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Adaptive Mesh Refinement Strategies for a Novel Model of Immiscible Fluid Flow in Fractures

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Abstract

In this paper, we consider two Adaptive Mesh Refinement (AMR) methods to simulate flow through fractures using a novel multiphase model. The approach represents the fluid using a two-dimensional parallel-plate model that employs techniques adapted from lattice-Boltzmann simulations to track the fluid interface.

Here, we discuss different mesh refinement strategies for the model and compare their performance to that of a uniform grid. Results from the simulations are demonstrated showing excellent agreement between the model and analytical solutions for both unrefined and refined meshes. We also present results from the study that illustrate the behaviour of the AMR front-tracking method. The AMR model is able to accurately track the interfacial properties in cases where uniform fine meshes would significantly increase the simulation cost. The ability of the model to dynamically refine the domain is demonstrated by presenting the results from an example with evolving interfaces.

Keywords: Multicomponent flow, Mesh refinement, Numerical Modelling

1. Introduction

Multiphase fracture flow is encountered in several different geo-engineering contexts (geothermal energy [1, 2], oil and gas production [3, 4], carbon sequestration [5, 6], and hydraulic fracturing [7, 8], for example). Nevertheless, our understanding of flow through fractures remains limited – particularly when compared to our knowledge of multiphase flows in three-dimensional pore networks. While experimental studies are invaluable in understanding these systems, these studies are limited by the difficulties in monitoring the

9 interface between the phases and detailed flow properties in controlled exper-
10 imental conditions [9]. Thus, robust numerical models are required to gain
11 insight into the behaviour of this class of fluid systems.

12 The ability of the lattice Boltzmann method (LBM) to simulate com-
13 plex and moving boundaries, combined with its ease of implementation, has
14 made it a popular method for modelling multi-phase flow [10, 11, 12, 13, 14].
15 There are several lattice Boltzmann methods to simulate such flow systems
16 including interaction potential models [15], color-gradient models [16], free-
17 energy formulations [17], and kinetic-equation based models [18]. However,
18 lattice Boltzmann modelling can be computationally expensive in fractured
19 media, where the apertures and flow properties may vary by orders of mag-
20 nitude [19]. This problem is compounded by the need to faithfully track
21 the immiscible fluid interface – high-resolution lattice sizes are required to
22 resolve the forces on the interface, adding to the computation cost.

23 In this paper, we use an intermediate model that explicitly represents the
24 changes in the fracture aperture or flow properties, while implicitly solving
25 the cross-sectional flow [19]. This model addresses many of the issues arising
26 due to the difference in length scales between the fracture aperture and the
27 in-plane flow. Nevertheless, the thickness of the immiscible fluid interface
28 remains tied to the in-plane mesh resolution. Here we demonstrate how
29 different Adaptive Mesh Refinement (AMR) strategies may be integrated
30 into the model to alleviate the difficulty of resolving the fluid interface.

31 In AMR, refined meshes are introduced as needed in certain numerically-
32 sensitive parts of the simulation domain (*e.g.* the interface region), while
33 coarser meshes are retained in other areas [20, 21]. The mesh resolution is
34 dynamically updated as the solution proceeds. This strategy retains numer-
35 ical accuracy while reducing memory and time requirements [22, 20, 23].

36 Broadly speaking, there are three ways to implement the AMR: block-
37 based, cell-based, and patch-based [24, 25, 26]. In block-based (also known
38 as tile-based) refinement, the domain is divided into several predefined non-
39 overlapping, fixed-size blocks [27, 28]. In this method, when a cell is tagged
40 for refinement, the whole block which the cell belongs to is refined. In con-
41 trast, in cell-based refinement, the refinement strategy is implemented on a
42 cell by cell basis which reduces the refined region [29]. Although the cell-
43 based method avoids over refinement, it loses the advantage of using struc-
44 tured meshes. In patch-based AMR, cells that are tagged for refinement are
45 grouped into a new (structured) level overlapping the coarse meshes [30, 31].
46 Thus, patch-based AMR retains much of the selectivity of cell based refine-

47 ment, while benefiting from structured meshes similar to block-based tech-
48 niques.

49 Here we compare the performance of cell-based and patch-based refine-
50 ment and consider their implications for the novel immiscible-fluid fracture
51 flow model [19]. The remainder of this paper is structured as follows: Section
52 2 is dedicated to the description of the immiscible multiphase flow model and
53 the implemented AMR techniques. In Section 3, the simulation results of
54 multiphase flow with different AMR strategies are compared to each other
55 and to those performed on uniform meshes. Where applicable, the results
56 are compared to the available analytical solution to validate the accuracy
57 of the model. In addition, the results of a case study is presented to show
58 the capability and performance of the AMR model to dynamically refine the
59 domain. The main findings and potential future works are summarized in
60 the final section.

