Centroid Approximation by use of Bernstein Polynomials for Multi-material Cell Interface Reconstruction

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Outline

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Introduction — Context

1. Fluid flow within Lagrangian, Eulerian, ALE context + complex meshes $\Rightarrow$ multi-material cells $\Rightarrow$ complex interfaces to reconstr.
2. Bad interfaces $\Rightarrow$ Bad material advection

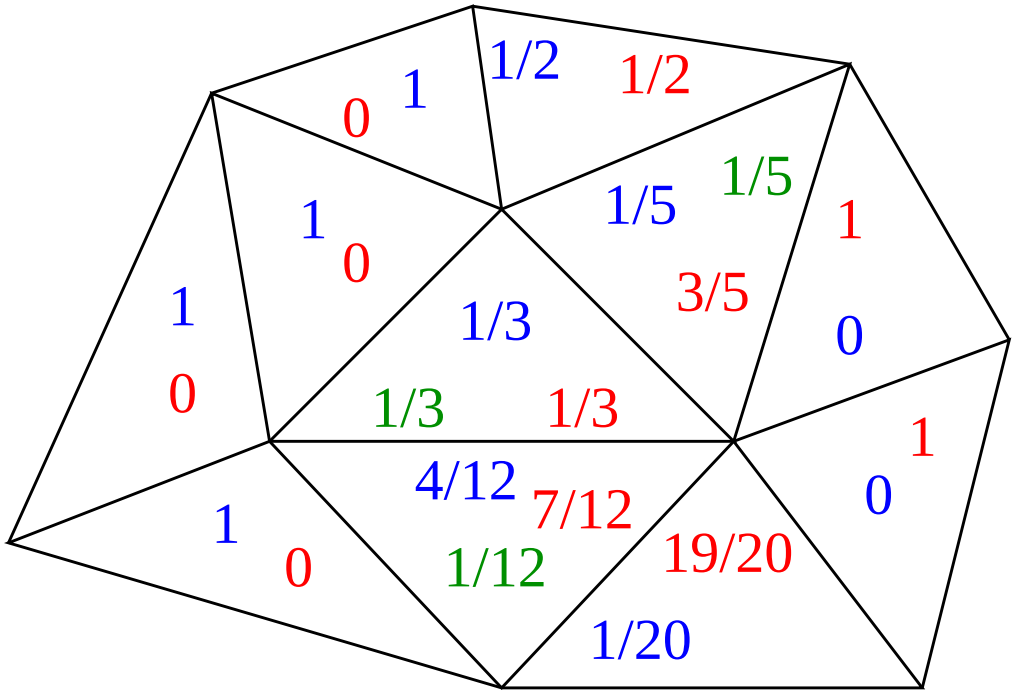
$N_{mat} = 2$: Youngs, VOF, PLIC $\rightarrow$ fine

Introduction — Context

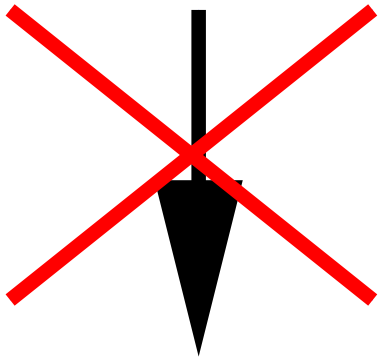
1. Fluid flow within Lagrangian, Eulerian, ALE context + complex meshes $\Rightarrow$ multi-material cells $\Rightarrow$ complex interfaces to reconstr.
2. Bad interfaces $\Rightarrow$ Bad material advection

$N_{mat} > 2$: partial solutions but...

- Known: Onion-skin, Nested-dissect., Youngs, Mosso and Clancy, Benson $\longrightarrow$ problem with T-junction, material order-dependency
- New: MOF, Power-Diagram $\longrightarrow$ Approx. of material centroids must be good enough

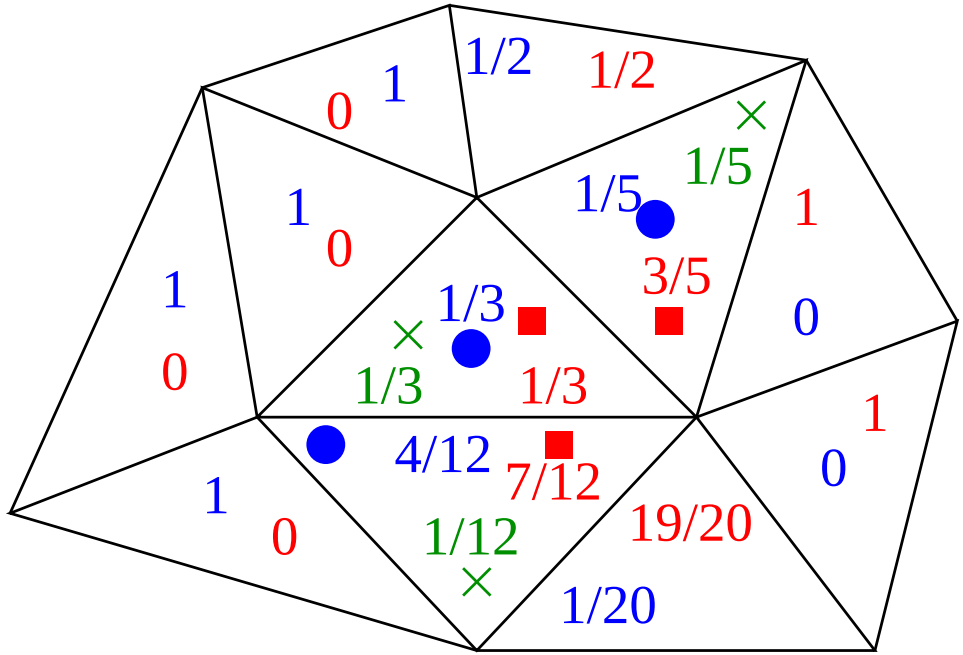


Good Volume Fractions



(Youngs, Mosso& Benson, ND...)

Good Interfaces



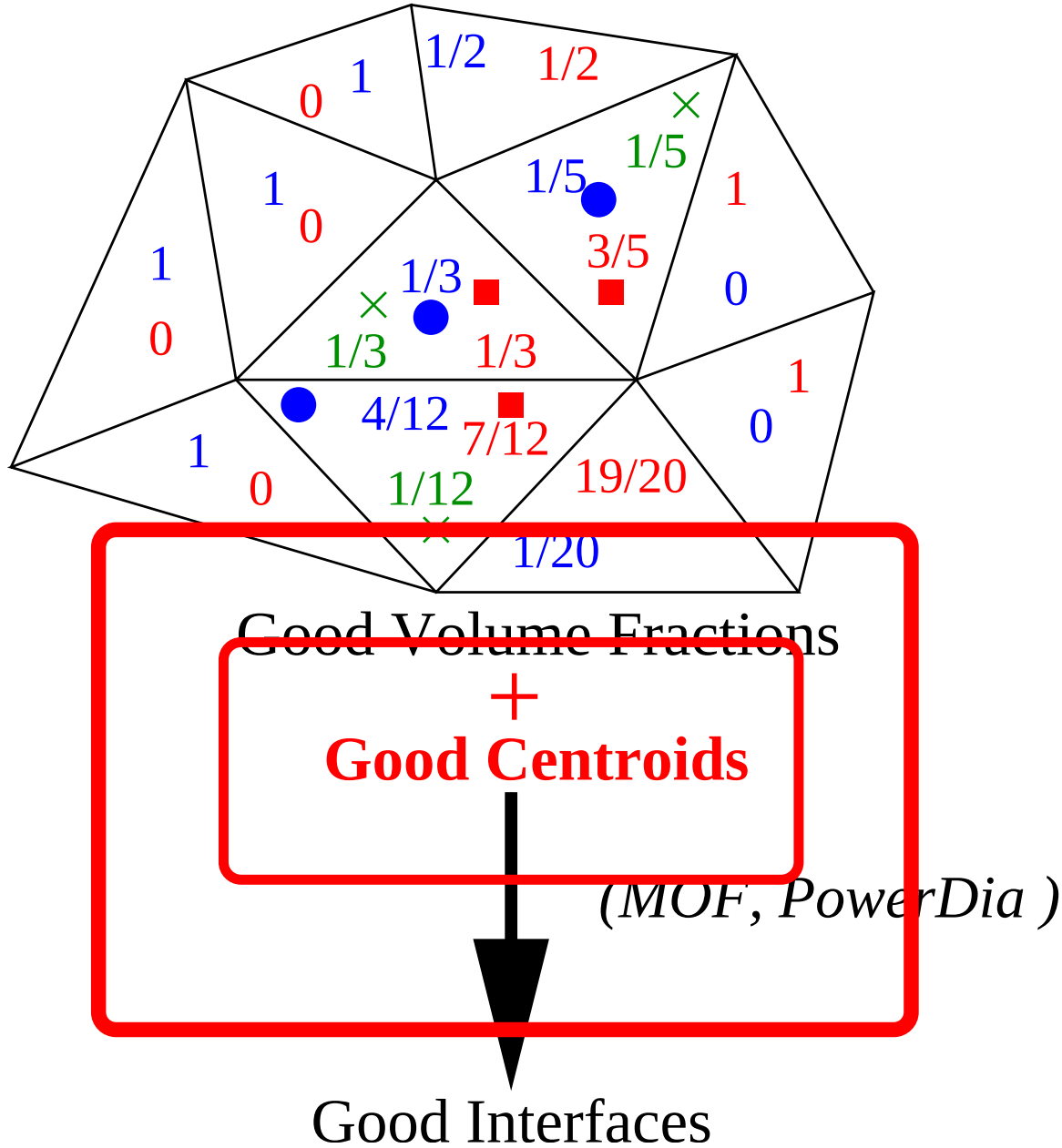
Good Volume Fractions

+

Good Centroids

↓ *(MOF, PowerDia)*

Good Interfaces



Introduction

Our goal is to develop methods to reconstruct material centroids within multi-material cells knowing

- Volumes fractions at t_n
- Mesh topology at t_n

Such that

- Independent of number of material, of the order, of the dimensionality, of the cell type, but...
- "High-order accurate"

Volume fractions in cell Ω

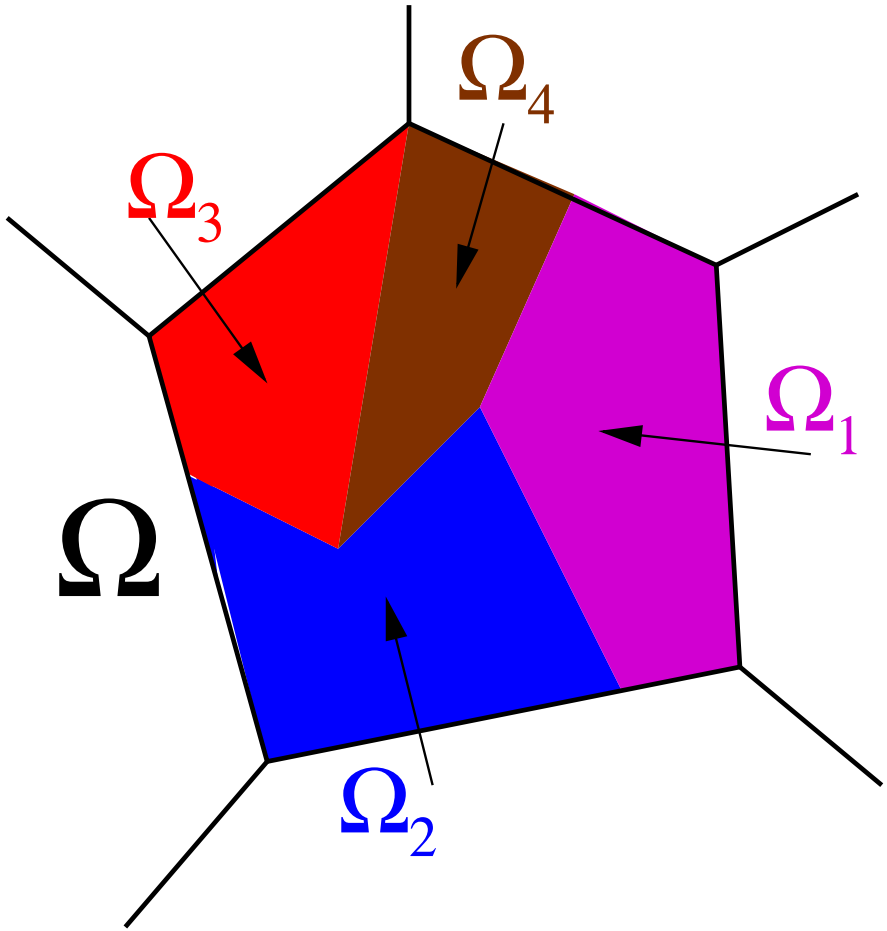
Ω_m: vol. occupied by material m

Volume fraction of material m:

$$\alpha_m = \frac{|\Omega_m|}{|\Omega|}$$

<u>Properties</u>: $\forall m$

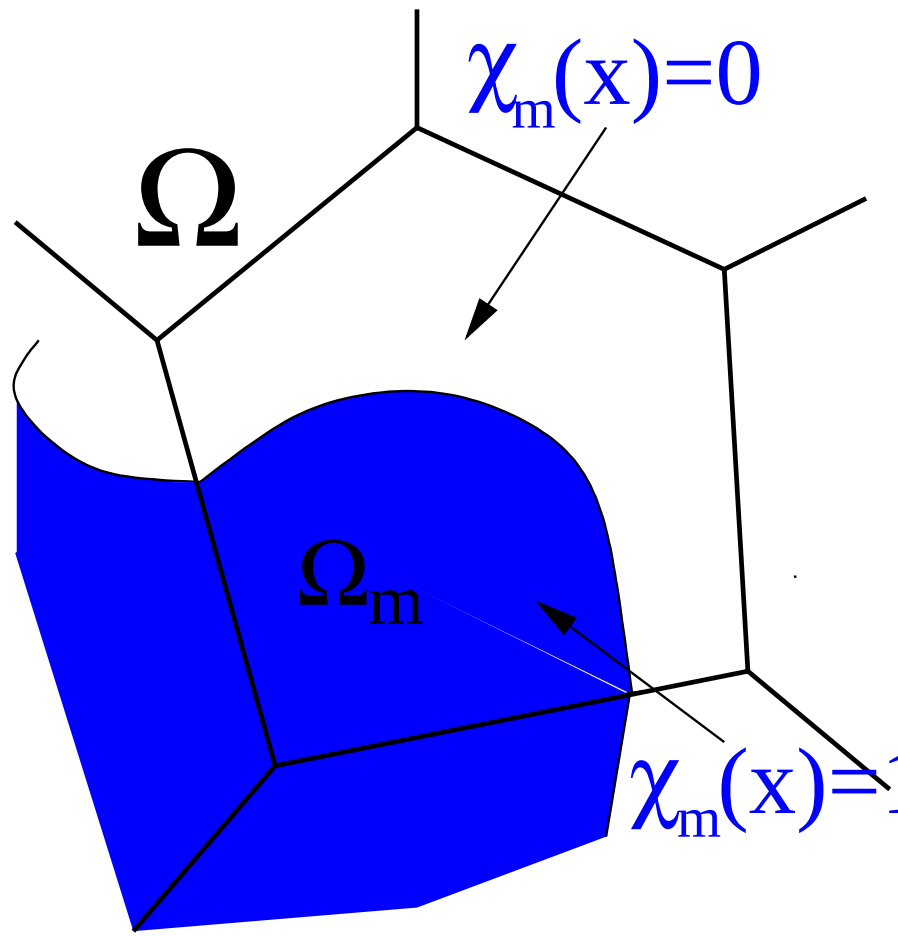
$$\sum_m \alpha_m = 1, \text{ and, } 0 \leq \alpha_m \leq 1$$



Volume fraction function $\chi_m(\mathbf{x})$

Characteristic function

$$\chi_m(\mathbf{x}) = \begin{cases} 1 & \text{if} \quad \mathbf{x} \in \Omega_m \\ 0 & \text{if} \quad \mathbf{x} \notin \Omega_m \end{cases}$$



Properties:

$$\int_\Omega \chi_m(\mathbf{x})d\mathbf{x} = \int_{\Omega_m} d\mathbf{x} = |\Omega_m|$$

$$\forall \mathbf{x} \in \Omega, \quad \sum_m \chi_m(\mathbf{x}) = 1$$

Material Centroid Approx.

