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Journal Pre-proof

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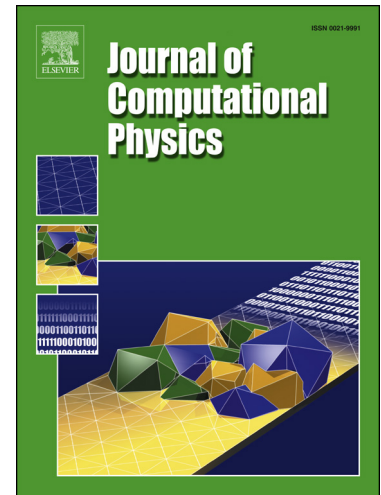
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Highlights

- Adaptive mesh refinement is implemented with the filament moment-of-fluid method.
- Mass conservative algorithms are proposed for MOF at different adaptive level.
- Centroid error is used as the mesh refinement criterion.
- High accuracy validated with benchmarks using symmetric filament reconstruction.
- Unrestricted CFL using Lagrangian backtracking for AMR.

Journal Pre-proof

1 A quadtree-based adaptive moment-of-fluid method for
2 interface reconstruction with filaments

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4 **Abstract**

5 Implementation of quadtree adaptive mesh refinement (AMR) to the
6 moment-of-fluid (MOF) method is presented in the context of an interface
7 capturing method. Filaments, thinner than a cell size, are resolved using a
8 computationally efficient technique on an unconstrained quadtree structure.
9 The centroid defect relative to its cell size is used as the refinement criterion,
10 together with an enhanced refinement calculation and subsequently its vol-
11 ume conservation. In addition, different approaches are proposed to ensure
12 mass conservation during the computation. This MOF-AMR framework is
13 validated for a range of benchmark problems which are studied widely in
14 the literature. There is no restriction on the choice of CFL number for the
15 purely Lagrangian advection method considered here and this has advantages
16 when combined with AMR. The current quadtree MOF-AMR method leads
17 to much improved computational efficiency and accuracy relative to its grid
18 size compared with a uniform grid. Higher levels of refinement can be costly,
19 therefore the efficiency of mesh resolution is further discussed in relation to
20 the choice of time step and number of AMR levels.

21 *Keywords:*

22 multiphase flow, MOF method, filament capturing, interface reconstruction,
23 adaptive mesh refinement, quadtree

24 *PACS:* 0000, 1111

25 *2000 MSC:* 0000, 1111

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26 1. Introduction

27 Multiphase flow modelling has been widely used in many engineering ap-
28 plications. Whilst it is important, representing the interface between two or
29 more materials to provide accurate prediction of complex topological struc-
30 tures is technically challenging. For simulation of natural flow processes or
31 industrial applications such as wave breaking, droplet behaviour or bubble
32 dynamics, highly deformable materials are of interest, which often involved
33 curved interfaces due to surface tension. Accurate prediction of these evol-
34 ving interfaces requires considerable computational resources.

35 To effectively improve models' computational efficiency, adaptive mesh
36 methods have been applied in many complex and large-scale engineering
37 modelling applications, including fluid dynamics, climate modelling and solid
38 structure analysis. Examples include adaptive unstructured mesh [1, 2],
39 adaptive polynomial degree [3] and adaptive mesh refinement [4, 5, 6, 7, 8,
40 9, 10, 11] methods. The purpose of adaptive mesh methods is to adjust dy-
41 namically the resolution of a grid in regions of interest or rapid change whilst
42 maintaining coarse grid resolution in the regions where the solution "stag-
43 nates". Grid adaptation is triggered using a specified refinement criterion.
44 Through "optimising" the number of grid cells used in the computation, such
45 a grid adaptation strategy may effectively enhance computational efficiency
46 while maintaining overall solution accuracy [9].

47 Methods for predicting the behaviour of fluids with complex interfaces
48 include marker-and-cell method [12], front tracking method [13], level-set
49 method [14, 15], volume-of-fluid (VOF) method [16, 17], and some meshless
50 methods such as the smooth particles hydrodynamics (SPH) [18]. Some
51 numerical techniques might be easier to implement than others, some might
52 have better mass conservation property, and some might resolve complex
53 interfaces in a superior way. Overall, all these techniques have been adopted
54 widely in the literature for interface calculation.

55 The moment-of-fluid (MOF) method belongs to the class of methods
56 known as interface capturing techniques and has been used to capture the
57 interface between two materials [19]. It can be considered as an extension
58 of the VOF method, in which the volume fraction as well as the centroid
59 are advected to reconstruct an interface within a cell independent of neigh-
60 bouring cells [19, 20, 21]. Recently, the standard MOF method [19] has been
61 improved using symmetric reconstruction [22] and its capability has been
62 extended to multi-materials [23, 24] which has enabled filaments and thin

63 structures to be reconstructed [25, 26].

64 Several techniques have been used over the years to capture interfaces
65 in the context of adaptive mesh refinement (AMR) [4]. These may be
66 broadly categorised as either patch-based AMR or quadtree(octree)-based
67 AMR. Patch-based AMR involves dividing the computational domain into
68 a set of refinement patches. This allows for local control over the mesh
69 resolution, and the patches can be refined or coarsened dynamically based
70 on the numerical solution being computed. The main advantage of patch-
71 based AMR is its flexibility. However, it can lead to increased complexity
72 in the maintenance of the grid being created [27]. On the other hand, a
73 quadtree(octree)-based AMR uses a tree-based hierarchical data structure.
74 The computational domain is recursively divided into four subcells (in 2D),
75 or eight for octree (in 3D) when the refinement criteria are met. This ap-
76 proach has the advantage of being computationally efficient and easier to
77 implement due to having a well-defined data structure [9]. This method is
78 typically implemented on Cartesian grids, and also used to support some
79 finite element simulations on tetrahedral meshes [28] and particle methods
80 [29].

81 In the past, AMR has been adopted to simulate interfacial flows using
82 volume-of-fluid [7, 10] and level-set [5, 11] methods. Local grid refinement has
83 been confirmed to be effective in reducing the computational cost compared
84 to refining the entire grid [30, 31, 32]. Furthermore, unphysical material
85 break-up might be avoided through local refinement techniques. The refine-
86 ment criterion is typically based on the volume fraction or level set function
87 in a cell. But the estimated curvature [33] and interface gradient have also
88 been used as refinement criteria.

89 Despite the potential gain in efficiency, using adaptive mesh refinement
90 in the context of MOF has not been sufficiently explored. Undoubtedly, the
91 associated complexity and natural computational cost of the MOF method
92 itself is the reason why AMR has been limited in this context. In MOF
93 situations, where zeroth and first moments are computed for interface recon-
94 struction, the latter is used as a refinement criterion. Indeed, the centroid
95 approximation is an estimate of the quality of the interface reconstruction.
96 This adaptive mesh refinement method combined with the original MOF
97 method was first developed in 2009 by Ahn & Shashkov [34]. This involved
98 the use of an unconstrained quadtree structure with up to five levels of re-
99 finement. In addition, the refinement criterion was set to be unique for all
100 levels and to a value smaller than machine precision. Later, Jemison et al.

101 [25] proposed for the first time a filament MOF approach in a patch-based
 102 AMR framework. In the advection process, their approach reached up to
 103 two levels of refinement and their criterion included a tolerance taking into
 104 account the relative subcell size. Recently, a standard MOF-AMR using a
 105 patch-based grid has been used in the flow simulation of droplets [35]. How-
 106 ever, no attempt has been reported to combine the quadtree-based AMR and
 107 filament MOF approaches to explore their advantages in improving model
 108 performance.

109 The main objective of this paper is to develop a novel MOF method that
 110 can reconstruct under-resolved structures, mainly filaments, at any level of
 111 refinement in a quadtree-based AMR structure using a newly developed effi-
 112 cient symmetric MOF scheme [26]. Using a Lagrangian pre-image, materials
 113 are advected at a base level and then refined locally to allow for a CFL num-
 114 ber much larger than unity. Therefore, the coarsening procedure becomes
 115 irrelevant. Fig. 1 highlights the key steps in the AMR reconstruction. In
 116 addition, a novel treatment within the MOF environment is also proposed to
 117 ensure the mass conservation property is satisfied to machine accuracy using
 118 a uniform redistribution procedure [36].

119 This paper is organised as follows. Section 2 describes the standard MOF
 120 method including how filaments are reconstructed within a cell on a fixed
 121 grid. Then, the adaptive mesh refinement structure and its advection pro-
 122 cedure are presented in Section 3. Section 4 gives an insight into several
 123 volume redistribution techniques designed to conserve volume exactly in dy-
 124 namic cases. In Section 5, results and analysis of several benchmark problems
 125 are presented. Finally, the efficiency and accuracy of the AMR is discussed
 126 in Section 6 and compared to a uniform grid approach. Some concluding
 127 remarks are included in Section 7.

128 2. MOF method

129 2.1. Interface reconstruction

130 Reconstructing a standard interface of a desired material using the MOF
 131 method requires the computation of the zeroth and first moments, M_0 and
 132 \mathbf{M}_1 , respectively, within a convex cell Ω . These quantities are given by the
 133 following expressions :

$$M_0 = \int_{\Omega} dV = \frac{1}{2} \sum_{i=1}^n (x_{i-1}y_i - x_iy_{i-1}) \quad (1)$$

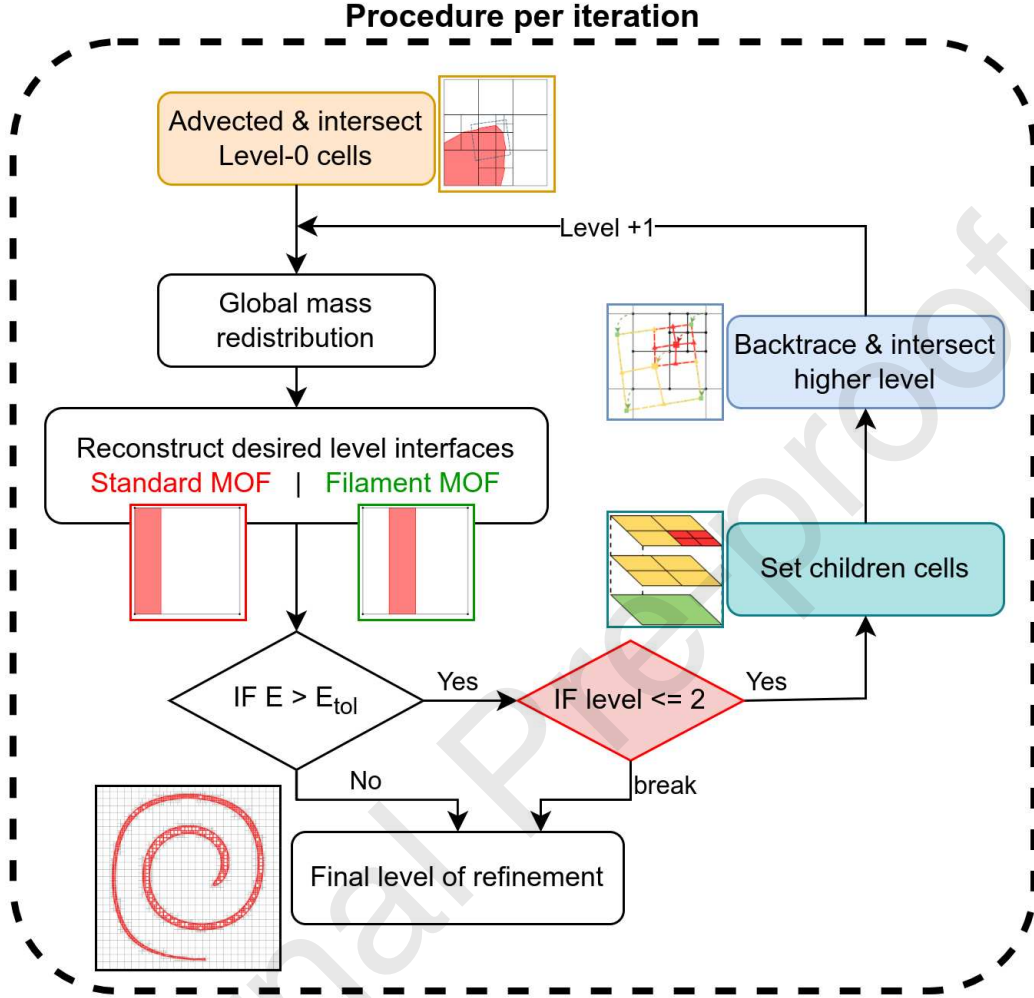


Figure 1: Flowchart highlighting the key steps to MOF-AMR reconstruction.

$$\mathbf{M}_1 = \int_{\Omega} \mathbf{x} dV = \begin{bmatrix} \frac{1}{6} \sum_{i=1}^n (x_{i-1} + x_i) (x_{i-1}y_i - x_iy_{i-1}) \\ \frac{1}{6} \sum_{i=1}^n (y_{i-1} + y_i) (x_{i-1}y_i - x_iy_{i-1}) \end{bmatrix} \quad (2)$$

134 where (x_i, y_i) , $i = 1, \dots, n$, are the co-ordinates of the vertices of a poly-
 135 gonal cell. Note that the reference volume fraction F_{ref} corresponds to the
 136 zeroth moment relative to the convex cell area and the reference centroid

137 \mathbf{x}_{ref} corresponds to the first moment relative to its zeroth moment.

