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

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Introduction — Context

1. Fluid flow within Lagrangian, Eulerian, ALE context + complex meshes ⇒ multi-material cells ⇒ complex interfaces to reconstr.

2. Bad interfaces ⇒ Bad material advection

\( N_{\text{mat}} = 2: \) Youngs, VOF, PLIC → fine
Introduction — Context

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

- **Known:** Onion-skin, Nested-dissect., Youngs, Mosso and Clancy, Benson → problem with T-junction, material order-dependency

- **New:** MOF, Power-Diagram → Approx. of material centroids must be good enough
Good Volume Fractions

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

Good Interfaces
Outline

Introduction
- Volume Fraction
- Volume Fraction Function
- Material Centroid Approx.
- via Particle System
- via Smooth Function
- Why so? Better
- Bernstein basis
  - Bernstein basis: basics
  - Bernstein basis: control pts
  - Bernstein basis: properties
- Bernstein basis: Function
  - B-coeff: Node
  - B-coeff: Edge
  - B-coeff: Int.
- Final Centroid
- Numerical result
  - Line
  - Node
  - Edge
  - Int.
  - Final centroid
- Good Volume Fractions
  - Good Interfaces
  - (MOF, PowerDia)
- Good Centroids
- Conclusion
  - Perspectives
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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 $\Omega$

$\Omega_m$: vol. occupied by material $m$

Volume fraction of material $m$:

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

Properties: $\forall m$

$$\sum_m \alpha_m = 1, \text{ and, } 0 \leq \alpha_m \leq 1$$
Volume fraction function $\chi_m(x)$

Characteristic function

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

Properties:

$$\int_{\Omega} \chi_m(x) \, dx = \int_{\Omega_m} \, dx = |\Omega_m|$$

$$\forall x \in \Omega, \quad \sum_m \chi_m(x) = 1$$
Material Centroid Approx.

- Center of mass of material $m$

\[ \tilde{x}_m = \frac{\int_{\Omega_m} x \, dx}{\int_{\Omega_m} dx} = \frac{\int_{\Omega} \chi_m(x) x \, dx}{\int_{\Omega} \chi_m(x) \, dx} \]

1. $\tilde{x}_m$ approx. via attract/repel Particle System with ad hoc BCs

2. $\tilde{x}_m$ approx. via $f_m$ smooth approx. of $f_m \simeq \chi_m$

\[ \tilde{x}_m = \frac{\int_{\Omega} f_m(x) x \, dx}{\int_{\Omega} f_m(x) \, dx} = \left\{ \begin{array}{l} \text{Exact int.} \\ \text{Numer.int.} \end{array} \right\} \simeq \tilde{x}_m \]
Material Centroid Approx

• Center of mass of material $m$

\[
\tilde{x}_m = \frac{\int_{\Omega_m} x \, dx}{\int_{\Omega_m} dx} = \frac{\int_{\Omega} \chi_m(x) x \, dx}{\int_{\Omega} \chi_m(x) \, dx}
\]

1. $\tilde{x}_m$ approx. via attract/repel Particle System with ad hoc BCs

2. $\hat{x}_m$ approx. via $f_m$ smooth approx. of $f_m(x) \approx \chi_m$

\[
\hat{x}_m = \frac{\int_{\Omega} f_m(x) x \, dx}{\int_{\Omega} f_m(x) \, dx} = \left\{ \begin{array}{ll} \text{Exact int.} & \\
\text{Numer. int.} & \end{array} \right\} \sim \tilde{x}_m
\]
Centroids via Particle system

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

$$\bar{x}_m = \frac{1}{N_m} \sum_{p=1}^{N_m} x_m^p \approx \tilde{x}_m$$
Centroids via Particle system

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$$\overline{x}_m = \frac{1}{N_m} \sum_{p=1}^{N_m} x_m^p \approx \tilde{x}_m$$

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

BUT
- $\overline{x}_m$ approximates location of fluid $m$ in $\Omega$ but is not per se an approximation of $\tilde{x}_m$
- Particle syst. is expensive
Centroid approx. via $f_m \in P_1$

Assume $f_m$ is a piecewise linear polynomial

- Green-Gauss or Least-Square to get $\nabla f$

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

- Barth-Jeperson limitation of $\nabla f$ to ensure

$$\forall \mathbf{x} \in \Omega \quad 0 \leq f_m(\mathbf{x}) \leq 1$$
Centroid approx. via \( f_m \in \mathbb{P}_1 \)