61 2. Model Description

62 The immiscible-fluid model used in this paper is based on the approach
63 outlined in Walsh & Carroll [19]. This model has three main components:
64 I) a parallel plate model to provide the cross-sectional flow, II) a lattice-
65 Boltzman-like color-gradient model to provide phase separation, and III) a
66 surface tension model to track the interface between the fluids. Below, we
67 first provide a brief description of the modelling approach. We then discuss
68 the AMR strategies used and how they were implemented into the model.

69 2.1. Parallel plate model

70 The general form of single phase flow through fracture can be expressed
71 using the following equation [32]:

$$\frac{\partial}{\partial x} \left(T_x \frac{\partial P}{\partial x} \right) dx + \frac{\partial}{\partial y} \left(T_y \frac{\partial P}{\partial y} \right) dy = \frac{\partial}{\partial t} (\rho V) , \quad (1)$$

72 in which x and y denote direction, t is time, and P , V , ρ , and T are pres-
73 sure, volume, density, and transmissibility. Using the parallel plate model,
74 transmissibility is calculated as [33]:

$$T = \frac{h^3 w}{12\nu} \quad (2)$$

75 where h is fracture aperture, w is fracture width, and ν is the kinematic
 76 viscosity. At the interface of two adjacent cells (*e.g.* a and b in Figure 1), the
 77 transmissibility is calculated using the harmonic average:

$$T_{ab} = \frac{T_a T_b}{T_a + T_b} \quad (3)$$

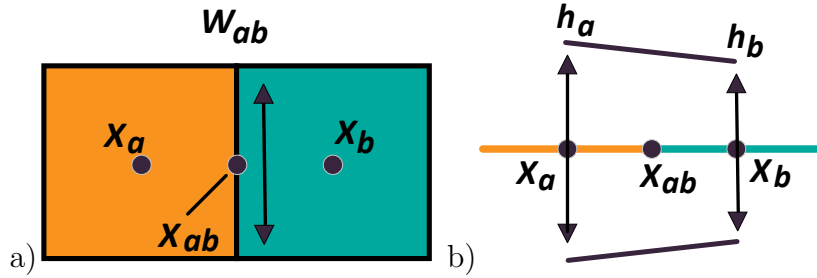


Figure 1: Top-down (a) and side (b) views of adjacent cells showing: the cell centers x_a and x_b , the edge center x_{ab} , the edge length w_{ab} , and the cell apertures h_a and h_b .

78

79 Multiphase flow in the fracture is simulated by coupling the parallel plate
 80 model with a recoloration technique. The separate fluid components are
 81 tracked using a color function, ϕ , that represents the saturation of one of the
 82 fluid phases. The recoloration strategy allows the fluid components to mod-
 83 erately mix, producing a diffusive interface. In a lattice Boltzmann model,
 84 mixing of the components occurs naturally, as a consequence of the inter-
 85 actions between the packets used to represent fluid momentum components.
 86 Phase separation is then enforced through the recoloration scheme that seg-
 87 regates the two phases. However, there is no self-diffusion in parallel plate
 88 models. Instead the intrinsic mixing of lattice-Boltzmann fluid packets is
 89 replicated by introducing an artificial diffusive flux, $\delta\Phi^{diff}$, between adja-
 90 cent cells. Once this is introduced, the same recoloration strategies used in
 91 lattice Boltzmann methods can be applied to the parallel plate flow model.

92 The recoloration strategy used here is based on that presented by Lattva-
 93 Kokko [34]. The strategy introduces a reflection term, β , that determines the
 94 interface width. For each timestep, the change in the color function consists
 95 of a diffusive component and an advective component:

$$\delta\Phi_a = \sum_b \left(\delta\Phi_{ab}^{diff} + \delta\Phi_{ab}^{adv} \right). \quad (4)$$

96 For the adjacent cells a and b in Figure 1, the diffusive term is defined by

$$\delta\Phi_{ab}^{diff} = \frac{D}{w_{ab}^2} \left(\Phi_b [1 - \beta(1 - \Phi_b) \cos(\theta)] - \Phi_a [1 + \beta(1 - \Phi_a) \cos(\theta)] \right) \delta t, \quad (5)$$

