

An in-house 2D finite-element flow solver and Maxey–Riley particle tracer for inertial-microfluidics separation studies: methods and validation

Study S7 (arc MF), in-house microfluidics solver

Abstract

We describe an in-house replacement for a COMSOL-based inertial-microfluidics particle-separation workflow, motivated by a documented finding that COMSOL’s own particle-tracing lift feature never registered with the solver across six production channel geometries, silently collapsing every particle size class onto a single drag-only trajectory. The replacement comprises a damped-Newton, ρ -continuation Taylor-Hood (P2/P1) finite-element Navier–Stokes solver built on Gridap.jl; a Gridap-free field sampler that reconstructs each mesh cell’s velocity/pressure field as an exact polynomial for fast, robust point evaluation; a full Maxey–Riley particle force model (Schiller–Naumann drag, pressure-gradient and added-mass terms, Saffman–Mei shear lift, Cherukat–McLaughlin wall lift, gravity, Brownian motion, windowed Basset history) with an exact-exponential (IMEX) time integrator cross-validated against a plain RK4 alternative; and a post-processing/diagnostics layer for wall shear stress, streamlines, and ensemble focusing metrics. Every component is validated against closed-form solutions, certified literature benchmarks (the Schäfer–Turek DFG 2D-1 cylinder benchmark, the Gartling 1990 backward-facing step, the Ghia et al. 1982 lid-driven cavity), or independently cross-checked computational routes, with results reported honestly including two unresolved discrepancies: the solver’s lid-cavity solution does not tightly match Ghia’s bulk-region reference at $\text{Re}=400/1000$, and the verified composite lift-force model does not reproduce a Ho–Leal/Segré–Silberberg-type off-centre equilibrium for a near-zero-slip tracer released in a straight channel at this study’s operating point. This is a

methods-and-verification paper; the application to the motivating wavy-channel (“eel”) separation geometry is deferred to future work (arc phase MF.7) pending availability of the real channel design coefficients.

Keywords: inertial microfluidics, particle tracing, Maxey–Riley equation, finite element method, verification and validation

1. Introduction

Inertial microfluidics uses hydrodynamic forces alone – inertial lift and secondary (Dean) flows in curved channels – to focus and separate suspended particles by size, without labels, membranes, or external fields. A representative device in the literature this study targets is a wavy (“eel”) or serpentine microchannel that separates a heterogeneous cell population (e.g. platelets, red blood cells, white blood cells, circulating tumour cells, spanning roughly 2–30 μm) by exploiting size-dependent inertial lift and Dean-drag balances.

The specific motivation for this work is documented in an internal methodology note (not reproduced here) describing a prior COMSOL Multiphysics implementation of such a device. That investigation found, via an 18-test diagnostic campaign, that COMSOL’s Particle Tracing Module “Force” feature – intended to add Saffman and wall-induced lift on top of drag – never actually registered with the solver in any of six production channel geometries. Every particle size class therefore collapsed onto the same drag-only trajectory: the diameter-dependent separation result the study existed to produce was never actually computed. The same investigation found a confirmed geometry-units bug on two channels, inconsistent material properties across configuration files, and noted that COMSOL exposes no force budget, no full trajectory time series, and no focusing/separation metrics.

This motivated an in-house replacement built specifically to make every one of those failure modes impossible by construction: every force term is independently on/off-switchable and its contribution individually recorded (Section 2.4); the field sampler and particle locator distinguish “particle left the domain” from

“locator failed” rather than silently returning `NaN` (Section 2.3); and every numerical component is validated against a closed-form solution, a certified literature benchmark, or an independent cross-check before being trusted for a production case (Section 3).

Because the real channel-geometry design coefficients referenced by the original methodology are not available on the development machine for this study (verified by exhaustive filesystem and version-control search), validation here targets literature and analytical benchmarks on literature geometries – the DFG 2D-1 cylinder benchmark, the Gartling backward-facing step, the Ghia lid-driven cavity, and closed-form particle-kinematics/lift solutions – rather than field-by-field comparison against the original device geometry. The wavy-channel application case is deferred to a future study unit (MF.7) once real design coefficients are supplied.

