Analytic Gradient for the Moment-of-Fluid Method in Axisymmetric and on General Polyhedrons in Any Dimension

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Abstract

The moment-of-fluid method (MOF) is an interface reconstruction method similar to the volume-of-fluid method with piecewise linear interface reconstruction (VOF-PLIC). In the MOF method, the normal to the interface is found by minimizing the distance between the centroid of the polyhedron below the interface and a reference centroid under a volume constraint. To solve this minimization problem, the gradient of the objective function must be evaluated. Analytic formulas have been proposed by many authors to compute the gradient in 2D on general polygons with a polar parametrization and in 3D on convex polyhedrons with a spherical parametrization. In this short note, we propose a more general formula that covers non-convex polyhedrons in any dimension and axisymmetric coordinates. Furthermore, this formula does not depend on the parametrization of the normal to the interface. We also provide some practical way to use the formula in a code.

Keywords: Moment-of-Fluid, interface reconstruction, analytic derivatives, polyhedron, axisymmetric coordinates

1. Introduction

The moment-of-fluid method (MOF) is an interface reconstruction method where the interface is represented by an hyperplane and where the volume is enforced below the interface. This method was introduced in 2D on polygonal cells by Dyadechko & Shashkov [1], extended to 3D on polyhedral cell by Ahn & Shashkov [2] and to axisymmetric coordinates by Anbarlooei & Mazaheri [3]. For a polyhedral cell $\Omega \subset \mathbb{R}^n$ as represented in figure 1, the reconstructed interface denoted $\mathcal{F}$ can be seen as the intersection of the boundary of a half-space $\mathrm{H}(\boldsymbol{n}, d)$ and the cell Ω, where $\boldsymbol{n} \in \mathbb{S}^{n-1}$ denotes the normal to the interface and $d \in \mathbb{R}$ represents the signed distance of the interface to the origin. The intersection of the half-space and the cell will be referred to as the *reconstructed polyhedron* and will be denoted $\mathcal{R}(\Theta)$ with $\Theta = (\Theta_1, \ldots, \Theta_{n-1}) \in \mathbb{R}^{n-1}$ a parametrization of $\boldsymbol{n}$, for instance, the polar angle in 2D and the spherical angles in 3D.

We denote as $\mathcal{C}(\Theta)$ the centroid of the reconstructed polyhedron $\mathcal{R}(\Theta)$ defined by:

$$\mathcal{C}(\Theta) = \frac{1}{|\mathcal{R}(\Theta)|} \int_{\mathcal{R}(\Theta)} \boldsymbol{x} \, d\boldsymbol{x} \qquad \text{where} \qquad |\mathcal{R}(\Theta)| = \int_{\mathcal{R}(\Theta)} d\boldsymbol{x} \tag{1}$$

The moment-of-fluid problem consists to find Θ such that the distance between the centroid of $\mathcal{R}(\Theta)$ and a *reference centroid* $\mathcal{C}^\star$ is minimum under the constraint $|\mathcal{R}(\Theta)| = \mathcal{V}^\star$, that is:

$$\text{Minimize} \quad \mathcal{M}(\Theta) = |\mathcal{C}(\Theta) - \mathcal{C}^\star|^2 \quad \text{such that} \quad |\mathcal{R}(\Theta)| = \mathcal{V}^\star \tag{2}$$

where $\mathcal{V}^\star \in \mathbb{R}_+$ is a fixed given parameter called the *reference volume*. The function $\mathcal{M}$ will be referred to as the *objective function*.

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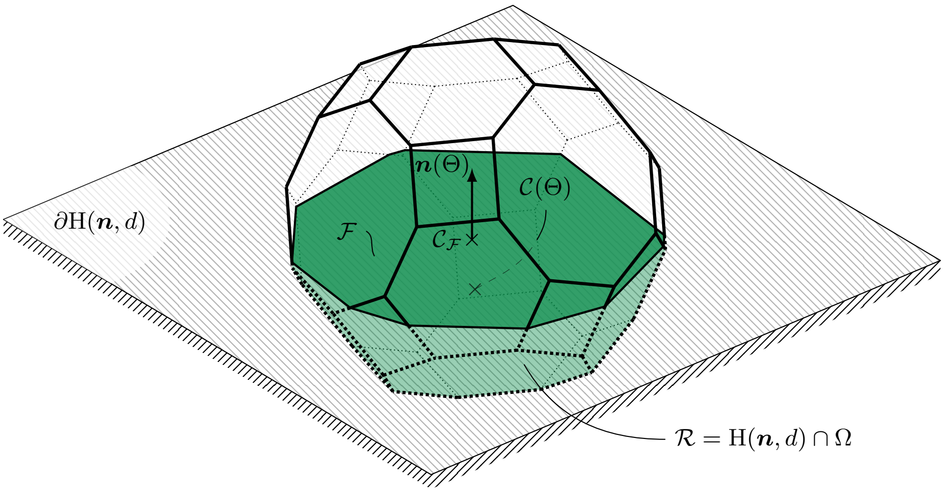

