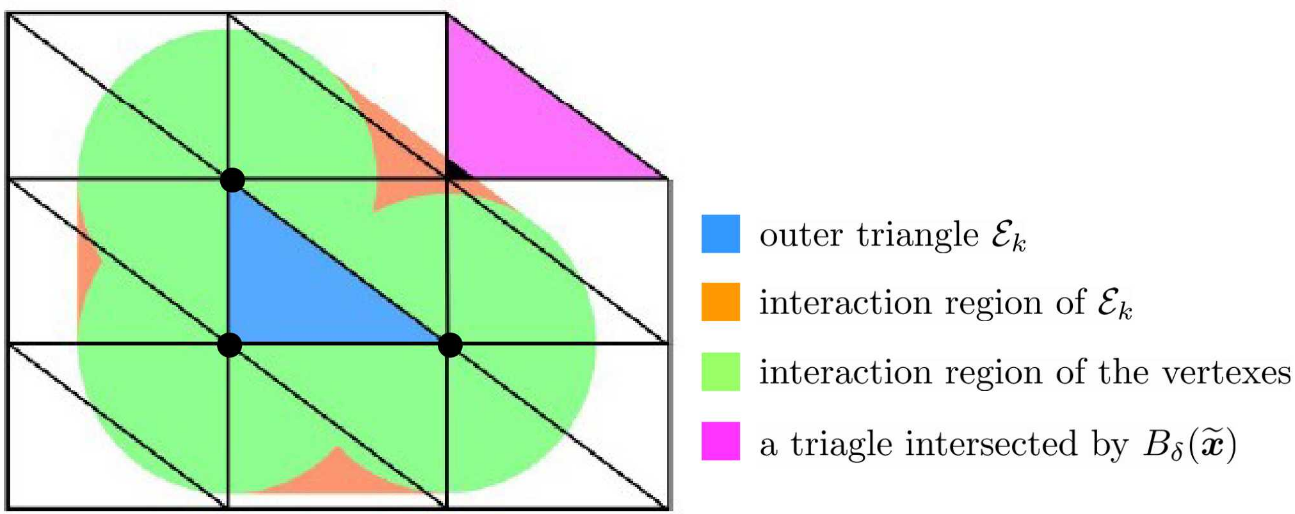

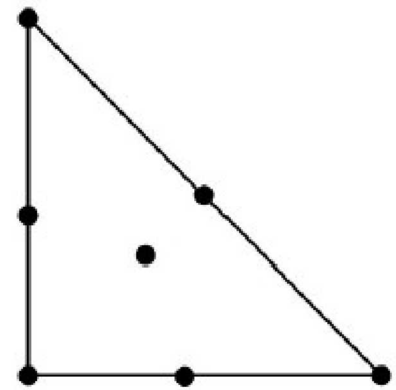

quadrature points for $\mathcal{E}_k$: integrates cubics exactly and takes care of missing triangles

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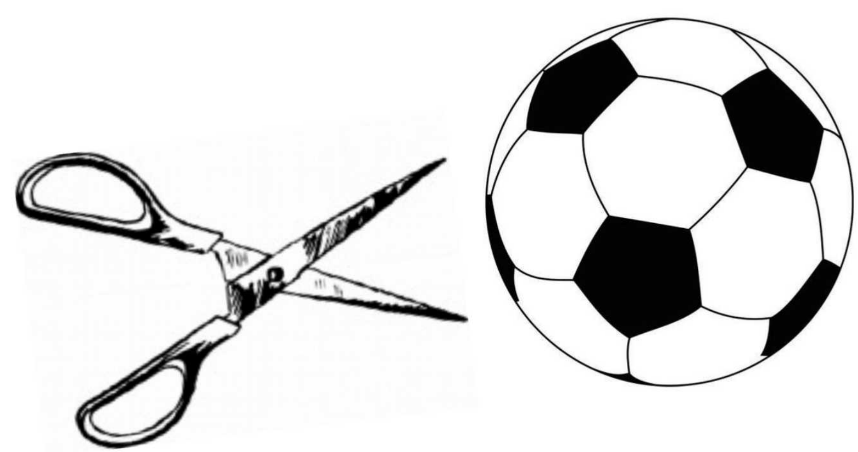
Note! Inner quadrature rules are also needed

(way too messy, not reported)