97 where D is the diffusion coefficient, w_{ab} is the distance between the cells' center, β is the anti-diffusion coefficient which controls the interface width, 98 and θ is the angle between the color function gradient and the normal to the cell's face (*i.e.* $\cos(\theta) = \frac{\nabla\phi \cdot \hat{\mathbf{n}}}{|\nabla\phi|}$). 99

100 An upwind scheme is used to calculate the advective term:
101

$$\delta\Phi_{ab}^{adv} = \frac{T_{ab}}{V} (P_b - P_a - \Delta P_{ab}) \phi_{ab}^{up}, \quad (6)$$

102 where

$$\phi_{ab}^{up} = \begin{cases} \phi_a & \text{if } P_b - P_a - \Delta P_{ab} \leq 0 \\ \phi_b & \text{if } P_b - P_a - \Delta P_{ab} > 0 \end{cases}. \quad (7)$$

103 Here V is the volume of the cell and ΔP_{ab} is the pressure differential at the interface. The pressure differential is determined by the surface tension, σ , 104 the curvature κ , and the change in color function, $\Delta\phi$:
105

$$\Delta P_{ab} = -\sigma\kappa\Delta\phi \quad (8)$$

106 The interface curvature, κ , is comprised of two parts, the out-of-plane curvature, κ_{\perp} , and the in-plane curvature, κ_{\parallel} :
107

$$\kappa = \kappa_{\perp} + \kappa_{\parallel} = \frac{1}{r_{\perp}} + \frac{1}{r_{\parallel}}, \quad (9)$$

108 where r_{\perp} and r_{\parallel} are the out-of-plane and in-plane radius of curvature, respectively. The out-of-plane radius of curvature is calculated as follows [35]:
109

$$r_{\perp} = \frac{h}{2 \cos(\alpha_w + \alpha_c)}, \quad (10)$$

110 in which h is the fracture aperture, α_w is the wetting angle, and α_c is the convergence angle of the fracture planes as illustrated in Figure 2. The in-plane curvature (*i.e.* parallel to the fracture surface)
111
112

$$\kappa_{\parallel} = -\nabla \cdot \left(\frac{\nabla\phi}{|\nabla\phi|} \right), \quad (11)$$

113 is determined from the color function distribution using the MAC scheme
114 provided in [36].

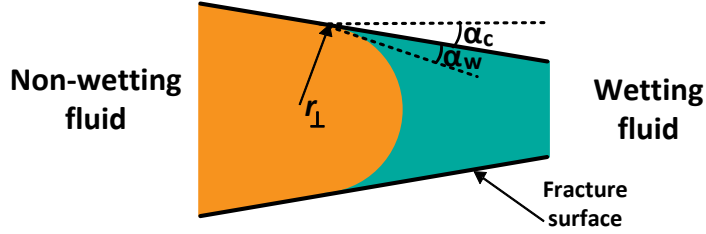


Figure 2: The radius of curvature normal to the fracture surface, r_{\perp} is a function of wetting angle α_w and the angle of convergence α_c .

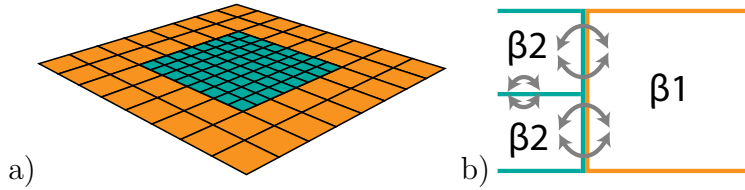


Figure 3: a) Mesh distribution in the cell-based AMR strategy where fine and coarse meshes are adjacent to each other. b) β value is to be changed based on the length scale to provide smooth connection between meshes.

115 *2.2. AMR strategies*

116 Accurate simulation of highly unsteady-state fluid-flow problems, such
 117 as those involving shock waves or moving interfaces, requires a fine mesh
 118 resolution around key areas of interest. However, if a uniform mesh is used
 119 throughout, significant computational effort may be wasted on areas where
 120 nothing occurs. Adaptive mesh refinement provides a solution to this prob-
 121 lem by refining the mesh in active regions while maintaining coarse meshes
 122 elsewhere. Here, we outline cell-based and patch-based refinement strategies
 123 for the immiscible multiphase flow model.

124 Figure 3a is an illustration of the mesh distribution in the cell-based
 125 refinement. In this case, the finer meshes lay adjacent to the coarser ones.
 126 Because individual cells are tagged for refinement, the footprint of the refined
 127 region is less than that for block-based refinement.