Assume \( f_m \) is a piecewise linear polynomial

- Green-Gauss or Least-Square to get \( \nabla f \)

\[
\forall \mathbf{x} \in \Omega \quad f_m(\mathbf{x}) = \alpha_m + \nabla f \cdot (\mathbf{x} - \tilde{x}_\Omega)
\]

- Barth-Jeperson limitation of \( \nabla f \)

- Approximate center of mass of material \( m \) by integrating over \( \Omega \)

\[
\hat{x}_m = \frac{\int_{\Omega} f_m(\mathbf{x}) \mathbf{x} d\mathbf{x}}{\int_{\Omega} f_m(\mathbf{x}) d\mathbf{x}} \simeq \tilde{x}_m
\]
Centroid approx. via $f_m \in \mathbb{P}_1$
Centroid approx. via $f_m \in \mathbb{P}_1$

T-junction

Zoom
Centroid approx. via $f_m \in \mathbb{P}_1$
Centroid approx. \( \text{via } f_m \in \mathbb{P}_1 \)
Why is it so? How to do better?

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Linear app.
Interface

Exact centroid
Approx. centroid
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Linear app.
Interface
Spline 4 pts:
Why is it so? How to do better?

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Linear app.
Interface
Spline 13 pts
Bernstein polynomial basis

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

\[
p(x) = \sum_{i,j,k \geq 0, i+j+k=n} p_{i,j,k} B_{i,j,k}^{(n)}(x)
\]

\[
B_{i,j,k}^{(n)}(x) = \binom{n!}{i!j!k!} \lambda_1^i(x) \lambda_2^j(x) \lambda_3^k(x)
\]

- \( B_{i,j,k}^{(n)} \leftarrow \) expansion \(( \lambda_1(x) + \lambda_2(x) + \lambda_3(x) )^n = 1 \)
- \( \lambda_1, \lambda_2, \lambda_3 \) barycentric coordinates of \( x \in \Omega \)
- Limited to Triangles so far
Bernstein basis: Control pts

Control point: \[ z \backslash B_{i,j,k}^{(n)}(z) = \max_x \left( B_{i,j,k}^{(n)}(x) \right) \]

\[ z = \frac{1}{n} (ix_i + jx_j + kx_k) \]
Bernstein basis: Properties

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

1. **Positivity:** \(0 \leq B_{i,j,k}^{(n)}(\mathbf{x}) \leq 1 \ \forall \mathbf{x} \in \Omega\)

2. **Partition of unity:**

\[
\sum_{i,j,k} B_{i,j,k}^{(n)}(\mathbf{x}) = 1 \ \forall \mathbf{x} \in \Omega
\]

3. **Integral weight:**

\[
\int_{\Omega} B_{i,j,k}^{(n)}(\mathbf{x}) d\mathbf{x} = |\Omega| / N_n
\]

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

\[
\min(q_{i,j,k}) \leq q(\mathbf{x}) \leq \max(q_{i,j,k})
\]
Bernstein basis: Properties

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

1. Positivity: \(0 \leq B_{i,j,k}^{(n)}(x) \leq 1 \quad \forall x \in \Omega\)

2. Partition of unity:

   \[\sum_{i,j,k} B_{i,j,k}^{(n)}(x) = 1 \quad \forall x \in \Omega\]

3. Integral weight:

   \[\int_{\Omega} B_{i,j,k}^{(n)}(x) dx = |\Omega|/N_n\]

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

   \[0 \leq \min(q_{i,j,k}) \leq q(x) \leq \max(q_{i,j,k}) \leq 1\]
Approx. of $\tilde{x}_m$ via $f_m \in \mathbb{P}_n(\Omega)$

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

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

- Approximate centroid

$$\hat{x}_m = \frac{\int_{\Omega} f_m(x) x \, dx}{\int_{\Omega} f_m(x) \, dx} \equiv \sum_{i,j,k} f_{i,j,k} \gamma_{i,j,k} \approx \tilde{x}_m$$