138 In order to reconstruct a piece-wise linear interface in the context of the
 139 MOF method, the distance between the reference and reconstructed centroids
 140 is minimised while preserving the value of the zeroth moment. Eq. (3)
 141 describes the objective function $E_c(\mathbf{n})$ to be minimised, where \mathbf{n} defines the
 142 unit outward normal to the interface. A minimisation algorithm is needed
 143 for non-rectangular cells, and a novel bisection method is used herein [26].
 144 For rectangular cells, in particular Cartesian cells, an analytical solution is
 145 available, which eliminates the need to use a minimisation algorithm.

$$E_c(\mathbf{n}) = |\mathbf{x}_{ref} - \mathbf{x}_{act}| \quad (3)$$

146 where \mathbf{x}_{act} refers to the reconstructed centroid.

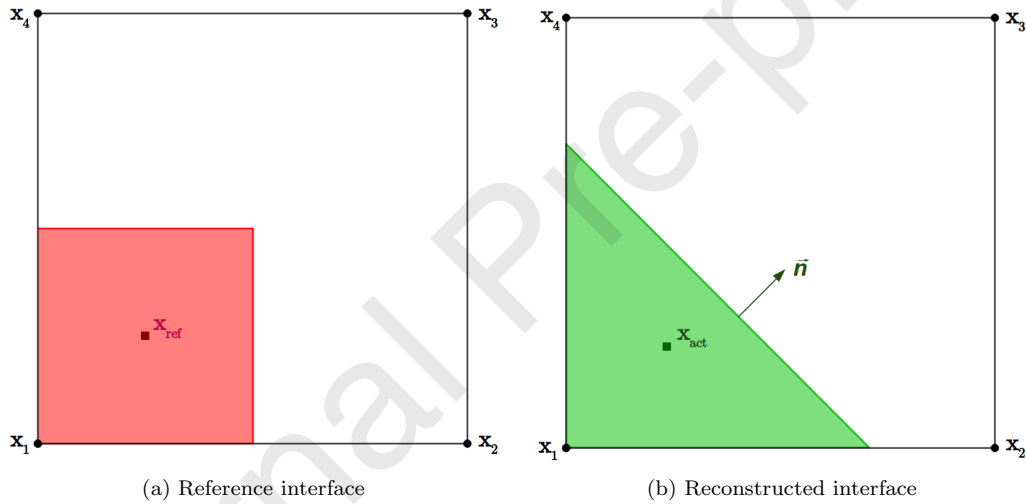


Figure 2: Reference vs. reconstructed interface using a standard MOF approach. $\mathbf{x}_1, \dots, \mathbf{x}_4$ represent the cell vertices. $\hat{\mathbf{n}}$ denotes the outward normal of the reconstructed interface.

147 2.2. Filament reconstruction

148 Filaments are thin structures created during material deformation. Since
 149 they are usually smaller than a cell size, some special treatment has been
 150 developed [37, 38]. It is worth noting that a standard MOF approach can-
 151 not resolve their exact topology. When considering filaments, two interfaces
 152 appear within a cell, one on each side of the thin structure, which means
 153 that two reconstructions are needed to capture the topology accurately. In

154 this approach, the thin structure needs to be detected before it can be re-
 155 constructed, creating the need of an extra step in the MOF reconstruction
 156 procedure. This extra step involves the use of the conglomeration algorithm
 157 detailed in Hergibo et al. [26]. This conglomeration algorithm detects the
 158 number of groups, i.e. conglomerates, that are present in a cell by collect-
 159 ing all sub-polygons adjacent to each other. A multi-material reconstruction
 160 procedure is needed when filaments are involved. Therein, a symmetric
 161 reconstruction is used in the paper, which minimises both conglomerates
 162 considered. This reduces the number of combinations and is therefore computationally
 163 more efficient. Eq. (4) refers to the objective function E_c^{sym} in
 164 a symmetric reconstruction process:

$$E_c^{sym}(\mathbf{n}) = |\mathbf{x}_{ref} - \mathbf{x}_{act}| + |\mathbf{x}_{ref}^{rem} - \mathbf{x}_{act}^{rem}| \quad (4)$$

165 where the superscript *rem* denotes the remaining conglomerates in a cell.

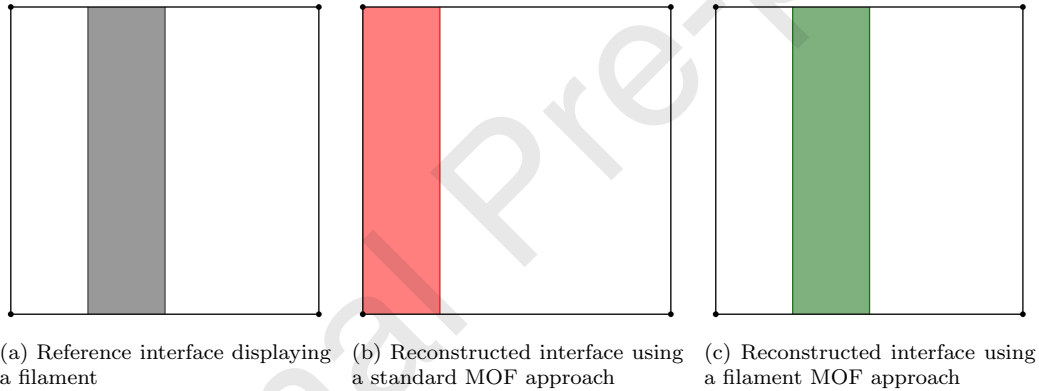


Figure 3: Schematic diagrams showing the different MOF reconstruction approaches. Filament MOF has the potential to offer exact reconstruction.

166 Note that the number of conglomerates is capped at three for the sake of
 167 computational efficiency. A sequential reconstruction is needed to minimise
 168 the centroid error regardless of the reconstruction of the other conglomerates
 169 considered [22]. By definition, all the possible combinations of material are
 170 tested to find the reconstruction that minimises all centroids present in a
 171 cell. The total centroid defect E can be calculated using:

$$E = \sqrt{\sum_i^n |\mathbf{x}_{ref}(\mu_i) - \mathbf{x}_{act}(\mu_i)|^2} \quad (5)$$

172 where μ_i characterises each material in a cell. In filament reconstructions, μ_i
 173 refers to each conglomerates until the fictitious material is assigned.

174 *2.3. Advection on a uniform mesh*

175 Advection of a material defines the process of its dynamic evolution
 176 through translation, rotation, and deformation. These are of particular in-
 177 terest when evaluating the precision of an interface tracking/capturing tech-
 178 nique/method. This paper uses a purely Lagrangian approach as opposed
 179 to a mixed Eulerian-Lagrangian approach [21, 26]. The benefits of using a
 180 Lagrangian approach include a less restrictive choice of Courant-Friedrichs-
 181 Lewys (CFL) number and an unsplit advection approach in which a La-
 182 grangian pre-image is used to capture the volume fraction and centroid of a
 183 material at the previous time step.

184 The vertices of a cell are advected backwards in time using a second order
 185 Runge-Kutta scheme (RK2) before determining its intersection with the pre-
 186 image. Advection forwards is then performed for centroids and reconstruction
 187 using the relevant volume fraction. The key steps of the advection procedure
 188 are summarised as follows:

- 189 (i) Backtrace any cells that may contain the desired material using RK2.
- 190 (ii) Intersect the backtrace cell with any material encountered to evaluate
 191 the reference volume fractions.
- 192 (iii) Advect individual centroids and compute their weighted average to ob-
 193 tain the reference centroid.
- 194 (iv) Reconstruct using one of the following techniques.
 - 195 (a) Standard MOF using a piecewise linear interface between two ma-
 196 terials.
 - 197 (b) Filament MOF using conglomeration algorithm to reconstruct a
 198 filament.

199 Despite showing a refined grid, Fig. 5 demonstrates visually the steps for
 200 MOF advection and is valid for a uniform grid.

201 **3. Adaptive mesh refinement**

202 The main motivation for using AMR is to balance the trade-off between
 203 solution accuracy and computational cost. High deformation regions are of

204 interest for AMR in order to produce high-resolution prediction in these com-
 205 plex areas. The process of mesh refinement must be informed by an appro-
 206 priate criterion and the reconstruction error is used to inform grid adaptation
 207 in the current MOF method [34]. Typically, the refinement process involves
 208 splitting each cell into 4 subcells in 2D, and 8 subcells in 3D; coarsening
 209 involves merging subcells into a larger (sub)cell when the specific condition
 210 is met. Generally, the refinement and coarsening processes are repeated un-
 211 til either a desired accuracy is achieved or a certain level of refinement is
 212 reached.

213 3.1. Data structure

214 This work adopts the quadtree-based AMR and the data structure is
 215 designed to store and manipulate the hierarchy of meshes with ease and effi-
 216 ciency, as well as allowing communication between levels [9]. The quad-tree
 217 data structure forms a tree where the root node represents the coarsest mesh
 218 (base mesh), and each additional level of refinement creates four children
 219 nodes to their parent node. This work introduces a simplified approach in
 220 which the data structure replicates a quad-tree algorithm up to two levels
 221 of refinement such that children cells can be accessed from a parent cell at
 222 every level up to two. The other advantage is that no subroutines are needed
 223 to find or access neighbours. In addition, unlike many other AMR codes, the
 224 new approach does not constrain the refinement level of neighbouring cells
 225 or subcells.

226 An arbitrary cell on the quad-tree mesh generated using the new approach
 227 is indexed as (i, j, is, js) where (i, j) represents the base mesh indices and
 228 $is = 1, \dots, Ms$ and $js = 1, \dots, Ms$ are the subcells indices, with $Ms = 2^{lev}$
 229 and lev denoting the level of refinement starting at 0 for the base mesh.
 230 Subsequently, the size of the new subcells is defined by $dx(lev) = \Delta x / 2^{lev}$ and
 231 $dy(lev) = \Delta y / 2^{lev}$ with lev being 0, 1 or 2. Naturally, at Level-0, $dx(0) = \Delta x$.
 232 In addition, the cell-centre coordinates can be directly decided through the
 233 following relationships $x_c = x(i) + (is - 1) \cdot dx(lev)$ in the x -direction and
 234 $y_c = y(j) + (js - 1) \cdot dy(lev)$ in the y -direction. The cell area $|\Omega|(lev)$ is
 235 then defined by $|\Omega|(lev) = dx(lev)dy(lev)$, and for uniform mesh, the cell
 236 area is simply defined as $|\Omega|$. Accessing children cells uses the logic from a
 237 parent cell's index parity is . Children subcells indices can be called using
 238 $(2is, 2is - 1)$ when the parent index is is even, and $(is, is + 1)$ when is is odd.
 239 This logic is valid up to level 2 and works in both horizontal and vertical
 240 directions. The data structure and index system are highlighted in Fig. 4.

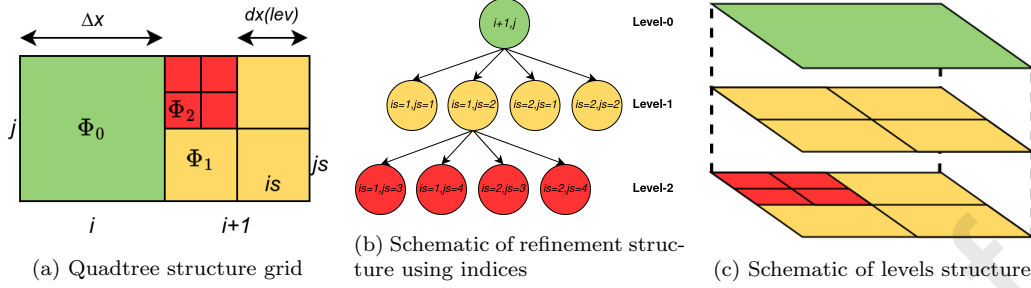


Figure 4: General idea of data structure used in an AMR framework

241 In order to allow for the manipulation of variables, an additional index
 242 representing the level of refinement is used in the data structure. Because
 243 the data structure may contain several variables accounting for volume frac-
 244 tion, centroid or polygon representation at different levels of refinement, a
 245 specific variable is used in the code for identifying which level of refinement
 246 is reached. The logical variable $last_lev_refinement(i, j, is, js, lev)$ allows to enable
 247 or disable any values of unused level of refinement. A true value means that
 248 subcell i, j, is, js at level lev is the last refinement and contains a valid vol-
 249 ume fraction to be intersected. A false value shows that the subcell i, j, is, js
 250 at level lev is not the last level of refinement and values are ignored. In
 251 general, when a higher level of refinement is triggered, the logical value of
 252 $last_lev_refinement$ of the corresponding parent subcell at a lower level is set to
 253 false. The value of this logical variable is set to true for all children subcells.
 254 Mathematically, the set Φ_{lev} , including subsets Φ_0 , Φ_1 and Φ_2 , respectively,
 255 represents all cells at their finest refinement i.e. $\Phi_{lev} = \Phi_0 \cup \Phi_1 \cup \Phi_2$ with
 256 $\Phi_i \cap \Phi_j = \emptyset$ for $i \neq j$. This means, with reference to the color scheme of Fig.
 257 4, Φ_0 corresponds to green cells, Φ_1 to yellow subcells and Φ_2 to red subcells.
 258 Algorithm 1 details how to loop and access any variables in our code.

