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ABSTRACT

We introduce two new approaches, called A-LSOB and N-MR, for boundary and interface-conjugate conditions on flat or curved surface shapes in the advection-diffusion lattice Boltzmann method (LBM). The Local Second-Order, single-node A-LSOB enhances the existing Dirichlet and Neumann normal boundary treatments with respect to locality, accuracy, and Péclet parametrization. The normal-multi-reflection (N-MR) improves the directional flux schemes via a local release of their nonphysical tangential constraints. The A-LSOB and N-MR restore all first- and second-order derivatives from the nodal non-equilibrium solution, and they are conditioned to be exact on a piece-wise parabolic profile in a uniform arbitrary-oriented tangential velocity field. Additionally, the most compact and accurate single-node parabolic schemes for diffusion and flow in grid-inclined pipes are introduced. In simulations, the global mass-conservation solvability condition of the steady-state, two-relaxation-time (S-TRT) formulation is adjusted with either (i) a uniform mass-source or (ii) a corrective surface-flux. We conclude that (i) the surface-flux counterbalance is more accurate than the bulk one, (ii) the A-LSOB Dirichlet schemes are more accurate than the directional ones in the high Péclet regime, (iii) the directional Neumann advective-diffusive flux scheme shows the best conservation properties and then the best performance both in the tangential no-slip and interface-perpendicular flow, and (iv) the directional non-equilibrium diffusive flux extrapolation is the least conserving and accurate. The error Péclet dependency, Neumann invariance over an additive constant, and truncation isotropy guide this analysis. Our methodology extends from the d2q9 isotropic S-TRT to 3D anisotropic matrix collisions, Robin boundary condition, and the transient LBM.

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I. MOTIVATION

Recent physical, biomechanical, and engineering research, and especially solute and heat transfer modeling in porous networks, intensively apply the lattice Boltzmann method (LBM) in complex problems for solving linear, non-linear, isotropic or anisotropic advection-diffusion equation (ADE) with homogeneous or heterogeneous coefficients and sources. Although the coordinate d2q5/d3q7 discrete velocity stencil is sufficient to match the diagonal diffusion tensors, the specific combinations of the coordinate and diagonal equilibrium weights are appealing for their truncation isotropy and advanced stability. In bulk, the standard LBM guarantees the local and global mass conservation, which is defined from the zero-moment (sum) of its real variables, called populations, allowing for a regular, cuboid control-volume interpretation of the LBM mass-balance. The simplest heterogeneity treatment–do nothing algorithm, and the Maxwell, bounce-back (BB), and mirror (specular-forward) population reflections on the impermeable boundary preserve the global conservation property at the cost of only approximately
mid-node, implicit location of the grid-aligned walls and interfaces.\textsuperscript{16,29,32,34,97}

However, it was recognized\textsuperscript{14,107} that although the mirror reflection is suitable, the BB and “local” specular reflection (which returns the mass to departure node), enforce to zero not only the normal but also the tangential mass-flux components through the wall-inclined discrete-velocities.\textsuperscript{16,29} The implicit interface tracking shares a similar tangential deficiency, because its advective-diffusive flux and scalar-field continuity conditions intrinsically couple\textsuperscript{16} the BB and the (anti-BB) ABB Dirichlet rule\textsuperscript{26,56}. The distribution moments can be regarded as the best indicators of the nonphysical solution behavior. So that, when the solute travels along an impermeable straight tubular conduit, the BB spurious effects on the first and second Gaussian moments, leading to (i) a retardation of the mean advection velocity $\mathcal{U}$ and (ii) a decrease in the molecular diffusion coefficient $D_0$, grow with a free-tunable diagonal weight-value and decay only linearly with the space resolution.\textsuperscript{16,29} Gebäck and Heintz\textsuperscript{2} extended the mirror reflection for curved wall on the $d3q7$ and $d3q19$ lattices, and improved the BB in the presence of the tangential wall flux in the diffusion problems. However, on the one side, the global accuracy worsens when the populations reflected by the same ghost solid node conserve its incoming mass; on the other side, the BB behaves as accurately as the mass-conserving mirror schemes, and much better than the non-conserving ones, for the zero tangential boundary flux.

Our boundary value problems are delivered by the extended method of moments (EMM),\textsuperscript{37,84} which is the mathematical algorithm for the recursive prediction of the distribution moments: dispersion, skewness, kurtosis, … The EMM extends the Brenner’s generalized dispersion approach\textsuperscript{2} and the volume averaging boundary-value formulation,\textsuperscript{93} from the second-order microscopic spatial Taylor moment to any-order, spatial or temporal, moment. The EMM applies in any nature multi-scale streamwise-periodic stationary d-dimensional, Newtonian or non-Newtonian, velocity field resolved in the piecewise continuous heterogeneous porousity field, where it simultaneously builds two systems of moments: the spatial (mean-concentration, due to 'Taylor & Aris'\textsuperscript{17}) and the temporal (residence time distribution, due to Danckwerts\textsuperscript{18}) The high-order moments characterize the non-Gaussian behavior, the EMM is hence appealing to classify them, particularly in porous and composite materials. Other utility is that the method builds recursively the steady-state ADE with the non-uniform, global-mass conserving sources; the ADE is closed by an impermeable Neumann boundary or periodic interface, and its symbolic solutions are available\textsuperscript{37,94} for benchmarking purpose.\textsuperscript{8}

The flow and the associated heat transport are often modeled with the so-called (multiple-relaxation-time thermal) MRT-TLBM, e.g., in a very recent work\textsuperscript{19} using the BB and ABB straight-wall rules. However, the MRT-TLBM operates the $d2q9$ flow collision with only two distinctive relaxation rates: the symmetric one for the fluid viscosity and the anti-symmetric one for the second-order BB accuracy using the exact Poiseuille flow solution,\textsuperscript{20,21} whereas the energy conservation equation is modeled with the $d2q5$ isotropic MRT-ADE. Indeed, these two collision models automatically reduce to the two-relaxation-time TRT collision,\textsuperscript{20,29} which is simpler, lattice independent, and more computationally efficient; additionally, the TRT allows for the solution parametrization, stability, and boundary/interface control with the help of the specific combination $\Lambda$ of its two relaxation rates; moreover, the optimal TRT-ADE stability choice\textsuperscript{31} $\Lambda = \frac{1}{2}$ remains robust in high Reynolds fluid flow modeling.\textsuperscript{79} The methodology developed in the present work is especially compact with the TRT collision but it extends for any linear collision operator. Numerically, we solve steady-state linear ADE with the recent (stationary) S-TRT formulation\textsuperscript{49} where (i) an arbitrary physical and model parameter range is available, because the S-TRT is quite insensitive to the transient stability restrictions and Péclet range, and (ii) the modeled solution is fixed by the grid Péclet number $\mathcal{W}/D_0$ and $\Lambda$ for any diffusion collision rate.

We apply the $d2q9$ with the free-tunable advection-diffusion equilibrium weights but, since the weight-stencils remains invisible for a stationary scalar field in the straight channels,\textsuperscript{38} in contrast with the aforementioned transient transport, we focus on the grid-rotated homogeneous and heterogeneous slabs, where all discrete directional effects “come to the surface.” To give one impressive example, the effective diffusivity of two diagonal heterogeneous blocks in series differs from its classical harmonic-mean value with the full $d2q9$ stencil. This happens because its intrinsic equilibrium accommodation on the implicit interface, called the A-layer,\textsuperscript{19} spoils the canonical piece-wise linear Chapman–Enskog prediction. The A-layer is much more harmful than its non-equilibrium B-layer counterpart, responsible for the BB moments corrections,\textsuperscript{33,34} because on top of the spurious weight-dependency, the A-layer is capable to modify the physical Péclet scale of the modeled solution, which is mandatory with the EMM for a proper prediction of the Péclet Ansatz in dispersion coefficient and higher order moments. Therefore, we aim to verify the performance of the advanced boundary and interface rules to reduce strong accommodation weight- and grid-inclined effects.

The “linear-interpolation” LI and “multi-reflection” MR ADE approach\textsuperscript{48} originates from its fluid flow counterparts\textsuperscript{22} and prescribes the Dirichlet scalar condition with the linear combination of three (LI) or five (MR) populations moving along the same wall-cut link, featuring, respectively, the exact linear or parabolic diffusion solutions in arbitrary oriented channels. Li and coworkers\textsuperscript{62} built several $d2q5/d3q7$ Dirichlet LI schemes and introduced flux LI scheme, hereafter referred to as FLI, which comes down to BB on a mid-grid wall. The Cartesian decomposition method\textsuperscript{62} involves the population interpolations and estimates the lacking tangential boundary flux value from the actual solution, with the help of the two intersecting coordinate linear MR Dirichlet conditions. This method however sacrifices the assets of the LI/MR link-wise implementation and its transparency for the discrete velocity set, because the $d2q9$ and $d3q19$ reduce the coordinate-set convergence by one-order.\textsuperscript{64} Then only the $d2q5/d3q7$ schemes\textsuperscript{62} were coupled for the scalar field and diffusive-flux interface-conjugate continuity\textsuperscript{65} and jumps\textsuperscript{65} these schemes were successfully evaluated against the semi-implicit interface methods.\textsuperscript{33,34} The coordinate, linear Dirichlet, Neumann, and Robin directional boundary schemes\textsuperscript{33,34} were combined for the interface diffusion conditions\textsuperscript{65} and further extended\textsuperscript{66} to account for the normal-vector variation along the shaped boundary.

Indeed, the transform of the Neumann and interface-flux conditions to their Dirichlet counterparts (like BB to ABB) has inspired many techniques on straight,\textsuperscript{19} stair-wise\textsuperscript{66} or curved\textsuperscript{67} surfaces. In an early work, the Neumann condition is simply plugged\textsuperscript{68} into the three-point back-sided normal Dirichlet extrapolation, whereas the interface-normal and bilinear extrapolations for curved shapes require even larger stencils.\textsuperscript{97,101} A very recent $d2q5$ scheme\textsuperscript{19} is more compact: it operates the solid bisection node with the two-node linear
(but again not directional) population interpolations and expresses the lacking boundary-flux from the obtained non-equilibrium solution, involving the ABB only for ghost population solution. However, the advection regime validation is commonly limited to a relatively small Péclet number (about twenty), whereas the ABB completely degrades its second-order accuracy for a mid-grid surface location in an interface-perpendicular plug flow at Pe \( \approx 10^3 \),\(^{33}\) because its directional closure relation interferes with the advective projections,\(^{33}\) overlooked by the later asymptotic analysis.\(^{106}\)

With these ideas in mind, the ABB, the equivalent LI schemes\(^ {40,106}\) and the MR Dirichlet schemes\(^ {40}\) have been recently extended\(^ {33}\) to “linear” [ABB/MPLI/PLI] and “parabolic” accurate [KMR/PP] Dirichlet families, improving their accuracy and parametrization by the grid Péclet number in the presence of the velocity field \([PABI/PSLI/KMR/PP]\) and space-variable mass-source, such that every family contains an infinite number of members (coefficients) of equivalent spatial accuracy; only the parametrized LMK scheme\(^ {26}\) enters the MPLI family. The LI can be operated in-node, whereas the MR requires the next directional fluid neighbor; both LI and MR cope with any discrete-velocity set but require, as a minimum, the TRT collision constraints into its global linear system. It should be emphasized that the A-LSOB has been developed independently of the single-node approach,\(^ {104,105}\) recently extended for the Dirichlet, Neumann and Robin conditions from its flow counterpart\(^ {103}\) with the d2q5 BGK\(^ {104}\) and d2q9 anisotropic matrix collision.\(^ {105}\) These two, flow and transport, methods adopt the original “Lwall” formulation\(^ {21}\) and the Chapman–Enskog solution through the surface variables but, "for the sake of simplicity", they drop all second-order derivatives. The methodology\(^ {104,105}\) is elaborated for the straight in-node wall and, in the curvilinear coordinates, for a circular surface. The method is reported to support the second-order accuracy through the benchmark simulations (i) in straight wall-node coincident surface, whereby the spatial variation vanishes from the closure relations, and (ii) in heat conduction inside a circle, where the diffusive flux only varies along the surface. Hence, the A-LSOB is expected to enhance those methods, principally, by now considering the spatial flux variation through the parabolic terms in the Chapman–Enskog solution. Several numerical examples will delineate the difference between the parabolic and linear-accurate A-LSOB.

Another point of focus is put on the comparison of the LI, MR, N-MR, and A-LSOB for their mass-balance properties. In fact, the solvability condition of the EMM boundary problems requires the mass-source distribution \( A(F) \) to conserve the global mass, say \( \langle A(F) \rangle \equiv 0 \). We prescribe it exactly and adjust the S-TRT with two heuristic solvability techniques: (i) a grid-uniform mass-source \( M_0 \) following,\(^ {40}\) then \( \langle A(F) + M_0 \rangle \equiv 0 \) in any geometry, or (ii) a non-conserving corrective flux \( \pm \Phi_0 \) prescribed on two parallel delimiting surfaces. The two variables, \( M_0 \) or \( \Phi_0 \), join the list of the global S-TRT unknowns and their solution measures the mass-balance property of the given scheme. Roughly speaking, these two experiments compare the uniform bulk distribution of the mass-leakage with its surface counterbalance.

We address them with the Taylor dispersion Ansatz\(^ {24,92}\) where the adjacent EMM problem combines the parabolic tangential velocity and mass-source fields. We will show that in the presence of the rotated advection, the quartic polynomial solution becomes only available with the hydrodynamic advection-diffusion weights, and it incorporates an anisotropic truncation correction; the latter obeys the
spurious non-linear Péclet scale and vanishes only with a particular choice of two remaining free model parameters. The constructed effective solution is first validated with the specific, fourth-order accurate Dirichlet and Neumann conditions, and then examined for its deviations due to generic schemes in open flow and at the diffusive interface. In parallel, a simultaneous truncation and mass-balance effect will be quantified exactly in straight heterogeneous blocks in series. This is a tough test, where the interface-normal Darcy plug flow induces asymmetry across the implicit interface, and although all MR schemes handle the diffusion problem exactly, they asymptotically decay only with the first-order accuracy, the BB alike, in advection dominant grid-inclined flows. At last, we will aim to understand whether the N-MR is able to reduce their accommodation.

This paper is organized as follows: Sec. II recalls the ADE-LBM and MR, and introduces N-MR, A-LSOB, and the 2D TRT reconstruction. Section III formulates the S-TRT, discusses its solvability, and recasts it the N-MR, interface-conjugate, and A-LSOB. Section IV validates N-MR and A-LSOB on the heterogeneous rotated parabolic profiles and also addresses their modeling with the lower-order treatment. Section V constructs the effective rotated quartic-polynomial solution and employs it for boundary and interface analysis. Section VI addresses the heterogeneous blocks in series and proposes an inverse 1d mapping from the A-LSOB to MR. In the Appendix, Subsection A summarizes the LI and MR families; Subsection B exemplifies the reconstruction step; Subsection C builds the corrective flux for the exact parabolic solutions; and Subsection D examines the mass-balance within the grid-shifted straight interface.

II. THE MR, N-MR, AND A-LSOB

We define the LBM framework in Sec. II.A, introduce the MR and A-LSOB closure relation in Sec. II.B, reconstruct all first- and second-order 2D derivatives in Sec. II.C, and then build tangential-flux N-MR corrections in Sec. II.D. Section II.E embeds the reconstruction process into N-MR and A-LSOB numerical algorithms. Section II.F summarizes the new methods and discusses their extensions. The notations employed for Dirichlet and Neumann schemes are gathered in Tables I and II, respectively; the reconstructions are specified in Table III.

**TABLE I.** The Dirichlet schemes are classified with respect to their exactness for piece-wise parabolic pure diffusion and constant-velocity rotated parabolic profiles modeled in an arbitrary inclined channel. (a) and (b) MPLI/LMKC and ABB are exact in the grid-aligned symmetric parabolic profiles with (a) $\Lambda = \frac{\delta}{2} \forall \delta$ and (b) $\Lambda = \frac{1}{2} \forall \delta$ (c) PPLI and KMR1 are exact on an inclined diffusion profile and grid-aligned advection velocity field $\forall \Lambda; (a)-(c)$ using $b_0 = 0$ in Eq. (A4) and $b_{0e} = 1$ in Eq. (37a) [see also Tables III and IV, Eqs. (121) and (122) in Ref. 46].

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Single-node</th>
<th>Exact parabolic rotated diffusion</th>
<th>Exact parabolic rotated advection-diffusion $\vec{u} = \vec{u}_i \vec{I}_i$</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPLI/PLI</td>
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<td></td>
<td>Equation (6a), Tables X–XIV</td>
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<tr>
<td>LMKC ∈ MPLI</td>
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<td>−(a)</td>
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<tr>
<td>ABB ∈ MPLI</td>
<td>✔</td>
<td>−(a)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PPLI ∈ LI</td>
<td>✔</td>
<td>✔</td>
<td>−(c)</td>
<td>Equation (6b), Tables XII–XIV</td>
</tr>
<tr>
<td>KMR1 ∈ MR</td>
<td>–</td>
<td>✔</td>
<td>−(c)</td>
<td>Equation (6b), Tables XI–XIV</td>
</tr>
<tr>
<td>PP ∈ MR</td>
<td>–</td>
<td>✔</td>
<td></td>
<td></td>
</tr>
<tr>
<td>T-PP ∈ A-LSOB</td>
<td>✔</td>
<td>✔</td>
<td></td>
<td>Equation (12a)</td>
</tr>
</tbody>
</table>
TABLE II. The Neumann schemes are classified with respect to their exactness for pure diffusion ad constant tangential velocity $\bar{u} = u_1 \hat{t}_1$, grid-rotated piece-wise parabolic profiles; (a): when $u_1 \neq 0$, FLI is exact only on the grid-aligned interface; (b): when $u_1 = 0$, FMR is also exact on the grid-rotated continuous interface solution or for specific jumps, as $\delta_{\perp}^q = \delta_{\parallel}^q = 0$ in Eq. (38) (see Eq. (102) in Ref. 40). The mass-conservation in the grid-shifted straight slab is indicated with respect to its exact solvability condition in the interface-perpendicular flow $\bar{u} = u_0 \hat{t}_u$, where N-MR reduces to MR.

<table>
<thead>
<tr>
<th>Flux scheme</th>
<th>Exact parabolic rotation diffusion in rotated $\bar{u} = u_i \hat{t}_i$</th>
<th>Exact mass-balance in surface perpendicular flow $\bar{u} = u_0 \hat{t}_u$</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>FLI $\in$ MR</td>
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<td>✓</td>
<td>$-\langle a \rangle$</td>
</tr>
<tr>
<td>FMR $\in$ MR</td>
<td>-</td>
<td>✓</td>
<td>$-\langle b \rangle$</td>
</tr>
<tr>
<td>DFLI $\in$ MR</td>
<td>-</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>N-FLI $\in$ N-MR</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>N-FMR in N-MR</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>N-DFLI in N-MR</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>T-DFLI in A-LSOB</td>
<td>✓</td>
<td>✓</td>
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</table>

B. Closure relations

We numerate the one-half of the discrete velocities $\sum_{i=1}^{N_q} \vec{c}_q$ with the positive numbers $q \in Q_+ \{ \text{sgn}_q = 1 \}$ and their opposite vectors with the negative numbers $-q \in Q_- \{ \text{sgn}_q = -1 \}$. When the population $f_q(\vec{r}, t + 1)$ leaves the computational domain at the boundary node $\vec{r}_b$, the opposite (incoming) population $f_{-q}(\vec{r}_b, t + 1)$ is prescribed by the boundary rule (see Fig. 1). The directional boundary rule computes $f_{-q}(\vec{r}_b, t + 1)$ from the known or already updated solution components (populations, their post-collision, equilibrium and non-equilibrium) moving along the same link ($\vec{c}_q, \vec{c}_{-q}$); this link-wise component is termed through $\text{MR}_q(\vec{r}_b, t)$; the boundary value is prescribed by the term $w_q(\vec{r}_b, t)$ in wall point $\vec{r}_q = \vec{r}_b + \delta_q \vec{c}_q \in V_p$, $\delta_q \in [0, 1]$, at some suitable time instance $t$

$$f_{-q}(\vec{r}_b, t + 1) = \text{MR}_q(\vec{r}_b, t) + w_q(\vec{r}_b, t), \quad q \in Q_+ \cup Q_-.$$

(4)

The content of MPLI/PLI is exemplified for the multi-reflection (MR) in Eqs. (A1) and (A2); their particular reduction to “linear-interpolation” LI is given by Eq. (A3); the $w_q$ is provided in Eq. (A4) for the Dirichlet rules and it makes the core subject of our discussion for the Neumann rules.

The associated (intrinsic, implicitly prescribed) closure relation $\text{CL}_q(\vec{r}_b, t)$ is expressed through the directional derivatives

$$\partial_{\perp} \psi = \nabla \psi \cdot \hat{c}_q$$

and $\partial_{\parallel}^2 \psi = \nabla^2 \psi \cdot \hat{c}_q$ [hereafter, cut link number $q$ is dropped in $\partial_{\perp}$ and the coefficients $\tau_{\parallel}^{(p)} - \tau_{\parallel}^{(a)}$, unless indicated];

$$-w_q(\vec{r}_b, t) = \text{CL}_q(\vec{r}_b, t),$$

$$\text{CL}_q(\vec{r}_b, t) := \left[ \tau_{\parallel}^{(p)} \vec{c}_q + \tau_{\parallel}^{(a)} \vec{c}_q + \beta_{\parallel}^{(p)} \partial_{\parallel} \vec{c}_q + \beta_{\parallel}^{(a)} \partial_{\parallel} \vec{c}_q \right]$$

$$+ \left[ \tau_{\perp}^{(p)} \partial_{\perp} \vec{c}_q + \tau_{\perp}^{(a)} \partial_{\perp} \vec{c}_q + \tau_{\perp}^{(p)} \partial_{\perp} \vec{c}_q + \tau_{\perp}^{(a)} \partial_{\perp} \vec{c}_q \right] (\vec{r}_b, t).$$

(5)

In this work, we focus us on the spatial component and refer to Ref. 40 for the temporal coefficients $\tau_{\parallel}^{(p)}$ and $\tau_{\parallel}^{(a)}$. The parametrized schemes produce identical steady-state solutions when Péclet number $\text{Pe} = \frac{\| \vec{L} \| / \delta_0}$ and the specific combinations of the symmetric/anti-symmetric relaxation rates are fixed, regardless the particular values assigned to $\text{Pe}$ and $\delta_0$ on given grid $\mathcal{L}$. The LI and MR schemes are all parametrized for any geometry. The following Dirichlet families apply here: the one-node “linear” [MPLI/PLI] and the two-node “parabolic” [PP/KMR] fit $\text{CL}_q$ to, respectively, the linear and parabolic, directional Taylor expansion from $\vec{r}_b$ to $\vec{r}_q = \vec{r}_b + \delta_q \vec{c}_q$.

$$\text{MPLI/PLI} : \Delta_{\parallel}^{(p)} (P + \delta_{\parallel} \vec{c}_q) \vec{P}_{\text{num}} \approx \Delta_{\parallel}^{(p)} \vec{P}(\vec{r}_b),$$

$$\text{PP/KMR/PLI} : \Delta_{\parallel}^{(p)} (P + \delta_{\parallel} \vec{c}_q + \frac{1}{2} \Delta_{\parallel}^2 \vec{P}) \vec{P}_{\text{num}} \approx \Delta_{\parallel}^{(p)} \vec{P}(\vec{r}_b).$$

(6a)

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<tr>
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<tr>
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<tr>
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<td>q = 1</td>
<td>q = 2</td>
<td>(q = 3)</td>
<td>(q = 4)</td>
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<tr>
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The Dirichlet family contains an infinite number of members parametrized by the link-wise free parameter $\chi^{(l)}$; the MPLI family improves LI schemes\cite{33,62} for parametrization and includes one of three schemes, called LMKC; the PLI family corrects MPLI for the cut link projection of the advective gradient $\mathbf{I}_{q}^{(l)}(\Delta \cdot \mathbf{q})$ in the 3D inclined or interface-perpendicular velocity field. The PP family is exact on the piece-wise parabolic profiles in the presence of the uniform grid-rotated velocity field; the two-node KMR1 and the novel single-node PPLI retain this accuracy in grid-rotated diffusion slabs and the grid-aligned advection velocity. The coefficients of the linear and parabolic Dirichlet MR are exemplified in Tables X and XII, respectively. The members of the same family produce identical stationary solutions provided that their effective steady-state closure relations, exactly expressed through $c_{\alpha}^{\sigma}$ and $n_{\alpha}^{\sigma}$, are equivalent; their coefficients can be found in Table XIII, whereas those of their approximation with Eq. (5) are gathered in Table XIV. The Dirichlet schemes are classified in Table I.

The MR$_q$ coefficients of the advective-diffusive flux FLI and FMR schemes are presented in Table XV, for an infinite diffusive-flux family DFLI in Table XVI; the internal coefficients of the stationary closure are all gathered in Table XVII, and those of the second-order accurate approximation with Eq. (5) are specified in Table XVIII. The one-node FLI and the two-node FMR fit CL$_q$ to the directional Taylor expansion for the projection of the advective-diffusive flux $\mathbf{B}(\mathbf{r})$:

$$\Phi_{\alpha}^{num}(\mathbf{r}_b) := t_{\alpha}^{(l)} \mathbf{P} \cdot \mathbf{\epsilon}_{\alpha} - t_{\alpha}^{(m)} \mathbf{\omega} \cdot \mathbf{P}_{\alpha}^{num},$$

$$\Phi_{q}(\mathbf{r}_b) := t_{q} \Phi(\mathbf{r}_b) \cdot \mathbf{\epsilon}_{q}, \quad \Phi := \mathbf{u} \mathbf{P} \cdot \mathbf{\omega} \nabla \mathbf{P}.$$  \hspace{1cm} (7b)

The flux linear interpolation (FLI) reduces to the BB for half-distance $\delta = \frac{1}{2}$; the FMR improves FLI for the parabolic advection term $\gamma(\alpha)_{q} \mathbf{I}_{q}^{(l)}(\mathbf{P} \cdot \mathbf{\epsilon}_{q})$ in Eq. (5); the scale factor $\gamma(\alpha)$ is fixed in these two schemes. Typically, the boundary accommodation simplifies with the same weight $t_{q}^{(m)} = t_{q}^{(l)} = t_{q}$ in Eq. (2). In turn, the diffusive-flux MR DFLI family vanishes all advection terms in Eq. (5) and it prescribes the linear continuation of the diffusive flux governed by an arbitrary linkwise scale factor $\beta$:

$$DFLI : \mathbf{B} \left( t_{q} \mathbf{D}_{q} + \delta \partial_{q} \mathbf{D}_{q} \right)_{\mathbf{r}}^{num} \approx \beta \mathbf{D}_{q}(\mathbf{r}_{b}),$$

$$D_{q}^{num}(\mathbf{r}_b) := -t_{q}^{(m)} \mathbf{\omega} \cdot \mathbf{P}_{\alpha}^{num},$$

$$D_{q}(\mathbf{r}_b) := t_{q}^{(l)} \mathbf{B}(\mathbf{r}_b) \cdot \mathbf{\epsilon}_{q}, \quad \mathbf{B} := -\mathbf{u} \mathbf{P} \cdot \mathbf{\omega} \nabla \mathbf{P}. \hspace{1cm} (8b)$$

The MR$_q$ schemes are quite natural for LBM because they supply the unknown populations directly, the BB alike. However, Eqs. (7) and (8) need to prescribe not only the normal (physical) flux component $\Phi_{n}(\mathbf{r}_b)$ but also its (unknown a priori) tangential component $\Phi_{t}(\mathbf{r}_b)$, given that $\Phi_{q}(\mathbf{r}_b) = (\Phi_{n}, \Phi_{t}) \cdot \mathbf{\epsilon}_{q}$ with $\mathbf{\Phi} = \Phi_{n} \mathbf{I}_{n} + \Phi_{t} \mathbf{I}_{t}$, in the unit (tangential, normal) surface-aligned coordinate system $(\mathbf{I}_{n}, \mathbf{I}_{t})$, traced at the bisection point $\mathbf{r}_{b} = \mathbf{r}_{b} + \delta \mathbf{\epsilon}_{q}$ of the cut link and a given surface; Fig. 2 illustrates flux decomposition for a constant flux $\mathbf{F}$ prescribed on the flat grid-inclined surface.