- Center of mass of material m

$$\widetilde{\mathbf{x}}_m = \frac{\int_{\Omega_m} \mathbf{x} d\mathbf{x}}{\int_{\Omega_m} d\mathbf{x}} = \frac{\int_{\Omega} \chi_m(\mathbf{x}) \mathbf{x} d\mathbf{x}}{\int_{\Omega} \chi_m(\mathbf{x}) d\mathbf{x}}$$

1. $\widetilde{\mathbf{x}}_m$ approx. *via* attract/repel Particle System with ad hoc BCs
2. $\widetilde{\mathbf{x}}_m$ approx. *via* f_m smooth approx. of $f_m \simeq \chi_m$

$$\widehat{\mathbf{x}}_m = \frac{\int_{\Omega} f_m(\mathbf{x}) \mathbf{x} d\mathbf{x}}{\int_{\Omega} f_m(\mathbf{x}) d\mathbf{x}} = \left\{ \begin{array}{c} \text{Exact int.} \\ \text{Numer.int.} \end{array} \right\} \simeq \widetilde{\mathbf{x}}_m$$

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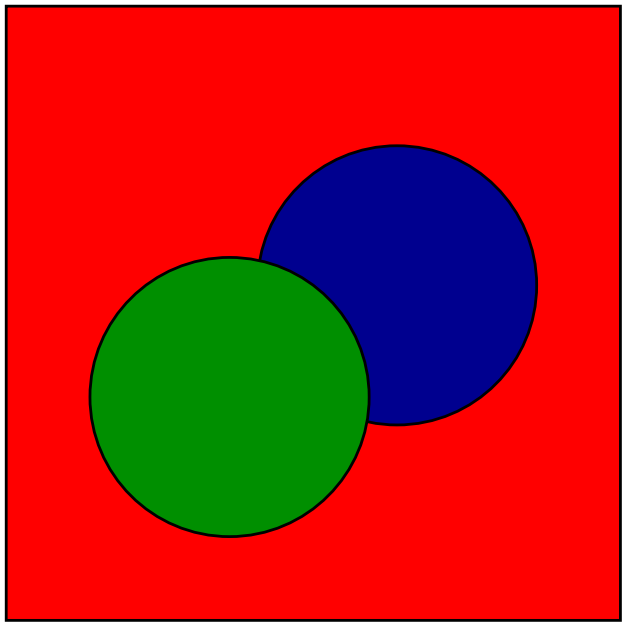
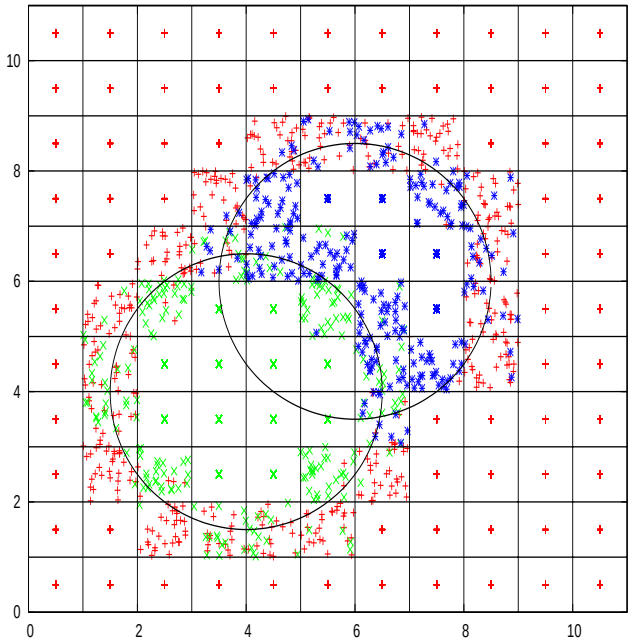
Centroids *via* Particle system

- Particles of diff. nature attract/repel each others
- System cools down, N_m part. of nature m gather

$$\bar{\mathbf{x}}_m = \frac{1}{N_m} \sum_{p=1}^{N_m} \mathbf{x}_p^m \simeq \tilde{\mathbf{x}}_m$$





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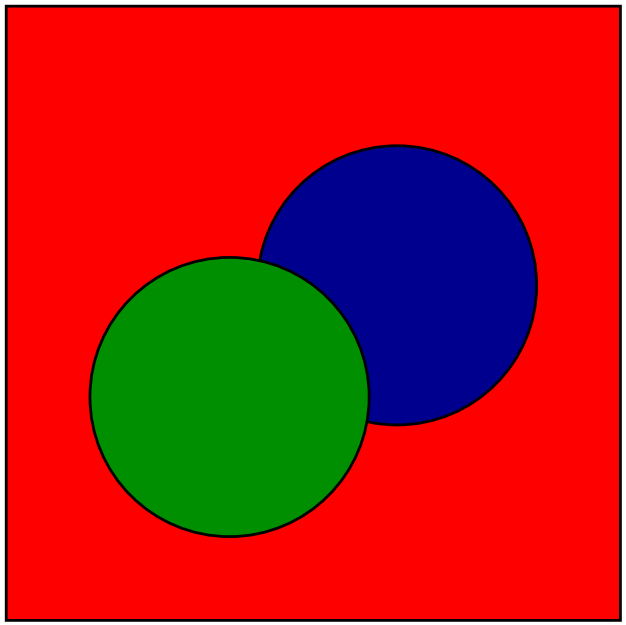

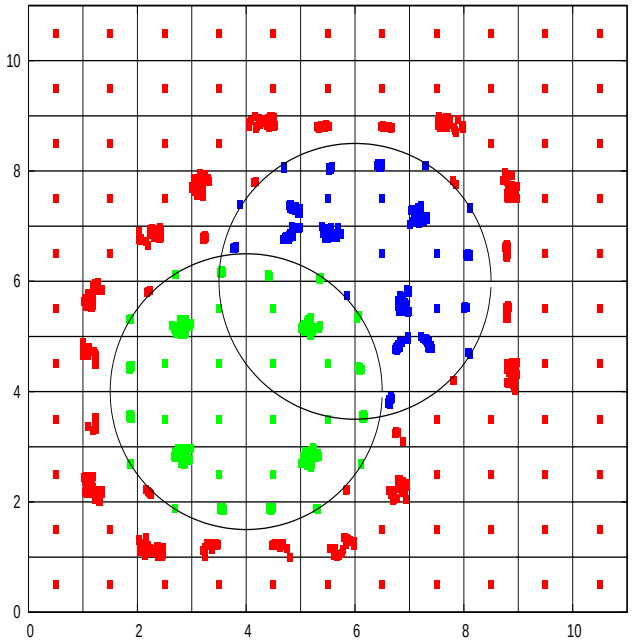

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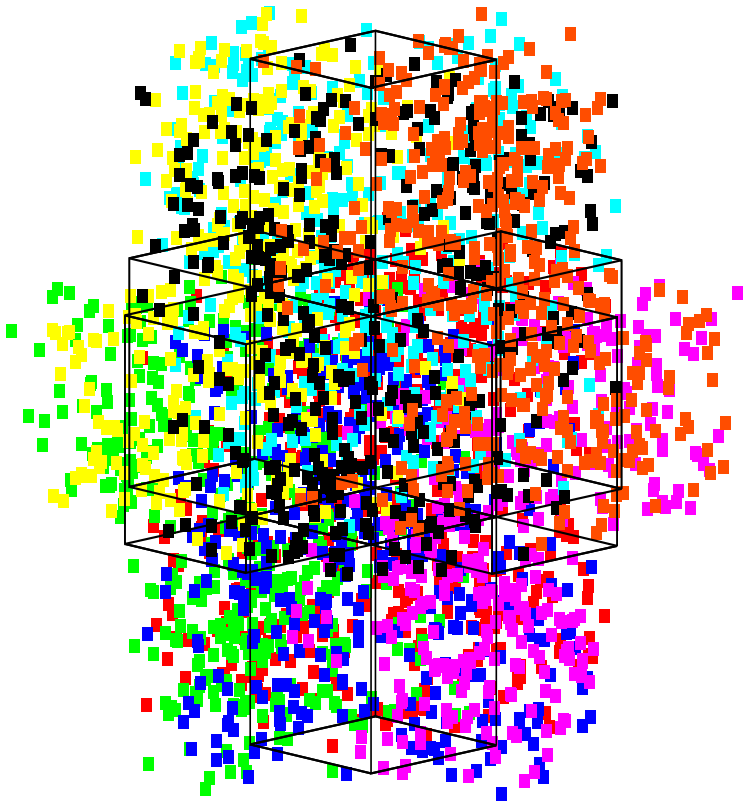

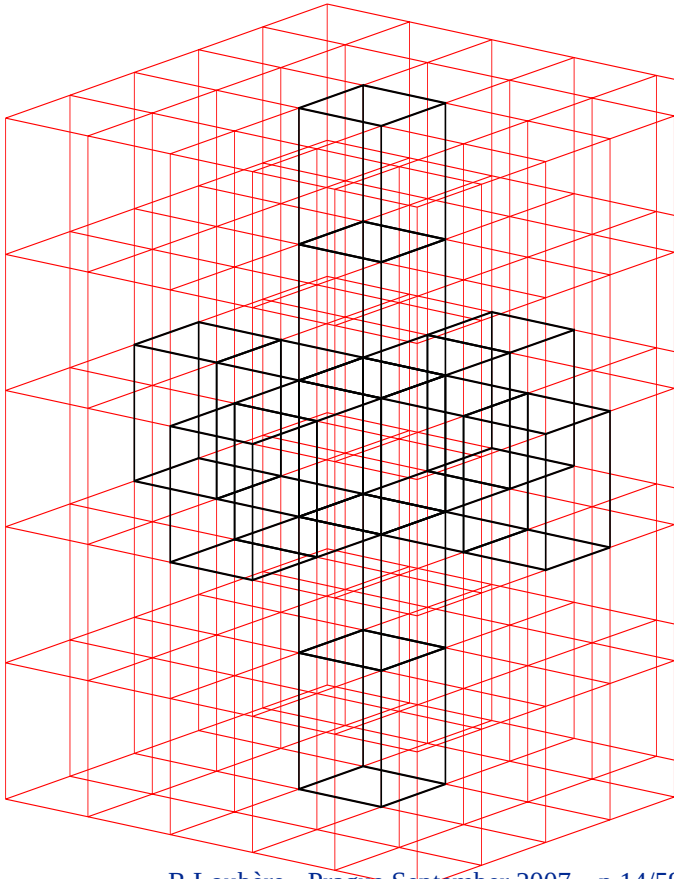

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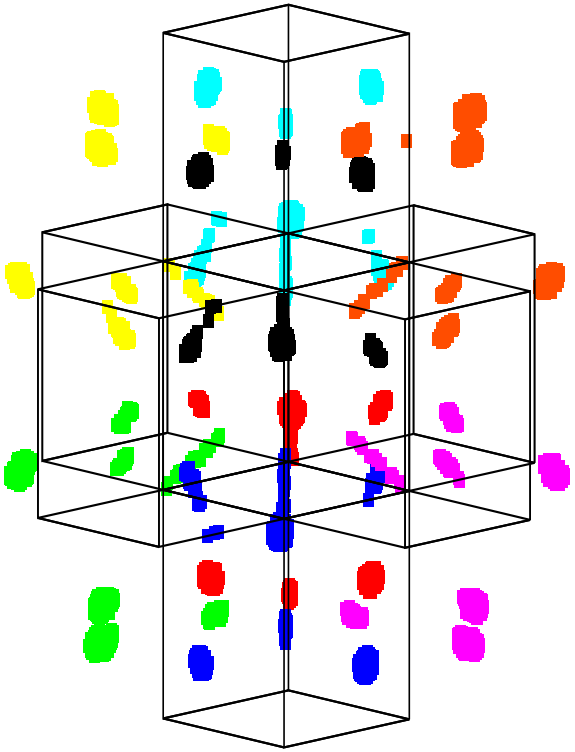

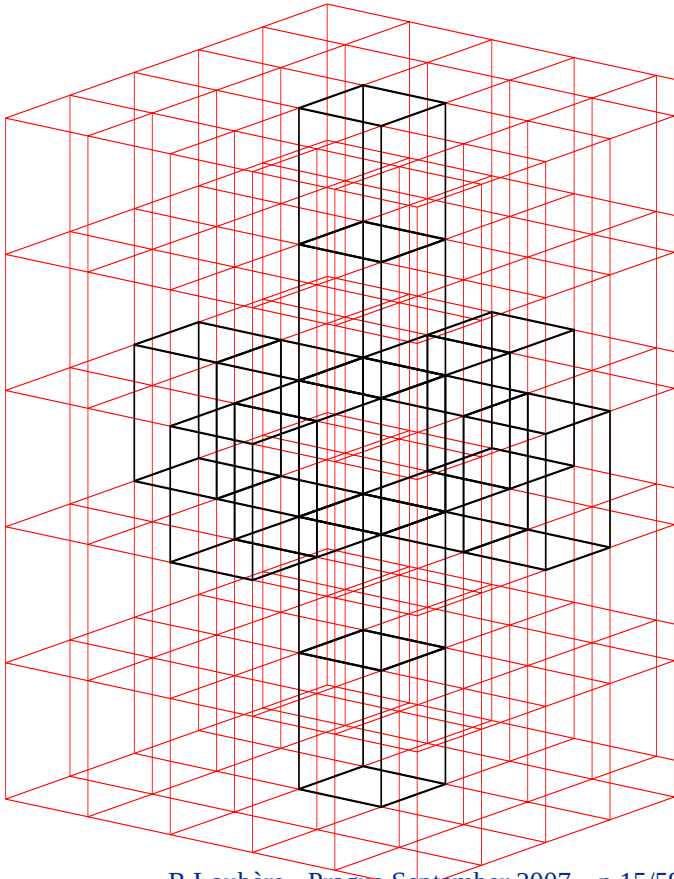

Centroids *via* Particle system

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$$\overline{\mathbf{x}}_m = \frac{1}{N_m} \sum_{p=1}^{N_m} \mathbf{x}_p^m \simeq \widetilde{\mathbf{x}}_m$$

Properties: 2D/3D, order-indep, // easy, indep. m

BUT

- $\overline{\mathbf{x}}_m$ approximates location of fluid m in Ω but is not *per se* an approximation of $\widetilde{\mathbf{x}}_m$
- Particle syst. is expensive

Centroid approx. *via* $f_m \in \mathbb{P}_1$

Assume f_m is a piecewise linear polynomial

- Green-Gauss or Least-Square to get ∇f

$$\forall \mathbf{x} \in \Omega \qquad f_m(\mathbf{x}) = \alpha_m + \nabla f \cdot (\mathbf{x} - \widetilde{\mathbf{x}}_\Omega)$$

- Barth-Jeperson limitation of ∇f to ensure

$$\forall \mathbf{x} \in \Omega \qquad 0 \leq f_m(\mathbf{x}) \leq 1$$

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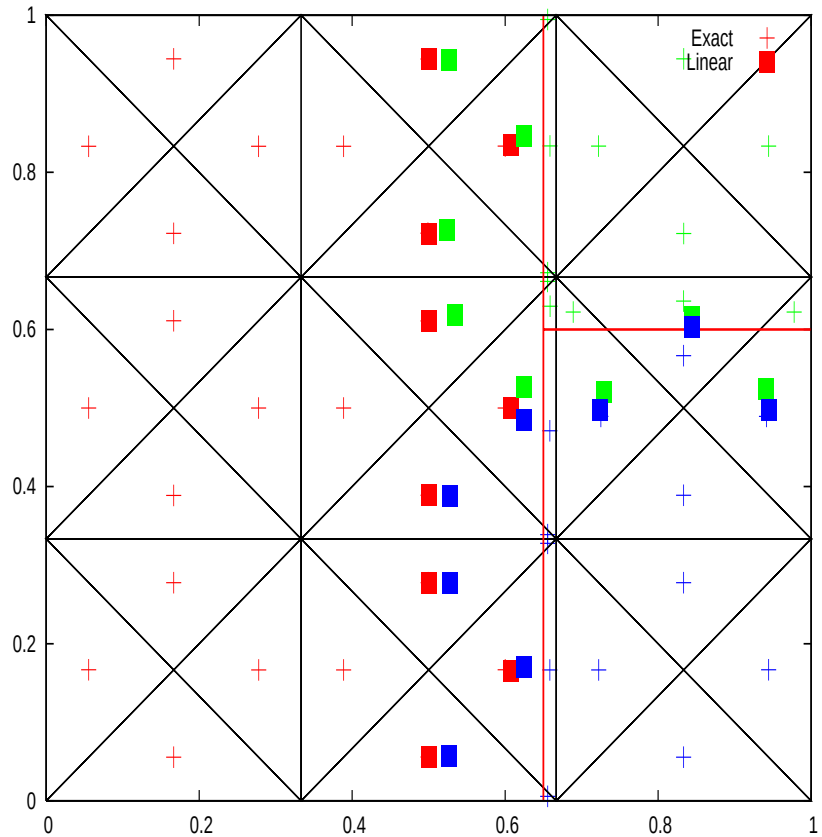
- Barth-Jeperson limitation of ∇f
- Approximate center of mass of material m by integrating over Ω

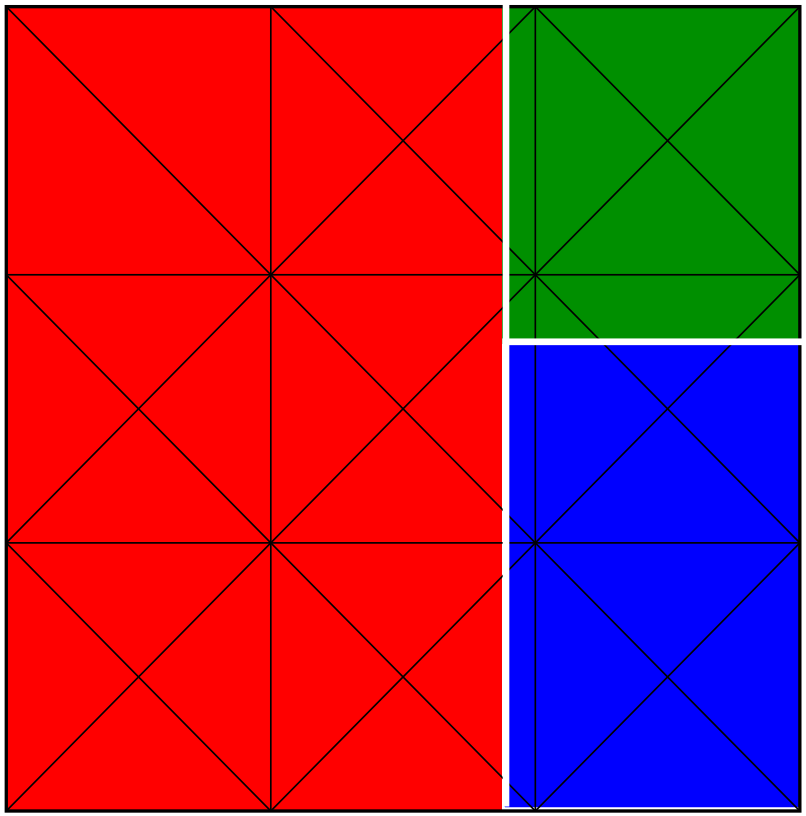
$$\widehat{\mathbf{x}}_m = \frac{\int_\Omega f_m(\mathbf{x})\mathbf{x}d\mathbf{x}}{\int_\Omega f_m(\mathbf{x})d\mathbf{x}} \simeq \widetilde{\mathbf{x}}_m$$