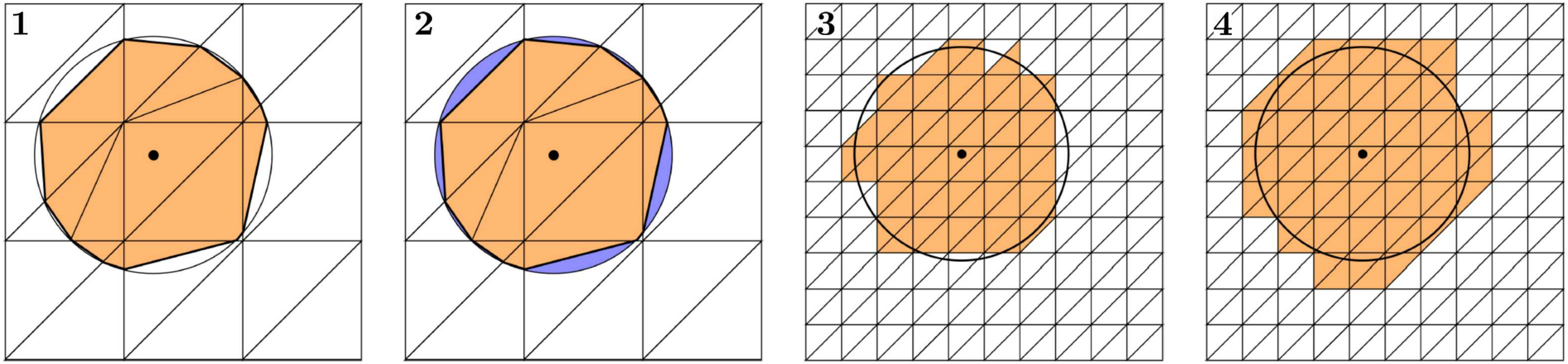
but luckily not as troublesome

APPROXIMATE BALLS

– C. Vollman, M. D'Elia, M. Gunzburger, V. Schulz, Reducing the cost of nonocal FEM via approximation of nonlocal neighborhoods, *in progress.*



GEOMETRIC APPROXIMATION



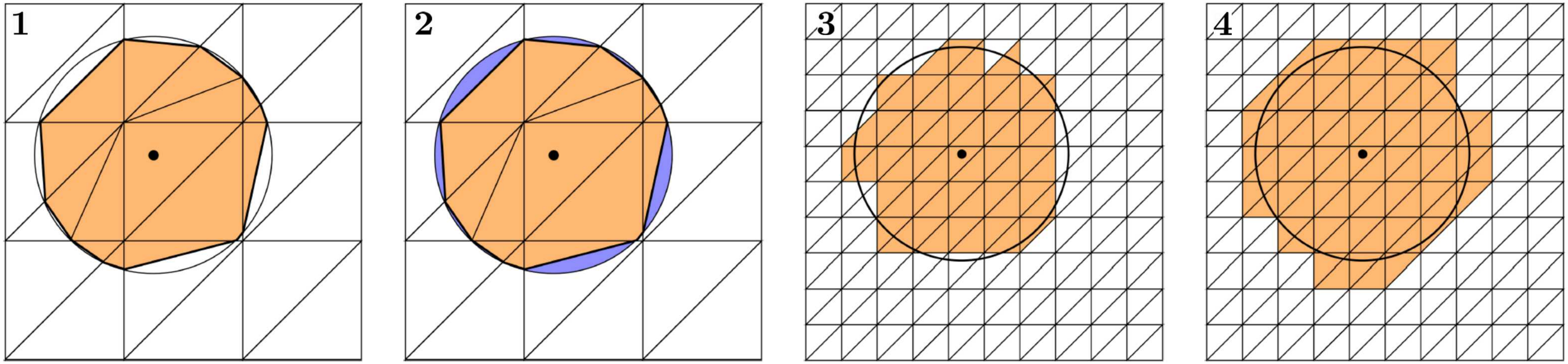
1 Inscribed triangle-based **polygonal approximation** of balls

