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1 **A theoretical analysis of mass leakage at boundaries within the lattice Boltzmann**  
2 **method**

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11 Mass leakage at boundaries can be a critical issue for reliability of the lattice Boltzmann  
12 (LB) method based on Cartesian grids. Despite numerous work based on the LB method,  
13 the intrinsic macroscopic mechanisms causing mass leakage are still not fully charac-  
14 terised, but are essential to improve the mass conservation of LB simulations. In this paper,  
15 an original theoretical investigation of mass leakage at boundaries is proposed within the  
16 general LB framework. It is demonstrated that the mass leakage originates from the in-  
17 trinsic deficiency of the wall-cut LB links at boundary nodes in recovering macroscopic  
18 momenta. From a mesoscopic-level definition, i.e. the net loss of distribution functions  
19 during the streaming process, the local mass leakage at individual boundary nodes and its  
20 averaged value along smooth boundaries are mathematically expressed using macroscopic  
21 variables. The local mass leakage is shown to be dominated by terms proportional to the  
22 tangential momentum component. In contrast, the averaged mass leakage is shown to be  
23 contributed from various terms including the boundary curvature, the tangential momen-  
24 tum, and the gradients of density, momentum and momentum flux. Meanwhile, amplitude  
25 of the averaged mass leakage is theoretically estimated to be proportional to the local grid  
26 spacing, based on which a first-order accurate correction scheme is proposed. In addition,  
27 both the local and averaged mass leakage are demonstrated to be significantly dependent  
28 on boundary orientation with respect to the grid. The proposed theoretical analysis is  
29 assessed by performing numerical experiments. Two-dimensional weakly compressible  
30 flows through straight and curved moving channels are considered to estimate each term  
31 appearing in the theoretical analysis. The numerical results are in very good agreement  
32 with the proposed analysis, and the proposed mass correction scheme based on the av-  
33 eraged mass leakage effectively cures the mass leakage problems in the considered test  
34 cases.

## 35 I. INTRODUCTION

36 During the last three decades, the lattice Boltzmann (LB) method has received a growing inter-  
37 est as an alternative computational fluid dynamic (CFD) tool, and it is nowadays widely applied  
38 in various problems<sup>1-3</sup>. Compared to the conventional CFD techniques the LB method is praised  
39 for its linear convective term, simple parallel implementation and high computational efficiency  
40 for unsteady flow simulations. However, since the LB method is usually implemented on Carte-  
41 sian grids, the stair-wise Cartesian grid boundaries (defined by “boundary nodes”) near curved  
42 and/or inclined solid walls raise challenges for accurate boundary treatments. Especially, the mass  
43 conservation (or inversely the mass leakage minimization) at boundary nodes is of fundamental  
44 importance to guarantee reliable and accurate solutions, in particular in internal flows, but it is still  
45 not fully understood and requires to be theoretically addressed.

46 Despite the stair-wise distribution of boundary nodes, various boundary treatments have been  
47 developed within the LB framework. The simplest and most commonly used boundary method is  
48 the bounce-back (BB) scheme in which the distribution functions streaming towards boundaries  
49 are directly returned to the boundaries node along the reversed directions to mimic particles col-  
50 lision dynamics on non-slip interfaces<sup>4-6</sup>. Although this method is simple to implement for arbi-  
51 trary geometries and satisfies the mass conservation well, it has a zero-order accuracy for pressure  
52 and first-order accuracy for velocity only when non-aligned boundaries involved<sup>7-9</sup>, while the LB  
53 method itself is of second-order accurate<sup>10,11</sup>. To develop more accurate boundary treatments,  
54 Chen *et al.*<sup>12</sup> proposed an extrapolation scheme to reconstruct the unknown distribution functions  
55 directly from their neighbouring counterparts. Filipova and Hanel<sup>13</sup> proposed a scheme to recon-  
56 struct the unknown distribution functions from macroscopic variables and their gradients, which  
57 are extrapolated from those known in the fluid domain. These two schemes are expected to ex-  
58 hibit a second-order accuracy, but suffer from numerical instability in some situations due to the  
59 extrapolation operations. The extrapolation-caused instability was cured by Mei *et al.*<sup>14</sup> by ad-  
60 justing the extrapolation stencil properly. Later, Bouzidi *et al.*<sup>15</sup> proposed a second-order accurate  
61 method which avoids extrapolation by combining the bounce-back concept with interpolation.  
62 This is achieved by extending the interpolation stencil for a prescribed LB link reversely to the  
63 fluid domain when a node in the non-fluid region is required. The scheme was further improved  
64 by Ginzburg and d’Humières<sup>16</sup> who proposed a more general framework from which a third-order  
65 accurate multi-reflection scheme was derived. These schemes have been demonstrated to be ap-

66 parently more accurate than the BB method. However, except in some special cases (e.g. simple  
67 steady Stokes flow simulations where the LB process is purely linear<sup>7,17,18</sup>), the mass conservation  
68 is generally compromised by the applied interpolation or extrapolation operations<sup>19,20</sup>.

69 Apart from the above mentioned schemes focusing on the reconstruction of the unknown distri-  
70 bution functions, there is another kind of boundary treatment relying on the use of an external body  
71 force tuned to enforce some constrains on the macroscopic quantities. Following the seminal work  
72 on immersed boundary method by Peskin<sup>21</sup>, many variants and improvements have been proposed  
73 and extensively applied within the LB framework, e.g.<sup>22,23</sup>. Usually, this boundary strategy uses  
74 lattice nodes in non-fluid regions so that the streaming process can be implemented without sens-  
75 ing the boundaries. On the one hand this feature is very favourable for moving and/or deformable  
76 boundary interfaces, but on the other hand it allows for local non-physical information leakage,  
77 e.g. mass and momentum, to the non-fluid regions.

78 Many research efforts have been devoted to studying the mass leakage in LB simulations. Con-  
79 ceptually, the LB method relies on the preservation of conservativity, i.e. preserving the zeroth  
80 and first-order moments of the distribution function to recover density and momentum, along with  
81 the associated collision invariants to recover the correct macroscopic mass and momentum con-  
82 servation equations.

83 Ginzburg & d’Humières<sup>7</sup> proposed a local second order accurate boundary (LSOB) treatment  
84 reconstructing unknown distribution functions from macroscopic variables and their gradients ac-  
85 cording to Chapman-Enskog analysis up to second order. In the analysis of simple Stokes flows  
86 (Reynolds number much less than unit), including the Couette and Poiseuille flow, using linear  
87 LB simulations, the LSOB method gave exact results without mass leakage. Meanwhile, the lo-  
88 cal mass leakage along aligned boundaries was analysed to be linearly dependant on the normal  
89 momentum as well its high order ( $\geq 2$ ) normal gradients. In a more general background beyond  
90 Stokes flow, Lallemand and Luo<sup>19</sup> pointed out that interpolation during the reconstruction of un-  
91 known distribution functions could lead to a breakdown of mass conservation, thus yielding mass  
92 leakage. To avoid interpolation-related issues, Kao and Yang<sup>24</sup> proposed an interpolation-free  
93 scheme based on the grid refinement concept<sup>13</sup> without refining the grid in practice. However,  
94 this scheme still does not guarantee mass conservation<sup>25</sup>. Rohde *et al.*<sup>26</sup> observed mass leak-  
95 age in LB simulations applying finite-volume flux techniques at moving boundaries. Bao *et al.*<sup>27</sup>  
96 observed apparent mass leakage in simulating flow through a U-shaped tube using interpolation-  
97 based boundary methods, and proposed a scheme to enforce mass conservation by directly ad-

TABLE I. Examples of mass leakage observation using the BGK lattice Boltzmann model. "FH" refers to the method proposed by Filipova and Hanel<sup>13</sup>, "MLS" refers to the boundary treatment proposed by Mei *et al.*<sup>14</sup>, "IPF" refers to the interpolation-free method proposed by Kao and Yang<sup>24</sup>, "NEE" is short for "Non-equilibrium extrapolation", "Bouzidi" refers to the schemes proposed by Bouzidi *et al.*<sup>15</sup>, "ZY" refers to the scheme proposed by Zhao and Yong<sup>33</sup>, "LSOB" refers to the scheme proposed by Ginzburg<sup>7</sup>, and "MR" refers to the scheme proposed by Ginzburg and d'Humieres<sup>16</sup>.

Ref.	Boundary methods	Configurations
Bao <i>et al.</i> <sup>27</sup>	FH, MLS	U-shaped channel
Oulaid&Zhang <sup>11</sup>	Density extrapolation	Aligned boundaries
Sanjeevi <i>et al.</i> <sup>25</sup>	IPF	Aligned boundaries, sharp corners
Feng&Lim <sup>30</sup>	NEE	Aligned boundaries , sharp corners
Yu <i>et al.</i> <sup>29</sup>	MLS, Bouzidi, ZY	Aligned boundaries
Ginzburg <i>et al.</i> <sup>7,17,18</sup>	LSOB, MR	Straight channel, curved boundaries

98 justing local density values. Similar mass correction schemes are also proposed and tested by  
99 other researchers<sup>28,29</sup>. There are also some mass-conservative strategies specifically valid for flat  
100 walls aligned with coordinate axes<sup>11,28,30</sup>. Especially, Feng and Lim<sup>30</sup> reported that mass leak-  
101 age around sharp boundary corners is much more significant than along aligned walls in their LB  
102 simulations. In addition, it was reported that mass leakage in LB simulations of Stokes flow is so  
103 low that local mass correction is not necessary and even harmful in some situations<sup>31,32</sup>, which is  
104 consistent with the observation that mass leakage is more significant at high Reynolds numbers  
105 and/or at moving boundaries<sup>25</sup>. More recently, Ginzburg<sup>17</sup> proposed to include mass sources in  
106 the multi-reflection boundary scheme within a two-relaxation-time LB framework, and it was suc-  
107 cessfully applied to achieve mass balance across interfaces in advection-diffusion and Stokes flow  
108 simulations. Besides, within the same LB framework, a uniform normal mass flux was demon-  
109 strated to outperform a uniform mass-source in advection-diffusion simulations<sup>18</sup>. Some examples  
110 of mass leakage observation are summarised in Table I. Apparently, the observed mass leakage  
111 is supposed to depends on many factors, such as the boundary orientation, the Reynolds number  
112 value and specific flow characteristics. However, mechanisms responsible for the mass leakage at  
113 boundaries within the LB framework are still not clearly and rigorously characterised, which is the  
114 motivation of this paper.

115 This paper is focused on macroscopic mechanisms of mass leakage in LB simulations. Firstly,  
116 some basic characteristics of the LB method are presented in §II. Secondly, the mass leakage is  
117 defined as the net loss of distribution functions from a mesoscopic view in §III. Thirdly, local mass  
118 leakage at individual boundary nodes is mathematically expressed using macroscopic variables in  
119 §IV. Based on the local mass leakage analysis, averaged mass leakage over smooth boundaries  
120 is theoretically investigated in §V. After that, a mass correction scheme based on the averaged  
121 mass leakage is proposed in §VI. To validate the proposed theoretical analysis and assess the mass  
122 correction scheme, numerical experiments dealing with two-dimensional flows through straight  
123 and curved channels with moving boundaries are simulated using an in-house LB solver in §VII.  
124 Finally, some conclusions are drawn in §VIII.

## 125 II. FUNDAMENTALS OF THE LB METHOD

126 As a fundamental basis to study mass leakage in LB simulations, some key features of the LB  
127 method are reminded with an emphasis on the mass conservation issue in this section. The LB  
128 method models fluid dynamics by considering a finite set of discrete velocities  $e_i$  and distribution  
129 functions  $f_i$  defined at a mesoscopic level. Specifically, the distribution functions are assumed to  
130 obey a set of coupled advection-relaxation partial differential equations, which can be interpreted  
131 as a discretisation in space, time and velocity space of the original continuous Boltzmann equation  
132 in kinetic theory. The relaxation term is a model of the exact collision term that appears in the  
133 Boltzmann equation, stemming from the idea that the net statistical effect of collisions is to drive  
134 the flow toward thermodynamic equilibrium.

135 Generally, the LB method can be formulated as follows:

$$136 \quad f_i(\mathbf{x}, t) - f_i(\mathbf{x} - \mathbf{e}_i \Delta t, t - \Delta t) = \ell_i(\mathbf{f} - \mathbf{f}^{eq}) \quad (1)$$

137 where  $\Delta t$  is the time step,  $\mathbf{f}$  and  $\mathbf{f}^{eq}$  are vectors containing  $f_i(\mathbf{x} - \mathbf{e}_i \Delta t, t - \Delta t)$  and the equi-  
138 librium distribution functions  $f_i^{eq}$ , respectively, and  $\ell_i$  is a scalar collision function of  $\mathbf{f} - \mathbf{f}^{eq}$  for  
139  $f_i$ . Each component of  $\mathbf{e}_i$  is equal to either 0 or  $\pm c$  with  $c = \Delta x / \Delta t$  and  $\Delta x$  being the grid spacing.  
140 The left-hand side of Eq. (1) originates in a Lagrangian implementation of the linear convective  
141 streaming process, while the right-hand side is generally a nonlinear collision process (might also  
142 be linear when the physics is linear, e.g. advection-diffusion Stokes flow). By selecting adequate  
143 collision operator  $\ell_i$ , Eq. (1) is able to recover the classic single-relaxation-time (SRT)<sup>34</sup>, the

144 multiple-relaxation-times (MRT)<sup>35</sup>, and the regularised (RLB)<sup>36</sup> LB methods. The most widely  
 145 applied definition of  $f_i^{eq}$  is a truncated polynomial expansion of the original Maxwell-Boltzmann  
 146 equilibrium distribution function, i.e.

$$147 \quad f_i^{eq} = \omega_i \rho \left[ 1 + \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^2} + O(Ma^3) \right]. \quad (2)$$

148 where  $\omega_i$  is the  $i^{th}$  weighting factor,  $c_s$  is the lattice sound speed,  $\rho = \sum f_i$ ,  $\mathbf{u} = \sum f_i \mathbf{e}_i / \rho$ , and  
 149  $Ma$  is the local Mach number  $\|\mathbf{u}\|/c_s$ . It should be noticed that  $c_s/c$  is a tunable parameter de-  
 150 pending on the lattice configuration as well as the adopted discrete velocities (e.g.,  $c_s/c = \frac{1}{\sqrt{3}}$  for  
 151 regular lattices using the D2Q9 model)<sup>16,37</sup>. By using terms up to the first-order in  $f_i^{eq}$  (i.e. without  
 152 non-linear terms in Eq. (2)) the LB method could restore to linear advection-diffusion equations.  
 153 Considering that mass leakage in this kind of linear LB processes has been well analysed by  
 154 Ginzburg<sup>7</sup>, and demonstrated to be fully avoidable by choosing proper high order accurate bound-  
 155 ary treatments in simple Stokes flow simulations<sup>7,17</sup>, hereafter this paper will be focused on more  
 156 general and complex situation. Usually, by using terms up to second-order in  $f_i^{eq}$ , the LB method  
 157 is sufficient to recover the low-Mach weakly compressible Navier-Stokes equations<sup>35</sup>. The higher  
 158 order terms, e.g.  $O(Ma^3)$  in Eq. (2), can be used to account for thermal and compressible effect<sup>38</sup>.  
 159 Particularly, the LB equation (1) can be directly restored to the macroscopic mass equation by  
 160 taking its zeroth moment, i.e.,

$$161 \quad \partial \rho / \partial t + \nabla \cdot (\rho \mathbf{u}) = 0. \quad (3)$$

162 However, it should be pointed out that this restoration is based on a complete stream process,  
 163 i.e., all the neighbouring nodes are within the fluid domain, thus not taking boundary conditions  
 164 into consideration. In addition, as discussed in the introduction, the reported boundary treatments  
 165 within LB framework are not designed to directly satisfy the mass equation but are more likely  
 166 focused on the boundary velocity condition. Consequently, mass leakage usually occurs along  
 167 boundaries and cannot be directly described by the macroscopic mass equation.