Centroid approx. *via* $f_m \in \mathbb{P}_1$

T-junction



Initial and Mesh



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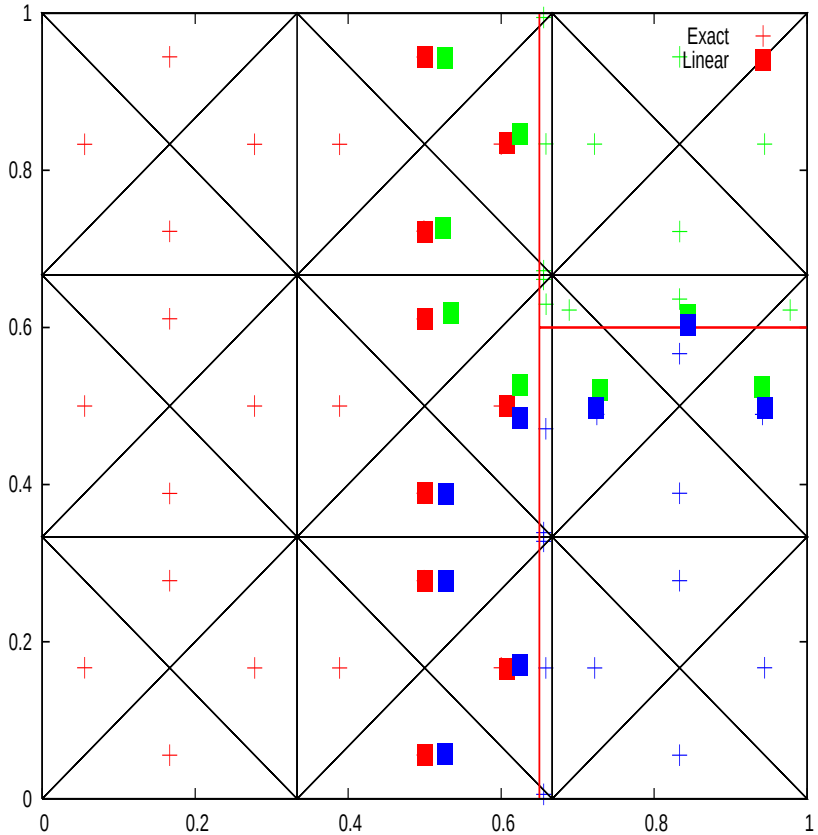
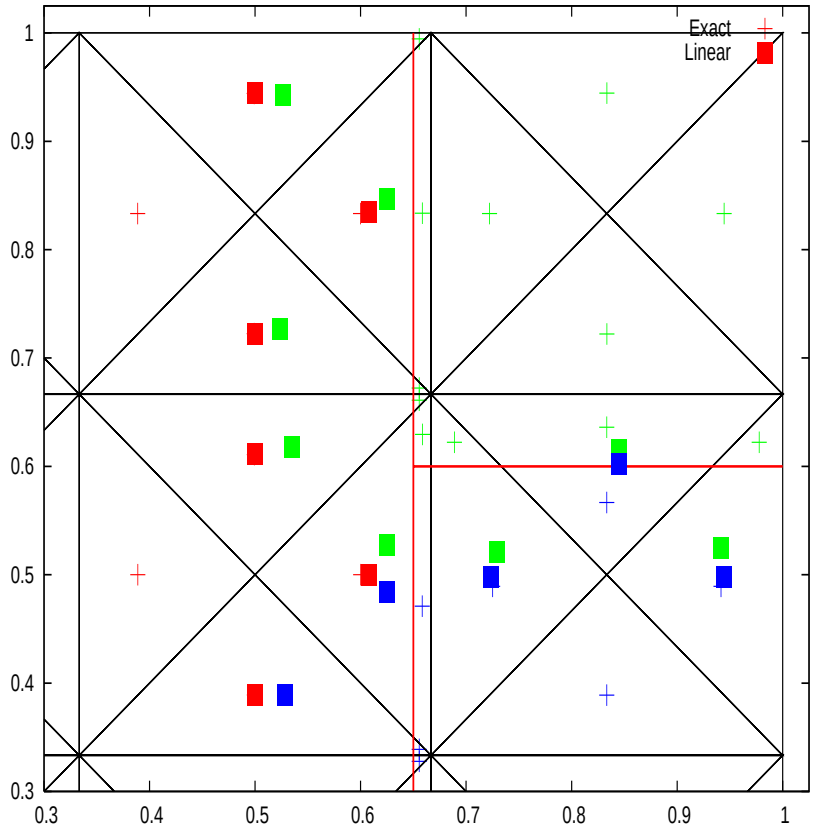
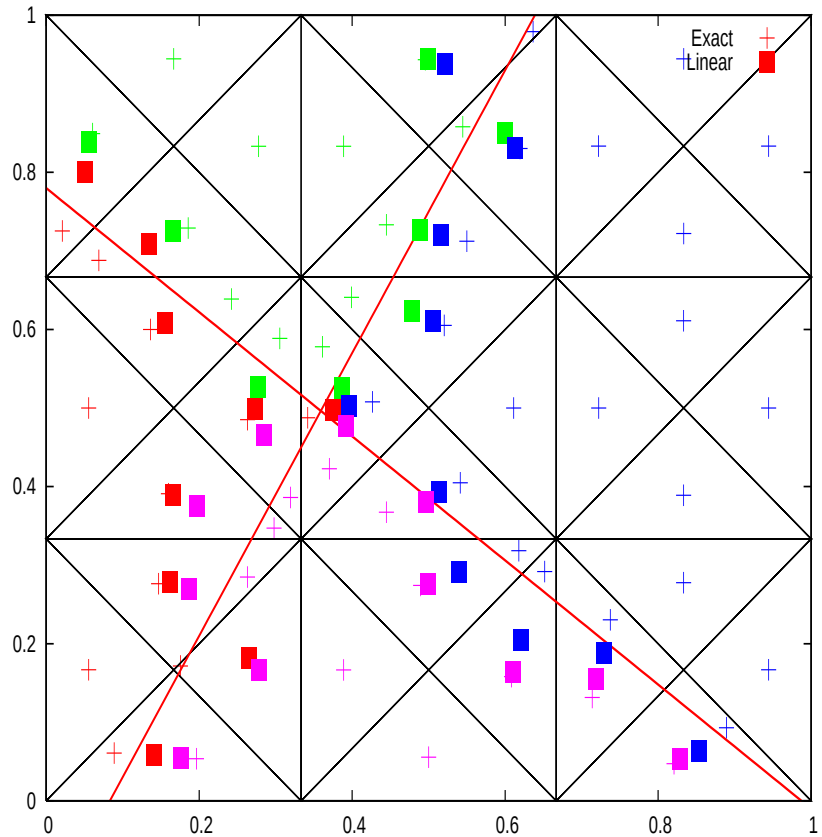


Zoom

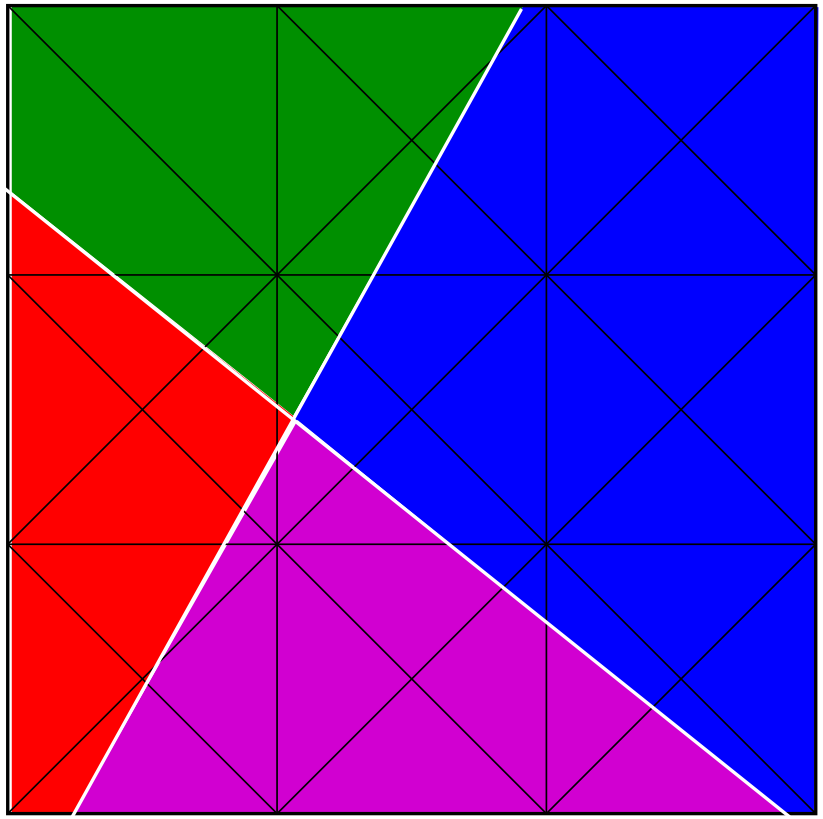


Centroid approx. *via* $f_m \in \mathbb{P}_1$

X-junction



Initial and Mesh



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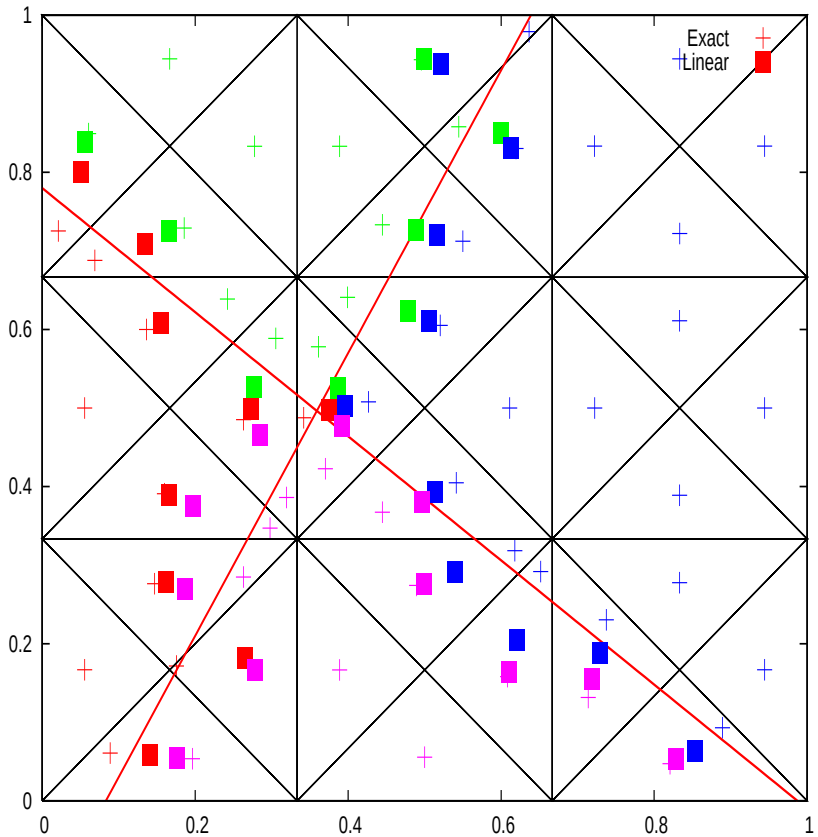

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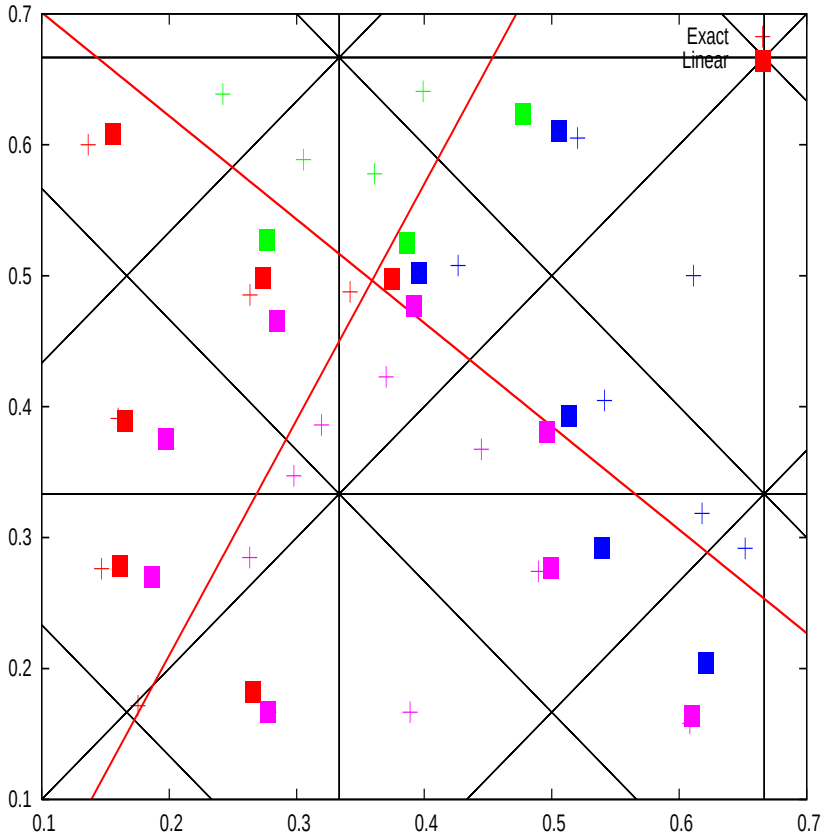
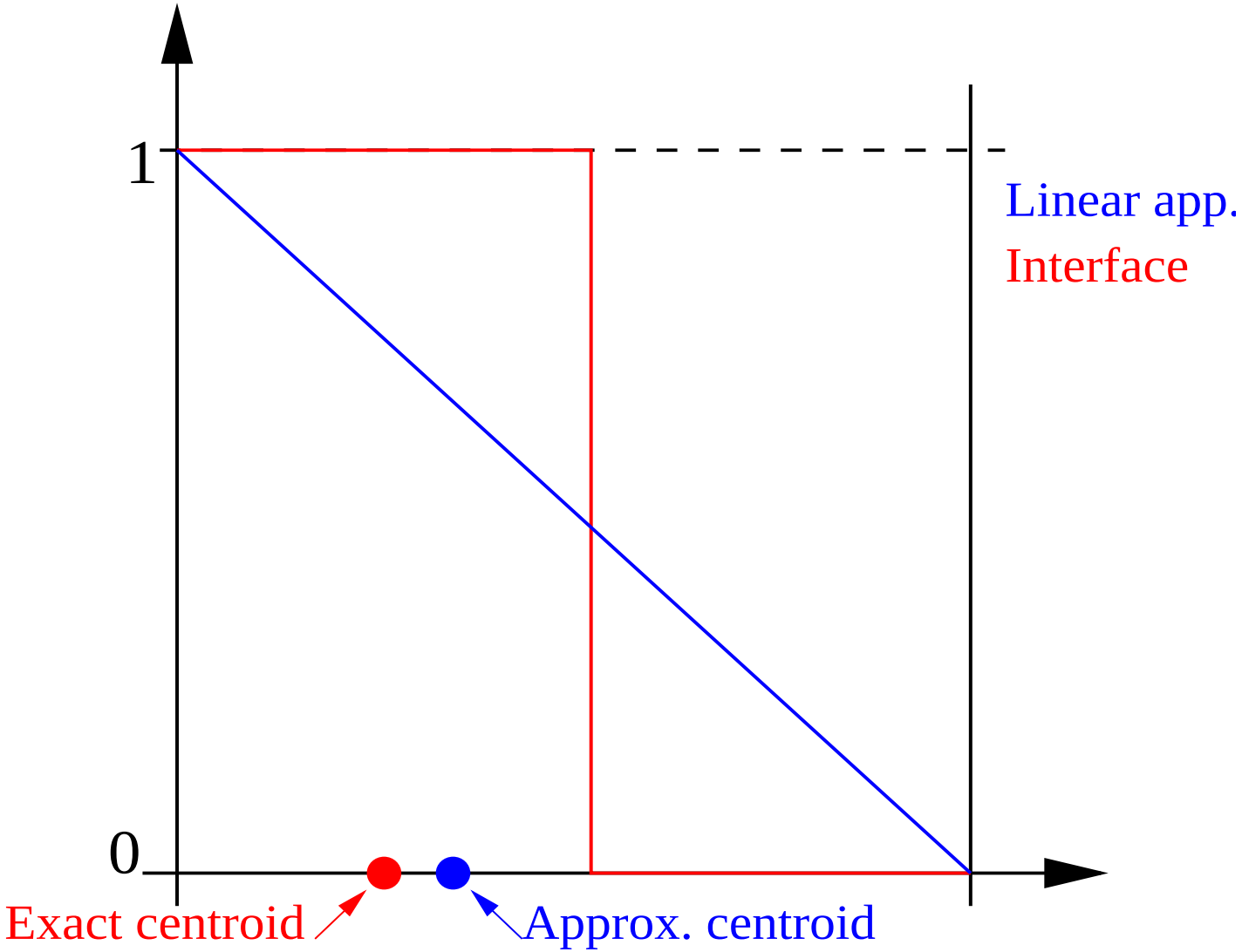


Why is it so? How to do better?



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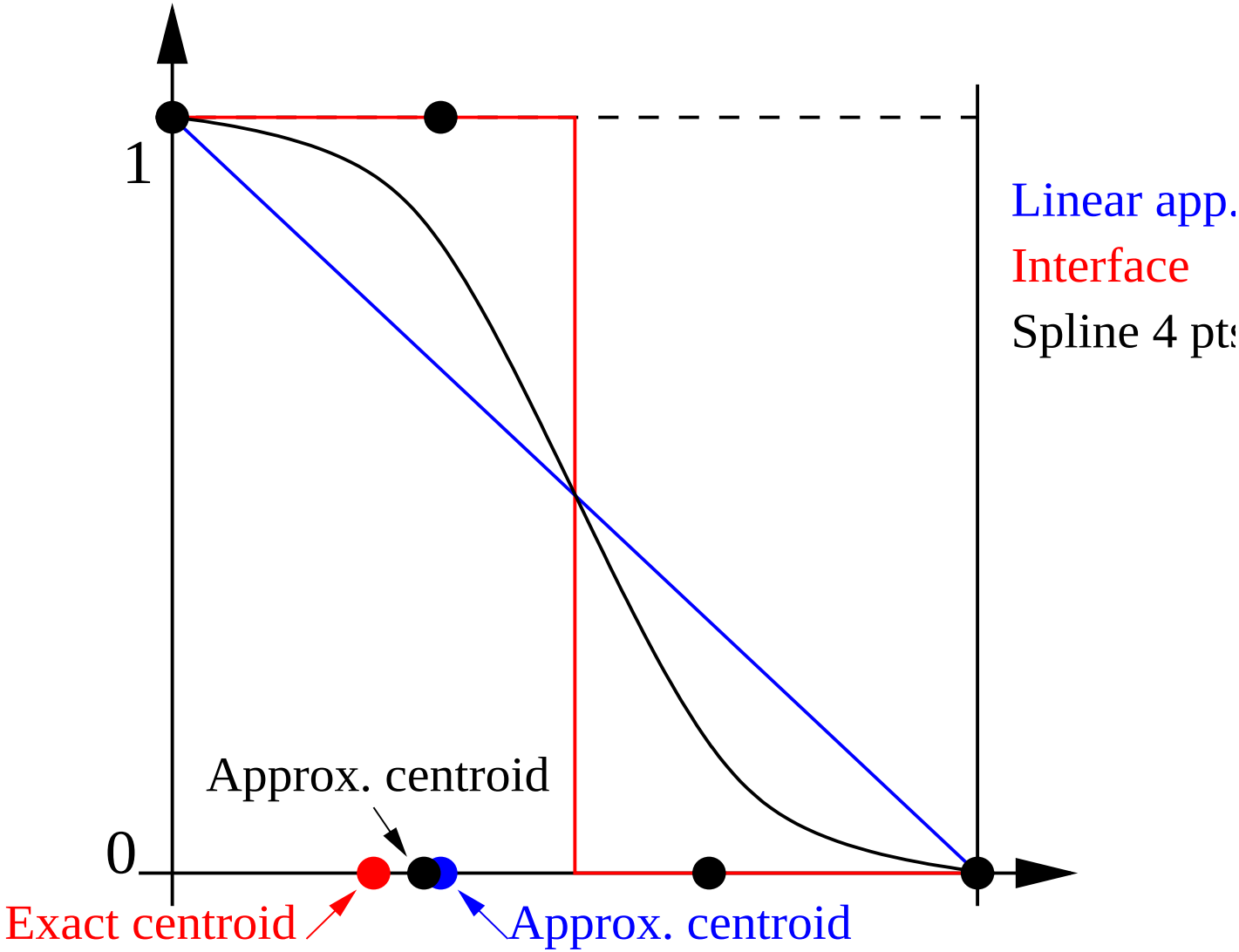