2 Inscribed cap-based **polygonal approximation** of balls

3 **Whole-triangle** approximation based on barycenter location

4 **Whole-triangle** approximation based on overlap with ball

GEOMETRIC APPROXIMATION



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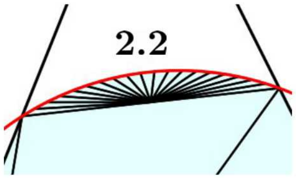
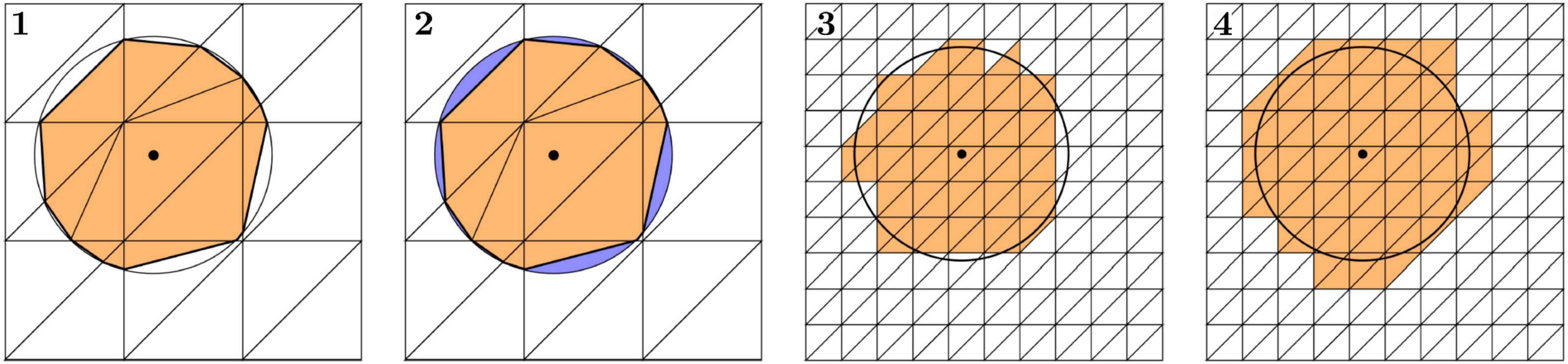
2.1 quadrature rules for caps

2.2 re-triangulation of caps



GEOMETRIC APPROXIMATION



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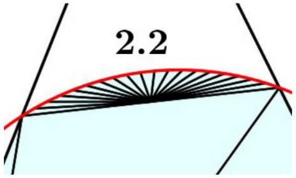

Are we losing accuracy?

ACCURACY OF THE APPROXIMATION

Lemma:

Let $B_\delta(\boldsymbol{x})$ be the ℓ^2 ball and $B_{\delta,h}(\boldsymbol{x})$ be an approximation, and let u_h and $\widetilde{u}_h$ be the corresponding finite element solutions. Then, for exact outer and inner quadrature rules,

$$|||u_h - ||| \leq K \, |\Delta B_\delta(\bar{\boldsymbol{x}})| \, |||_{L^2(\Omega\cup\Omega_I)},$$

where K is a positive constant independent of δ and h, $\bar{\boldsymbol{x}} \in \Omega$ and ΔB_δ is the "difference ball":

$$\Delta B_\delta = (B_\delta \setminus (B_\delta \cap B_{\delta,h})) \cup (B_{\delta,h} \setminus (B_\delta \cap B_{\delta,h}))$$

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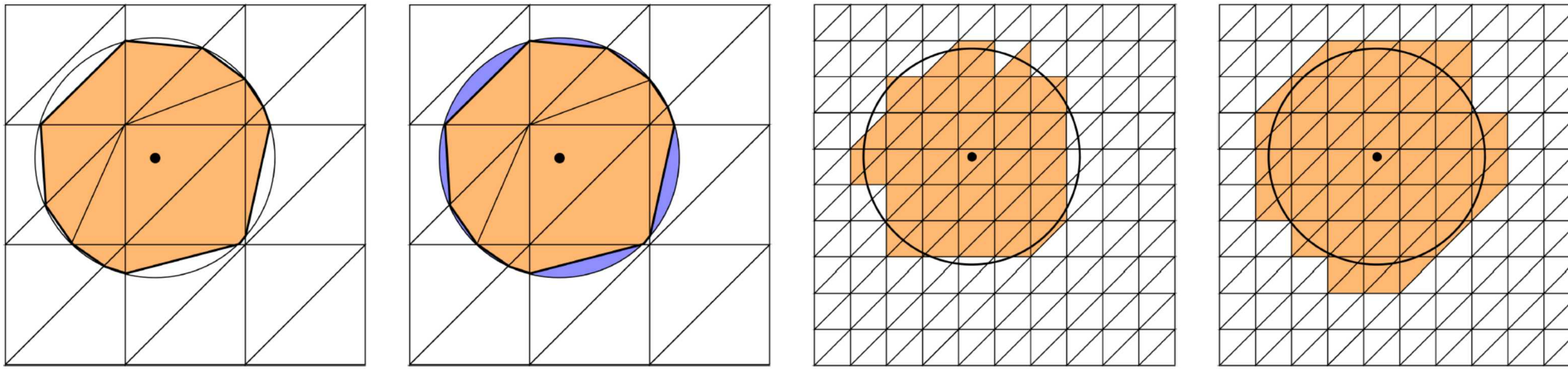
the overall accuracy depends on the volumeof the difference ball !