168 To unveil the macroscopic mechanisms of mass leakage, it is important to express the non-  
 169 equilibrium parts of the distribution functions,  $f_i^{ne} = f_i - f_i^{eq}$ , as functions of their macroscopically  
 170 determined equilibrium counterparts  $f_i^{eq}$ . By applying Taylor's series expansion, the LB equation  
 171 (1) can be rewritten as:

$$172 \quad \frac{D\mathbf{f}}{Dt} + \frac{\Delta t}{2} \frac{D^2 \mathbf{f}}{Dt^2} + O(\Delta t^2) = \frac{1}{\Delta t} \mathcal{L}(\mathbf{f}^{ne}) \quad (4)$$



173 where  $\mathbf{f}^{ne} = \mathbf{f} - \mathbf{f}^{eq}$ ,  $D/Dt$  is a diagonal matrix spanned by material derivative operators,  
 174 e.g.  $\partial/\partial t + \mathbf{e}_i \cdot \nabla$  along  $\mathbf{e}_i$ , and  $\mathcal{L}$  is a matrix that contains all the linear collision operators  $\ell_i$ .  
 175 Applying  $D/Dt$  to both sides of Eq. (4), one obtains:

$$176 \quad \frac{D^2 \mathbf{f}}{Dt^2} = \frac{1}{\Delta t} \mathcal{L} \left( \frac{D \mathbf{f}^{ne}}{Dt} \right) - \frac{\Delta t}{2} \frac{D^3 \mathbf{f}}{Dt^3} + O(\Delta t^2). \quad (5)$$

177 Substituting  $\mathbf{f} = \mathbf{f}^{eq} + \mathbf{f}^{ne}$  and Eq. (5) into Eq. (4), the non-equilibrium part can be expressed  
 178 as follows

$$179 \quad \mathbf{f}^{ne} = \Delta t \mathcal{L}^{-1} \left( \frac{D \mathbf{f}^{eq}}{Dt} \right) + \Delta t \left( \mathcal{L}^{-1} + \frac{1}{2} \mathbf{Id} \right) \left( \frac{D \mathbf{f}^{ne}}{Dt} \right) + O(\Delta t^2) \quad (6)$$

180 where  $\mathbf{Id}$  is the identity matrix. Applying  $D/Dt$  to both sides of this equation, it comes:

$$181 \quad \frac{D \mathbf{f}^{ne}}{Dt} = \Delta t \mathcal{L}^{-1} \left( \frac{D^2 \mathbf{f}^{eq}}{Dt^2} \right) + \Delta t \left( \mathcal{L}^{-1} + \frac{1}{2} \mathbf{Id} \right) \left( \frac{D^2 \mathbf{f}^{ne}}{Dt^2} \right) + O(\Delta t^2) \quad (7)$$

182 Now substituting Eq. (7) into Eq. (6), one obtains:

$$183 \quad \mathbf{f}^{ne} = \Delta t \mathcal{L}^{-1} \left( \frac{D \mathbf{f}^{eq}}{Dt} \right) + O(\Delta t^2) \quad (8)$$

184 This relation shows that  $\mathbf{f}^{ne}$  contains time-dependent informations. Based on Eq. (8),  $\mathbf{f}$  can be  
 185 expressed as a function of  $\mathbf{f}^{eq}$  :

$$186 \quad \mathbf{f} = \mathbf{f}^{eq} + \mathbf{f}^{ne} = \mathbf{f}^{eq} + \Delta t \mathcal{L}^{-1} \left( \frac{D \mathbf{f}^{eq}}{Dt} \right) + O(\Delta t^2) \quad (9)$$

187 where  $\mathbf{f}^{eq}$  is explicitly determined by  $\rho$  and  $\mathbf{u}$  through Eq. (2). According to Eq. (8), amplitude  
 188 of the non-equilibrium distribution functions  $\mathbf{f}^{ne}$  scales as  $O(\Delta t \frac{D \mathbf{f}^{eq}}{Dt})$ , which is consistent with the  
 189 widely used Chapman-Enskog analysis<sup>35</sup>. Noticeably, external body force is not included from Eq.  
 190 (1) to (9) because its effect on mass leakage can be directly expressed by the change of  $\mathbf{f}^{eq}$  due  
 191 to the induced change of  $\rho \mathbf{u}$ . This is reasonable considering that the LB simulations have been  
 192 verified to be insensitive to the adopted external force models<sup>39</sup>.

193 At boundary nodes, reconstruction of  $\mathbf{f}$  using Eq. (9) represents a second-order accurate  
 194 boundary treatment. The mass leakage analysis presented hereafter is related to second-order  
 195 accurate boundary treatments based on this equation in 2D.

### 196 III. DEFINITIONS OF MASS LEAKAGE

197 The mass leakage at boundaries in LB simulations is defined in this subsection. For the sake  
 198 of convenience, a discrete velocity together with the associated distribution function is referred to  
 199 as a LB link hereafter, and a fluid lattice node with wall-cut LB links is referred to as a boundary  
 200 node (e.g. node  $B_1$  shown in Fig. 1(a)).

201 Following the widely applied conception<sup>40–45</sup>, the mass leakage is defined as the difference  
 202 between the sum of the distribution functions streaming out from the fluid domain ( e.g.  $f_1$  and  $f_3$   
 203 in Fig. 1(a)) and that of those streaming into the fluid domain (e.g.  $f_2$  and  $f_4$  Fig. 1(a)). In addition,  
 204 the normal mass flux due to the movement of the boundary should be deducted. Consequently, the  
 205 local mass leakage per time unit per area unit can be defined as

$$206 \quad E(\mathbf{x}) = \frac{\Delta x^D}{\Delta S \Delta t} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} [f_i(\mathbf{x}) - f_{\bar{i}}(\mathbf{x} + \mathbf{e}_i \Delta t)] + \rho_w \mathbf{U} \cdot \mathbf{n} \quad (10)$$

207 where  $\mathbf{x}$  is the coordinate vector of a boundary node,  $D$  is the number of spatial dimensions  
 208 ( $D = 2$  here),  $S$  is the solid side of the boundary,  $f_i$  and  $f_{\bar{i}}$  corresponds to discrete velocities in  
 209 opposite directions, i.e.  $\mathbf{e}_i$  and  $-\mathbf{e}_i$ , respectively,  $\rho_w$  and  $\mathbf{U}$  are the fluid density and velocity at  
 210 the projection of  $\mathbf{x}$  onto the boundary,  $\mathbf{n}$  is the unit normal vector (pointing to the fluid side) at  
 211 the projection point,  $\Delta x$  is the local grid spacing, and  $\Delta S$  is the projection area of a lattice on the  
 212 boundary. Clearly, the mass leakage  $E$  defined in Eq. (10) is a density flux. Actually, it can be  
 213 considered as an approximation to the conventional density flux loss  $(-\rho \mathbf{u} + \rho_w \mathbf{U}) \cdot \mathbf{n}$ :

$$214 \quad \begin{aligned} E(\mathbf{x}) &= \frac{\Delta x^D}{\Delta S \Delta t} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} [f_i(\mathbf{x}) - f_{\bar{i}}(\mathbf{x} + \mathbf{e}_i \Delta t)] + \rho_w \mathbf{U} \cdot \mathbf{n} \\ &\approx -\frac{\Delta x^D}{\Delta S \Delta t} \sum_i f_i \text{Sign}(\mathbf{e}_i \cdot \mathbf{n}) + \rho_w \mathbf{U} \cdot \mathbf{n} \\ &\approx -\sum_i f_i \mathbf{e}_i \cdot \mathbf{n} + \rho_w \mathbf{U} \cdot \mathbf{n} = (-\rho \mathbf{u} + \rho_w \mathbf{U}) \cdot \mathbf{n} \end{aligned} \quad (11)$$

215 It should be noticed that Eq. (11) is an effective but not the unique measurement of the potential  
 216 mass leakage, for example, at a steady flow state the density at  $t - \Delta t$  could be directly used to  
 217 determine the mass leakage as  $\rho(t - \Delta t) - \sum_i f_i(t)$ . By implicitly included this measurement as  
 218 a correction source term within a two-relaxation-time LB framework, Ginzburg<sup>46</sup> proposed a LB  
 219 scheme successfully reproducing the Poiseuille flow without mass leakage. Apparently, the steady  
 220 state intended measurement is not suitable for general LB simulations as concerned in this paper.

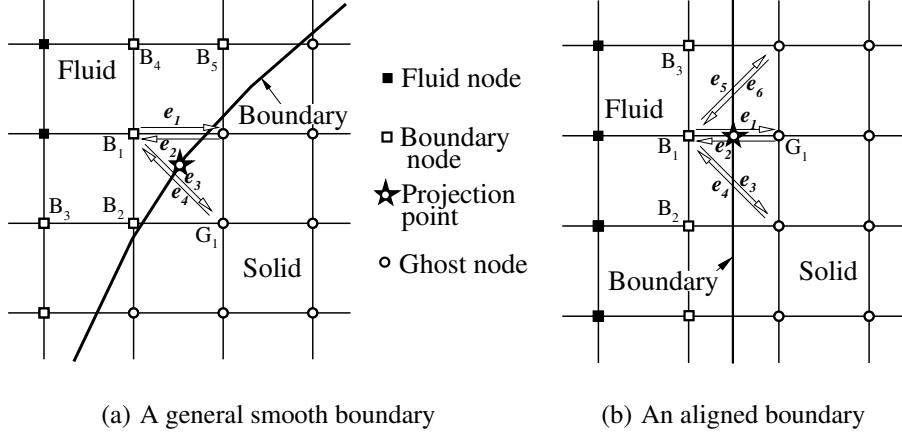


FIG. 1. Sketches of the streaming process at boundary nodes considering a D2Q9 lattice: (a) boundary nodes with LB links irregularly cut by a general smooth boundary and (b) boundary nodes with LB links regularly cut by an aligned planar boundary. Nodes in the solid area, e.g.  $G_1$ , are not necessary.

221 Based on the local mass leakage at individual boundary nodes defined in Eq. (10), the averaged  
 222 mass leakage over a smooth boundary can be now expressed as:

$$223 \quad \bar{E} = (\sum E \Delta S) / \sum \Delta S \quad (12)$$

224 where the summation is conducted over all the involved boundary nodes.

#### 225 IV. LOCAL MASS LEAKAGE AT INDIVIDUAL BOUNDARY NODES

226 Based on the fundamentals of the LB method presented in §II, the local mass leakage at indi-  
 227 vidual boundary nodes defined by Eq. (10) is now theoretically expressed in terms of macroscopic  
 228 variables in this section. Firstly, mass leakage at boundary nodes with LB links regularly cut by  
 229 aligned planar boundaries (referred to as “regular boundary nodes”, see Fig. 1(b)) is analysed in  
 230 §IV A. Based on that, mass leakage at boundary nodes with LB links irregularly cut by general  
 231 smooth boundaries (referred to as “irregular boundary nodes”, see Fig. 2(a)-(c)) is considered in  
 232 §IV A.

##### 233 A. Regular boundary nodes

234 Due to the symmetry of wall-cut LB links at a regular boundary node, the zero and first order  
 235 moments of the links can be directly expressed by macroscopic variables. Hence, regular boundary

236 nodes are an ideal starting point to express the mass leakage by macroscopic variables.

237 By applying the symmetry of the wall-cut LB links at regular boundary nodes, the mass leakage  
238 can be expressed as (see Appendix A for details):

$$\begin{aligned}
 E(\mathbf{x}) \approx & -\rho u_m + \frac{\Delta x}{6} c \partial_m \rho + \frac{\Delta x}{3} \partial_m (\rho u_m) + \frac{\Delta x}{6} \nabla \cdot (\rho \mathbf{u}) \\
 & + \frac{\Delta x}{4c} [\partial_m (\rho u_m^2) + \nabla \cdot (\rho u_m \mathbf{u})] + \rho_w \mathbf{U} \cdot \mathbf{n}
 \end{aligned} \tag{13}$$

240 where the sub-index  $m$  indicates components along the symmetry axis of the wall-cut LB links  
241 (referred to as “main direction” with a unit vector  $\mathbf{n}_m$  pointing to the fluid domain). It is worth  
242 noticing that  $\rho u_m$  is the major part of the momentum recovered by the wall-cut LB links, and  
243 expression (13) is accurate without requiring  $\mathbf{n}_m = \mathbf{n}$  and will be used for irregular boundary  
244 nodes in the next subsection.

245 Considering that  $\mathbf{n}_m = \mathbf{n}$  is satisfied for aligned boundaries, Eq. (13) can be further simplified  
246 as:

$$E(\mathbf{x}) = \left( \frac{\Delta x}{3} - \Delta w \right) \partial_n (\rho u_n) + \frac{\Delta x}{6} c \partial_n \rho + \frac{\Delta x}{6} \nabla \cdot (\rho \mathbf{u}) + \frac{\Delta x}{4c} [\partial_n (\rho u_n^2) + \nabla \cdot (\rho u_n \mathbf{u})] \tag{14}$$

248 where  $\Delta w$  is the wall distance ( $\Delta w < \Delta x$ ), and  $\partial_n$  and  $u_n$  are the normal gradient and velocity  
249 components, respectively.

250 The last relation (14) clearly shows that the mass leakage along aligned boundaries mainly  
251 arises from the normal gradient of density  $\rho$ , normal momentum  $\rho u_n$ , and the corresponding  
252 kinetic energy  $\rho u_n^2$ , as well as the divergence of the momentum  $\nabla \cdot (\rho \mathbf{u})$  (compressibility effect)  
253 and the normal momentum flux  $\nabla \cdot (\rho u_n \mathbf{u})$ . Moreover, amplitude of the mass leakage is in the  
254 order of  $O(\Delta x)$ . As a consequence, in the case of weakly compressible flows with fixed non-slip  
255 boundaries, all the terms in Eq. (14) are all supposed to be negligibly small, as is the resultant  
256 local mass leakage. It should be noticed that this conclusion does not conflict with the reported  
257 mass leakage along aligned boundaries<sup>11,29</sup> because they adopted an external force at boundary  
258 nodes, thus yielding a significant  $\partial_n (\rho u_n)$  in Eq. (14).

## 259 B. Irregular boundary nodes

260 The mass leakage at irregular boundary nodes is now addressed. The analysis is conducted by  
261 approximating irregular boundary nodes as regular ones, and then estimating the mass leakage by

262 applying the analysis proposed for regular nodes in §IV A.

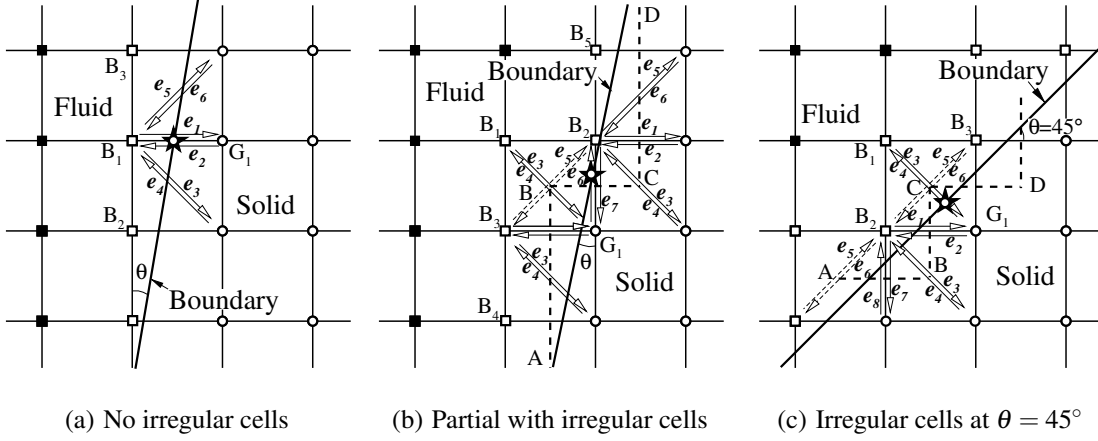


FIG. 2. Irregular boundary nodes at a smooth boundary. The symbols are the same with those in Fig. 1(a). Lattice cells with boundary going through two perpendicular edges, e.g. B in (b) and C (c), are referred to as “irregular cells”. Three typical cases are illustrated: boundary node irregularly cut with the cut-links similar to those cut by aligned boundaries in Fig. 1(b), without irregular cells involved (a); part of the boundary nodes are involved with irregular cells (b); and all boundary nodes are involved with irregular cells when a straight boundary is inclined at  $45^\circ$  (c),

263 Firstly, some basic characteristics of irregular boundary nodes are emphasised. As shown in  
 264 Fig. 2(a)-(c), irregular boundary nodes are distinguished by an angle deviation  $\theta$  ( $0^\circ \leq \theta \leq 45^\circ$ )  
 265 between  $\mathbf{n}$  and the coordinate axes. Noticeably, when the boundary goes through two perpendicular  
 266 edges of a lattice cell (referred to as “irregular cell”, e.g. the one containing B and C shown  
 267 in Fig. 2(b)-(c)), the cut links change rapidly by every node. For a well resolved smooth boundary  
 268 wall (without sharp corners) in 2D, irregular cells always occur in pairs (e.g. B and C), with three  
 269 irregular boundary nodes (e.g.  $B_1, B_2$  and  $B_3$ ) involved.

270 For irregular boundary nodes not associated with irregular cells ( e.g.  $B_1$  shown in Fig. 2(a)),  
 271 they can be directly approximated as regular boundary nodes because the cut links are exactly the  
 272 same as those cut by aligned boundaries (see  $B_1$  shown in Fig. 1(b) and Fig. 2(a)). The main  
 273 difference is that the main direction  $\mathbf{n}_m$  of the approximated regular boundary node is different  
 274 from the local normal vector  $\mathbf{n}$ . By applying Eq. (13), the mass leakage can be estimated as (see  
 275 Appendix B):

$$276 \quad E(x) = \pm \rho u_t \tan \theta + O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho \mathbf{u})\|) + O\left[\Delta x \frac{\|\nabla(\rho \mathbf{u})\|}{c_s}\right] \quad (15)$$

277 where  $u_t$  is the tangential velocity component.