128 At coarse-fine mesh interfaces, the flux of particles should be adjusted
 129 to get a consistent flux across the two meshes. This can be accomplished
 130 by changing the value of β – the anti-diffusion parameter controlling the
 131 number of particles crossing the interface (Figure 3b). Thus the key is to
 132 find a relationship between the length scale and β to ensure consistency
 133 between the different mesh scales.

134 Figure 4a shows the shape of the fully developed interface for different
 135 β values ranging from 0.3 to 1.2 using a uniform mesh structure throughout
 136 the domain. Like the other diffusive-interface methods [37, 38], use of a color
 137 function causes the interface to spread over a portion of the domain. Larger
 138 β values result in a greater portion of the color particles being reflected over
 the cell length – producing a narrower interface.

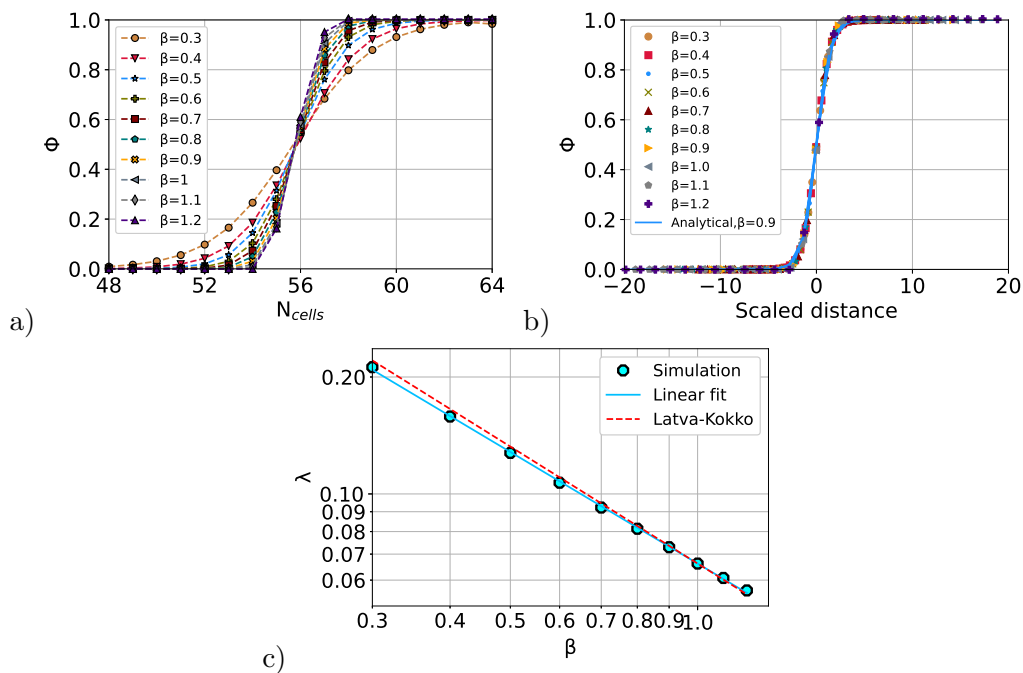


Figure 4: Effect of β on interface width: a) Fully developed interface profiles for different β values versus cell's number, b) The same profiles as in figure a and the profile for quasi-analytical solution with $\beta = 0.9$ c) Length scale, λ , versus β profile along with the Latva-Kokko quasi-analytical solution.

139

140 Latva-Kokko [34] derived a quasi-analytical solution which describes the
 141 shape of the fully developed interface:

$$\phi = \frac{e^{k(\beta)(x-x_0)}}{1 + e^{k(\beta)(x-x_0)}} \quad (12)$$

$$k(\beta) = \frac{2}{3}(1 + \sqrt{2})\beta, \quad (13)$$

142 in which ϕ is colour function, $x - x_0$ is the distance from the interface location,
 143 and β is the anti-diffusion coefficient. The interface profiles in Figure 4a were

144 fitted to the quasi-analytical interface profile corresponds to $\beta = 0.9$ (see
145 Figure 4b), yielding the following empirical equation:

$$\ln(\lambda) = -0.957677 \ln(\beta) - 2.578139, \quad (14)$$

146 where λ denotes the length scale. Figure 4c illustrates the length scale, λ , and
147 β relationship from the simulation results along with those obtained from the
148 linear fit and quasi analytical solution. As can be seen, the quasi-analytical
149 solution deviates from the simulation results. Although this inconsistency
150 is small, capturing the non-linearity is important to accurately match the
151 interface behaviour at different scales. Hence, equation 14 was incorporated
152 into the model to change the β values according to the length scale in the
153 case of cell-based refinement.