APPROXIMATION ERROR

Discretization: piecewise linear FEM spaces, optimal accuracy (h^2)



no caps	quad rules for caps or retriangulation	whole triangles based on barycenters	whole triangles based on overlap
$\lvert\Delta B_\delta\rvert = \mathcal{O}(h^2)$	$\lvert\Delta B_\delta\rvert = \mathcal{O}(h^2)$	$\lvert\Delta B_\delta\rvert = \mathcal{O}(h)$	$\lvert\Delta B_\delta\rvert = \mathcal{O}(h)$

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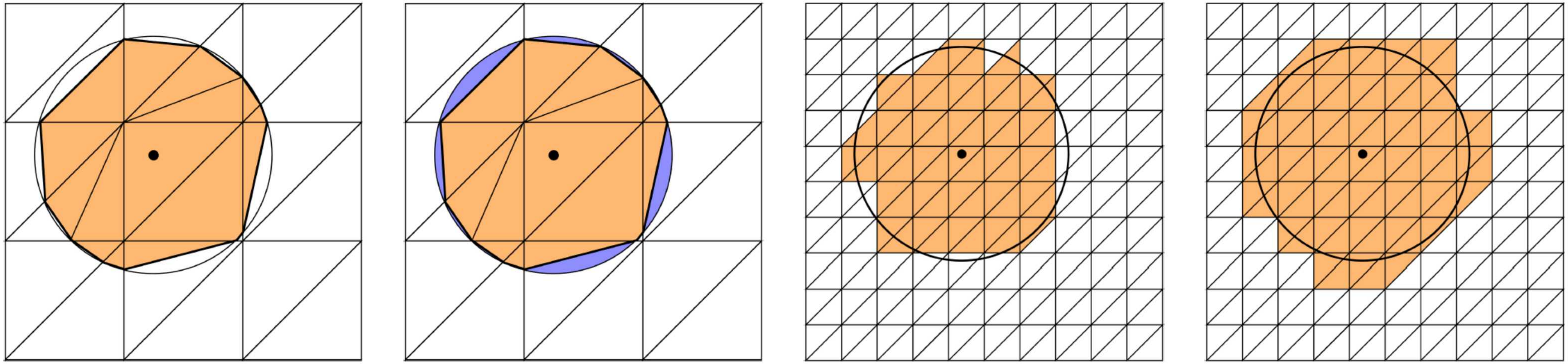
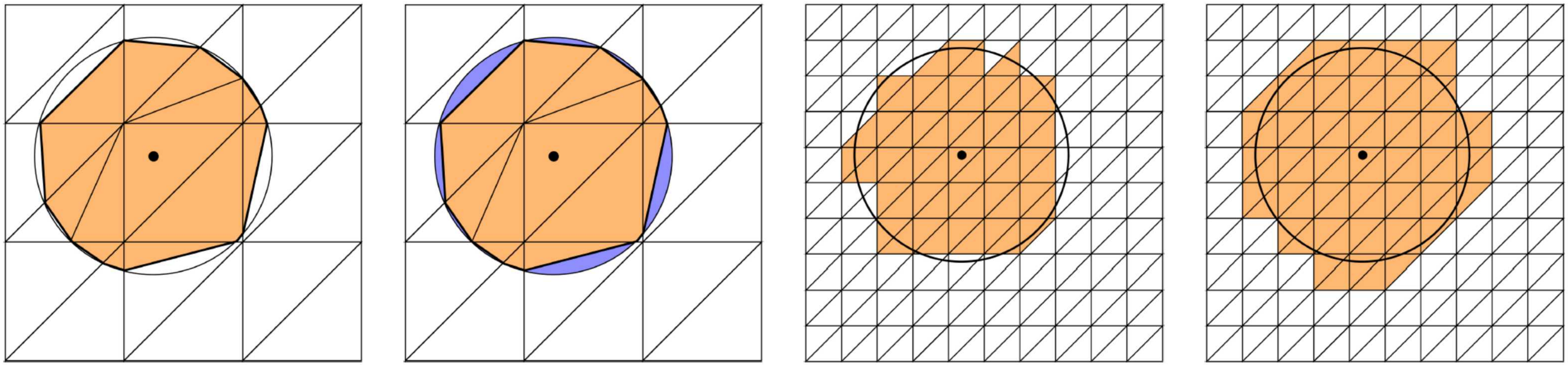