Hence, one of our objectives is to relax the continuation of $\Phi_{n}, \mathbf{\epsilon}_{q}$ and $\mathbf{D}_{q}, \mathbf{\epsilon}_{q}$ from the closure relation CL$_q$ in the normal N-MR flux schemes, where MR$_q$ in Eq. (4) becomes replaced by MR$_{q,n}$:

$$N-MR : MR_{q,n} = MR_{q} - CL_{q,n}. \hspace{1cm} (9)$$

When Eq. (5) is expressed in the 2D rotated frame $(\mathbf{I}_{n}, \mathbf{I}_{t})$ using decomposition $\mathbf{u}(\mathbf{r}_b) = (u_{n}, u_{t})$ and $\mathbf{\epsilon}_{q} = \{\mathbf{q}_{n}, \mathbf{q}_{t}\}$, the CL$_{q,n}$ reads

\[ \Phi_{q,n}(\mathbf{r}_b) := \Phi_{n} \mathbf{I}_{n} + \Phi_{t} \mathbf{I}_{t}, \]

\[ \Phi_{q,t}(\mathbf{r}_b) := t_{q} \Phi(\mathbf{r}_b) \cdot \mathbf{\epsilon}_{q}, \quad \Phi := \mathbf{u} \mathbf{P} \cdot \mathbf{\omega} \nabla \mathbf{P}. \hspace{1cm} (7b) \]

The flux linear interpolation (FLI) reduces to the BB for half-distance $\delta = \frac{1}{2}$; the FMR improves FLI for the parabolic advection term $\gamma(\alpha)_{q} \mathbf{I}_{q}^{(l)}(\mathbf{P} \cdot \mathbf{\epsilon}_{q})$ in Eq. (5); the scale factor $\gamma(\alpha)$ is fixed in these two schemes. Typically, the boundary accommodation simplifies with the same weight $t_{q}^{(m)} = t_{q}^{(l)} = t_{q}$ in Eq. (2). In turn, the diffusive-flux MR DFLI family vanishes all advection terms in Eq. (5) and it prescribes the linear continuation of the diffusive flux governed by an arbitrary linkwise scale factor $\beta$:

$$DFLI : \mathbf{B} \left( t_{q} \mathbf{D}_{q} + \delta \partial_{q} \mathbf{D}_{q} \right)_{\mathbf{r}}^{num} \approx \beta \mathbf{D}_{q}(\mathbf{r}_{b}),$$

$$D_{q}^{num}(\mathbf{r}_b) := -t_{q}^{(m)} \mathbf{\omega} \cdot \mathbf{P}_{\alpha}^{num},$$

$$D_{q}(\mathbf{r}_b) := t_{q}^{(l)} \mathbf{B}(\mathbf{r}_b) \cdot \mathbf{\epsilon}_{q}, \quad \mathbf{B} := -\mathbf{u} \mathbf{P} \cdot \mathbf{\omega} \nabla \mathbf{P}. \hspace{1cm} (8b)$$

The MR$_q$ schemes are quite natural for LBM because they supply the unknown populations directly, the BB alike. However, Eqs. (7) and (8) need to prescribe not only the normal (physical) flux component $\Phi_{n}(\mathbf{r}_b)$ but also its (unknown a priori) tangential component $\Phi_{t}(\mathbf{r}_b)$, given that $\Phi_{q}(\mathbf{r}_b) = (\Phi_{n}, \Phi_{t}) \cdot \mathbf{\epsilon}_{q}$ with $\mathbf{\Phi} = \Phi_{n} \mathbf{I}_{n} + \Phi_{t} \mathbf{I}_{t}$, in the unit (tangential, normal) surface-aligned coordinate system $(\mathbf{I}_{n}, \mathbf{I}_{t})$, traced at the bisection point $\mathbf{r}_{b} = \mathbf{r}_{b} + \delta \mathbf{\epsilon}_{q}$ of the cut link and a given surface; Fig. 2 illustrates flux decomposition for a constant flux $\mathbf{F}$ prescribed on the flat grid-inclined surface.

Hence, one of our objectives is to relax the continuation of $\Phi_{n}, \mathbf{\epsilon}_{q}$ and $\mathbf{D}_{q}, \mathbf{\epsilon}_{q}$ from the closure relation CL$_q$ in the normal N-MR flux schemes, where MR$_q$ in Eq. (4) becomes replaced by MR$_{q,n}$:

$$N-MR : MR_{q,n} = MR_{q} - CL_{q,n}. \hspace{1cm} (9)$$

When Eq. (5) is expressed in the 2D rotated frame $(\mathbf{I}_{n}, \mathbf{I}_{t})$ using decomposition $\mathbf{u}(\mathbf{r}_b) = (u_{n}, u_{t})$ and $\mathbf{\epsilon}_{q} = \{\mathbf{q}_{n}, \mathbf{q}_{t}\}$, the CL$_{q,n}$ reads

\[ \Phi_{q,n}(\mathbf{r}_b) := \Phi_{n} \mathbf{I}_{n} + \Phi_{t} \mathbf{I}_{t}, \]

\[ \Phi_{q,t}(\mathbf{r}_b) := t_{q} \Phi(\mathbf{r}_b) \cdot \mathbf{\epsilon}_{q}, \quad \Phi := \mathbf{u} \mathbf{P} \cdot \mathbf{\omega} \nabla \mathbf{P}. \hspace{1cm} (7b) \]
Linear formulation assumes that $\vec{u}(\vec{r})$ is independent of $P(\vec{r})$. Equation (10) can be then readily expressed through the local vector $Y[5]$:

$$2d \cdot Y[5] = \left\{ \partial_J P, \partial_J P, \partial_J^2 P, \frac{\partial}{\partial n} P \right\}_n^{(num)}.$$  \hfill (11)

The idea is to reconstruct $Y[5]$ locally, based on the in-node LSOb approach,\textsuperscript{21,67} and to compute CL$_Q(\vec{P}, \vec{u}, P)$ explicitly; the one-node N-NR, as N-FLI, then remains local but it loses its directional implementation.

The alternative in-node A-LSOb approach assumes the surface-aligned ($I, I_u$)$_n$ unit coordinate system to be traced at the bisection point $\vec{r}_n(\vec{r}_B) = \vec{r}_B + \alpha_n \vec{I}_u$ (see Figs. 1 and 2), and it employs the reconstructed nodal derivatives to build the parabolic-accurate Taylor closure relation along the normal direction from $\vec{r}_B$ to $\vec{r}_n$ for Dirichlet [T-PP], diffusive flux [T-DFLI] and advective-diffusive flux [T-FLI]:

\begin{align}
\text{T-PP} : \ & \nabla \cdot P(\vec{r}_B) + \sum_{m=1}^{2} \frac{\delta^m}{m!} \partial_m P(\vec{r}_n) = P(\vec{r}_B), \quad \text{(12a)} \\
\text{T-DFLI} : \ & \sum_{m=1}^{2} \frac{\delta^m}{m!} \partial_m P(\vec{r}_n) = P(\vec{r}_B), \quad \text{(12b)} \\
\text{T-FLI} : \ & (u_n(\vec{r}_B) \times \text{T-PP}) + \text{T-DFLI} = \Phi_n(\vec{r}_B), \quad \text{(12c)}
\end{align}

Assuming a constant normal velocity $u_n$, Eq. (12c) computes the advection component $u_n P$ with $P$ replaced by the LHS of Eq. (12a); Eq. (12c) reduces to Eq. (12b) when the normal velocity $u_n$ is zero (typically on the solid wall), or when $u_n$ and $P$ are continuous on the interface provided that scalar-field continuity is prescribed with Eq. (12a). An extension to space-variable $u_n(\vec{r})$ is straightforward giving its normal Taylor expansion.

At this point, we should recognize that the A-LSOb extension to interface is less evident than with the MB, because the interface points $\{\vec{r}_n\}$ do not overlap, except for a grid-aligned interface. For that reason, the Taylor schemes will be only considered for grid-rotated walls and grid-aligned interface.

The flux schemes are summarized in Table II; just to fix ideas, we propose to “interpret” FLI and FMR as the linearly and parabolically interpolated BB, whereas T-DFLI and DFLI can be thought as the local and back-sided extrapolations of the diffusive flux and its non-equilibrium term, respectively. We will show that these internal characteristics determine their mass-balance properties.

### C. Local reconstruction

The reconstruction procedure restores the first- and second-order derivatives from the non-equilibrium solution based on the LSOb ideas.\textsuperscript{21,67} We demonstrate this procedure for TRT operator, but it extends under the symmetry argument\textsuperscript{32,40} for any standard isotropic or anisotropic collision matrix, giving the associated third-order accurate Chapman-Enskog non-equilibrium solution.

#### 1. Reconstruction with the TRT collision

The TRT update applies in the following form:

$$f_j(\vec{r} + \text{sgn} \vec{e}_j, t + 1) = f_j(\vec{r}, t) + \tilde{n}_q^\pm(\vec{r}, t) + \text{sgn} \tilde{n}_q^\pm(\vec{r}, t),$$

$$\forall j \in Q, q \in \{\text{sgn} \vec{e}_j, 0\} \subset Q_0,$$

$$\{\vec{r}, \vec{r} + \text{sgn} \vec{e}_j \} \subset V_p, \quad \text{with}$$

$$\tilde{n}_q^\pm := - \frac{1}{\tau} \left( \tilde{n}_q^\pm - e_q^\pm \right), \quad f_j^\pm(\vec{r}, t + 1) := f_j(\vec{r}, t) + \tilde{n}_q^\pm(\vec{r}, t),$$

$$\tilde{n}_0^\pm := - \tilde{n}_q^\pm(\vec{r}, t) - 2 \sum_{q=1}^Q \tilde{n}_q^\pm(\vec{r}, t).$$  \hfill (13a)

$$e_q^\pm(\vec{r}) := \tilde{t}_q(\vec{r}) \tilde{P}_q^\pm, \quad P_q^\pm = P(\vec{r}) + \Lambda^\pm \cdot \tilde{M}(\vec{r}),$$

$$\Lambda^\pm(\vec{r}) := \left( \tau^\pm(\vec{r}) - \frac{1}{\tau} \right), \quad \Lambda(\vec{r}) = \Lambda^+(\vec{r}) \Lambda^-(\vec{r}).$$  \hfill (14a)

A free-tunable collision parameter $\Lambda(\vec{r})$ should remain fixed to obtain the same steady-state solution for any diffusion coefficient $\tilde{D}_0 = c_0 \Lambda$ given the grid Péclet number $\tilde{P}_e / \tilde{D}_0$ and, in general case, $c_0$ value. At steady-state, the non-equilibrium solution obeys the recurrence equations\textsuperscript{46,51} exactly expressed through the directional central-differences: $\Delta \tilde{f}_q^\pm(\vec{r}) = \frac{1}{2} \left( \tilde{f}_q^\pm(\vec{r} + \vec{e}_q) - \tilde{f}_q^\pm(\vec{r} - \vec{e}_q) \right)$ and $\Delta \tilde{f}_q^\pm(\vec{r}) = \left( \tilde{f}_q^+(\vec{r} + \vec{e}_q) - \tilde{f}_q^-(\vec{r} - \vec{e}_q) \right)$, as

$$\text{RE-a : } \tilde{n}_q^\pm = \Lambda^\pm \tilde{P}_q^\pm - \Lambda^\pm \tilde{P}_q^\pm, \quad \Lambda^\pm \tilde{P}_q^\pm = -\frac{1}{\tau} \tilde{P}_q^\pm,$$  \hfill (15a)

$$\text{RE-b : } \tilde{A}^\pm \tilde{n}_q^\pm = \Delta^\pm \tilde{P}_q^\pm - \tilde{n}_q^\pm, \quad \Lambda^\pm \tilde{n}_q^\pm = 0,$$  \hfill (15b)

$$\text{RE-c : } \Delta^\pm \tilde{n}_q^\pm = \tilde{A}^\pm \tilde{n}_q^\pm - \frac{1}{\tau} \tilde{P}_q^\pm.$$  \hfill (15c)

Equation (15c) is obtained by expressing $\Delta^\pm \tilde{n}_q^\pm$ from RE-b and inserting it into RE-a. We restrict RE-a to its second-order accurate approximation [A-RE]:

$$\Lambda = \text{RE : } \tilde{n}_q^\pm(\vec{r}) \approx \partial \tilde{P}_q^\pm - \Lambda^\pm \partial \tilde{P}_q^\pm, \quad \forall \vec{r}.$$  \hfill (16)

Given the post-collision solution $\tilde{n}_q^\pm$ at boundary node $\vec{r}_B$ or at interface node $\vec{r}_I$, $Y[5]$ from Eq. (11) solves the local linear system:

$$B \cdot [Y[5] = \alpha, \quad B = \{B_0^\pm, B_j^\pm = \partial e_j q^\pm(\vec{r}_B)^2, \}$$

$$\{R_0^\pm, R_j^\pm = \tilde{n}_q^\pm(\vec{r}_B)^2 \} \text{for } R = \{R_0^\pm, R_j^\pm = \tilde{n}_q^\pm(\vec{r}_B)^2 \}, \quad Y[5] = B^{-1} R.$$

\hfill (17a)

\hfill (17b)

\hfill (17c)
The term \( n_q^{(2)} |_{Y=0} \) may differ from zero when \( \vec{u}(r) \) and/or \( \vec{q}(r) \) vary in space, e.g., \( n_q^{(2)} |_{Y=0} \) includes \( P(\vec{r}, t) \partial_\vec{u} \cdot \vec{c}_q \) and \( P(\vec{r}, t) \partial_\vec{q} \cdot \vec{c}_q \) in a parabolic velocity profile.

Remark. In the transient case, the RHS in Eq. (16) sums with \( \partial_t c_q^+ (r, t) \) which can be estimated locally from \( n_q(t) = \partial_t P(r, t) \).

2. Reconstruction in constant velocity field

Let us illustrate the reconstruction procedure for a constant velocity field \( \vec{u} = (u_i, u_j) \). When the mass-source is set piece-wise constant, Eq. (16) becomes

\[
\dot{n}_q^{(2)} (P, \vec{u} P) = \left( \gamma_{q,p} u_i + c_{q,u} \right) \partial_{\vec{u}} \left( \gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}} \right) \frac{1}{\gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}}} - \gamma_{q,p} \partial_{\vec{u}} \left( \gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}} \right).
\]

Eq. (17) can be expressed in the Cartesian coordinate system through \( \gamma_{q,p} \partial_{\vec{q}} \) with the help of the posterior mapping given in Eq. (B1). The alternative reconstructions, when the fifth component is available, are

\[
\begin{align*}
\dot{n}_q^{(2)} (P, \vec{u} P) &= \left( \gamma_{q,p} u_i + c_{q,u} \right) \partial_{\vec{u}} \left( \gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}} \right) \frac{1}{\gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}}} - \gamma_{q,p} \partial_{\vec{u}} \left( \gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}} \right), \\
&= \left( \gamma_{q,p} u_i + c_{q,u} \right) \partial_{\vec{u}} \left( \gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}} \right) \frac{1}{\gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}}} - \gamma_{q,p} \partial_{\vec{u}} \left( \gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}} \right), \\
&= \left( \gamma_{q,p} u_i + c_{q,u} \right) \partial_{\vec{u}} \left( \gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}} \right) \frac{1}{\gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}}} - \gamma_{q,p} \partial_{\vec{u}} \left( \gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}} \right), \\
&= \left( \gamma_{q,p} u_i + c_{q,u} \right) \partial_{\vec{u}} \left( \gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}} \right) \frac{1}{\gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}}} - \gamma_{q,p} \partial_{\vec{u}} \left( \gamma_{q,p} \partial_{\vec{q}} + c_{q,p} \partial_{\vec{P}} \right).
\end{align*}
\]

Remark. In the transient case, the RHS in Eq. (16) sums with \( \partial_t c_q^+ (r, t) \) which can be estimated locally from \( n_q(t) = \partial_t P(r, t) \).

Finally, the whole rectangular matrix ("RM" hereafter) can be pseudo-inverted in Eq. (17):

\[
RM^* : B[8 \times 5] \cdot Y[5] = R[8], \quad R = \vec{n} - \vec{n}_q^{(2)} |_{Y=0}.
\]

(20)

D. The N-MR flux schemes

Gathering that \( Y[5] \) is reconstructed with Eq. (17), the N-MR applies the correction \( \dot{\epsilon}_q^{(n)} (\vec{r}, t) \) to the MR rule as

\[
f_{q,\dot{q}}(\vec{r}, t + 1) = (C_{q,\dot{q}} - \dot{\epsilon}_q^{(n)})(\vec{r}, t) + w_q(\vec{r}, t),
\]

\[
\dot{\epsilon}_q^{(n)} = I_1 c_q |_{\vec{r}, t} + \dot{I}_1^{(n)} c_q |_{\vec{r}, t},
\]

(21)

We distinguish three optional and independent directional corrections: \( C_{q,\dot{q}}(P, u, P) \) for the tangential projection of the advective-diffusive flux; \( \dot{I}_1^{(n)} c_q |_{\vec{r}, t} \) for the tangential and normal variation of the mass-source. The boundary term \( w_q(\vec{r}, t) \) prescribes the projection of \( F_{\vec{r}, t} = \partial_t c_q |_{\vec{r}, t} \), respectively.

N-FI/FMR: \( w_q(\vec{r}, t) = -\alpha^{(n)} \partial_t F_{\vec{r}, t} I_1(\vec{r}, t) \cdot \vec{c}_q \),

(22a)

N-DFLI: \( w_q(\vec{r}, t) = -\beta^{(n)} D_{\vec{r}, t} I_1(\vec{r}, t) \cdot \vec{c}_q \),

(22b)

When \( B = 1 \), Eq. (5) reproduces the directional Taylor expansion for the link projection of the normal flux \( \Phi_{q,n} \) or \( D_{q,n} \), and Eqs. (7) and (8) then read as, accordingly;

\[
\Phi_{q,n}^{(num)} := \frac{\tilde{t}_q^{(n)} (u, \partial_\vec{q} P_{\vec{q}, \dot{\vec{r}}, t})}{\tilde{t}_q^{(n)} (u, \partial_\vec{q} P_{\vec{q}, \dot{\vec{r}}, t})} \approx \alpha^{(n)} \Phi_{q,n}(\vec{r}, t),
\]

(23a)

\[
\Phi_{q,n}^{(num)} := \frac{\tilde{t}_q^{(n)} (u, \partial_\vec{q} P_{\vec{q}, \dot{\vec{r}}, t})}{\tilde{t}_q^{(n)} (u, \partial_\vec{q} P_{\vec{q}, \dot{\vec{r}}, t})} \approx \beta^{(n)} \Phi_{q,n}(\vec{r}, t),
\]

(23b)

When \( \vec{a}(\vec{r}) \), its tangential and normal variations modify the flux closure condition, and they can be removed from it in Eq. (21), e.g., giving their (known) derivatives.
5. If the tangential-flux N-MR correction is not needed, go to the next boundary node when all values \( f_{q}(\vec{r}_{b}, t + 1) \) are updated.

Note: In this work only a constant flat-surface boundary flux is simulated, where the flux boundary values \( \Phi_{n} \) and \( D_{n} \) in Eqs. (22)–(23) can be set equal to \( \Phi_{n}(\vec{r}_{q}) \) and \( D_{n}(\vec{r}_{q}) \), respectively (see Fig. 2). This enables us to perform one reconstruction procedure per boundary node in the wall-aligned coordinate system. Otherwise, when \( \Phi_{n}(\vec{r}_{q}) \) or the coordinate system \( \{ \vec{T}_{c}, \vec{T}_{a} \} \) \( (\vec{r}_{q}) \) varies along the surface, the N-MR may perform the reconstruction in the Cartesian coordinates, applying then the individual mapping from Eq. (B1) to compute the term of \( \ell_{d}^{(-)} \) in Eq. (21) for the given cut link.

The reconstruction step may be performed as the following:

1. Select a subset \( \bar{\eta}_{q} \) for the square reconstruction of \( \mathcal{Y}(\bar{\eta}_{q}) \) (e.g., with Eq. (19)), unless when the rectangular reconstruction is applied with Eq. (20) giving all \( \bar{\eta}_{q} \) values \( \eta_{q} \).

2. Select the coordinate system, e.g., the Cartesian or the wall-aligned \( \{ \vec{T}_{c}, \vec{T}_{a} \} \). From Table X or the parabolic PP/KMR1 from Table XI, the matrix entries \( \mathbf{B}_{q}(\vec{r}_{b}, t) \) and the right-hand-side (RHS) vector \( \{ \bar{n}_{q}^{(2)}(\bar{\eta}_{q})/q_{\text{in}} \} \) in Eq. (17); the examples are provided by Eqs. (18) and (B3).

Note: The matrix \( \mathbf{B} \) and \( \{ \bar{n}_{q}^{(2)}(\bar{\eta}_{q})/q_{\text{in}} \} \) can be precomputed prior to the iterative update provided that the relaxation rates, velocity and source fields do not vary in time.

3. Compute vector \( \mathbf{R}(\vec{r}_{b}, t) \) from \( \{ \bar{n}_{q}^{(2)}(\bar{\eta}_{q}), t \} \) and solve Eq. (17) or Eq. (20) for \( \mathcal{Y}(\vec{r}_{b}, t) \).
point MR rule in Eqs. (A1) and (A2). Generalizing the common procedure, Eq. (5) includes not only the first-order equilibrium derivatives but also the second-order ones, and it also accounts for the non-equilibrium neighbor variation in two-point rules. The coefficients in Eq. (5) are provided in Sec. A for the Dirichlet and Neumann ADE rules, but they are also tabulated for the Dirichlet velocity, pressure and normal stress LI and MR rules; the LI and MR also extend for the slip-flow regime. Practically, any directional boundary or interface rule fits Eq. (5) with some coefficients; for example, the free-interface pressure/stress scheme corresponds to the Dirichlet family MPLI ($\chi^{2} = -1$) [see Eq.(61) in Ref. 40].

We then identify the deficient projections in Eq. (5) for the given boundary rule; Eq. (19) exemplifies the deficient advective-diffusion tangential projection with respect to the normal Neumann flux condition in a constant velocity ADE. Once the deficient term is formulated, the idea is to re-build it from the in-node non-equilibrium solution $\bar{n}_q^-$, and to subtract it from the MR incoming population. Again, this type of correction can be built-in into any directional rule. The proposed algorithms are all summarized in Sec. II E and they do not need to resort to any off-grid interpolations. The subsequent analysis extends straightforwardly for any linear collision operator by replacing Eq. (16) by its associated Chapman-Enskog approximate.

The current reconstruction assumes that $\bar{e}_q^-$ is linear with respect to the macroscopic variables, as the concentration, diffusive-flux variable (in the linear or non-linear ADE), or pressure and velocity in the fluid Stokes/Brinkmann flow modeling. The 2D ADE system then requires the restoring of the five derivatives; they are exemplified in the wall-aligned coordinate system by Eq. (11) but the coordinate system can be assigned arbitrarily, and it may vary from one node to another. We propose then either to preselect the five values $\bar{n}_q^-$ and to invert the square system in Eq. (17), or to give all $Q_w$ values $\bar{n}_q^-$ and to (approximately) solve the rectangular system with Eq. (20). We note that the second strategy is geometry and problem independent, but it may not maintain exactly the TRT parametrization by the physical dimensionless numbers at fixed $\Lambda$. The reconstruction was introduced with the LB flow matrix method and it has been recently optimized with the 2D/3D TRT collision for Stokes flow. In turn, the A-LSOB closure equations (12) are formulated here as an alternative, normal Taylor single-node parabolic closure of the ADE system. Once the macroscopic variables and derivatives are reconstructed, the incoming populations are consequently prescribed by Eq. (16).

We note that the N-BB prototype of N-FLI was successfully applied to release the tangential advective-diffusive flux, and hence to compute correctly the two first moments, in solute transition along the flat surface, and on the heterogeneous anisotropic interface. The numerical simulations in this work will be performed with the steady-state formulation, which enables us to verify all new bounding techniques through a quite arbitrarily, parameter range (physical contrasts, Péclet number), without concerns from stability. However, the transient MR ADE interface-conjugate has been also developed, its update to N-MR is identical with the boundary counterpart, and it is exemplified with the steady-state interface-conjugate treatment in Sec. II D. The MR interface-conjugate is also formulated for the velocity and normal-stress continuous flow conditions; their release from the tangential stress projection shell becomes possible following the N-MR path. Conversely, the LSOB approach demonstrates how to insert the physical, normal and tangential, free-surface flow stress conditions directly into the Chapman-Enskog multiple-relaxation-time (MRT) population reconstruction in the filling process, either at high Reynolds number or for Bingham fluid.

A preliminary MR analysis demonstrated that the parabolic velocity scheme MR1 (which is the original flow counterpart of the Dirichlet scalar scheme KMR1 from Table XI) is much more accurate than the linear ones, not only for porous media later confirmed, but also for the pressure fluctuations in a newborn fluid node, improving them for the mass conservation and the Galilean invariance in the static/moving frames. These properties have been recently carefully evaluated, leading however partly to a different conclusion on the competition between the linear CL1 scheme (which is in turn the flow counterpart of LMKC) and MR1. In our belief, the parabolic MR scheme shall handle more accurately pressure fluctuations because MR vanishes the pressure terms of $\beta^{(1)}$ (as MR1) and also $\gamma^{(1)}$ (with new PM schemes) in Eq. (5), which are both non-zero in the linear (LI) Dirichlet velocity schemes including their new member IPLI from Table XII.

Finally, it is well known that the local mass adjustment spoils body-fitted boundary rules. Differently from a mechanical mass conservation account, the steady-state formulation will express it through the body-fitted global solvability condition, providing interesting hints for mass-balance properties of the linear and parabolic ADE flux schemes. We expect to extend this approach in a near future to flow schemes.

III. STEADY-STATE TRT FORMULATION

We recall the steady-state TRT formulation and specify its bulk-uniform $M_0$—solvability condition in Sec. III. The alternative corrective boundary-flux approach is introduced in Sec. III B. Section III C recasts steady-state MR and N-MR; Sec. III D applies them with the interface-conjugate; Sec. III E provides the steady-state MR, N-MR and A-LSOB algorithms; and Sec. III F resumes these techniques.

A. Bulk system

The TRT bulk steady system is composed from two equations per every internal link connecting $\bar{r} \in V_, \bar{r} + \bar{c}_q \in V_p, q \in Q_2$:

$$S_q(\bar{r}) = S_{-.q}(\bar{r} + \bar{c}_q), \quad G_q(\bar{r}) = -G_{-.q}(\bar{r} + \bar{c}_q),$$

with

$$S_q(\bar{r}) = \left[ e_q^+ + \frac{1}{2} \bar{n}_q^- - \Lambda^+ \bar{n}_q^+ \right](\bar{r}),$$

$$S_{-.q}(\bar{r} + \bar{c}_q) = \left[ e_q^+ - \frac{1}{2} \bar{n}_q^- - \Lambda^- \bar{n}_q^+ \right](\bar{r} + \bar{c}_q),$$

$$G_q(\bar{r}) = \left[ e_q^+ + \frac{1}{2} \bar{n}_q^- - \Lambda^+ \bar{n}_q^+ \right](\bar{r}),$$

$$-G_{-.q}(\bar{r} + \bar{c}_q) = \left[ e_q^+ - \frac{1}{2} \bar{n}_q^- - \Lambda^- \bar{n}_q^+ \right](\bar{r} + \bar{c}_q).$$

This system is complemented with the local mass-conservation equation given by

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The local (linear) MR operates with zero coefficients \( m_b \) is local. The correction \( \Phi_b \) applies with Eq. (21), where \( \Phi_b \) is expressed with Eq. (17c) through the in-node variables \( n = \sum_{q} \tilde{n}_q^n \) (cf. Eqs. (B3)–(B4a)). Equations (34) and (35) complete the bulk system for \( \sum_{q} Q_b \) wall-cut links. The steady-state algorithm then solves the global linear system with respect to all unknowns \( \text{Var} \) from Eq. (29) or Eq. (33).

\begin{equation}
\text{Var} = \Phi_b \sum_{q} Q_b \left( P(\tilde{r}_b) \cup \tilde{n}(\tilde{r}_b) \right), \quad M_b = 0. \tag{33}
\end{equation}

The rationale behind of the corrective flux is to verify whether Eq. (32) is more accurate than the \( M_b \) source, because the modeled bulk equation remains not modified.

### C. The steady-state MR and N-MR

The bulk system (26) is not defined for the cut links \( q_b \in Q_b(\tilde{r}_b) \) when Eq. (21) reduces to linear equation with respect to \( X_q[8] \):

\begin{align}
M_q \cdot X_q - \Phi_b^{(\pm)}(\tilde{n}) &= -w_q^n(\tilde{r}_q^n), \quad M_q[8] = \{ m_1, m_2, m_3, m_4 \} \nonumber \\
&\quad \cup \{ m_5, m_6, m_7, m_8 \} \quad q, \tag{34}
\end{align}

The coefficients \( m_j \) are computed from MR in Eq. (A1):

\begin{align}
m_1 &= \tilde{\alpha} + \beta - \beta - 1, \quad m_2 = (\tilde{\alpha} + \beta - \beta + 1), \nonumber \\
m_3 &= -\tilde{\tau} m_1 + \tilde{\alpha} + \beta, \quad m_4 = -\tilde{\tau} m_2 + \tilde{\alpha} - \beta + K^+, \quad m_7 = \gamma + \tilde{\gamma}, \quad m_5 = -\tilde{\tau} m_3 + \gamma, \quad m_6 = -\tilde{\tau} m_4 - \gamma, \tag{35}
\end{align}

The local (linear) MR operates with zero coefficients \( m_5 - m_8 \), so that \( M_q \) reduces to \( M_q[4] = \{ m_1, m_2, m_3, m_4 \} q \) and the unknown vector \( X_q[4] \) is local. The correction \( \Phi^{(\pm)}_b \) applies with Eq. (21), where CLQ(\( \tilde{r}_b \)) is expressed with Eq. (17c) through the in-node variables \( n = \sum_{q} \tilde{n}_q^n \) (cf. Eqs. (B3)–(B4a)). Equations (34) and (35) complete the bulk system for \( \sum_{q} Q_b(\tilde{r}_b) \) wall-cut links. The steady-state algorithm then solves the global linear system with respect to all unknowns \( \text{Var} \) from Eq. (29) or Eq. (33).