Figure 1: Illustration of the notations used to define the MOF problem: Ω a polyhedron, $\mathrm{H}(\boldsymbol{n}, d)$ the half-space of normal $\boldsymbol{n}$ and distance d, Θ the parametrization of the normal, $\mathcal{R}$ the region of Ω below the interface and $\mathcal{C}$ its centroid, $\mathcal{F}$ the interface in the polyhedron, and $\mathcal{C}_\mathcal{F}$ its centroid.

The classic strategy to solve this problem consists in using a minimization algorithm on the parameters Θ where the reconstructed polyhedron is constructed at each iteration using a volume enforcement algorithm such as the Brent's based method [4] or the method of Diot & François [5]. The minimization algorithm requires the evaluation of the gradient of the objective function with respect to Θ which can be approximated by a finite-differences scheme that requires several calls to the volume enforcement algorithm and introduces inaccuracies that can slow down the convergence of the minimization algorithm or let it fall into some local minima. Many authors have found analytic formulas for the gradient in particular cases based on the geometry of the reconstructed interface $\mathcal{F}$ meaning that the volume enforcement algorithm can be used to evaluate simultaneously the objective function and its gradient. Dyadechko & Shashkov [6] provides two formulas for polygonal cells in 2D where the first can be used if the reconstructed interface is composed of one line segment and the second when the interface is composed of several line segments, which may happen when the cell is non-convex. Later, Chen & Zhang [7] have developed an analytic formula on convex polyhedrons where the normal to the interface is parametrized by the spherical angles. In more specific a context, the gradient of the objective function can be evaluated without a prior call to the volume enforcement algorithm, such as the formulas proposed on rectangular cells in 2D by Lemoine *et al.* [8] and on rectangular hexahedral cells in 3D by Milcent & Lemoine [9].

In this short note, we develop a general formula that can be applied to any regular set of $\mathbb{R}^n$ which covers two cases that remain without analytic formulas: MOF in axisymmetric coordinates and in 3D on non-convex polyhedrons. Furthermore, the proposed formula does not depend on the parametrization of the normal to the interface. In section 2, we give the proof of our analytic formula. In section 3, we provide a practical way to use this formula on polygon in 2D and axisymmetric coordinates and in 3D on polyhedrons.

2. Analytic gradient of the centroid

2.1. Analytic gradient

Consider the normal vector $\boldsymbol{n} \in \mathbb{S}^{n-1}$ parametrised by $\Theta = (\Theta_1, \ldots, \Theta_{n-1}) \in \mathbb{R}^{n-1}$. The gradient of the objective function (2) is given by:

$$\nabla_\Theta \mathcal{M}(\Theta) = 2\left[\nabla_\Theta \mathcal{C}(\Theta)\right]^\mathsf{T} \left(\mathcal{C}(\Theta) - \mathcal{C}^\star\right) \tag{3}$$

where $[\nabla_\Theta \mathcal{C}(\Theta)]$ denotes the gradient — or Jacobian matrix — of the centroid with respect to Θ. Using the partial derivatives of the centroid, it can be written in terms of coordinates:

$$\forall i \in [\![1, n-1]\!] \qquad \big[\nabla_\Theta \mathcal{M}(\Theta)\big]_i = 2\sum_{j=1}^{n} \big(\partial_{\Theta_i}\mathcal{C}_j(\Theta)\big)\big(\mathcal{C}_j(\Theta) - \mathcal{C}_j^\star\big) \tag{4}$$