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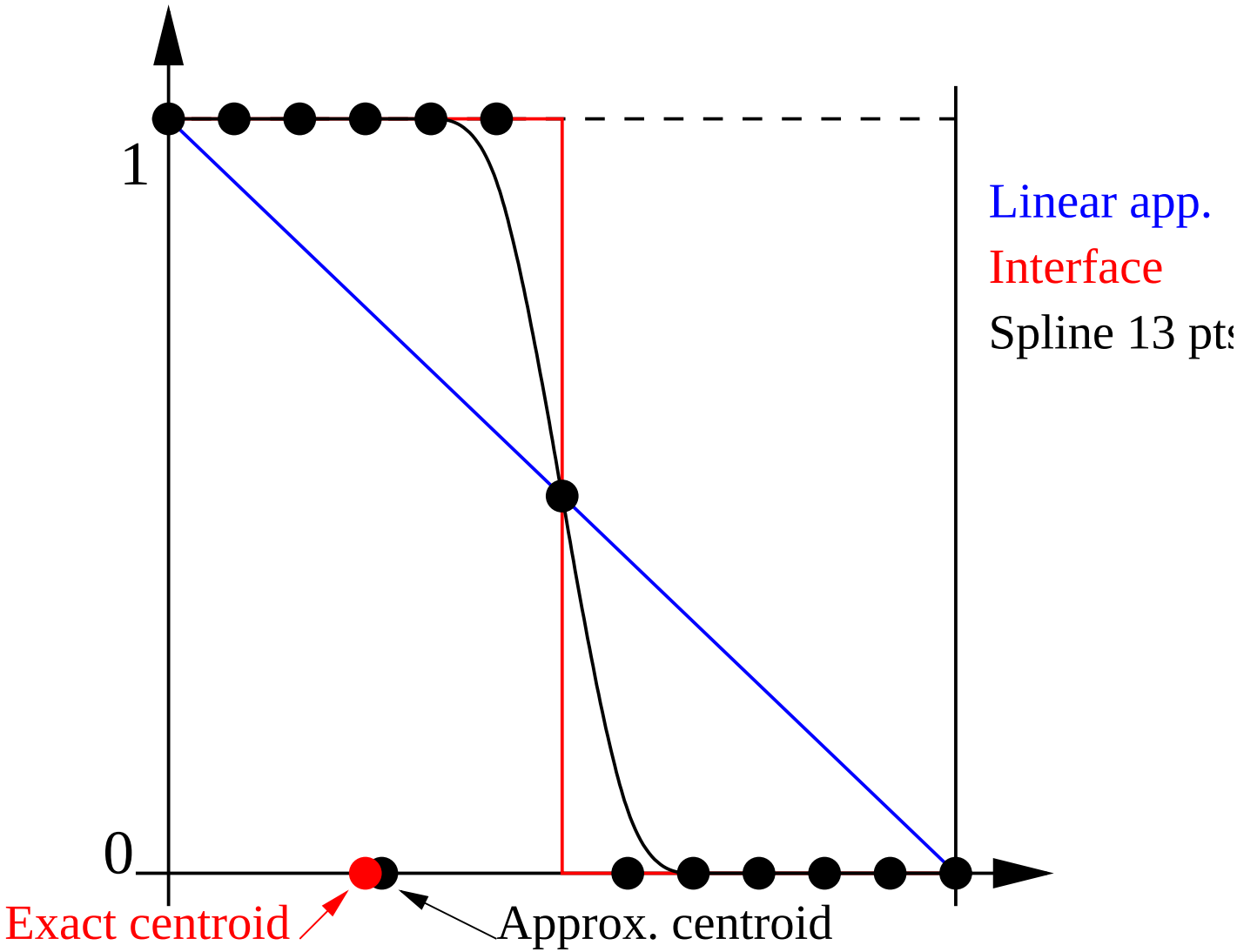


Bernstein polynomial basis

- $\forall p \in \mathbb{P}_n(\Omega)$ polynomial of deg. n

$$p(\mathbf{x}) = \sum_{i,j,k \geq 0,\ i+j+k=n} p_{i,j,k}\, B^{(n)}_{i,j,k}(\mathbf{x})$$

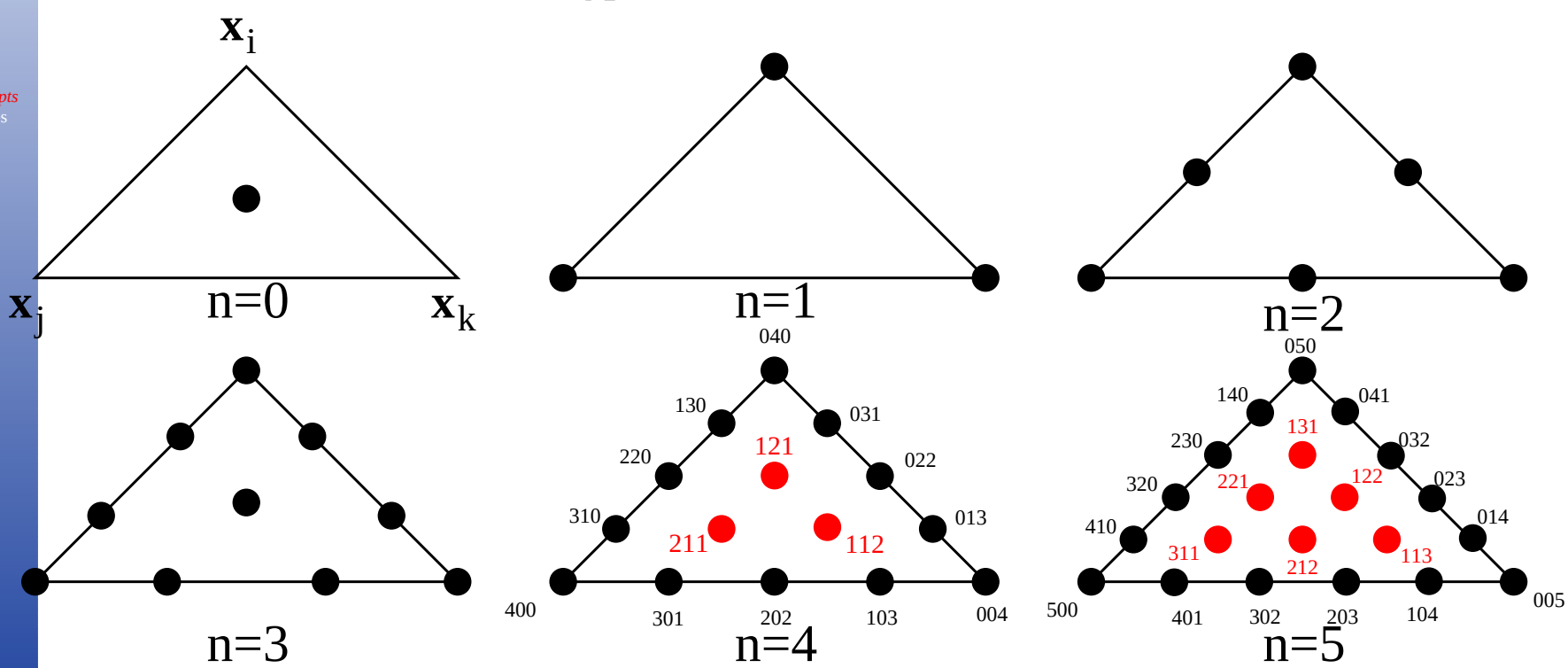
$$B^{(n)}_{i,j,k}(\mathbf{x}) = \left(\frac{n!}{i!\,j!\,k!}\right) \lambda_1^i(\mathbf{x})\, \lambda_2^j(\mathbf{x})\, \lambda_3^k(\mathbf{x})$$

- $B^{(n)}_{i,j,k}$ $\leftarrow$ expansion $(\lambda_1(\mathbf{x}) + \lambda_2(\mathbf{x}) + \lambda_3(\mathbf{x}))^n = 1$
- $\lambda_1, \lambda_2, \lambda_3$ barycentric coordinates of $\mathbf{x} \in \Omega$
- Limited to Triangles so far

Bernstein basis: Control pts

Control point: $\mathbf{z} \setminus B^{(n)}_{i,j,k}(\mathbf{z}) = \max_{\mathbf{x}} \left(B^{(n)}_{i,j,k}(\mathbf{x}) \right)$

$$\mathbf{z} = \frac{1}{n} \left(i\mathbf{x}_i + j\mathbf{x}_j + k\mathbf{x}_k \right)$$



Bernstein basis: Properties

The Bernstein basis functions of degree $(n) > 0$ verify

1. Positivity: $0 \leq B^{(n)}_{i,j,k}(\mathbf{x}) \leq 1 \; \forall \mathbf{x} \in \Omega$
2. Partition of unity:

$$\sum_{i,j,k} B^{(n)}_{i,j,k}(\mathbf{x}) = 1 \quad \forall \mathbf{x} \in \Omega$$

3. Integral weight:

$$\int_{\Omega} B^{(n)}_{i,j,k}(\mathbf{x}) d\mathbf{x} = |\Omega| / N_n$$

4. Convex hull: If $q \in \mathbb{P}_n(\Omega)$

$$\min(q_{i,j,k}) \leq q(\mathbf{x}) \leq \max(q_{i,j,k})$$

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Approx. of $\widetilde{\mathbf{x}}_m$ *via* $f_m \in \mathbb{P}_n(\Omega)$

- Def. $f_m \in \mathbb{P}_n(\Omega) \Longleftrightarrow$ Def. $0 \leq f_{i,j,k} \leq 1$ such that

$$f_m(\mathbf{x}) = \sum_{i,j,k} f_{i,j,k}\, B^{(n)}_{i,j,k}(\mathbf{x})$$

- Approximate centroid

$$\widehat{\mathbf{x}}_m = \frac{\int_\Omega f_m(\mathbf{x})\mathbf{x}d\mathbf{x}}{\int_\Omega f_m(\mathbf{x})d\mathbf{x}} \equiv \underbrace{\sum_{i,j,k} f_{i,j,k}\, \gamma_{i,j,k}}_{\text{Convex combination}} \simeq \widetilde{\mathbf{x}}_m$$

where

$$\gamma_{i,j,k} = \frac{N_n}{\sum_{i,j,k} f_{i,j,k}} \frac{\int_\Omega B^{(n)}_{i,j,k}(\mathbf{x})\mathbf{x}d\mathbf{x}}{|\Omega|} \geq 0$$

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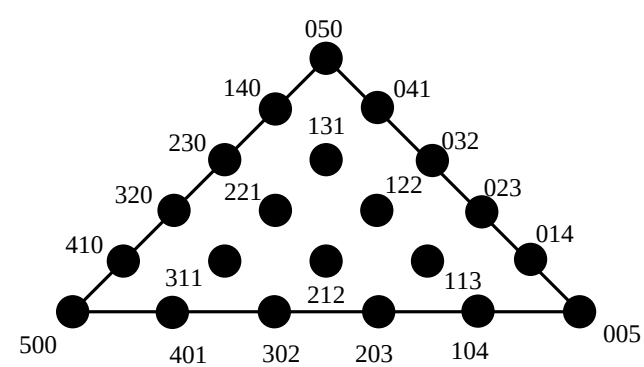
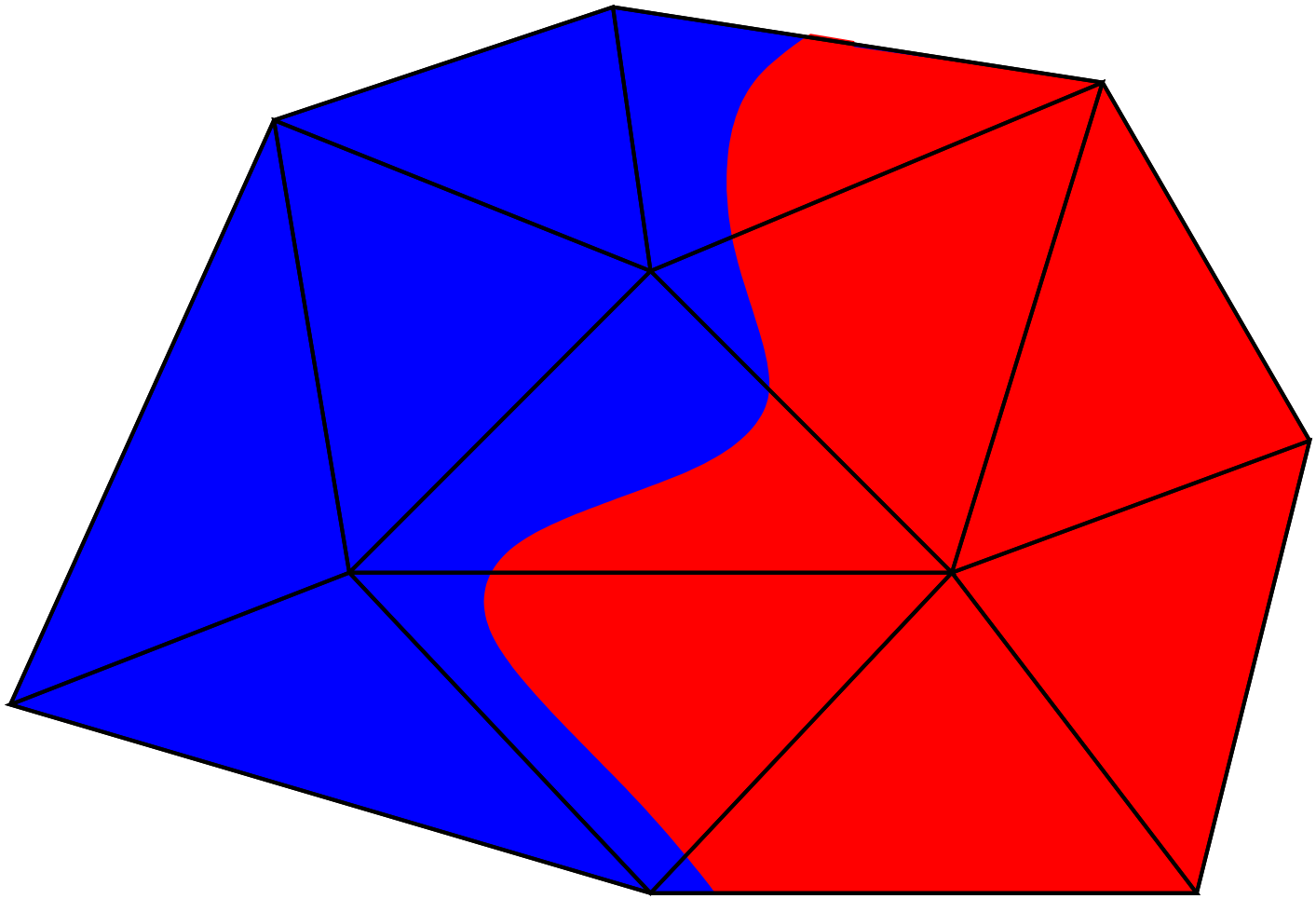
Unknowns:

$f_{i,j,k}$ "$\Longleftrightarrow$" value of $\chi_m(\mathbf{z}_{i,j,k})$



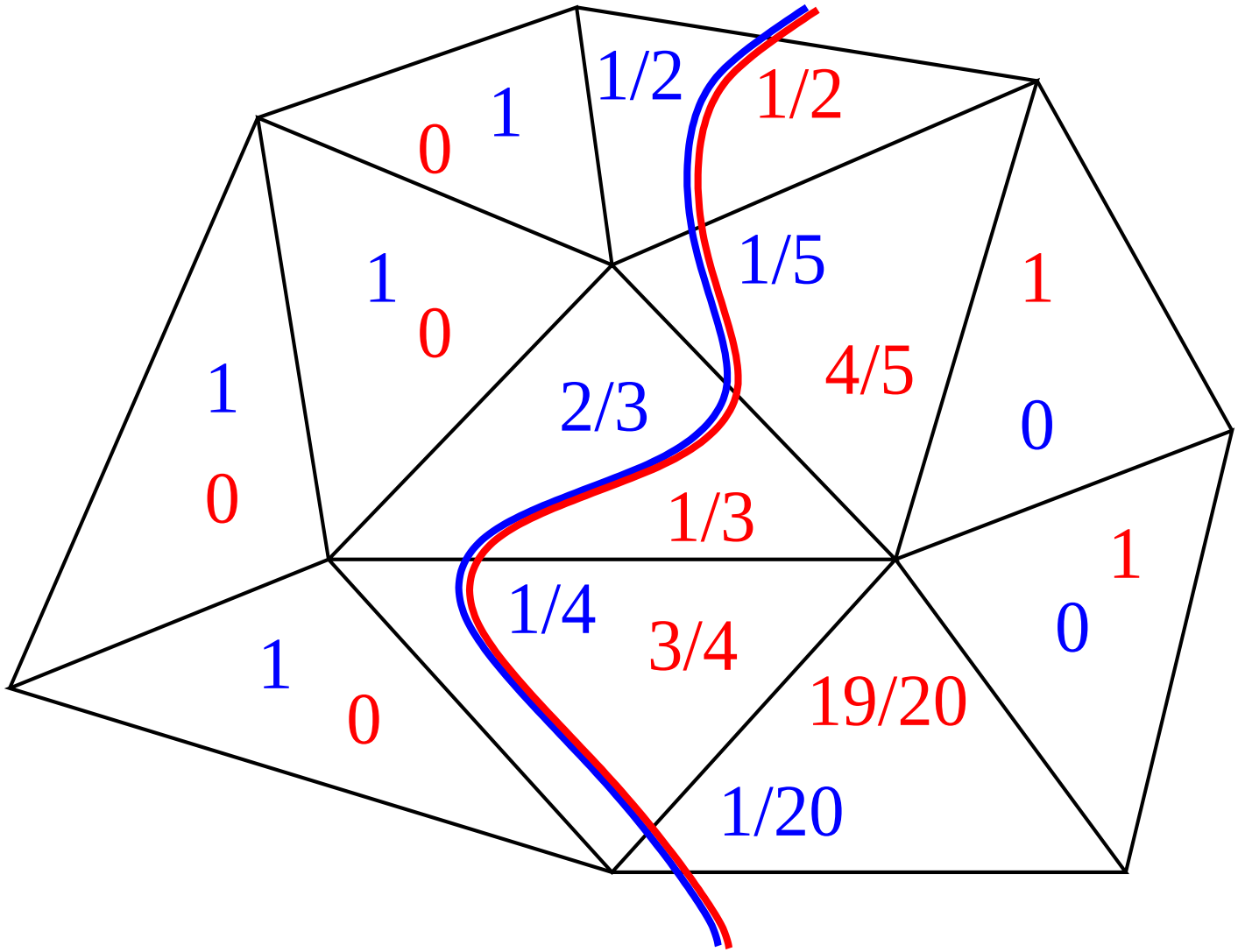
Approx. of $f_m \in \mathbb{P}_n(\Omega)$