### D. The MR and N-MR interface-conjugate

Following \(^{40,42,63}\) assume now that \( P_\text{L}(\tilde{r}_\text{int}) \) and \( D^{(k)}_\text{L}(\tilde{r}_\text{int}) \) are subject to continuity or jump conditions on the interface \( \tilde{r}_\text{int} \):

\begin{align}
P^{(\pm)}_\text{L} &\big|_{\tilde{r}_\text{int}} = \sigma^{(\pm)P} D^{(s)}_\text{L} + \eta^{(s)} \quad (36a) \\
D^{(k)}_\text{L} &\big|_{\tilde{r}_\text{int}} = \sigma^{(\pm)D} D^{(s)}_\text{L} + \eta^{(s)} \quad (36b)
\end{align}

Based on Eq. (34), the interface-conjugate directional closure between the two neighbors \( \tilde{r}_i \) and \( \tilde{r}_i = \tilde{r}_i + \tilde{e}_{\tilde{q}_j} \) is accordingly expressed by the Dirichlet \( M^{(k)}_q(\tilde{a}^{(k)}_q) \) rule for Eq. (36a) and by the flux \( D^{(k)}_\text{L}(\tilde{r}_\text{int}) \) rule for Eq. (36b):

\begin{align}
\frac{M^{(k)}_q \cdot X_q - \Phi^{(\pm)}_b}{\tilde{a}^{(k)}_q} \bigg|_{\tilde{r}_i}^{(1)} &= \sigma^{(\pm)} \left[ M^{(k)}_q \cdot X_q - \Phi^{(\pm)}_b \right]_{\tilde{r}_i}^{(2)} + \eta^{(s)} \quad (37a)
\end{align}
or periodic-interface systems. In such cases, \( M_0 \) from Eq. (28) enters the list of the global variables; otherwise \( M_0 = 0 \) is substituted there. Alternatively, the boundary flux can be prescribed with the corrective flux variable \( \Phi_0 \) from Eq. (32); an extension for periodic interface is exemplified by Eq. (64).

Note: a posteriori, the normalized procedure shall remove the solution dependency on the prescribed value. We will examine the proposed flux schemes with respect to this property.

1. Steady-state N-MR boundary algorithm

The N-MR tangential correction \( \text{CL}_{\text{T}}(P, u; P) \) from Eq. (10) is embedded via \( \delta_{\text{T}}(\hat{\mathbf{n}}) \) in Eq. (34), following Eq. (21). In that, \( \text{CL}_{\text{T}}(P, u; P) \) is expressed through \( \mathbf{Y}[1] = \mathbf{B}^{-1}\mathbf{R} \), \( \mathbf{R}_q^\perp = \hat{n}_q^\perp - \hat{n}_q^{(2)} \vert_{\text{Y}=0} \), and \( \{ \hat{n}_q^{\pm} \} \) belong to the list of unknowns \( \text{Var} \). In that, one computes \( \mathbf{B}^{-1} \) and \( \hat{n}_q^{(2)} \vert_{\text{Y}=0} \) following the Reconstruction step from the transient algorithm in Sec. II E.

2. Steady-state N-MR interface-conjugate algorithm

The interface-conjugate applies with Eq. (37) where, similarly, the tangential corrections are introduced by \( \delta_{\text{T}}(\hat{\mathbf{n}}) \) and \( \delta_{\text{T}}(\hat{\mathbf{n}}) \) in Eq. (37b). They are expressed, respectively, through \( \mathbf{Y}[1] = \mathbf{B}^{-1}\mathbf{R}^\perp \) and \( \mathbf{Y}[1] = \mathbf{B}^{-1}\mathbf{R}^{(2)} \) in two interface nodes.

3. Steady-state A-LSOB boundary algorithm

Similarly with the N-MR, the normal derivatives in the Taylor conditions from Eq. (12) are expressed through \( \mathbf{Y}(\hat{\mathbf{n}}(\hat{\mathbf{r}}_b)) \) and the prescribed Taylor condition is embedded into the global system. Then, giving \( N_b \) cut links \( \{ q_b \} \), one adds to the global system \( N_b - 1 \) closure “expansions” in the form

\[
\hat{n}_q^+ = \hat{n}_q^{(2)}(\hat{\mathbf{r}}_b), \quad \hat{n}_q^- = \hat{n}_q^{(2)}(\hat{\mathbf{r}}_b), \quad q = \text{sgn}_q q_b,
\]

where \( \hat{n}_q^+ \) belongs to \( \text{Var} \), and \( \hat{n}_q^{-2}(\hat{\mathbf{r}}_b) \) is prescribed as given by Eq. (16) in terms of \( \mathbf{Y}(\hat{\mathbf{n}}(\hat{\mathbf{r}}_b)) \).

Note: The choice of \( N_b - 1 \) Eq. (40) is not defined uniquely: one can prescribe \( N_b - 1 \) relations for the symmetric or anti-symmetric components alone, as \( \hat{n}_q^+ = \hat{n}_q^{(2)}(\hat{\mathbf{r}}_b) \) or \( \hat{n}_q^- = \hat{n}_q^{(2)}(\hat{\mathbf{r}}_b) \), or combine these two. In principle, any combination of the reconstruction subset with \( N_b - 1 \) closure relations is suitable provided that, respectively, Eq. (17) and the global linear system are well defined. Our optional semi-heuristic algorithm is detailed by Example 4 in Sec. B.

4. Steady-state A-LSOB interface-conjugate algorithm

This algorithm is only applied in Sec. VI A 3 for a straight interface in interface-perpendicular plug flow. The couple of the interface conditions (36a) and (36b) is then expressed through their normal Taylor approximate with Eqs. (12a) and (12b), and it replaces the couple of the bulk equations for interface-cut link.

F. Summary on the steady-state formulation

The steady-state TRT formulation operates with the non-equilibrium post-collision variables \( \hat{n}_q^{\pm}(\hat{\mathbf{r}}) \) and the conserved quantity...
They solve the linear algebraic bulk system composed of Eqs. (26)–(28). In a continuous problem, the solvability condition of the Neumann problem is guaranteed by the global mass conservation condition; however, since the continuous condition may not be assured in the discrete system, we propose to adjust it either with a single variable \( M_0 \) from Eq. (28), in any geometry, or with the corrective boundary flux \( \pm \Phi_0 \) from Eq. (32), in specific channel-like slabs. These variables are automatically obtained by solving the global Neumann or interface-constrained system, where solution \( P(\vec{r}) \) is defined to an additive constant. Our next experiments will compare the respective accuracy of the two solvability techniques, whereas \( [M_0] \) and \( [\Phi_0] \) will measure the mass imbalance of the proposed flux schemes.

The key point is that the MR, N-MR, and A-LSOB are very similar to their transient formulation, but these algorithms are directly expressed in terms of the steady-state local variables, \( \{\hat{n}^\pm\} \) and \( P \). The bulk linear system is then closed by the compact MR closure equations (34), and it may incorporate the compact MR interface-conjugate (37). Equations (34) and (37) are optionally amended with the corrections for mass-source variation and tangential-flux release; the N-MR is specified with the FLI, FMR, and DFLI. Alternatively, the bulk system can be closed by the A-LSOB closure equations; they prescribe the normal Taylor equation (12) and \( \hat{n} = \hat{n}^{[2]} \) for the incoming links with Eq. (40); these equations are all retained in node variables through the reconstruction. The algorithms are all formulated in Sec. III; they are built within the symbolic software and solved with its numerical solver.

IV. ROTATED PARABOLIC SOLUTIONS WITH THE TANGENTIAL ADVECTIVE MODEL

We introduce the stratified Darcy system and outline its previous analysis in Sec. IV A. Section IV B demonstrates that (i) the N-MR makes the two advective-flux schemes FLI and FMR exact for any interface diffusive-flux jumps in the presence of the grid-rotated Darcy velocity, and that (ii) the A-LSOB Dirichlet scheme T-PP and the diffusive-flux T-DFLI support this problem exactly. We then intentionally degrade the parabolic Dirichlet and Neumann accuracy to the linear one following the existing (similar in spirit) approaches\(^{26,62,104,105}\) and demonstrate their respective solutions in Sec. IV C. Section IV D discusses obtained results and outlines the similarity/distinctness with their rotated Poiseuille flow counterpart. The Dirichlet and Neumann schemes are, respectively, classified in Tables I and II according to the presented analysis.

A. Stratified Darcy layers

We consider a stratified two-layered rotated system of width \( h = h_1 + h_2 \); \( \phi = \phi_1 \) when \( y' \in [-h_1, 0] \) and \( \phi = \phi_2 \) when \( y' \in [0, h_2] \). The system is aligned with the axis \( x' = \tilde{I}_1 \cdot (x, y) \), and the diffusion process develops along the normal axis \( x' = \tilde{I}_n \cdot (x, y) \) [cf. Eq. (18c)]; the two layers are either periodic or bounded by two parallel walls. The interface-parallel (Darcy) velocity \( \vec{u} = u \hat{\vec{e}} \) is constant; the mass-source \( \mathcal{M}(\vec{u}) \) is set piece-wise constant and hence, the profile \( P(y') \) is piece-wise parabolic:

\[
\partial_\varepsilon u_i P_k(y') - \mathcal{M}(y') = \mathcal{D}_k \partial_{y'}^2 P_k(y'), \quad \mathcal{D}_k := \phi_k \mathcal{D}_0 = c_k \Lambda_k^\varepsilon, \quad \mathcal{M}(y') := \partial_y \hat{u}_j - u_j, \tag{41a}
\]

The constants \( \{a_k, b_k\} \) are set by Eq. (36) provided that the solvability condition is satisfied. The periodic continuous condition with \( \mathcal{U}^{[0]} = 1 \), \( \eta^{[0]} = 0 \) in Eq. (36b) is satisfied when \( \Psi = \Psi^{[0]} \) in Eq. (41a), thanks to the global mass conservation:

\[
\langle \partial_y \hat{u}_j \rangle = 0 \text{ with } \Psi^{[0]} := \langle \frac{u_j}{\phi} \rangle = \frac{u_j \Lambda_1}{\phi_1 h_1 + \phi_2 h_2}. \tag{42}
\]

Equations (41) and (42) with the \( y' \)–periodic, continuous solution \( P(y') \) and continuous diffusive flux \( -\mathcal{D}_k \partial_{y'} P(y') \) match the EMM boundary problem\(^{37,94}\) for the (rotation-invariant) Taylor dispersion problem when \( f(x) \) and the periodic, continuous solution \( f(y') \) match the EMM boundary problem with the help of the interface-conjugate treatment in the rotated channels by\(^{37,94}\). The TRT-EMM numerical solution for \( D_\tau \) has been examined with the implicit interface tracking in the straight system,\(^{38}\) where the exact piecewise parabolic profile is available thanks to \( \Lambda = \frac{1}{\tilde{I}_1 - \tilde{I}_2} \), because this choice\(^{25,26}\) locates midway the ABB implicit surface that corresponds to \( I_0 = 1 \) in Eq. (44) and \( I_{int} = 0 \) in Eq. (37a); otherwise, \( \Lambda = \frac{1}{\tilde{I}_2} \) with \( I_0 = 0 \) in Eq. (44) and \( I_{int} = 1 \) in Eq. (37a), as in Table I. The stratified Darcy modeling has been also extended\(^{39}\) for the cubic and quartic polynomial solution due to the recursive polynomial mass-source expansion; these solutions provide, respectively, the skewness and kurtosis. Further extension\(^{39}\) to the diagonally-rotated d2q9 system with the implicit interface tracking revealed that the non-equilibrium B-layer accommodation and the truncation parabolic component \( t_\tau \partial_\varepsilon^2 P_{\varepsilon} \) produce a non-zero local gradient estimate in the translation invariant solution, as \( c_\varepsilon \partial_y \varepsilon \approx \sum_{q=1}^{Q-1} \hat{n}_q \varepsilon_q \). Moreover, the equilibrium A-layer accommodation perturbs the predicted Pe\(^2\) scale of the modeled dispersion coefficient and retards its convergence from the second to first order, unless with the d2q5 in the diagonal stratified system. We examine now the interface-conjugate treatment in the rotated channels by extending the MR simulations\(^{37}\) to N-MR and A-LSOB.

B. Piece-wise parabolic solutions with MR, N-MR, and A-LSOB

We formally extend the EMM problem for suitable combinations of the interface jumps and boundary conditions. Equation (42) presents the solvability condition for the \( y' \)–periodic but also constant-flux bounded system; in these two problems, \( P(y') \) is defined up to an additive constant. Equation (36) with the continuous and jump conditions has been addressed\(^{36}\) with the help of the interface-conjugate treatment from Eq. (37), but without the tangential-flux correction \( \varepsilon^{[0]}_q \) in Eq. (37b). In theory, the solution in Eq. (41b) is expected to be the same with and without tangential velocity field when \( \mathcal{M}_k \) is fixed with Eq. (41a). However, the numerical computations in pure-diffusion \( [c_q] \equiv 0 \) and in the presence of the advective velocity \( [c_q] = [d_0] u_0 \tilde{I}_1 \cdot \hat{c}_q \), \( \hat{c}_q \), may produce different results because of the closure relations. That is because their non-equilibrium solutions differ, e.g., on the exact advection-diffusion solution \( \hat{n}_q \) reads

\[
\hat{n}_q^{[0]} = \sum_{q=1}^{Q-1} \hat{n}_q^{[0]} u_0 \tilde{I}_1 \cdot \hat{c}_q \partial_y \hat{c}_q - \sum_{q=1}^{Q-1} \hat{n}_q^{[0]} \hat{c}_q \varepsilon_q \tilde{I}_n \cdot \hat{c}_q \partial_y \hat{c}_q, \tag{43a}
\]

\[
\hat{n}_q^{[0]} = \sum_{q=1}^{Q-1} \hat{n}_q^{[0]} u_0 \tilde{I}_1 \cdot \hat{c}_q \partial_y \hat{c}_q - \sum_{q=1}^{Q-1} \hat{n}_q^{[0]} \hat{c}_q \varepsilon_q \tilde{I}_n \cdot \hat{c}_q \partial_y \hat{c}_q + \sum_{q=1}^{Q-1} \hat{n}_q^{[0]} \hat{c}_q \varepsilon_q \tilde{I}_n \cdot \hat{c}_q \partial_y \hat{c}_q, \tag{43b}
\]
with
\[
\partial_1 p = b_2 + 2c_2 y', \quad \partial_2^2 p = 2c_2, \\
\partial_2 p = \partial_2^2 p = \partial_2^3 p = 0.
\] (43c)

Since \(a_k\) is piece-wise constant, the mass-source corrections vanish in Eqs. (24a) and (24b). The tangential-flux correction \(\text{CL}_{\text{cl}}\) in Eq. (10) implicitly reduces to its *advective flux* counterpart on the exact profile:
\[
\text{CL}_{\text{cl}}(y') = \frac{1}{q_{\text{nl}}}(y') u_t(y') y_{\text{cl}} + \frac{\theta_{\text{nl}}}{q_{\text{nl}}}(y') u_t \partial_n p(y') y_{\text{cl}}^2 + \frac{\theta_{\text{nl}}^2}{q_{\text{nl}}^2}(y') u_t^2 \partial_n^2 p(y') y_{\text{cl}}^2.
\] (44)

Hence, although in theory the advective-diffusive flux and diffusive flux continuity conditions are equivalent, this is not the case with the MR flux schemes, because the tangential advection term is projected onto the interface-cut links with Eq. (44). In other words, Eq. (44) is expected to spoil the linear diffusive flux, unless when \(x^{(u)} = y^{(u)} = 0\), as for example, in DFLI from Tables XVI–XVIII. Indeed, it has been confirmed that PP-DFLI is exact in Eq. (36) for any scalar profiles and flux grid-oriented conditions [recall, the Dirichlet family PP assures the continuity or jump in Eq. (36a) on the parabolic profiles]. In pure-diffusion and grid-aligned slabs, the PPLI-FLR, PP-FLR and PPLI-FLI, PP-FLI are also exact. However, among these schemes, only PP-FLR is exact in grid-inclined advection restricted to the “proportional” jump, as \(x^{(u)} = y^{(u)} = 1\). At the same time, the FLI closure in Eq. (5) is built with \(\theta_{\text{nl}} = \frac{1}{\lambda}\), like FMR, but with \(y^{(u)} = \frac{1}{\lambda}\), instead of \(y^{(u)} = \frac{1}{\lambda}\) (see Table XVIII). Consequently, FLI cannot assure an exact continuation of the (last) parabolic advection term in Eq. (44); however, PP-FLI remains second-order accurate in the rotated slabs (see Figs. 5–7 in Ref. 40). By construction, N-FLI aims to vanish Eq. (44) from the closure relation, and then it is expected to become exact on the piece-wise parabolic rotated solutions for (i) a constant flux Neumann boundary and (ii) for any interface-conjugate with Eq. (35).

In detail, the grid-inclined streamwise-periodic channel is discretized hereafter following, such that the boundary/interface bisects a prescribed point \((x_0, y_0)\) on the bottom. The \(L_2\)-error metric \(E_2\) is employed hereafter to estimate the relative root squared error to exact solution; \(E_2\) is computed over all grid points. We apply the generic procedure and reconstruct \(\mathbf{Y}[5]\) in Eq. (10) with Eq. (17) and (18). Equation (19) or Eq. (B2) [with non-zero determinant] then exactly reproduce all derivatives in Eq. (43c). This exact solution is also matched with the rectangular subsets, as \(B[6 \times 5]\) or \(B[8 \times 5]\) from Eq. (20). When \(\mathbf{Y}[5]\) is expressed through the local unknowns, N-FLI and N-FMR apply with Eq. (21) for the boundary flux and Eq. (37b) for the interface flux.

Figure 3 addresses the computations in the bounded inclined channel \(\theta = \arctan[\frac{h}{20}] \approx \frac{h}{20}\) closed by the constant diffusive flux and the continuous interface (left diagram), or Dirichlet boundary and interface jumps from Eq. (36) (right diagram). The PP scheme reproduces the interface scalar continuity condition from Eq. (36a). The boundary and interface flux-conditions are first modeled with the three MR schemes, FLI, FMR and DFLI. In agreement with our predictions, FLI and FMR produce very large errors, but DFLI is exact. In fact, the FMR is exact here for the *continuous interface advective-diffusive flux* but it cannot prescribe correctly the rotated diffusive boundary flux alone. Next, on the left diagram of Fig. 3, we replace the FMR by N-FMR for the boundary flux, and the obtained solution then becomes exact in agreement with our expectations. Accordingly, \(P(y')\) becomes exact when N-FLI replaces FMR both on the boundary and the interface (left diagram). Finally, the combinations of the exact schemes, as the single-node A-LSOB T-DFLI on the boundary, with the DFLI, N-FLI or N-FMR on the interface, all reproduce the exact profile. In turn, the single-node T-PP operates exactly the Dirichlet boundary (right diagram), where FLI and FMR are not able to reproduce the diffusive-flux interface jump because of their advection components. In contrast, DFLI, N-FLI and N-FMR are exact.

C. Inexact solutions with the linear schemes

We model a very sharp variation (of three orders of magnitude) at high Péclet number \(Pe = 10^3\) in a small inclined channel \(h = 10 \cos \theta\), as displayed in Fig. 3, but replace the parabolic Dirichlet and linear flux schemes by the linear Dirichlet boundary and interface continuity conditions, and constant-flux schemes. We consider first the linear LMKC scheme; \(E_2\) the LMKC is the member of the infinite MPLI family from Table X and they share the same steady-state solution. These schemes are parametrized but their accuracy degrades in the presence of the advection velocity, because the advection \(\hat{n}_d\) term \(\theta_{\text{nl}}^2 \hat{\sigma}_{\text{nl}}^2 \partial_n \hat{u} \hat{u} \hat{c}_n^2\) is non-zero in Eq. (5) in the inclined channels. Consequently, the \(E_2\) grows almost linearly with \(Pe\) but still converges with second-order rate (see Figs. 5–8 in Ref. 40 for the MPLI-FLI interface conjugate in continuous straight/diagonal/rotated systems).

Figure 4 (left diagram) follows Fig. 3 but LMKC replaces PP for the continuity condition in the interface-conjugate. Recall that only the FLI-FLI and the FMR-FMR (boundary-interface) treatment is inexact in Fig. 3 (left diagram). Now, also the four others, exact flux combinations, display highly inaccurate solutions, N-FLI-N-FLI shows the smallest but still unacceptable error. Remarkably that FLI-
FLI and FMR-FMR are almost unaffected by this intentional interface discontinuity; we will show later that their mass-balance properties (and then accuracy) are independent of the scalar-continuity scheme in basic configurations. Figure 5 (right diagram) demonstrates that LMKC also completely destroys the expected Dirichlet boundary location, hence $Pe^{-1}P(y') \approx 0$, when it replaces the parabolic A-LSOB T-PP scheme (12a).

Figure 5 displays the results of the linearly-truncated normal Taylor conditions, when T-DFLI from Eq. (12b) (left diagram) and T-PP from Eq. (12a) (right diagram) become depleted from their parabolic terms. The T-DFLI then degrades from the linear to the constant-flux condition, and it spoils all exact parabolic solutions. In turn, the degraded T-PP cannot support the exact solutions but its boundary location is much more accurate than with the LMKC in Fig. 4 (right diagram). This confirms that the principal MPLI/LMKC deficiency at high $Pe = 10^3$ is due to the linear advection correction $\beta^{(1)}v_0P_{\text{in}}\lambda_{\text{in}}$, which is absent in the degraded normal Taylor T-PP in Fig. 5 (right diagram).

**D. Summary on the piece-wise parabolic solutions**

The piece-wise parabolic solution allows us to validate exactly the N-FLI and N-FMR in the presence of constant Darcy velocity field of an arbitrary amplitude. Since the obtained profiles $P(y')$ are exact, only $\partial_y P(r_0)$ and $\partial^2_y P(r_0)$ are non-zero on the obtained solution $Y(\bar{r}_1, \bar{r}_2)$, giving an efficient reconstruction test-case. In turn, $d_0q$ is also able to produce the exact rotated channel solution with $B[4 \times 4]$ provided that $\partial_y^n P = 0$ or $\partial^2_y P = 0$ is substituted into Eq. (18). Moreover, giving zero tangential and mixed solution derivatives, the $d_0q$ is able to derive $Y[2] = \{\partial_y P, \partial^2_y P\}$ from the same link $c_{\text{in}} \neq 0$. Altogether, we confirm that DFLI, N-FLI and N-FMR are exact for the boundary and interface piece-wise linear rotated diffusion-flux in the presence of a uniform grid-inclined tangential advection velocity and jumps, provided that the interface scalar condition is modeled exactly with the MR PP. We also validate the exactness of the one-node Taylor boundary schemes from Eq. (12), T-PP and T-DFLI. In principle, Eq. (12) might be applied exactly on the interface in the rotated channel solutions due to their translation invariance.

Except the parabolic MR and A-LSOB T-PP, the existing Dirichlet ADE schemes are commonly restricted to only leading-order accuracy in the grid-inclined velocity field. Although PPLI is exact in the rotated pure-diffusion slab and the grid-aligned velocity field, it shares the MPLI/LMKC deficiency in the grid-rotated advection velocity field, because their closure relation in Eq. (5) reads with $\beta^{(1)} \neq 0$ and $\gamma^{(1)} \neq 0$ in Table XIV. Methodologically, the degraded T-J-PP extends the Dirichlet flat-wall scheme [85,105] from the in-node placement $\delta \equiv 0$ to an inclined flat wall; obviously, when $\delta \equiv 0$, the linear and parabolic terms vanish in the normal Taylor expansion (12), but $\delta \equiv 0$ cannot address the grid-inclined walls. The degraded T-J-PP, fits then only the first-order accurate normal Taylor relation but it locates much more accurately the boundary values thanks to the absence of the velocity projections in its well-normal Dirichlet Taylor prescription.

Let us mention that the force-driven Poiseuille flow modeling follows the same path: whereas a rotated parabolic no-slip and slip solutions are available for any two-point multi-reconstruction [20,40,83] and single-node LSOB [12,14] they cannot be matched by the moment-based on-grid boundary methods [7,27] with $\delta \equiv 0$. The recent LI scheme [97] pursues the exact inclined Poiseuille flow modeling but, in reality, its solution is exact only in a straight channel, extending the BB solution [32,62] and MGLI schemes [31,64] to any distance $\delta$ and to any (stable) $\Lambda$. Yet, this Poiseuille channel problem is a pure-diffusion counterpart of the ADE problem (41). To this end, we complement PPLI with its flow counterpart IPLI in Table XII; the IPLI is exact for the force-driven Poiseuille flow in a grid-inclined channel and it is parabolic-accurate for any uniform-density Stokes flow, at least. We emphasize that the IPLI prescribes the forcing term $t_qA_{\text{in}}$ in $\bar{v}_q$ in both bulk and boundary equilibrium $e_q^{(1)}$ otherwise, when expressing [20,25,96] the force term from the momentum equation, IPLI becomes anisotropic, i.e., cut-link direction dependent. The PPLI/IPLI derivation straightforwardly applies Eq. (5), a result that will be reported elsewhere.

Finally, concerning the Neumann condition, the Cartesian decomposition method [22,62] assumes that the linear interpolations along two grid axes produce the “same” Dirichlet value; we have shown that they fail on the parabolic profiles and, especially, in the
inclined velocity field. Hence, although the original FLI scheme is able to support the rotated parabolic diffusion profile, the Cartesian decomposition method is not expected to extend this property to a constant rotated velocity. Purposely, we also degraded the A-LSOB flux scheme T-DFLI following and rendered it only suitable for a constant normal-flux; obviously, this scheme cannot then support a linear diffuse flux on the parabolic profiles and it produces the relaxation-dependent, wrong solutions.

To sum up, the parabolic, N-FLI and T-DFLI and two-point N-FMR are expected to enhance the similarly constructed, but lower-order Neumann schemes. The single-node Dirichlet PPLI extends MPLI/PLI to rotated diffusion slabs and grid-aligned tangential velocity. These schemes do not restrict the free parameter range.

V. Rotated quartic solution with the tangential advection

We extend the stratified rotated system to the presence of the parabolic velocity-field and mass-source. In this context, Sec. VA describes the model equation and its analytical solution; Sec. VB constructs the effective rotated TRT bulk solution and determines the free-parameter range when it is either exact or obeys the exact solvability condition. Section VC extends the reconstruction procedure for a space-variable velocity and mass-source; Sec. VD validates the bulk solution and determines the effective rotated TRT bulk solution and determines the same in pure diffusion and in the presence of the tangential advection velocity. Moreover, the discrete solvability condition and the effective solution will differ giving two quartic (numerical) dispersion, skewness and kurtosis, by extending the EMM to the fourth-order approximate of the modeled macroscopic equation; (ii) to estimate the D_t deviations induced by the tangential velocity constraint; and (iii) to examine the convergence delay due to the weighted accommodation on the diagonal interface. However, although the particular optimal A solutions have been derived to minimize these numerical artifacts, the effective advection-diffusion bulk solution of the scheme has not yet been constructed in arbitrary rotated channels.

In theory, when \( H(y') \) is prescribed with Eq. (45), \( P^{(v)}(y') \) is the same in pure diffusion and in the presence of the tangential advection velocity \( u_i(y') \). However, the discrete solvability condition and the effective solution will differ giving two quartic (numerical) dispersion, skewness and kurtosis, by extending the EMM to the fourth-order approximate of the modeled macroscopic equation; (ii) to estimate the D_t deviations induced by the tangential velocity constraint; and (iii) to examine the convergence delay due to the weighted accommodation on the diagonal interface. However, although the particular optimal A solutions have been derived to minimize these numerical artifacts, the effective advection-diffusion bulk solution of the scheme has not yet been constructed in arbitrary rotated channels.

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The case \( u_3 = 0 \) \([\Psi = 0 \text{ in Eq. (45)}\] corresponds to pure diffusion with a given parabolic mass source, where the quartic polynomial solution exists for any rotation. The case \( \sin[4\theta] = 0 \) covers the grid-aligned, straight/diagonal, orientation where the effective quartic solution exists for any \( \Lambda \) and advection-weight \( \{t_i^{(n)}\} \). The case \( \Lambda = \frac{1}{2} \) vanishes the third-order truncation spatial error (see and reference therein). The case \( \{t_i^{(0)} = \frac{1}{6}, t_j^{(0)} = \frac{1}{12}\} \) corresponds to the isotropic (hydrodynamic) \( \Delta \psi \) weight obeying the additional constraint \( \sum_{i=1}^{N_{\Omega}} (t_i^{(0)})^2 = 1 \). We prescribe \( t_i^{(0)} = t_i^{(m)} = \frac{1}{2} \) and keep \( \Lambda \) free.