In the remainder of this section, we will prove that the gradient of the centroid with respect to Θ is given by:

$$\nabla_\Theta \mathcal{C}(\Theta) = \frac{|\mathcal{F}|}{\mathcal{V}^\star}\big(\mathcal{C}_\mathcal{F} \otimes \mathcal{C}_\mathcal{F} - \mathcal{S}_\mathcal{F}\big)\nabla_\Theta \boldsymbol{n}(\Theta) \tag{5}$$

where $\mathcal{F}$ denotes the reconstructed interface and

$$|\mathcal{F}| = \int_\mathcal{F} d\boldsymbol{x} \qquad \mathcal{C}_\mathcal{F} = \frac{1}{|\mathcal{F}|}\int_\mathcal{F} \boldsymbol{x}\, d\boldsymbol{x} \qquad \mathcal{S}_\mathcal{F} = \frac{1}{|\mathcal{F}|}\int_\mathcal{F} \boldsymbol{x}\otimes\boldsymbol{x}\, d\boldsymbol{x} \tag{6}$$

where $|\mathcal{F}|$ is the area of the interface, $\mathcal{C}_\mathcal{F}$ is the centroid of the interface, and $\mathcal{S}_\mathcal{F}$ is a quadratic momentum of the interface.

2.2. Proof of the analytic gradient

To prove this formula, consider $\Theta(t)$ that varies smoothly with respect to a real parameter $t \in \mathbb{R}$ and call $\mathcal{R}^t = \mathcal{R}(\Theta(t))$ and $\mathcal{F}^t = \mathcal{F}(\Theta(t))$.

Let $\mathbf{X}\colon \mathbb{R}^n \times \mathbb{R}_+ \to \mathbb{R}^n$ be the application that transforms the reconstructed polyhedron at $t = 0$ to the reconstructed polyhedron at any t such that $\mathbf{X}(\mathcal{R}^0, t) = \mathcal{R}^t$. Consider any vector field $\boldsymbol{u}\colon \mathbb{R}^n \times \mathbb{R}_+ \to \mathbb{R}^n$ that satisfies the following Cauchy problem:

$$\begin{cases} \partial_t \mathbf{X}(\boldsymbol{\xi}, t) = \boldsymbol{u}(\mathbf{X}(\boldsymbol{\xi}, t), t) \\ \mathbf{X}(\boldsymbol{\xi}, 0) = \boldsymbol{\xi} \end{cases} \tag{7}$$

The vector field $\boldsymbol{u}$ can be seen as the Eulerian velocity that transforms $\mathcal{R}^0$ into $\mathcal{R}^t$. In particular, the normal velocity on the boundary of the cell Ω is zero since it does not move during the transformation meaning that $\boldsymbol{u}\cdot\boldsymbol{n} = \mathbf{0}$ on $\partial\mathcal{R}^t \cap \partial\Omega$. The derivative of the centroid with respect to t is given by:

$$\frac{d}{dt}\mathcal{C}(\Theta(t)) = \big[\nabla_\Theta \mathcal{C}(\Theta(t))\big]\Theta'(t) = \frac{1}{\mathcal{V}^\star}\frac{d}{dt}\int_{\mathcal{R}^t} \boldsymbol{x}\, d\boldsymbol{x} \tag{8}$$

The middle term is obtained using the chain rule and right-hand side of this formula is obtained using (1) bearing in mind that the volume of the reconstructed polyhedron $|\mathcal{R}^t| = \mathcal{V}^\star$ does not vary with t. Any point $\boldsymbol{x} = \mathbf{X}(\boldsymbol{\xi}, t)$ of the reconstructed interface verifies the following equation:

$$\mathbf{X}(\boldsymbol{\xi}, t)\cdot\boldsymbol{n}(\Theta(t)) = d(t) \tag{9}$$

Differentiating this equation with respect to t gives:

$$\boldsymbol{u}(\mathbf{X}(\boldsymbol{\xi}, t), t)\cdot\boldsymbol{n}(\Theta(t)) + \mathbf{X}(\boldsymbol{\xi}, t)\cdot\big([\nabla_\Theta \boldsymbol{n}(\Theta(t))]\Theta'(t)\big) = d'(t) \tag{10}$$

Calling $\boldsymbol{x} = \mathbf{X}(\boldsymbol{\xi}, t)$ and re-organizing this equation gives:

$$\boldsymbol{u}(\boldsymbol{x}, t)\cdot\boldsymbol{n}(\Theta(t)) = d'(t) - \boldsymbol{x}\cdot\big([\nabla_\Theta \boldsymbol{n}(\Theta(t))]\Theta'(t)\big) \tag{11}$$