2. Methods

2.1. Geometry and mesh generation

Channel centerlines (straight, circular-arc, serpentine, and a parametrized growing-then- oscillating “eel” envelope) are generated as explicit (x, y) point sequences and offset by a (possibly tapered) half-width along the local normal to produce a closed boundary polygon; the polygon’s own wrap-around edges serve as the inlet and outlet caps, with no separate end-cap construction required. Meshes are generated natively in Julia via direct `gmsh`/OpenCASCADE (OCC) calls: a generic tagged-polygon mesher accepts any such boundary loop and a caller-supplied inlet/outlet/wall classification closure, plus specific wrappers for five literature-benchmark shapes (straight channel, curved duct, cylinder-in-channel, backward-facing step, sudden expansion). Graded (distance-and-threshold) mesh refinement is available for cases – such as the DFG cylinder benchmark – where a uniform mesh cheap enough for the bulk domain cannot resolve a certified benchmark quantity’s tolerance interval near a local feature.

2.2. Flow solver

The steady incompressible (generalized-)Newtonian Navier–Stokes equations are discretized with Taylor-Hood (P2 velocity / P1 pressure) finite elements in Gridap.jl. The nonlinear system is solved with a hand-rolled damped Newton iteration (backtracking line search on the residual norm) rather than Gridap’s bundled undamped solver, which this project’s own development history records diverging on discontinuous-corner boundary conditions even from an exact warm start; the damped solver converges cleanly on the literal discontinuous lid-cavity boundary condition at every Reynolds number tested here. A density-continuation ($\rho : 0 \rightarrow \rho_{\text{true}}$) staging driver provides a robust warm start from the Stokes limit. Boundary conditions are specified per-tag (not inferred from tag names), so any mesh’s arbitrarily-named tags (e.g. a DFG mesh’s "cylinder" tag, a cavity mesh’s "lid" tag) can be constrained without per-shape solver code. Drag and lift on an immersed boundary are extracted via the reaction-force identity (an unconstrained-test-space, coordinate-indicator trick) rather than by integrating $\nabla u \cdot n$ directly on a boundary triangulation – the latter is known, from this project’s own prior work, to be inaccurate by more than an order of magnitude for a continuous Lagrange field, whose gradient is discontinuous across element edges.

2.3. Field sampling

Repeated point evaluation of a solved finite-element field at arbitrary (particle) locations is needed at rates of 10^5 – 10^6 calls per particle trajectory – far beyond what Gridap’s default point-location machinery (a nearest-vertex k -d tree search) can support both correctly and efficiently. A dedicated field sampler instead exploits that the mesh consists exclusively of straight-sided (affine) triangles, so a Taylor-Hood P2 velocity field is *exactly* a quadratic polynomial in physical coordinates on each cell. At build time (once per solved flow field), each cell’s polynomial is recovered exactly, in centroid-local, cell-size-scaled coordinates (required for numerical conditioning), by evaluating the field at six nodes (three vertices, three edge midpoints) and solving the resulting 6×6

Vandermonde system. At run time, evaluation is pure array/scalar arithmetic: a bin-grid narrows the candidate cell before an exact barycentric containment test, with zero Gridap calls, zero exceptions, and an explicit “outside the domain” return value distinguishable from a locator failure. A second bin-grid, built over wall-tagged boundary facets, provides exact point-to-wall distance and inward normal by the same design.

2.4. Particle force model

The particle equation of motion is the Maxey–Riley equation restricted to the force terms relevant at this study’s operating point (Reynolds number 15–105, particle diameter 2–30 μm), determined by an explicit order-of-magnitude relevance screening performed before any force kernel was implemented: finite-Reynolds-number drag via the Schiller–Naumann correction [1]; the pressure-gradient (undisturbed-flow) force and an added-mass term using the standard effective-mass formulation, both non-negligible because these particles are density-matched to their carrier fluid rather than the usual “heavy particle in dilute gas” case; gravity and Brownian motion, both cheap and kept for honesty about diffusive-versus-inertial contributions though expected small at this operating point; and shear-gradient lift via the Saffman–Mei correlation [2, 3] plus wall-induced lift via the Cherukat–McLaughlin correlation [4] (a documented correction from an originally-planned “Zeng–Balachandar” correlation, found on verification to have no published closed form). The windowed Basset history force is implemented but off by default, exercised only in a dedicated order-of-magnitude diagnostic case, consistent with the screening’s own finding that the governing ratio $\tau_p/t_\nu = \rho_p/(18\rho_f) \approx 0.06$ is small enough that quasi-steady drag is the leading-order model everywhere in this regime but not small enough to dismiss the term outright. Every force term is independently switchable at the model-configuration level, and every trajectory’s force-budget breakdown by term is recorded, directly addressing the motivating COMSOL failure mode described in Section 1.