259 3.2. Refinement criterion

260 In the previous VOF methods or level set methods, refinement was trig-
 261 gered when the volume fraction is in a certain range or when the estimated
 262 curvature gradient reaches a certain value. In the adopted MOF method, the
 263 centroid error is used as the criterion for refinement. Indeed, when a standard
 264 MOF or a filament MOF procedure is used in a cell, reconstruction error is
 265 a good indicator of how accurate the reconstruction is. Eq. (5) includes ma-
 266 terial centroid error and fictitious material in a filament case. In this paper,

Algorithm 1 AMR data structure

```

for lev = 0,2 do
  for i = 1, N_cell_x do
    for j = 1, N_cell_y do
      Ms = 2lev; dx(lev) = Δx/2lev; dy(lev) = Δy/2lev
      for is = 1, Ms do
        for js = 1, Ms do
          % EXAMPLE : accessing the volume fraction of a subcell
          volume_fraction(i,j,is,js,lev)
          % EXAMPLE : checking the last level of refinement of a subcell
          last_lev_refinement(i,j,is,js,lev) ← true
        end for
      end for
    end for
  end for
end for

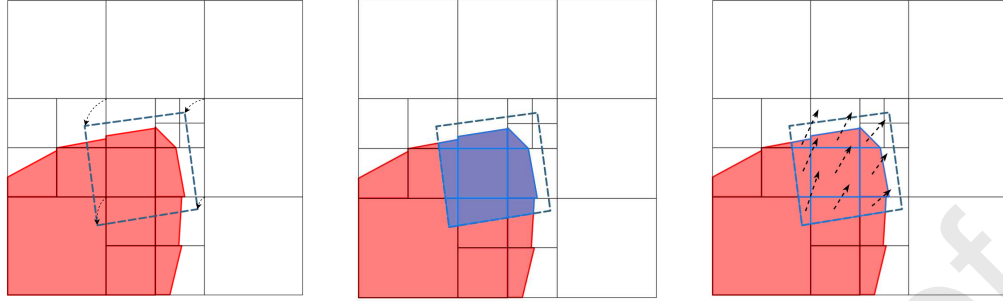
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267 the refinement criterion is dependent on the cell size, here $10^{-9}dx(lev)$, finer
 268 than [25] and not set to a fixed tolerance, which is different from the previous
 269 MOF-AMR schemes [34].

270 3.3. Advection procedure on a refined mesh

271 Similar to advection on a uniform mesh, the advection on a refined mesh
 272 entails the use of a Lagrangian pre-image. This requires intersecting the
 273 material at the previous time step without omitting the different levels of
 274 refinement. All levels of refinement needs to be intersected. As per the
 275 uniform approach, the backtrace cell is advected backwards using RK2, and
 276 the area intersected in this pre-image relative to the subcell area corresponds
 277 to the volume fraction of the refined subcell. Eventually, the centroids of all
 278 polygons intersected forming the volume fraction are advected forward using
 279 the same scheme and the weighted average will define the new reference
 280 centroid. The respective reference volume fraction and centroid are used for
 281 reconstruction.

282 Our approach differs from other general MOF-AMR schemes since here
 283 filament MOF is enabled. The ability to capture filaments has significant
 284 advantages over a standard MOF method and has been shown to generate
 285 high accuracy on a uniform mesh [26]. For the sake of capturing filaments, the



(a) Lagrangian backtracking pre-image (b) Intersection between backtrace and material at all levels (c) Forward advection of individual centroids

Figure 5: Schematic showing advection of moments in an AMR framework

286 base mesh is used as the backtracking level, meaning that Level-0 is advected
 287 first at all time. To determine which cells need advecting, neighbouring
 288 volume fractions are used at Level-0 to evaluate its potential of being an
 289 interface, similar to a uniform advection.

290 In the case of a cell being refined, the backtrace at a defined level of
 291 refinement is performed as follows. The central point common to all child
 292 subcells is advected using the usual RK2 subroutine. All other vertices are in-
 293 terpolated from the backtrace at Level-0. This will guarantee exact material
 294 intersection with the level of refinement below, hence exact mass conserva-
 295 tion. This is performed in a similar fashion for Level-2.

- 296 (i) Backtrace the four vertices from a Level-0 cell using RK2.
- 297 (ii) Advect the common node using RK2.
- 298 (iii) Interpolate the four mid-points from the Level-0 backtrace cell
- 299 (iv) Create four new subcells

300 Fig. 6 shows the procedure in place for backtracking a subcell in this
 301 refinement framework. This ensures the intersection with a refined backtrace
 302 cell with the interface. This approach differs from the one introduced by
 303 [34] where a simplified backtracking approach is used. As stated above, our
 304 approach does not create gaps and overlaps, and therefore a simpler mass
 305 redistribution procedure can be implemented.

306 3.4. Time-step on a refined mesh

307 In numerical simulations, the typical time step is determined according
 308 to the CFL condition. In this paper, the CFL number is chosen to be unity

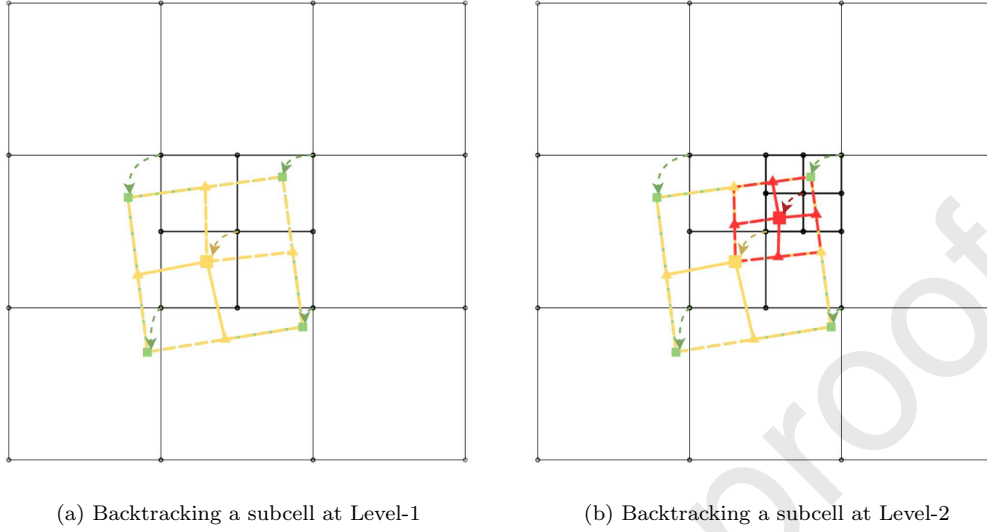


Figure 6: Schematic showing backtracking of moments in an AMR framework. (\square) symbols refer to vertices advected using RK2. (\triangle) symbols refer to mid-point vertices being interpolated. Color scheme shows green vertices for Level-0; Yellow vertices and dashed lines for Level-1 vertices and subcells; Level-2 vertices and subcells are in red.

309 unless stated otherwise. The Lagrangian approach enables an unrestricted
 310 choice of the CFL number [26]. Specifically, the time step is chosen with
 311 respect to the base mesh. When refining a mesh locally, the time step used
 312 at a refined cell is the same as the one adopted at the base mesh, and so the
 313 CFL number is 2 for Level-1 and 4 for Level-2 cells. Alternative time step
 314 strategies such as adaptive time stepping can be employed, but for simplicity
 315 these were not adopted here as no instability issues were encountered using
 316 the present approach.

317 4. Mass conservation during advection

318 4.1. Uniform global mass redistribution

319 Mass conservation is difficult to enforce in a grid refinement procedure.
 320 Local redistribution in a refinement step can lead to a large deformation of
 321 the interface, hence global redistribution is used in this paper. When using a
 322 global redistribution approach, over/under-filled cells are considered. These
 323 cells are formed by only one material, however their area intersected lead to a
 324 volume fraction being either less or greater than unity. These cells have their

325 volume fraction set to unity and the difference to unity multiplied by the cell
 326 area $|\Omega| (lev)$ is added to a global variable. Let us call the global redistribu-
 327 tion variable δ . On a uniform approach, δ is redistributed to N mixed cells,
 328 i.e. cells with an interface. In fact, the $\delta/(|\Omega| N)$ amount is redistributed to
 329 mixed cells. In the case that not all of the mass is redistributed, an iterative
 330 procedure is enacted to ensure all mass is redistributed. Indeed, lack of mass
 331 redistribution can penalise mass conservation at other levels.

332 At other levels of refinement, over/under-filled cells may also occur in
 333 the intersection process, meaning that mass needs to be redistributed at
 334 all levels. However, on a refined mesh, mass has been redistributed at a
 335 lower level with cells needing refinement. Therefore, another local variable
 336 “*distributed*” is considered in the redistribution process corresponding to the
 337 mass redistributed in each cell/subcell at a lower level. It allows to keep
 338 track of redistribution to cells that may trigger refinement, with the sum of
 339 them all being δ_{low_lev} . Indeed, mass may be redistributed to cells that will
 340 be refined, hence that amount needs to be shared to the next refinement
 341 level. All cells needing refinement have their mass redistributed at a lower
 342 level added to the δ of the refinement level. Then, the new amount of mass
 343 redistributed is $\delta + \delta_{low_lev}$. Therefore, for each cell, the new volume fraction
 344 F_i is calculated using

$$F_i \leftarrow F_i + \frac{(\delta + \delta_{low_lev})}{|\Omega| (lev) N_{mix}} \quad (6)$$

345 where N_{mix} corresponds to the number of mixed cells in the domain at a
 346 certain level. The following subroutine gives more insight into the redistribu-
 347 tion procedure 2. In this subroutine, the amount of mass that is not repaired
 348 “*not_repaired*” is taken into account because some “almost” full/empty cells
 349 may not be able to receive/give their contribution. In these instances, the
 350 redistribution subroutine is repeated until the amount of mass is close to
 351 machine precision. The amount redistributed is kept in the variable “*dis-*
 352 *tributed*”.

353 Several approaches can be used when redistributing the mass globally.
 354 Two of them are presented in this section, these are termed the directly
 355 proportional and inversely proportional distribution approaches.

356 4.2. Directly proportional global mass redistribution

357 Amongst redistribution procedures, the directly proportional redistribu-
 358 tion seems intuitive. The redistribution occurs in a similar fashion as the

Algorithm 2 Redistribution in a refined mesh