The volume of the reconstructed polyhedron does not depend on t meaning that $\frac{d}{dt}|\mathcal{R}^t| = 0$. Using successively the Reynolds' transport theorem, the Stokes' theorem, $\boldsymbol{u}\cdot\boldsymbol{n} = \mathbf{0}$ on $\partial\mathcal{R}^t \cap \partial\Omega$, equation (11), and the definition (6) of the centroid of the face $\mathcal{C}_\mathcal{F}$ gives:

$$\begin{aligned} 0 &= \frac{d}{dt}\int_{\mathcal{R}^t} d\boldsymbol{x} = \int_{\mathcal{R}^t} \operatorname{div}\big(\boldsymbol{u}(\boldsymbol{x}, t)\big) d\boldsymbol{x} = \int_{\partial\mathcal{R}^t} \boldsymbol{u}(\boldsymbol{x}, t)\cdot\boldsymbol{n}(\Theta(t))\, d\boldsymbol{x} = \int_{\mathcal{F}^t} \boldsymbol{u}(\boldsymbol{x}, t)\cdot\boldsymbol{n}(\Theta(t))\, d\boldsymbol{x} \\ &= \int_{\mathcal{F}^t} \big(d'(t) - \boldsymbol{x}\cdot([\nabla_\Theta \boldsymbol{n}(\Theta(t))]\Theta'(t))\big) d\boldsymbol{x} = |\mathcal{F}^t|\big(d'(t) - \mathcal{C}_\mathcal{F}\cdot[\nabla_\Theta \boldsymbol{n}(\Theta(t))]\Theta'(t)\big) \end{aligned} \tag{12}$$

Finally, we obtain a relation between the derivative of the signed distance with the centroid of the reconstructed interface and the derivative of the normal:

$$d'(t) = \mathcal{C}_{\mathcal{F}} \cdot [\nabla_\Theta \boldsymbol{n}(\Theta(t))]\Theta'(t) \tag{13}$$

Now, let us develop the right-hand side of equation (8). Apply successively the Reynold's transport theorem, the Stokes' theorem, $\boldsymbol{u} \cdot \boldsymbol{n} = \boldsymbol{0}$ on $\partial\mathcal{R}^t \cap \partial\Omega$, equations (11) and (13), $\boldsymbol{u}(\boldsymbol{v} \cdot \boldsymbol{w}) = (\boldsymbol{u} \otimes \boldsymbol{v})\boldsymbol{w}$ where $\otimes$ denotes the tensor product, and the definitions in equation (6) gives:

$$\begin{aligned}
\frac{d}{dt}\mathcal{C}(\Theta(t)) &= \frac{1}{\mathcal{V}^\star}\frac{d}{dt}\int_{\mathcal{R}^t} \boldsymbol{x}\, d\boldsymbol{x} = \frac{1}{\mathcal{V}^\star}\int_{\mathcal{R}^t} \operatorname{div}(\boldsymbol{x} \otimes \boldsymbol{u}(\boldsymbol{x},t))d\boldsymbol{x} = \frac{1}{\mathcal{V}^\star}\int_{\mathcal{F}^t} \boldsymbol{x}\big(\boldsymbol{u}(\boldsymbol{x},t)\cdot \boldsymbol{n}\big)d\boldsymbol{x} \\
&= \frac{1}{\mathcal{V}^\star}\int_{\mathcal{F}^t} \boldsymbol{x}\big(\mathcal{C}_{\mathcal{F}} \cdot [\nabla_\Theta \boldsymbol{n}(\Theta(t))]\Theta'(t) - \boldsymbol{x} \cdot [\nabla_\Theta \boldsymbol{n}(\Theta(t))]\Theta'(t)\big)d\boldsymbol{x} \\
&= \frac{|\mathcal{F}^t|}{\mathcal{V}^\star}\mathcal{C}_{\mathcal{F}}\big(\mathcal{C}_{\mathcal{F}} \cdot [\nabla_\Theta \boldsymbol{n}(\Theta(t))]\Theta'(t)\big) - \frac{1}{\mathcal{V}^\star}\int_{\mathcal{F}^t} \boldsymbol{x}\big(\boldsymbol{x} \cdot [\nabla_\Theta \boldsymbol{n}(\Theta(t))]\Theta'(t)\big)d\boldsymbol{x} \\
&= \frac{|\mathcal{F}^t|}{\mathcal{V}^\star}\left(\mathcal{C}_{\mathcal{F}} \otimes \mathcal{C}_{\mathcal{F}} - \frac{1}{|\mathcal{F}^t|}\int_{\mathcal{F}^t} \boldsymbol{x} \otimes \boldsymbol{x}\, d\boldsymbol{x}\right)[\nabla_\Theta \boldsymbol{n}(\Theta(t))]\Theta'(t)
\end{aligned} \tag{14}$$