The effective solution (48a) is then given as

\[
\begin{align}
\rho_1^{(0)} &= \rho_2^{(0)} = \rho_3^{(0)} = \frac{m_0}{2}, \\
\delta_2 &= \mu^2 \psi(\Lambda, c_4) + \frac{\zeta(\Lambda)}{864} \left(6\mu^2 u_4 + 2\mu^2 u_4\right), \\
p_3^{(0)} &= \frac{p_3^{(0)}}{\mu^2} = \frac{m_0}{6}, \\
\delta_3 &= \mu^2 u_4^2 \zeta(\Lambda) \sin[4\theta], \\
p_v^{(0)} &= \frac{p_v^{(0)}}{\mu} = \frac{m_0}{12}, \text{ with} \\
\psi_{\Lambda, c_4} &= \mu_{\mu}, \quad \mu_{\mu} = \mu_{\mu}, \quad \delta = c_4 \Lambda^2, \\
\psi(\Lambda, c_4) &= \frac{1}{6} + \Lambda(c_4 - 1), \quad \zeta(\Lambda) = 1 + 30\Lambda(-1 + 4\Lambda).
\end{align}
\] (51a, 51b, 51c)

Hence, \( p_v^{(0)}(y') \) is anisotropic and it becomes exact, and hence isotropic, only provided that \( \Lambda \) and \( c_4 \) are inter-related, as

\[
p^{(0)}(y') = p^{(0)}(y'), \quad \text{if only} \quad \psi(\Lambda^{0}(c_4), c_4) = 0:
\]

(a) \( \theta = 0 \), \( \forall t_i^{(m)} \), or \( \theta = \frac{\pi}{4} \), \( t_i^{(m)} = \frac{1}{3} \), or \( c_i^{(m)} = 0 \),

\[
\Lambda^{(0)}(c_4) = \frac{1}{6(1 - c_4)} , \quad \forall c_4 \in [0, 1];
\]

(b) \( \forall \theta \) if \( t_i^{(0)} = \frac{1}{3} \), \( \zeta(\Lambda^{(0)}(c_4)) = 0, \quad \psi(\Lambda^{(0)}(c_4), c_4^{(0)}) = 0,
\]

then \( \Lambda^{(0)}(c_4^{(0)}) = \Lambda^{(0)}(c_4) \), with

\[
\Lambda^{(0)} = \sqrt{105 + 15} \approx 0.210391, \\
c_4^{(0)} = \sqrt{105 - 5} \approx 0.207825.
\] (53)

The pure diffusion rotated solution is exact with \( \Lambda = \Lambda^{(0)}(c_4) \), Eq. (52). In the presence of advection, the diagonal channel \( \theta = \frac{\pi}{4} \) also gets the exact solution with \( \Lambda^{(0)}(c_4) \), giving the hydrodynamic mass-weight. However, in the rotated system, \( \Lambda^{(0)}(c_4) \) is restricted to \( \Lambda^{(0)}(\theta) \) with the particular solution \( c_4(\theta) \) from Eq. (53). We substitute now velocity and mass-source profiles from Eq. (45); Eq. (51) then reads with \( \{p_v^{(0)}\} \) from Eq. (46), and \( \mathcal{M}(\gamma)(y') \) gets the effective correction \( \delta(y') = -\mathcal{D}^{(0)} p_v^{(0)}(y') - \mathcal{M}(\gamma) \).

\[
\delta^{(0)}(y') = \mathcal{M}(\gamma^{(0)}(\theta), c_4(\theta), Pe, h); \quad \mathcal{M}(\gamma^{(0)}(\Lambda^{(0)}, c_4^{(0)})) = \Lambda^{(0)}(\gamma^{(0)}), \quad \forall \theta, Pe, h;
\]

(54)

Given that \( \mathcal{M}(\gamma^{(0)}(\theta), c_4^{(0)})) = 0 \), the effective profile \( p_v^{(0)}(y') \) may satisfy the impermeable condition on the two walls only provided that

\[
\langle \delta^{(0)}(y') \rangle = 0 \quad \text{with} \quad \Lambda^{(0)}(\theta, c_4, Pe, h);
\]

\[
\Lambda^{(0)}_{\Gamma_{\gamma=0}} = \Lambda^{(0)}(\gamma^{(0)}(c_4^{(0)})) = \Lambda^{(0)}(\gamma^{(0)}), \quad \forall \theta, Pe, h.
\] (55)

Here, \( \Lambda^{(0)} \) solves the quartic polynomial equation \( \langle \delta^{(0)}(y') \rangle = 0 \), and it reduces to Eq. (52) in the grid-aligned case. Figure 6 displays the suitable real root to Eq. (55) in the advection-dominant limit \( c_4 \rightarrow 0 \) when \( Pe = 10^3 \), \( \forall \psi \in [0, \frac{\pi}{2}] \) (left diagram) and \( vs \) \( H \) (right diagram, with \( H = H \cos(\theta) \), \( \theta = \arctan(\frac{h}{L}) \)). This root is delineated by a narrow (suitable) interval \( \Lambda^{(0)}(\gamma^{(0)}(c_4^{(0)})) \), where \( \Lambda^{(0)}(\gamma^{(0)}(c_4^{(0)})) \) rapidly reduces to \( \Lambda \approx \zeta(\Lambda) \) when \( Pe \) is small or when \( H \) increases. The difference with respect to the exact solution in Eq. (47) reads on the normalized profiles:

\[
\frac{P_v^{(0)}(y') - P_v^{(0)}(y')}{P_e h} = (1 - 3Y)^2 \left(\psi(\Lambda, c_4) + \frac{P_e^2 \zeta(\Lambda)^2 \sin[4\theta]}{12h^2} \right.
\]

\[
\left. - \frac{1 - 6Y^2 + 4Y^2}{8h^4} Pe^3 \zeta(\Lambda) \sin[4\theta]. \right)
\] (56)

Equation (56) only vanishes with \( \{\Lambda^{(0)}(\gamma^{(0)}(c_4^{(0)})) \) from Eq. (53), and Eq. (56) is exactly asymmetric with respect to exchange \( Y \rightarrow -Y \) only with \( \Lambda^{(0)}(c_4^{(0)}) \). Figure 7 displays the anisotropic asymmetric solution \( h^2 Pe^{-2}(P_v^{(0)} - P_v^{(0)}(Y)) \) using \( \Lambda^{(0)} \); we find that this distribution becomes practically \( h \) – and \( Pe \)-independent when \( \Lambda^{(0)} \) approaches its asymptotic values, e.g., when \( H \geq 10, Pe = 10^2 \) or \( H \geq 20, Pe = 10^3 \) in Fig. 6.
To sum up, our analysis suggests that when using $\Lambda^{(eff)}(c_i)$, the bulk system may satisfy the exact solvability condition, but one should expect the (anisotropic, asymmetric) discrete effects, which scale nonlinearly with Pe and decay for finer resolutions when Pe grows. Clearly, this advection-diffusion rotated discrete behavior is very different from the isotropic symmetric pure-diffusion or grid-aligned profiles obeying the linear Pe-scale with Eq. (46). The effective solution becomes exact only with $\Lambda^{(ex)}$ and $c_i^{(ex)}$ from Eq. (53).

**C. Reconstruction step**

The standard reconstruction step is computed with Eq. (17) where the prescribed post-collision solution in Eq. (18) becomes modified according to Eq. (16), because $\vec{u} = u_r(y')\hat{1}$, and $\mathcal{S}(y')$ vary along the normal direction:

$$\nabla^{(2)}(\vec{r}) = f^{(a)} [\nabla_i \partial_i + c_{qi} \partial_q] (Pu_{c_i}) - f^{(a)} \nabla_i \lambda_{q_i} \nabla_i \nabla_i \nabla_{m_i} (P + \Lambda^{K(\mathcal{S})} + \mathcal{S}) + 2\varepsilon q_i \nabla_i \nabla_i \nabla_{m_i} P + 2c_i \nabla_i \nabla_{m_i} P),$$

(57a)

$$\nabla^{(2)}(\vec{r}) = f^{(a)} (\nabla_i \lambda_{q_i} \nabla_i \nabla_i \nabla_{m_i} (P + \Lambda^{K(\mathcal{S})} + \mathcal{S}) + 2\varepsilon q_i \nabla_i \nabla_i \nabla_{m_i} P + 2c_i \nabla_i \nabla_{m_i} P),$$

(57b)

where the matrix $\mathbf{B}(\vec{r}_b)$ from Eq. (17) then becomes space-dependent and $\mathbf{R}(\vec{r}_b)$ comprises the known terms due to the velocity and mass-source variation, hence $\mathbf{R}(\vec{r}_b)$ then linearly depends upon $\vec{P}(\vec{r}_b)$ due to the advection term, as exemplified by Eqs. (B3) and (B4). The closure conditions are expressed locally through $\mathbf{Y}^b = \mathbf{B}^{-1} \mathbf{R}(\vec{r}_b)$, with Eq. (21) in N-MR and Eqs. (12) and (40) in A-LSOB. The whole linear system is solved with the constructed unknown list $\mathbf{V}$ from Eq. (29) or (33).

**D. Exact validation of the effective solution**

The effective solution from Eqs. (51)–(56) is first validated numerically with the help of the fourth-order accurate Dirichlet [T-PP($\Lambda^{(eff)}$)] and Neumann [T-DFLI($\Lambda^{(eff)}$)] Taylor conditions:

$$\text{D-DFLI}^{(eff)} : D_{\mathbf{P}}^{\partial(M-1)/m} P^{\partial(M-1)/m} |_{t=0} = D_{\mathbf{P}}^{\partial(M-1)/m} P^{\partial(M-1)/m} |_{t=0},$$

(58a)

$$\text{T-PP}^{(eff)} : P^{\partial(M-1)/m} |_{t=0} = P^{\partial(M-1)/m} |_{t=0}.$$  

(58b)

The Dirichlet solution is defined for any $\Lambda$; the constant-flux Neumann solution is defined with $\Lambda^{(eff)}$ from Eq. (55); their boundary conditions complete the bulk system. Additionally, following the A-LSOB in Sec. III E, the effective equations: $\nabla^{(2)}(\vec{r}_b) = \nabla^{(2)}(\vec{r}_b)$ and/or $\nabla^{(2)}(\vec{r}_b) = \nabla^{(2)}(\vec{r}_b)$ are prescribed for $N_0 = 1$ cut links; $\{\nabla^{(2)}(\vec{r}_b)\}^{(eff)}$ obeys Eq. (48b) with Eq. (51) and, giving $\{\nabla^{(2)}(\vec{r}_b)\}^{(eff)}$ and $\{\nabla^{(2)}(\vec{r}_b)\}^{(eff)}$, $\{\nabla^{(2)}(\vec{r}_b)\}^{(eff)}$ is derived with Eq. (15c), using there Eq. (49).

The effective solution is validated when it coincides with the numerical solution $P^{\partial(M-1)/m}(y')$ in all grid points; to get rid of the additive constant, the normalization $(P) = 0$ of the predicted effective and numerical Neumann profiles is performed by summation. We first prescribe the effective solution for all derivatives in Eq. (58) and confirm that, when using $\{\Lambda^{(ex)}, c_i^{(ex)}\}$, the numerical Neumann solution is exact and given by Eq. (46). Using $\Lambda^{(eff)}(c_i)$, the difference between the numerical and exact solutions then coincides with Eq. (56).

We now make use of this benchmark to validate the reconstruction procedure. The first- and second-order derivatives in Eq. (58) are then extracted with Eq. (17) giving there $R^2 (\vec{r}_b) = (\nabla^{(2)}(\vec{r}_b) - \nabla^{(2)}(\vec{r}_b))$, where the last term accounts for the fourth-order difference between the effective solution and its second-order approximate. Figure 8 displays the difference between the numerical solution obtained in two configurations: $\{\Lambda^{(eff)}(Pe), c_i = \frac{1}{2}\}$ and $\{\Lambda^{(ex)}, c_i^{(ex)}\}$ for Neumann (left diagram) and Dirichlet (right diagram) Taylor conditions from Eq. (58). Here, the rectangular and square reconstructions give the same (effective) solution where $E^{(eff)} = E_{\text{est}}$. In the error-estimate $E_2$ with respect to exact solution is non-zero unless when using $\{\Lambda^{(ex)}, c_i^{(ex)}\}$ from Eq. (53). Figure 8 (left diagram) confirms Eq. (56); the difference with the exact profile is asymmetric in the grid-symmetric channel using $\Lambda^{(eff)}$, the Dirichlet system (right diagram) shares the same property of $\Lambda^{(eff)}$, otherwise effective solution loses asymmetry.

It is worthwhile to note that the Neumann numerical solution with $\Lambda^{(eff)}$ finds $\theta = 0$ in Eq. (28) [because $\langle \mathcal{S}(y') \rangle = 0$ thanks to $\Lambda^{(eff)}$]. However, when $\Lambda \neq \Lambda^{(eff)}$ and hence $\langle \mathcal{S}(y') \rangle \neq 0$, the
condition \( \langle \hat{\mathbf{u}}^{(\alpha)} = \mathbf{M}_{\zeta} \rangle = 0 \) becomes satisfied in the grid-aligned system or pure-diffusion problem thanks to the established numerical solution \( \mathbf{M}_{\zeta} = -\hat{\mathbf{u}} \). Using the exact closure with Eq. (58a), the obtained numerical solution is then exact, as

\[
\theta = \frac{\pi n}{4} \quad \text{or} \quad \epsilon_q^C \equiv 0 : P(y') = P^{(\alpha)}(y'),
\]

with \( \mathbf{M}_{\zeta} = -\hat{\mathbf{u}} = -\frac{12\text{Pe}}{\text{h}^3} \psi(\Lambda, c_\zeta), \quad \forall \Lambda, \forall \epsilon_q^C. \tag{59}
\]

### E. Exact solutions with inexact boundary schemes

We examine the straight system using \( \mathbf{M}_{\zeta}^{(\alpha)} \) from Eq. (52); the bulk solution is then exact, \( E_2 = E_2^{(\zeta)} \), and any eventual deviation is due to the boundary closure. Its solvability condition is adjusted with one of the two mechanisms: (i) via \( \mathbf{M}_{\zeta} \neq 0 \) in Eq. (28), and (ii) via the corrective flux \( \pm \Phi_0 = \pm \phi \) in Eq. (32). We first examine the difference between these two techniques for a midway impermeable boundary \( \delta = \frac{1}{2} \), where FLI reduces to BB and the numerical solution reads with

\[
\mathbf{M}_0 - \mathbf{BB} : E_2 \neq 0, \quad \mathbf{M}_0 = \mathbf{M}(\hat{\mathbf{u}}^{(\text{num})}) - \mathbf{M}(\hat{\mathbf{u}}^{(C)}) \\
= \hat{\mathbf{u}}^{(\text{num})} - \hat{\mathbf{u}}^{(C)} = \frac{C_{17}}{C_{19}}.
\]

\[
\Phi_0 - \mathbf{BB} : E_2 = 0, \quad \chi = \frac{\text{Pe}}{4\text{h}} \quad \text{or} \quad \Phi_0 = \frac{1}{4\text{h}^2}.
\]

Equation (60a) means that the BB system adjusts the exact (integration) solvability condition to summation in Eq. (45), in agreement with our prediction in Eq. (31), but the numerical solution is then inexact. The magnitude of \( \mathbf{M}_0 \) scales with the mean-velocity amplitude, similarly to the case of grid-oriented constant velocity; when \( \mathbf{u} \) is kept constant, \( |\mathbf{M}_0| \) reduces as \( \text{h}^{-2} \) at fixed Pe. In contrast, BB - \( \Phi_0 \) produces the exact solution because the corrective flux in Eq. (60b) compensates the BB error with respect to the fourth-order accurate Neumann condition; this result is derived by Eqs. (C1)-(C7). Equation (60b) shows that \( \chi \) reduces with second-order rate at fixed Pe. The total corrective flux, \( 2\Phi_0 = \frac{\text{Pe}}{2\text{h}} \), is then equal to \( \langle \mathbf{M}_0 \rangle = \mathbf{M}_0 \). However, only the corrective flux reproduces the exact profile, because it does not modify the mass-source \( \mathbf{M}(\hat{\mathbf{u}}^{(C)}, \gamma) \). Equation (C8) extends \( \chi(\delta) \) to an arbitrary distance \( \delta \) with FLI, and Eq. (C14) generalizes this construction for FLI, FMR, and DFLI, as

\[
\text{FLI} : \chi(\delta) = \frac{\text{Pe}}{\text{h}^2} \left( 3\delta^2 - \frac{1}{2} + \frac{\delta(1 - 4\delta^2)}{\text{h}} \right), \tag{61a}
\]

\[
\text{FMR} : \chi(\delta) = \chi_{\text{FLI}} + \frac{3\text{Pe}(\text{h} - 1 - 2\delta)(2\Lambda^{(\alpha)} - \delta^2)}{\text{h}^2}, \tag{61b}
\]

\[
\text{DFLI} : \chi(\delta) = \chi_{\text{FLI}} + \frac{3\text{Pe}(\text{h} - 1 - 2\delta)(1 + \delta)}{\text{h}^2}, \tag{61c}
\]

\[
|x|_{\text{DFLI}} > |x|_{\text{FMR}} \quad \text{when} \quad h \geq 4, \quad \delta > 0,
\]

\[
\chi_{\text{DFLI}} > \chi_{\text{FMR}} \quad \text{when} \quad \delta = 0.
\]

These results show that DFLI needs a larger amplitude \( \Phi_0 \) than FMR, except when \( \delta = 0 \). The interrelation between FLI and DFLI is more complicated, but typically \( |x|_{\text{DFLI}} > |x|_{\text{FLI}} \), e.g., \( \delta^2 \approx 0.09 \) when \( h \approx 4 \), and \( \delta^2 \approx 0.03 \) when \( h \approx 10 \). Figure 9 (left diagram) compares the three schemes in the limit \( c_\zeta \rightarrow 0 \), featuring the high Pe regime. The results are displayed for \( \Phi_0 = \frac{\text{Pe}}{\text{h}^3} \), when \( \delta = \left\{ \frac{1}{2}, \frac{1}{4}, \frac{1}{8} \right\} \).

They show that DFLI requires a much larger amplitude \( \Phi_0 \) to adjust the exact straight quartic solution, and confirm that DFLI approaches FMR when \( \delta \) tends to zero. In turn, FMR shows an almost \( \delta \)-independent amplitude \( \Phi_0 \). The FLI also approaches FMR when \( \delta \rightarrow 0 \), but FLI is more accurate than the two other formally higher-order accurate schemes, when it comes down to BB for \( \delta = \frac{1}{2} \). The FLI, FMR, and DFLI are supplemented with the normal mass-source correction \( \mathbf{M}_{\zeta}(\delta) = 1 \) in Eq. (21) because \( \mathbf{M}(y') \) varies along the normal direction (see Table III). The steady-state MR closure from Eq. (34) then reads with \( \delta^2 < \frac{1}{2} \) by C in Eq. (24b). This correction modifies \( \chi(\delta) \) equally with the three schemes and it is given by Eq. (C11):

\[
\chi(\delta) \rightarrow \chi(\delta) + \chi_{\delta}, \quad \chi_{\delta} < 0 \quad \text{with}
\]

\[
\chi_{\delta} = \frac{\delta^{(\delta)}(y^1)\mathbf{L}_{\text{eff}}(\phi_{\text{eff}}^2)}{\mathbf{F}_{\text{eff}}(\phi_{\text{eff}}^2)} \left( \Lambda - \Lambda^{(\alpha)} \right) = -\frac{c_\zeta \text{Pe}}{(1 - c_\zeta) \text{h}^2}. \tag{62}
\]

Since \( \Phi_0 \) is positive in Eq. (60b), and it is mostly positive in Eq. (61) when \( h \geq 4 \), the mass-source correction reduces the amplitude \( |\chi| \). The derived solution \( |\chi| \) is in exact agreement with the FLI, FMR, and DFLI numerical solutions displayed in Fig. 9 (right diagram). Additionally, Eq. (C12) demonstrates that the Taylor scheme T-DFLI produces the unknown vertical population with Eq. (57), according to example 4 in Subsection B of the Appendix.

The MR solutions with the three basic flux schemes are weight-independent in the straight channel, so that they are the same with \( \delta_{2}\text{q5} \) and \( \delta_{2}\text{q9} \). In other words, the accommodation of the advective flux by the diagonal links is invisible on the profiles due to the symmetry. The N-MR complements FLI, FMR, and DFLI with the tangential correction \( \mathbf{C}_{\text{tan}}(P, u, P) \) from Eq. (57) \( |P = 1 \) in Eq. (21). We observe that their profiles \( \phi^{(\text{num})(y')} \) remain exact, but the reconstructed tangential and mixed derivatives in \( \mathbf{Y}[5] \) are due to the non-equilibrium accommodation, and they depend on the reconstruction subset. Figure 9 (right diagram) compares \( \Phi_0 \) between MR, and N-MR using rectangular reconstruction with Eq. (20). We observe that on the coarse grids N-FLI, and N-FMR, reduce \( \Phi_0 \) of their counterparts, FLI, and FMR, while the N-DFLI, and DFLI, behave...
very similarly. All schemes approach their MR counterparts when 

\[ H \approx 30, \] 

and then monotonically reduce \( |\Phi_0| \) with second-order rate.

To sum up, the corrective flux from Eq. (32) is able to adjust 

the exact quartic Neumann solution of the inexact flux schemes 

provided that the two straight walls are placed symmetrically. 

Although DFLI is exact on the parabolic rotated solutions, it is 

expected to behave worst on the quartic solutions because of its 

larger deviations from the exact solvability condition; consequently, 

N-DFLI, does not improve DFLI. The MRs typically decreases \( |\Phi_0| \) 

and hence, it improves for the conservation properties. The 

diffusive-flux A-LSOB T-DFLI from Eq. (12b) produces an identi-

fication with two strategies: \( \Phi_0(\delta) \) with FLL1 used the standard reconstruction 

algorithm; hence, T-DFLI shows smaller amplitude \( |\Phi_0(\delta)| \) than 

DFLI, which is its MR counterpart. The N-MR releases the 
diagonal-link accommodation of the tangential advective flux; it 

retains the exact solution and further reduces \( |\Phi_0| \), at least with 

the N-FLI and N-FMR, on the coarse grids. Finally, the MRs and their 

N-MR counterparts decay \( |\Phi_0(\delta)| \) altogether with second-order rate.

**F. Grid-shifted and diagonal channels**

When the distances to the top and bottom walls differ, say \( \delta_1 \neq \delta_2 \), Eq. (32) should be modified by prescribing \( \{ \chi(\delta_0), -\chi(\delta_1) \} \), and the numerical solution then remains exact. However, we restrict this work to an equal amplitude corrective flux with Eq. (32), where the numerical solution is then not exact. Figure 10 compares the results obtained with \( M_0 \) and \( \Phi_0 \) when the whole slab is shifted with respect to the grid. We observe that T-DFLI and FLL1 continue to produce 

the same solutions. On the whole, \( E_2(\Phi_0) \) is one order of magnitude 

smaller than \( E_2(M_0) \), especially with FMRs – \( \Phi_0 \) where \( E_2 \) is the 

smallest and it converges faster, with third-order rate; otherwise, \( E_2 \) 

\( M_0 \) and \( \Phi_0 \) converge with second-order rate with all schemes. The 

FMRs is much more accurate than FLL1 because it vanishes the 

second-order advection accommodation term but FLL1 demonstrates 

the best solvability properties, with the smallest amplitudes of \( [M_0] \) 

and \( [\Phi_0] \). In addition, Fig. 10 displays the N-MR results using the rect-

angular reconstruction from Eq. (20). The N-FLI, then improves FLL1 

for \( E_2, M_0 \) and \( \Phi_0 \) but only on coarse grids \( H \leq 20 \), and the two 

schemes decay together on the finer grids. Similarly, N-FMR improves 

FMRs for \( M_0 \) and \( \Phi_0 \), but \( E_2(N-FMRs) \) is not regular. This 

confirms our suggestion that FMR does not need any second-order 

tangential advection corrections in the straight channels, in agreement 

with the exactness of its parabolic solution. Like FMR, the DFLI copes 

better with \( \Phi_0 \), where N-DFLI, reduces the error on coarse grids but 

again, the DFLI– based schemes show much larger errors and one-

order larger amplitude for \( [M_0] \) and \( [\Phi_0] \) against FLL and FMR. In 

turn, N-MR produces similar results using the square-matrix recon-

struction, where it maintains the parametrization, meaning that \( E_2 \) 

is fixed by the grid Pe number \( \sqrt{\delta_i} \), \( c_1 \) and \( \Lambda(c_1) \). In contrast, 

the rectangular reconstruction loses the bulk parametrization property, 

unless on the exact solutions.

Another important property refers the weight-independence and 

the linear Pe-scale of the numerical solutions. The unmodified MR 

schemes and T-DFLI produce weight-independent results in the 

straight grid-shifted channels, where they also retain the linear Pe-

dependency of the analytical profile. These two features are not sup-

ported by the N-MR on the quartic profiles, either with the square- 

or rectangular reconstructions. We suggest that this spurious effect is 

induced via a complex accommodation dependency upon the weights 

and Pe inserted by the diagonal links into reconstructed tangential cor-

rections. It follows that the results displayed in Fig. 10 are weight- 

and Pe-independent only with FLL1 = T-DFLI, FMRs and DFLI. These 

results confirm our expectation that the d2q9 MR flux schemes do not 

need any tangential corrections in the steady-state straight homoge-

neous solutions, to be contrasted with their necessity in the presence of 

the non-zero tangential boundary flux, the heterogeneous interface 

weights or for the transient BB simulations in the uniform velocity 

field. Indeed, one should keep in mind that the harmful tangential 

boundary effect is much smaller on the parabolic profile \( u_i(y) \) consid-

ered here than when \( u_i \) is constant, because \( u_i(y) \) vanishes on the 

wall. This difference was clearly quantified and on the effective retarda-

tion of the mean velocity, which is the first-order distribution 

moment.

We extend now these simulations to the symmetric diagonal slab, 

where the d2q9 weight-stencil excites the A – layer equilibrium 

accommodation on the implicit-interface quartic profiles. The 

homogeneous solution remains exact using the fourth-order accurate 

boundary closure from Eq. (58), thanks to \( \Lambda(c_1) \) and isotropic weights. 

Figure 11 addresses \( M_0 \) and \( \Phi_0 \) results obtained with the second-

order schemes: the straight channel alike, \( \Phi_0 \) produces better accuracy 

and exhibits the third-order convergence rate [this is obtained with the second-

order schemes: the straight channel alike, \( \Phi_0 \) produces better accuracy 

and exhibits the third-order convergence rate [this is obtained with the second-

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and exhibits the third-order convergence rate [this is obtained with the second-

order schemes: the straight channel alike, \( \Phi_0 \) produces better accuracy 

and exhibits the third-order convergence rate [this is obtained with the second-
irregular on the coarse grid; the DFLI continues to show the worst results. The T-DFLI, behaves similarly to FLI, when \( H \geq 20 \) but it is very inaccurate when \( H = 10 \) because of the rectangular reconstruction. We will systematically observe that T-DFLI is much less accurate on the coarse grids compared to the square reconstruction, but the latter one is geometry-dependent.

### C. Rotated channels

We model now a rotated channel \( \theta = \arctan\frac{h}{l} \) with the isotropic (hydrodynamic) advection-diffusion weights. Unless indicated, we prescribe \( \{\Lambda^{(x)}, c_r^{(x)}\} \) from Eq. (53), so that \( P^{(x)}(y') \) is exact in bulk and \( E_2 = E_2^{(x)} \). However, inexact boundary schemes do not reproduce the exact solution and hence, they are subject to truncation effects, such as the anisotropy and the loss of symmetry; also, \( E_2 \) becomes Pe- and weight-dependent with all schemes. According to Fig. 6, one might expect that the anisotropic bulk effect is still relatively weak when \( \text{Pe} \ll 10^2 \), but it rapidly increases on the coarse grid when \( \text{Pe} = 10^3 \). Figures 12 and 14 display the numerical profiles with the Dirichlet and Neumann conditions, respectively, on the coarse grid \( H = 20 \) when \( \text{Pe} = 10^2 \) and \( \text{Pe} = 10^3 \). The fourth-order accurate Taylor schemes T-PP\(^{(d)}\) and T-DFLI\(^{(d)}\) from Eq. (58) match \( P^{(x)}(y') \) exactly; otherwise, \( E_2 \) is given in Tables IV and V.