154 The patch-based refinement was conducted using the AMReX library [39].
155 AMReX provides a framework for building parallel, block-structured AMR
156 for solving system of partial differential equations (PDEs). Figure 5a illus-
157 trates an example of mesh distribution for patch-based strategy where a finer
158 level is created on top of the coarser level out of the patches tagged for refine-
159 ment. Each patch contains the ghost cells storing the necessary information
160 from the neighbours needed for computation. A hierarchical sub-cycling with
161 time algorithm is used – in which the finer level is advanced with smaller time
162 step than the coarse level. For example, as is shown in Figure 5b, if the new
163 level 2 is refined by a factor of two, it advances for two steps with each time
164 step half of that for the coarser level. Finally the two levels are synchron-
165 ized and the color distribution is updated throughout the domain. The
166 sub-cycling process removes the need for a $\lambda - \beta$ relationship like the earlier
167 model.

168 3. Simulation results

169 In this section, simulation results for the cell-based and patch-based
170 refinement strategies are presented and compared to those from uniform
171 meshes. Next an example is given showing how the model can accurately
172 track the interfacial properties of small droplets where using the uniform
173 meshes deviates significantly from the analytical solution. Finally, a case
174 study is presented showing the ability of the model to dynamically refine the
175 domain as the interface moves across the fracture space.

176 Figure 6a shows the steady state color distribution profile of a droplet
177 simulated on a uniform mesh. The radial distribution of the colour function

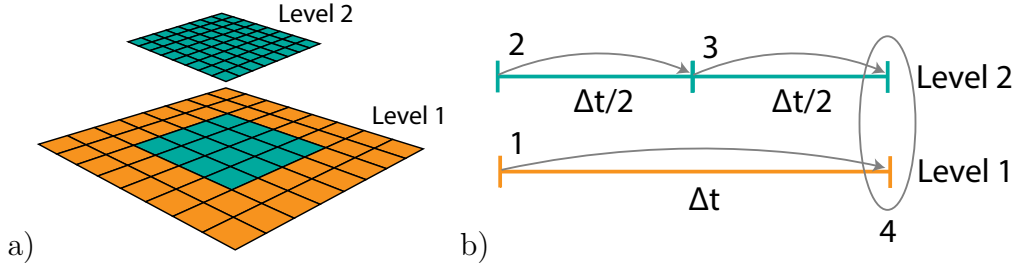


Figure 5: Mesh distribution in overlapping mesh refinement strategy. A finer level is defined on the top of the coarser level. b) The sub-cycling stages when the new level is refined by a factor of two: 1) integrate level 1 over Δt , 2,3) integrate level 2 over $\Delta t/2$, 4) synchronize levels 1 and 2.

178 over a horizontal cross section passing through the center of the droplet is
 179 illustrated in Figure 6b. As already mentioned, the width of the interface
 180 is governed by β parameter. For this paper the typical β value of 0.9 [34]
 181 was used unless explicitly mentioned otherwise. Periodic boundary conditions
 182 applied to both x and y boundaries. Two separate sets of simulations
 183 were conducted to test both the cell-based refinement and the patch-based
 refinement strategies.

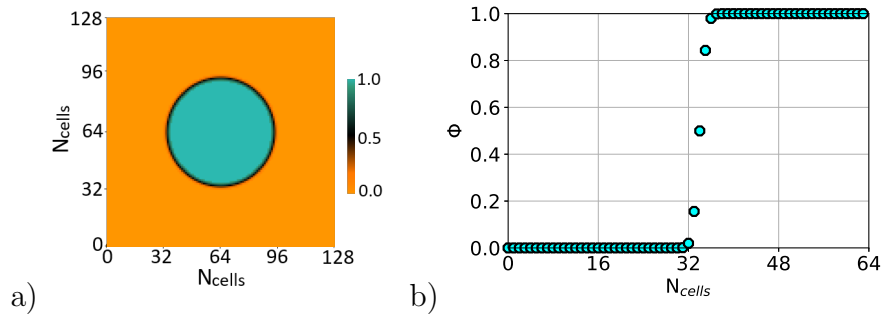


Figure 6: a: Top view of the colour function distribution at the steady state condition for $\beta = 0.9$. b: Radial distribution of the color function versus the cell's number.