278 For irregular boundary nodes associated with irregular cell pairs, they can be approximated as  
 279 regular boundary nodes through two kinds of operations. Firstly, the links between neighbouring  
 280 boundary nodes could be treated as virtual cut links without causing extra net mass leakage. For  
 281 example, as shown in Fig. 2(a), by considering the virtually cut links  $e_5$  and  $e_6$  between  $B_2$  and  
 282  $B_3$ , the node  $B_3$  can be treated as an approximated regular boundary node with a horizontal main  
 283 direction. Secondly, wall-cut LB links at one boundary node can be shifted to its neighbouring  
 284 boundary nodes to complete the remained approximation to regular boundary nodes. For example,  
 285 as shown in Fig. 2(a), by shifting the cut links  $e_3$  and  $e_4$  at  $B_1$  to  $B_2$ , the total cut links, including  
 286 the virtual  $e_5$  and  $e_6$ , exactly approximate  $B_2$  as two regular boundary nodes with different main  
 287 directions (one is horizontal and the other is vertical). Mass leakage at the approximated regular  
 288 node pairs, e.g. those at  $B_2$  as analysed, can be estimated by Eq. (13) as (see Appendix B):

$$289 \quad E(\boldsymbol{x}) = \rho u_t \tan(\pm\theta \mp 45^\circ) + O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho \boldsymbol{u})\|) + O\left[\Delta x \frac{\|\nabla(\rho \boldsymbol{u} \boldsymbol{u})\|}{c_s}\right] \quad (16)$$

290 Clearly, relations (15) and (16) shows that the mass leakage at both kinds of irregular boundary  
 291 nodes are dominated by terms proportional to  $\rho u_t$ . Recalling Eq. (13), it can be concluded that the  
 292 dominating terms in Eqs. (15) and (16) are due to  $\rho u_m \neq \rho_w \boldsymbol{U} \cdot \boldsymbol{n}$  when  $\boldsymbol{n} \neq \boldsymbol{n}_m$ , indicating that the  
 293 mass leakage is mainly caused by the intrinsic deficiency of the wall-cut LB links in recovering the  
 294 momenta. Meanwhile, these terms depends on the boundary orientation significantly. Particularly,  
 295 for  $\theta \rightarrow 0$ , only the first kind of irregular boundary nodes emerges, and the dominating term  
 296  $\rho u_t \tan \theta \rightarrow 0$ ; For  $\theta \rightarrow 45^\circ$ , only the second kind of irregular boundary nodes emerges, and the  
 297 dominating term  $\rho u_t \tan(\pm\theta \mp 45^\circ) \rightarrow 0$ .

298 To this point it should be pointed out that, from Eq. (13) to (16), the potential significant  
 299 mass leakage  $\propto \rho u_t$  is inevitable for general non-aligned boundaries because it originates from  
 300 the intrinsic deficiency of the incomplete distribution functions at boundary nodes in restoring the  
 301 momentum vector properly. In addition, the dependence of mass leakage on different boundary  
 302 treatments is supposed to be included in the potentially different coefficients before the qualitative  
 303 terms (e.g.  $O(\Delta x c \|\nabla \rho\|)$ ), and this can be expected to holds for the corresponding averaged mass  
 304 leakage discussed in the followed §V.

## V. AVERAGED MASS LEAKAGE OVER SMOOTH BOUNDARIES

### A. Estimates of the averaged mass leakage

Based on the estimates for local mass leakage at individual boundary nodes derived in §IV, the averaged mass leakage over smooth boundaries is analysed in this section.

Firstly, for aligned boundaries, regular boundary nodes are uniformly distributed, and the averaged mass leakage is exactly the same as the local value at an individual node given by Eq. (14).

Secondly, for 45° inclined boundaries, all the boundary nodes are associated with irregular cells, and the mass leakage can be estimated by Eq. (16) taking  $\theta = 45^\circ$ , i.e.

$$\bar{E} = O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho u_n)\|) + O\left[\Delta x \frac{\|\nabla(\rho \mathbf{u})\|}{c_s}\right] \quad (17)$$

Finally, for general smooth boundaries, the boundary nodes can be decomposed into a series of serrated cells (see Fig. 3(a)-(d)), and the overall averaged mass leakage can be estimated from that of the serrated cells. Specifically, a general serrated cell can be deemed as a linear superposition of four basic types, and so is the averaged mass leakage.

Figures 3(a)-(d) display the four basic kinds of serrated cells, i.e. an ideal serrated cell with the two sawtooth tip nodes exactly on a planar boundary (see Fig. 3(a)), an ideal serrated cell shifted from the planar solid boundary by a distance  $\Delta s$  (see Fig. 3(b)), an ideal serrated cell rotated from the planar boundary by an angle of  $\Delta\theta$  (see Fig. 3(c)), and an ideal serrated cell with the sawtooth tip nodes on a boundary with a curvature radius  $R_c$  (see Fig. 3(d)).

By combining the local mass leakage (Eqs. (15) and (16)), the definition of averaged mass leakage (Eq. (12)) and the geometry relationships shown in Fig. 3(a)-(d), the averaged mass leakage of an ideal serrated cell, and those caused by  $\Delta s$ ,  $\Delta\theta$  and  $R_c$  are estimated as (see Appendix C for details):

$$\begin{cases} E_{sc} = O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho \mathbf{u})\|) + O\left[\Delta x \frac{\|\nabla(\rho \mathbf{u})\|}{c_s}\right] \\ E_{\Delta s} = \Delta s \partial_n(\rho u_n), \quad E_{\Delta\theta} = \rho u_t \tan \Delta\theta = O(\rho u_t \frac{\Delta x}{L}), \quad E_{R_c} = O\left(\rho \|\mathbf{u}\| \frac{\Delta x}{R_c}\right) \end{cases} \quad (18)$$

It should be noted that  $E_{\Delta s}$ ,  $E_{\Delta\theta}$  and  $E_{R_c}$  are not just for a local serrated cell, but have taken the whole smooth boundary into consideration (see Appendix C). Consequently, the resultant averaged mass leakage for smooth boundaries can be estimated as the sum of Eq. (18):

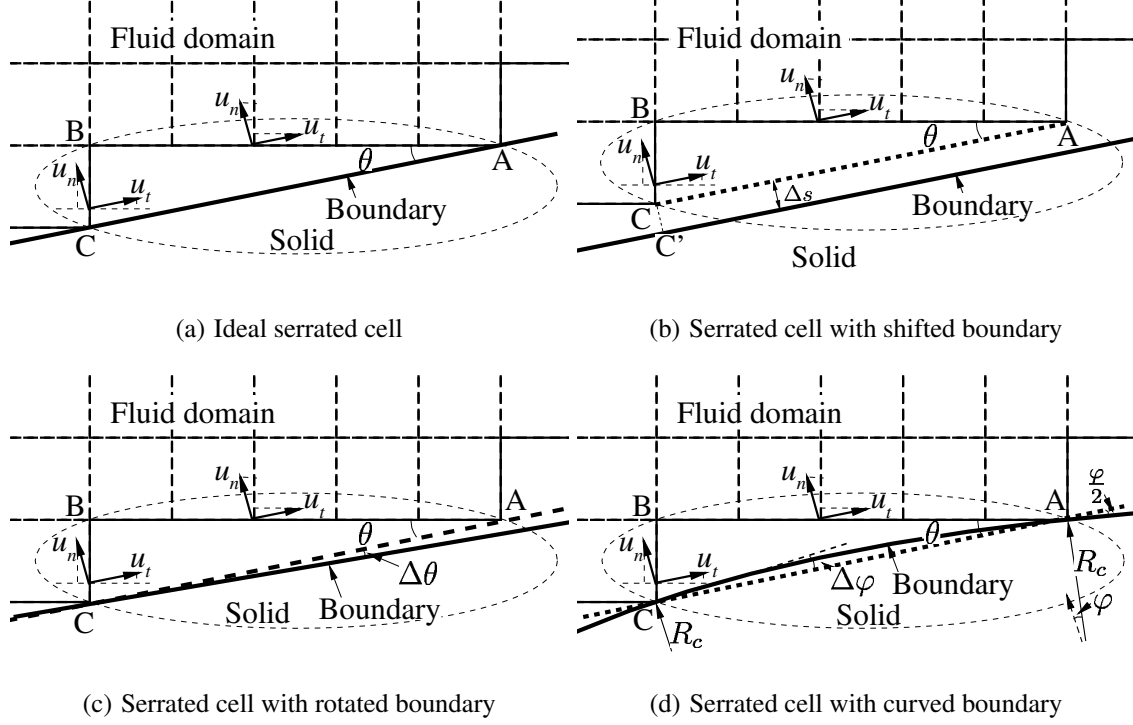


FIG. 3. Sketches of serrated cells including boundary nodes between two successive “sawtooth tips” (e.g. A and C). Four basic types are shown: an ideal serrated cell with the two sawtooth tips (A and C) on a planar boundary (a), an ideal serrated cell shifted from a planar boundary by  $\Delta s$  (b), an ideal serrated cell deviating from a planar boundary by an angle of  $\Delta\theta$  (c), and an ideal serrated cell with the sawtooth tips on a curved boundary. AC is a real (solid) or virtual (dashed) planar boundary.  $\theta$  is the minimal angle between AC and the coordinate axes.  $u_t$  and  $u_n$  are the tangential and normal velocity components, respectively. In (d),  $R_c$  is the local boundary curvature,  $\varphi$  is angle corresponding to the arc  $\widehat{AC}$ , and  $\Delta\varphi$  is angle between AC and the local tangential direction.

$$332 \quad \bar{E} = O(\rho u_t \frac{\Delta x}{L}) + O\left(\rho \|\mathbf{u}\| \frac{\Delta x}{R_c}\right) + O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho \mathbf{u})\|) + O\left[\Delta x \frac{\|\nabla(\rho \mathbf{u} \mathbf{u})\|}{c_s}\right] \quad (19)$$

333 As shown by this relation, the averaged mass leakage mainly originates in several sources,  
 334 including the tangential momentum  $\rho u_t$ , the boundary curvature and the momentum  $\rho \mathbf{u}/R_c$  and  
 335 the gradients of density  $\rho$ , momentum  $\rho \mathbf{u}$  and momentum flux tensor  $\rho \mathbf{u} \mathbf{u}$ . Moreover, all the  
 336 terms are proportional to the grid spacing  $O(\Delta x)$ , indicating that the averaged mass leakage can  
 337 be reduced by refining grids. In addition, it should be noticed that all the terms appearing in Eq.  
 338 (19) are significantly dependent on the boundary orientation. For example, the first term caused  
 339 by  $\Delta\theta$  is zero when the boundary is inclined at  $\theta = \arctan \frac{1}{N}$  with  $N = 1, 2, 3 \dots$ , e.g.  $\theta = 45^\circ$



340 corresponding to  $N = 1$ .

341 Physically, moving boundaries induce significant velocities at boundary nodes, and high  
 342 Reynolds numbers are associated with strong gradients near the boundaries. According to Eq.  
 343 (19), these two situations are expected to induce significant averaged mass leakage, which is  
 344 consistent with the previous observations reported in<sup>25</sup>.

## 345 B. Examples on two academic cases: Poiseuille and Taylor-Couette flows

346 The above expressions for mass leakage can be used to analyse the behaviour of mass leakage  
 347 in simple flow configurations, for which analytical solutions are available. Hereafter, averaged  
 348 mass leakage along boundaries for steady laminar Poiseuille flow and Taylor-Couette flow are  
 349 estimated thanks to Eq. (19).

350 For Poiseuille flow, considering  $\nabla\rho = 0$ ,  $u_n = 0$ ,  $\partial_t u_t = 0$  and  $\nabla \cdot (\rho\mathbf{u}) \approx 0$ , the averaged mass  
 351 leakage along the straight walls can be expressed as:

$$352 \quad \bar{E} = O(\rho u_t \frac{\Delta x}{L}) + O(\Delta x \rho \partial_n u_t) + O\left(\Delta x \frac{\rho u_t \partial_n u_t}{c_s}\right) \quad (20)$$

353 For the steady laminar weakly compressible Taylor-Couette flow with a static outer cylinder  
 354 (pressure gradient offsetted by external body force), one has  $\nabla\rho = 0$ ,  $u_n = 0$  and  $\nabla \cdot (\rho\mathbf{u}) \approx 0$ , and  
 355 the averaged mass leakage along the curved inner wall can be expressed as:

$$356 \quad \bar{E} = O(\Delta x \rho \Omega) + O\left(\Delta x \frac{\rho r_1 \Omega^2}{c_s}\right) \quad (21)$$

357 where the reference length  $L$  in Eq. (19) is represented by the inner radius  $r_1$ , and  $\Omega$  is the  
 358 angular velocity of the inner cylinder.

## 359 VI. A FIRST-ORDER ACCURATE MASS CORRECTION SCHEMES

360 Corresponding to the local and averaged mass leakage estimates, there are two mass correction  
 361 schemes, i.e. the local mass correction (LMC) scheme and the averaged mass correction (AMC)  
 362 scheme.

363 With the LMC, the local mass leakage is used to satisfy mass conservation by applying a cor-  
 364 rection as:

$$\Delta\rho(\boldsymbol{x}) = \frac{\Delta t \Delta S}{\Delta x^D} E(\boldsymbol{x}) = \sum_{\boldsymbol{x} + \boldsymbol{e}_i \Delta t \in \mathcal{S}} [f_i(\boldsymbol{x}) - f_{\bar{i}}(\boldsymbol{x} + \boldsymbol{e}_i \Delta t)] + \frac{\Delta t \Delta S}{\Delta x^D} \rho_w \boldsymbol{U} \cdot \boldsymbol{n} \quad (22)$$

where  $E$  is defined in Eq. (10). For static or tangentially moving boundaries (i.e.  $\boldsymbol{U} \cdot \boldsymbol{n}$ ), this scheme complies with the way of mass conservation of the well-known bounce-back method, has been used by Sanjeevi *et al.*<sup>25</sup>, and is similar to most of the reported mass correction schemes<sup>27–29</sup>. According to the analysis in §IV, the local mass leakage could be proportional to the tangential velocity amplitude, and thus the LMC scheme adds a zero-order perturbation to the solution of density.

In contrast, the averaged mass leakage is promising to facilitate a first-order accurate correction scheme because it has an amplitude in the order of  $O(\Delta x)$ . With the AMC, the mass correction can be formulated as:

$$\Delta\rho(\boldsymbol{x}) = \frac{\Delta t \Delta S}{\Delta x^D} \bar{E} = \frac{\sum_{\Omega} \sum_{\boldsymbol{x} + \boldsymbol{e}_i \Delta t \in \mathcal{S}} [f_i(\boldsymbol{x}) - f_{\bar{i}}(\boldsymbol{x} + \boldsymbol{e}_i \Delta t)]}{\sum_{\Omega} \Delta S} + \frac{\Delta t \Delta S}{\sum_{\Omega} \Delta S} \sum_{\Omega} (\rho_w \boldsymbol{U} \cdot \boldsymbol{n} \Delta S) \quad (23)$$

where  $\bar{E}$  is defined in Eq. (12), and  $\Omega$  represents a concerned boundary. It should be noticed that  $\Delta\rho(\boldsymbol{x})$  is implied locally, but the AMC only provide a global mass conservation, which is consistent with local mass flux correction proposed by Ginzburg<sup>17</sup>. The two schemes will be compared in the followed §VII.

## VII. NUMERICAL VALIDATION ON THE CHANNEL AND TAYLOR-COUETTE FLOWS

A preliminary validation of the proposed scaling laws for the mass leakage error is achieved by performing 2D simulations of two academic flows with straight and curved boundaries, e.g. the Poiseuille flow and the Taylor-Couette flow, respectively. Meanwhile, the influence of mass leakage on the numerical solutions as well as the effectiveness of the LMC and AMC schemes are investigated. Without loss of generality, the multiple-relaxation-times (MRT) LB method together with a second-order accurate immersed boundary method will be used for the validation.

An in-house C/C++ solver<sup>22</sup> applying the LB method based on multi-block Cartesian grids is used to perform the simulations until otherwise specified. In this solver, the multiple-relaxation-times (MRT)<sup>47</sup> method together with the D2Q9 lattice is used for two-dimensional simulations. The no-slip boundary condition is implemented by an interpolation-based scheme similar to the

392 one discussed in Ref.<sup>13,38</sup>. In this approach, as shown in Fig. 4, the macroscopic variables ( $\rho$  and  
 393  $\mathbf{u}$ ) at a boundary node are reconstructed from quadratic interpolation using a stencil including the  
 394 six nearest fluid domain nodes (the projection point on the boundary is also used for  $\mathbf{u}$ ). Then, the  
 395 equilibrium parts of the distribution functions are calculated based on the obtained macroscopic  
 396 variables, while the non-equilibrium parts are the averaged values of those at the neighbouring  
 397 fluid domain nodes. All the considered simulations are converged to steady states.

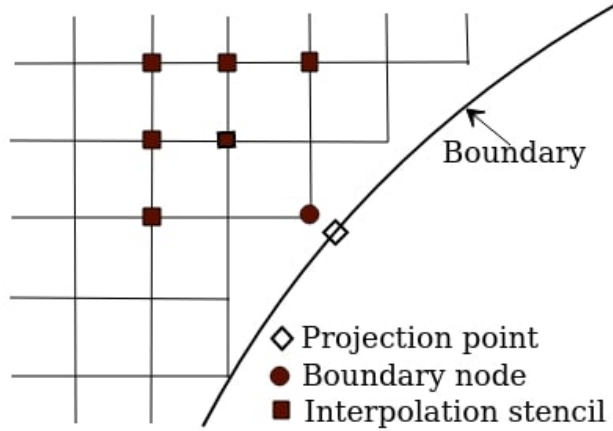


FIG. 4. Sketch of the interpolation based IB method. For interpolation of velocity, the projection point is  
 398 also used.