We examine first the Dirichlet boundary schemes prescribing \( P|_{y=0,H} = \text{Pe} \); the exact profile \( P(y')/\text{Pe} \) is then Pe-independent. Figure 12 displays the ADE results of (i) linear, one-node MPLI/LMKC and PLI families from Table XI; (ii) parabolic in pure diffusion, new single-node PPLI scheme from Table XII; and (iii) parabolic in constant velocity field, two-node PP family from Table XI; the variation of the mass-source is accounted for by using \( B_0 = 1 \) in Eq. (A4). Additionally, the single-node Taylor schemes T-PP, and T-PP from Eq. (12a) are examined using, respectively, rectangular and (mainly) square reconstructions. Again, we intentionally degrade Eq. (12a) to the first order with the T-I-PP, scheme but address it with the parabolic-accurate rectangular reconstruction.

Figure 12 (left diagram) shows that all schemes match the quartic profile on the relatively coarse grid when \( \text{Pe} = 10^2 \). However, unlike in pure-diffusion, the profiles are not symmetric and they do not scale exactly with Pe. These effects grow rapidly with Pe and only those schemes where the leading-order advection projections are absent, like the PP, T-PP, \( n \), and T-PP, but also a less accurate T-I-PP, retain the profile shape when \( \text{Pe} = 10^3 \). The PLI is expected to overcome MPLI when Pe grows, because PLI removes the first-order advection gradient from its closure relation.\(^{40} \) Table IV confirms that although MPLI is more accurate than the two other linear schemes, PLI and T-I-PP, in pure diffusion and Pe = \( 10^2 \), the T-I-PP, gains over them at \( \text{Pe} = 10^3 \). In turn, according to Table IV, the PPLI overpasses not only MPLI/PLI but also PP and A-LSOB T-PP/T-PP, in the pure-diffusion regime. However, as was expected, the PPLI accuracy worsens in the presence of a grid-inclined velocity field, very similarly to MPLI/LMKC.

Figure 13 displays \( E_2(H) \); it confirms that when \( \text{Pe} = 10^2 \), PLI gains over MPLI/PPLI only for \( H = 10 \), but it is more accurate over the long interval \( H < 80 \) when \( \text{Pe} = 10^3 \). In turn, the PPLI asymptotically approaches PP and converges with the third-order rate when \( \text{Pe} = 10^2 \), but it decays slower together with MPLI when \( \text{Pe} = 10^3 \). The PP systematically gains over the LI schemes, especially when Pe increases, and converges smoothly. The T-PP, and T-PP behave very similarly, they are the most accurate on the finer grids, here when \( H \geq 20 \) with \( \text{Pe} = 10^2 \), because their closure relation is free of the advection projection; however, their reconstruction is not smooth when \( \text{Pe} = 10^3 \). The employed LI and MR Dirichlet schemes are all parametrized, and their results are set by \( \text{Pe}, \), \( \Lambda \), and \( H \). The T-PP, does not maintain the parametrization; the T-PP is parametrized when it employs only square subsets in Eq. (17); otherwise, T-PP loses the parametrization property when it (optionally) uses the rectangular matrix in single cut link nodes following the algorithm from example 4 in Subsection B of the Appendix.

Figure 14 shows similar results with the Neumann schemes; here we additionally consider the degraded T-I-DFLI, where we omit the parabolic term in Eq. (12b) but retain the reconstruction process. Figure 14 (left diagram) shows that the T-I-DFLI is the least accurate at \( \text{Pe} = 10^2 \), and its \( E_2 \) exceeds FLI, by about two orders of magnitude in pure diffusion according to Table V. When \( \text{Pe} = 10^3 \), all schemes become affected by the loss of symmetry, and this effect becomes most noticeable with the diffusive-flux parabolic schemes, DFLI, and T-DFLI, [T-DFLI produces similar results], whereas the degraded
TABLE IV. Quartic-polynomial rotated Dirichlet numerical solution when \( H = 20 \) using \( \{ \Lambda^{(a)}, c_0^{(a)} \} \) (i) in pure diffusion [top line: \( E_2 \) is Pe-independent] and (ii) in ADE [\( \text{Pe} = 10^3 \) and \( \text{Pe} = 10^4 \) from Fig. 12]; E2 is fixed by the grid Pécel number except T-I-PP, [the first-order degradation of Eq. (12a)], T-PP, and T-PP.

<table>
<thead>
<tr>
<th>Pe</th>
<th>MPLI</th>
<th>PLI</th>
<th>PPLI</th>
<th>PP</th>
<th>T-I-PP</th>
<th>T-PP</th>
<th>T-PP</th>
<th>T-PP(df)</th>
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<tbody>
<tr>
<td>(\lambda)</td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>(\text{Pe} = 10^2)</td>
<td>(1.1 \times 10^{-2})</td>
<td>(7 \times 10^{-4})</td>
<td>(5.2 \times 10^{-3})</td>
<td>(3 \times 10^{-2})</td>
<td>(9.5 \times 10^{-4})</td>
<td>(10^{-3})</td>
<td>(5 \times 10^{-15})</td>
<td></td>
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<tr>
<td>(\text{Pe} = 10^3)</td>
<td>(8.8 \times 10^{-3})</td>
<td>(1 \times 10^{-2})</td>
<td>(5.5 \times 10^{-3})</td>
<td>(1.6 \times 10^{-2})</td>
<td>(9.8 \times 10^{-4})</td>
<td>(1.2 \times 10^{-3})</td>
<td>(6.9 \times 10^{-15})</td>
<td></td>
</tr>
<tr>
<td>(\text{Pe} = 10^4)</td>
<td>(1.7 \times 10^{-1})</td>
<td>(7.5 \times 10^{-2})</td>
<td>(1.6 \times 10^{-1})</td>
<td>(1.9 \times 10^{-2})</td>
<td>(2.9 \times 10^{-2})</td>
<td>(1.2 \times 10^{-2})</td>
<td>(1.2 \times 10^{-15})</td>
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<p>| (E_2) using Eq. (28) |</p>
<table>
<thead>
<tr>
<th>Pe</th>
<th>FMR(_n)</th>
<th>DFLI(_n)</th>
<th>T-I-DFLI</th>
<th>T-DFLI</th>
<th>T-DFLI</th>
<th>T-DFLI(df)</th>
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<td>(\lambda)</td>
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<tr>
<td>(\text{Pe} = 10^2)</td>
<td>(1.8 \times 10^{-3})</td>
<td>(4.7 \times 10^{-3})</td>
<td>(2.2 \times 10^{-2})</td>
<td>(-0.12)</td>
<td>(6.6 \times 10^{-3})</td>
<td>(6.8 \times 10^{-3})</td>
</tr>
<tr>
<td>(\text{Pe} = 10^3)</td>
<td>(1.8 \times 10^{-3})</td>
<td>(4.7 \times 10^{-3})</td>
<td>(2.3 \times 10^{-2})</td>
<td>(-7.04 \times 10^{-2})</td>
<td>(4.6 \times 10^{-3})</td>
<td>(4.7 \times 10^{-3})</td>
</tr>
<tr>
<td>(\text{Pe} = 10^4)</td>
<td>(1.3 \times 10^{-1})</td>
<td>(6 \times 10^{-3})</td>
<td>(1.2 \times 10^{-1})</td>
<td>(-1.22 \times 10^{-1})</td>
<td>(1.2 \times 10^{-1})</td>
<td>(5.8 \times 10^{-2})</td>
</tr>
</tbody>
</table>

T-I-DFLI worsens by a smaller extent because its principal inaccuracy is due to the constant diffusive-flux approximation. Table IX confirms that FFLI, overheads all other schemes, including FMR\(_n\), and produces two-order magnitude smaller \(M_0\) than DFLI\(_n\) and T-DFLI\(_n\) when \(\text{Pe} = 10^3\).

Figure 15 addresses the convergence of \(M_0\) and \(\Phi_0\) strategies when \(\text{Pe} = 10^2\); the basic MR schemes are displayed here together with the N-MR and Taylor schemes T-DFLI and T-DFLI. The results show that all schemes obey a second-order rate and, except FFLI\(_n\) and DFLI\(_n\) in ADE, they almost overlap when \(H \geq 20\); FFLI\(_n\) gains again by a large extent and shows much smaller values of \([M_0]\) and \([\Phi_0]\). In this respect, DFLI\(_n\) and N-DFLI remain the least accurate. We note that \(E_2\) is very similar with the two-node FMR/N-FMR and the single-node T-DFLI/T-DFLI, but the MR schemes show better conservation properties.

We employ now \(\Lambda^{(df)}\) from Eq. (55), where the exact solvability condition remains formally valid but the effective profile does not scale with \(\text{Pe}\) exactly, because of the truncation correction in Eq. (48). Figure 16 compares FFLI\(_n\) with its five N-MR counterparts from Table III, and with the two Taylor schemes, T-DFLI and T-I-DFLI. The results are restricted to \(\text{Pe} = 10\) because the reconstruction is not always regular at higher \(\text{Pe}\). All schemes decay similarly with second-order rate and here only N-DFLI improves FFLI\(_n\) in accuracy and convergence due to the smaller amplitude and faster decay of \(\Phi_0(h)\). Recall, N-DFLI\(_2\), is exact, [the first-order degradation of Eq. (12a)], T-DFLI\(_2\) and T-DFLI\(_{df}\).

![FIG. 13. Quartic-polynomial rotated Dirichlet numerical solution. Left: \(\text{Pe} = 10^2\). Right: \(\text{Pe} = 10^3\). The exact (solid line) and numerical (symbols) solutions with \(M_0\) from Eq. (28) and the flux schemes: MPLI\(_n\), PLI\(_n\), PPLI\(_n\), PP\(_n\), T-PP\(_n\), T-PP\(_n\), H\(_n\). Data from Fig. 12.](image)

![FIG. 14. Quartic-polynomial rotated Neumann solution when \(H = 20\). Left: \(\text{Pe} = 10^2\). Right: \(\text{Pe} = 10^3\). The exact (solid line) and numerical (symbols) solutions with \(M_0\) from Eq. (28) and the flux schemes: PLI\(_n\), PLI\(_n\), PPLI\(_n\), T-PP\(_n\), T-PP\(_n\), H\(_n\). Data from Fig. 12.](image)
passes condition \( h \) on the normalized analytical and numerical solutions, e.g., obeying the local tangential gradient \( c_i \) changes non-zero in the translation-invariant direction even with the implicit interface treatment. This effect is attributed to the anti-symmetric truncation correction contained in \( \tilde{h} \), which contributes to the local gradient estimate.

We note that the term \( \tilde{h} \) is different in FLI, FMR and DFLI closure relations, and also, that it depends upon a solution constant in the parabolic velocity profile. Figure 18 demonstrates the difference in the error estimate and \( M_0 \) when two arbitrary values are fixed in one point. A very interesting result is that not only FMR, DFLI and T-DFLI, but also all N-MR schemes N-FLI, N-DFLI from Table III produce consistent solutions. In contrast, the FLI and FLI are produce different normalized solutions with two different values, where the displayed difference in \( E_l \) and \( M_0 \) approximately decays in-between second/third rate and third-order rate, respectively. The FLI and FLI manifest this artifact not only in the grid-shifted rotated channels, but also in the grid-symmetric ones; the results with \( \Phi_0 \) follow along this line. Hence, it is suggested that the N-MR removes this free-dependent dependency with the help of its tangential corrections of \( \tilde{h} \) in terms (10).

To sum up, the N-FLI does not improve FLI and FLI regularly for accuracy in the parabolic no-slip velocity profiles because of the relatively weak tangential advection effects against the advection truncation and its accommodation. However, it appears that the N-FLI removes the principal advection terms in the non-equilibrium

\[ \text{FIG. 15. Quartic-polynomial rotated Neumann solution. Top row: } E_l(H) \text{ and } M_0(H) / H. \text{ Bottom row: } E_l(H) \text{ and } (2\Phi_0/H)(\psi h). \text{ Flux schemes: FLI, FMR, DFLI, N-DFLI, N-FLI, N-FMR, N-FLI. } H^2 \text{ Data: } Pe = 10^2, \theta = \arctan(k/4), \{x_0, y_0\} = \{0, 0\}, c_0 = \pi^2 \Lambda^0(\phi_0) \text{ obeys Eq. (55).} \]

\[ \text{FIG. 16. Quartic rotated Neumann solutions at } Pe = 10. \text{ } E_l^0/(H) \text{ (left) and } 2\Phi_0/(H)/(\psi h). \text{ Flux schemes: FLI, FMR, DFLI, N-DFLI, N-FLI, N-FMR, N-FLI. } H^2 \text{ Data: } \theta = \arctan(k/4), \{x_0, y_0\} = \{0, 0\}, c_0 = \pi^2 \Lambda^0(\phi_0) \text{ obeys Eq. (55).} \]

\[ \text{FIG. 17. Quartic rotated Neumann solutions. } E_l(H) \text{ with the FLI using } M_0 \left[ Pe = 10, \Phi_0 \right] \text{ and } (2\Phi_0/H)(\psi h). \text{ Flux schemes: FLI, FMR, DFLI, N-DFLI, N-FLI. } H^2 \text{ Data: } \theta = \arctan(k/4), \{x_0, y_0\} = \{0, 0\}, c_0 = \pi^2 \Lambda^0(\phi_0) \text{ obeys Eq. (55).} \]

\[ \text{FIG. 18. Dependency upon an additive constant in quartic rotated Neumann profiles: the difference } \Delta E_l \text{ and } \Delta M_0 \text{ with } \Delta E_l \text{ and } \Delta M_0 \text{ when } \Phi_0 = Pe = 10^2. \text{ FLI, FMR, DFLI, N-DFLI, N-FLI. } H^2 \text{ Data: } Pe = 10^2, \theta = \arctan(k/4), \{x_0, y_0\} = \{0, 0\}, \{\Lambda^0(\phi_0), c_0(\phi_0)\}. \]

\[ \text{FIG. 19. Flux schemes: FLI, FMR, DFLI, N-FLI, N-DFLI. } H^2 \text{ Data: } Pe = 10^2, \theta = \arctan(k/4), \{x_0, y_0\} = \{0, 0\}, \{\Lambda^0(\phi_0), c_0(\phi_0)\}. \]

\[ \text{FIG. 20. Flux schemes: FLI, FMR, DFLI, N-FLI, N-DFLI. } H^2 \text{ Data: } Pe = 10^2, \theta = \arctan(k/4), \{x_0, y_0\} = \{0, 0\}, \{\Lambda^0(\phi_0), c_0(\phi_0)\}. \]
expansion responsible for the FLI inconsistency. Otherwise, the FLI and FLI₂ normalized solution and error-estimate vary together with the solution constant, and therefore, these schemes are to be considered as not reliable, despite their very good conservation properties.

I. Rotated heterogeneous system

We extend now the boundary problem37 from the grid-aligned implicit-interface TRT-EMM scheme38,39 to the grid-rotated interface-conjugate treatment. The bulk equation remains the same as described by Eq. (41a), but the stratified system combines now the diffusive porous layer \( \phi = \phi_1 \in [0,1] \) with the open (Poiseuille) profile \( \phi_2 = 1 \):

\[
\begin{align*}
    u_c(y') &= 0, \quad \phi = \phi_1, \quad y' \in [-h_1, 0], \\
    u_c(y') &= -\frac{1}{2} \Psi y'(y' - h_2), \quad \phi = 1, \quad y' \in [0, h_2], \\
    \Psi &= \frac{\Psi_{13}^3}{12(\phi_1 h_1 + \phi_2 h_2)}, \quad \rho_e = \frac{\Psi(h_1 + h_2)}{c_1}.
\end{align*}
\]

The two layers are either periodic [OPL] or impermeable [B – OPL]; the B – OPL reduces to the above considered Poiseuille flow problem when the diffusion-layer vanishes \([h_1 = 0]\). The diffusion coefficients are discontinuous: \( \Lambda_1 = \phi_1 \Lambda \) and \( \Lambda_2 = \phi_2 \Lambda \); the scalar field \( P(y') \) and the diffusive flux \( -\phi \partial_y P(y') \) are set continuous on the interface \( y' = 0 \). The advective flux remains discontinuous:

\[
    \Psi_{13} = \frac{\Psi_{13}^3}{12(\phi_1 h_1 + \phi_2 h_2)}, \quad \rho_e = \frac{\Psi(h_1 + h_2)}{c_1}.
\]

We apply the interface-conjugate from Eq. (37) with the two-node parabolic PP family for the scalar-field continuity condition and compare it with (i) its MR counterparts involving the normal mass-source correction, as FLI₂, FMR₂ and DFLI₂; (ii) the N-MR partners, as N-FLI₂ or N-FLI from Table III, and (iii), the single-node combinations of the Taylor and N-MR schemes, where T-DFLI applies for boundary and N-FLI [or N-FLI] adjusts the interface. Figures 19 and 20 employ the square and rectangular reconstructions, respectively. We recall that all examined schemes are exact for the boundary and interface in two adjacent diffusive layers (STRD restricted to pure-diffusion).

Figure 19 shows that the FLI₂ is by far the most accurate and it decays with third-order rate thanks to its best conservation property, while the DFLI₂ behaves as the worst, due to its significant deviation from the exact solvability condition manifested again by the large \( M_0 \) and \( \Phi_0 \) magnitudes. All other flux schemes show very similar results of intermediate accuracy: N-FLI₂ behaves slightly better than FLI₂ with \( M_0 \) and slightly worse than with \( \Phi_0 \), but FLI₂ surpasses FMR₂ and the two mixed combinations of the Taylor and MR schemes: T-DFLI₂, FLI₂, and T-DFLI₂ – FLI₂, which are formally more accurate. The \( M_0 \) and \( \Phi_0 \) techniques also show close results for the \( E_2 \) and their respective amplitudes of \( M_0/\Psi \) and 2\( M_0/\Psi \).

When \( \Psi = 10^2 \), the truncation and accommodation grow non-linearly against \( \Psi = 10 \) in Fig. 19. Figure 20 shows that all schemes then decay with second-order rate; the rectangular reconstruction is not accurate on the coarsest grid, here with a width \( h_0 = 10 \cos \theta \approx 8.9 \) node per layer. The finer grids show results which are similar with \( \Psi = 10 \) and confirm the advanced precision of the FLI₂ interface/boundary treatment. However, we should emphasize again that the reported values of \( E_2 \) depend upon an additive constant in FLI₂ and FLI₂.

To sum up, we used the piece-wise parabolic solutions and confirmed the suitability of the MR and N-MR for the continuous-flux interface-conjugate in the non-uniform velocity profile. The N-FLI₂
might offer an interesting compromise to FLI$^2$ and FLI$^3$, because it (i) needs only one interface or boundary point; (ii) shares with FLI$^2$ similar mass-conservation, and (iii) improves FLI$^2$ and FLI$^3$ for their tangential constraints and a free-constant dependency. However, we find that the important role of the truncation and accommodation at higher Pe, here typically Pe $\geq 10^3$, corrupts the second-order reconstruction procedure.

2. Periodic open-porous layered system, OPL

We consider now a fully periodic system where the corrective flux from Eq. (32) is extended for interface system and $\Phi_0$ strategy prescribes

$$ M_0 = 0, $$

$$ || - \partial_y \partial_y P ||_{y=0} = || \mathcal{D}_y || + \Phi_0, $$

$$ || - \partial_y \partial_y P ||_{y=\h} = || \mathcal{D}_y || - \Phi_0, $$

(64)

Like with Eq. (32), Eq. (64) is expected to produce the most accurate results when the two interfaces are placed symmetrically. In the OPL system, the diffusion-flux is continuous, then $|| \mathcal{D}_y || = 0$. The OPL is run with $M_0$ from Eq. (28) and $\Phi_0$ from Eq. (64). Figure 21 addresses the pure diffusive system $c_e^2 = 0$ but applies the same mass-source as in Eq. (41a). We confirm that all numerical solutions formally scale with the Pe number and then produce Pe-independent error-estimates. It is interesting to note that $M_0 / \h = 2 \Phi_0 / (U \h)$ with all schemes, the straight symmetric Poiseuille flow alike [cf. Eq. (60)]. We observe that $\Phi_0 - \text{FMR} = \Phi_0 - \text{N-FMR}$ decay with a third-order rate in the absence of the advection terms. Due to the same reason, the N-MR$_3$ and N-MR$_4$, exemplified for the square and rectangular reconstruction, show similar results to their counterparts, such as FLI$_n$ and FMR$_n$. It is curious that, unlike in all previous results, $\Phi_0 - \text{DFLI}_3$ clearly surpasses $\Phi_0 - \text{DFLI}_n$ in pure diffusion. This indicates that although DFLI$_n$ vanishes the uniform-velocity advection terms from its closure relation on the parabolic profiles, its accuracy is impacted by them in the general cases. All $M_0 -$ schemes decay with a second-order rate because of the mass-source correction in Eq. (28). On the whole, these results are similar to those in the diagonal flow displayed in Fig. 11 at Pe = $10^3$. The last diagram in Fig. 21 confirms that among the $\Phi_0-$ schemes, DFLI$_n$ and FMR$_n$ produce, respectively, the largest and smallest deviations from the exact profile.

Figure 22 examines the $E_2-$ dependency over Pe with two basic schemes, as FLI$_n$ (left diagram) and FMR$_n$ (right diagram); their results are displayed together using $M_0$ and $\Phi_0$ when Pe = $\{10, 10^2, 10^3\}$. When Pe $\leq 10^2$, $\Phi_0 - \text{FMR}$ monotonously decays with third-order rate, in pure diffusion alike; but $M_0$, Pe $\to \infty$, and the two FLI schemes, $M_0 - \text{FLI}_n$, and $\Phi_0 - \text{FLI}_n$, decay with second-order rate in agreement with the expectations and previous results. In these simulations, $E_2$ remains almost Pe-independent, whereas $M_0 / (U \h)$ and $2 \Phi_0 / (U \h)$ practically coincide between them in all these schemes. However, again, when $\text{Pe} = 10^3$, the $M_0$ and $\Phi_0$ solutions behave similarly and produce much larger errors on the same grids.

To sum up, these observations confirm that $M_0 - \text{FMR}$ is dominated by the second-order bulk accuracy of the $M_0-$ strategy in the pure diffusion and intermediate Pe range, but both $M_0$ and $\Phi_0$ solutions are dominated by the Pe-dependent truncation and its interface-accommodation at high Pe. We note that the boundary systems alike, (i) the results of FLI and FLI$_n$ depend upon an additive constant in the fully periodic OPL, and (ii) the N-MR removes this deficiency but becomes irregular when Pe grows.

3. Summary

The rotated quartic solution due to the parabolic velocity and mass-source fields extends our previous analysis on the numerical modeling of the Taylor dispersion problem. We confirm that the pure-diffusion grid-rotated solution can be matched exactly with the help of the fourth-order accurate Neumann and Dirichlet Taylor schemes using $\Lambda^{(s)}(c_e)$ from Eq. (52), $\forall c_e$. When $\Lambda \neq \Lambda^{(s)}$, the effective diffusion solution is isotropic only with the hydrodynamic mass-weight $\Lambda^{(m)}$, but it retains the symmetry. In contrast, the effective advection-diffusion solution is anisotropic and not symmetric with the hydrodynamic weights unless when it is tuned to be exact with the singular choice of the two remaining free parameters, as given by $\{\Lambda^{(s)}(c_e), \text{c}_e^{(\alpha)}\}$ from Eq. (53). Using the fourth-order accurate Dirichlet closure, the effective solution is validated exactly with free-tunable values of these two parameters. In the Neumann system, $\Lambda^{(\alpha)}(c_e)$ from
Eq. (55) becomes mandatory for the exact solvability condition \( \mathcal{M}(\psi(\alpha_{ex}), y') = 0; \Lambda^{(0)}(\alpha_e) \) reduces to \( \Lambda^{(0)} \) when \( c = c_{\alpha_{ex}}^{(0)} \).

The exact bulk-parameter choice is employed to validate all proposed Dirichlet and Neumann schemes. We confirmed their second and, partly, third-order, convergence order in arbitrary-oriented, uniform and heterogeneous channels, and related their accuracy with the mass balance metrics. The interesting result is that the corrective flux \( \Phi_0 \) is able to adjust the exact straight quartic solution for any flux scheme. Its analytical solution \( |\Phi_0(\delta)| \) clearly indicates that the diffusive-flux DFLI family, which is built to be exact on the grid-rotated parabolic profiles in uniform tangential velocity field, deviates most significantly from the exact solvability condition on the quartic solution. This DFLI feature is then observed through all examined solutions, which undoubtedly explains its worst accuracy. In contrast, the FLI and FLL, behave most accurately despite their lower formal Taylor-accuracy order; this happens because their single-node flux continuation, as \(- A \tilde{n}_y + \delta \tilde{n}_x \), fits the mid-grid LBM bulk-flux discretization in Eqs. (27). These suggestions are further confirmed through the exact mass-balance analysis in Sec. D.

Unfortunately, due to this semi-implicit discretization, FLI and FLL may do not respect the additivity of a free constant in the Neumann or periodic solutions. All other schemes, including N-FLI, are consistent in our simulations. Also, the MR, but also N-MR and A-LSOB with the square-matrix reconstruction are all parameterized by grid Pe number and \( A \); the rectangular reconstruction loses this property but it avoids the problem of the subset choice in Eq. (17), and hence it can be regarded as geometry- and problem-independent.

We recognize that the coarse grid solution may become spoiled by the truncation and its accommodation, growing very rapidly with Pe; the rectangular reconstruction becomes then not sufficiently accurate on the coarse grids. In this respect, when the tangential advective boundary flux is very small due to the no-slip velocity or a diffusive interface, the preselected candidates are the two-node FMR, and the one-node N-FLI, which show similar accuracy at the intermediate Pe range, e.g., Fig. 15. The FMR converges faster, with third-order rate in the grid-aligned channels, it is simpler and more robust for the high Pe range. However, N-FMR or N-FLI should replace FMR, in the case of the (nearly) uniform rotated tangential flow and in the presence of the diffusive-flux jumps, as demonstrated for STRD, and as also expected for problems with the non-zero tangential diffusive boundary/interface flux.

Concerning the single-node A-LSOB flux schemes, the T-DFLI and T-DFLL, are interesting because they (i) share with FLI, the same (good) solvability condition in the straight grid-shifted systems, (ii) respect there, together with the unmodified MR, the weight-independence and linear Pe-scale, and (iii) show comparable to two-node FMR, conservation properties in the inclined channels. On the negative side, they are affected by strong truncation and accommodation errors through the reconstruction procedure at high Pe. The Taylor Dirichlet schemes T-PP and T-PP, are not impacted by Pe-dependent effects, and they even surpass the parabolic PP family (cf. Figs. 12 and 14, Table IV) because their normal Taylor condition is not affected by the advection projections. This is confirmed by the results of the degraded (linear) T-T-PP, scheme, which behaves much more accurately at high Pe than its linear MR counterparts, MPLI/LMKC, PLI and PPLI. In turn, the novel single-node parabolic PPLI

from Table XII is the most accurate in the pure-diffusion and it approaches PP in the intermediate Pe range.

Finally, concerning the EMM – TRT application with the no-slip velocity field, we highlight that the parametrized schemes should be preferred to assure the solution control by the Pelet number at fixed \( A \), and that the grid shall be refined approximately linearly when Pe grows to get rid of the nonphysical Pe-dependency due to the interface/boundary high-order accommodation. It should be said that the transient ADE solvers meet even stronger limitations for the Taylor moments prediction, because both the translation length and the computational time toward the steady Taylor regime grow with Pe. Moreover, whereas the transient ADE solvers become unstable with Pe, the steady-state EMM – TRT is not affected by the stability issue and the interface-conjugate MR steady-state treatment allows to accelerate the convergence by one or two orders with respect to their implicit tracking in rotated slabs.40

VI. ROTATED EXPONENTIAL SOLUTION IN PLUG FLOW

The two stratified heterogeneous layers of width \( h_1, h_2 \) are again arbitrary rotated and placed with respect to the grid, but now the constant (Darcy) advection velocity \( \bar{u} = u_{\bar{y}} \bar{y} \) is perpendicular to the interface in “series.” The system is periodic along \( y' \), it is abbreviated DS, and its modeled equation reads

\[
\begin{align*}
L_y u_y &= \phi_y, \\
\phi_y &= D_y \phi_y, \\
\phi_y &= 0.
\end{align*}
\]

Solvability condition \( \langle \mathcal{M} \rangle = 0 \) is adjusted with the mean-velocity \( \bar{u} \).