```

Initialise  $\delta, \delta_{low\_lev}$ 
 $repair \leftarrow \delta + \delta_{low\_lev}$ 
 $not\_repaired \leftarrow repair$ 
%Note :  $\delta_{low\_lev} = 0$  at Level-0
while ( $not\_repaired > 10^{-13}$ ) do
  if ( $mixed\_cell \leftarrow \mathbf{true} \text{ .AND. } repair < 0$ ) then
    %REPAIR IS NEGATIVE - REMOVE VOLUME FRACTION
    if ( $volfrac(i, j, is, js, lev) + repair / (|\Omega| (lev)N\_mix) < 0$ ) then
      %CELL VOLUME FRACTION CANNOT BE NEGATIVE - RESET TO 0
       $not\_repaired = not\_repaired + volfrac(i, j, is, js, lev) *$ 
 $(|\Omega| (lev)N\_mix)$ 
    else
       $volfrac(i, j, is, js, lev) = volfrac(i, j, is, js, lev) +$ 
 $repair / (|\Omega| (lev)N\_mix)$ 
       $distributed(i, j, is, js, lev) = distributed(i, j, is, js, lev) +$ 
 $repair / N\_mix$ 
       $not\_repaired = not\_repaired - repair / N\_mix$ 
    end if
  else if ( $mixed\_cell \leftarrow \mathbf{true} \text{ .AND. } repair > 0$ ) then
    %REPAIR IS POSITIVE - ADD VOLUME FRACTION
    if ( $volfrac(i, j, is, js, lev) + repair / (|\Omega| (lev)N\_mix) > 1$ ) then
      %CELL VOLUME FRACTION CANNOT MORE THAN UNITY - RESET TO 1
       $not\_repaired = not\_repaired + (1 - volfrac(i, j, is, js, lev)) *$ 
 $(|\Omega| (lev)N\_mix)$ 
    else
       $volfrac(i, j, is, js, lev) = volfrac(i, j, is, js, lev) +$ 
 $repair / (|\Omega| (lev)N\_mix)$ 
       $distributed(i, j, is, js, lev) = distributed(i, j, is, js, lev) +$ 
 $repair / N\_mix$ 
       $not\_repaired = not\_repaired - repair / N\_mix$ 
    end if
  end if
end while
% WHEN REDISTRIBUTION IS TRIGGERED AT NEW REFINEMENT LEVEL
 $\delta_{low\_lev} = \sum distributed(i, j, is, js, lev)$  if( $last\_lev\_refinement(i, j, is, js, lev) ==$ 
false)

```

359 uniform case. However, the mass is redistributed proportional to the volume
 360 fraction in a cell. Hence, the total volume fraction of all mixed cells is calcu-
 361 lated. The repair is then performed using the redistribution process in which
 362 the new volume fraction is given by

$$F_i \leftarrow F_i + \frac{(\delta + \delta_{low_lev})}{|\Omega|(lev)} \frac{F_i}{\sum_{i=1}^{N_{mix}} F_i} \quad (7)$$

363 This approach may alter the shape of the interface to a lesser extent.

364 4.3. Inversely proportional global mass redistribution

365 Opposite to the previous concept, mass is redistributed inversely pro-
 366 portional to its volume fraction in this approach. Conceptually, a propor-
 367 tional approach may lead to several iterations of redistribution because a
 368 large mass is redistributed to an “almost” full/empty cell, and therefore the
 369 mass that is not repaired may be large. By using the inversely proportional
 370 approach, more mass is redistributed to those almost empty cells which in-
 371 tuitively would reduce the number of redistribution iterations, but may alter
 372 the shape of the interface more. The repair would be redistributed as follows

$$F_i \leftarrow F_i + \frac{(\delta + \delta_{low_lev})}{|\Omega|(lev)} \frac{(1 - F_i)}{\sum_{i=1}^{N_{mix}} (1 - F_i)} \quad (8)$$

373 5. Results

374 5.1. Error evaluation

375 Computing errors play an important part of interface capturing methods
 376 as it is the primary indicator of the relevance of a method. Comparing errors
 377 enables one to evaluate the merits of different methods. The L_1 error norm
 378 E_{L_1} , which is based on a volume fraction approach, is one of these numerical
 379 indicators. On a refined grid, the L_1 error is evaluated on the base mesh,
 380 which means that refined subcells are grouped together to form a single
 381 volume fraction on the base mesh. Using the data structure described in
 382 Section. 3, the error can be evaluated using

$$E_{L_1} = \sum_{i,j} |(F_{final}(i,j) - (F_{initial}(i,j)))| |\Omega|(0) \quad (9)$$

383 where $|\Omega|(0)$ represents the cell area at Level-0, $F_{final}(i,j)$ and $F_{initial}(i,j)$
 384 are calculated in similar fashion :

$$F_{final}(i, j) = \sum_{lev} \sum_{is, js \in \{\Phi_{lev}\}} \frac{F(i, j, is, js, lev) |\Omega| (lev)}{|\Omega| (0)} \quad (10)$$

385 where F represents the volume fraction in a subcell and Φ_{lev} corresponds
 386 to the set including subsets Φ_0 , Φ_1 and Φ_2 , respectively. If a cell contains
 387 subcells at level 1 and level 2, then Eq. (10) aims at summing up their
 388 volume fraction with respect to their subcell grid size. If a cell has not been
 389 refined, then level 0 remains and $F_{final}(i, j)$ is the volume fraction at level 0.
 390 The relative error norm E_r is given by

$$E_r = \frac{E_{L_1}}{\sum_{i,j} |(F_{initial}(i, j))| |\Omega| (0)} \quad (11)$$

391 The symmetric error is another indicator of the error in reconstruction.
 392 This error indicator provides an estimation of the discrepancy in the area
 393 between the initial and final states. The symmetric error E_{sym} is similarly
 394 given by

$$E_{sym} = \sum |\omega^{ref} \cup \omega^{act} - \omega^{ref} \cap \omega^{act}| \quad (12)$$

395 where ω^{ref} denotes the initial state reference interface, which is potentially
 396 curved, and ω^{act} denotes the final state reconstructed polygon.

397 Eventually, the mass difference is also used as an indicator. Mass conser-
 398 vation is critical during dynamic cases. In this paper, mass corresponds to
 399 the area encompassed within the original interface i.e.

$$\Delta m = \sum |F_{final}| |\Omega| (lev) - \sum |F_{initial}| |\Omega| (lev) \quad (13)$$

400 While the order of convergence is always calculated on a uniform mesh, an
 401 attempt at finding the pseudo-order of convergence of the mesh is presented
 402 here. Indeed, the order of convergence calculated with a uniform mesh is
 403 related to the mesh size but also to the ratio of number of cells between
 404 refinement levels. In that respect, we aim to give a ratio of maximum grid
 405 cells. The pseudo-order of convergence OC is given by

$$OC = \log \left(\frac{E_1^{sym}}{E_2^{sym}} \right) / \log \left(\sqrt{\frac{n_2^{max}}{n_1^{max}}} \right) \quad (14)$$

406 where E^{sym} corresponds to the symmetric difference error of a particular grid
 407 and n^{max} its maximum number of grid cells. Note that Eq. (14) is valid for

408 a uniform mesh and so the ratio of maximum number of cells in a constant
 409 environment gives the same order of convergence equation as in a uniform
 410 mesh.

411 5.2. Static reconstruction

412 Static reconstruction consists of reconstructing the interface of a material
 413 using the same AMR logic as that described in Section. 3. The only variation
 414 is that no advection is necessary. The refinement procedure still applies and
 415 the refinement criterion remains. The intersection of a circle of radius $r =$
 416 0.15 centred at $[0.5, 0.75]$ in a unit domain on a finer grid is determined using
 417 the exact interface rather than the material configuration at the previous time
 418 step. Exact mass conservation is achieved at all levels. Fig. 7 highlights the
 419 difference in precision during reconstruction when refining the interface using
 420 zero, one or two levels of refinement. The symmetric difference error gives a
 421 good insight into the increased precision and accuracy obtained when using
 422 a higher level of refinement.

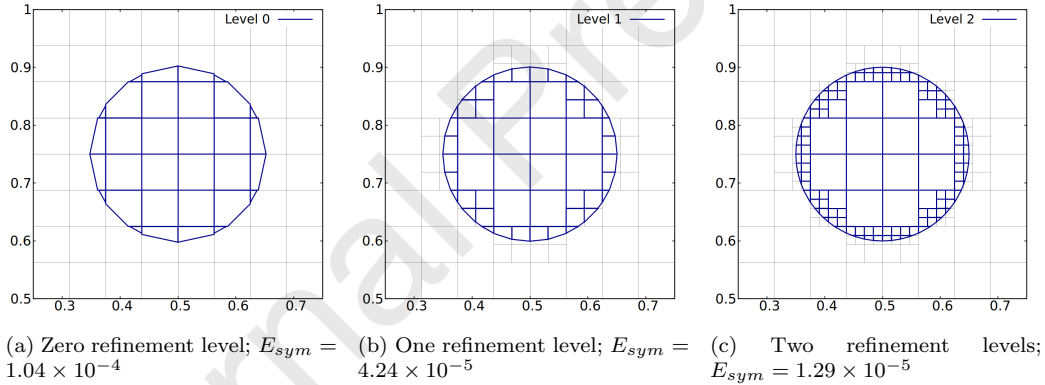


Figure 7: Static reconstruction for a 16×16 base grid with zero, one and two levels of refinement and the associated symmetric difference error

423 5.3. Benchmark: Zalesak slotted disc

424 This benchmark test case involves a slotted disc which is rotated anti-
 425 clockwise in a rigid body rotation around the centre of the domain [39]. The
 426 circle of radius $r = 0.15$ has a rectangular slot of width $w = 0.05$ in its centre
 427 part with a maximum height of $h = 0.85$. The velocity field for this test case
 428 is given by

$$\mathbf{u}(x, y) = \begin{bmatrix} 0.5 - y \\ x - 0.5 \end{bmatrix} \quad (15)$$

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430

431 Even though no filaments are formed during the advection process, the
 432 filament capability of our code is still enabled. The rotational nature of this
 433 test case also highlights the fact that no deformation occurs in the material,
 434 hence the mass redistribution algorithms are enabled but not used as the
 435 backtrace is always of the same size as the cell area. This highlights the
 436 powerful choice of backtrace when refining a mesh as described in Section.
 437 3. Three different grids are presented, explicitly 32×32 as base mesh and a
 438 Level-1 and Level-2 of refinement. The number of iterations is $n_{it} = 300$ and
 439 $\Delta t = 2\pi/n_{it}$.

Table 1: Dependence of the L_1 error, E_{L_1} , and relative error, E_r , on refinement level for the Zalesak slotted disc problem using a 32×32 base mesh

Refinement level	E_{L_1}	E_r
0	2.55×10^{-3}	4.38×10^{-2}
1	5.31×10^{-4}	9.13×10^{-3}
2	1.98×10^{-4}	3.41×10^{-3}