184

185 The first set of simulations evaluated the cell-based refinement strategy.
 186 Three different cases were considered to test if the same interface profiles can
 187 be generated using $\lambda - \beta$ relationship (equation 14):

- 188 1. In the first case, the cell size is uniform throughout the domain;
- 189 2. In the second, the cell size in half of the interface region was refined by
 190 a factor of two; and

191 3. In the third, all of the interface was refined by a factor of two.

192 For the first case, $\beta = 0.9$ was used in all cells, while in the last two cases,
 193 β was changed in the refined cells according to Equation 14. The three
 194 simulations began with the same initial conditions and were advanced until
 195 the steady state condition was achieved. The results of these simulations are
 196 presented in Figure 7a. The three plots are in good agreement, demonstrating
 197 the smooth communication between the different levels provided by the $\lambda - \beta$
 relationship.

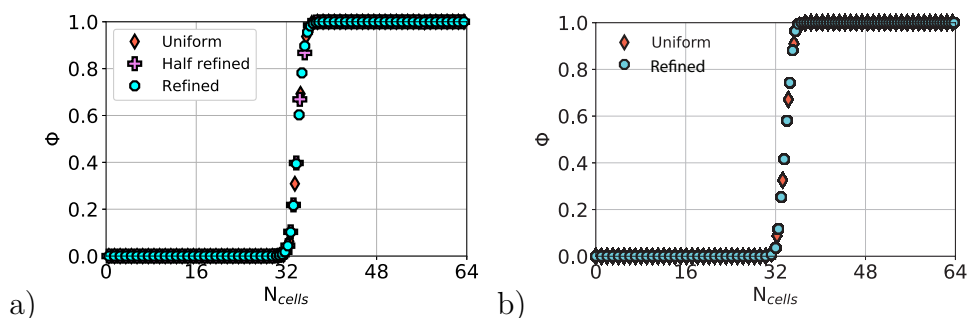


Figure 7: Steady-state interface profile versus cell's number for uniform and refined meshes: a) cell-base AMR; b) patch-based AMR.

198

199 Two cases are considered in the second example, which demonstrates
 200 the patch-based refinement strategy. In the first, uniform meshes were used
 201 throughout the domain and in the second, a refined region was defined on top
 202 of the coarse level just at the droplet region. As is presented in Figure 7b,
 203 the fully developed interface profiles for both cases match quite well which
 204 confirms the accuracy of the patch-based refinement strategy.

205 As noted earlier, one of the main challenges in immiscible multiphase flow
 206 is tracking the interface properties between the phases. Fine mesh resolution
 207 is normally needed to accurately resolve the forces exerting on the interface
 208 which can make the simulation computationally expensive, particularly when
 209 only a small portion of the domain is occupied by one of the phases. In these
 210 cases using AMR can significantly cut the simulation costs by selectively
 211 refining the domain as is depicted in Figure 8.

212 Figure 9a shows the pressure differential across the boundary of a single
 213 droplet defined on a uniform mesh as a function of the droplet radius. Here r_D
 214 is dimensionless droplet radius which is defined as the droplet radius divided
 215 by the length of the coarsest mesh ($r_D = \frac{r}{l}$ where r is droplet radius and

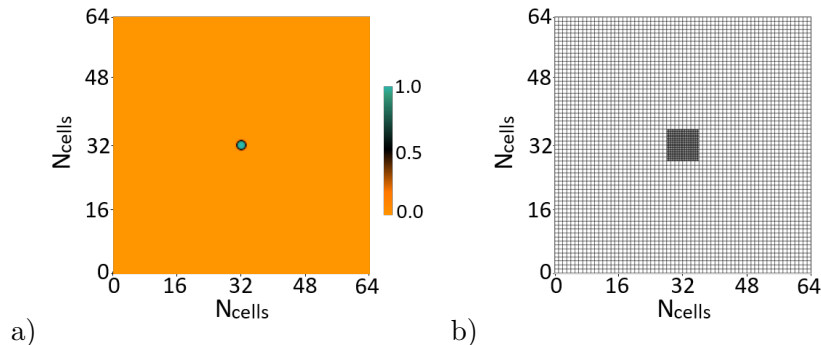


Figure 8: a) Colour distribution profile for a small droplet with the radius equal to the length of a coarse cell. b) A refined level is created on top of the coarse level at the droplet region with cell sizes that are four times smaller.