The interface conditions are described by Eq. (36): the scalar field is continuous \( (\phi_s = 1, \eta_s = 0) \) but the normal diffusive-flux is subject to the jump condition: \( \phi_n^{(0)} = 1, \eta_n^{(0)} = \| \mathcal{S} \| \bar{y} \cdot \bar{y} \). In theory, the diffusive flux is continuous on the interface and hence it vanishes from the flux closure relation. A continuous periodic solution \( \phi(y') \) is defined up to an additive constant. Solution of Eq. (65) allows to predict the effective diffusivity (at zero velocity, thanks to the interface-diffusive-flux jump) and the dispersion coefficient \( D_y = (\phi_y)^{-1} (u_{\bar{y}} P) \) in the plug flow due to the structure heterogeneity, the EMM also extends this procedure to the high-order moments.37 The symbolic and numerical analysis of the EMM – TRT scheme is developed for the straight (the diffusivity, dispersion, skewness and kurtosis) and the diagonal (the second-order moments) implicit-jump tracking. These results (i) produce exact solutions for the three moments in the pure diffusion with the help of the specific dependency \( \Lambda(c) \) for kurtosis (given by the third-order polynomial solution \( P(y) \)) and (ii) show that the implicit-interface ABB – continuity condition produces Pe-growing errors and an anisotropic interface location due to the presence of the advective term of \( P(\eta, \eta^2) = -A \phi^{(0)} \) in Eq. (5), as \( -A' \Delta_{\bar{y}} \bar{y} \propto -\Delta_{\bar{y}} \bar{y} \Delta_{\bar{y}} \Delta_{\bar{y}} \phi_{\bar{y}} \phi_{\bar{y}} \), in the perpendicular flow \( \bar{u} = u_{\bar{y}} \bar{y} \). This term is vanished in PLI/PAB with the help of the post-collision correction \( F_y \) and, together with the next-order term of \( \gamma^{(0)} \), in the parabolic MR PP family (see Table XIV). In the diagonal slab, both pure diffusion and plug flow are affected by the implicit interface accommodation.

In the present work, the “internal” \( y' = 0 \) and “periodic” \( y' = h_1 \) interfaces are modeled with the interface-conjugate from Eq. (37). When the proposed schemes are not exact on the discrete-exponential profile, we adjust their solvability condition with \( M_0 \) from Eq. (28) and the corrective interface jump \( \Phi_0 \) from Eq. (64).
Our analysis undertakes a symbolic procedure in the straight geometry, and the numerical computations in the diagonal and rotated slabs.

A. Effective symbolic solutions

We construct and examine the effective solutions of the MR and A-LSOB interface-conjugate, and their combinations, in the straight interface-perpendicular plug flow. We also build the effective Taylor equivalents of the MR schemes and develop their inverse mapping, from the parabolic Taylor closure to its local MR equivalent.

1. Symbolic procedure

Our symbolic analysis follows and develops with d2q5, because the steady-state profile \( P(y) \) is weight-independent in the straight geometry; the extension for d2q9 solution and the diagonal orientation may follow. We apply \( M_0 \) strategy, then Eq. (28) determines d2q5 solution for \( \mathbf{y} \):\n\[
\mathbf{y} = \mathbf{y}_0 + \mathbf{u}_0(t)\mathbf{u}.
\]
\[
\mathbf{u}_0(t) = \mathbf{M}_0 = 0, \quad \forall \mathbf{y},
\]
(66b)
\[
\mathbf{M}_0 = 0, \quad \forall \mathbf{y}\) if only \( \delta^{(i)} = \delta^{(p)} \).
\]

Conversely, plugging Eq. (66) into Eqs. (15a)–(15c), \( \mathbf{y} \) reads with \( \mathbf{P} = \mathbf{P}_0 \):
\[
\mathbf{y} = \mathbf{y}_0 + \mathbf{u}_0(t)\mathbf{u},
\]
\[
\mathbf{u}_0(t) = \mathbf{M}_0 = 0, \quad \forall \mathbf{y},
\]
(66a)
\[
\mathbf{M}_0 = 0, \quad \forall \mathbf{y}\) if only \( \delta^{(i)} = \delta^{(p)} \).
\]

Equation (28) equates the sums of Eqs. (67a) and (66a), and provides the central-difference form of the modeled equation:
\[
u_0 \Delta P - (\mathcal{H}_k + M_0) = \mathcal{D}_k \Delta^2 P, \quad \mathcal{D}_k = c_i \Lambda_k.
\]
(68)

Clearly, when \( \mathbf{M}_0 \neq 0 \), the solution gradient gets modified as
\[
\mathbf{P} = \mathbf{P}_0 + \mathbf{u}_0(t)\mathbf{u}, \quad \mathbf{u}_0(t) = \mathbf{M}_0 = 0, \quad \forall \mathbf{y},
\]
(69)

The two-layered solution is determined up to an additive constant \( a_1 \) [or \( a_2 \)]. The three coefficients from the set \{ \( a_1, a_2, c_1, c_2 \) \} and \( M_0 \) are determined giving the two couples of the interface-conjugate conditions (37), e.g., with PP – FLI, FLI – FLI, and other MR combinations. The MR, and N-MR reduce to MR because the tangential advective-diffusive flux is zero in d2q5. Their interface-closure relations are all expressed exactly through Eqs. (66a) and (67b) plugging their Eq. (69). In turn, the A-LSOB Taylor schemes (12) become expressed through the four couples of the grid unknowns \( \{ \Delta P, \Delta^2 P \} \), T-DFLI (diffusive flux) or T-FLI (advective-diffusive flux) are substituted into the interface-flux equation (36b). Equation (67) closes the A-LSOB system by equating the RHS of Eq. (67) to its solution expressed on the profile (69) for vertical links in the interface grid nodes \( \mathcal{M} \); this procedure mimics the reconstruction of \( \{ \Delta P, \Delta^2 P \} \) with the \( \mathcal{B} \) \( \mathbf{[}2 \times 2\mathbf{]} \) matrix in Eq. (17). We also combine the MR and A-LSOB interface-conjugate relations, as T-PP-FLI or PP – T-DFLI.

Our symbolic procedure does not involve the truncation approximation from Eq. (16). The constructed solution then presents the effective numerical solution of a given scheme.

2. Solvability conditions

Assume that the "internal" \( y' = 0 \) and "periodic" \( y' = \h_2 \) interfaces are shifted from their mid-grid position at the distance \( \delta^{(i)} \) and \( \delta^{(p)} \), respectively, giving \( h_1 = h_1 + \delta^{(i)} - h^{(p)} \), \( h_2 = h_2 + \delta^{(i)} - h^{(p)} \), but keeping the total length \( h = h_1 + h_2 = h_1 + h_2 = h \). The following results are obtained on the symbolic solutions and confirmed numerically:

- Both FLI and FMR satisfy the exact solvability condition \( \langle \mathcal{H}(\varphi^{(ex)}) \rangle = 0 \) with \( M_0 = 0 \):
\[
\mathcal{H}_k(y') = \mathbf{y}_0 = 0, \quad \forall y',\]
(70)

This property is independent of the continuity scheme applied for a scalar-field in the interface-conjugate.

- Otherwise, when for example \( \varphi \) is prescribed in Eq. (63b) via summation, FLI and FMR adjust \( M_0 \) according to the derivation in Subsection D 1 of the Appendix, as
\[
M_0 = -\frac{\mathcal{H}_k - \mathcal{H}_k(y') + \mathcal{H}_k(y)}{H}, \quad \mathcal{H}_k(y') = \mathbf{y}_0 + \mathbf{u}_0(t)\mathbf{u}, \quad \mathcal{H}_k(y) = \mathbf{y}_0 + \mathbf{u}_0(t)\mathbf{u},
\]
(71)

The case \( \delta^{(i)} = 0 \) corresponds to the uniform vertical shift of the whole slab from its mid-grid position.

- Conversely, if one adjusts \( c_1 \Lambda_1 \) and prescribes the same values \( \varphi^{(ex)} = \varphi^{(sum)} \) at the fixed grid Péclet number \( \mathbf{p} = \mathbf{p}_0 \), then \( \mathcal{H}_k(y') = \mathbf{y}_0 + \mathbf{u}_0(t)\mathbf{u}, \quad \mathcal{H}_k(y) = \mathbf{y}_0 + \mathbf{u}_0(t)\mathbf{u},
\]
(72)

The proof is based on Eq. (71). However, \( P(y') \) is distinguished in these two configurations, because \( u_0(\varphi^{(ex)} \neq \varphi^{(sum)}) \).

- Unlike the FLI/FMR, the DFLI and T-DFLI produce \( M_0 \neq 0 \) either with \( \varphi^{(ex)} \) or \( \varphi^{(sum)} \) for any interface position, including its midway \( \delta^{(i)} = 0 \) or the uniformly-shifted \( \delta^{(i)} = 0 \) placements. The effective solution of \( M_0 \) with \( \varphi^{(sum)} \) is expressed in Eq. (71). The symbolic solutions confirm it and show that, in contrast to Eq. (71), \( M_0 \) depends on the scalar-field continuity scheme \( M^{(p)}_0 \) applied in Eq. (37a), both with the DFLI and the Taylor scheme T-DFLI. That means these two parabolic schemes do not satisfy the exact solvability condition in a series of straight blocks in the presence of the interface-normal velocity. Moreover, it is shown in Subsection D 2 of the Appendix that the vertical DFLI closure relation in Eq. (8) is equivalent with the back-sided non-equilibrium extrapolation of the diffusive-flux component – \( \Lambda \mathbf{\Lambda} \mathbf{n} \mathbf{q} \), as
\[
\mathbf{D}_{\mathcal{L}}(\mathbf{r} + \delta \mathbf{q}) = -\Lambda \mathbf{\Lambda} \mathbf{n} \mathbf{q} (\mathbf{r} - \mathbf{n} \mathbf{q} (\mathbf{r} - \delta \mathbf{q})).
\]
(73)
In contrast, T-DFLI in Eq. (12b) presents the locally expressed normal Taylor extrapolation of the diffusive flux.

- All these results are also valid in parallel Darcy flow $\mathbf{u} = u_{r} \mathbf{i}_{r}$ [STRD]. However, since the STRD solution $P(y)$ to Eq. (41a) is determined by $\mathcal{H}(\mathbf{u}) + M_{0}$, it is the same when $\mathcal{H}(\mathbf{u}_{\text{l}}) = \mathcal{H}(\mathbf{u}_{\text{sam}})$ but $u_{r}(\mathbf{u}_{\text{l}})$ and $c_{A}^\Lambda$ differ. In these cases, the T-DFLI and DFLI are also exact, because Eqs. (12b) and (73) are exact when the diffusive flux is linear in space.

To sum up, when the mass-source is piece-wise constant, the DFLI “straight” closure relation is equivalent with the back-sided normal extrapolation of $-\Lambda \cdot \mathbf{n}_{\text{g}}$, whereas FLI and FMR operate its continuation locally via $\delta \mathbf{n}_{\text{g}}^{0}$, the BB alike, and they are then able to satisfy the exact solvability condition $\langle \mathcal{H}(\mathbf{u}_{\text{sam}}) \rangle = 0$ with plug flow in series; this conservation property is unavailable with the DFLI and T-DFLI, even on the uniformly shifted interface $\delta^{(h)} = \delta^{(0)}$.

### 3. The exact Taylor MR form

We build now the Taylor equivalents of the MR schemes in the plug flow. This analysis is based on the exact central-difference solution in Eq. (67); the effective MR closure is then not identical with its second-order approximation in Eq. (5). This analysis allows us to compare the Taylor and MR closure relations in terms of the exact central-difference gradients $\Delta \mathbf{P}$ and $\Delta_{c}^{2} \mathbf{P}$ according to Eq. (67). The key point is that the neighbor components $P(\tilde{r}_{b} - \tilde{c}_{y})$ and $\tilde{n}_{y}(\tilde{r}_{b} - \tilde{c}_{y})$ in two-node MR schemes are expressed from Eqs. (26a) and (26b) through $P(\tilde{r}_{b})$ and $\tilde{n}_{y}^{0}(\tilde{r}_{b})$, where we take into account that $\tilde{n}_{y}^{0}$ is the same inside one layer thanks to Eq. (66). The MR Taylor form then reads as

$$
T_{n}(\tilde{r}_{b}) = t_{1} M_{0} + t_{2} P + m_{e} c_{y}^{0}(t_{3} P + t_{4} \Delta \mathbf{P} c_{y}^{0} + t_{5} \Delta_{c}^{2} \mathbf{P} c_{y}^{0}) + t_{6} \Delta_{c} \mathbf{P} c_{y}^{0} + t_{7} \Delta_{c}^{2} \mathbf{P} c_{y}^{0}|_{r_{b}}.
$$

(74)

### Table VI. The coefficients of the effective interface Taylor closure in Eq. (74) along the vertical cut are derived from Eq. (34) [It is subdivided by $x^{(0)} c_{y}^{0}$, and reads with $\Lambda = \{\Lambda_{r}\}$. Equation (74) with the MR and normal Taylor Dirichlet schemes in the straight geometry. The MR coefficients of Eq. (34) are subdivided by $x^{(0)} c_{y}^{0}$.

<table>
<thead>
<tr>
<th>$t_{i}$</th>
<th>MR</th>
<th>PLI</th>
<th>PP/KMR1</th>
<th>T-PP</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_{1}$</td>
<td>$(1 - \Lambda c_{y}^{0}) \Delta_{c} \mathbf{P}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$t_{2}$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>$t_{3}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>$t_{4}$</td>
<td>$(1 + \Lambda c_{y}^{0}) \Delta_{c} \mathbf{P}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$t_{5}$</td>
<td>$\Lambda \cdot \mathbf{n}_{\text{g}}^{0}$</td>
<td>$\delta$</td>
<td>$\delta$</td>
<td>$\delta$</td>
</tr>
<tr>
<td>$t_{6}$</td>
<td>$\Delta_{c} \mathbf{P} c_{y}^{0}$</td>
<td>$\delta$</td>
<td>$\delta$</td>
<td>$\delta$</td>
</tr>
<tr>
<td>$t_{7}$</td>
<td>$(1 + \Lambda c_{y}^{0}) \Delta_{c} \mathbf{P} c_{y}^{0}$</td>
<td>0</td>
<td>$\delta^{2}$</td>
<td>$\delta^{2}$</td>
</tr>
</tbody>
</table>

### TABLE VII. Equation (74) with the MR and normal Taylor flux schemes in the straight geometry. The coefficients of Eq. (34) are subdivided by $x^{(0)}$ in FLI/FMR and $\Delta_{c}^{2} \mathbf{P} c_{y}^{0}$ in DFLI.

<table>
<thead>
<tr>
<th>$t_{i}$</th>
<th>FLI/FMR</th>
<th>T-FLI</th>
<th>DFLI</th>
<th>T-DFLI</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_{1}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$t_{2}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$t_{3}$</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$t_{4}$</td>
<td>$\delta$</td>
<td>$\delta$</td>
<td>$\delta$</td>
<td>$\delta$</td>
</tr>
<tr>
<td>$t_{5}$</td>
<td>$\frac{1}{4}$</td>
<td>$\frac{1}{2}$ $\delta^{2}$</td>
<td>$\frac{1}{4}$</td>
<td>$(1 + 2\delta)$</td>
</tr>
<tr>
<td>$t_{6}$</td>
<td>$-c_{A}^\Lambda$</td>
<td>$-c_{A}^\Lambda$</td>
<td>$-c_{A}^\Lambda$</td>
<td>$-c_{A}^\Lambda$</td>
</tr>
<tr>
<td>$t_{7}$</td>
<td>$-c_{A}^\Lambda \cdot \delta$</td>
<td>$-c_{A}^\Lambda \cdot \delta$</td>
<td>$-c_{A}^\Lambda \cdot \delta$</td>
<td>$-c_{A}^\Lambda \cdot \delta$</td>
</tr>
</tbody>
</table>

Tables VII and VII give, respectively, the coefficients for the Dirichlet and Neumann, MR and A-LSOB basic schemes. They remain valid for the pure diffusion and in straight parallel flow giving $u_{n} = 0$ in Eq. (74). We first note that according to these two tables, all MR schemes are incorrect for the term of $t_{5} u_{s} \Lambda \Delta_{c} \mathbf{P} c_{y}^{0}$. In detail, the effective diffusive-flux interface condition reads as

$$
T-DFLI \equiv \left\| P + \delta \mathbf{P} c_{y}^{0} + \frac{\delta^{2}}{2} \Delta_{c}^{2} \mathbf{P} c_{y}^{0} \right\| = \| \mathcal{S} \|, \quad DFLI \equiv \left\| P + \delta \mathbf{P} c_{y}^{0} + \frac{\delta^{2}}{2} \Delta_{c}^{2} \mathbf{P} c_{y}^{0} \right\| = \| \mathcal{S} \||

(75a)

(75b)

Thus, DFLI modifies the prescribed jump condition with respect to T-DFLI in the normal flow, to be contrasted with the second-order approximation in Eq. (5), which vanishes all velocity terms in DFLI closure thanks to its coefficients, $x^{(u)} = \beta^{(u)} = \gamma^{(0)} = 0$. In turn, the PP/KMR1 – FLI/FMR interface-conjugate reads with

$$
PP/KMR1 \equiv \| P + \delta \mathbf{P} c_{y}^{0} + \frac{\delta^{2}}{2} \Delta_{c}^{2} \mathbf{P} c_{y}^{0} \| = \left\| \frac{\delta(1 + \delta) \mathbf{P} c_{y}^{0}}{4} \right\|, \quad FLI/FMR \equiv \| u_{s} \mathbf{P} c_{y}^{0} + \frac{1}{4} \Delta_{c}^{2} \mathbf{P} c_{y}^{0} \| = \| \mathcal{S} \|. \quad (75c)
$$

(76a)

(76b)

These results show first that the parabolic schemes PP and KMR1 are equivalent on the straight interface, and they both modify the Taylor continuity relation in the interface-normal flow $\mathcal{P} e_{\|} \neq 0$; again, this is despite that the PP closure in Eq. (5) is predicted to be velocity-independent. Second, FLI and FMR produce identical closure relations and hence, the same solutions in the basic straight configurations, although their form in Eq. (5) is distinct for the coefficient of $\gamma^{(u)}$. Namely, their common deficient advection term $\frac{1}{4} \Delta_{c}^{2} \mathbf{P} c_{y}^{0}$ in Eq. (76b) is $\delta-$independent and hence, it is the same as with the BB or implicit-interface tracking. Hence, Eq. (76b) comes down to T-DFLI from Eq. (75a) only provided that the scalar interface-continuity condition in Eq. (37a) is modeled with the incorrect, modified Taylor scheme, replacing $\frac{\delta}{2}$ by $\frac{\delta}{4}$ in the parabolic term:

$$
M-PP \equiv \left\| P + \delta \mathbf{P} c_{y}^{0} + \frac{1}{4} \Delta_{c}^{2} \mathbf{P} c_{y}^{0} \right\| = 0. \quad (77)
$$

(77)
To sum up, the second-order “correct” Taylor interface-conjugate T-PP – T-DFLI produces \( M_0 \neq 0 \) according to above analysis, and hence it does not support the exact solvability condition, whereas the “incorrect” interface-conjugate M-T-PP – T-DFLI respects \( \langle M \rangle_{\langle \mathcal{N}^{(n)} \rangle} = 0 \) thanks to its equivalence with M-T-PP – FLI/FRM. This example clearly shows that the best mass-balance and the best Taylor accuracy are not equivalent for LBM flux schemes.

4. The \( M_0 \) and \( \phi_0 \) in plug flow

Let us exemplify the symbolic solutions for several basic interface combinations, like PP – FLI, PP – DFLI and T-PP – T-DFLI, where we now compare the two strategies, \( M_0 \) from Eq. (28) and the corrective interface-jump \( \Phi_0 \) from Eq. (64). Figure 23 displays \( E_2 \) when the interface is shifted uniformly (left diagram) and when the “internal” and “periodic” interfaces move one to another; on the whole, we observe that these two “opposite” configurations produce very similar results. In accord with the above analysis, PP-FLI and PP-FMR produce identical and the most accurate results; they solve the system with \( M_0 = 0 \) and \( \Phi_0 = 0 \). Otherwise, with both DFLI and T-DFLI, the effective solution \( M_0 \) and \( \Phi_0 \) depends on the scalar-continuity scheme. It is confirmed that \( M_0 = 0 \) – DFLI is the least accurate, and it is surpassed by the \( \Phi_0 = 0 \) – DFLI over a long interval \( H < \approx 3 \times 10^4 \); the two techniques then decay together on the finer grids. In turn, T-PP – T-DFLI behaves similar to PP – DFLI on the coarsest grids, where it is not accurate; however, T-PP – T-DFLI converges faster and decays almost in parallel with PP – FLI/FMR, both with \( M_0 = 0 \) and \( \Phi_0 = 0 \). The “mixed” single-node pair T-PP-FLI is also interesting: it behaves as the T-PP – T-DFLI on the coarse grid, but then very rapidly (with a rate about 2.4) joins PP-FLI. These observations confirm that the mass conservation, or the exact solvability, pre-determines the asymptotic accuracy, whereas the joined combination of the two interface conditions determines it on the realistic grids.

B. Inverse mapping in the straight system

A very interesting property of the examined above effective closure relations and their solutions is that they are \( \Lambda - \) independent. This property is not automatic, for example \( E_2 \) linearly grows with \( \Lambda \) using the implicit ABB – BB interface-tracking,\(^{38,40}\) where ABB differently shifts the midway interface position on two interface sides to \( \frac{1}{2} + \Lambda \frac{1}{2} (1 - \Lambda) \) \( PE \). The PAB scheme (which is PLI(\( \frac{1}{2} \)) radical improves for this property with the leading-order post-collision advection correction, and makes the solution \( \Lambda - \) independent; the parabolic PP and T-PP schemes examined above share the same property in the straight series. However, we have seen that the MR and Taylor schemes are not equivalent there. The idea of the “inverse mapping” is to construct the I-MR equivalents of the Taylor schemes. The I-MR is searched in its steady-state one-node form in Eq. (34):

\[
M_0 (\phi_0) = (m_1 e_{q1} + m_2 e_{q2} + m_3 \phi_0 + m_4 \phi_0^2) |_{\phi_0^0}. \tag{78}
\]

Equations (66a) and (67b) are substituted into Eq. (78) for \( n_{\phi^0}; M_0 (\phi_0) \) then becomes expressed through the local variables \{\( M_0, \mathcal{P}, \Lambda_\mathcal{P}, \Lambda_\mathcal{Y}, \mathcal{P}_{\mathcal{Y}} \}\). The four coefficients \( m_4 \) are then adjusted to one of the three Taylor schemes (12); the obtained coefficients are gathered in Table VIII for their three (inverse) equivalents: I-PP, I-FLI and I-DFLI. Usually, the MR coefficients only depend upon the directional distance \( \delta \) to the interface/boundary. However, the I-MR coefficients also depend on (a) the sign of (cut) link \( \mathcal{P}_{\mathcal{Q}} \) and (b), grid Pécellet number \( \mathcal{P}_{\mathcal{Q}} \). Hence, the inverse mapping automatically detects the anisotropy and Pécellet–dependency of the effective closure. We have verified that the I-MR numerical solution coincides with the symbolic solution of its Taylor counterpart. Hence, the single-node I-MR reproduces the A-LSOB in straight series without any reconstruction. At zero \( \mathcal{P}_{\mathcal{Q}} \), the local I-MR reduces to Table IX and it applies exactly on the vertical cut link for piece-wise parabolic straight profile [STRD problem above]. To sum up, the I-MR delivers the methodological example on how one should combine equilibrium and non-equilibrium components in single interface-neighboring nodes to make the interface-

![FIG. 23. The Darcy in series system [DS] in two equal straight blocks when the “internal” and “periodic” interfaces are shifted at \( \delta^{(1)} \) and \( \delta^{(2)} \), respectively, from the mid-grid position. PP – FLI/FMR and T-PP – FLI/FMR with \( M_0 = \phi_0 = 0 \), then M – DFLI \( \Phi_0 = M \), T – T-DFLI \( \Phi_0 = M \), T – PP – T-DFLI \( \Phi_0 = 0 \). Left: \( \delta^{(1)} = \delta^{(2)} = \frac{1}{2} \); \( E_2 \) – rate \( r = [2.37, 2.23, 1.56, 1.47, 1.77, 1.77] \). Right: \( \delta^{(1)} = -\delta^{(2)} = -\frac{1}{2} \); \( E_2 \) – rate \( r = [2.37, 2.23, 1.55, 1.45, 1.75, 1.74] \). Data: \( \mathcal{P}_{\mathcal{Q}} = 10^7 \), \( \mathcal{P}_{\mathcal{Q}} = 8 \).](https://example.com/fig23.png)

| Table VIII. The coefficients \( m_1 \) – \( m_4 \) of the “inverse” single-node I-MR in Eq. (78), equivalent with the Taylor schemes from Eq. (12) in straight plug flow in series. The table reads with \( X = 2 \mathcal{P}_{\mathcal{Q}} \mathcal{P}_{\mathcal{Y}} \), \( Y = -4 - \mathcal{P}_{\mathcal{Q}} - \mathcal{P}_{\mathcal{Y}} \), \( Z = -2 + \delta \mathcal{P}_{\mathcal{Q}} \mathcal{P}_{\mathcal{Y}} \), \( \delta = \delta_k \) in phase \( k \) and \( c_{\mathcal{Q}} \) corresponds to interface cut link \( \mathcal{Q} \). The I-PP applies flag \( Y_{\mathcal{Q}} \) = 1 in interface-conjugate in Eq. (37a). |
|----------------|----------------|----------------|----------------|
| I-MR = A-LSOB  | \( m_1 \) | \( m_2 \) | \( m_4 \) |
| I-PP = T-PP    | 1               | \( \delta (2 + \delta)(\mathcal{P}_{\mathcal{Q}} + c_{\mathcal{Q}}(4\delta + \mathcal{P}_{\mathcal{Q}}^2)) \) | 0               | \( -2\delta (2 + c_{\mathcal{Q}} \mathcal{P}_{\mathcal{Q}})(2c_{\mathcal{Q}} + \delta \mathcal{P}_{\mathcal{Q}}) \) |
| I-FLI = T-FLI  | 0               | \( c_{\mathcal{Q}}(-1 + 2\delta^2) \mathcal{P}_{\mathcal{Q}} + c_{\mathcal{Q}} \delta \mathcal{Y} \) | 1               | \( -2c_{\mathcal{Q}} \Lambda_\mathcal{Y}^2 (2 + c_{\mathcal{Q}} \mathcal{P}_{\mathcal{Q}})Z \) |
| I-DFLI = T-DFLI| 0               | \( -2(1 + 2\delta \mathcal{P}_{\mathcal{Q}}) \mathcal{Y} + c_{\mathcal{Q}}(8\delta + \mathcal{P}_{\mathcal{Q}}^2) \) | 0               | \( 4c_{\mathcal{Q}} \Lambda_\mathcal{Y}^2 (2 + c_{\mathcal{Q}} \mathcal{P}_{\mathcal{Q}})(1 + c_{\mathcal{Q}} \delta \mathcal{P}_{\mathcal{Q}}) \) |
conjugate in Eq. (36) equivalent with the Taylor interface closure from Eq. (12) on the straight interface in series. This approach may find its utility for construction of the MR schemes.

**Remark.** In principle, giving $m_1 - m_4$ in Eq. (78), one can try to invert the system (35) and to find the corresponding coefficients \(\{\tilde{a}, \tilde{b}, \tilde{c}, \tilde{d}, \tilde{e}\}\) in the standard (transient) MR, Eq. (A1). When $Pe_0 \neq 0$, the obtained coefficients depend upon $c_0$. For example, the I-PP and I-FLI can be, respectively, reproduced by the ABB and BB supplemented with two local specific post-collision corrections $K^\pm$.

### C. Diagonal interface

The symbolic and numerical results\(^{39}\) show that the d2q5 tackles the implicit diagonal mid-way interface without accommodation layers and retains the second-order convergence in series of two heterogeneous blocks. In contrast, the full weight-stencil d2q9 model suffers from the equilibrium discrete-exponential A-layer accommodation; its amplitude depends on the weight distribution, $A$, $Pe$, and porosity contrast. The error estimates\(^{39}\) address the two solution functionalities, like the effective diffusivity and the Taylor dispersion coefficient $D_T$ the A-layer slows their error convergence to the first order (see Fig. 10 in Ref. 39) We extend this analysis to the grid-shifted interface-conjugate treatment and employ the standard error-estimate metric.

Our steady-state simulations are performed in a single column delimited by the diagonal periodic interface. The PP is prescribed for the scalar-continuity in Eq. (37a); in flux schemes, MR delimits by the diagonal periodic interface. The PP is prescribed for the straight interface in series. This approach may find its utility for construction of the MR schemes.

**Remark.** In principle, giving $m_1 - m_4$ in Eq. (78), one can try to invert the system (35) and to find the corresponding coefficients \(\{\tilde{a}, \tilde{b}, \tilde{c}, \tilde{d}, \tilde{e}\}\) in the standard (transient) MR, Eq. (A1). When $Pe_0 \neq 0$, the obtained coefficients depend upon $c_0$. For example, the I-PP and I-FLI can be, respectively, reproduced by the ABB and BB supplemented with two local specific post-collision corrections $K^\pm$.