Convex combination

where

$$\gamma_{i,j,k} = \frac{N_n}{\sum_{i,j,k} f_{i,j,k}} \frac{\int_{\Omega} B_{i,j,k}^{(n)}(x) x \, dx}{|\Omega|} \geq 0$$
Approx. of $\tilde{x}_m$ via $f_m \in \mathbb{P}_n(\Omega)$

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**Unknowns:**

$f_{i,j,k}$ \iff "value of $\chi_m(z_{i,j,k})$"
Approx. of $f_m \in \mathbb{P}_n(\Omega)$
Approx. of $f_m \in \mathbb{P}_n(\Omega)$

Volume Fractions

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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

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

- Mean value

$$\overline{\alpha} = \frac{\sum_j |\Omega_j| \alpha^j}{\sum_j |\Omega_j|}$$

$$g = \begin{cases} 
1 & \text{if } \overline{\alpha} > 1/2 \\
0 & \text{if } \overline{\alpha} < 1/2 \\
1/2 & \text{if } \overline{\alpha} = 1/2 
\end{cases}$$

<table>
<thead>
<tr>
<th>$\alpha^+$</th>
<th>$\alpha^- = 0$</th>
<th>$\alpha^- &gt; 0$</th>
</tr>
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<tbody>
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<td>$\alpha^+ = 1$</td>
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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 $f_m \in \mathbb{P}_n(\Omega)$

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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 $\implies$ assoc. 1 or 0 to all B-coeff.

**Command 2:** Apply 9 rules

<table>
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<tr>
<th>$[n^-;n^+]$</th>
<th>$f_{n^-} = 0$</th>
<th>$f_{n^-} = \frac{1}{2}$</th>
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<td>$f_{n^+} = 0$</td>
<td>$f_e = 0$</td>
<td>$f_e = \frac{1}{2} \rightarrow 0$</td>
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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 $\rightarrow$ assoc. 1 or 0 to all B-coeff.

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

Case: $f_e = 0 \rightarrow 1$?

$K$ control points $z_k$ unif. distrib. along edge $[n^-, n^+]$

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

$$\left\{ \begin{array}{l}
    f_{ek} = 1 \text{ up to } z_k / \frac{k}{K} \leq \alpha_e \\
    f_{ek} = 0 \text{ beyond }
\end{array} \right.$$ 

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. $f_{\text{node}}, f_{\text{edge}}$: local
Approx. of $f_m \in \mathbb{P}_n(\Omega)$: Internal

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

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

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

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

\[
\tilde{X}_m \simeq \begin{cases} 
\hat{X}_m = \frac{\int_\Omega f_m(x) x \, dx}{\int_\Omega f_m(x) \, dx} & \text{if } \alpha_m \geq \frac{1}{M} \quad \text{Dominant} \\
\hat{\hat{X}}_m = \frac{\sum f_{i,j,k} z_{i,j,k}}{\sum f_{i,j,k}} & \text{if } \alpha_m < \frac{1}{M} \quad \text{Subordinate}
\end{cases}
\]

- For small $\alpha_m$, $\hat{\hat{X}}_m$: sharper approximation than $\hat{X}_m$
- $n = 4, 5$ is usually used
Results: Line

Current method

\[ P_1 \text{ approximation} \]
Results: Line — Comparison

- Comparison of different methods for calculating the centroid of a line segment.

- Four methods are compared:
  - $\mathbb{P}_1$ (polynomial of degree 1)
  - Current method
  - Exact solution

- The graph shows the comparison for different line segments.

- T junction, X junction, and disks are used as test cases.

- Conclusion and perspectives are outlined.
Results: T junction

Current

\( P_1 \) approximation
Results: T junction

Current: zoom

\[ P_1: \text{Zoom} \]
Results: X Junction

Current method

$P_1$ approximation

Numerical result

Perspectives
Results: X Junction — Comparison

- : $P_1$
- : current
+ : exact
Results: X Junction unstruct.

Current method

Zoom
Results: Disks

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- : current
- + : exact
Results: Disks

1st triple point

2nd triple point

Numerical results:
- Line
- T-junction
- X-junction

Conclusion
Perspectives
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 \( \text{via } \mathbb{P}_4/\mathbb{P}_5 \) Bernstein polynomial
  - According to neighborhood define Node \( \rightarrow \) Edge \( \rightarrow \) 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
- Reconstruct. 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:

- Centroid approximation by Bspline in multi-material cells, R.L *et al*, *LAUR* (2007)