no caps	quad rules for caps or retriangulation	whole triangles based on barycenters	whole triangles based on overlap
$\lvert\Delta B_\delta\rvert = \mathcal{O}(h^2)$	$\lvert\Delta B_\delta\rvert = \mathcal{O}(h^2)$	$\lvert\Delta B_\delta\rvert = \mathcal{O}(h)$	$\lvert\Delta B_\delta\rvert = \mathcal{O}(h)$
$\lvert\lvert\lvert e\rvert\rvert\rvert = \mathcal{O}(h^2)$	$\lvert\lvert\lvert e\rvert\rvert\rvert = \mathcal{O}(h^2)$	$\lvert\lvert\lvert e\rvert\rvert\rvert = \mathcal{O}(h)$	$\lvert\lvert\lvert e\rvert\rvert\rvert = \mathcal{O}(h)$

APPROXIMATION ERROR

Discretization: piecewise linear FEM spaces, optimal accuracy (h^2)



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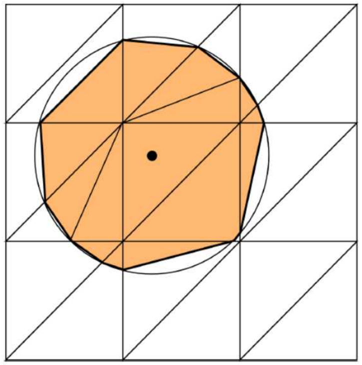
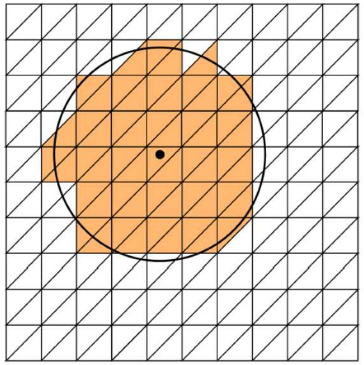
APPROXIMATION ERROR



1 No caps

3 Barycenter



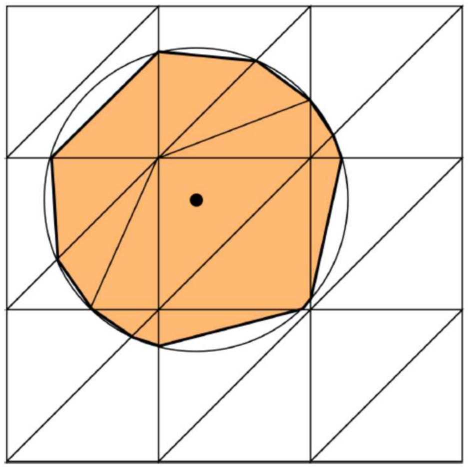
h	L^2	rate	energy	rate
0.1	2.75e-2	-	1.29e-1	-
0.05	3.86e-3	2.83	1.88e-2	2.77
0.025	4.00e-4	3.26	3.37e-3	2.48
0.0125	2.60e-4	0.61	1.20e-3	1.48
0.00625	7.00e-5	1.86	3.20e-4	1.92
		2.09		**2.13**

h	L^2	rate	energy	rate
0.1	1.71e-1	-	7.8e-1	-
0.05	6.00e-2	1.51	2.64e-1	1.56
0.025	1.51e-2	1.99	6.85e-2	1.94
0.0125	2.30e-3	2.71	1.07e-2	2.68
0.00625	4.60e-4	2.33	2.19e-3	2.29
		2.17		**2.15**

Note 1: rate seem erratic, an adaptive quad rule for the outer integral fixes this issue