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The error indicator used in this test case is the interpolated L_1 error. Table 1 presents the error for different levels of refinement. Fig 8 emphasises the difference between initial and final reconstructions, as well as the intermediate reconstructions captured during the full rigid body rotation. The shape of the interface is maintained well, except around the sharp edges of the rectangular slot. The MOF method, as it stands, is not able to reconstruct these sharp edges even when refining the grid locally. Note, however, that the straight interface around the longer edges of the rectangle is not refined during the initial condition. Indeed, because MOF reconstructs these cells exactly, the refinement criterion is not triggered. The main difference compared with the method of Ahn et al. [34] is that the tolerance used in that paper is independent of the cell dimension. This means that, with a tolerance set to be smaller than machine precision, even cells that are reconstructed exactly will be refined. Fig. 9 taken from Ahn et al.[34] shows that

454 the neighbourhood of slots are refined while it is not in our initial reconstruction.
 455 tion.

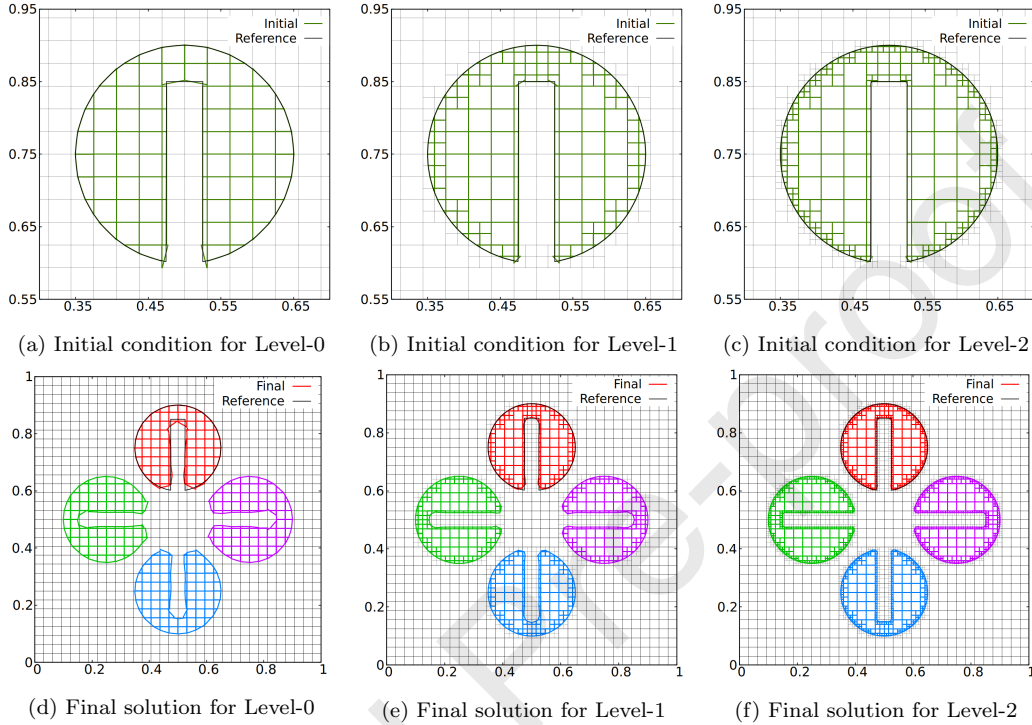


Figure 8: Zalesak slotted disc test case for a 32×32 base grid and one and two levels of refinement. Top row of figures shows the initial reconstruction. Bottom row of figures shows the evolution of the shape of the interface.

456 The Zalesak slotted disc is also a good benchmark to evaluate the effi-
 457 ciency of the method through a time distribution. The time investigation is
 458 an average percentage of time per iteration. Five main blocks exist in this
 459 code, the first involves identifying level 0 cells that will need to be advected.
 460 This second and third part involves backtracking cells at any levels and also
 461 the intersection procedure. The final blocks involves global mass redistribu-
 462 tion and interface reconstruction. Fig.10 highlights the percentage of time
 463 taken in each block of the code both for a 32×32 and 64×64 grid. The second
 464 plot shows data for the same finest level of refinement. Note the advection
 465 identification subroutine is insignificant, so is the redistribution procedure.
 466 Most of the time is taken in the intersection procedure as expected due to
 467 looping through all cells and subcells. As more levels are considered, the

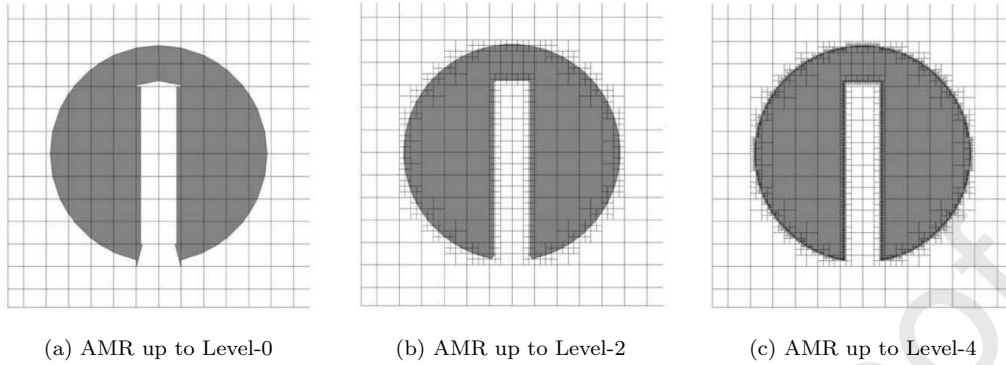


Figure 9: Figure taken from Ahn et al. [34] highlighting their initial reconstruction and choice of refinement for the Zalesak slotted disc.

468 percentage of time increases in the intersection procedure. However, the
 469 time spent in reconstruction does not increase significantly because of limited
 470 number of cells reaching higher levels. In addition, the likelihood of them
 471 not being filament reconstruction cells mitigates the computational cost.

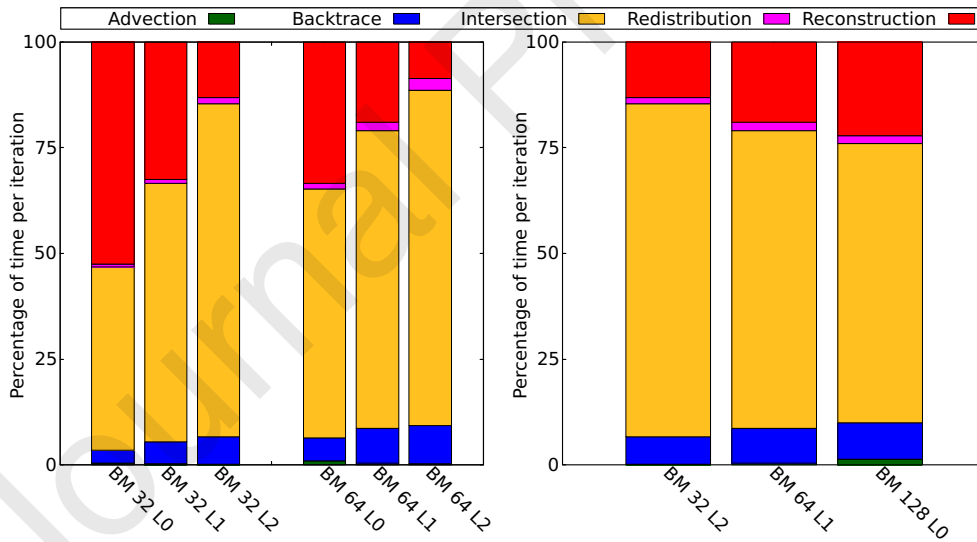


Figure 10: Percentage of time spent on key MOF processes per iteration for a 32×32 and 64×64 grid for level 0, level 1 and level 2, respectively. Comparison of time distribution for same finest level of refinement.

472 5.4. Benchmark: Reversible vortex $T=8$

473 The reversible vortex is an advection benchmark that has been widely
 474 studied in the literature [40]. This deformation case sees a circle of radius
 475 $r = 0.15$ within a unit domain and centered at $[0.5, 0.75]$ shearing its body
 476 along a divergence-free velocity field given by

$$\mathbf{u}(x, y, t) = \begin{bmatrix} -\sin^2(\pi x) \sin(2\pi y) \\ \sin^2(\pi y) \sin(2\pi x) \end{bmatrix} \cos(\pi t/T) \quad (16)$$

477 in which T represents the full period. In most cases, $T = 8$ and in our case,
 478 the Courant-Friedrichs-Lewy (CFL) number is 1. In that respect, the number
 479 of iterations $n_{it} = 256$ and $\Delta t = \Delta x$. The structure of the deformed interface
 480 exhibits filaments which indicates that the filament procedure is activated
 481 within our AMR scheme. Fig. 11 highlights the results for a base mesh of
 482 32×32 with 0, 1 and 2 levels of refinement. The maximum deformation at
 483 $t = T/2$ is shown as well as the final state at $t = T$. Indeed, during the
 484 final state, the symmetric difference error can be used when comparing with
 485 the initial reconstruction. It is important to note that during the refinement
 486 process, the local CFL number reaches 2 and 4, respectively, for refinement at
 487 Level-1 and Level-2. Mass difference and runtime are also explicitly displayed
 488 in Table 2.

Table 2: Symmetric difference error, order of convergence, mass difference and runtime for the reversible vortex test case at final reconstruction using a filamentary approach. The pseudo-order of convergence is given in parenthesis.

Refinement level	0	1	2
E_{sym}	3.05×10^{-3}	1.14×10^{-3}	8.93×10^{-4}
Order of convergence	-	1.41(4.25)	0.35(0.77)
Mass difference	3.3×10^{-15}	-6.7×10^{-15}	2.5×10^{-13}
Runtime (s)	15.7	35.2	92.2

489 The evolution of the number of cells is displayed in Fig. 12. As expected,
 490 Level-0 offers a constant number of cells throughout the iterations, while the
 491 number of cells for Level-1 and Level-2 increase gradually until the vortex
 492 is reversed. Note the small drop in the number of cells in the final iteration
 493 before reversal. At this instant in time the magnitude of the velocity field
 494 vanishes which limits the error in reconstruction.

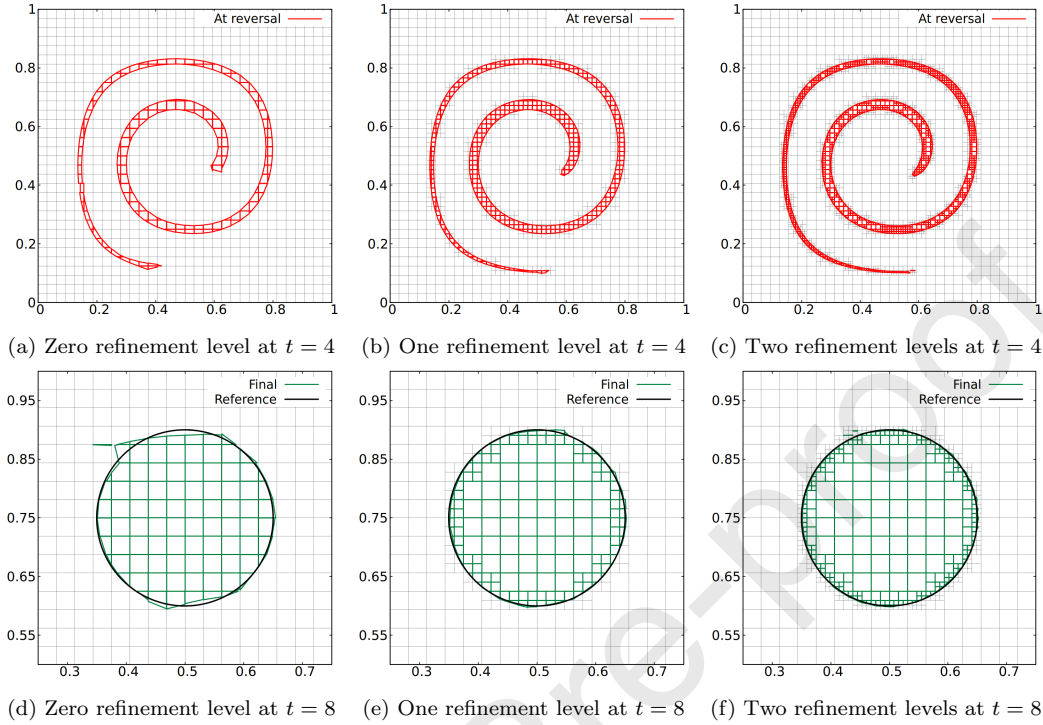


Figure 11: Reversible vortex test case using $T = 8$ for the base grid 32×32 with zero, one and two levels of refinement. Top row of figures shows the maximum deformation. Bottom row of figures shows the final interface.

495 5.4.1. Influence of the mass redistribution procedure

496 In this section the influence of the mass redistribution procedure is exam-
 497 ined. In most cases, mass is redistributed uniformly. However, as discussed
 498 in Section 4, directly proportional and inversely proportional redistributions
 499 are implemented and explored in this paper. Fig. 13 shows the seemingly
 500 marginal differences between these approaches in terms of reconstruction.
 501 Runtime are also comparable with a uniform distribution. However, in terms
 502 of mass conservation, machine precision is not achieved. The main difference
 503 lies in the way the redistribution of mass is achieved. While a directly propor-
 504 tional approach seems to be a natural way to follow, the number of iterations
 505 necessary to redistribute mass is increased compared to a uniform approach.
 506 Similarly, the inversely proportional approach iterates more times without
 507 increasing the runtime significantly.

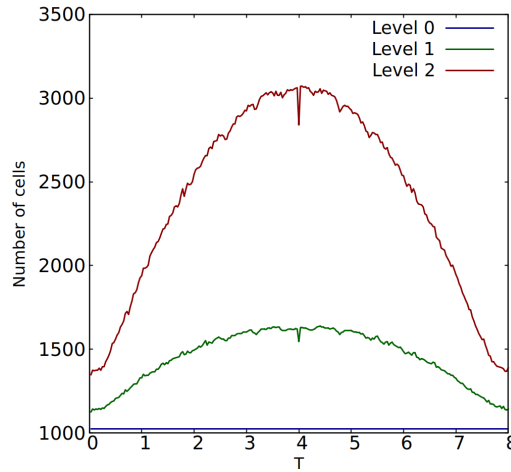


Figure 12: Evolution of the number of cells when using different levels of refinement during the reversible vortex test case.

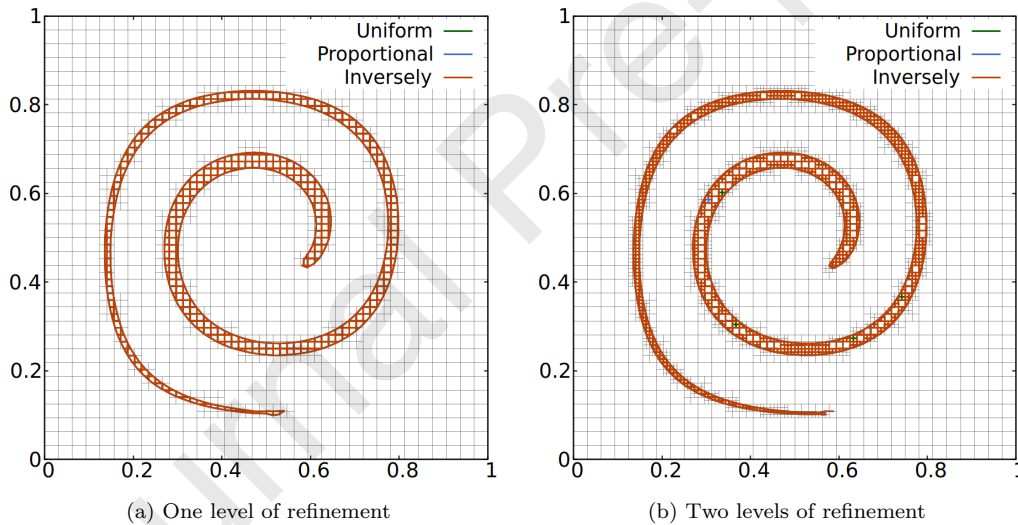


Figure 13: Visual comparison between a uniform, directly proportional and inversely proportional mass redistribution at maximum deformation.

508 5.4.2. Influence of the initial refinement

509 The initial reconstruction is the lower limit of error possible when recon-
 510 structing the interface. Indeed, it may differ between the initial reconstruc-
 511 tion and the dynamic case. In general, when using a refinement structure, the

512 initial refinement is the same as the advection process. This is the case for all
 513 other cases in this present study. Hence, this section assesses the influence of
 514 the initial refinement on the final reconstruction. In the following case, the
 515 circle is reconstructed using different levels of refinement at the initial stage,
 516 then advected using either level 0, level 1 or level 2. Fig. 14 shows the final
 517 reconstruction for different levels of refinement at the initial stage.

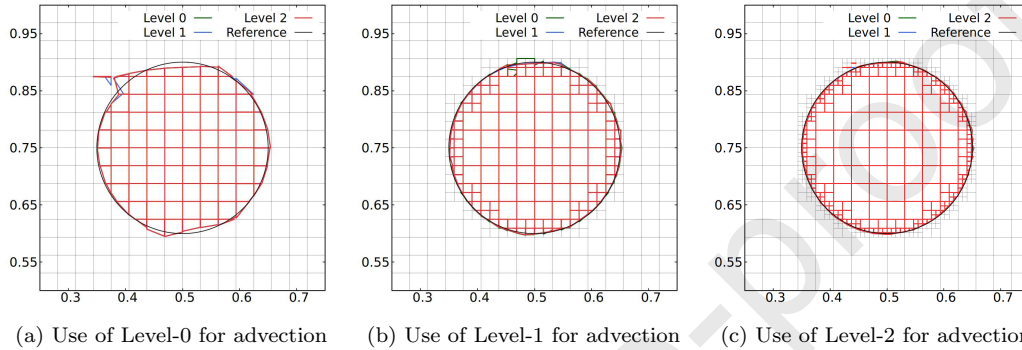


Figure 14: Final reconstruction for the reversible vortex test case using $T = 8$ for the base grid 32×32 , one and two levels of refinement. Levels indicate the level of refinement at the initial stage.

518 A slightly adapted data structure is used to accommodate the correct
 519 segmentation. In our code, (i, j, is, js, lev) is the data structure used for
 520 adaptive mesh refinement. However, space allocation is performed at the
 521 start using the desired maximum refinement level div_max , i.e. is has an
 522 allocation of 2^{div_max} and so has js . Note that this allocation would not
 523 work if the maximum level was 0 at the initial stage but then 2 during the
 524 advection process as the allocation would not be performed. This allows us
 525 to use any initial condition in terms of refinement levels as one can see in
 526 Fig. 7. Note that the final state is not highly dependent on the initial level