### D. Rotated series of porous blocks

The rotated system of two heterogeneous blocks in series has been examined\(^{37}\) with the MR interface-conjugate schemes (see there Fig. 14). When $Pe = 10$, the FLI and FMR, combined with PP in Eq. (37a), converge with rate $r \approx 1.8$, and they clearly overpass their combinations with the linear scalar-continuity schemes, like FLI and MPLI, which demonstrate the expected linear decay. These computations are run with $M_0 \neq 0$ in Eq. (28). It has been observed that the advection accommodation effect rapidly amplifies between $Pe = 10$ and $Pe = 10^3$: the solution dependency over the equilibrium weights then becomes highly irregular, and the convergence rate becomes halved, both for $E_2$ and $M_0$. Moreover, d2q5 loses its advanced accuracy, which is observed in the grid-aligned and, for small $Pe$ range, rotated systems. At the same time, the BB flux condition, combined either with the implicit interface scalar-continuity condition (ABB), linear or parabolic Dirichlet schemes, retains its first-order convergence when $Pe = 10^3$, and then ABB-BB even slightly supersedes the formally most accurate PP-FMR interface-conjugate on the finest grids $H \geq 3 \times 10^3$. In agreement with our conclusions above with respect to FLI/FMR straight system, this advanced BB performance might be related to its mass-conservation ($M_0 = 0$) because the solvability condition\(^{37}\) is prescribed via summation, as $\langle \mathcal{H}(\Phi^{(\text{sum})}) \rangle = 0$.

We apply here the exact condition $\langle \mathcal{H}(\Phi^{(\text{sum})}) \rangle = 0$, which is equivalent to the summation in constant velocity field when the discrete phase distribution respects the porosity ratio $r_0$ exactly. Figure 25 presents in the left diagram the error decay in the same geometry considered previously, but using the two solvability strategies, $M_0$ and $\Phi_0$. The corrective interface flux-jump $\Phi_0$ shows slightly better accuracy in all simulations, and slightly better convergence rate (DFLI excepted); $\Phi_0 - FF$ is again the most accurate. The PP – DFLI remains one-order magnitude less accurate than its FLI and FMR counterparts, but it converges slightly faster. The two linear schemes $M_0 - PLI - FLI$ and $\Phi_0 - PLI$ halve the PP convergence rate.
The (normal) N-MR follows another path to prescribe the parabolic-accurate Neumann condition. The N-MR restores locally, but precisely, the actual directional projection of the tangential advective-diffusive flux, built-in to a given MR flux closure relation, and simply deducts it from the incoming-population solution. Also, the in-node correction of the normal mass-source variation improved accuracy of the MR, and N-MR flux schemes for all reported results. In this work, the A-LSOB and N-MR shared the same reconstruction procedure, delivering the same results in the Cartesian and flat-surface aligned coordinates. The N-MR extension to 2d/3d curved boundaries and corner geometries with a non-zero boundary flux value is thought to be more efficient in the fixed coordinate system, because the normal direction is distinct for different cut-links. This next step might adapt the recent LSOB formulation\textsuperscript{87} for the curved cross-section duct Stokes flow.

In the presence of a grid-rotated high Pe velocity field, the single-node parabolic Dirichlet A-LSOB T-PP shows better accuracy level than the two-node parabolic MR PP; in turn, a linear normal Taylor condition behaved more accurately than its single-node MR counterparts MPLI/PPLI. This Dirichlet A-LSOB enhancement is because the MR directional closure relations are affected by the advection projections, e.g., at the first order with MPLI/PPLI, the second order with PLI and the third-order with PP; however, the A-LSOB reconstruction process is not smooth at high Pe. The MR, N-MR and A-LSOB expand straightforwardly for the Robin condition by combining their Dirichlet and normal Neumann counterparts. The A-LSOB is expected to extend easier its parabolic accuracy to the full-matrix and anisotropic collisions, but, like the MR, the N-MR operates directly on any-shape interface-conjugate and it applies very similarly in transient and steady-state algorithms. The two methods follow the so-called Lnode approach\textsuperscript{12,13,104,105} whereas the ideas of the “Lwall” approach\textsuperscript{87} might become beneficial for (i) their reduction to the coordinate stencils, thanks to additional surface information, and (ii) their interface extensions, by re-formulating A-LSOB and N-MR in terms of the surface derivatives. Finally, the reconstruction procedure was elaborated for the linear ADE; we assume that the transient non-linear problems might adapt the linearization of the Chapman-Enskog solution around the previous step.

We have shown that the BB, its linear [FLI] and parabolic [FMR] advective-diffusive MR flux counterparts should be corrected in the steady-state problems in the presence of the grid-rotated tangential constant velocity field. The previous research delivered similar conclusions in the wall-parallel transient advection\textsuperscript{17,42,62–64} and for the non-zero tangential diffusive boundary flux;\textsuperscript{33,36,39} indeed, the accommodation mechanism is equivalent for tangential, constant-velocity and linear diffusive, fluxes.\textsuperscript{33,36,39} The N-MR and Neumann A-LSOB are constructed to resolve these two problems together, for any velocity field; their formulation is equivalent for advective and diffusive flux components, and their concept was validated through the exactness of their piece-wise parabolic, bounded, periodic, continuous and discontinuous, profiles in the grid-inclined uniform velocity field, extending this solution class for the single-node Dirichlet and Neumann A-LSOB schemes, and the single-node N-FLI scheme. We note that the N-FLI improves the FLM scheme\textsuperscript{82} for any weight-stencil without need for resorting to the heuristic Dirichlet and off-grid interpolations. Conversely, we have demonstrated that the linearly accurate Dirichlet LIfamilies, and the intentionally degraded A-LSOB Dirichlet and

![Figure 25](right diagram) then compares PP-FLI and PP-FMR with their N-MR partners on the finest grids. In fact, we observed that N-MR is rather irregular on the coarser grids, most likely because of

\begin{equation}
\begin{aligned}
\rho_0 &= \text{the usual,}
\end{aligned}
\end{equation}

The DS in the inclined series of two porous blocks. Left: PP continuity scheme is combined with $M_0 = \text{FLI}$, $\Phi_0 = \text{FLI}$, $M_0 = \text{FMR}$, $\Phi_0 = \text{FMR}$, $r = 10^{-1} \times \{8.7, 8.9, 8.1, 8.3\}$, followed by FLI continuity combined with, $M_0 = \text{FLI}$, $\Phi_0 = \text{FLI}$, $M_0 = \text{FMR}$, $\Phi_0 = \text{FMR}$, $r = (0.49, 0.5)$; and then by (the least accurate) $M_0 = \text{PP} - \text{DPLI}$ and $\Phi_0 = \text{FLI}$, $r = (1.3, 1.2)$. Right: The PP is combined with $M_0 = \text{FLI}$, $\Phi_0 = \text{FLI}$, $M_0 = \text{FMR}$, $\Phi_0 = \text{FMR}$, $r = (0.49, 0.5)$; and then by (the least accurate) $M_0 = \text{PP} - \text{DPLI}$ and $\Phi_0 = \text{FLI}$, $r = (1.3, 1.2)$.

![Figure 25](right diagram) then compares PP-FLI and PP-FMR with their N-MR partners on the finest grids. In fact, we observed that N-MR is rather irregular on the coarser grids, most likely because of the strong interface-accommodation advection effect. We optionally apply (i) the reduced rectangular reconstruction N-FLI3 and N-FMR3 with Eq. (17), reducing $n_B$ that, as usual, applies (i) the reduced rectangular reconstruction N-FLI3 and N-FMR3 with Eq. (17), reducing $n_B$ that, as usual, $M_0 = \text{FLI}$, $\Phi_0 = \text{FLI}$, $M_0 = \text{FMR}$, $\Phi_0 = \text{FMR}$, $r = (0.49, 0.5)$; and then by (the least accurate) $M_0 = \text{PP} - \text{DPLI}$ and $\Phi_0 = \text{FLI}$, $r = (1.3, 1.2)$.

The DS in the inclined series of two porous blocks. Left: PP continuity scheme is combined with $M_0 = \text{FLI}$, $\Phi_0 = \text{FLI}$, $M_0 = \text{FMR}$, $\Phi_0 = \text{FMR}$, $r = 10^{-1} \times \{8.7, 8.9, 8.1, 8.3\}$, followed by FLI continuity combined with, $M_0 = \text{FLI}$, $\Phi_0 = \text{FLI}$, $M_0 = \text{FMR}$, $\Phi_0 = \text{FMR}$, $r = (0.49, 0.5)$; and then by (the least accurate) $M_0 = \text{PP} - \text{DPLI}$ and $\Phi_0 = \text{FLI}$, $r = (1.3, 1.2)$. Right: The PP is combined with $M_0 = \text{FLI}$, $\Phi_0 = \text{FLI}$, $M_0 = \text{FMR}$, $\Phi_0 = \text{FMR}$, $r = (0.49, 0.5)$; and then by (the least accurate) $M_0 = \text{PP} - \text{DPLI}$ and $\Phi_0 = \text{FLI}$, $r = (1.3, 1.2)$.

The DS in the inclined series of two porous blocks. Left: PP continuity scheme is combined with $M_0 = \text{FLI}$, $\Phi_0 = \text{FLI}$, $M_0 = \text{FMR}$, $\Phi_0 = \text{FMR}$, $r = 10^{-1} \times \{8.7, 8.9, 8.1, 8.3\}$, followed by FLI continuity combined with, $M_0 = \text{FLI}$, $\Phi_0 = \text{FLI}$, $M_0 = \text{FMR}$, $\Phi_0 = \text{FMR}$, $r = (0.49, 0.5)$; and then by (the least accurate) $M_0 = \text{PP} - \text{DPLI}$ and $\Phi_0 = \text{FLI}$, $r = (1.3, 1.2)$.

The DS in the inclined series of two porous blocks. Left: PP continuity scheme is combined with $M_0 = \text{FLI}$, $\Phi_0 = \text{FLI}$, $M_0 = \text{FMR}$, $\Phi_0 = \text{FMR}$, $r = 10^{-1} \times \{8.7, 8.9, 8.1, 8.3\}$, followed by FLI continuity combined with, $M_0 = \text{FLI}$, $\Phi_0 = \text{FLI}$, $M_0 = \text{FMR}$, $\Phi_0 = \text{FMR}$, $r = (0.49, 0.5)$; and then by (the least accurate) $M_0 = \text{PP} - \text{DPLI}$ and $\Phi_0 = \text{FLI}$, $r = (1.3, 1.2)$.
Neumann schemes, fail to reproduce interface and boundary behavior correctly in the benchmark configurations tested herein.

All parabolic-accurate schemes behaved well on the quartic profiles in the diffusion-dominant regimes and intermediate Pe-range, suggesting them to be suitable for heat and mass transfer applications in composite materials. In particular, the most simple single-node Dirichlet PPLI shows the best diffusion accuracy; its Dirichlet velocity counterpart IPI is expected to share these properties in the pipe fluid flow modeling; their further validation is required because of the restricted heuristic stability range. Some reservations should be made for the advection-dominant regime. In practice, both the Cartesian-decomposition method and N-MR considerably complicate the simple directional MR concept; it is legitimate to understand when they are necessary for the realistic solute transport. We have shown that the tangential grid-inclined no-slip velocity field induces relatively small boundary and open-porous diffusive-interface errors, as compared to the truncation and its accommodation effects caused by the inexactness of the boundary rules. The latter was demonstrated on the parabolic-accurate schemes excite the anisotropic advection truncation, which non-linearly grows with Péclet number, violates the linear Pe-scale of the modeled equation and makes the error-estimates Pe-dependent. A similar deficiency is provoked by the accommodation layers in the grid-inclined interface-perpendicular plug flow, rendering the N-MR solutions irregular in the high Péclet regime. Given that the diffusive-flux effects must become negligible when the advection is strong, we suggest to give the preference to the unmodified MR schemes, and in particular, the two-node FMR/FMR, for the interface-continuous Neumann problems in the high Pe problems. The N-MR or A-LSOB may substitute it there for the discontinuous solutions with the diffusive-flux jumps.

We also examined all flux schemes with respect to the exact, “body-fitted”, mass-conservation solvability condition $\langle \mathcal{M} \rangle = 0$ using either the (i) artificial uniform mass-source $M_0$, suitable in any geometry or (ii) corrective surface-flux $\pm \Phi_0$, applicable on two parallel surfaces; these unknown variables are automatically obtained on the global S-TRT solution. Their respective amplitudes $|M_0|$ and $|\Phi_0|$ served us as mass-balance metrics. Although the two techniques decay closely with second-order rate, the corrective flux is more accurate, especially with MR, because it does not modify the bulk equation. As one illustrative example, the corrective flux is able to adjust the grid-shifted symmetric MR, because it does not modify the bulk equation. As one illustrative example, the corrective flux is able to adjust the grid-shifted symmetric MR, because it does not modify the bulk equation. As one illustrative example, the corrective flux is able to adjust the grid-shifted symmetric MR, because it does not modify the bulk equation.

Along these lines, our results undoubtedly show that the inherent mass-balance dominates the formal accuracy with the Neumann LBM. In particular, the FLI/FLL exhibits the smallest mass leakage and, together with the FMR/FMR, assures the exact mass-balance for any straight interface position in the plug flow. This happens because FLI describes the total local mass-flux as $-\Lambda n_q$, and its continuation toward the delimiting surface as $\delta \mathcal{M}$, which comes down to the regular bulk-flux discretization for $\delta = \frac{1}{2}$. However, due to this semi-implicit discretization, FLI/FLL, does not guarantee to respect a free additive constant in the Neumann solutions, in the presence of the parabolic tangential velocity field at least. This truncation feature is inline with the deficient local-gradient estimate dependency upon an additive constant. On the positive side, all other examined flux schemes, as the FMR, DFLI, N-MR and Taylor scheme T-DFLI, are consistent with respect to additive constant independence in our examples. The FMR, N-MR and T-DFLI report a comparable mass-balance in the grid-inclined situations, but the example of the parabolic diffusive-flux MR scheme DFLI shows that its intrinsic back-sided extrapolation of $-\Lambda n_q$ along the characteristic is extremely non-conserving, except the linear diffusive-flux case where it is exact. These observations might become fruitful for many non-equilibrium interpolation approaches.

Concerning the presented analytical work, we (i) derived the solvability conditions on the equilibrium weights or free TRT parameter $\Lambda$, when the quartic polynomial may satisfy the discrete system in the presence of the grid-rotated parabolic advection profile, (ii) constructed the associated effective solution with the hydrodynamic weights, (iii) delineated the particular dependency $\Lambda(\epsilon)$ where the effective solution becomes exact and hence, isotropic and linearly scaling with Pe, and (iv) built the corrective boundary flux which adjusts the global mass conservation for all examined flux schemes. We also constructed the effective symbolic solutions in the interface-perpendicular straight plug flow and applied them to compare exactly all schemes for their mass balance; the FLI and FMR are found to be conservative on the grid-shifted straight interface. Finally, we built the single-node MR counterparts of the Taylor schemes and demonstrated that, unlike in the current MR approach, their coefficients should become anisotropic and account for the cut link direction with respect to the surface-perpendicular plug velocity field. We believe that our methodology will be helpful to advance the LBM analysis and to delineate the most optimal closure schemes.

In conclusion, the Neumann boundary and interface-flux conditions should combine the compactness, accurate mass-balance, physical parametrization, correct Pe-scale and free-constant independence with the release of the tangential constraints and efficient reduction of the accommodation layers. We have shown that the proposed approaches progress along all these directions, and we expect that they will bring some new ideas for two-phase and fluid-solid, stress and slip Lattice Boltzmann models.

**APPENDIX A: THE LI AND MR MULTI-REFLECTION SCHEMES**

We consider the MR in two-node directional form:

$$f_{-\gamma}(\vec{r}_b, t + 1) = \text{MR}_q(\vec{r}_b, t) + w_{\gamma}(\vec{r}_q, t), \quad \vec{r}_q = \vec{r}_b + \vec{e}_q \notin V_p,$$

$$\text{MR}_q = \hat{F}_q(\vec{r}_b, t) + \hat{\beta} f_q(\vec{r}_b, t + 1) + \hat{\beta} \hat{f}_{-\gamma}(\vec{r}_b, t)$$

$$+ \hat{\gamma} f_q(\vec{r}_b - \vec{e}_q, t + 1) + \hat{\gamma} \hat{f}_{-\gamma}(\vec{r}_b - \vec{e}_q, t)$$

$$+ \hat{F}_q(\vec{r}_b, t), \quad \hat{F}_q = \hat{K}^{+} n_q^{+} + \hat{K}^{-} n_q^{-}. \tag{A1}$$

Equation (A1) gives solution for unknown population $f_{-\gamma}(\vec{r}_b, t + 1)$ in boundary node $\vec{r}_b$ in terms of (i) three postcollision populations: $f_{\gamma}(\vec{r}_b, t), f_{-\gamma}(\vec{r}_b, t), f_{-\gamma}(\vec{r}_b - \vec{e}_q, t)$; (ii) two after-streaming populations: $f_q(\vec{r}_b, t + 1) = f_q(\vec{r}_b - \vec{e}_q, t)$ and $f_q(\vec{r}_b - 2\vec{e}_q, t + 1) = f_q(\vec{r}_b - 2\vec{e}_q, t)$; (iii) local post-collision correction $\hat{F}_q(\vec{r}_b, t)$ and (iv), the prescribed boundary term $w_{\gamma}(\vec{r}_b, t)$. Alternatively, one may adopt the time-explicit algorithm by replacing $\hat{\beta} f_q(\vec{r}_b, t + 1)$ and $\hat{\gamma} \hat{f}_{-\gamma}(\vec{r}_b, t + 1)$ by their previous time step solution: $\beta f_q(\vec{r}_b, t)$ and
TABLE X. The three-population families MPLI(\(\varepsilon^{(p)}\)) and PLI(\(\varepsilon^{(p)}\)) with free coefficient \(\varepsilon^{(p)}\) and \(\gamma = \dot{\gamma} = 0\); \(w_0\) obeys Eq. (A4); the two schemes differ for \(K_+\); \(\beta\) or \(K_+\) can be set equal to zero with the specific \(\varepsilon^{(p)}\). Heuristic stability: \(\{\dot{x}, \beta, K\} \in [-1, 1]\) when \(\varepsilon^{(p)} \in [-1, 0], \forall \delta\). The coefficients of the three Dirichlet families are matched with \(\varepsilon^{(p)} = \frac{1}{2}(1 - 2 \xi_0 - \frac{\xi_0}{1 - e^{2\delta}})\); these two first schemes are not parametrized; the LMKC refers to their third scheme which belongs to MPLI with \(K^- = 0\) and \(\dot{x} = -1\). The (anti-bounce-back) ABB (and implicit interface) correspond to MPLI with \(\delta = \frac{1}{2}\) and \(F_q = 0\); PAB = PLI(\(\delta = \frac{1}{2}\)) is the pressure scheme (see also Table XI in Ref. 40).

The Dirichlet linear one-node families

\[
\begin{array}{|c|c|c|c|}
\hline
\text{MPLI} & \varepsilon^{(p)} & \dot{x} & \beta \\
\hline
\forall \varepsilon^{(p)} & 1 + \varepsilon^{(p)} & \frac{1}{2} + \delta & -(1 + \varepsilon^{(p)}) \delta \\
\hline
\text{PLI} & \varepsilon^{(p)} & 1 + \varepsilon^{(p)} & \frac{1}{2} + \delta & -(1 + \varepsilon^{(p)}) \delta \\
\hline
\end{array}
\]

\[
\begin{align*}
\text{Li} & = \text{MR with } \gamma = \dot{\gamma} = 0.
\end{align*}
\]

The Dirichlet parabolic two-node schemes

\[
\begin{align*}
\text{KMRI} & \quad \text{SMR} \in \text{PP family} \\
\dot{x} & = -1 \\
\beta & = \frac{1}{2}(1 + \dot{\delta}) \\
\dot{\beta} & = \frac{1}{4}(4 + \varepsilon^{(p)}(2 - \dot{\delta}^2 + 2\dot{\Delta}\lambda)) \\
\gamma & = \frac{1}{4}(\varepsilon^{(p)} \delta(\lambda + 2\dot{\Delta}\lambda)) \\
\dot{\gamma} & = \frac{1}{4}(\varepsilon^{(p)} \delta(\lambda + 2\dot{\Delta}\lambda)) \\
\dot{F}_q & = \frac{(4 + \varepsilon^{(p)}(1 + \dot{\delta}))}{(1 + \dot{\delta})^2} \\
\lambda & = \frac{4(1 + \dot{\delta})^2}{\varepsilon^{(p)}}
\end{align*}
\]

The Dirichlet parabolic single-node ADE and flow schemes

\[
\begin{align*}
\text{PPLI} & \quad \text{IPLI} \\
\dot{x} & = 1 + \varepsilon^{(p)} \left(1 - \frac{1}{2} + \dot{\delta}\right) \\
\beta & = -(1 + \varepsilon^{(p)} \delta) \\
\dot{\beta} & = 1 - \varepsilon^{(p)} \delta \\
\gamma & = 0 \\
\dot{\gamma} & = 0 \\
\dot{F}_q & = 0 \\
\varepsilon^{(p)} & = 0 \\
\lambda & = 0 \\
w_q & = 0
\end{align*}
\]

We provide the coefficients for several linear and parabolic Dirichlet families, advective-diffusive flux schemes and diffusive-flux family. An MR family with infinite number of members is controlled by the free-tunable coefficient as, typically, the scale factor of the underlying closure relation, \(\varepsilon^{(p)}\) in Dirichlet families. The coefficients of (i) the exact steady-state MR form in Eq. (34) and (ii) the corresponding second-order closure approximate in Eq. (5), are tabulated for all schemes. The mixed (Robin) schemes can be built as the linear combinations of the Dirichlet and diffusive-flux MR following. All provided MR schemes support the bulk parametrization of the ADE solutions by the grid Peclet number and free collision product \(\Lambda\) using TRT. When the MR coefficients depend upon \(\Lambda\), they should be computed with the free-tunable collision rate of the symmetric modes in TRT(1) \(\cup\) MRT(1) collision operators, which are sufficient for isotropic and anisotropic diagonal tensors. Accordingly, \(\Lambda = \Lambda^+ \Lambda^-\) is defined in TRT or TRT(1) \(\cup\) MRT(1) isotropic collisions, where \(\Lambda^-\) corresponds to the common rate of the discrete-velocity eigenvectors. In the
TABLE XIII. Equations (34) and (35) are specified for Dirichlet schemes from Tables X-XII.

Exact steady-state form in Eqs. (34) and (35)

<table>
<thead>
<tr>
<th>MPLI</th>
<th>PLI</th>
<th>PPLI</th>
<th>KMR1</th>
<th>PP</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_1/\varphi^{(p)}$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$m_3/\varphi^{(p)}$</td>
<td>$-\Lambda$</td>
<td>0</td>
<td>$-\frac{1}{2}\delta^2$</td>
<td>$\frac{1}{2}\delta^2$</td>
</tr>
<tr>
<td>$m_5/\varphi^{(p)}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$\frac{1}{2}\delta^2$</td>
</tr>
<tr>
<td>$m_7/\varphi^{(p)}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$\frac{1}{2}\delta^2$</td>
</tr>
<tr>
<td>$m_9/\varphi^{(p)}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$-\frac{1}{2}\delta^2$</td>
</tr>
</tbody>
</table>

TABLE XIV. The coefficients of the approximate closure relation in Eq. (5) with the Dirichlet schemes from Table XIII. The ABB and implicit interface correspond to MPLI with $\delta = \frac{1}{2}$; PAB = PLI($\delta = 1$) is the pressure scheme. 30

Directional closure relation in Eq. (5)

<table>
<thead>
<tr>
<th>Eq. (5)</th>
<th>MPLI</th>
<th>PLI</th>
<th>PPLI</th>
<th>KMR1</th>
<th>PP</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varphi^{(p)}/\varphi^{(p)}$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$\varphi^{(p)}/\varphi^{(p)}$</td>
<td>$\delta$</td>
<td>$\delta$</td>
<td>$\delta$</td>
<td>$\delta$</td>
<td></td>
</tr>
<tr>
<td>$\varphi^{(p)}/\varphi^{(p)}$</td>
<td>$\Lambda$</td>
<td>0</td>
<td>$\frac{1}{2}\delta^2$</td>
<td>$\frac{1}{2}\delta^2$</td>
<td></td>
</tr>
<tr>
<td>$\varphi^{(p)}/\varphi^{(p)}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$\varphi^{(p)}/\varphi^{(p)}$</td>
<td>$-\Lambda^+$</td>
<td>0</td>
<td>$\frac{1}{2}\delta^2$</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$\varphi^{(p)}/\varphi^{(p)}$</td>
<td>$-\Lambda^+$</td>
<td>$-\Lambda^+$</td>
<td>$-\Lambda^+$</td>
<td>$-\Lambda^+$</td>
<td></td>
</tr>
</tbody>
</table>

TABLE XV. The single-node FLI and two-node FMR advective-diffusive flux families; $w_0$ obeys Eq. (22a), FLI : $\{\hat{x}, \hat{\beta}, \hat{\gamma}\} \in [-1, 1]$; FMR : $\{\hat{x}, \hat{\beta}, \hat{\gamma}\} \in [-1, 1]$ when $\Lambda \in [0, \frac{3}{4}]$, $\frac{1}{2}\delta$. The advective-diffusive flux schemes

<table>
<thead>
<tr>
<th>FLI</th>
<th>FMR</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\hat{x}$</td>
<td>$1$</td>
</tr>
<tr>
<td>$\hat{\beta}$</td>
<td>$\frac{1 - 2\delta}{1 + 2\delta}$</td>
</tr>
<tr>
<td>$\hat{\gamma}$</td>
<td>$-\hat{\beta}$</td>
</tr>
</tbody>
</table>

TABLE XVI. The diffusive-flux DFLI family preserves $w_0(r_0)$ with Eq. (22b); the DFLI reduces to back-sided $\hat{n}_q$—extrapolation in 1D, Eq. (73). The SFLI has several heuristic sub-domains $\{\hat{x}, \hat{\beta}, \hat{\gamma}\} \in [-1, 1]$, they include: $(\Lambda > 3\delta)$ $(\Lambda < \frac{1}{4})$; the SFLI is able to adjust $\hat{K}$ to $[-1, 1]$. The AFLI is more restrictive. We apply SFLI and refer to it as DFI because steady-state solution are the same with any DFLI member.

<table>
<thead>
<tr>
<th>FLI</th>
<th>FMR</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\hat{K} = -K</td>
<td>_{AFLI}$</td>
</tr>
</tbody>
</table>

TABLE XVII. The single-node FLI and two-node FMR advective-diffusive flux families, $w_0$ is given there, and diffusive-flux family DFLI from Table XVI [s' is free-tunable]. The exact steady-state form in Eqs.(34)-(35)

<table>
<thead>
<tr>
<th>FLI</th>
<th>FMR</th>
<th>DFLI, $\forall \beta'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_1/(\Lambda \varphi^{(u)})$</td>
<td>0</td>
<td>$m_1/(\Lambda \varphi^{(u)})$</td>
</tr>
<tr>
<td>$m_3/\varphi^{(u)}$</td>
<td>$\delta$</td>
<td>$m_3/\varphi^{(u)}$</td>
</tr>
<tr>
<td>$m_5/(\Lambda \varphi^{(u)})$</td>
<td>0</td>
<td>$m_5/(\Lambda \varphi^{(u)})$</td>
</tr>
<tr>
<td>$m_7/\varphi^{(u)}$</td>
<td>$-2\delta$</td>
<td>$m_7/\varphi^{(u)}$</td>
</tr>
<tr>
<td>$m_9/\varphi^{(u)}$</td>
<td>1</td>
<td>$m_9/\varphi^{(u)}$</td>
</tr>
</tbody>
</table>

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The exact steady-state form in Eqs.(34)-(35)

<table>
<thead>
<tr>
<th>FLI</th>
<th>FMR</th>
<th>DFLI, $\forall \beta'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_m / z^{(u)}$</td>
<td>0</td>
<td>$\frac{1}{2} \delta^2 - \Lambda$</td>
</tr>
<tr>
<td>$m_m / (\Lambda - z^{(u)})$</td>
<td>0</td>
<td>$-\Lambda$</td>
</tr>
</tbody>
</table>

Directional closure relation in Eq. (5)

<table>
<thead>
<tr>
<th>Eq. (5)</th>
<th>FLI</th>
<th>FMR</th>
<th>DFLI($\beta'$), $\forall \beta'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha'^{(u)} / z^{(u)}$</td>
<td>1</td>
<td>1</td>
<td>$\alpha'^{(u)} = 0$</td>
</tr>
<tr>
<td>$\beta'^{(u)} / z^{(u)}$</td>
<td>$\delta$</td>
<td>$\delta$</td>
<td>$\beta'^{(u)} = 0$</td>
</tr>
<tr>
<td>$\gamma'^{(u)} / z^{(u)}$</td>
<td>$\Lambda$</td>
<td>$\frac{1}{2} \delta^2$</td>
<td>$\gamma'^{(u)} = 0$</td>
</tr>
<tr>
<td>$\alpha'^{(u)} / z^{(u)}$</td>
<td>$-\Lambda$</td>
<td>$-\Lambda$</td>
<td>$\alpha'^{(u)} = 0$</td>
</tr>
<tr>
<td>$\beta'^{(u)} / z^{(u)}$</td>
<td>$-\Lambda - \delta$</td>
<td>$-\Lambda - \delta$</td>
<td>$\beta'^{(u)} = 0$</td>
</tr>
<tr>
<td>$\gamma'^{(u)} / z^{(u)}$</td>
<td>$-\delta$</td>
<td>$-\delta$</td>
<td>$\gamma'^{(u)} = 0$</td>
</tr>
</tbody>
</table>

Hence, unlike in Eq. (19), $\det[\mathbf{B}]$ vanishes when $\bar{u}$ and $\bar{c}_q$ are orthogonal.