399

#### 400 **A. The Poiseuille flow through straight channels with variously inclined and translating** 401 **boundaries**

402 To validate our analysis of mass leakage at planar wall boundaries (§IV A-IV B), the laminar  
 403 steady Poiseuille flow through straight channels inclined at different angles are simulated. Both  
 404 walls of the channel are set to move in translation to emphasised the role of the tangential velocity  
 405 ( $u_t$ ) on the mass leakage. As shown in Fig. 5,  $h$  is the half height of the channel,  $L$  is the channel  
 406 length ( $L/h = 80$ ), and a prescribed parabolic velocity profile is imposed at inlet on the left bound-  
 407 ary. A reference velocity ( $U_{ref}$ ) is chosen to satisfy a low Reynolds number  $Re = U_{ref}h/\nu = 25$   
 408 and Mach number  $Ma = U_{ref}/c_s = 0.0866$ . The flow is driven by an external body force. A  
 409 minimum grid spacing  $\Delta x/h = 0.025$  is applied unless otherwise specified.

410 The averaged mass leakage for the Poiseuille flow is estimated by Eq. (20). Since the serrated  
 411 cell at the lower and upper walls (denoted by indices  $l$  and  $u$ , respectively) are rotational symmet-

412 rical by  $180^\circ$ , the tangential velocity  $u_t$  in Eq. (20) is in opposite signs to estimate their averaged  
 413 mass leakage. Therefore,  $\bar{E}_l - \bar{E}_u$  is supposed to be contributed by the linear terms  $O(\rho u_t \frac{\Delta x}{L})$  and  
 414  $O(\Delta x \rho \partial_n u_t)$ , and the net mass leakage  $\bar{E}_l + \bar{E}_u$  is supposed to be contributed by the non-linear term  
 415  $O(\Delta x \rho u_t \partial_n u_t / c_s)$  as well as the coupling between the linear terms and the asymmetrical geometry  
 416 uncertainties (e.g.  $\Delta s$  in Eq. (18) could be different for the two walls).

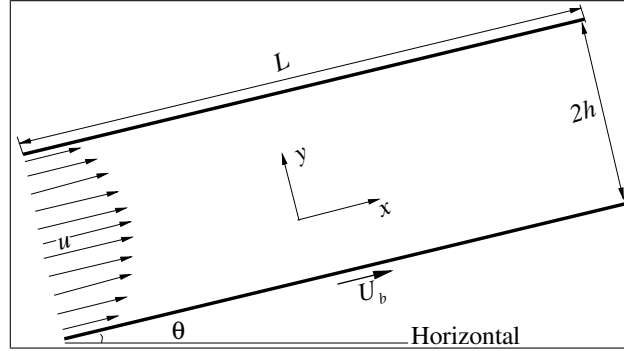


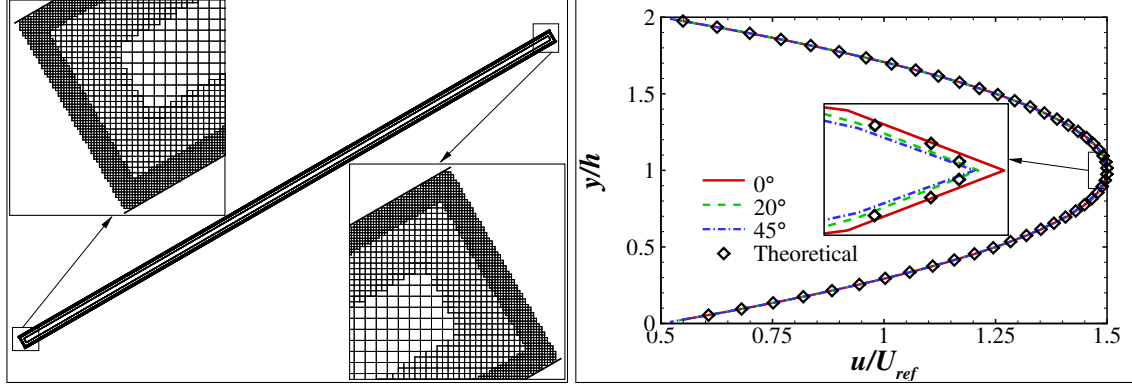
FIG. 5. Sketch of the Poiseuille flow through a straight channel inclined at  $\theta$ .  $U_b$  is the translating velocity of both walls.

### 417 1. Effect of geometry orientation

418 To investigate the mass leakage dependence on geometry orientation, the Poiseuille flow with  
 419 tangentially moving walls inclined from  $\theta = 0^\circ$  to  $45^\circ$  by an increment of  $5^\circ$  is simulated. A finite  
 420 boundary velocity  $U_b = 0.5U_{ref}$  is enforced to provide significant velocity at the boundary nodes.

421 To illustrate and validate the numerical solution, grid distribution at  $\theta = 30^\circ$  and streamwise  
 422 velocity profiles (at  $x/L = 0.5$ ) at different  $\theta$  are shown in Fig. 6(a) and (b), respectively. It  
 423 can be observed the multi-block grid refinement has no spurious effect on the solution, making it  
 424 possible to measure boundary-condition-based errors in a clean way. The velocity profiles shown  
 425 in Fig. 6(b) with  $\theta = 0^\circ, 20^\circ$  and  $45^\circ$  correspond to an aligned boundary (§IV A), a general  
 426 irregularly-oriented boundary and a  $45^\circ$  inclined boundary (§IV B), respectively. It is seen that  
 427 the solved velocity profiles exhibit good agreement with the theoretical results, indicating that the  
 428 flow is well reproduced by the solver. All the Poiseuille flow in the rest of this paper are accurately  
 429 simulated similarly unless further specified.

430 Fig. 7(a) displays the local mass leakage amplitude  $|E|_{max}$  at each wall as a function of the  
 431 inclined angle  $\theta$ . As can be observed,  $|E|_{max}$  at the two walls varies significantly with  $\theta$  in a



(a) Grid at  $\theta = 30^\circ$

(b) Velocity profiles

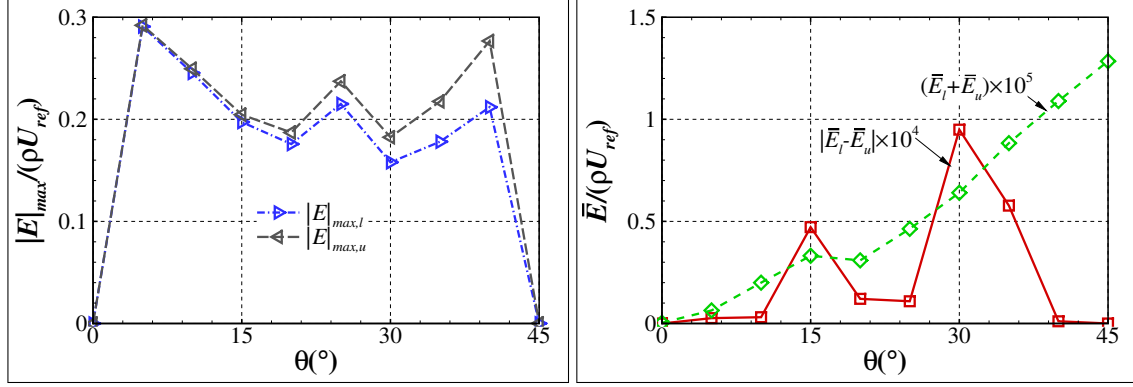
FIG. 6. Grid distribution at  $\theta = 30^\circ$  (a) and streamwise velocity profile at different  $\theta$  (b).

432 similar manner. Specifically,  $|E|_{max}$  approaches zero at  $\theta = 0^\circ$  and  $45^\circ$ , and hold a significant  
 433 amplitude around  $0.2\rho U_{ref}$  with a decreasing trend over  $5^\circ \leq \theta \leq 20^\circ$  and an increasing trend  
 434 over  $30^\circ \leq \theta \leq 40^\circ$ . These observations can be well explained by the theoretical analysis of local  
 435 mass leakage in §IV B, i.e. the dominating terms is zero at  $0^\circ$  ( $\rho u_t \tan \theta = 0$  in Eq. (15)) and  $45^\circ$   
 436 ( $\rho u_t \tan(45^\circ - \theta) = 0$  in Eq. (16)), and otherwise  $|E|_{max}$  is dominated by a U-shaped function  
 437 determined by  $\max[\rho u_t \tan \theta, \rho u_t \tan(45^\circ - \theta)]$ .

438 Fig. 7(b) shows the averaged mass leakage  $\bar{E}$  as a function of  $\theta$ . The linear part  $|\bar{E}_l - \bar{E}_u|$   
 439 approaches zero at  $\theta = 0^\circ$  and  $45^\circ$ , and displays significant oscillations over  $0^\circ < \theta < 45^\circ$ . This  
 440 indicates that  $|\bar{E}_l - \bar{E}_u|$  is dominated by the term  $O(\rho u_t \frac{\Delta x}{L})$  which is zero at  $\tan \theta = 1/N$ , e.g.  
 441  $0^\circ$ ,  $26.6^\circ$  and  $45^\circ$  (see §V). In contrast, the net mass leakage  $\bar{E}_l + \bar{E}_u$  generally increases with  
 442  $\theta$ , indicating that the term  $O(\Delta x \rho u_t \partial_n u_t)$  has a positive reliance on  $\theta$ . The observable average  
 443 mass leakage is consistent with the analysis in Ref.<sup>46</sup> that the non-linear terms in the equilibrium  
 444 definition of distribution functions cause unavoidable mass leakage.

## 445 2. Effect of tangential velocity

446 To emphasise the effect of tangential velocity on the mass leakage, simulations with the walls  
 447 translating at a finite tangential velocity  $U_b$  varying from 0 to  $0.5U_{ref}$  are performed in this sub-  
 448 section. The normal gradient of tangential velocity  $\partial_n u_t$  is set to be constant so that  $u_t$  is the sole  
 449 changing variable in Eq. (20). In addition, to clarify effect of the angle bias  $\Delta\theta$ , i.e. the term  
 450  $O(\rho u_t \frac{\Delta x}{L})$  in Eq. (20), configurations at  $\theta = \arctan \frac{1}{2}$  ( $\approx 26.6^\circ$ ,  $\Delta\theta = 0$ ) and  $\theta = 30^\circ$  ( $\Delta\theta \neq 0$ ) are  
 451 simulated and compared.



(a) Local mass leakage

(b) Averaged mass leakage

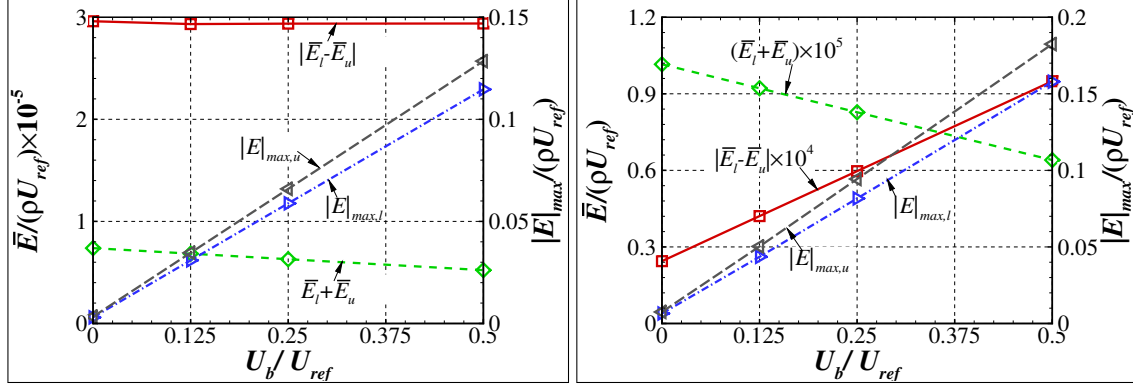
FIG. 7. Mass leakage as a function of the inclined angle  $\theta$ . The sub-indices  $l$  and  $u$  indicate the lower and upper walls, respectively. In (a),  $|E|_{max}$  is the local mass leakage amplitude. In (b),  $\bar{E}_l - \bar{E}_u$  and  $\bar{E}_l + \bar{E}_u$  correspond to the averaged mass leakage due to the linear terms in Eq. (20) and the net averaged mass leakage, respectively.

452 Fig. 8(a) and (b) display the mass leakage as functions of  $U_b$  for  $\theta = \arctan \frac{1}{2}$  and  $30^\circ$ , respec-  
 453 tively. As can be observed, for both values of  $\theta$ , the local amplitude  $|E|_{max}$  at both walls is almost  
 454 proportional to the boundary velocity  $U_b$ , which can be related to the dominating terms  $\propto \rho u_t$   
 455 in Eqs. (15) and (16). Meanwhile, the net mass leakage  $\bar{E}_l + \bar{E}_u$  in both figures exhibits similar  
 456 linear dependence versus  $U_b$ , which can be explained by the nonlinear term  $O(\Delta x \rho u_t \partial_n u_t)$  in Eq.  
 457 (20). The main difference between the two figures is that  $\bar{E}_l - \bar{E}_u$  remains almost unchanged about  
 458  $3 \times 10^{-5} \rho U_{ref}$  for  $\theta = \arctan \frac{1}{2}$  (Fig. 8(a)), while that shows a significant linear dependence on  $U_b$   
 459 for  $\theta = 30^\circ$  (Fig. 8(a)). This clearly confirms the effect of  $\Delta\theta$  is definitely well estimated by the  
 460 term  $O(\rho u_t \frac{\Delta x}{L})$ .

### 461 3. Effect of velocity gradient

462 To measure the effect of velocity gradient on the mass leakage, simulations with the maximum  
 463 relative incoming velocity  $u_{max} - U_b$  varying from 0 to  $U_{ref}$  are now performed. Without loss of  
 464 generality, the solid walls are set to move tangentially at  $U_b/U_{ref} = 0.5$  so that  $\partial_n u_t$  is the sole  
 465 changing variable in Eq. (20).  $\theta = \arctan \frac{1}{2}$  is chosen to vanish the term  $O(\rho u_t \Delta x)$  in Eq. (20),  
 466 and thus to avoid the uncertainty induced by  $\Delta\theta$ .

467 Figure 9(a) and (b) display the computed streamwise velocity profiles and the mass leakage over  
 468  $0 \leq (u_{max} - U_b)/U_{ref} \leq 1$ , respectively. As shown in Fig. 9(a), profiles of the relative streamwise



(a)  $\theta = \arctan 0.5$

(b)  $\theta = 30^\circ$

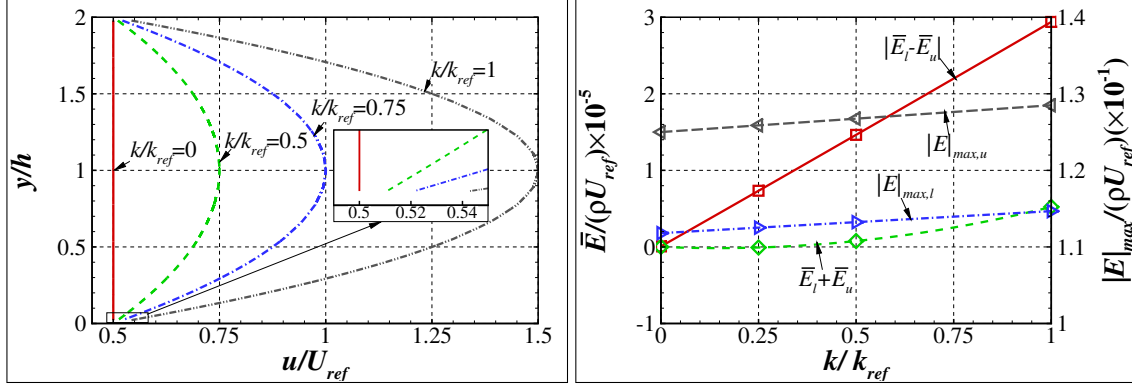
FIG. 8. Mass leakage at  $\theta = \arctan 0.5$  (a) and  $\theta = 30^\circ$  (b) for  $0 \leq U_b/U_{ref} \leq 0.5$ . The sub-indices  $l$  and  $u$  indicate the lower and upper walls, respectively.

469 velocity  $(u - U_b)$  is well reproduced as expected. For the mass leakage shown in Fig. 9(b), the local  
 470 amplitude  $|E|_{max}$  at both walls exhibits linear dependence on  $\partial_n u_t$  with a small amplitude variation  
 471 (2%). This is consistent with that  $\partial_n u_t$  only emerges linearly in minor terms in Eqs. (15) and (16).  
 472 Comparatively, the linear averaged mass leakage  $\bar{E}_l - \bar{E}_u$  is almost proportional to  $\partial_n u_t$ , which  
 473 could be attributed to the linear term  $O(\Delta x \rho \partial_n u_t)$  in Eq. (20). Differently, the net mass leakage  
 474  $\bar{E}_l + \bar{E}_u$  is well described by a parabolic curve, which can be explained by the considerable increase  
 475 of  $u_t$  due to  $\partial_n u_t$  in the nonlinear term  $O(\Delta x \rho u_t \partial_n u_t)$ . By taking this increment into consideration,  
 476 the nonlinear term is changed to  $O[\Delta x \rho (u_t + \Delta w \partial_n u_t) \partial_n u_t]$ , including eventually a quadratic term  
 477 for significant  $\partial_n u_t$  (the relative increase of  $u_t$  at  $(u_{max} - U_b)/U_{ref} = 1$  reaches a considerable  
 478 amplitude of about  $10\% U_b$  in Fig. 9(a)).