216 l is length of the coarsest cell). The value of $r_D=1$ means that the droplet
 217 radius is equal to the size of the coarsest mesh. The simulation results are
 218 compared to the Young-Laplace analytical solution for the capillary pressure
 219 across the interface of two static phases:

$$\Delta P = -\sigma \left(\frac{1}{r_1} + \frac{1}{r_2} \right), \quad (15)$$

220 where σ is the interfacial tension and r_1 and r_2 are the principal radii of cur-
 221 vature. As can be seen in the figure, for the droplet radius smaller than four
 222 coarse grid size, the simulation results deviate from the analytical solution
 223 which is similar to what is observed in similar lattice Boltzmann models with
 224 diffusive interfaces [34, 37, 22, 19]. When the droplet radius equals the size
 225 of the coarse simulation cell, the the analytical solution and the simulation
 226 results differ by more than 120%. Figure 9b shows the AMR simulation re-
 227 sults for similar droplet radii as in Figure 9a. A refined level is defined on
 228 top of the coarse level at the droplet boundary (see Figure 8). This provides
 229 sufficient resolution to accurately capture the interface properties. In this
 230 case, even for the smallest droplet radius, the simulation results are in good
 231 agreement with the analytical solution.

232 In the final example, merging droplets are considered to test the ability of
 233 the model in dynamic tracking of moving interfaces. Using the patch-based
 234 AMR model, four droplets with different radius were introduced at the center
 235 of the domain (see Figure 10a). Figure 10b shows the mesh distribution
 236 over the domain. In this case two refined levels were considered. The first

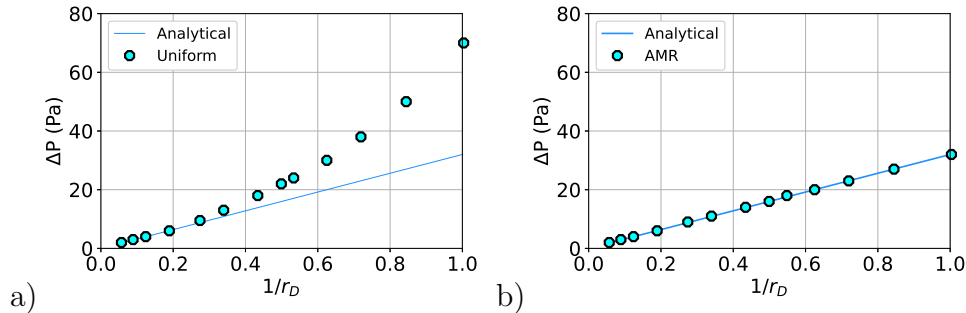


Figure 9: Pressure differential (ΔP) as a function of droplet radius for neutrally wetting fracture surface ($\alpha_w = 90^\circ$), fracture aperture of $1 \mu m$, and surface tension of 50 dyne/cm : a) uniform mesh, b) AMR. The solid line shows Young-Laplace analytical solution.

237 level was set to be defined at the regions with $0.01 < \phi < 0.99$ and the
 238 second one at the regions with $0.2 < \phi < 0.8$. The color distribution profile
 239 along a horizontal line through the center of the domain is also depicted in
 240 Figure 10c. As Figure 10d illustrates the interfaces evolve as the simulation
 241 proceeds and the smaller droplets merge into the largest one. Figure 10e and
 242 Figure 10f show the updated refined levels and the color profile, respectively.
 243 The simulation proceeded until the steady state condition was achieved. At
 244 this point, a single droplet was created out of the small droplets as is depicted
 245 in Figure 10g along with the corresponding mesh distribution in Figure 10h
 246 and color profile in Figure 10i. This demonstrates the ability of the AMR
 247 model to dynamically track evolving interfaces. As the figures show, the
 248 refined levels are continuously updated in accordance to the new color distri-
 249 bution to accurately capture the interfacial properties – providing sufficient
 250 resolution in those regions and reducing the total computational cost.

251 4. Conclusions

252 Accurate tracking of interfacial properties remains a key challenge when
 253 simulating immiscible multiphase flows in fractures. A fine uniform-mesh
 254 defined throughout the domain can accurately resolve the forces exerting on
 255 fluid interfaces. However, this strategy is computationally inefficient, as a
 256 coarser mesh resolution is often sufficient for most of the domain.