Finally, using equation (8), we obtain for any $\Theta'(t)$:

$$\left[[\nabla_\Theta \mathcal{C}(\Theta(t))] - \frac{|\mathcal{F}^t|}{\mathcal{V}^\star}\big(\mathcal{C}_{\mathcal{F}} \otimes \mathcal{C}_{\mathcal{F}} - \mathcal{S}_{\mathcal{F}}\big)[\nabla_\Theta \boldsymbol{n}(\Theta(t))]\right]\Theta'(t) = 0 \tag{15}$$

This is verified if and only if the matrix in factor of $\Theta'(t)$ is the null matrix, which proves equation (5).

2.3. Remarks

We remark that the formula (5) can be separated into a product of two terms. The first one depends only on the geometry of the reconstructed interface $\mathcal{F}$ but not on the parametrization of the normal to the interface. The second one, the gradient of the normal, depends only on the parametrization Θ. This formula is very similar to the formula obtained by Chen & Zhang [7] except it does not require any changes of coordinates, it depends on the parametrization of the normal only in the gradient of the normal, and can be applied to any dimensions. Furthermore, we did not use the fact that the cell is a polyhedron, convex or simply connected. It can be any regular shape smooth enough to use the Stokes' theorem.

3. Applications on 2D polygons, axisymmetric coordinates, and 3D polyhedrons

3.1. In dimension 2 on polygons

In this section, we will simplify the formula (5) to obtain the short formula given by Dyadechko & Shashkov [6]. Consider that the interface is the line segment $[\boldsymbol{p}_1, \boldsymbol{p}_2]$ which is always the case when the cell is convex. The centroid of the interface is given by $\mathcal{C}_{\mathcal{F}} = \frac{\boldsymbol{p}_1+\boldsymbol{p}_2}{2}$. To compute the quantity $\mathcal{S}_{\mathcal{F}}$ we can use the three point Simpson's quadrature which is exact for any polynomial function of degree smaller or equal to 3. For any real function f, the Simpson's formula is given by:

$$\int_{-1}^{1} f(x)\, dx \approx \frac{1}{3}(f(-1) + 4f(0) + f(1)) \tag{16}$$

Applied on $\mathcal{S}_{\mathcal{F}}$, the quadrature rule gives:

$$\begin{aligned}
\mathcal{S}_{\mathcal{F}} &= \frac{1}{|\mathcal{F}|}\frac{|\boldsymbol{p}_2 - \boldsymbol{p}_1|}{2}\frac{1}{3}\left(\boldsymbol{p}_1 \otimes \boldsymbol{p}_1 + 4\frac{\boldsymbol{p}_1+\boldsymbol{p}_2}{2} \otimes \frac{\boldsymbol{p}_1+\boldsymbol{p}_2}{2} + \boldsymbol{p}_2 \otimes \boldsymbol{p}_2\right) \\
&= \frac{1}{6}\big(\boldsymbol{p}_1 \otimes \boldsymbol{p}_1 + \boldsymbol{p}_2 \otimes \boldsymbol{p}_2 + (\boldsymbol{p}_1 + \boldsymbol{p}_2) \otimes (\boldsymbol{p}_1 + \boldsymbol{p}_2)\big)
\end{aligned} \tag{17}$$

Gathering all the terms in equation (5) and simplifying gives:

$$\begin{aligned}\nabla_\Theta \mathcal{C}(\Theta) &= \frac{|\mathcal{F}|}{\mathcal{V}}\left(\frac{\boldsymbol{p}_1+\boldsymbol{p}_2}{2}\otimes\frac{\boldsymbol{p}_1+\boldsymbol{p}_2}{2} - \frac{1}{6}\left(\boldsymbol{p}_1\otimes\boldsymbol{p}_1+\boldsymbol{p}_2\otimes\boldsymbol{p}_2+(\boldsymbol{p}_1+\boldsymbol{p}_2)\otimes(\boldsymbol{p}_1+\boldsymbol{p}_2)\right)\right)\nabla_\Theta\boldsymbol{n}(\Theta)\\ &= -\frac{1}{12}\frac{|\mathcal{F}|}{\mathcal{V}}(\boldsymbol{p}_2-\boldsymbol{p}_1)\otimes(\boldsymbol{p}_2-\boldsymbol{p}_1)\nabla_\Theta\boldsymbol{n}(\Theta)\end{aligned} \tag{18}$$