#### 479 4. Effect of grid spacing $\Delta x$

480 To examine effect of  $\Delta x$  on the mass leakage, simulations using four different grid spacings  
 481 near the solid walls, i.e.  $\Delta x/h = 0.025, 0.0125, 0.00625$  and  $0.0003125$ , are performed. Without  
 482 loss of generality,  $U_b$  is taken equal to  $0.5 U_{ref}$ , and the channel is inclined at  $\theta = 30^\circ$  to include  
 483 all the terms in Eq. (20).

484 Figure 10 displays the mass leakage as functions of  $\Delta x$ . The local amplitude of the mass  
 485 leakage  $|E|_{max}$  at both walls is slightly affected (1%) in a linear way, which can be attributed to the  
 486  $\Delta x \partial_n u_t$ -related terms in Eqs. (15) and (16). Meanwhile, the averaged mass leakage at both walls  
 487 exhibits a general linear versus  $\Delta x$  with some observable deviations. This can be deemed



(a) Velocity profiles

(b) Mass leakage

FIG. 9. Velocity profiles (a) and mass leakage (b) for  $0 \leq (u_{max} - U_b)/U_{ref} \leq 0.5$ .  $k$  is the value of  $\partial_n u_t$  at the walls, and  $k_{ref}$  is associated with  $u_{max} - U_b = U_{ref}$ . In (b),  $\bar{E}_l + \bar{E}_u$  can be described by a parabolic curve.

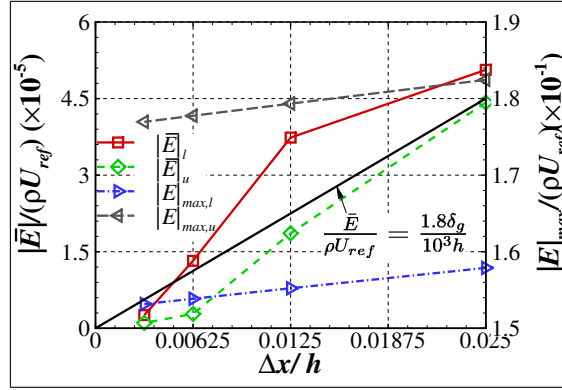


FIG. 10. Mass leakage with  $0.0003125 \leq \Delta x/h \leq 0.025$ . The sub-indices  $l$  and  $u$  denote the lower and upper walls, respectively.

488 as reasonable validation of  $\bar{E} \propto \Delta x$  (Eq. (20)) considering that refining the grid could generate  
 489 substantial uncertainties to the boundary node distribution, e.g.  $\Delta s$  and  $\Delta\theta$  in Eq. (18).

## 490 5. Effect of mass leakage on wall-modelled turbulent flow through straight channel

491 As demonstrated above (§VII A 1-VII A 4), mass leakage in the laminar Poiseuille flow simula-  
 492 tions is well predicted by the proposed theory, but the amplitude is too low (0.01%) to significantly  
 493 impact the solution. Thus, to emphasise the effect of mass leakage, a wall-modelled RANS simu-  
 494 lation of turbulent flow at  $Re = 5 \times 10^4$  ( $Re_{tau} \approx 2000$ ) is performed. At steady state, this solution



495 is similar with the Poiseuille flow in terms of mass leakage estimate, i.e. still described by Eqs.  
496 (15), (16) and (20). Moreover, the velocity and its gradients at the boundary nodes are supposed to  
497 be large enough to involve a significant mass leakage. Finally, the use of wall function increases  
498 the sensitivity of the solution to the boundary treatment. Without loss of generality, the channel is  
499 inclined at  $\theta = 30^\circ$  with  $L/h = 200$ , and a uniform grid spacing  $\Delta x/h = 0.05$  is used. Instead of a  
500 parabolic velocity profile at the inlet, a uniform inlet velocity is imposed.

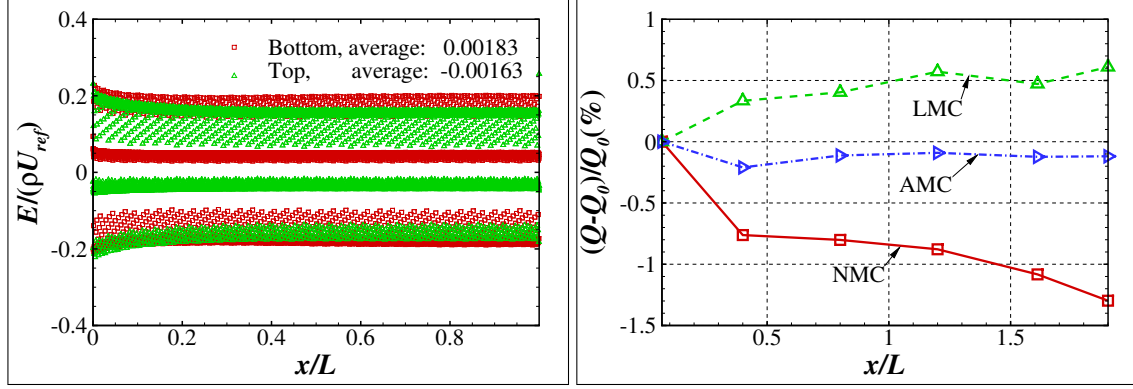
501 The simulation is conducted using the ProLB software<sup>38</sup> in 2D by extending one layer of grid  
502 along the third axis with periodic setup. In ProLB, the D3Q19 LB model is solved for the fluid  
503 dynamics by applying the hybrid recursively regularised strategy<sup>38</sup>. The one-equation Spalart-  
504 Allmaras turbulence model is used to model the turbulence in the fluid domain, and the power-law  
505 wall function<sup>48</sup> is adopted to model the near-wall turbulence effect. Meanwhile, an interpolation-  
506 based second-order accurate immersed boundary treatment is applied to implement the non-slip  
507 boundary condition. Similar to the boundary treatment used for the above laminar simulations, the  
508 macroscopic variables are interpolated from the Lagrangian boundary points and the neighbouring  
509 fluid domain nodes. Differently, the non-equilibrium distribution functions are reconstructed from  
510 the macroscopic gradient information<sup>48</sup>.

511 Fig. 11(a) and (b) display the local mass leakage and sectional mass flux variation, respectively.  
512 As can be observed, without mass correction, the local mass leakage varies significantly with  
513 an amplitude about two orders higher than the averaged values. This observation can be well  
514 explained by the proposed theory ( Eqs. (15), (16) and (19) ). Meanwhile, the sectional mass flux  
515 shown Fig. 11(b) exhibits a loss up to 1.3%, and the AMC scheme apparently outperforms the  
516 LMC scheme in controlling the mass flux loss.

518 Fig. 12(a)-(b) display the friction coefficient and sectional velocity profile, respectively. As  
519 can be observed, without mass correction, the mass leakage causes significant error to the solution,  
520 e.g. the flow symmetry is ruined and both the friction and streamwise velocity significantly deviate  
521 from the reference data. Notably, these problems are well cured by the AMC scheme, while the  
522 LMC scheme leads to worse result.

## 524 B. Taylor-Couette flow

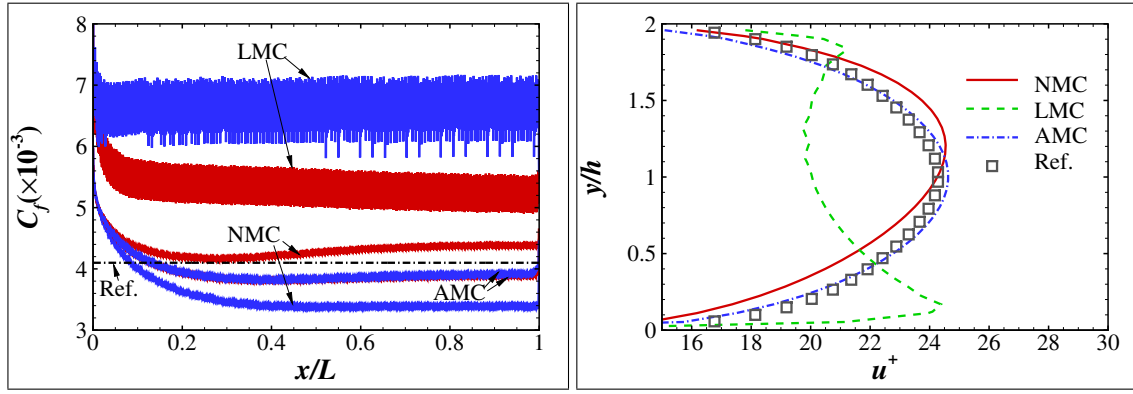
525 In order to validate the proposed theoretical analysis of mass leakage on curved boundaries, the  
526 steady laminar Taylor-Couette flow is considered. The boundary set up is shown in Fig. 13(a). The



(a) Mass leakage without mass correction

(b) Sectional mass flux

FIG. 11. Local mass leakage (a) and sectional mass flux (b). “NMC” is short for “no mass correction”.



(a) Friction coefficient

(b) Velocity profiles

FIG. 12. Friction coefficient (a) and sectional velocity profiles (b). The DNS data reported by Hoyas<sup>49</sup> is used as reference data.

527 inner and outer cylinders’ radii are denoted as  $r_1$  and  $r_2$ , respectively. The inner cylinder rotates  
 528 clockwise at an angular velocity  $\Omega$ . The half channel height, i.e.  $h = (r_2 - r_1)/2$ , is used as the  
 529 reference length. A reference value of angular velocity  $\Omega_{ref}$  is defined as  $Re = \Omega_{ref}h/\nu = 50$ .  
 530 Accordingly, a reference velocity is defined as  $U_{ref} = \Omega_{ref}h$ . A volumic forcing term equal to  
 531  $\rho u_t^2/r$  (with  $r$  being the local radial distance) is used to ensure negligible density gradients. The  
 532 minimum grid spacing is fixed at  $\Delta x/h = 0.02$  unless otherwise specified. The generated multi-  
 533 block grid is shown in Fig. 13(b).

534 The averaged mass leakage is assumed to be described by Eq. (21). Due to the symmetry of the  
 535 geometry setup, the serrated cells are symmetrically distributed around every line inclined at  $0^\circ$  or  
 536  $45^\circ$ . Therefore, the linear averaged mass leakage (denoted as  $\bar{E}_L$ , corresponding to  $O(\Delta x \rho \Omega)$  in

Eq. (21)) is evaluated as the difference between two adjacent  $45^\circ$  arcs. In contrast, the net mass leakage of a  $90^\circ$  arc is denoted as  $\bar{E}_{NL}$ , corresponding to  $O(\Delta x \rho r_1 \Omega^2)$  in (21).

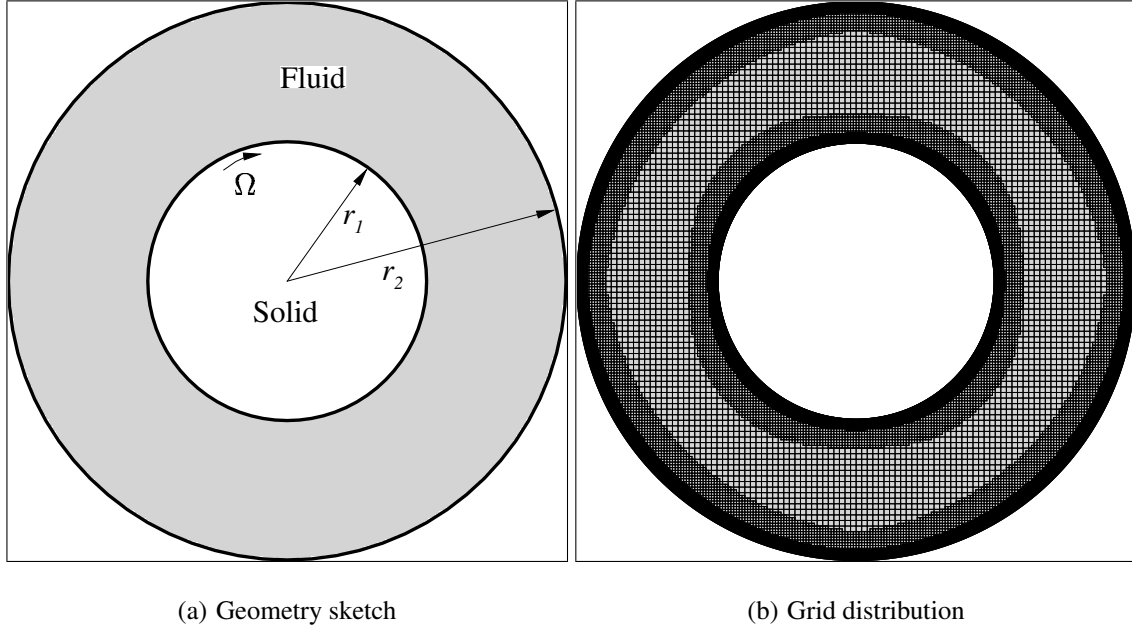
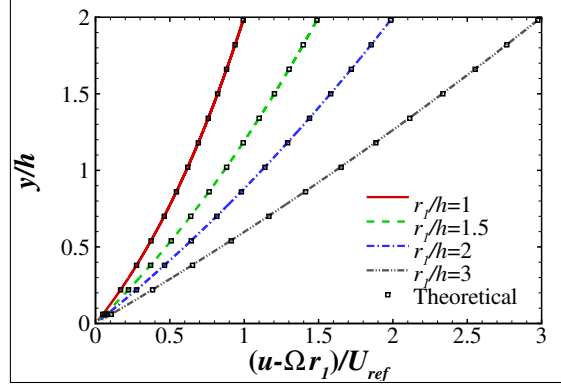


FIG. 13. Sketch of Taylor-Couette flow through a circular channel (a) and the adopted grid distribution (b).

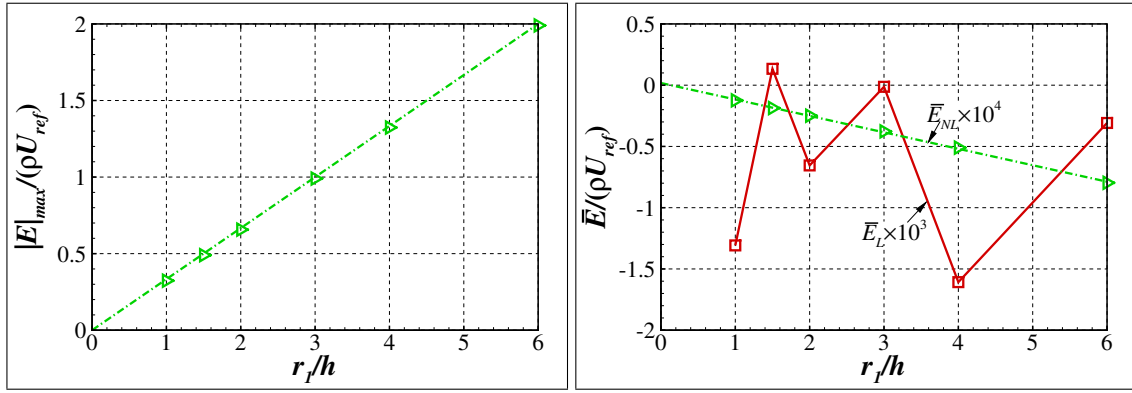
### 539 1. *Effect of boundary curvature*

540 To validate effect of boundary curvature on the mass leakage, simulations with  $r_1$  ranging from  
 541  $h$  to  $6h$  are performed in this subsection. The angular velocity is set as  $\Omega = \Omega_{ref}$ .

542 Figure 14(a), (b) and (c) display the computed velocity profiles, the local and averaged mass  
 543 leakage, respectively. As shown in Fig. 9(a), profiles of the relative velocity  $(u - \Omega r_1)$  agree well  
 544 with the analytical solutions. All the Taylor-Couette flow in the rest of this paper is accurately  
 545 reproduced similarly without showing. For the mass leakage shown in Fig. 14(b)-(c), the local  
 546 amplitude  $|E|_{max}$  is almost proportional to  $r_1$ . Considering  $r_1$  is proportional to the tangential ve-  
 547 locity  $u_t = \Omega r_1$  and  $\Omega$  is fixed, this observation can be explained by the leading terms ( $\propto \rho u_t$ ) in  
 548 Eqs. (15) and (16). Meanwhile, the linear averaged mass leakage  $\bar{E}_L$  exhibits significant oscilla-  
 549 tions without an obvious increasing or decreasing trend. The oscillations can be attributed to the  
 550 substantial uncertainties associated with the boundary node distribution caused by the change of  
 551 geometry configuration. The unclear trend is consistent with the term  $O(\rho \Delta x \Omega)$  (see Eq. (21))  
 552 which is independent of  $r_1$ . In contrast, the net averaged mass leakage  $\bar{E}_{NL}$  shown in Fig. 14(c) is



(a) Velocity profiles



(b) Local mass leakage

(c) Averaged mass leakage

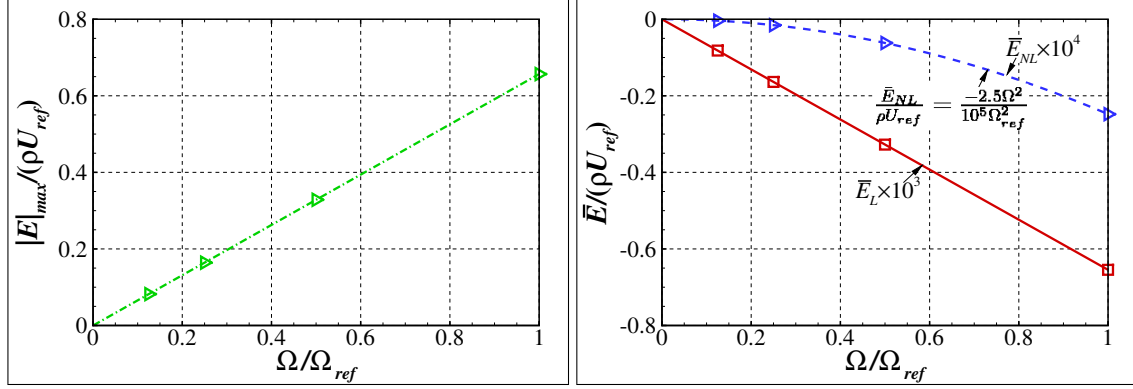
FIG. 14. Velocity profiles (a), local mass leakage (b) and averaged mass leakage (c) for  $1 \leq r_1/h \leq 6$ .