 527 of refinement.

528 5.4.3. Influence of the mesh refinement criteria

529 As described above the refinement criteria in a MOF framework is the
 530 discrepancy between the reference and reconstructed centroid. This section
 531 discusses the influence of having a finer or coarser criterion. Note that the
 532 criterion is non-dimensionalised by the cell size so that it is more meaningful
 533 use than using machine precision. A lower tolerance has a great influence on
 534 the reconstruction precision, but it also has implications on the number of

535 cells in the domain and indeed the runtime. In setting a suitable tolerance,
 536 one has to consider the trade-off between accuracy and runtime. Runtime is
 537 comparable for all test cases and a significant difference is not found. Fig.
 538 15 shows the intermediate and final reconstruction as well as the evolution
 539 of the number of cells in the domain. The maximum number of cells is also
 540 comparable, however the evolution shows an interesting feature where the last
 541 iteration before reversal exhibits a large drop in the number of cells. Indeed,
 542 the last iteration corresponds to the $\cos(\pi t/T)$ term vanishing, meaning the
 543 reconstruction is an almost-static reconstruction. The Level-0 advection will
 544 be able to reconstruct more filaments. Combined with a low tolerance, the
 545 number of cells in the domain decreases significantly.

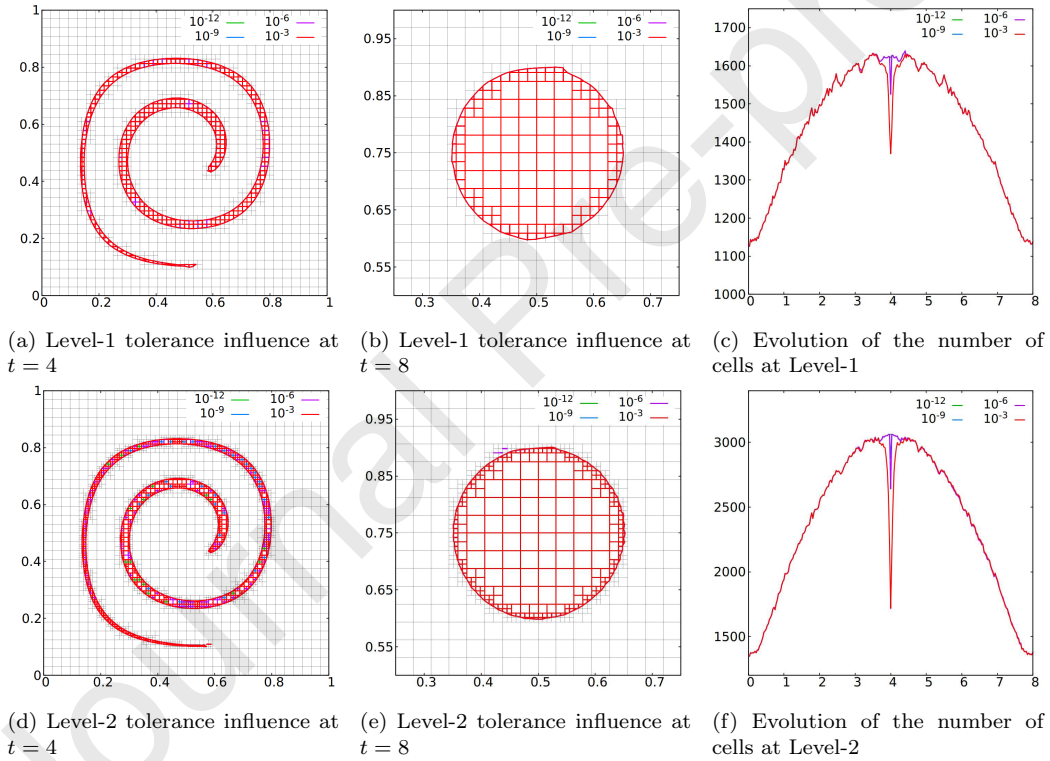


Figure 15: Influence of the mesh refinement criterion tolerance on intermediate and final reconstruction and evolution of the number of cells in the domain.

546 *5.4.4. Influence of the backtrace on interface reconstruction*

547 The choice of backtrace within a refinement framework can influence re-
 548 sults greatly. Indeed, the natural choice is to perform backtracking on the
 549 subcell itself, ascribed here as *Regular*. However, there are some advantages
 550 and disadvantages which are explained below. On the one hand, the inter-
 551 section procedure of our approach must intersect the entirety of the desired
 552 material at all times. In this regard, our backtracking approach is to use
 553 Level-0 as reference and make sure that all refined levels intersect the same
 554 area as previous levels. This ensures exact mass conservation. However, the
 555 refined backtrace subcells are slightly deformed, which means the reference
 556 volume fraction and centroid are somewhat distorted. On the other hand,
 557 the regular backtrace creates gaps and overlaps that are very small [34]. This
 558 does not guarantee a full intersection of the material, leading to poor con-
 559 servation of mass. Despite this loss of mass, the interface reconstruction is
 560 not distorted which may indicate a smoother interface reconstruction. The
 561 correct backtracking consisting of advected hanging nodes may also create
 562 non-convex cells, which means more complex algorithms are needed. This
 563 approach has been discarded. Fig. 16 emphasises the difference between a
 564 regular backtrace and our proposal for one and two levels of refinement.

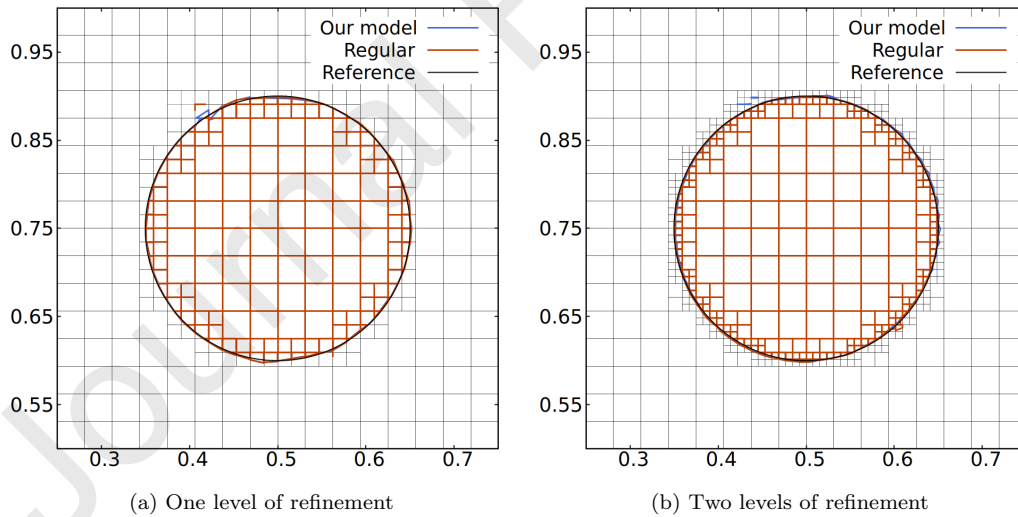


Figure 16: Comparison between a regular backtrace and our choice of backtracking a refined subcell at the final state.

565 Table 3 shows that the error is smaller when using a regular backtrace.

566 Yet, having a smaller symmetric difference error may not guarantee good
 567 mass conservation. In addition, the regular backtrace choice seems to be
 568 computationally faster. Indeed, the backtracking procedure is only relevant
 569 for the subcell itself, whereas in our model, higher levels need to account for
 570 the previous levels of refinement for its backtracking procedure.

Table 3: Comparison between our model and a regular backtrace regarding interface reconstruction.

	Our model	Regular backtrace
Level-1		
E_{sym}	1.14×10^{-3}	7.84×10^{-4}
Mass difference	-6.7×10^{-15}	9.8×10^{-5}
Runtime (s)	35.3	31.0
Level-2		
E_{sym}	8.93×10^{-4}	6.26×10^{-4}
Mass difference	2.5×10^{-13}	-2.6×10^{-4}
Runtime (s)	92.2	75.2

571 5.5. Benchmark: Droplet flow

572 Originally proposed by Ahn and Shashkov [34] and further developed by
 573 Jemison et al. [25], the droplet flow test case deforms an initial circle of
 574 radius $r = 0.125$ centred in a unit domain using a nonlinear divergence-free
 575 velocity field given by

$$\mathbf{u}(x, y, t) = \begin{bmatrix} 0.125(8x - 4) \\ 0.125 [-(8y - 4) - 4 - (1 - (8x - 4)^2 - (8x - 4)^4)] \end{bmatrix} f(t) \quad (17)$$

576 where

$$f(t) = \begin{cases} 1 & 0 \leq t < T_{max} - t_\epsilon/2 \\ \cos\left(\frac{\pi(t - T_{max} + t_\epsilon/2)}{t_\epsilon}\right) & T_{max} - t_\epsilon/2 \leq t \leq T_{max} + t_\epsilon/2 \\ -1 & T_{max} + t_\epsilon/2 < t \leq 2T_{max} \end{cases} \quad (18)$$

577 represents the amplitude of the velocity field which varies in time so that at
 578 time $t = T_{max}$ the initial droplet is recovered to its original position.

579 Filaments are formed during the advection process. A leading tip is gen-
 580 erated, making this case challenging. The base mesh is 32×32 , the number
 581 of iterations is $n_{it} = 160$ and $\Delta t = 0.01$. Two levels of refinement are tested.
 582 Fig. 17 highlights the shape of the intermediate $t = T_{max}$ and final inter-
 583 face using different levels of refinement. All figures show adequate results
 584 compared to the original circle. In addition, filaments are well reconstructed
 585 except when the tip needs to be reconstructed using refinements. This tends
 586 to lead to spurious break ups in the material.

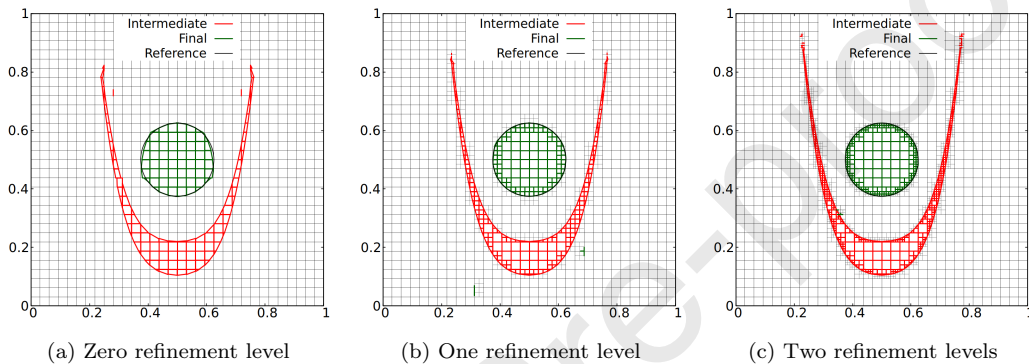


Figure 17: Droplet flow test case for a 32×32 grid with zero, one and two levels of refinement. Figures shows the maximum deformation and the final interface.

Table 4: Symmetric difference error, mass difference and runtime for the droplet flow test case at final reconstruction using a 32×32 base mesh compared to reference solutions.

Refinement level	0	1	2
E_{sym} in [25]	2.48×10^{-3}	6.37×10^{-4}	2.96×10^{-4}
Order of convergence	-	1.96	1.10
Runtime (s)	191.3	529.3	940.4
E_{sym}	1.53×10^{-3}	2.55×10^{-4}	1.90×10^{-4}
Mass difference	-2.82×10^{-4}	-4.78×10^{-7}	-4.92×10^{-16}
Runtime (s)	2.9	7.8	21.2

587 Table 4 provides the information on the symmetric difference error, mass
 588 difference and runtime. Note that the mass difference is not as accurate as
 589 expected. Indeed, for the coarser refinement, some material tends to leave the
 590 domain near the bottom edge. The Level-1 figure shows that some material

591 at the final state was advected very near the edge of domain, suggesting
 592 that for levels 0 and 1, some has left the domain. This highlights a major
 593 drawback of our approach. Indeed, when using a Level-0 advection scheme
 594 combined with filaments, material that breaks away from the main material
 595 tends to stay detached, or is reconstructed poorly even when using some
 596 levels of refinement.

597 5.6. Benchmark: S-shape

598 First tested by Ahn and Shashkov [34] and Jemison et al. [25], the S-
 599 shape benchmark case is a challenging material deformation test where an
 600 initial circle of radius $r = 0.25$ centred in a unit domain is deformed in a
 601 nonlinear divergence-free velocity field given by

$$\mathbf{u}(x, y, t) = \begin{bmatrix} 0.25[(4x - 2) + (4y - 2)^3] \\ -0.25[(4y - 2) + (4x - 2)^3] \end{bmatrix} f(t) \quad (19)$$

602 where $f(t)$ is given in Eq. (18). In this case, $T_{max} = 4$ and $t_\epsilon = 2$. The total
 603 number of iterations for a base mesh 32×32 is $n_{it} = 320$ and $\Delta t = 0.025$.

604 The deformation creates a highly deformed material creating thin fila-
 605 mentary structures in the centre of the domain. For this benchmark, our
 606 filament capable MOF procedure is used. Fig. 18 shows the maximum de-
 607 formation of the material and its final state. The Level-0 grid shows poor
 608 reconstruction because the thin strand of material in the centre of the domain
 609 is difficult to reconstruct even with a filament approach using three conglom-
 610 erates. When more than three conglomerates exist, a standard MOF recon-
 611 struction is used which tends to merge materials together [26]. Using one or
 612 two levels of refinement exhibits a better reconstructed interface. However,
 613 mass conservation is not well maintained for this challenging case due to the
 614 reversion of large portion of thin filamentary structures. The significant loss
 615 of mass affects the symmetric difference error at Level-2, which is larger than
 616 the reconstruction at Level-1.

617 6. Discussion on the efficiency of MOF-AMR filament capability

618 Any AMR framework is known to use a reasonable trade-off between ac-
 619 curacy and runtime, refining regions of interest while decreasing the total