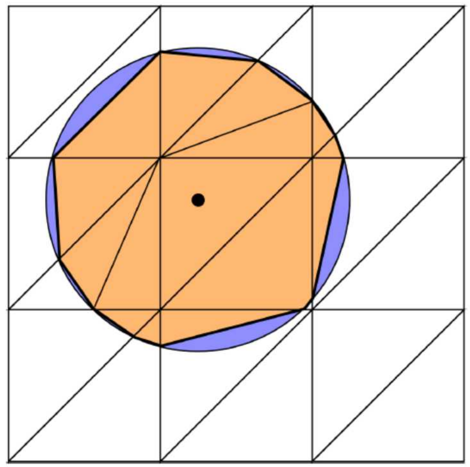
Note 2: CPU(no caps) $\sim 3\times$CPU(barycenter)

APPROXIMATION ERROR



no caps

$$|||e||| = \mathcal{O}(h^2)$$



quad rules for caps or retriangulation

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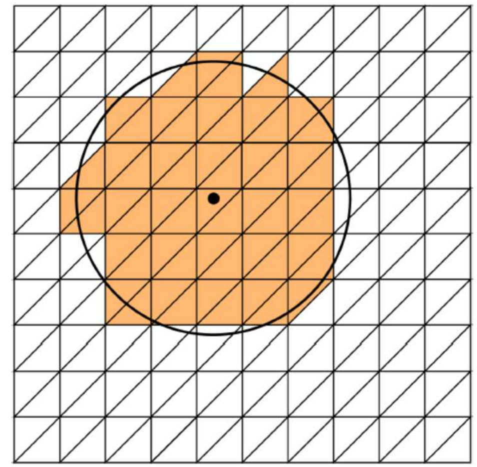

whole triangles based on barycenters

$$|||e||| = \mathcal{O}(h)$$

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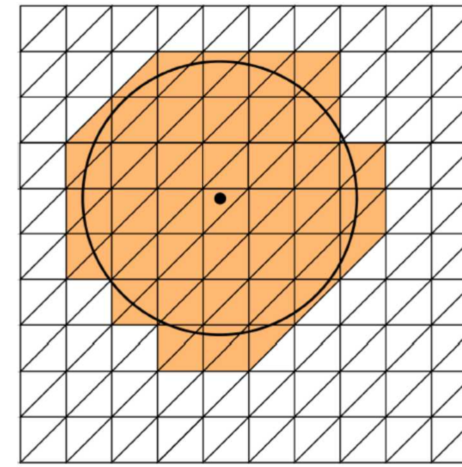


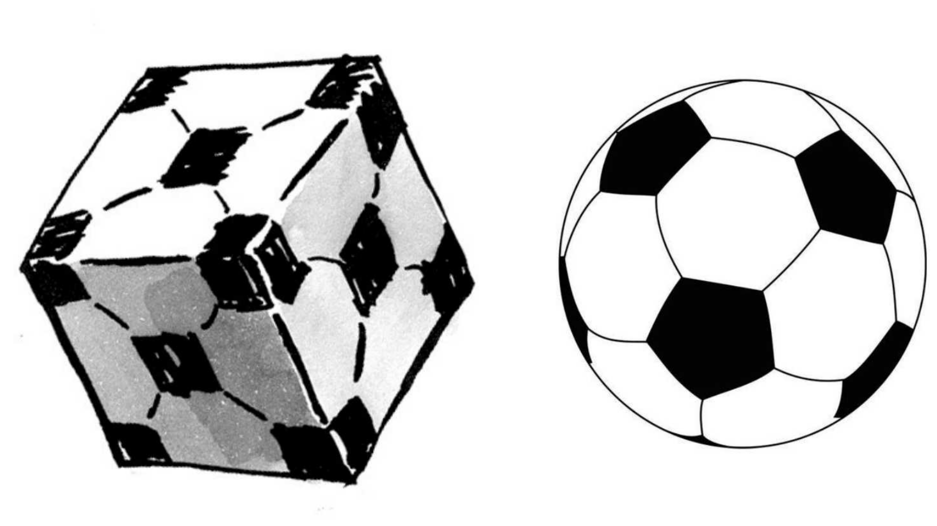
whole triangles based on overlap

$$|||e||| = \mathcal{O}(h)$$

RELATED WORK

C. Vollman, M. D'Elia, M. Gunzburger, V. Schulz,

Nonlocal Continuum Models with Nonstandard Interaction Domains, *Book in progress*.