553 almost proportional to  $r_1/h$ , which can be well explained by the term  $O(\Delta x r_1 \Omega^2/c_s)$  in Eq. (21).

## 554 2. Effect of angular velocity

555 To quantify effect of the angular velocity on the mass leakage, simulations with  $\Omega$  ranging from  
 556  $0.125\Omega_{ref}$  to  $\Omega_{ref}$  are performed with  $r_1 = 2h$ .

557 Figure 15(a) and (b) display the local and averaged mass leakage over  $0.125 \leq \Omega/\Omega_{ref} \leq 1$ ,  
 558 respectively. As can be observed, the local amplitude  $|E|_{max}$  (Fig. 15(a)) and the linear averaged  
 559 mass leakage  $\bar{E}_L$  (Fig. 15(b)) are almost proportional to  $\Omega$ . The former can be well explained  
 560 by the leading error terms ( $\propto \rho u_t$ ) in Eqs. (15) and (16), and the later is consistent with the term  
 561  $O(\Delta x \rho \Omega)$  in Eq. (21). In contrast, the net averaged mass leakage  $\bar{E}_{NL}$  shown in Fig. 15(b) is  
 562 almost proportional to  $\Omega^2$ , which is consistent with the term  $O(\Delta x \rho r_1 \Omega^2)$  in Eq. (21).



(a) Local mass leakage

(b) Averaged mass leakage

FIG. 15. Local (a) and averaged mass leakage (b) for  $0.125 \leq \Omega/\Omega_{ref} \leq 1$ .

### 563 3. Effect of grid spacing $\Delta x$

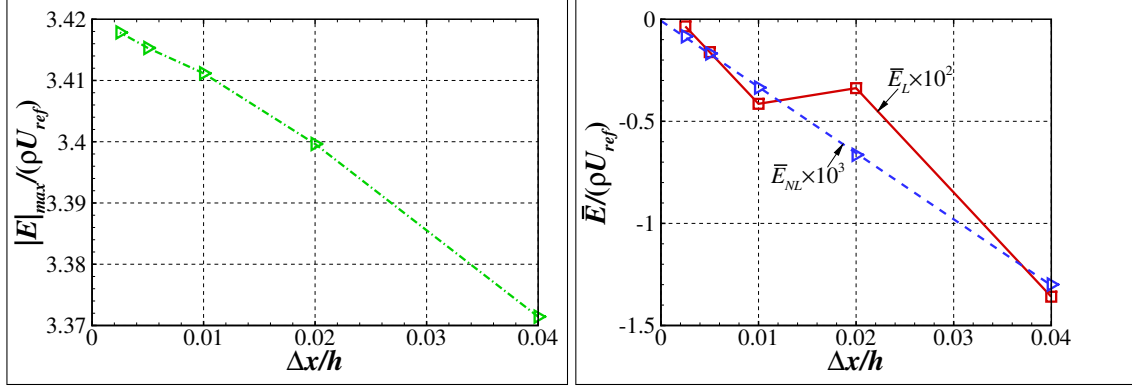
564 In order to measure the effect of grid spacing  $\Delta x$  on the mass leakage, simulations are performed  
 565 considering five different values of  $\Delta x$  at the wall, i.e.  $\Delta x/h = 0.04, 0.02, 0.01, 0.005$  and  $0.0025$ .  
 566  $r_1$  and  $\Omega$  are set equal to  $h$  and  $\Omega_{ref}$ , respectively.

567 Figure 16(a) and (b) display the local and averaged mass leakage over  $0.0025 \leq \Delta x/h \leq 0.04$ ,  
 568 respectively. As can be observed, the local amplitude  $|E|_{max}$  (Fig. 16(a)) is slightly affected within  
 569 2%, which is consistent with Eqs. (15) and (16) where the  $\Delta x$ -related terms are of relatively minor  
 570 amplitude. In contrast, the net mass leakage  $\bar{E}_{NL}$  (Fig. 16(b)) is almost proportional to  $\Delta x$ , and  
 571 the linear averaged mass leakage  $\bar{E}_L$  (Fig. 16(b)) exhibits a similar trend with some oscillations.  
 572 Considering the substantial uncertainties associated with boundary node distribution caused by  
 573 the grid refinement, behaviours of both  $\bar{E}_{NL}$  and  $\bar{E}_L$  reasonably validate the theoretical prediction  
 574  $\bar{E} \propto \Delta x$  (Eq. (21)).

### 575 4. Effect of mass leakage on the solution

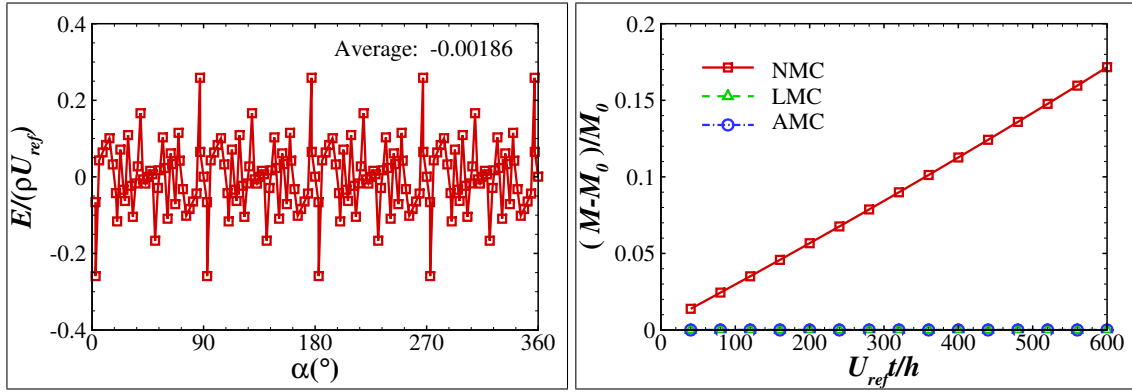
576 To emphasise the effect of mass leakage on the simulation of Taylor-Couette flow, a case with-  
 577 out body force using a uniform coarse grid spacing  $\Delta x/h = 0.1$  is conducted. The body force is  
 578 cancelled to clarify the influence on the pressure estimate. Other parameters are set as:  $r_1 = h$  and  
 579  $\Omega = \Omega_{ref}$ .

580 Fig. 17(a) and (b) display the local mass leakage along the inner cylinder and time history of  
 581 the total mass  $M$ , respectively. As shown in Fig. 17(a), the local mass leakage varies significantly



(a) Local mass leakage

(b) Averaged mass leakage

FIG. 16. Local (a) and averaged mass leakage (b) for  $0.0025 \leq \Delta x/h \leq 0.04$ .

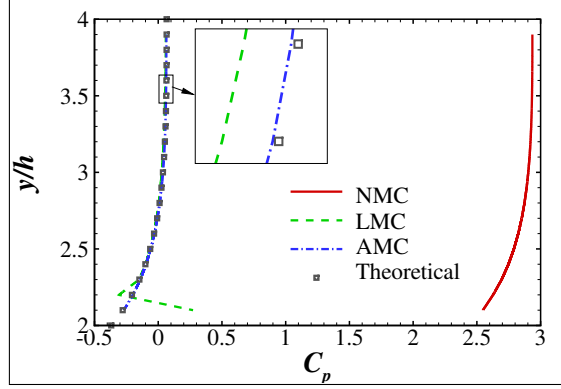
(a) Local mass leakage

(b) Total mass

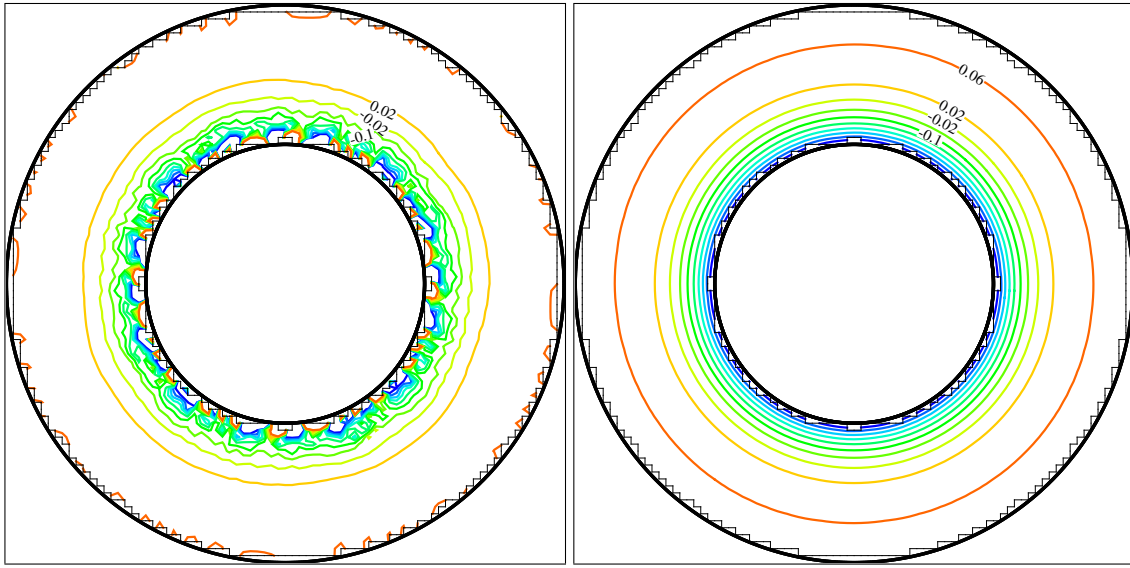
FIG. 17. Local mass leakage (a) and history of total mass (b). In (b),  $M_0$  is the total mass at  $t = 0$ , “NMC” is short for “no mass correction”.

582 with an amplitude comparable to  $\rho U_{ref}$ , but the negative averaged value has an amplitude about  
 583 three order lower than  $\rho U_{ref}$ . These observations can be well explained by the proposed theory  
 584 ( Eqs. (15), (16) and (21) ). Consistent with the negative average mass leakage in Fig. 17(a),  
 585 without mass correction, the total mass  $M$  within the circular channel increases linearly with time,  
 586 to an increment of 17% at  $U_{ref}t/h = 600$ . In contrast, both the local and averaged schemes are  
 588 effective to remove the total mass leakage.

589 Fig. 18(a) displays the pressure coefficient profile at  $x/h = 0$ . As can be observed, without  
 590 mass correction, a significant shift of pressure is produced due to the significant mass increment  
 591 shown in Fig. 17(b). In contrast, both the local and averaged correction schemes successfully  
 592 remove the pressure shift. However, the AMC scheme performances much better than the LMC



(a)  $C_p$  profile



(b)  $C_p$ , LMC

(c)  $C_p$ , AMC

FIG. 18. Comparison of pressure coefficient profiles (a) and the corresponding contour lines with LMC (b) and AMC (c).

593 scheme in terms of accuracy and smoothness. The superiority of the averaged scheme is further  
 594 corroborated by the pressure coefficient contours shown in Fig. 18(b) and (c).

## 595 VIII. CONCLUSIONS

596 In this paper, mass leakage within the general lattice Boltzmann framework is theoretically  
 597 analysed for boundary treatments of at least second-order accuracy. The local mass leakage, de-  
 598 fined from a mesoscopic viewpoint, is theoretically approximated using macroscopic variables at  
 599 regular (aligned boundaries) and irregular boundary nodes. Based on that, the averaged mass leak-

600 age over smooth boundaries is mathematically estimated from that of a basic serrated structure of  
601 boundary nodes.

602 The present theoretical results show that the mass leakage in LB simulations originates from the  
603 deficiency of the wall-cut links in recovering momenta at the boundary nodes. Unexpectedly, from  
604 the macroscopic point of view, the local mass leakage at individual boundary nodes is dominated  
605 by terms proportional to the tangential momentum (i.e.  $\rho u_t$ ). In contrast, the averaged mass  
606 leakage involves several different terms related to the tangential momentum  $\rho u_t$ , product of the  
607 boundary curvature and the momentum  $\rho u/R_c$  and the gradients of density  $\rho$ , momentum  $\rho u$  and  
608 momentum flux tensor  $\rho uu$ . Moreover, the present analysis shows its amplitude is proportional  
609 to the local grid spacing. Based on that, a mass correction scheme is proposed. Besides, both the  
610 local and averaged mass leakage significantly depends on the boundary orientation. Particularly,  
611 the mass leakage at fixed no-slip aligned boundaries is negligibly small.

612 The good agreement between the proposed theoretical estimates and numerical results extracted  
613 from the simulations of the two-dimensional weakly compressible flows through moving straight  
614 and curved channels provides a preliminary validation of the theory. In addition, the numerical  
615 results show that LB solutions can be significantly impacted by mass leakage. However, the av-  
616 eraged mass correction scheme designed from the present theoretical analysis performs well in  
617 curing the mass leakage problems in the considered cases.

618 The theoretical analysis proposed in this paper unveils the basic mechanisms of mass leakage  
619 in the LB framework. However, its validity is limited to 2D flow academic configurations and its  
620 validation in more complex situations as well as its extension to 3D still requires future research  
621 efforts as its validation. In addition, the complex dependance of the evitable local mass leakage  
622 on local flow characteristics indicates that it might be necessary to includes specific characteristic  
623 like "steady flow" into the configuration of boundary treatments as preliminarily demonstrated by  
624 Ginzburg & d'Humières<sup>7,46,50</sup>.

## 625 ACKNOWLEDGEMENTS

626 This work was funded by ANR Industrial Chair ALBUMS (grant ANR-18-CHIN-0003-01).



627 **Appendix A: Local mass leakage at regular boundary nodes**

628 Theoretically, mass leakage defined by Eq. (10) can be decomposed into three parts by splitting  
 629  $\mathbf{f}$  into then equilibrium  $\mathbf{f}^{eq}$  and non-equilibrium  $\mathbf{f}^{ne}$  parts, i.e.

$$630 \quad E(\mathbf{x}) = E^{eq}(\mathbf{x}) + E^{ne}(\mathbf{x}) + \rho_w \mathbf{U} \cdot \mathbf{n} \quad (\text{A1})$$

631 with

$$632 \quad \begin{cases} E^{eq}(\mathbf{x}) = \frac{\Delta x^D}{\Delta S \Delta t} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} [f_i^{eq}(\mathbf{x}) - f_i^{eq}(\mathbf{x} + \mathbf{e}_i \Delta t)] \\ E^{ne}(\mathbf{x}) = \frac{\Delta x^D}{\Delta S \Delta t} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} [f_i^{ne}(\mathbf{x}) - f_i^{ne}(\mathbf{x} + \mathbf{e}_i \Delta t)] \end{cases} \quad (\text{A2})$$

633 It should be noted that  $f_i^{ne}$  could contribute to mass leakage during the stream process (involv-  
 634 ing two neighbouring nodes) despite that its zero and first order moments are theoretically zero at  
 635 a given node.