 620 number of cells used in computation compared to a uniform grid. In gen-
 621 eral AMR practices, runtime increases with refinement levels while the error

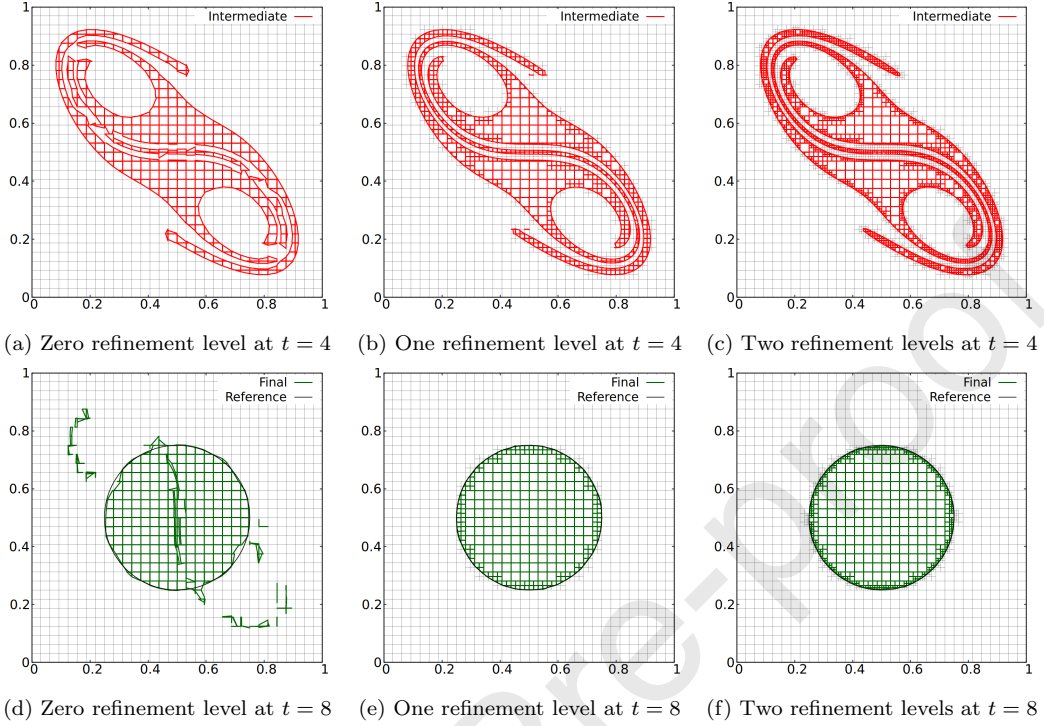


Figure 18: S-shape test case for a 32×32 base grid with zero, one and two levels of refinement. Top row of figures shows the maximum deformation. Bottom row of figures shows the final interface.

Table 5: Symmetric difference error, mass difference and runtime for the S-shape test case at final reconstruction compared to Jemison et al. [25].

Refinement level	0	1	2
E_{sym} in [25]	2.11×10^{-2}	1.34×10^{-3}	4.74×10^{-4}
Runtime (s)	157.2	773.1	1871.5
E_{sym}	1.57×10^{-2}	1.11×10^{-3}	1.41×10^{-3}
Mass difference	-3.47×10^{-10}	-2.44×10^{-4}	3.30×10^{-3}
Runtime (s)	35.9	61.7	180.7

622 decreases (or the region of interest becomes more accurately defined). How-
 623 ever, in the MOF context, regions of high deformation can be reconstructed
 624 with ease using filaments while maintaining a reasonable computational cost.
 625 In this regard, one can try to compare the efficiency of different levels of a

626 MOF-AMR filament capable procedure. Indeed, a filament reconstruction
 627 with a higher base resolution but with a lower level of refinement may be
 628 equivalent to a lower base resolution reconstruction but with a higher level
 629 of refinement. This section tries to give an insight into compromising run-
 630 time and error for the well-known reversible vortex benchmark. At first we
 631 use a constant unity CFL number on the base mesh, meaning the local CFL
 632 number for refined grids is 2 and 4, respectively, for Level-1 and Level-2. Sec-
 633 ondly, we consider an effective CFL number for the finest resolution meaning
 634 that the number of iterations is constant for all three configurations. The
 635 base mesh CFL number for one level of refinement is 0.5 and for two levels
 636 of refinement 0.25.

Table 6: Efficiency table testing three different grids with the same maximum level of refinement. BM 128 relates to Base Mesh and its resolution. CFL numbers are expressed for the base mesh.

	BM 128 Level-0	BM 64 Level-1	BM 32 Level-2
CFL	1.0	1.0	1.0
E_{sym}	1.56×10^{-4}	2.36×10^{-4}	8.93×10^{-4}
Max number of cells	16384	5530	3061
Number of iterations	1024	512	256
Runtime (s)	115.3	81.2	92.9
CFL	1.0	0.5	0.25
E_{sym}	1.56×10^{-4}	1.65×10^{-4}	2.42×10^{-4}
Runtime (s)	115.3	165.5	296.9

637 One can see from Table 6 that with a constant CFL number, runtime
 638 is better for one level of refinement, which is also better than two levels of
 639 refinement. This is due to the fact that Level-1 has to be reconstructed first.
 640 In addition, the number of cells used is very small compared to a uniform
 641 mesh even with the highest refinement levels. When using the same effective
 642 CFL number, i.e. equivalent at the finest resolution, runtime increases sig-
 643 nificantly with the increased number of iterations. Similarly, the symmetric
 644 difference error increases. Fig. 19 shows the improved final reconstruction.
 645 Comparison of performance on a fine uniform grid and a grid using one level
 646 of refinement, both using filament capable methods, shows that there is a
 647 significant improvement in runtime and number of cells for the latter while
 648 the error is very similar in both cases. This solution may be a more desirable

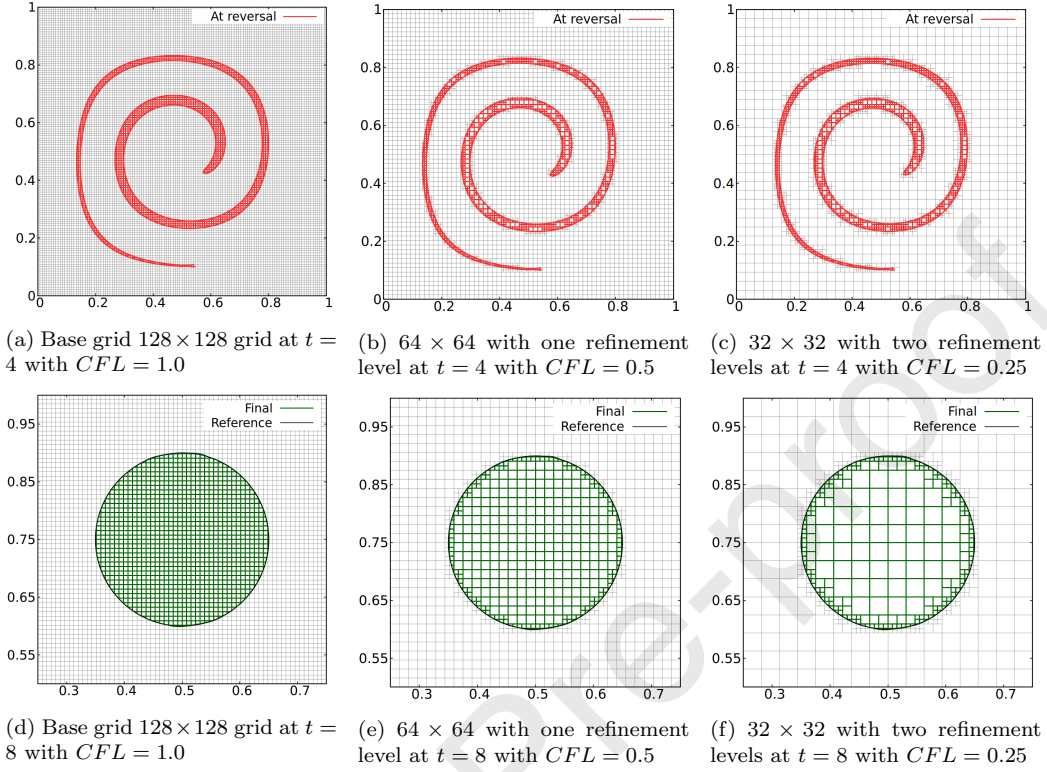


Figure 19: Visual results of the efficiency test of the MOF-AMR filament capable procedure using different CFL numbers therefore a constant number of iterations.

option. Fig. 20 shows a significantly smaller number of cells used. In addition, much better reconstruction is achieved with a smaller CFL number. The influence of high CFL numbers (> 2) on interface accuracy has not been demonstrated.

7. Conclusions

In this paper, a new quadtree-based adaptive MOF method has been presented where filament structures are resolved using a symmetric multi-material approach on a refined grid. A simplified quadtree structure has been implemented with logical connection between parent and children cells up to two levels of refinement. A Lagrangian backtracking approach for refined grids is proposed that enables exact material intersection during the advection process, hence ensuring mass conservation. The refinement crite-

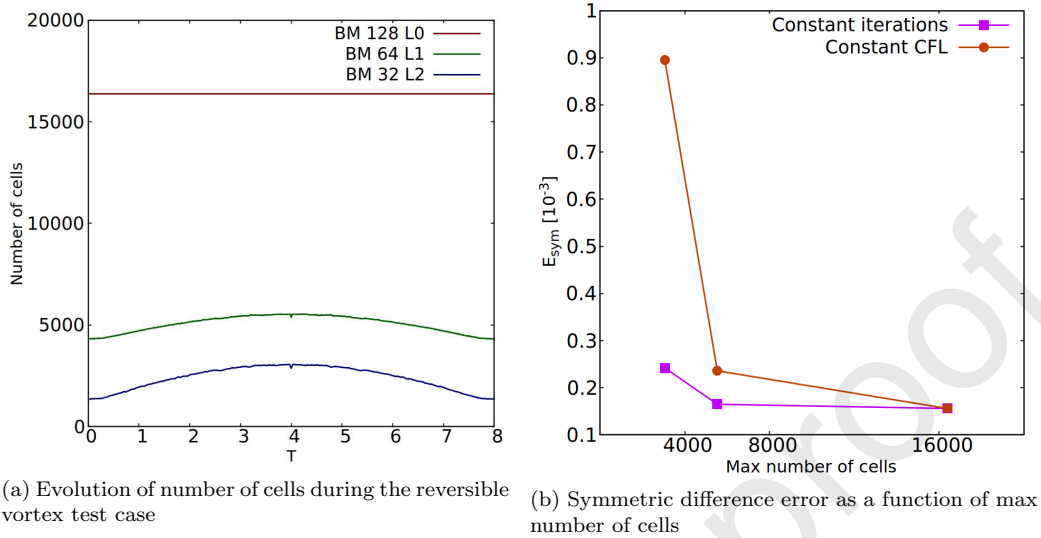


Figure 20: Number of cells and symmetric difference error for the efficiency test.

661 rion is based on the centroid defect relative to the cell or subcell size, ensuring
 662 linear interfaces are reconstructed exactly without the need for refinement.
 663 As a result, the proposed framework achieved good results in terms of accu-
 664 racy and runtime while using computational resources in a more efficient
 665 manner. Comparison between different levels of refinement for the same mini-
 666 mum cell size provides insight into the most efficient use of this framework
 667 and the MOF method in general.

668 This MOF-AMR method is tested on several benchmark problems with
 669 high material deformation. All of these benchmark problems are compared
 670 with a couple of similar MOF approaches using refinement. First, the Zale-
 671 sak slotted disc shows less refined cells at the initial stage and achieved good
 672 qualitative results. Other benchmarks such as the reversible vortex show
 673 highly precise reconstruction at maximum deformation under different levels
 674 of refinement. The droplet flow and the S-shape test case yielding highly de-
 675 formed structures are presented with filament reconstruction. Qualitatively,
 676 results are comparable to other MOF methods. The limitation of our method
 677 lies in the number of refinement levels available in an unconstrained adaptive
 678 grid structure. Our refinement approach differs from other MOF-AMR refer-
 679 ence methods [25, 34] but shows acceptable results. Machine precision mass
 680 conservation algorithms are achieved for benchmark problems such as the re-

681 versible vortex, whilst further improvements are required for other problems
682 such as the droplet flow or the S-shape case. Furthermore, runtime has been
683 significantly decreased compared to previous methods. In this study, no high-
684 performance libraries are used and calculations are carried out on a single
685 core. High-performance frameworks would offer strong scalability and effi-
686 cient algorithms for handling large parallel octree operations [37, 41, 42, 43].
687 Yet, complexity and potential resource requirements may be challenging. In
688 comparison, our data structure offers ease of use and accessibility, suitable
689 for smaller-scale efforts. Many advantages follow from this decision such as
690 the absence of load balancing, numbering, and neighbouring search. How-
691 ever, the authors are aware of potential issues related to limited scalability
692 and versatility, memory access, parent node data optimisation and general
693 computing performance.

694 The present MOF-AMR method tends to decrease the cross-stream diffu-
695 sion of advected material and can reconstruct sharp edges or tips of filaments
696 with greater accuracy using up to two levels of refinement. Further improve-
697 ment may be made to address these numerical issues by using the recent
698 new moment-of-fluid method [44] or the parabolic interface reconstruction
699 [45]. In addition, the number of conglomerates has less influence on the cen-
700 troid defect as these scenarios tend to trigger refinement. In future work
701 we would like to advect and reconstruct several materials within the same
702 domain which will most likely involve reconstructing more than three mate-
703 rials. In this AMR framework, optimising the levels of refinement could be
704 of interest to reduce the computational cost by using prediction algorithms.
705 Coupling our MOF-AMR framework with a fluid flow solver is our next aim
706 targeting complex multiphase flow problems, which can potentially reduce
707 the computational cost without sacrificing accuracy.

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717 **References**

- 718 [1] X. Zheng, J. Lowengrub, A. Anderson, V. Cristini, Adaptive unstruc-
719 tured volume remeshing-ii: Application to two-and three-dimensional
720 level-set simulations of multiphase flow, *Journal of Computational*
721 *Physics* 208 (2) (2005) 626–650.
- 722 [2] Z. Xie, D. Pavlidis, P. Salinas, J. R. Percival, C. C. Pain, O. K. Matar, A
723 balanced-force control volume finite element method for interfacial flows
724 with surface tension using adaptive anisotropic unstructured meshes,
725 *Computers & Fluids* 138 (2016) 38–50.
- 726 [3] C. Cantwell, D. Moxey, A. Comerford, A. Bolis, G. Rocco, G. Mengaldo,
727 D. De Grazia, S. Yakovlev, J.-E. Lombard, D. Ekelschot, B. Jordi, H. Xu,
728 Y. Mohamied, C. Eskilsson, B. Nelson, P. Vos, C. Biotto, R. Kirby,