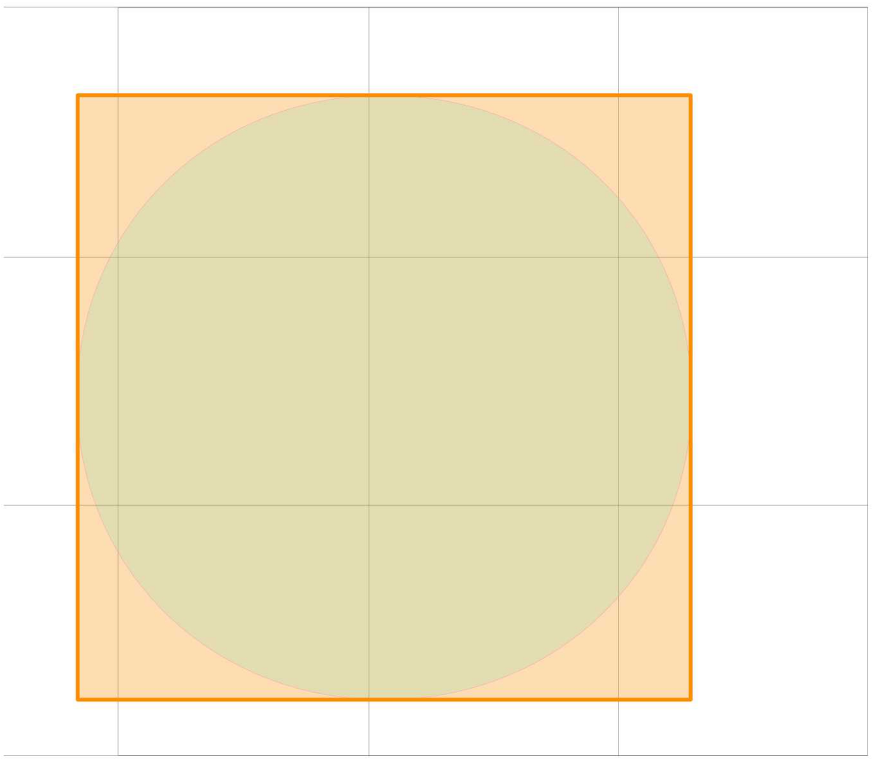


USING DIFFERENT BALLS

what if we consider a different ball?

$\Rightarrow$ triangulation w/o geometry errors

$\Rightarrow$ much easier re-triangulation!



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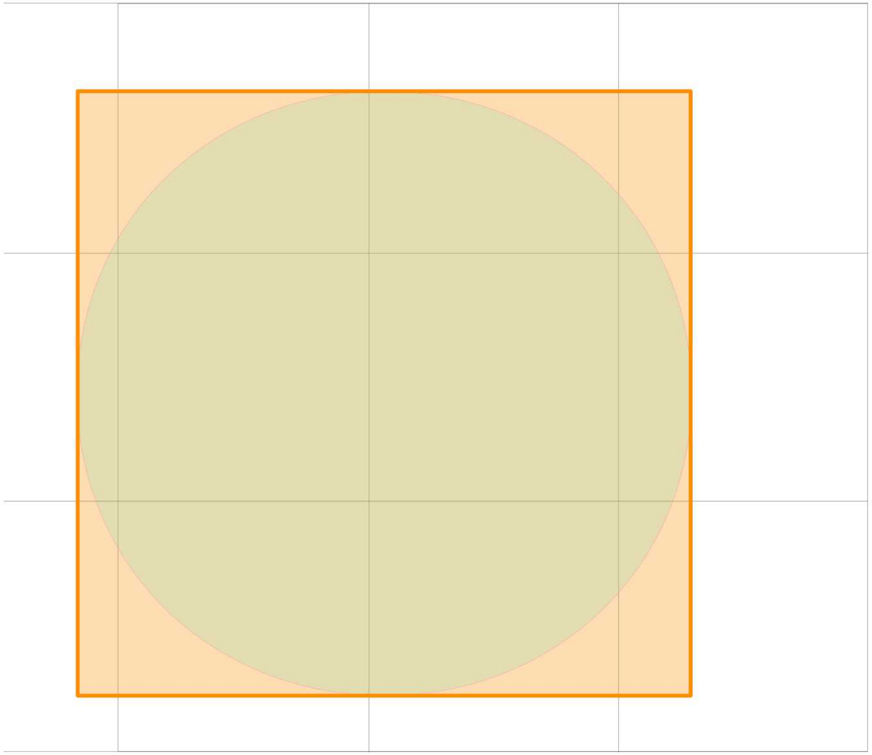

this can be a modeling choice!