636 Applying the definition of  $f_i^{eq}$  given by Eq. (2), the equilibrium error part  $E^{eq}$  can be expanded  
 637 as:

$$638 \quad \begin{aligned} E^{eq}(\mathbf{x}) &= \frac{\Delta x^D}{\Delta S \Delta t} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} \left[ 2\omega_i \frac{\rho \mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + 2\Delta t \omega_i \mathbf{e}_i \cdot \nabla \cdot \frac{\rho \mathbf{e}_i \cdot \mathbf{u}}{c_s^2} - \Delta t \mathbf{e}_i \cdot \nabla f_i^{eq} + O(\Delta t^2) \right] \\ &= \frac{\Delta x^D}{\Delta S \Delta t} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} \left\{ 2\omega_i \frac{\rho \mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \Delta t \omega_i \mathbf{e}_i \cdot \nabla \cdot \frac{\rho \mathbf{e}_i \cdot \mathbf{u}}{c_s^2} - \Delta t \omega_i \mathbf{e}_i \cdot \nabla \rho + O(\Delta t^2) \right\} \\ &\quad - \frac{\Delta x^D}{\Delta S} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} \left[ \omega_i \frac{\mathbf{e}_i \cdot \nabla (\rho \mathbf{e}_i \cdot \mathbf{u})^2}{2c_s^4} - \omega_i \rho \frac{\mathbf{e}_i \cdot \nabla (\rho \mathbf{u} \cdot \mathbf{u})}{2c_s^2} + O(\|\rho Ma^2 \nabla \mathbf{u}\|) \right] \end{aligned} \quad (\text{A3})$$

639 Clearly, Eq. (A3) shows that high-order terms  $O(\rho Ma^n)$  in  $f_i^{eq}$  could induce a mass leakage  
 640 that scales as  $O(Ma^{n-1} \rho \|\nabla \mathbf{u}\|)$ . Without loss of generality, in the rest of this paper,  $Ma$ -related  
 641 high-order terms, e.g.  $O(Ma^3)$ , will be neglected because their effect can be inferred from those of  
 642  $O(Ma)$  and  $O(Ma^2)$ . Hence, by omitting the high-order terms  $O(Ma^2 \rho \|\nabla \mathbf{u}\|)$  and  $O(\Delta t^2)$ , Eq.  
 643 (A3) simplifies as:

$$644 \quad \begin{aligned} E^{eq}(\mathbf{x}) &= \frac{\Delta x^D}{\Delta S \Delta t} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} \left[ 2\omega_i \frac{\rho \mathbf{e}_i \cdot \mathbf{u}}{c_s^2} - \Delta t \omega_i \mathbf{e}_i \cdot \nabla \rho + \Delta t \omega_i \mathbf{e}_i \cdot \nabla \frac{\rho \mathbf{e}_i \cdot \mathbf{u}}{c_s^2} \right] \\ &\quad - \frac{\Delta x^D}{\Delta S} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} \left\{ \omega_i \frac{\mathbf{e}_i \cdot \nabla [\rho (\mathbf{e}_i \cdot \mathbf{u})^2]}{2c_s^4} - \omega_i \frac{\mathbf{e}_i \cdot \nabla (\rho \mathbf{u} \cdot \mathbf{u})}{2c_s^2} \right\} \end{aligned} \quad (\text{A4})$$

645 As illustrated in Fig. 1(b), at a boundary node along an aligned boundary, the wall-cut LB links  
 646 is symmetrical around an axis, e.g. the  $m$ th axis, with a unit vector  $\mathbf{n}_m$  pointing to the fluid side  
 647 (referred to as “main direction”). Accordingly, all wall-cut links share a non-zero  $m$ th velocity  
 648 component  $e_{i,k} = \pm c$ , and the other components  $e_{i,j \neq m}$  are symmetrically distributed among  $-c, 0$   
 649 and  $c$ . Considering the symmetry of wall-cut links and  $\Delta S = \Delta x^{D-1}$ , the linear terms of  $\mathbf{u}$  on the  
 650 right-hand side of Eq. (A4) can be evaluated as:

$$\left\{ \begin{array}{l}
 \frac{\Delta x^D}{\Delta S \Delta t} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} \left( 2\omega_i \frac{\rho \mathbf{e}_i \cdot \mathbf{u}}{c_s^2} \right) = c \sum_{i=1}^Q \left( \omega_i \frac{-c \rho u_m}{c_s^2} \right) = -\rho u_m \\
 \frac{\Delta x^D}{\Delta S \Delta t} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} (\Delta t \omega_i \mathbf{e}_i \cdot \nabla \rho) = \frac{\Delta x}{2} \sum_{i=1}^Q (-c \omega_i \partial_m \rho) = -\frac{\Delta x}{6} c \partial_m \rho \\
 \frac{\Delta x^D}{\Delta S \Delta t} \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S} \left( \Delta t \omega_i \mathbf{e}_i \cdot \nabla \frac{\rho \mathbf{e}_i \cdot \mathbf{u}}{c_s^2} \right) = \\
 \frac{\Delta x}{2} \sum_{i=1}^Q \left[ \omega_i \frac{e_{i,m}^2 \partial_m (\rho u_m)}{c_s^2} \right] + \Delta x \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S, j \neq m} \left[ \omega_i \frac{e_{i,j}^2 \partial_j (\rho u_j)}{c_s^2} \right] \\
 = \frac{\Delta x}{2} \partial_m (\rho u_m) + \frac{\Delta x}{6} \partial_j (\rho u_j) = \frac{\Delta x}{3} \partial_m (\rho u_m) + \frac{\Delta x}{6} \nabla \cdot (\rho \mathbf{u})
 \end{array} \right. \quad (\text{A5})$$

652 where  $\partial_m = \mathbf{n}_m \cdot \nabla$ ,  $u_m = \mathbf{u} \cdot \mathbf{n}_m$ ,  $j$  denotes the axis perpendicular to the main direction (or the  
 653  $m$ th axis),  $Q$  is the number of the discrete velocities (e.g.  $Q = 9$  for the D2Q9 model), and the  
 654 following relations hold:

$$\left\{ \begin{array}{l}
 e_{i,m}^2 = c^2, \quad c_s^2 = c^2/3, \quad \sum_{i=1}^Q \omega_i \frac{e_{i,j}^2}{c_s^2} = 1 \\
 e_{i,m} \cdot \mathbf{n}_m = -c \quad \text{for } \mathbf{x} + \mathbf{e}_i \Delta t \in S \\
 2 \sum_{\mathbf{x} + \mathbf{e}_i \Delta t \in S, j \neq m} \left( \omega_i \frac{e_{i,j}^2}{c_s^2} \right) / \sum_{i=1}^Q \left( \omega_i \frac{e_{i,j}^2}{c_s^2} \right) = \frac{c_s^2}{c^2}
 \end{array} \right. \quad (\text{A6})$$

656 In the last relation of Eq. (A6), compared to the denominator, the nominator does not include  
 657 the discrete velocities perpendicular to the main direction, e.g. the links between  $B_1$  and  $B_2$  in Fig.  
 658 1(b). The relations in Eq. (A6) are valid for the D2Q5 and D2Q9 models as well as D3Q19 and  
 659 D3Q27 models when the solution is invariant along the third axis. Equation (A5) demonstrates  
 660 that the wall-cut LB links at a regular boundary node are only able to restore velocity and gradient  
 661 components along the main direction, while the other components are completely omitted. Still,  
 662 by applying Eq. (A6), the non-linear terms in Eq. (A4) can be simplified as:

$$\begin{aligned}
& \frac{\Delta x^D}{\Delta S} \sum_{\mathbf{x}+\mathbf{e}_i\Delta t \in S} \left\{ \omega_i \frac{\mathbf{e}_i \cdot \nabla [\rho(\mathbf{e}_i \cdot \mathbf{u})^2]}{2c_s^4} - \omega_i \frac{\mathbf{e}_i \cdot \nabla (\rho \mathbf{u} \cdot \mathbf{u})}{2c_s^2} \right\} \\
&= \frac{\Delta x}{2} \sum_{i=1}^Q \left[ \omega_i \frac{-c e_{i,m}^2 \partial_m (\rho u_m^2)}{2c_s^4} \right] + \Delta x \sum_{\mathbf{x}+\mathbf{e}_i\Delta t \in S, j \neq m} \left\{ \omega_i \frac{e_{i,m} e_{i,j}^2}{2c_s^4} [\partial_m (\rho u_j^2) + \partial_j (\rho u_m u_j)] \right\} \\
663 \quad & - \frac{\Delta x}{2} \sum_{i=1}^Q \left[ \omega_i \frac{-c \partial_m (\rho u_m^2 + \rho u_j^2)}{2c_s^2} \right] \tag{A7} \\
&= -\frac{\Delta x}{2} c \left[ \frac{\partial_m (\rho u_m^2)}{2c_s^2} + \frac{c_s^2}{c^2} \frac{\partial_m (\rho u_j^2) + \partial_j (\rho u_m u_j)}{2c_s^2} - \frac{\partial_m (\rho u_m^2 + \rho u_j^2)}{2c^2} \right] \\
&= -\frac{\Delta x}{2} c \left[ \frac{\partial_m (\rho u_m^2)}{3c_s^2} + \frac{\partial_j (\rho u_m u_j)}{6c_s^2} \right] = -\frac{\Delta x}{4c} [\partial_m (\rho u_m^2) + \nabla \cdot (\rho u_m \mathbf{u})]
\end{aligned}$$

664 Consequently, by substituting Eqs. (A5) and (A7) into Eq. (A3), the mass leakage directly  
665 induced by  $f^{eq}$  can be expressed as:

$$666 \quad E^{eq}(\mathbf{x}) = -\rho u_m + \frac{\Delta x}{6} c \partial_m \rho + \frac{\Delta x}{3} \partial_m (\rho u_m) + \frac{\Delta x}{6} \nabla \cdot (\rho \mathbf{u}) + \frac{\Delta x}{4c} [\partial_m (\rho u_m^2) + \nabla \cdot (\rho u_m \mathbf{u})] \tag{A8}$$

667 The mass leakage due to the non-equilibrium distribution function, i.e.  $E^{ne}$  in Eq. (A2), is now  
668 analysed. Still considering regular boundary nodes along aligned boundaries ( $\Delta S = \Delta x^{D-1}$ ), by  
669 applying the symmetry of discrete velocities, it can be rewritten as:

$$\begin{aligned}
670 \quad E^{ne}(\mathbf{x}) &= -\sum_{i=1}^Q [e_{i,m} f_i^{ne}(\mathbf{x})] - \frac{\Delta x}{\Delta t} \sum_{\mathbf{x}+\mathbf{e}_i\Delta t \in S} [f_i^{ne}(\mathbf{x} + \mathbf{e}_i\Delta t) - f_i^{ne}(\mathbf{x})] \\
&= -\Delta x \sum_{\mathbf{x}+\mathbf{e}_i\Delta t \in S} \left[ \frac{D f_i^{ne}(\mathbf{x})}{Dt} + \Delta t \frac{D^2 f_i^{ne}(\mathbf{x})}{Dt^2} + O(\Delta t^2) \right] \tag{A9}
\end{aligned}$$

671 Now using Eq. (8), one obtains :

$$672 \quad E^{ne}(\mathbf{x}) = -c \Delta x^2 \sum_{\mathbf{x}+\mathbf{e}_i\Delta t \in S} \mathcal{L}_i^{-1} \frac{D^2 f^{eq}(\mathbf{x})}{Dt^2} + O(\Delta x^3) \tag{A10}$$

673 Substituting Eqs. (A8) and (A10) into Eq. (A1) and omitting high order terms, the resultant  
674 mass leakage is dominated by  $E^{eq}$ , and can therefore be expressed as:

$$\begin{aligned}
675 \quad E(\mathbf{x}) &\approx -\rho u_m + \frac{\Delta x}{6} c \partial_m \rho + \frac{\Delta x}{3} \partial_m (\rho u_m) + \frac{\Delta x}{6} \nabla \cdot (\rho \mathbf{u}) \\
&+ \frac{\Delta x}{4c} [\partial_m (\rho u_m^2) + \nabla \cdot (\rho u_m \mathbf{u})] + \rho_w \mathbf{U} \cdot \mathbf{n} \tag{A11}
\end{aligned}$$

676 **Appendix B: Local mass leakage at irregular boundary nodes**

677 As depicted in §IV, irregular boundary nodes can be classified into two kinds regarding whether  
678 they are associated with irregular cells. Their mass leakage are analysed separately now.

679 For irregular boundary nodes not associated with irregular cells ( e.g.  $B_1$  shown in Fig. 2(a)),  
680 they can be directly approximated as regular boundary nodes because the cut links are exactly the  
681 same as those cut by aligned boundaries (see  $B_1$  shown in Fig. 1(b) and Fig. 2(a)). The main  
682 difference is that the main direction  $\mathbf{n}_m$  of the approximated regular boundary node is different  
683 from the local normal vector  $\mathbf{n}$ , i.e.

$$684 \quad \mathbf{n}_m = \cos \gamma \mathbf{n} - \sin \gamma \mathbf{n}_t \quad (\text{B1})$$

685 where  $\gamma$  is the angle rotating from  $\mathbf{n}$  to  $\mathbf{n}_m$  anti-clockwise, and  $\mathbf{n}_t$  is the tangential unit vector.  
686 By substituting Eq. (B1) into Eq. (A11), the mass leakage can be estimated as:

$$687 \quad E(\mathbf{x}, \gamma) = \frac{\Delta x^{D-1}}{\Delta S} \left\{ -\rho u_m + \frac{\Delta x c \partial_m \rho}{6} + \frac{\Delta x \partial_m (\rho u_m)}{3} \right. \\ \left. + \frac{\Delta x \nabla \cdot (\rho \mathbf{u})}{6} + \frac{\Delta x}{4c} [\partial_m (\rho u_m^2) + \nabla \cdot (\rho u_m \mathbf{u})] \right\} + \rho_w \mathbf{U} \cdot \mathbf{n} \quad (\text{B2})$$

688 which can be simplified as:

$$689 \quad E(\mathbf{x}, \gamma) = \rho u_t \tan \gamma + \frac{\Delta x c}{6} (\partial_n - \tan \gamma \partial_t) \rho + E_{sh} + E_{exp} + E_{div} \quad (\text{B3})$$

690 with

$$691 \quad \begin{cases} E_{sh} = -\frac{\Delta x \sin \gamma}{3} [\partial_t (\rho u_n) + \partial_n (\rho u_t)] - \frac{\Delta x \sin(2\gamma)}{8c} [2\partial_n (\rho u_n u_t) + \partial_t (\rho u_n^2)] \\ \quad + \frac{\Delta x \sin^2 \gamma}{4c} [2\partial_t (\rho u_n u_t) + \partial_n (\rho u_t^2)] \\ E_{exp} = \left[ \frac{\cos(2\gamma)}{3 \cos \gamma} \Delta x - \Delta w \right] \partial_n (\rho u_n) + \frac{\Delta x \cos^2 \gamma}{4c} [\partial_n (\rho u_n^2) - \tan^3 \gamma \partial_t (\rho u_t^2)] \\ E_{div} = \Delta x \left( \frac{\sin^2 \gamma}{3 \cos \gamma} + \frac{1}{6 \cos \gamma} \right) \nabla \cdot (\rho \mathbf{u}) + \frac{\Delta x \cos^2 \gamma}{4c} \nabla \cdot [\rho (u_n - \tan \gamma u_t) \mathbf{u}] \end{cases} \quad (\text{B4})$$

692 where  $\Delta S = \Delta^{D-1} x \cos \gamma$  and  $\partial_m = \cos \gamma \partial_n - \sin \gamma \partial_t$  are applied,  $u_n = \mathbf{u} \cdot \mathbf{n}$ ,  $u_t = \mathbf{u} \cdot \mathbf{n}_t$ , and  $E_{sh}$ ,  
693  $E_{exp}$  and  $E_{div}$  are the mass leakages associated with fluid shear rate, expansion rate and divergence  
694 of the involved first- and second-order momentum, respectively. Geometrically,  $\gamma$  is related to the  
695 angle  $\theta$  as  $\gamma = \pm \theta$ , and thus  $-45^\circ \leq \gamma \leq 45^\circ$ . Substituting  $\gamma = \pm \theta$  into Eq. (A11), it becomes:

$$E(\mathbf{x}) = \pm \rho u_t \tan \theta + O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho \mathbf{u})\|) + O\left[\Delta x \frac{\|\nabla(\rho \mathbf{u})\|}{c_s}\right] \quad (\text{B5})$$

For irregular boundary nodes associated with irregular cell pairs, they can be approximated as regular boundary nodes through two kinds of operations. Firstly, the links between neighbouring boundary nodes could be treated as virtual cut links without causing extra net mass leakage. For example, as shown in Fig. 2(a), by considering the virtually cut links  $e_5$  and  $e_6$  between  $B_2$  and  $B_3$ , the node  $B_3$  can be treated as an approximated regular boundary node with a horizontal main direction. Secondly, wall-cut LB links at one boundary node can be shifted to its neighbouring boundary node to complete the remained approximation to regular boundary node. For example, as shown in Fig. 2(a), by shifting the cut links  $e_3$  and  $e_4$  at  $B_1$  to  $B_2$ , the total cut links, including the virtual  $e_5$  and  $e_6$ , exactly approximate  $B_2$  as two regular boundary nodes with different main directions (one is horizontal and the other is vertical). Mass leakage at the approximated regular node pairs, e.g. those at  $B_2$  as analysed, can be estimated by Eq. (B3) with  $\gamma$  being  $\pm\theta$  and  $\pm\theta \mp 90^\circ$ , respectively, i.e.

$$E(\mathbf{x}) = \frac{E(\mathbf{x}, \pm\theta) \Delta x^{D-1} \cos \theta + E(\mathbf{x}, \pm\theta \mp 90^\circ) \Delta x^{D-1} \cos(\pm\theta \mp 90^\circ)}{\Delta x^{D-1} \cos \theta + \Delta x^{D-1} \cos(\pm\theta \mp 90^\circ)} \\ = \rho u_t \tan(\pm\theta \mp 45^\circ) + O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho \mathbf{u})\|) + O\left[\Delta x \frac{\|\nabla(\rho \mathbf{u})\|}{c_s}\right] \quad (\text{B6})$$

In addition, using shifted links to derive Eq. (B3) requires extra mass leakage correction terms. The required correction for shifting  $f_j$  from  $\mathbf{x} + e_i \Delta t$  to  $\mathbf{x}$  can be expressed as:

$$E_s(\mathbf{x}) = \frac{\Delta x^D}{\Delta S \Delta t} [f_j(\mathbf{x} + e_i \Delta t) - f_j(\mathbf{x})] \\ = \frac{\Delta x^D}{\Delta S} e_i \cdot \nabla f_j + O(\Delta x^2) = \frac{\Delta x^D}{\Delta S} e_i \cdot \nabla f_j^{eq} + O(\Delta x^2) \quad (\text{B7})$$

where the expression of  $f$  by  $f^{eq}$  (Eq. (9)) has been used. Omitting the high order term  $O(c \Delta x^2)$  and applying the analysis of  $e_i \cdot \nabla f_i^{eq}$  given in Eqs. (A3) to (A8), Eq. (B7) can be rewritten as:

$$E_s(\mathbf{x}) = O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho \mathbf{u})\|) + O\left[\Delta x \frac{\|\nabla(\rho \mathbf{u})\|}{c_s}\right] \quad (\text{B8})$$

Since all the terms in Eq. (B8) have been included in Eq. (B6), Eq. (B6) adequately describes the resultant mass leakage at the irregular boundary nodes associated with irregular cells.