Finally, use the fact that Θ is the polar angle ϕ, the normal can be expressed as $\boldsymbol{n}(\phi) = [\cos(\phi), \sin(\phi)]$ and its gradient by $\nabla\boldsymbol{n}(\phi) = [-\sin(\phi), \cos(\phi)]$. Denoting $\boldsymbol{t}(\phi)$ the tangent vector of the interface $\boldsymbol{t}(\phi) = \frac{\boldsymbol{p}_2-\boldsymbol{p}_1}{|\mathcal{F}|}$ also equal to $[-\sin(\phi), \cos(\phi)]$ gives the formula:

$$\mathcal{C}'(\phi) = -\frac{1}{12}\frac{|\mathcal{F}|^3}{\mathcal{V}}\boldsymbol{t}(\phi) \tag{19}$$

If the interface is composed of many parts, the Simpson's formula can be used on each line segments.

3.2. *In axisymmetric on polygons*

In axisymmetric coordinates, any point of the space can be written $\boldsymbol{r} = r\boldsymbol{e_r} + z\boldsymbol{e_z}$ where $\boldsymbol{e_r}$ and $\boldsymbol{e_z}$ are the radial and axial unit vectors. As presented by Anbarlooei & Mazaheri [3] the definition of the volume and the centroid must be slightly changed for the MOF problem to be defined:

$$\mathcal{C}(\Theta) = \frac{1}{|\mathcal{R}(\Theta)|}\int_{\mathcal{R}(\Theta)} r\boldsymbol{r}\; drdz \qquad \text{where} \qquad |\mathcal{R}(\Theta)| = \int_{\mathcal{R}(\Theta)} r\; drdz \tag{20}$$

Everything is the same as in the Euclidean plane except there is an extra r in all the integrals. Note that as everything is computed on the plane $(\boldsymbol{e_r}, \boldsymbol{e_z})$, the rotation around the axis is ignored. The proof given in section 2 remains unchanged except there is an extra r in all the integrals. Finally, we obtain the analytical formula (3) where $|\mathcal{F}|$, $\mathcal{C}_\mathcal{F}$, and $\mathcal{S}_\mathcal{F}$ are defined by:

$$|\mathcal{F}| = \int_\mathcal{F} r\; drdz \qquad \mathcal{C}_\mathcal{F} = \frac{1}{|\mathcal{F}|}\int_\mathcal{F} r\boldsymbol{r}\; drdz \qquad \mathcal{S}_\mathcal{F} = \frac{1}{|\mathcal{F}|}\int_\mathcal{F} r\boldsymbol{r}\otimes\boldsymbol{r}\; drdz \tag{21}$$

In these formulas, the integrands are polynomial functions of at most third degree, so we can use the Simpson's rule (16) to exactly evaluate the integrals. However, the formula cannot be simplified as in equation (19).