729 S. Sherwin, Nektar++: An open-source spectral/hp element framework,
730 *Computer Physics Communications* 192 (2015) 205–219.
- 731 [4] M. Berger, J. Olinger, Adaptive mesh refinement for hyperbolic partial
732 differential equations, *Journal of Computational Physics* 53 (3) (1984)
733 484–512.
- 734 [5] M. Sussman, A. S. Almgren, J. B. Bell, P. Colella, L. H. Howell, M. L.
735 Welcome, An adaptive level set approach for incompressible two-phase
736 flows, *Journal of Computational Physics* 148 (1) (1999) 81–124.
- 737 [6] H. D. Ceniceros, A. M. Roma, A. Silveira-Neto, M. M. Villar, et al., A ro-
738 bust, fully adaptive hybrid level-set/front-tracking method for two-phase
739 flows with an accurate surface tension computation, *Communications in*
740 *Computational Physics* 8 (1) (2010) 51–94.
- 741 [7] S. Popinet, An accurate adaptive solver for surface-tension-driven inter-
742 facial flows, *Journal of Computational Physics* 228 (16) (2009) 5838–
743 5866.
- 744 [8] D. Hartmann, M. Meinke, W. Schröder, A strictly conservative carte-
745 sian cut-cell method for compressible viscous flows on adaptive grids,
746 *Computer Methods in Applied Mechanics and Engineering* 200 (9-12)
747 (2011) 1038–1052.

- 748 [9] Q. Liang, A simplified adaptive Cartesian grid system for solving the 2D
749 shallow water equations, *International Journal for Numerical Methods*
750 *in Fluids* 69 (2) (2012) 442–458.
- 751 [10] X. Chen, V. Yang, Thickness-based adaptive mesh refinement methods
752 for multi-phase flow simulations with thin regions, *Journal of Compu-*
753 *tational Physics* 269 (2014) 22–39.
- 754 [11] M. Mirzadeh, A. Guittet, C. Burstedde, F. Gibou, Parallel level-set
755 methods on adaptive tree-based grids, *Journal of Computational Physics*
756 322 (2016) 345–364.
- 757 [12] F. H. Harlow, J. E. Welch, Numerical calculation of time-dependent
758 viscous incompressible flow of fluid with free surface, *Physics of Fluids*
759 8 (12) (1965) 2182–2189.
- 760 [13] S. O. Unverdi, G. Tryggvason, A front-tracking method for viscous,
761 incompressible, multi-fluid flows, *Journal of Computational Physics*
762 100 (1) (1992) 25–37.
- 763 [14] S. Osher, J. A. Sethian, Fronts propagating with curvature-dependent
764 speed: Algorithms based on Hamilton-Jacobi formulations, *Journal of*
765 *Computational Physics* 79 (1) (1988) 12–49.
- 766 [15] J. A. Sethian, P. Smereka, Level set methods for fluid interfaces, *Annual*
767 *Review of Fluid Mechanics* 35 (1) (2003) 341–372.
- 768 [16] C. W. Hirt, B. D. Nichols, Volume of fluid (VOF) method for the dynam-
769 ics of free boundaries, *Journal of Computational Physics* 39 (1) (1981)
770 201–225.
- 771 [17] R. Scardovelli, S. Zaleski, Direct numerical simulation of free-surface
772 and interfacial flow, *Annual Review of Fluid Mechanics* 31 (1) (1999)
773 567–603.
- 774 [18] J. J. Monaghan, Smoothed particle hydrodynamics, *Annual Review of*
775 *Astronomy and Astrophysics* 30 (1) (1992) 543–574.
- 776 [19] V. Dyadechko, M. Shashkov, Moment-of-fluid interface reconstruction,
777 *Los Alamos Report LA-UR-05-7571* (2005) 49.

- 778 [20] A. Lemoine, S. Glockner, J. Breil, Moment-of-fluid analytic reconstruction
779 on 2D Cartesian grids, *Journal of Computational Physics* 328 (2017)
780 131–139.
- 781 [21] A. A. Mukundan, T. Ménard, J. C. B. de Motta, A. Berlemont, A hybrid
782 moment of fluid–level set framework for simulating primary atomization,
783 *Journal of Computational Physics* 451 (2022) 110864.
- 784 [22] R. N. Hill, M. Shashkov, The symmetric moment-of-fluid interface re-
785 construction algorithm, *Journal of Computational Physics* 249 (2013)
786 180–184.
- 787 [23] H. T. Ahn, M. Shashkov, Multi-material interface reconstruction on gen-
788 eralized polyhedral meshes, *Journal of Computational Physics* 226 (2)
789 (2007) 2096–2132.
- 790 [24] V. Dyadechko, M. Shashkov, Reconstruction of multi-material interfaces
791 from moment data, *Journal of Computational Physics* 227 (11) (2008)
792 5361–5384.
- 793 [25] M. Jemison, M. Sussman, M. Shashkov, Filament capturing with
794 the multimaterial moment-of-fluid method, *Journal of Computational*
795 *Physics* 285 (2015) 149–172.
- 796 [26] P. Hergibo, T. N. Phillips, Z. Xie, A moment-of-fluid method for resolv-
797 ing filamentary structures using a symmetric multi-material approach,
798 *Journal of Computational Physics* 491 (2023) 112401.
- 799 [27] Y. Zeng, H. Liu, Q. Gao, A. Almgren, A. P. S. Bhalla, L. Shen, A
800 consistent adaptive level set framework for incompressible two-phase
801 flows with high density ratios and high Reynolds numbers, *Journal of*
802 *Computational Physics* 478 (2023) 111971.
- 803 [28] O. Antepara, N. Balcázar, A. Oliva, Tetrahedral adaptive mesh refine-
804 ment for two-phase flows using conservative level-set method, *Internation-*
805 *al Journal for Numerical Methods in Fluids* 93 (2) (2021) 481–503.
- 806 [29] L. Fu, S. Litvinov, X. Y. Hu, N. A. Adams, A novel partitioning method
807 for block-structured adaptive meshes, *Journal of Computational Physics*
808 341 (2017) 447–473.

- 809 [30] I. Ginzburg, G. Wittum, Two-phase flows on interface refined grids modeled with VOF, staggered finite volumes, and spline interpolants, *Journal of Computational Physics* 166 (2) (2001) 302–335.
810
811
- 812 [31] D. Greaves, A quadtree adaptive method for simulating fluid flows with moving interfaces, *Journal of Computational Physics* 194 (1) (2004) 35–56.
813
814
- 815 [32] M. Malik, E. S.-C. Fan, M. Bussmann, Adaptive VOF with curvature-based refinement, *International Journal for Numerical Methods in Fluids* 55 (7) (2007) 693–712.
816
817
- 818 [33] J. Wang, A. Borthwick, R. E. Taylor, Finite-volume-type VOF method on dynamically adaptive quadtree grids, *International Journal for Numerical Methods in Fluids* 45 (5) (2004) 485–508.
819
820
- 821 [34] H. T. Ahn, M. Shashkov, Adaptive moment-of-fluid method, *Journal of Computational Physics* 228 (8) (2009) 2792–2821.
822
- 823 [35] A. Islam, M. Sussman, H. Hu, Y. Lian, Simulation of drop impact on substrate with micro-wells, *Physics of Fluids* 34 (6) (2022) 062108.
824
- 825 [36] M. Shashkov, B. Wendroff, The repair paradigm and application to conservation laws, *Journal of Computational Physics* 198 (1) (2004) 265–277.
826
827
- 828 [37] K. Saurabh, M. Ishii, M. A. Khanwale, H. Sundar, B. Ganapathysubramanian, Scalable adaptive algorithms for next-generation multiphase flow simulations, in: *2023 IEEE International Parallel and Distributed Processing Symposium (IPDPS)*, IEEE, 2023, pp. 590–601.
829
830
831
- 832 [38] C. Harrison, J. Weiler, R. Bleile, K. Gaither, H. Childs, A distributed-memory algorithm for connected components labeling of simulation data, in: *Topological and Statistical Methods for Complex Data: Tackling Large-Scale, High-Dimensional, and Multivariate Data Spaces*, Springer, 2015, pp. 3–19.
833
834
835
836
- 837 [39] S. T. Zalesak, Fully multidimensional flux-corrected transport algorithms for fluids, *Journal of computational physics* 31 (3) (1979) 335–362.
838
839

- 840 [40] W. J. Rider, D. B. Kothe, Reconstructing volume tracking, *Journal of*
841 *Computational Physics* 141 (2) (1998) 112–152.
- 842 [41] C. Burstedde, L. C. Wilcox, O. Ghattas, p4est: Scalable algorithms for
843 parallel adaptive mesh refinement on forests of octrees, *SIAM Journal*
844 *on Scientific Computing* 33 (3) (2011) 1103–1133.
- 845 [42] M. Ishii, M. Fernando, K. Saurabh, B. Khara, B. Ganapathysubrama-
846 nian, H. Sundar, Solving pdes in space-time: 4d tree-based adaptivity,
847 mesh-free and matrix-free approaches, in: *Proceedings of the Interna-*
848 *tional Conference for High Performance Computing, Networking, Stor-*
849 *age and Analysis*, 2019, pp. 1–61.
- 850 [43] H. Sundar, R. S. Sampath, G. Biros, Bottom-up construction and 2: 1
851 balance refinement of linear octrees in parallel, *SIAM Journal on Scien-*
852 *tific Computing* 30 (5) (2008) 2675–2708.
- 853 [44] M. Shashkov, E. Kikinzon, Moments-based interface reconstruction,
854 remap and advection, *Journal of Computational Physics* 479 (2023)
855 111998.
- 856 [45] R. A. Remmerswaal, A. E. Veldman, Parabolic interface reconstruction
857 for 2d volume of fluid methods, *Journal of Computational Physics* 469
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Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Journal Pre-proof

P.H.: Methodology, Software, Data curation, Validation, Investigation, Visualization, Writing- Original draft, Writing- Reviewing and Editing.

Q.L.: Methodology, Software, Investigation, Writing- Reviewing and Editing.

T.N.P.: Conceptualization, Investigation, Writing- Reviewing and Editing, Supervision.

Z.X.: Conceptualization, Methodology, Validation, Investigation, Writing- Reviewing and Editing, Supervision, Funding acquisition.

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