719 **Appendix C: Averaged mass leakage over smooth boundaries**

720 As described in §V, the averaged mass leakage over general smooth boundaries can be estimated  
 721 from those of four basic kinds of serrated cells (see Fig. 3(a)-(d)), and they are quantified now.

722 Firstly, mass leakage of an ideal serrated cell is quantified by considering the one shown in Fig.  
 723 3(a) without loss of generality. Apparently, the averaged process is conducted over the boundary  
 724 nodes along  $AB$  (excluding A) and the one at C. According to the analysis proposed in §IV B, the  
 725 irregular boundary node at B and C can be approximated as two regular ones with a horizontal  
 726 and vertical main directions, respectively, and those along  $AB$  (except B) can be approximated as  
 727 regular ones with a vertical main direction. Accordingly, their mass leakage can be estimated by  
 728 Eq. (B3) with  $\gamma$  being equal to  $90^\circ - \theta$  and  $-\theta$ , respectively. Consequently, the averaged mass  
 729 leakage of an ideal serrated cell can be expressed as:

$$\begin{aligned}
 E_{sc,i} &= \frac{\Delta s_C E(\mathbf{x}_C) + \sum_{P=B}^A [\Delta s_P E(\mathbf{x}_P)]}{\|AC\|} \\
 &= \frac{\rho u_t \tan(90^\circ - \theta) \Delta x \sin \theta}{\|AC\|} + \frac{\sum_{n=1}^{\tan^{-1} \theta} \left[ \rho u_t + \frac{\partial \rho u_t}{\partial y} \Delta x + \frac{\partial \rho u_t}{\partial x} n \Delta x \right] \tan(-\theta) \Delta x \cos \theta}{\|AC\|} \\
 &\quad + O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho \mathbf{u})\|) + O\left[ \Delta x \frac{\|\nabla(\rho \mathbf{u} \mathbf{u})\|}{c_s} \right] \tag{C1} \\
 &= \rho u_t (\cos \theta \sin \theta - \cos \theta \sin \theta) - \left[ \frac{\partial \rho u_t}{\partial y} + \frac{\tan^{-1} \theta + 1}{2} \frac{\partial \rho u_t}{\partial x} \right] \Delta x \cos \theta \sin \theta \\
 &\quad + O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho \mathbf{u})\|) + O\left[ \Delta x \frac{\|\nabla(\rho \mathbf{u} \mathbf{u})\|}{c_s} \right] + O(\Delta x^2) \\
 &\approx O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho \mathbf{u})\|) + O\left[ \Delta x \frac{\|\nabla(\rho \mathbf{u} \mathbf{u})\|}{c_s} \right]
 \end{aligned}$$

731 where the macroscopic variables are evaluated at C, and the terms in the order of  $O(\Delta x^2)$  are  
 732 omitted.

733 Secondly, extra mass leakage of a serrated cell (see Fig. 3(b)) induced by a non-zero distance  
 734 shift  $\Delta s$  ( $\Delta s < \sqrt{D} \Delta x$ ) is estimated. As shown in Fig. 3(b),  $\Delta s$  causes a uniform wall distance  
 735 increase to the boundary nodes, e.g.  $\mathbf{x}_C = \mathbf{x}'_C + \Delta s \mathbf{n}$ , but does not affect  $n$  and the main direc-  
 736 tions of the approximated regular boundary nodes. Therefore,  $\Delta s$  could directly modify the term  
 737  $\Delta w \partial_n(\rho u_n)$ , and its influence on the other terms appearing in Eq. (C1) is the order of  $O(\Delta x^2)$ .  
 738 Consequently, the extra mass leakage caused by  $\Delta s$  can be expressed as:

739

$$E_{sc,s} = \Delta s \partial_n(\rho u_n) \quad (C2)$$

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Thirdly, extra mass leakage of a rotated serrated cell caused by an angle deviation  $\Delta\theta$  (see Fig. 3(c)) is quantified. The mass leakage can be estimated based on the virtual ideal serrated cell  $ABC$  with the normal velocity of the virtual boundary  $AC$  being:

743

$$u_{n,v} = -u_t \sin \Delta\theta + u_n \cos \Delta\theta \quad (C3)$$

744

745 as:

746

$$\begin{aligned} E_{sc,r} &= \frac{(E_{sc,i} - \rho u_{n,v}) \|AC\|}{\|AC\| \cos \Delta\theta} + \rho_w \mathbf{U} \cdot \mathbf{n} \\ &= \rho u_t \tan \Delta\theta + O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho \mathbf{u})\|) + O\left[\Delta x \frac{\|\nabla(\rho \mathbf{u} \mathbf{u})\|}{c_s}\right] \end{aligned} \quad (C4)$$

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Since the angle deviation  $\Delta\theta$  may vary significantly for each serrated cell, it is necessary to estimate averaged mass leakage of cascaded rotated serrated cells.

Firstly, two cascaded serrated cells are considered. As shown in Fig. 19(a), averaged mass leakage of two cascaded serrated cells can be estimated from those of each cells (see Eq. (C4)) as:

751

$$\begin{aligned} E_{sc,2rt} &= (\rho u_t \tan \Delta\theta_1)|_{x=x_C} \frac{\|AA'\|}{\tan \Delta\theta_1 \|AA'\| (\tan \Delta\theta_1 + \tan \Delta\theta_2)} \\ &\quad - (\rho u_t \tan \Delta\theta_2)|_{x=x_A} \frac{\|AA'\|}{\tan \Delta\theta_2 \|AA'\| (\tan \Delta\theta_1 + \tan \Delta\theta_2)} \\ &\quad + O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho \mathbf{u})\|) + O\left[\Delta x \frac{\|\nabla(\rho \mathbf{u} \mathbf{u})\|}{c_s}\right] \\ &= O(\Delta x c \|\nabla \rho\|) + O(\Delta x \|\nabla(\rho \mathbf{u})\|) + O\left[\Delta x \frac{\|\nabla(\rho \mathbf{u} \mathbf{u})\|}{c_s}\right] \end{aligned} \quad (C5)$$

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Interestingly, the averaged mass leakage of two cascaded serrated cells share a same formula with that of an ideal serrated cell (see Eq. (C1)). This similarity is important because it indicates that the mass leakage of two cascaded cells with an angle deviation can be directly described by that of a rotated cell given by Eq. (C4). Based on that, three cascaded serrated cells can be decomposed into one rotated serrated cell and two cascaded serrated cells with an angle deviation, and the total mass leakage is given by Eq. (C5). Recursively, a series of cascaded serrated cells with an angle deviation  $\Delta\theta$  (see Fig. 19(b)) can be estimated thanks to Eq. (C5).

759 Considering that the distance between the starting and ending "sawtooth" tip nodes (e.g. the  
 760 "Start" and "End" points in Fig. 19(b)) could be comparable with the macroscopic reference length  
 761  $L$ ,  $\tan\Delta\theta$  can scales like  $O(\Delta x/L)$ , and the averaged mass leakage of a series of cascaded rotated  
 762 serrated cells can be estimated as:

$$763 \quad E_{sc,rt} \approx O\left(\frac{\Delta x}{L}\rho u_t\right) + O(\Delta x c \|\nabla\rho\|) + O(\Delta x \|\nabla(\rho\mathbf{u})\|) + O\left[\Delta x \frac{\|\nabla(\rho\mathbf{u}\mathbf{u})\|}{c_s}\right] \quad (C6)$$

764 Comparing Eq. (C6) to Eq. (C1), the extra mass leakage term caused by  $\Delta\theta$  can be expressed  
 765 as:

$$766 \quad E_{sc,\theta} = E_{sc,rt} - E_{sc} = \rho u_t \tan\Delta\theta = O(\rho u_t \frac{\Delta x}{L}) \quad (C7)$$

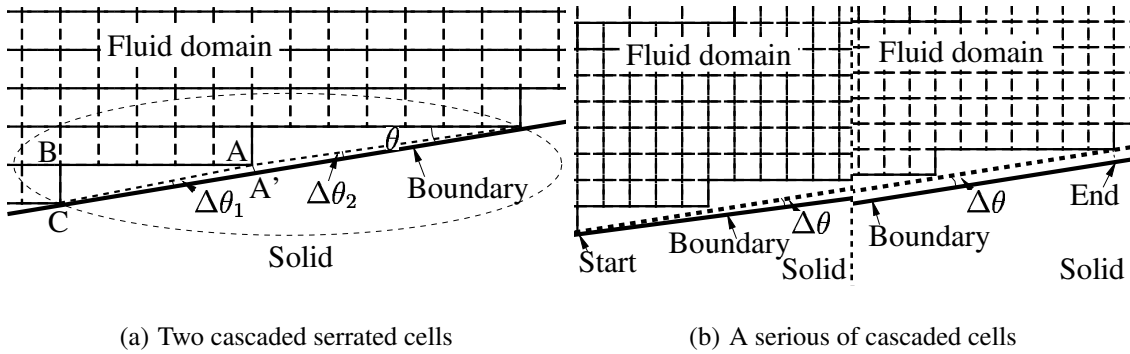


FIG. 19. Sketches of cascaded serrated cells at a smooth boundary: two cascaded serrated cells (a) and a series of cascaded serrated cells (b).

767 Finally, the mass leakage caused by boundary curvature is analysed. As shown in Fig. 3(d),  
 768  $R_c$  is the local curvature radius,  $\varphi$  is the angle corresponding to the arc  $\widehat{AC}$ , and  $\Delta\varphi$  is the angle  
 769 from the virtual planar boundary  $AC$  to the tangential direction at a point on the curved boundary  
 770 (positive if clockwise measured).

771 Before going further, two basic geometrical relationships are derived. First,  $\theta$  and  $\varphi$  are related  
 772 as:

$$773 \quad \|AC\| = 2R_c \sin \frac{\varphi}{2} = \frac{\Delta x}{\sin \theta} \quad (C8)$$

774 Second, to avoid another intersection point (except A) between the curved boundary and the  
 775 grid line  $AB$ ,  $R_c$  is constrained to be:



$$\frac{\|AC\|}{\sin \theta} \leq 2R_c \Rightarrow \sin \theta \geq \sqrt{\frac{\Delta x}{2R_c}} \Rightarrow \sin \frac{\varphi}{2} \leq \sqrt{\frac{\Delta x}{2R_c}} \text{ and } \varphi \sim O\left(\sqrt{\frac{\Delta x}{R_c}}\right) \quad (C9)$$

where  $\|AC\| = \frac{\Delta x}{\sin \theta}$  and  $2R_c \sin \frac{\varphi}{2} = \frac{\Delta x}{\sin \theta}$  are used.

Based on Eqs. (C8) and (C9), the extra mass leakage of a serrated cell caused by boundary curvature can be estimated in a way similar to the mass leakage of an ideal serrated cell (see Eq. (C1)). As a matter of fact, the extra mass leakage can be attributed to the associated velocity disturbances. Along a curved boundary, the tangential and normal (relative to the virtual planar boundary, e.g.  $AC$  shown in Fig. 3(d)) velocity disturbances at a boundary node due to the boundary curvature can be estimated as:

$$\Delta u_t = u_t(\cos \Delta \varphi - 1) - u_n \sin \Delta \varphi, \quad \Delta u_n = u_t \sin \Delta \varphi + u_n(\cos \Delta \varphi - 1) \quad (C10)$$

where  $u_t$  and  $u_n$  are the tangential and normal velocity components relative to the curved boundary, respectively. Applying Eq. C10, the mass leakage can be expressed as:

$$E_{sc,c} = \frac{E(x_C)\Delta s_C + \sum_{P=A}^B E(x_P)\Delta s_P}{R_c \varphi} = E_{sc,ct} + E_{sc,cn} \quad (C11)$$

with

$$\begin{cases} E_{sc,ct} = \frac{\rho \Delta u_t \cos \theta \Delta x - \sum_{n=1}^{\tan^{-1} \theta} \rho \Delta u_t \sin \theta \Delta x}{R_c \varphi}, \\ E_{sc,cn} = \frac{-\rho \Delta u_n \sin \theta \Delta x - \sum_{n=1}^{\tan^{-1} \theta} \rho \Delta u_n \cos \theta \Delta x}{R_c \varphi} \end{cases} \quad (C12)$$

where  $E_{sc,ct}$  and  $E_{sc,cn}$  are the mass leakage caused by the tangential and normal velocity disturbances, respectively, and terms in the order of  $O(\Delta x^2)$  are omitted. Substituting Eq. (C10) into Eq. (C12), one obtains :

$$\begin{cases} E_{sc,ct} = \frac{\rho [u_t(\cos \frac{\varphi}{2} - 1) - u_n \sin \frac{\varphi}{2}] \cos \theta \Delta x - \sum_{n=1}^{\tan^{-1} \theta} \rho [u_t(\cos \Delta \varphi - 1) - u_n \sin \Delta \varphi] \sin \theta \Delta x}{R_c \varphi}, \\ E_{sc,cn} = \frac{-\rho [u_t \sin \frac{\varphi}{2} + u_n(\cos \frac{\varphi}{2} - 1)] \sin \theta \Delta x - \sum_{n=1}^{\tan^{-1} \theta} \rho [u_t \sin \Delta \varphi + u_n(\cos \Delta \varphi - 1)] \cos \theta \Delta x}{R_c \varphi} \end{cases} \quad (C13)$$

In Eq. (C13), the angle variation  $\Delta \varphi$  can be approximated as:

$$\Delta \varphi \approx \frac{n \Delta x \cos \theta}{R_c} - \frac{\varphi}{2} \quad (C14)$$

796 Substituting  $\frac{\Delta x}{R_c} = 2 \sin \theta \sin \frac{\varphi}{2}$  (Eq. (C8)) and  $\sin \frac{\varphi}{2} = \frac{\varphi}{2} + O(\frac{\varphi^3}{8})$  into the above expression, it  
 797 comes :

$$798 \quad \Delta\varphi \approx 2n \sin \theta \cos \theta \sin \frac{\varphi}{2} - \frac{\varphi}{2} = [n \sin(2\theta) - 1] \frac{\varphi}{2} + O(\frac{\varphi^3}{8}) \quad (C15)$$

799 Now substituting (C15) along with  $\sin \frac{\varphi}{2} = \frac{\varphi}{2} + O(\frac{\varphi^3}{8})$ ,  $\cos \frac{\varphi}{2} = 1 - \frac{\varphi^2}{8} + O(\frac{\varphi^4}{16})$ ,  $\sin \Delta\varphi = \Delta\varphi +$   
 800  $O(\Delta\varphi^3)$  and  $\cos \Delta\varphi = 1 - \Delta\varphi^2/2 + O(\Delta\varphi^4)$  into Eq. (C12), the mass leakages  $E_{sc,ct}$  and  $E_{sc,cn}$  can  
 801 be simplified as:

$$802 \quad \begin{cases} E_{sc,ct} \approx -u_n \cos \theta (1 + \sin^2 \theta - \sin \theta \cos \theta) \frac{\Delta x}{R_c} + u_t \cos^2 \theta \frac{\Delta x}{4R_c} + O(u_t \frac{\Delta x^{3/2}}{R_c^{3/2}}) \\ E_{sc,cn} \approx -\rho u_t (\sin^3 \theta + \cos^3 \theta) \frac{\Delta x}{R_c} + \rho u_n \cos^2 \theta \frac{\Delta x}{4R_c} + O(\rho u_n \frac{\Delta x^{3/2}}{R_c^{3/2}}) \end{cases} \quad (C16)$$

803 Consequently, by omitting the terms in the order of  $O(\frac{\Delta x^{3/2}}{R_c^{3/2}})$ , the dominating parts of the total  
 804 mass leakage caused by boundary curvature can be estimated as:

$$805 \quad E_{sc,c} = E_{sc,ct} + E_{sc,cn} \approx O\left(\rho u_t \frac{\Delta x}{R_c}\right) + O\left(\rho u_n \frac{\Delta x}{R_c}\right) = O\left(\rho \|\mathbf{u}\| \frac{\Delta x}{R_c}\right) \quad (C17)$$

806 Notably, the above analysis of averaged mass leakage is derived from the mesoscopic view to  
 807 the macroscopic view, and thus is generally valid for LB simulation. Whereas, it should be noticed  
 808 that it is not the only way to quantify the averaged mass flux. For example, Ginzburg<sup>7</sup> proposed an  
 809 exact computation of mass leakage in inclined channel Stokes flow based on distribution functions  
 810 reconstructed by Chapman-Enskog analysis up to second order, and it has been already exemplified  
 811 analytically for stair-wise boundaries.

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