Initial State



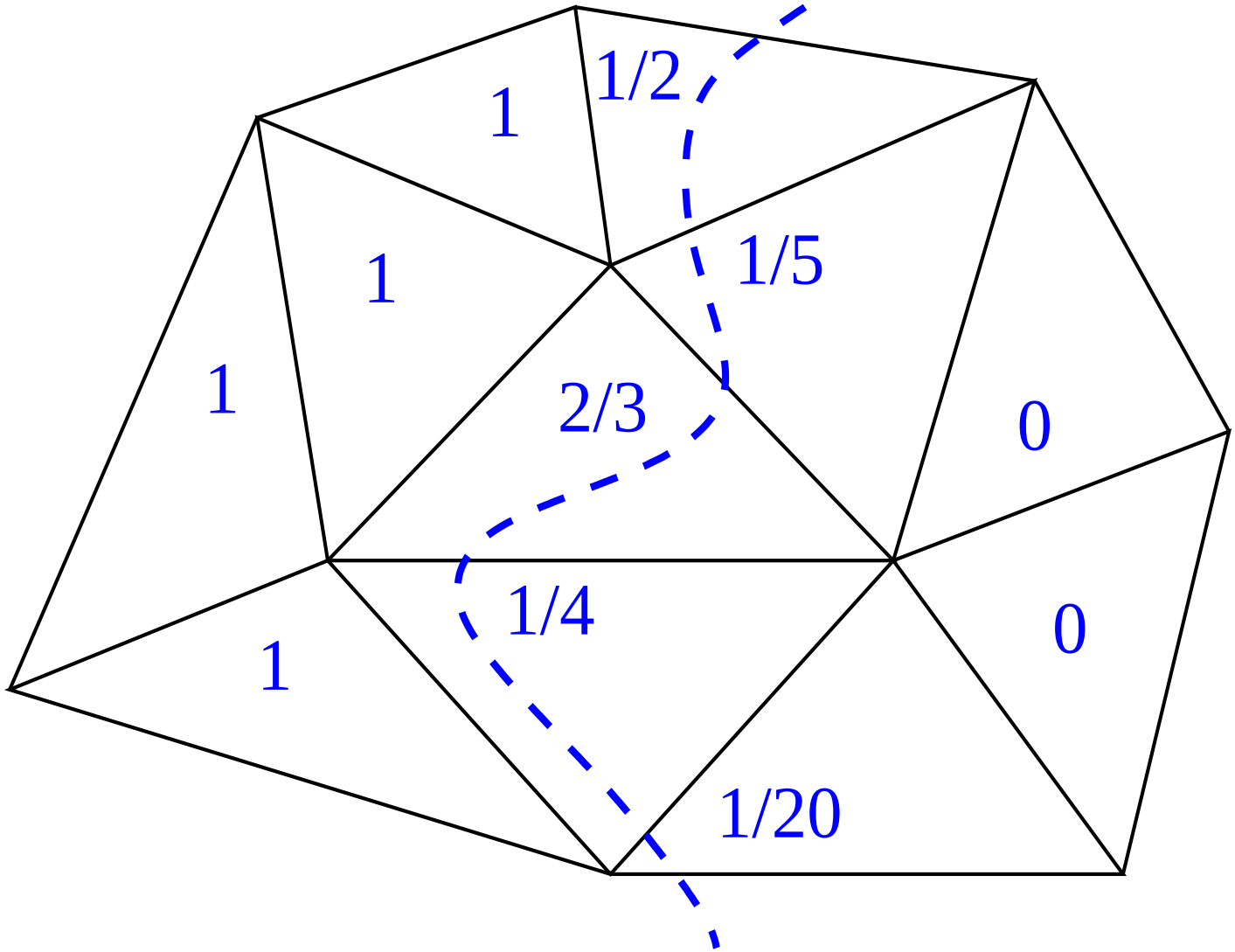
Approx. of $f_m \in \mathbb{P}_n(\Omega)$

Volume Fractions



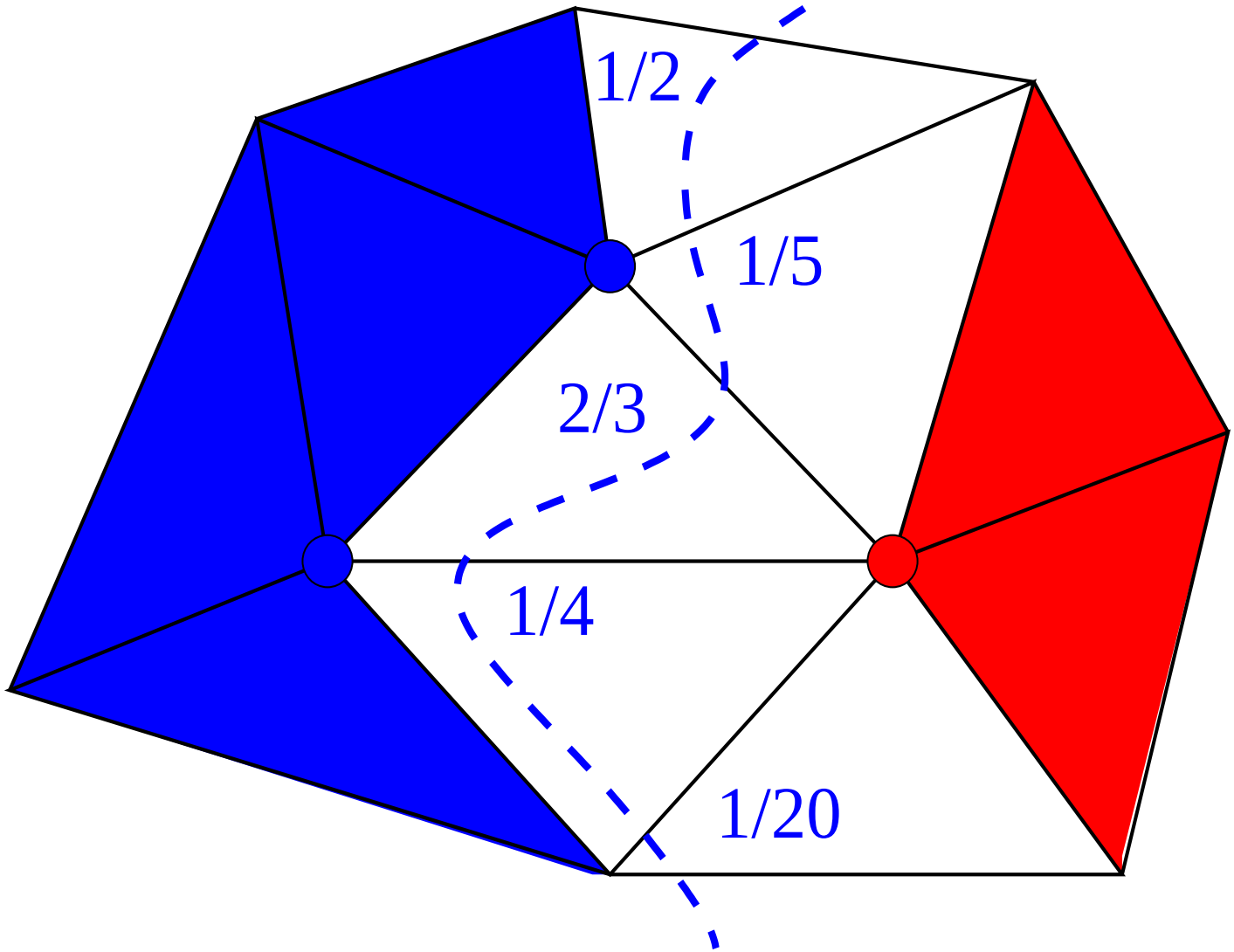
Approx. of $f_m \in \mathbb{P}_n(\Omega)$

Volume Fractions for blue fluid



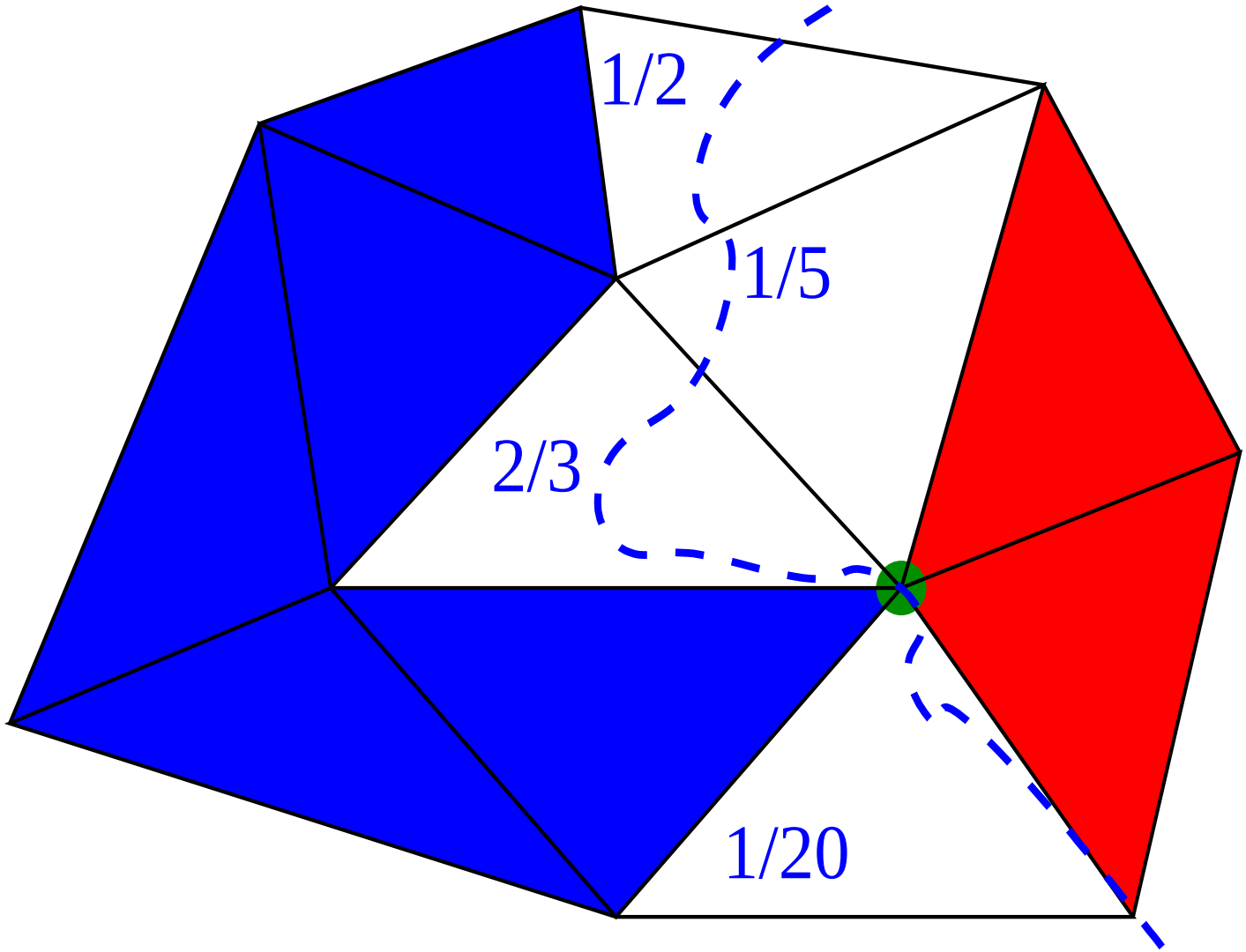
Approx. of $f_m \in \mathbb{P}_n(\Omega)$

"Pure" nodes: Nodal B-coeff.$\Rightarrow$ $f_{n,0,0} = 1$ or 0



Approx. of $f_m \in \mathbb{P}_n(\Omega)$

Ambiguous nodal B-coeff $\Rightarrow f_{n,0,0} = 1/2$



Approx. of $f_m \in \mathbb{P}_n(\Omega)$: Nodes

- Min/Max

$$\alpha^+ = \max_{j \in Neighb(\Omega)} (\alpha^j) \qquad \alpha^- = \min_j (\alpha^j)$$

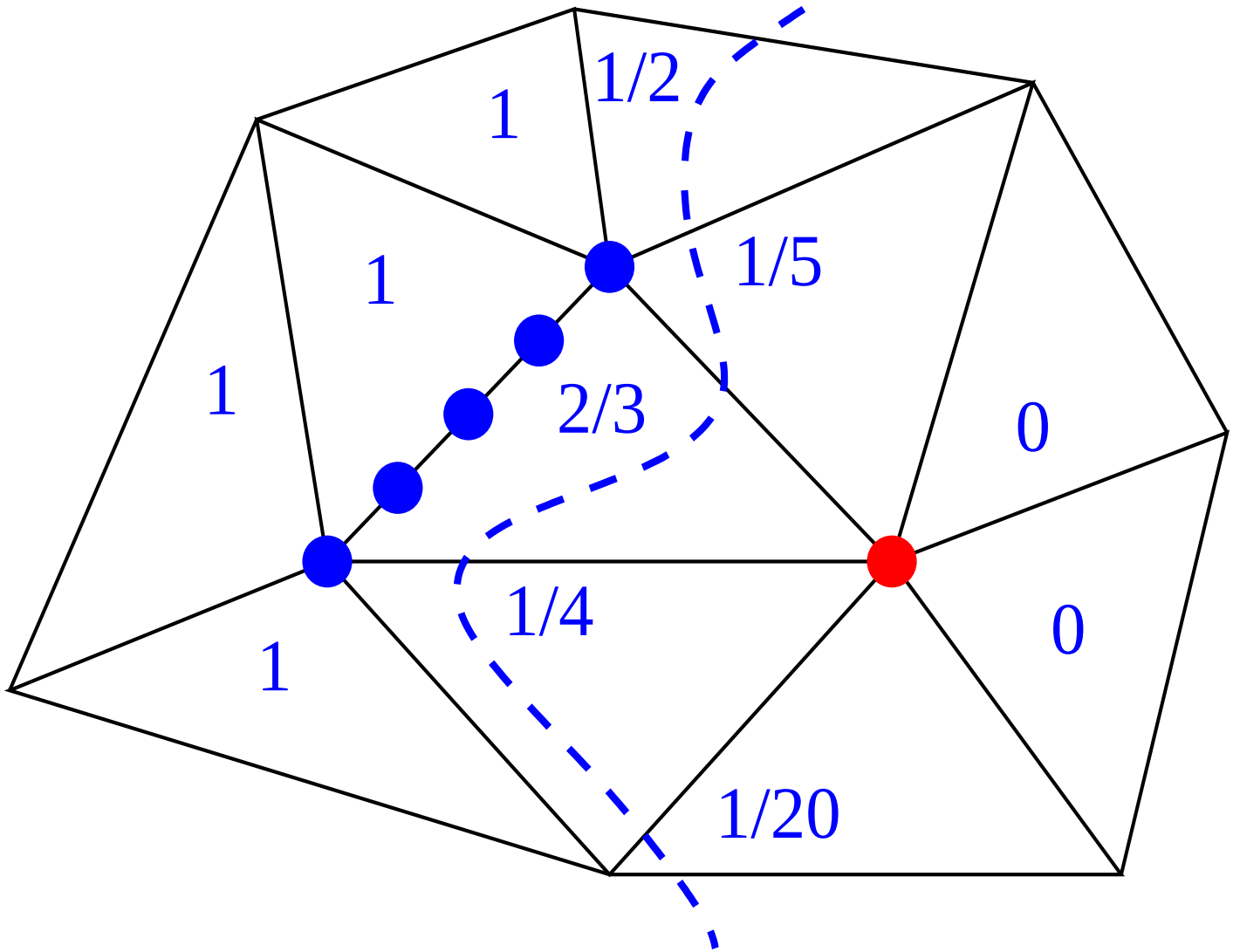
- Mean value

$$\overline{\alpha} = \frac{\sum_j |\Omega_j| \, \alpha^j}{\sum_j |\Omega_j|} \qquad g = \begin{cases} 1 & \text{if } \overline{\alpha} > 1/2 \\ 0 & \text{if } \overline{\alpha} < 1/2 \\ 1/2 & \text{if } \overline{\alpha} = 1/2 \end{cases}$$

	$\alpha^+ = \mathbf{1}$	$\alpha^+ < \mathbf{1}$
$\alpha^- = \mathbf{0}$	$f_{n,0,0} = 1/2$	$f_{n,0,0} = 0$
$\alpha^- > \mathbf{0}$	$f_{n,0,0} = 1$	$f_{n,0,0} = g$

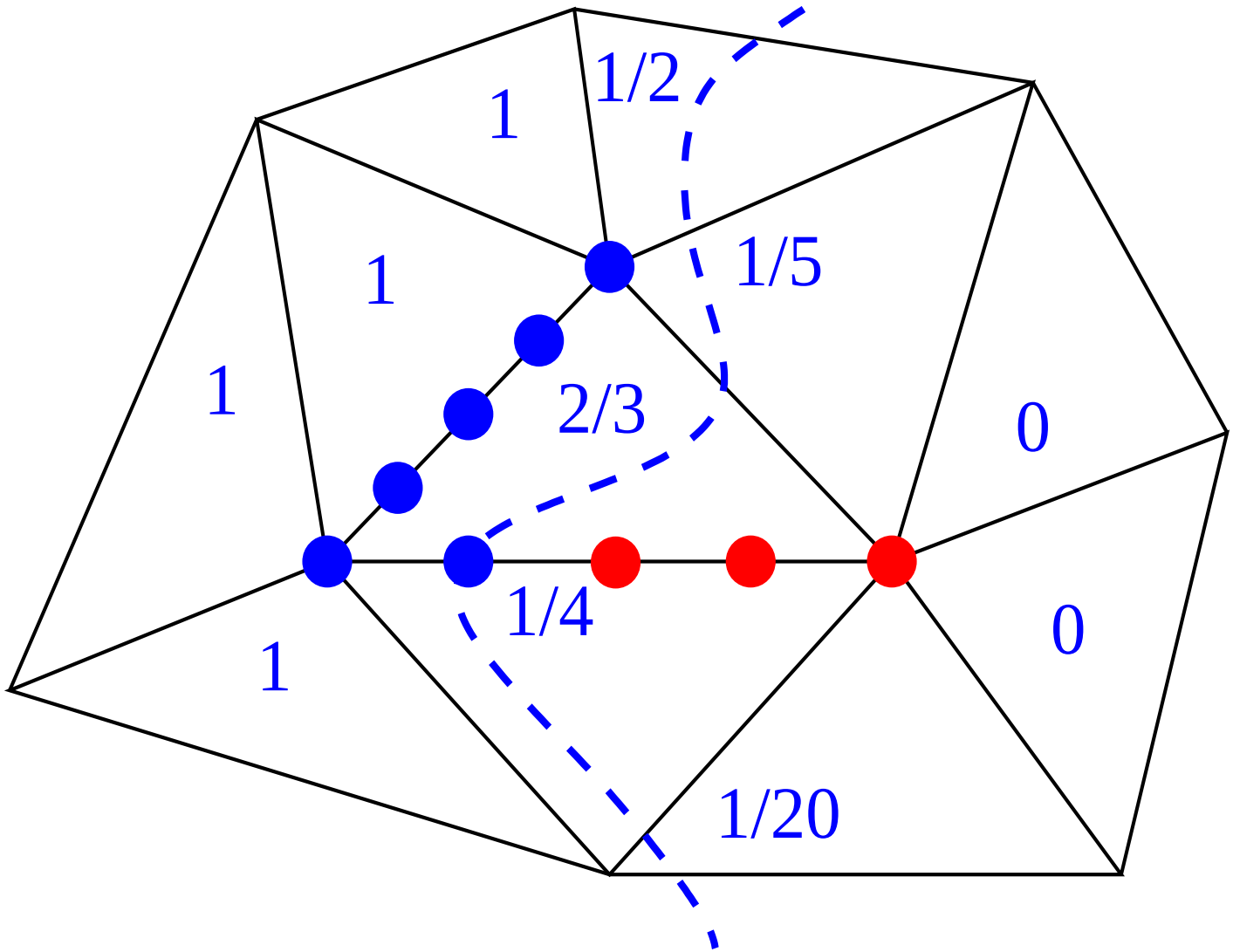
Approx. of $f_m \in \mathbb{P}_n(\Omega)$