- when even round balls are not required by physics
- when the nature of the problem calls for square balls

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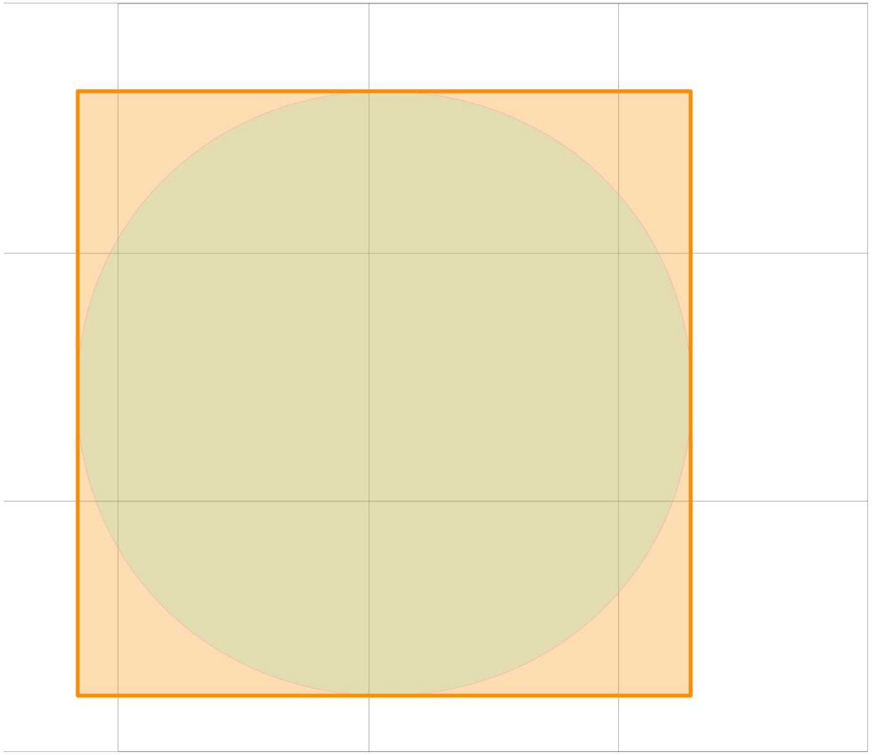

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Important questions

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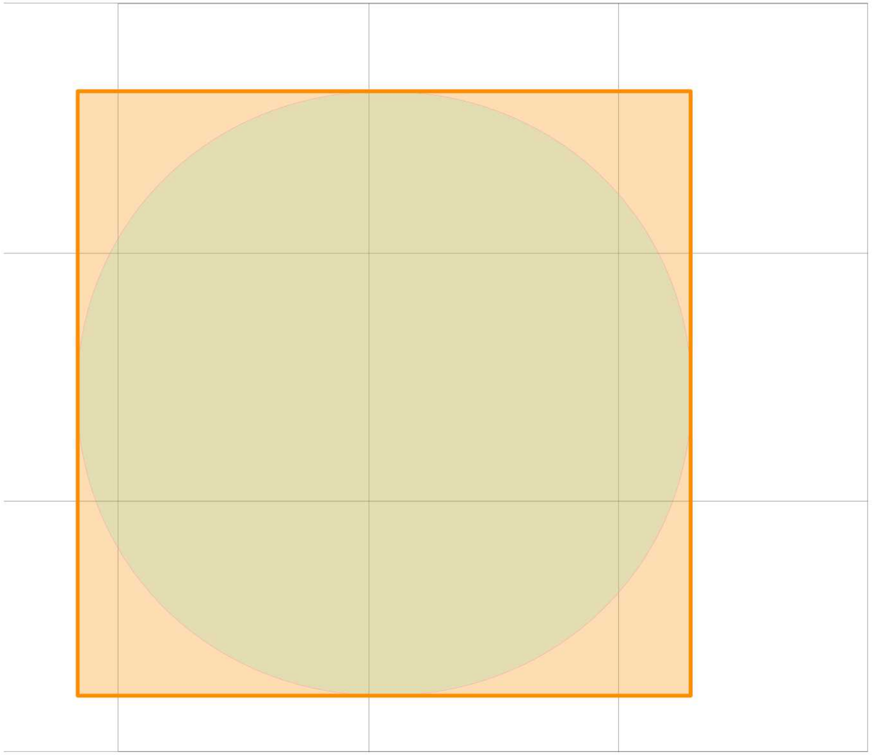

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Thank you