**Example 3:** We exemplify Eq. (17) with the velocity field from Eq. (45). For the sake of simplicity, we consider the straight stream $\bar{u} = u_t(y)\mathbf{I}$ and the weights $t^{(u)}_j = t^{(a)}_j = t_j = \{t_1, t_2\}$; since $u_t(y)$ and $A(y)$ are parabolic, Eq. (16) is expressed by Eq. (57). The weight $t_j$ is factorized and the reduced matrix $\tilde{\mathbf{B}}[6 \times 5]$ and RHS $\mathbf{R}[6]$ in Eq. (17) read with $\zeta = 2\Lambda^2 \partial \delta u_t$:

$$
\begin{align*}
\tilde{\mathbf{B}} &= \begin{pmatrix}
  u_t & u_t & -c_r \Lambda^- & -2c_r \Lambda^- & -c_r \Lambda^- \\
  u_t & -u_t & -c_r \Lambda^- & 2c_r \Lambda^- & -c_r \Lambda^- \\
  -c_r - \zeta & c_r - \zeta & -\Lambda u_t & -2\Lambda^2 u_t & -\Lambda u_t \\
  -c_r - \zeta & c_r - \zeta & \Lambda^2 u_t & -2\Lambda^2 u_t & \Lambda^2 u_t \\
  0 & -c_r \Lambda^- & 0 & 0 & 0
\end{pmatrix}
\end{align*}
$$

and

$$
\begin{align*}
\mathbf{R}[6] &= t_j^{-1} \mathbf{n}_t - t_j^{-1} \mathbf{n}_t |_{y=0}.
\end{align*}
$$

When $u_t(y)$ and $A(y)$ are constant, Eq. (B4b) vanishes. Equations (B3) and (B4) correspond to an ensemble of six components $\hat{n}_{t}^{(a)}$ in Eq. (19b). The two square $[5 \times 5]$ sub-systems $\mathbf{B}_y[5] = \mathbf{R}$ in Eq. (17), referred to as N-MR1 and N-MR2 in Table III, only differ for the two last lines, corresponding to $\hat{n}_{t}^{(a)} (q = 1)$ or $\hat{n}_{t}^{(a)} (q = 2)$, respectively, in Eqs. (B3) and (B4); the two sub-systems operate Eq. (17) with $\det[\mathbf{B}] = t_j t_j^{-1} \det[\mathbf{B}]$:

$$
\begin{align*}
\det[\mathbf{B}] &= 8c_r^{2} \Lambda^{-2} (c_r^{2} \Lambda^{-2} - 2c_r^{2} \Lambda (2(\partial \delta u_t^{2}) + u_t^2))
\end{align*}
$$

**Example 4:** The A-LSOB algorithm The steady-state A-LSOB formulation is resumed in Sec. III E. The Taylor schemes given in Eq. (12) prescribe one closure equation for the wall-normal direction traced from the boundary node $\tilde{n}_q$. Additionally, the $N - 1$ “expansions” are prescribed with Eq. (40) for the given $N_0$ cut links $q \in Q_{0}$, where $\hat{n}_{t}^{(a)} \odot$ obeys Eq. (16) and the five derivatives $\mathbf{Y}[5]$ are expressed linearly with Eq. (17). Let us exemplify (i) the “expansion” subset $Q$, in Eq. (40) and (ii), the “reconstruction” subset $Q_t$ in Eq. (17) assuming that $N_0 \leq 4$. Optionally, we set $Q_t \subset Q_0$.
and, when possible, prescribe $Q_c \cap Q_e = \emptyset$. Prior, we preselect the type of $\hat{n}_{rec}$, e.g., $\hat{n}_{rec} = \{\hat{n}_q^+\}$ or $\hat{n}_{rec} = \{\hat{n}_y^+\}$, then $Q_c$ is described with Eq. (19) or Eq. (B2), respectively. We prescribe Eq. (40) for the two components $\hat{n}_{rec}^{(2)}$ with the first link in $Q_c$ when $N_b = 1 \geq 2$, and then either $\hat{n}_{rec}^{(2)}$ if $\hat{n}_{rec} = \{\hat{n}_q^+\}$ or $\hat{n}_{rec}^{(2)}$ if $\hat{n}_{rec} = \{\hat{n}_y^+\}$ for the second link in $Q_c$ when $N_b = 1 \geq 3$. This last rule also applies if $N_b = 1 \geq 1$ and $Q_e$ prescribes only one equation. We operate with $q_{1c}, q_{2c}, q_{3c}$ for the links $c_q = \{(0, 0), (0, 1), (1, 1), (1, 1), (0, 1)\}$. We preselect the reconstruction default type $r$ – default. $Q_y$ and $Q_c(r_b)$ are optionally set as

1. If $N_b = 1$ then $r$ – default applies, $Q_c = \emptyset$ because $N_b = 1 \geq 0$, done is 1.
2. If $Q_c = \{q_1\},$ and $|\{c_q \cdot \hat{T}_q\}| > |\{c_q \cdot \hat{T}_c\}|$, then $Q_c = \{q_1\}$ and $Q_c = \{q_2, q_1, q_1\}$, else $Q_c = \{q_1\}$ and $Q_c = \{q_2, q_1, q_1\}$; done is 1.
3. If $Q_c = \{q_1, q_2, q_3\},$ then $Q_c = \{q_1, q_2, q_3\}$, i.e., $c_q$ in Eq. (19b) if $\hat{n}_{rec} = \{\hat{n}_q^+\}$ or IVb in Eq. (B2b) if $\hat{n}_{rec} = \{\hat{n}_y^+\}$; done is 1.
4. If $Q_c = \{q_1, q_2, q_3\},$ then $Q_c = \{q_1, q_2, q_3\}$, i.e., $c_q$ in Eq. (19b) if $\hat{n}_{rec} = \{\hat{n}_q^+\}$ or IVa in Eq. (B2b) if $\hat{n}_{rec} = \{\hat{n}_y^+\}$; done is 1.
5. If done is 0, $q_5 \in Q_b$ and $|\{c_q \cdot \hat{T}_c\}| > |\{c_q \cdot \hat{T}_c\}|$, then
   (a) If $N_b = 2$ or $N_b = 3$, then $Q_c = q_5$ for $n_{rec} = \{q_5\},$ $Q_c = \{q_1, q_5, q_3\}$, i.e., $c_q$ in Eq. (19b) if $\hat{n}_{rec} = \{\hat{n}_y^+\}$ or IVb in Eq. (B2b) if $\hat{n}_{rec} = \{\hat{n}_y^+\}$; done is 1.
   (b) If $N_b = 4$, then $Q_c = \{q_1, q_5, q_3\}$, $Q_c = \{q_1, q_5, q_3\}$; done is 1.
6. If done is 0, $q_5 \in Q_b$ and $|\{c_q \cdot \hat{T}_c\}| > |\{c_q \cdot \hat{T}_c\}|$, then the Step 5 exchanges $q_3$ and $q_4$.

In our examples, $r$-default is rectangular with Eq. (20) (T-PP) and T-DFLI apply the square reconstruction except when $N_b = 1$ (step 1); T-PP, and T-DFLI, apply Eq. (20) in all nodes but $Q_c$ is set according to the above algorithm. Let us exemplify the straight horizontal wall: $N_b = 3$, $Q_c = \{q_1, q_2, q_3\}$, then $Q_c = \{q_1, q_2, q_3\}$ according to Step 3. Equation (40) prescribes two “expansions” $\hat{n}_{rec}^{(2)}$, and reconstruction is performed using subset IIa in Eq. (19b) when $\hat{n}_{rec} = \{\hat{n}_y^+\}$, or subset IVa in Eq. (B2b) when $\hat{n}_{rec} = \{\hat{n}_y^+\}$.

**APPENDIX C: EXACT STRAIGHT QUARTIC SOLUTIONS DUE TO CORRECTIVE FLUX**

We prescribe $A_c^{(\alpha)} = \frac{[c_q \cdot \hat{T}_c]}{[c_q \cdot \hat{T}_q]}$ from Eq. (52) and consider the exact quartic solution from Eqs. (48a) and (48b) with an impermeable horizontal boundary. Example 1a derives Eq. (61a) where FLLI matches this solution exactly with the help of the corrective flux $\Phi_b = \partial \chi$ from Eq. (32); BB [FLLI with $\delta = \frac{1}{2}$] reduces this solution to Eq. (60b). Examples 2 and 3 demonstrate that FLLI, which is FLII with the normal-source correction from Eq. (24b) and the Taylor scheme T-DFLI, are exact with the same solution $|\Phi_b|$ reproduced in Eq. (62). Example4 generalizes these solutions for the MR flux schemes, like FLLI, FMR, or T-DFLI. In these derivations, $\hat{I}_q = \hat{I}_y$, the boundary nodes are $y_b = \delta_y$ (bottom) and $y_b = h - \delta_y$ (top), and the prescribed corrective flux reads with $\hat{I}_q = \hat{I}_y$, as

$$-\hat{I}_q \partial_y P_{y = h} = \hat{I}_y \partial_y \chi_{\delta_y} = -\hat{I}_y \partial_y \chi_{\delta_y}.$$  

(C1)

Equation (C1) reduces to Eq. (32) when $\delta_T = \delta_y = \delta$. Solution $P(y)$ is the same with $d2q5$ and $d2q6$ in the straight system; $d2q5$ satisfies Eq. (28) with

$$\hat{n}_q^+(y) = t_q \hat{M}(y) \hat{q}^2 \hat{y} = -t_q \hat{M}(y) \hat{q}^2 \hat{y}$$

(C2a)

$$\hat{q}^2 \hat{y} = -t_q \hat{M}(y) \hat{q}^2 \hat{y}$$

(C2b)

In this section, $\partial_T \Phi_b(y)$ denotes the exact derivatives on the quartic solution from Eq. (46). Equation (15c) gives, by replacing the central-difference $\Delta_u$ with its exact Taylor expression and using Eq. (C2b):

$$\Lambda^\top \hat{n}_y^+ = t_q \hat{M}(y) \hat{q}^2 \hat{y} + \Lambda^\top \hat{M}(y) \hat{q}^2 \hat{y}$$

(C3)

**Example 1a:** We apply FLII with the corrective flux from Eq. (C1). The exact closure from Eq. (34) reads with $c_q = 0$ on the vertical cut link $c_y = \{y_b = h - \delta_T\}$ and $c_y = \{-1 \geq \delta_y\}$. We substitute there $m_1 / \chi^{(u)} = \delta$ and $m_1 / \chi^{(u)} = \Lambda^\top$ from Table XVII, and the closure condition becomes

$$-\Lambda^\top \hat{n}_y^+ + \partial_T \hat{n}_y^+ = -t_q \partial \chi \partial \hat{y} = t_q \hat{M}(y) \hat{q}^2 \hat{y}$$

(C4)

Equation (C4) reads plugging there Eqs. (C2a) and (C3),

$$-\hat{I}_q \partial y \hat{M}(y) \hat{q}^2 \hat{y} - \hat{I}_y \partial T \hat{q}^2 \hat{y}$$

(C5)

Equation (C5) presents the fourth-order accurate Taylor closure relation provided that

$$\chi(\delta) \hat{q}^2 \hat{y} = -\left(\frac{1}{2} \delta^2 \hat{q}^2 \hat{y} \hat{p} + \frac{1}{6} \delta^3 \hat{q}^2 \hat{y} \hat{p}^2 - \delta T \right) \hat{y}$$

(C6)

Plugging the exact derivatives from Eq. (46) and Eq. (C3) for $\delta_T$, Eq. (C6) gives when $\delta = \frac{1}{2}$.

**BB** : $\chi(\delta = \frac{1}{2}) \hat{q}^2 \hat{y} = \psi_1^2 \hat{q}^2 \hat{y} \hat{p} + \psi_2^2 \hat{q}^2 \hat{y} \hat{p} - \psi_3^2 \hat{q}^2 \hat{y} \hat{p} - \delta T \hat{y}$

(C7)

then $\chi(\delta = \frac{1}{2}) \hat{q}^2 \hat{y} = \psi_1^2 \hat{q}^2 \hat{y} \hat{p} + \psi_2^2 \hat{q}^2 \hat{y} \hat{p} - \psi_3^2 \hat{q}^2 \hat{y} \hat{p} - \delta T \hat{y}$

(C7)

When $\delta_T = \delta_y = \delta$ and $\delta_T = \{\delta, \delta_y = \delta\}$, Eq. (C5) gives

**FLII** : $\chi(\delta) \hat{q}^2 \hat{y} = \frac{\psi_1^2 \hat{q}^2 \hat{y} \hat{p}}{12} + \frac{\psi_2^2 \hat{q}^2 \hat{y} \hat{p}^2}{12} - \frac{\psi_3^2 \hat{q}^2 \hat{y} \hat{p}^3}{12}$

(C8)

Equation (C8) reduces to Eq. (C7) when $\delta = \frac{1}{2}$. It is confirmed that the numerical solution with Eq. (32) reproduces the symmetric
solution from Eq. (C8) exactly. When $\delta_y \neq \delta_z$, this solution is not symmetric and it cannot be exactly reproduced with Eq. (32); it is then validated by prescribing Eq. (C1) for the boundary flux and reproducing the exact quartic profile.

**Example 2b:** Curiously, BB is able to reproduce the exact quartic solution for any symmetric walls thanks to $\Phi_y$. The derivation follows the same lines, replacing $\delta T$ from Eq. (C3) by $\delta T + \left( \frac{1}{2} - \delta \right) \partial_y^2 Pe_q$. Equation (C8) then becomes

$$
\chi(\delta) = \frac{Pe}{2 \delta^2} \left( \frac{1 + (1 - 2 \delta)}{h} \right)^2 (2 \delta - 1) \delta + (1 - 2 \delta) h.
$$

\textbf{Equation (C9)}

**Example 2:** When the MR is complemented with the normal mass-source correction $\left[ h_{1}^{d} \right] = 1$ in Eq. (21), the LHS of the closure relation in Eq. (C4) gets an additional term $\epsilon^{\text{(c)}} = \text{CL}_{\text{num}}(\lambda^+; h, 0) / \chi^{\text{(o)}}$ from Eq. (24b). It reads with $\beta^{(\text{c})} / \chi^{(\text{c})} = -\lambda^+ / \chi^{(\text{c})}$ from Table XVIII:

$$
\epsilon^{\text{(c)}} = t_q \lambda^+ \epsilon_q \left( \epsilon_q \partial_y P + \partial_{\delta} \partial_y P \right)
+ \partial_{\delta} \partial_y^2 P
+ \partial_{\delta} \partial_y P

\text{and then}

\text{(see Table XVIII). Equation (C10) gives then the same}

**Example 3:** We show that Eq. (C11) also satisfies the Taylor scheme T-DFLI provided that Eq. (57) applies on the vertical cut link, as for example with T-DFLI, or T-DFLI, using the notations from Table III and example 4 from Sec. B. We then equate Eq. (57) to $\hat{a}_{y}^{\text{ex}}$ and $\hat{a}_{x}^{\text{ex}}$ from Eqs. (C3) and (C2a), respectively; this gives

$$
\partial_y P = \partial_y P
+ \left( \chi^{(\text{c})} - \frac{1}{12} \partial_y^2 P \right)
+ \partial_{\delta} \partial_y P
+ \epsilon_q \left( \partial_{\delta} \partial_y P \right).
$$

\textbf{Equation (C12a)}

Equation (12b) becomes modified by the corrective flux from Eq. (C1) and it reads

$$
-\partial_{\delta} \partial_y P
+ \partial_{\delta} \partial_y P
+ \partial_{\delta} \partial_y P
+ \epsilon_q \left( \partial_{\delta} \partial_y P \right)

\text{Plugging Eq. (C12) into Eq. (C13), it reproduces Eq. (C11). Therefore, the T-DFLI is equivalent to FMM on these solutions. In contrast, T-DFLI produces the same solution for $\partial_{\delta} \partial_y P$ (num) and differs for $\partial_{\delta} \partial_y P$ (num) and then $\chi^{(\text{y})}$.

**Example 4:** We extend now Eqs. (C8) and (C11) to other MR flux schemes, as FMR and DFLI, prescribing Eq. (34) on the vertical cut link. The corrective flux presents the difference between the MR closure relation and the fourth-order accurate Neumann condition, as

$$
\left[ M_{y} + X_{y} - \delta^{(\text{c})} \right] - T^{(4)} \chi^{(\text{y})} = -\partial_{\delta} \partial_y P
+ \partial_{\delta} \partial_y P
+ \epsilon_q \left( \partial_{\delta} \partial_y P \right).
$$

**Equation (C14)**

The term $M_{y} + X_{y}$ is expressed with $M_{y} = \{ m \}$ in FLI/FMR and $W_{y} = \beta$ in T-DFLI [cf. Eq. (39)]; these coefficients are pre-computed in Table XVIII. The components $X_{y}[8]$ are expressed exactly: (i) $\epsilon_q$ in Eq. (46); (ii) $\epsilon_q = 0$; (iii) $\hat{a}_{y}^{\text{ex}}(y)$ with Eq. (C2a) and (iv), $\hat{a}_{x}^{\text{ex}}(y)$ with Eq. (C3). It is confirmed that FLI reduces Eq. (C14) to Eq. (C8); additionally, FMR and DFLI substitute the exact solution components in the neighbor node $f_{y} = q_{b}$. Equation (61) resumes their solutions with respect to FLI. Next, FMM, FMR, and DFLI apply the normal mass-source correction $\delta^{(\text{c})} = \text{CL}_{\text{num}}(\lambda^+; h, 0)$ from Eq. (24b) which reads with the same coefficients in three schemes: $\epsilon^{(\text{c})} / \chi^{(\text{c})} = -\lambda^+ / \chi^{(\text{c})}$ and $\epsilon^{(\text{c})} / \chi^{(\text{c})} = -\lambda^+ / \chi^{(\text{c})}$ (see Table XVIII). Equation (C10) gives then the same (negative value) correction $\delta^{(\text{c})}$, expressed with $\lambda^{(\text{ex})}$ in Eq. (62), and then $\chi$ in Eq. (C11).

**APPENDIX D: MASS-BALANCE OVER A GRID-SHIFTED STRAIGHT INTERFACE**

We construct FLI/FMR and DFLI solutions for $M_{a}$ from Eq. (28) in the straight grid-shifted layers subject to piece-wise constant mass-source and either interface-parallel or perpendicular velocity field. These results are resumed in Sec. VIA 2.

1. The advective-diffusive flux FLI/FMR

The macroscopic solution in the straight geometry is weight-independent, and it can be examined with the d2q5 exact recurrence solution from Eqs. (66) and (67). It can then be demonstrated that FLI and FMR have the same interface closure given in Eq. (76b). We examine their mass-balance with FLI, without construction of its symbolic solution; recall, FLI reduces to BB (implicit interface, or do nothing algorithm) on the mid-grid interface. Assume that the “internal” and “periodic” interface nodes are $\{ y, y_{1} = y_{1} + 1 \}$ and $\{ y_{1}, y_{1} = y_{1} + 1 \}$, respectively. The two flux continuity equations (37b) [without correction $\delta^{(\text{c})}$] read then with $\epsilon_{q} = 1$ by inserting FMM coefficients from Table XVIII:

$$
\Phi_{q}^{(\text{f})} = 0, \quad \text{with}
\Phi_{q}^{(\text{f})} = \left[ \epsilon_q + \left( \frac{1}{2} + \delta^{(\text{f})} \right) \hat{a}_{q}^{\text{ex}} - \lambda^{(\text{-ex})} \right]_{y_{1}}^{(1)}
$$

$$
- \epsilon_q - \left( \frac{1}{2} + \delta^{(\text{f})} \right) \hat{a}_{q}^{\text{ex}} - \lambda^{(\text{-ex})} \hat{a}_{q}^{\text{ex}}_{y_{1} + 1}
$$

$$
\Phi_{q}^{(\text{f})} = 0, \quad \text{with}
\Phi_{q}^{(\text{f})} = \left[ \epsilon_q + \left( \frac{1}{2} + \delta^{(\text{f})} \right) \hat{a}_{q}^{\text{ex}} - \lambda^{(\text{-ex})} \right]_{y_{1}}^{(2)}
$$

$$
- \epsilon_q - \left( \frac{1}{2} + \delta^{(\text{f})} \right) \hat{a}_{q}^{\text{ex}} - \lambda^{(\text{-ex})} \hat{a}_{q}^{\text{ex}}_{y_{1} + 1}
$$

The BB reads with $\delta^{(\text{f})} = 0$ in Eq. (D1). We consider the total flux $\partial_{\delta} \partial_y P$ across the domain given by the sum of Eqs. (D1a) and (D1b), $\partial_{\delta} \partial_y P = \Phi_{q}^{(\text{f})} + \Phi_{q}^{(\text{p})}$, and subtract from it the implicit-interface (BB) flux $\partial_{\delta} \partial_y P = \Phi_{q}^{(\text{f})} (\delta^{(\text{f})} = 0) + \Phi_{q}^{(\text{p})} (\delta^{(\text{p})} = 0) = 0$, which is zero due to the bulk flux discretization in Eq. (26b), provided that $\chi^{(\text{num})}$ is prescribed. This gives:
\[ \delta \Phi_{FLI} = \Phi_{FLI} - \Phi_{RB} = (\Phi_q^{(i)}(\delta^{(i)} - \Phi_q^{(i)}(\delta^{(i)} = 0)) + (\Phi_q^{(p)}(\delta^{(p)}) - \Phi_q^{(p)}(\delta^{(p)} = 0)). \] (D2)

Then,
\[ \delta \Phi_{FLI} = (n_q^{(1)} - n_q^{(2)})(\delta^{(i)} - \delta^{(p)}) = t^{(m)}_n (\mathcal{M}_1 - \mathcal{M}_2)(\delta^{(i)} - \delta^{(p)}), \] if \( n_q^+ = t^{(m)}_n \mathcal{M}_2 \mathcal{C}_q^m. \) (D3)

We equate Eq. (D3) to \(-n_q^{(m)} M_0 H\) and get \( M_0 \) from Eq. (71), which provides the solvability condition. This tells us that FLI/FMR conserves the population mass \([M_0 = 0]\) with \( \mathcal{M}(\mathcal{Y}^{(a)}) \) only when the two-layers are uniformly shifted from the midway interface position \([\delta^{(i)} = \delta^{(p)}]\). Otherwise, when using the exact definition \( M_0(\mathcal{Y}^{(a)}) \) in Eq. (68), \( M_0 = 0 \) with any interface position. These two findings are in agreement with the symbolic and numerical solutions, and they are resumed by Eqs. (70) and (71). These solutions are valid in the heterogeneous series subject to the plug flow \( \bar{u} = u_0 \bar{I}_0 \), but also in the stratified parabolic solutions with \( \bar{u} = u_0 \bar{I}_0 \), because \( \mathcal{M}(\mathcal{Y}) \) is piece-wise constant and Eq. (66) is valid in these two systems. We note that the total flux \( \Phi_q^{(i)} + \Phi_q^{(p)} \) remains the same in the presence of the “physical” interface jump in series, giving \( \sigma^{(o)} = 1, \eta^{(m)} = |(\mathcal{Z}_r)| \bar{I}_y \cdot \bar{I}_y \) in Eq. (36) (see next section).

2. The diffusive-flux FLI MR

We build the grid-shifted straight interface-flux mass-balance in Eq. (37b) [without correction \( \delta^{(i)} \)] with the diffusive-flux parabolic family FLI from Tables XVI and XVII. We follow Eq. (D1), where we also include the flux jump \( \pm f_q \) on the two interfaces, with \( f_q = t^{(m)}_n \mathcal{M}_2(\Phi_q - \Phi_{RB}) \) in series. We decompose \( \Phi_q \) in Eq. (D1) on the local and neighbor components \( \Phi_{loc} \) and \( \Phi_{qb} \), respectively, and it reads giving \( \Phi_{loc} = 1 \):
\[ \Phi_q^{(i)} = 0, \quad \Phi_q^{(p)} = \Phi_{loc} + \Phi_{qb} - f_q, \] (40)
\[ \Phi_{loc} = \frac{1}{2} \left( a_1 x_1 + a_2 x_2 \right), \] (41)
\[ \Phi_{qb} = \frac{1}{2} \left( A_1 X_1 + A_2 X_2 + A_3 \hat{n}_q^1 + A_4 \hat{n}_q^2 \right), \] (42)
\[ x_1 = c_q^1 - A^{(1)} \hat{n}_q^1 \hat{n}_q^1, \quad x_2 = c_q^1 - A^{(2)} \hat{n}_q^2 \hat{n}_q^2, \]
\[ X_1 = c_q^1 - A^{(3)} \hat{n}_q^1 \hat{n}_q^1, \quad X_2 = c_q^1 - A^{(4)} \hat{n}_q^2 \hat{n}_q^2, \]
where \( \{a, A\} \) are set by the MR coefficients from Table XVII. The idea is to express the neighbor solution \( c_q^{(1)} \) and \( c_q^{(2)} \) in the in-phase bulk relation in Eq. (27), as
\[ e_q^{(i)} = \frac{1}{2} \hat{n}_q - A^{(i)} \hat{n}_q \hat{n}_q, \quad e_q^{(i)} = e_q^{(i)} - \frac{1}{2} \hat{n}_q - A^{(i)} \hat{n}_q \hat{n}_q \] (43)
\[ e_q^{(i)} + e_q^{(i)} = e_q^{(i)} + e_q^{(i)} = e_q^{(i)} + e_q^{(i)} = e_q^{(i)} + e_q^{(i)}. \] (43)

Then, we first substitute the FMR coefficients and confirm that \( \Phi_q^{(i)} \) reduces to its FLI solution, given that \( \hat{n}_q^{(1)} \) is layer-wise constant according to Eq. (D3). In turn, DFLI holds

\[ \Phi_q^{(i)} = 0, \quad \Phi_q^{(i)} = \Phi_q^{(i)} - \Phi_q^{(1)} - f_q, \] (44)
\[ \Phi_q^{(2)} = -\Lambda^{-1} \hat{n}_q - (\delta^{(1)} + \delta^{(1)}) \hat{n}_q^{(1)} - \frac{1}{2} \delta^{(1)}, \] (45)
\[ \Phi_q^{(2)} = -\Lambda^{-1} \hat{n}_q - (\delta^{(2)} + \delta^{(2)}) \hat{n}_q^{(2)} - \frac{1}{2} \delta^{(2)}, \] (46)
\[ \delta \hat{n}_q^{(1)} \hat{n}_q^{(1)} = \hat{n}_q^{(1)} \hat{n}_q^{(1)} - \hat{n}_q^{(1)} \hat{n}_q^{(1)} - \delta^{(1)}, \] (47)
\[ \delta \hat{n}_q^{(2)} \hat{n}_q^{(2)} = \hat{n}_q^{(2)} \hat{n}_q^{(2)} - \hat{n}_q^{(2)} \hat{n}_q^{(2)} - \delta^{(2)}. \] (48)

Obviously, Eq. (D6) presents the back-sided in-phase extrapolations of the diffusive-flux non-equilibrium component \( \Phi_q^{(i)} = -\Lambda^{(i)} \hat{n}_q^{(i)}. \) Straightforwardly, the DFLI flux condition shares the same property on the periodic interface \( y_1 = y_2 + 1, \)
\[ \Phi_q^{(p)} = 0, \quad \Phi_q^{(p)} = \Phi_q^{(2)} - \Phi_q^{(1)} + f_q, \] (49)
\[ \Phi_q^{(2)} = -\Lambda^{-1} \hat{n}_q - (\delta^{(1)} + \delta^{(1)}) \hat{n}_q^{(1)} - \frac{1}{2} \delta^{(1)}, \] (50)
\[ \delta \hat{n}_q^{(1)} \hat{n}_q^{(1)} = \hat{n}_q^{(1)} \hat{n}_q^{(1)} - \hat{n}_q^{(1)} \hat{n}_q^{(1)} - \delta^{(1)}, \] (51)
\[ \Phi_q^{(1)} = -\Lambda^{-1} \hat{n}_q - (\delta^{(2)} + \delta^{(2)}) \hat{n}_q^{(2)} - \frac{1}{2} \delta^{(2)}, \] (52)
\[ \delta \hat{n}_q^{(2)} \hat{n}_q^{(2)} = \hat{n}_q^{(2)} \hat{n}_q^{(2)} - \hat{n}_q^{(2)} \hat{n}_q^{(2)} - \delta^{(2)}. \] (53)

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

REFERENCES