"Pure" edge: Edge B-coeff. $f_{n,0,0} \leq f_{i,j,0} \leq f_{0,n,0}$



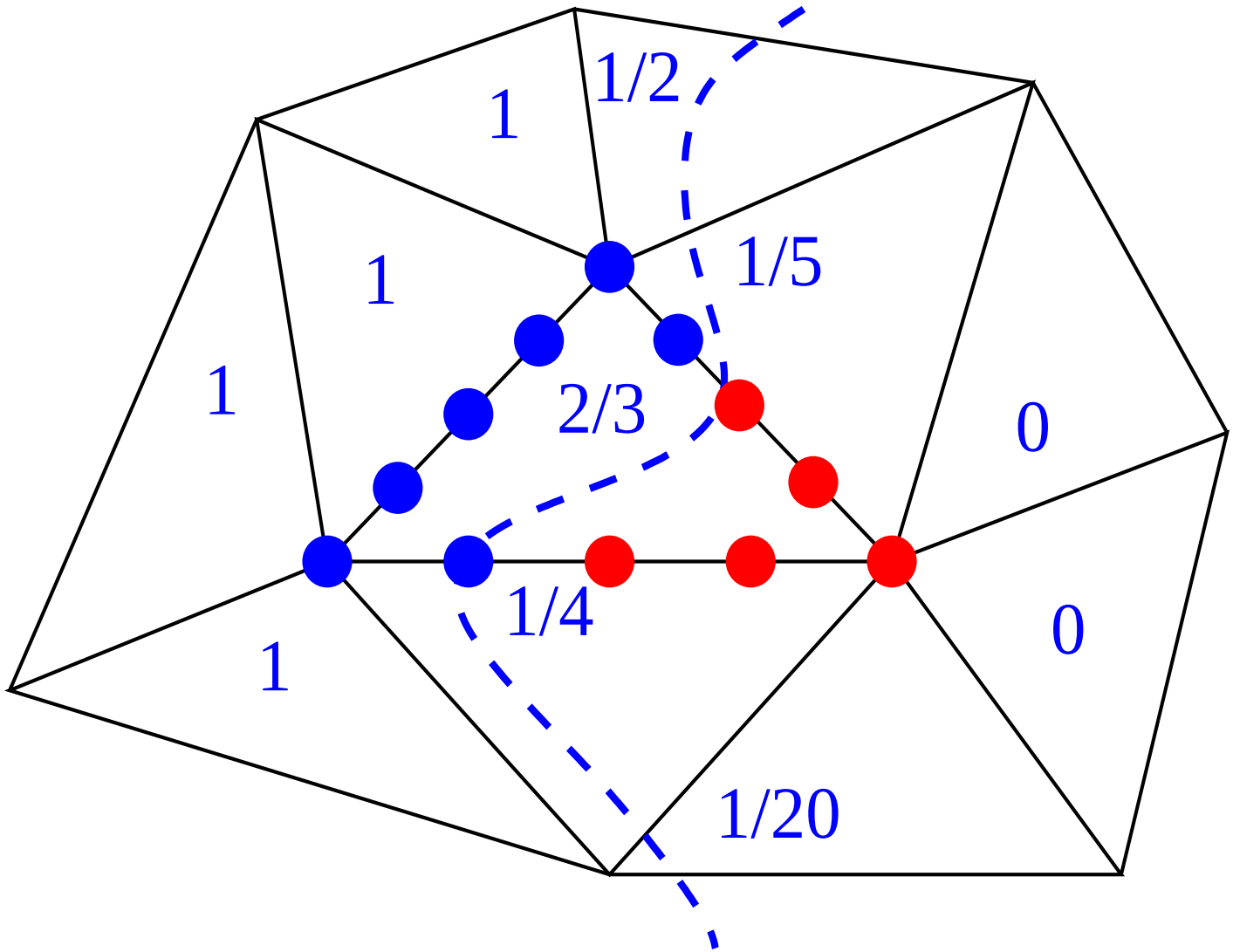
Approx. of $f_m \in \mathbb{P}_n(\Omega)$

"Mixed" edge: Edge B-coeff. $f_{0,0,n} \leq f_{i,0,j} \leq f_{n,0,0}$



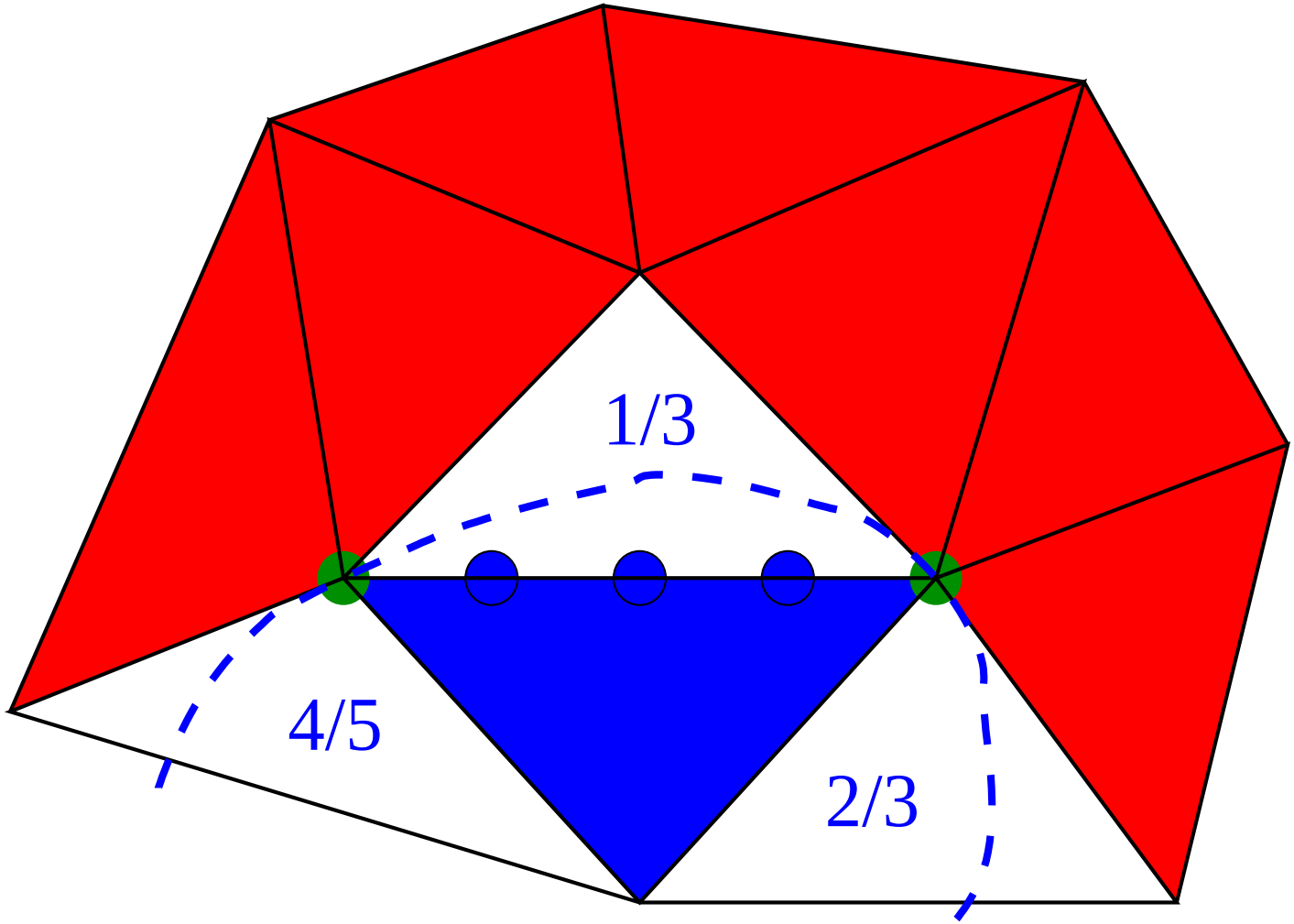
Approx. of $f_m \in \mathbb{P}_n(\Omega)$

"Mixed" edge: Edge B-coeff. $f_{0,0,n} \leq f_{0,i,j} \leq f_{0,n,0}$



Approx. of $f_m \in \mathbb{P}_n(\Omega)$

Ambiguous edge B-coeff $\Rightarrow$ $f_{i,j,0} = 0$ or 1



Approx. of $f_m \in \mathbb{P}_n(\Omega)$: Edge

Command 1: If a pure or empty cell is in contact with the current edge $\Longrightarrow$ assoc. 1 or 0 to all B-coeff.

Command 2: Apply 9 rules

$[n^-;n^+]$	$f_{n^-}=0$	$f_{n^-}=\frac{1}{2}$	$f_{n^-}=1$
$f_{n^+}=0$	$f_e=0$	$f_e=\frac{1}{2}\rightarrow 0$	$f_e=1\rightarrow 0$
$f_{n^+}=\frac{1}{2}$	$f_e=0\rightarrow\frac{1}{2}$	$f_e=\beta$	$f_e=\frac{1}{2}\rightarrow 1$
$f_{n^+}=1$	$f_e=0\rightarrow 1$	$f_e=\frac{1}{2}\rightarrow 1$	$f_e=1$

Approx. of $f_m \in \mathbb{P}_n(\Omega)$: Edge

Command 1: If a pure or empty cell is in contact with the current edge $\Longrightarrow$ assoc. 1 or 0 to all B-coeff.

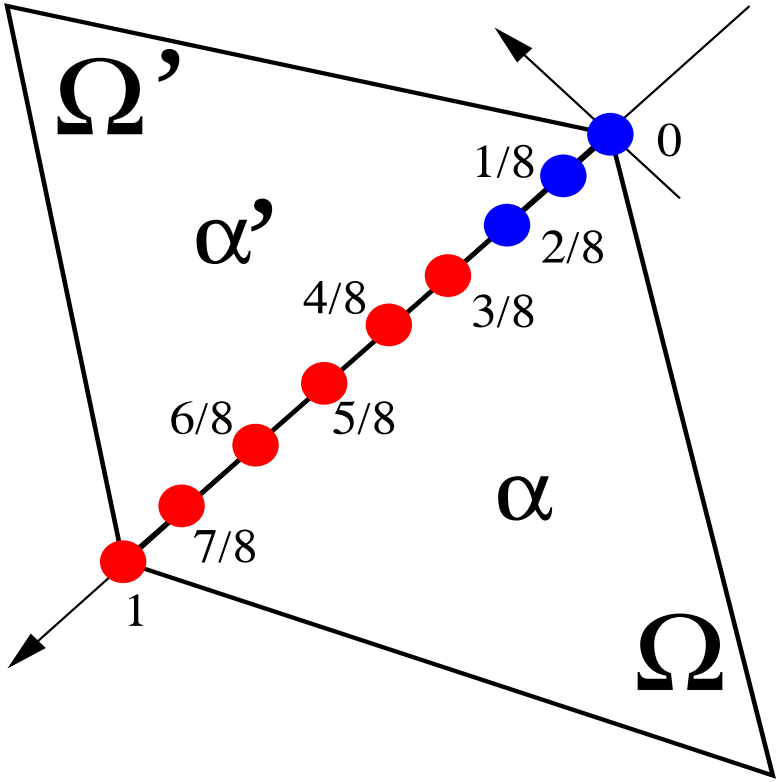
Command 2: Apply 9 rules

$[n^-;n^+]$	$f_{n^-}=0$	$f_{n^-}=\frac{1}{2}$	$f_{n^-}=1$
$f_{n^+}=0$	Obvious	Simple	$f_e=1\rightarrow 0$
$f_{n^+}=\frac{1}{2}$	Simple	Obvious	Simple
$f_{n^+}=1$	$f_e=0\rightarrow 1$	Simple	Obvious

Approx. of $f_m \in \mathbb{P}_n(\Omega)$: Edge

Case: $f_e = 0 \rightarrow 1$?

K control points $\mathbf{z}_k$ unif. distrib. along edge $[n^-, n^+]$



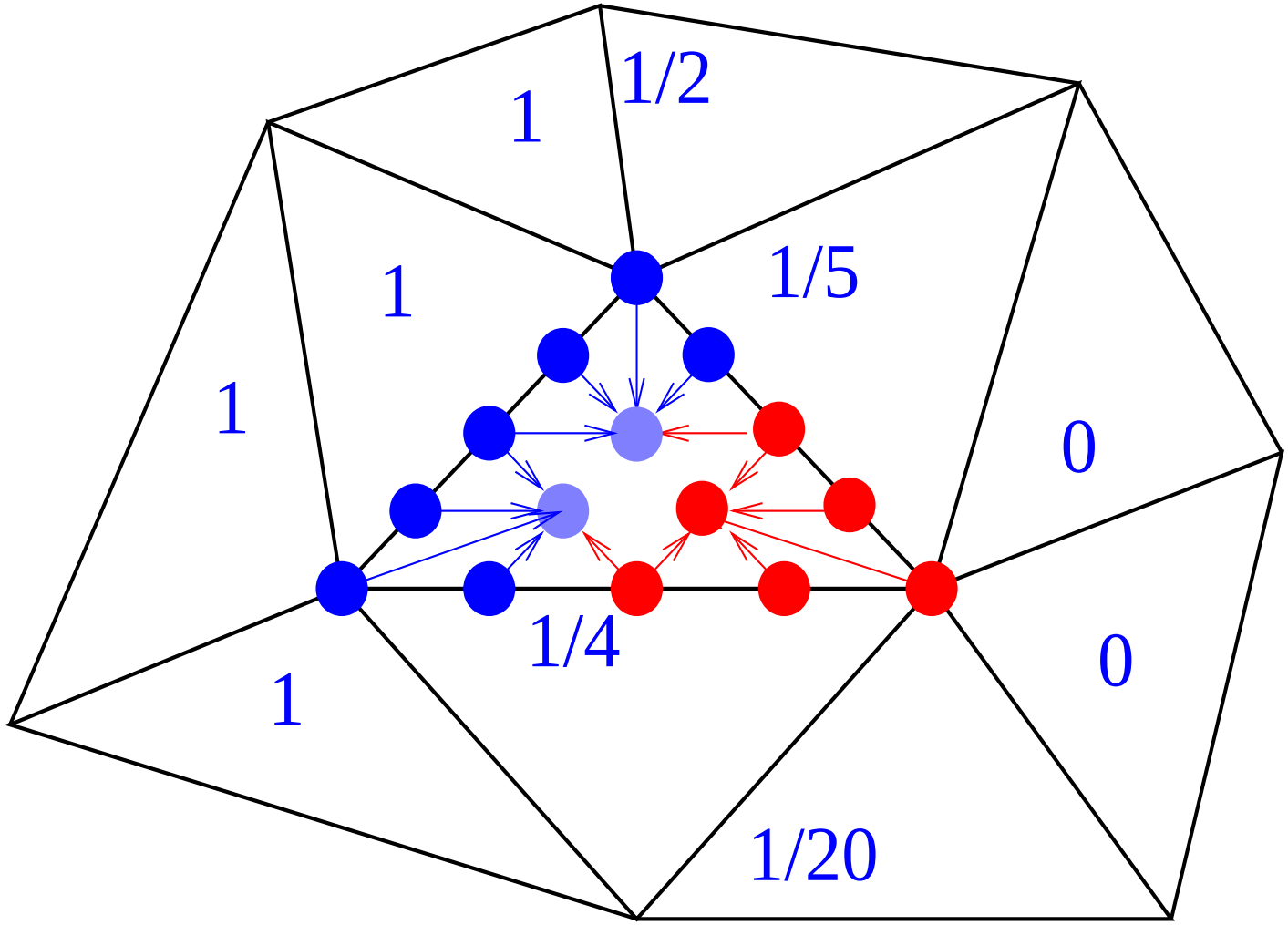
$$0 < \alpha_e = \frac{\alpha\,|\Omega| + \alpha'\,|\Omega'|}{|\Omega| + |\Omega'|} < 1$$

$$\begin{cases} f_{e_k} = 1 & \text{up to } \mathbf{z}_k \ / \ \frac{k}{K} \leq \alpha_e \\ f_{e_k} = 0 & \text{beyond} \end{cases}$$

ex: $\alpha = 1/4,\ \alpha' = 1/12 \Rightarrow 2/8 < \alpha_e = 1/6 < 3/8$

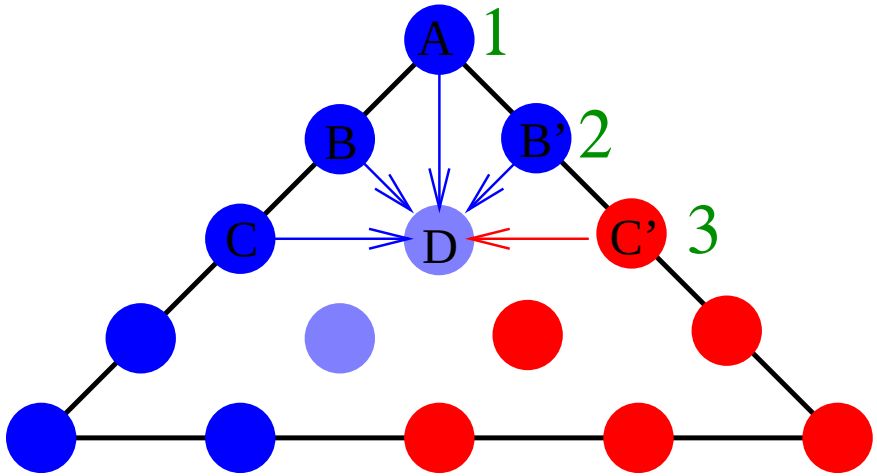
Approx. of $f_m \in \mathbb{P}_n(\Omega)$

Inside B-coeff: Weight.aver. f_{node}, f_{edge}: **local**



Approx. of $f_m \in \mathbb{P}_n(\Omega)$: Internal

Inside B-coeff: Weight.aver. f_{node}, f_{edge}: **local**



$$f_D = \frac{1}{11}\left(1 f_A + 2 f_B + 2 f_{B'} + 3 f_C + 3 f_{C'}\right)$$

- Same type of formula for degree $n > 4$

Centroid Approximation formula

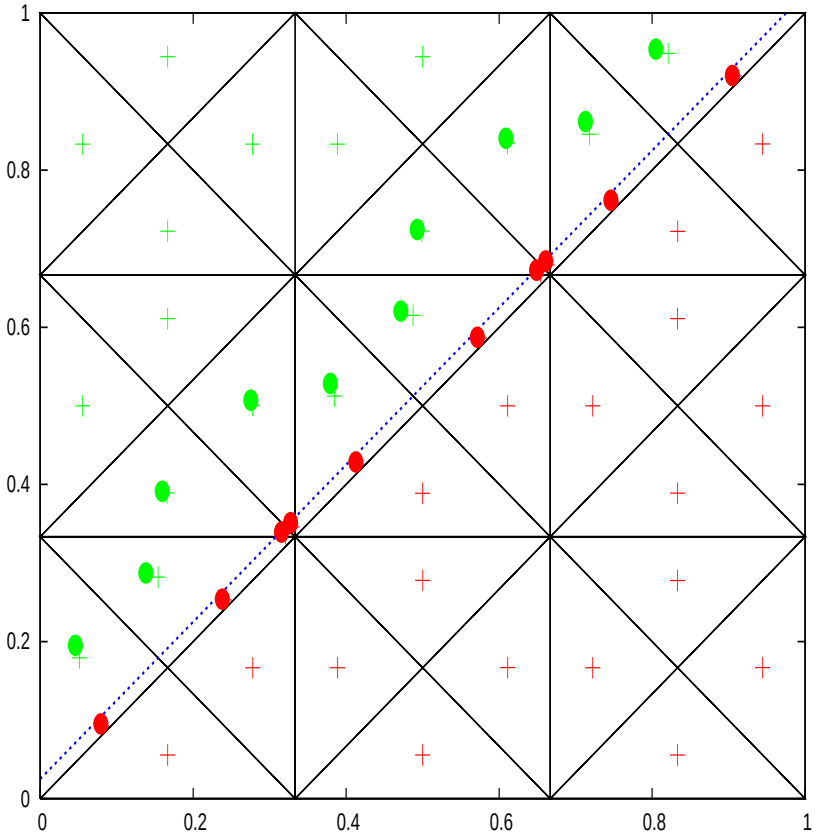
For all fluid $m = 1, \cdots M$ in Ω, $\chi_m \simeq f_m$ and the approximate centroid

$$\widetilde{\mathbf{x}}_m \simeq \begin{cases} \widehat{\mathbf{x}}_m = \dfrac{\int_\Omega f_m(\mathbf{x})\mathbf{x}d\mathbf{x}}{\int_\Omega f_m(\mathbf{x})d\mathbf{x}} & \text{if} \quad \alpha_m \geq \dfrac{1}{M} \quad \text{Dominant} \\[2ex] \widehat{\widehat{\mathbf{x}}}_m = \dfrac{\sum f_{i,j,k}\ \mathbf{z}_{i,j,k}}{\sum f_{i,j,k}} & \text{if} \quad \alpha_m < \dfrac{1}{M} \quad \text{Subordinate} \end{cases}$$