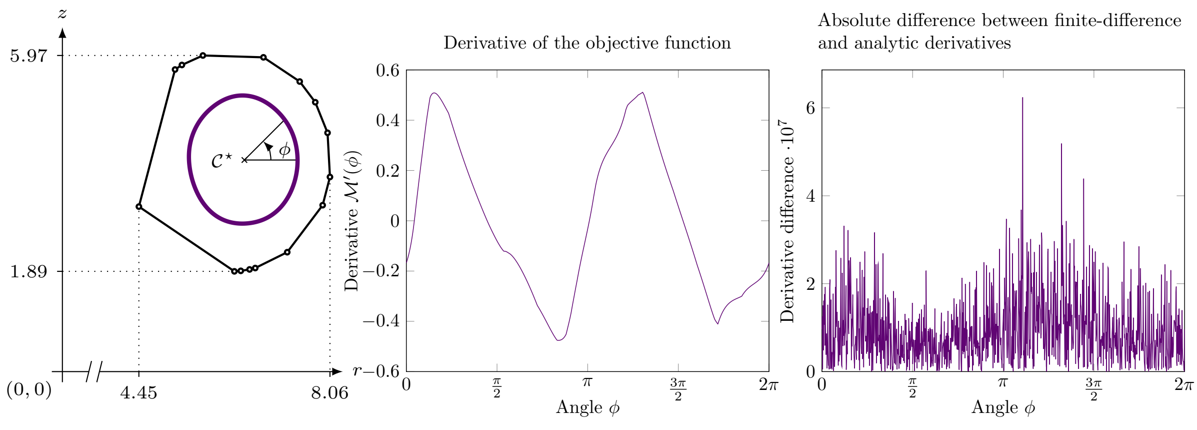

Figure 2: Numerical results on a 15-sided polygon (left) in axisymmetric. Analytic and finite-differences derivatives are almost superimposed (middle). The absolute difference is about 6×10^{-7} (right).

To illustrate equation (3) in axisymmetric coordinates, the formula is applied to a randomly generated 15-sided polygon and the results are compared to those obtained by computing the derivatives with a second order centered finite-differences scheme. On the left of figure 2, the polygon is represented together with the locus of the centroids for a volume fraction of 0.3. The middle of figure 2 represents the derivative of the objective function $\mathcal{M}'(\phi)$ as a function of the angle ϕ. The absolute difference between the derivatives given by the finite-difference scheme and the analytic formula is represented on the right of figure 2. For this test, the maximal value of the difference is about 6×10^{-7}.

3.3. In dimension 3 on polyhedrons

Let $T(\mathcal{F})$ be any triangulation of the interface $\mathcal{F}$. We denote $\boldsymbol{p}$ as the set of three points $\{\boldsymbol{p}_1, \boldsymbol{p}_2, \boldsymbol{p}_3\}$ defining a triangle. The area of the interface can be computed using the formula:

$$|\mathcal{F}| = \frac{1}{2} \sum_{\boldsymbol{p} \in T(\mathcal{F})} \big|(\boldsymbol{p}_2 - \boldsymbol{p}_1) \times (\boldsymbol{p}_3 - \boldsymbol{p}_1)\big| \tag{22}$$

where $\times$ denotes the cross product. The centroid of the interface can be computed by:

$$\mathcal{C}_{\mathcal{F}} = \frac{1}{6\mathcal{V}} \sum_{\boldsymbol{p} \in T(\mathcal{F})} \big|(\boldsymbol{p}_2 - \boldsymbol{p}_1) \times (\boldsymbol{p}_3 - \boldsymbol{p}_1)\big| \big(\boldsymbol{p}_1 + \boldsymbol{p}_2 + \boldsymbol{p}_3\big) \tag{23}$$

The 3-point Gauss quadrature formula on a triangle $\mathcal{T}$ for $f \colon \mathbb{R}^3 \to \mathbb{R}$ is given by:

$$\int_{\mathcal{T}} f(\boldsymbol{x})\, d\boldsymbol{x} \approx \frac{1}{6}\big|(\boldsymbol{p}_2 - \boldsymbol{p}_1) \times (\boldsymbol{p}_3 - \boldsymbol{p}_1)\big| \left(f\left(\frac{\boldsymbol{p}_1 + \boldsymbol{p}_2}{2}\right) + f\left(\frac{\boldsymbol{p}_2 + \boldsymbol{p}_3}{2}\right) + f\left(\frac{\boldsymbol{p}_3 + \boldsymbol{p}_1}{2}\right) \right) \tag{24}$$

To compute the matrix $\mathcal{S}_{\mathcal{F}}$, apply the previous formula for $\boldsymbol{x} \otimes \boldsymbol{x}$ on any triangle of the interface:

$$\mathcal{S}_{\mathcal{F}} = \frac{1}{|\mathcal{F}|} \sum_{\mathcal{T} \in T(\mathcal{F})} \int_{\mathcal{T}} \boldsymbol{x} \otimes \boldsymbol{x}\, d\boldsymbol{x} \tag{25}$$

Note that the interface is not required to be simply connected which may happen on non-convex polyhedrons.

4. Conclusion

In this short note, we give a short and simple proof of a general analytic formula to evaluate the gradient of the objective function of the MOF problem in any dimension. Few hypotheses are required on the geometry of the cell meaning that it can be applied on non-convex polyhedrons. Furthermore, the formula does not depend on the parametrization of the normal to the interface. We provide a practical way to use the formula on polygons in 2D and axisymmetric coordinates, and on 3D polyhedrons.

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