257 Adaptive Mesh Refinement offers a solution to this problem by dynam-
 258 ically increasing the mesh resolution as needed in different parts of the do-
 259 main. Thus the simulation accuracy is retained for reduced computational

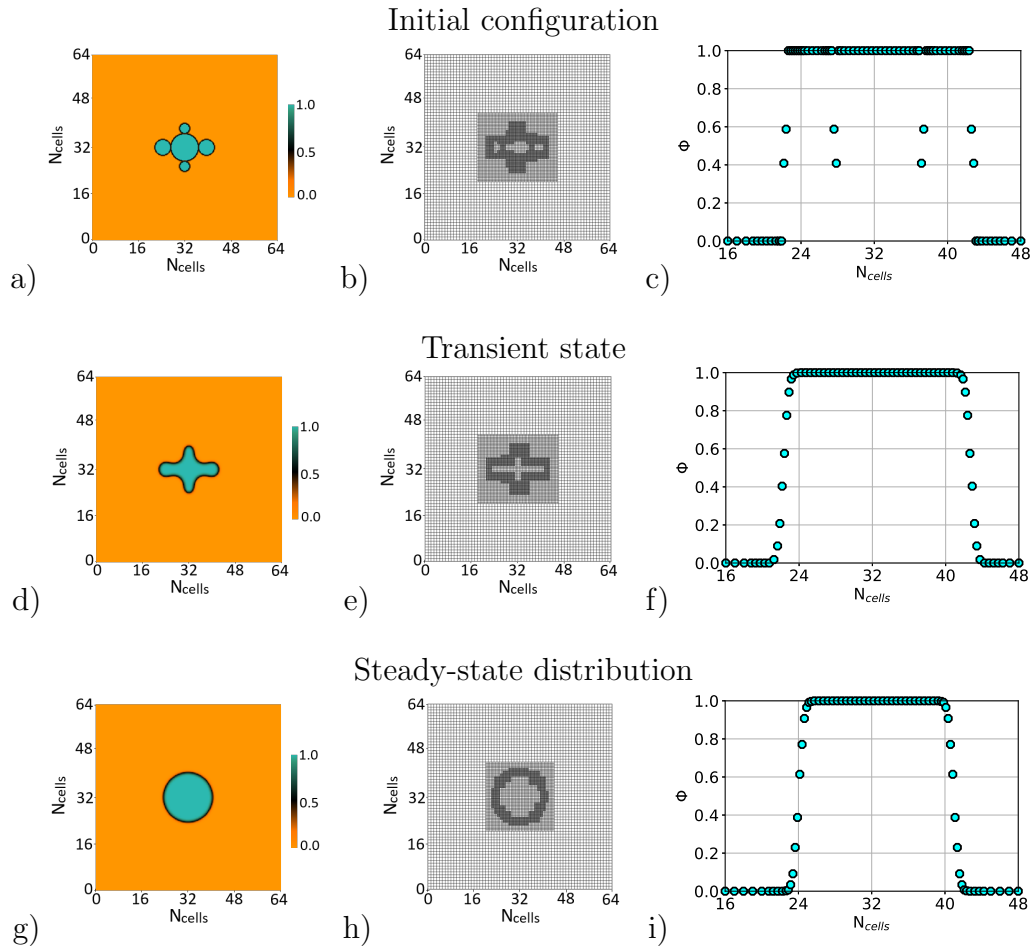


Figure 10: Different stages in a simulation tracking merging droplets (wetting angle $\alpha_w = 60^\circ$, fracture aperture $h = 1\mu\text{m}$, and surface tension $\sigma = 50\text{dyne/cm}$). a) shows the initial 2D color distribution profile, b) shows the corresponding mesh distribution, and c) shows the color distribution along the center line. Figures d), e) and f) show the same plots shortly after the start; while Figures g), h), and i) show the steady state distributions.

260 cost. In this paper, cell-based and patch-based AMR strategies were incor-
261 porated into a model that describes immiscible fracture flows by combining
262 a parallel-plate model with an lattice Boltzmann recoloration scheme.

263 The cell-based refinement strategy was implemented by introducing a
264 mathematical expression to relate the length scale to the anti-diffusion pa-
265 rameter that controls the interface width. In the patch-based refinement, a
266 recursive hierarchical sub-cycling in time is used where the finer level ad-
267 vances with smaller time step than the coarser level. The accuracy of both
268 methods was successfully tested by considering different cases and comparing
269 the results to those from uniform meshes.

270 For small droplets where uniform meshes are unable to resolve the in-
271 terface properties, the AMR model is able to successfully produce the same
272 results as those of the analytical solution. Finally, the ability of the model to
273 dynamically refine the domain was illustrated through an example in which
274 small droplets are joined together to create a large droplet. In this case, as
275 the interfaces evolved with time, the refined levels were updated based on the
276 new color distribution to both provide sufficient resolution at the interface
277 and reduce the computational effort.

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