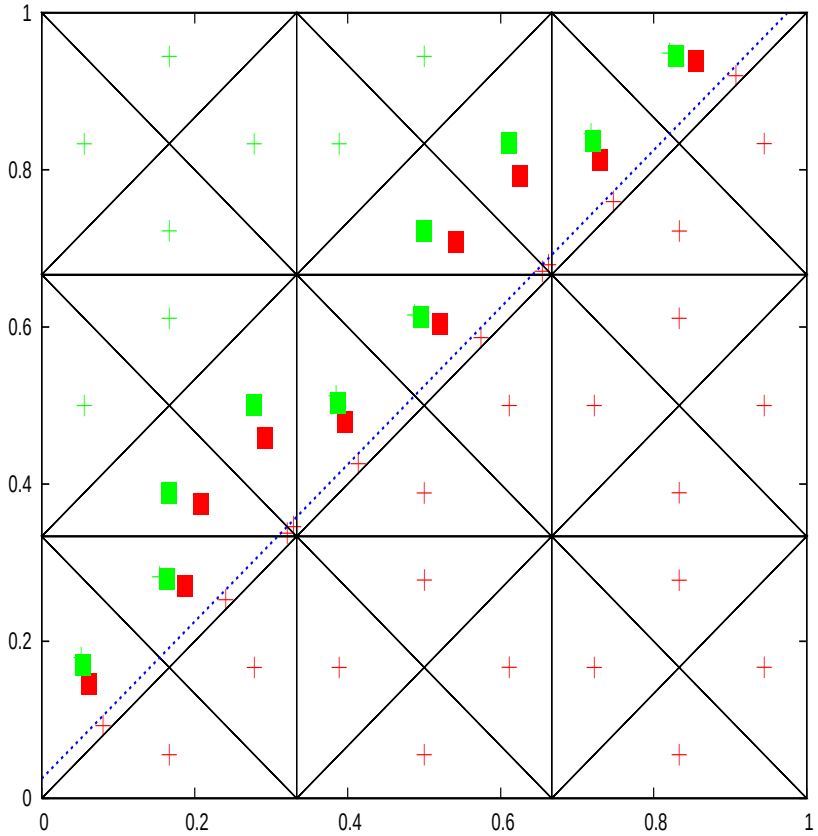
- For small α_m, $\widehat{\widehat{\mathbf{x}}}_m$: sharper approximation than $\widehat{\mathbf{x}}_m$
- $n = 4, 5$ is usually used

Results: Line

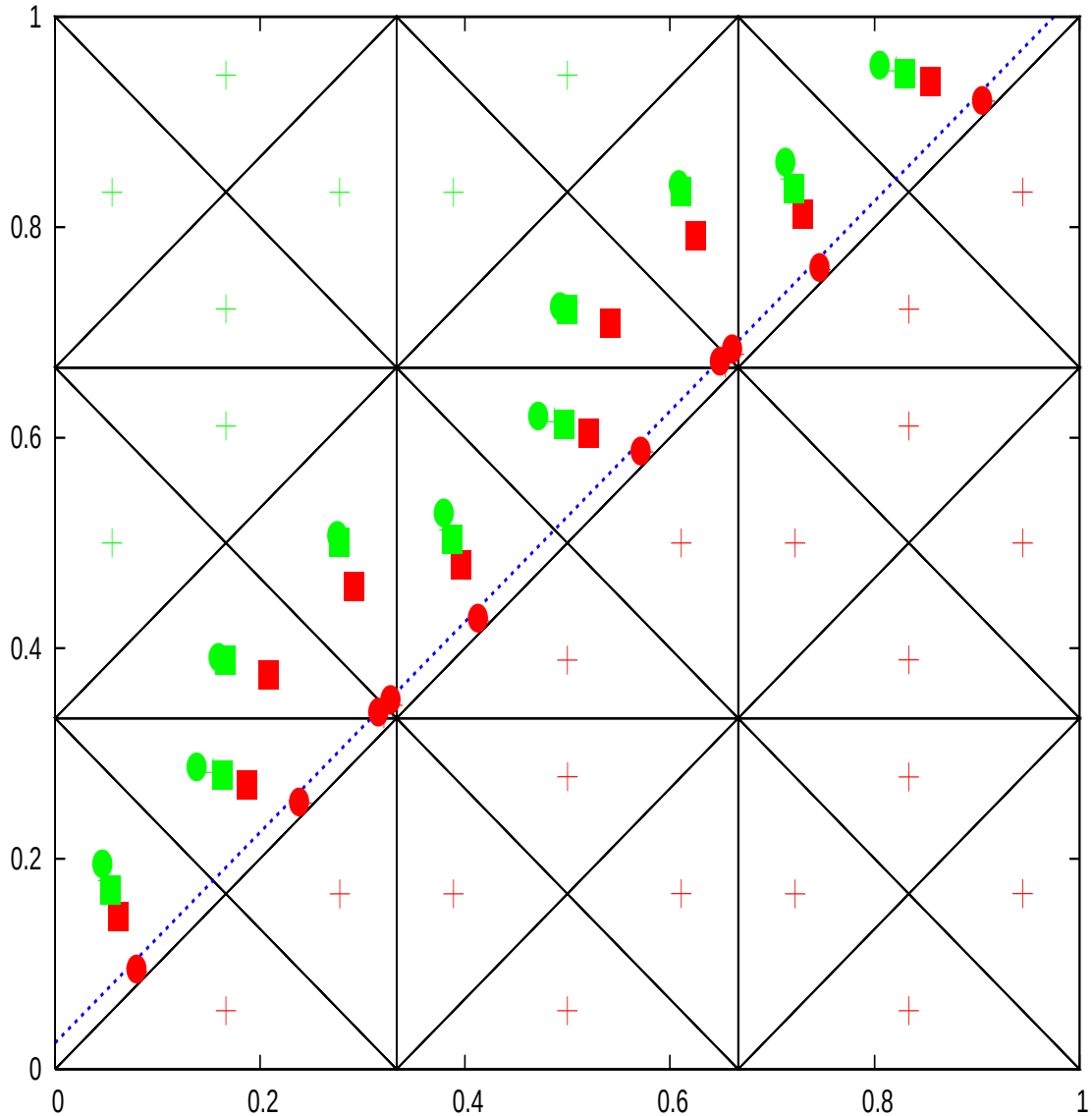
Current method



$\mathbb{P}_1$ approximation



Results: Line — Comparison



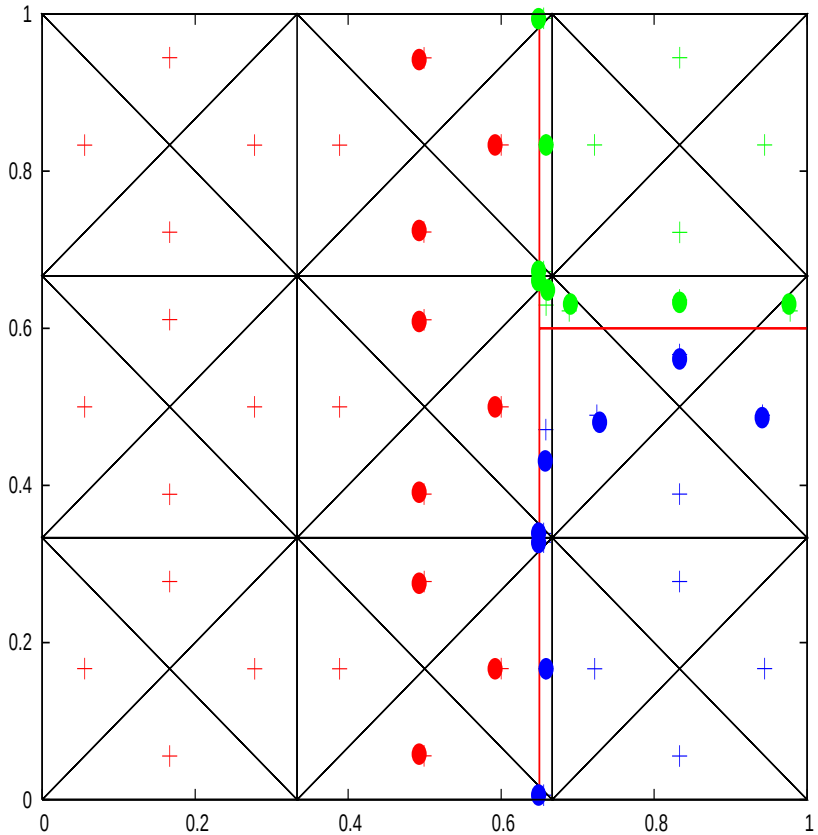
■ : $\mathbb{P}_1$

● : current

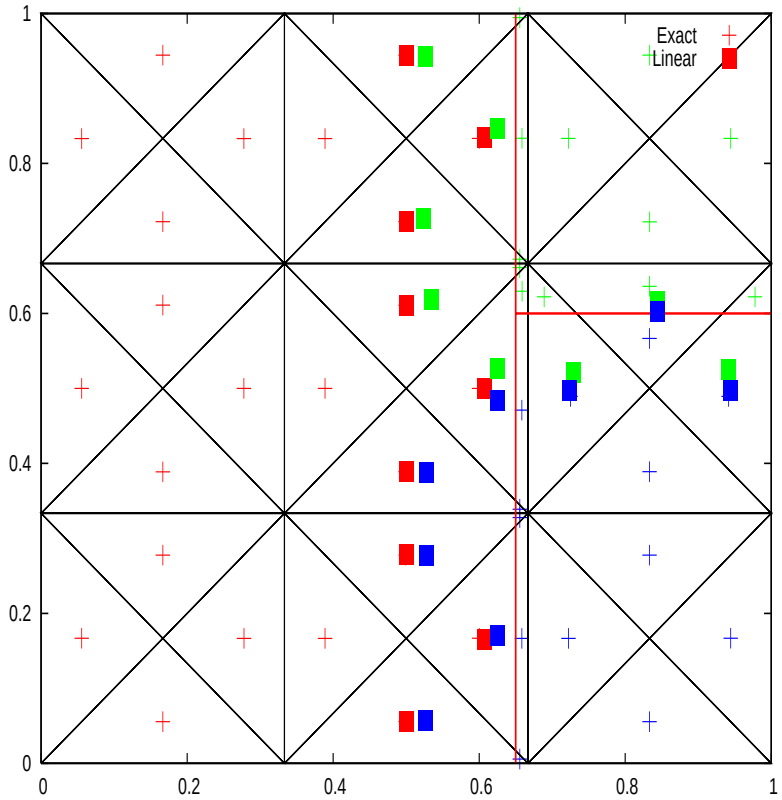
+ : exact

Results: T junction

Current

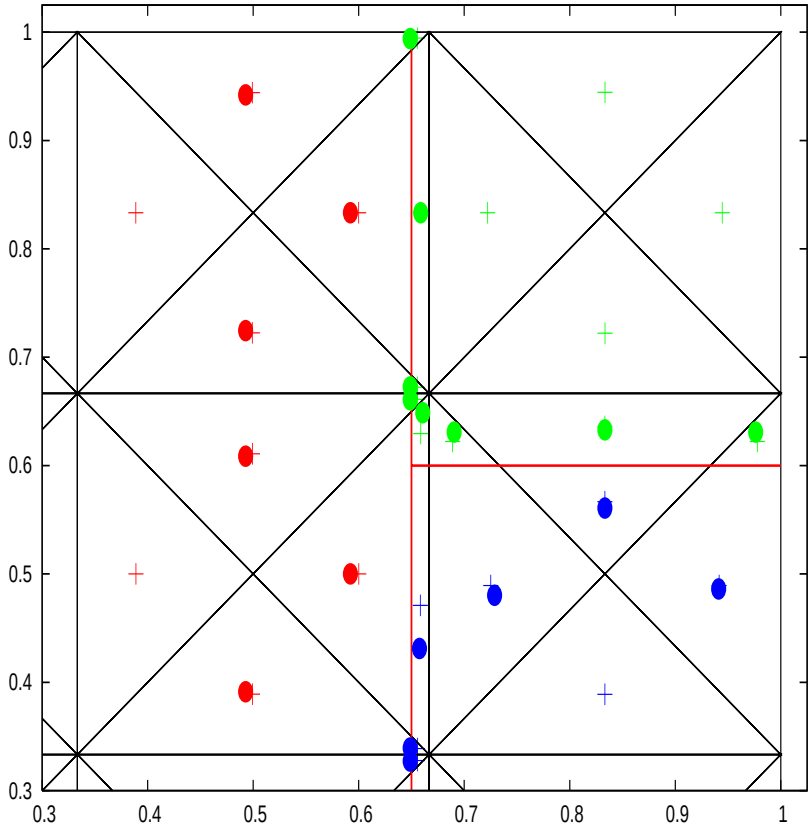


$\mathbb{P}_1$ approximation

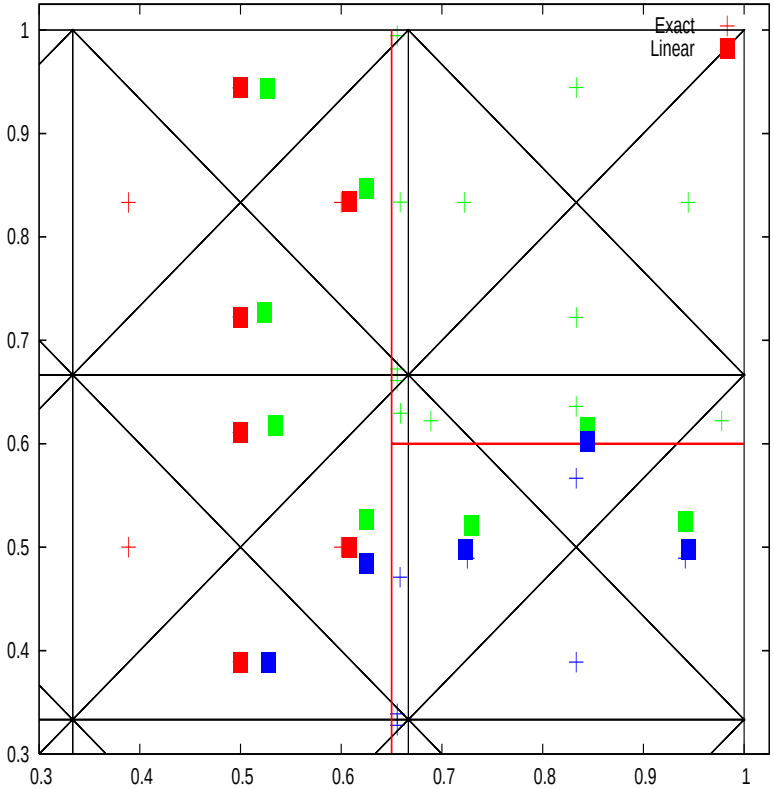


Results: T junction

Current: zoom

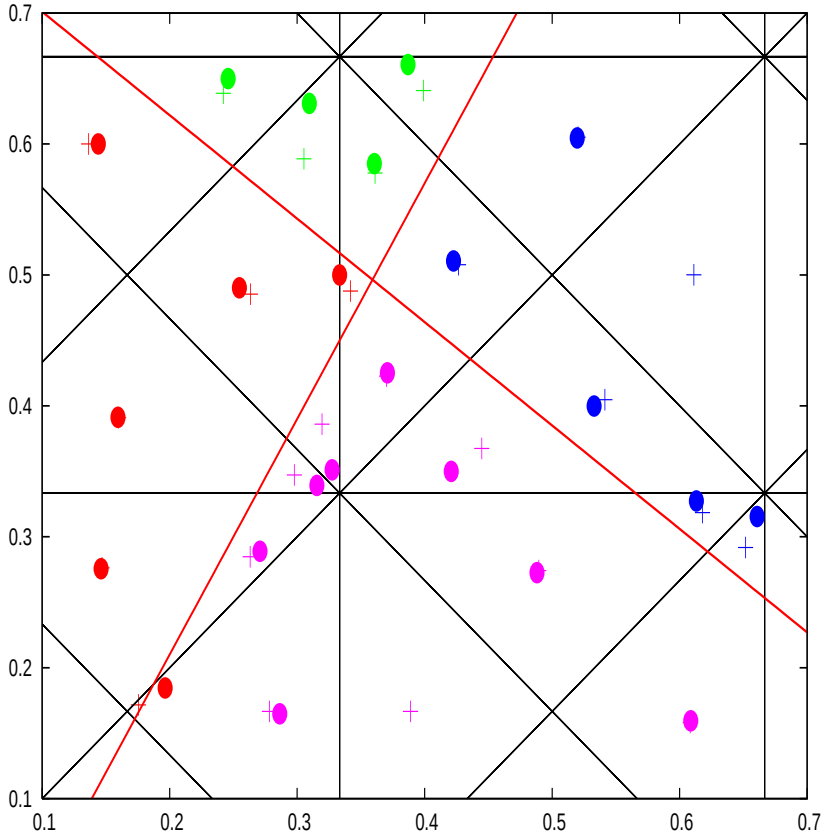


$\mathbb{P}_1$: Zoom

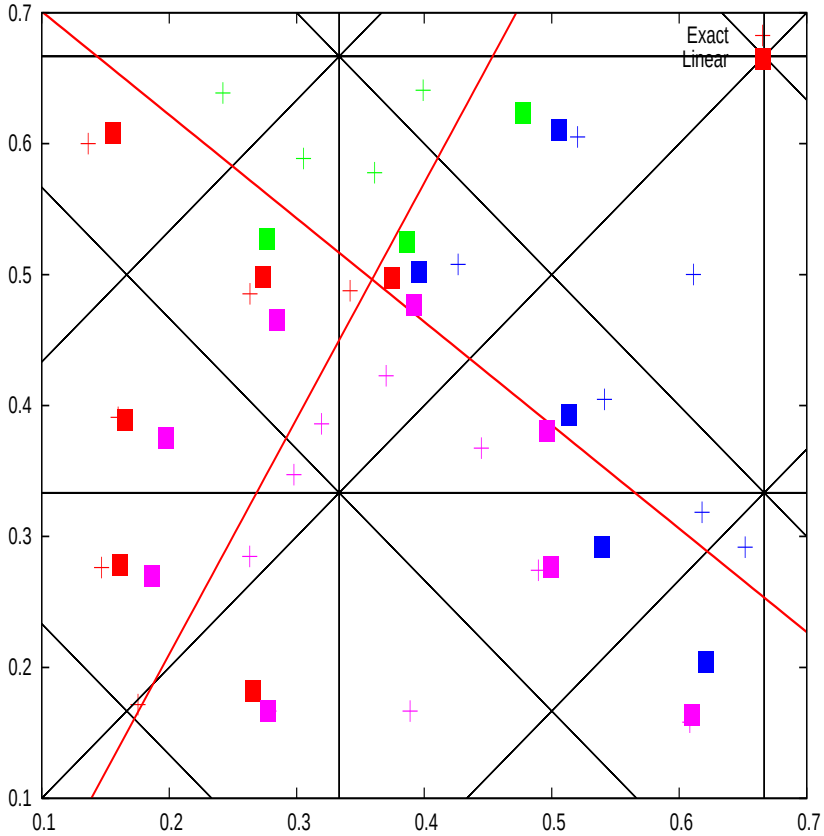


Results: X Junction

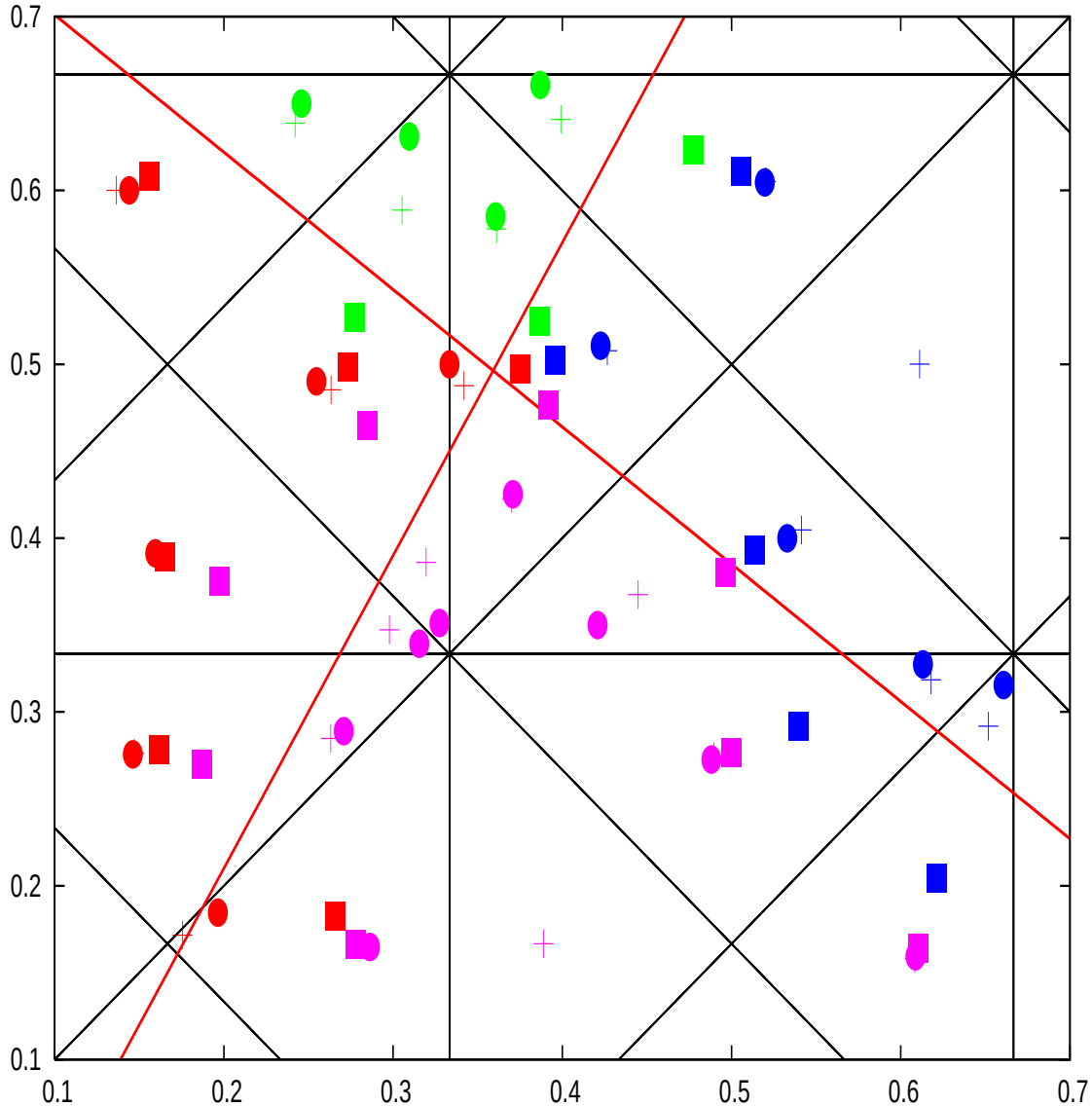
Current method



$\mathbb{P}_1$ approximation



Results: X Junction — Comparison



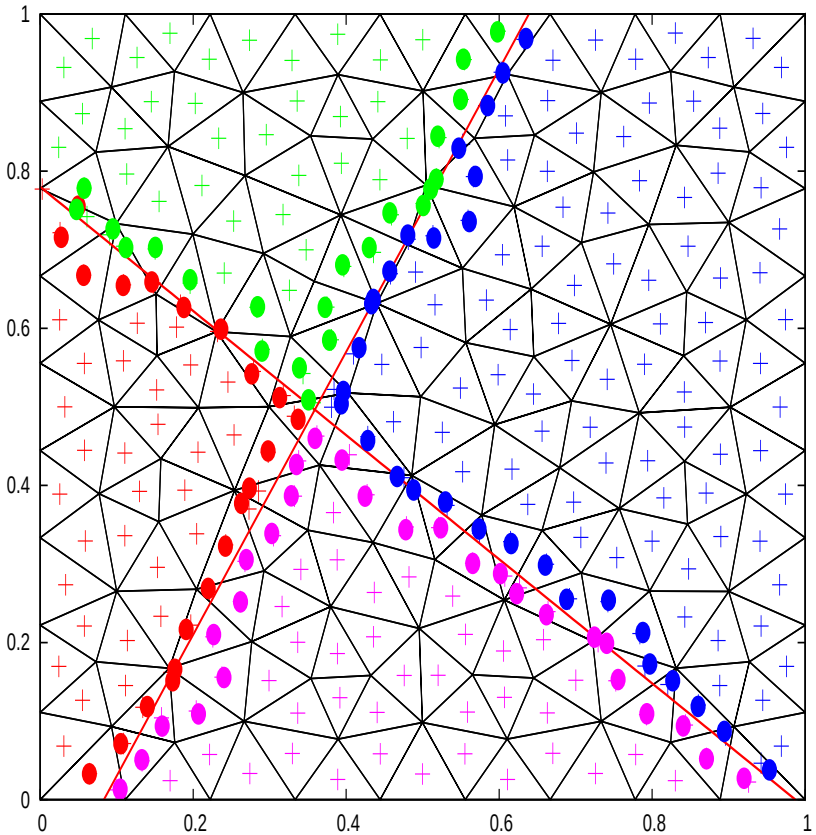
■ : $\mathbb{P}_1$

● : current

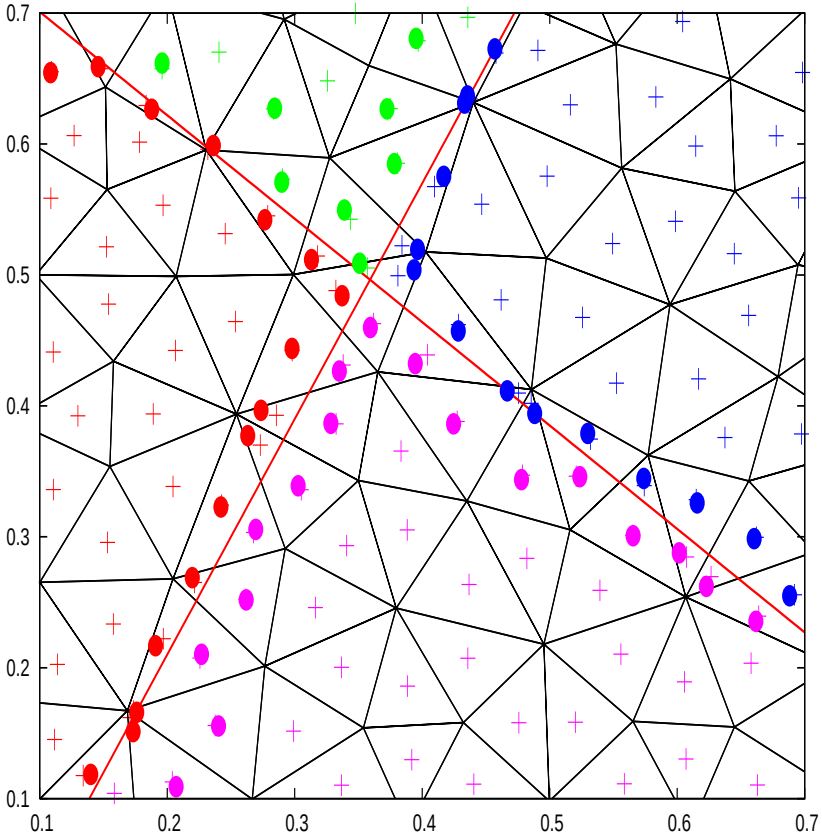
+ : exact

Results: X Junction unstruct.

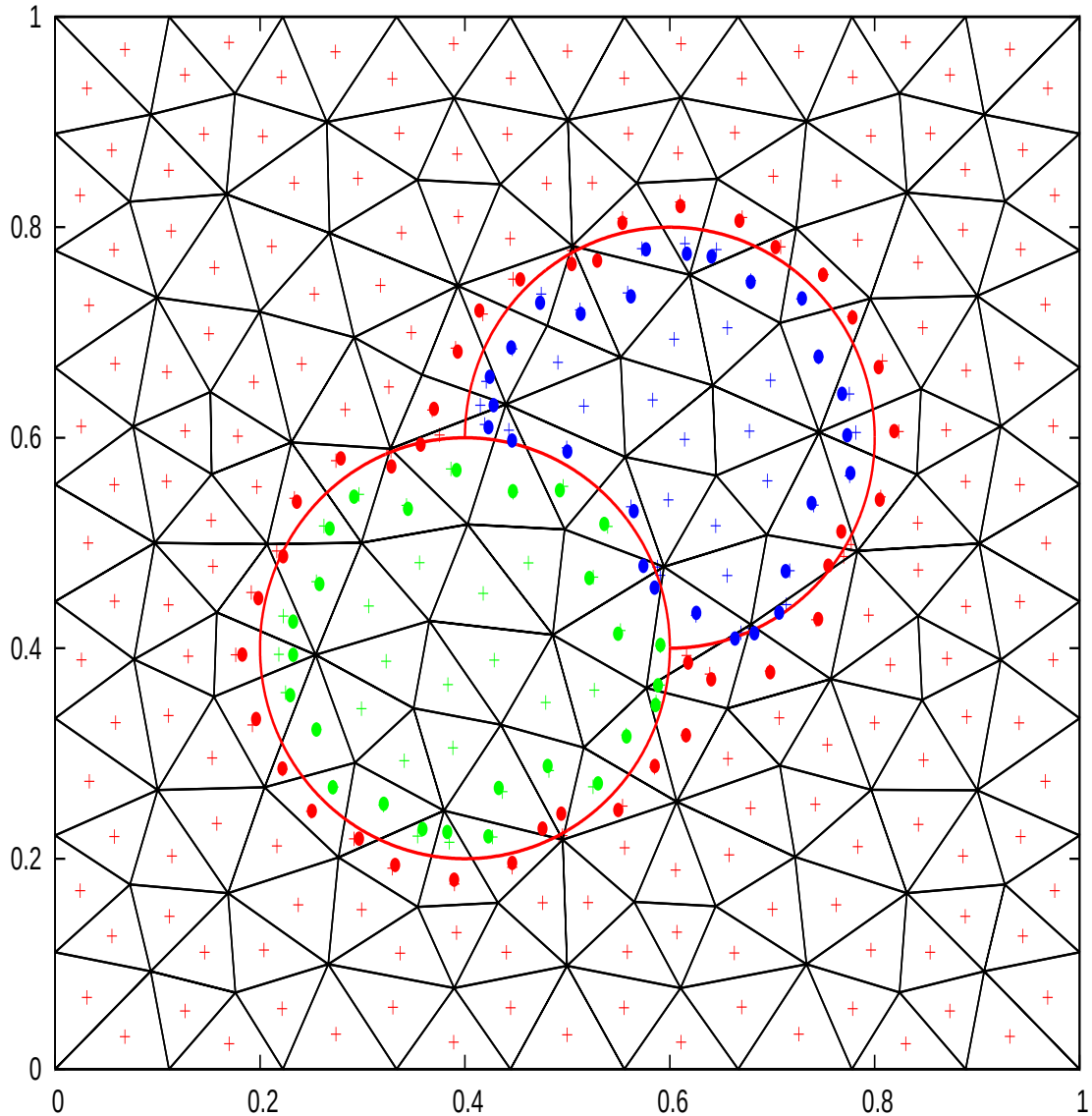
Current method



Zoom



Results: Disks

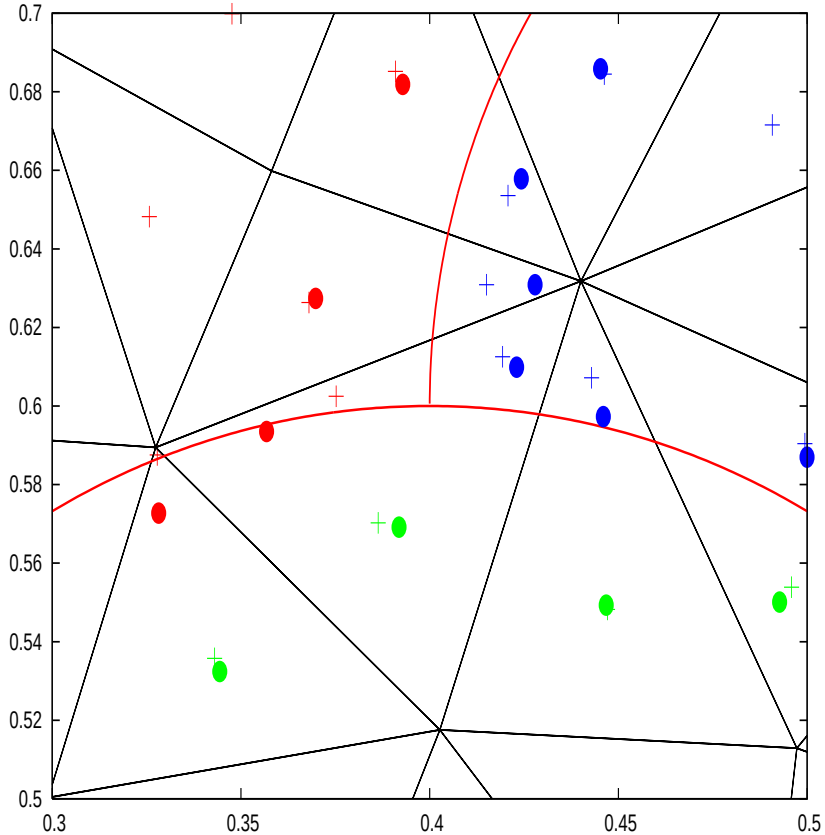


● : current

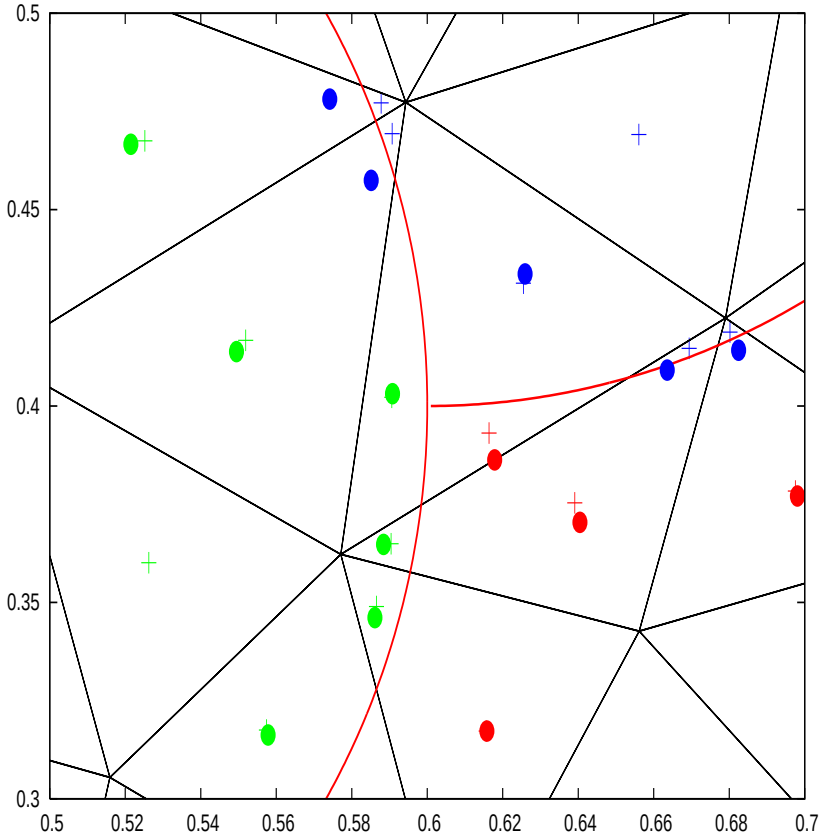
\+ : exact

Results: Disks

1st triple point



2nd triple point



Conclusion

What have you seen/heard?

- Approximate material centroids with Particle or linear approx. of the vol. frac. function may not be accurate enough
- To get higher-order of accuracy on triangles
  - Approx. vol.frac.function *via* $\mathbb{P}_4/\mathbb{P}_5$ Bernstein polynomial
  - According to neighborhood define Node $\longrightarrow$ Edge $\longrightarrow$ Intern. Bernstein coefficients
  - Integrate to get the centroids (pick best approximant)

Perspectives

What haven't you seen/heard?

- *Tricky:* How to deal with "pathology" like fragment, filament
- *Obvious:* How to extend to 3D tetrahedral
- Reconstr. Interfaces (see Rao's next talk)

What will you see/hear next time? (maybe)

- Extend to polygonal cells using Generalized Barycentric Coordinates
- Real context (hydro + advection + interface reconstruction)
- New ideas: automate, segregation,

Bibliography

Bibliography:

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- A Second-order Accurate Material-order-independent Interface Reconstruction. . ., *submitted JCP 2007*
- Centroid approximation by Bspline in multi-material cells, R.L *et al*, *LAUR (2007)*