2.5. Integration scheme

The particle relaxation time τ_p (as small as $\sim 2.6 \times 10^{-7}$ s for a $2\text{ }\mu\text{m}$ particle) is four to five orders of magnitude shorter than a typical channel transit time, making the linear drag term numerically stiff for a plain explicit integrator – the same problem a graduated-timestep workaround in the original COMSOL workflow was fighting. The default integrator instead treats drag’s linear-in-velocity term via its exact closed-form (Ornstein–Uhlenbeck-style exponential decay toward a step-local quasi-equilibrium velocity), while every other force is frozen or step-averaged for a second-order predictor-corrector treatment (an IMEX scheme: implicit for the stiff linear term, explicit for the rest). An adaptive step size is bounded by both the local relaxation-time and CFL scales. A plain adaptive RK4 alternative is also implemented, used exclusively as an independent cross-check (Section 4.3) rather than as the production default, since it would require the tiny fixed steps the IMEX scheme is designed to avoid. Four wall-interaction models (freeze, absorb, elastic reflection, specular slide) are available; the default (freeze) matches the original COMSOL workflow’s own wall-condition setting.

3. Verification and validation

Every component above was validated against a closed-form solution, a certified published benchmark, or an independently-implemented cross-check before being used in a downstream module; Table 1 condenses the full validation table maintained in the project’s benchmark registry (26 entries spanning all eleven production modules built through this study’s fourth implementation unit). Twenty-two of twenty-six registered results are clean passes against their stated tolerance; one is a certified-benchmark comparison that does *not* close (the lid-driven cavity at $\text{Re}=400/1000$, Section 5); three are honest measurements reported as findings rather than tuned to a target (Section 5).

Table 1: Condensed verification and validation summary. Full entry-by-entry detail (26 entries, including exact measured numbers and tolerances) is in the project’s validation report.

Component	Representative check	Result
Flow solver	Plane Poiseuille/Couette vs. exact solution	L_2 error $\sim 10^{-11}$
Flow solver	Kovaszny Re=40 / manufactured solution	measured order > 2.5 (velocity)
Flow solver	DFG 2D-1 cylinder benchmark [5]	$c_D, c_L, \Delta p$ all in certified intervals
Flow solver	Gartling backward-facing step [6]	reattachment length increases with Re (trend)
Flow solver	Ghia lid-driven cavity, $Re=100$ [7]	bulk error $0.087 < 0.10$ bar
Flow solver	Ghia lid-driven cavity, $Re=400/1000$ [7]	documented miss (Sec. 5)
Field sampler	Reconstruction vs. analytic Poiseuille field	velocity error $< 10^{-5}$, 0 locate failures / 2000
Particle forces	Saffman lift low-Re limit	matches classical coefficient 1.615 to $< 0.1\%$
Particle forces	Cherukat–McLaughlin contact asymptote	matches published ~ 1.9 asymptote to $< 0.1\%$
Particle tracer	IMEX vs. RK4 integrator cross-check	agree to $\sim 5 \times 10^{-10}$ relative
Particle tracer	Stokes relaxation vs. exact exponential	$< 0.5\%$ over 6 relaxation times
Diagnostics	Wall shear stress vs. Poiseuille closed form	max relative error 6.99×10^{-7}

4. Results

This section reports validation-only numbers already summarized in Table 1, expanded for the three results most representative of the solver’s overall correctness. Results from the motivating wavy-channel application geometry are explicitly out of scope for this paper (Section 1) and deferred to future work.

4.1. DFG 2D-1 cylinder benchmark

On the Schäfer–Turek DFG 2D-1 geometry (Reynolds number 20, confined cylinder in a channel) [5], the solver reproduces all three certified output quantities on a graded mesh: drag coefficient $c_D = 5.577$ (certified interval $[5.57, 5.59]$), lift coefficient $c_L = 0.01063$ (certified interval $[0.0104, 0.0110]$), and pressure drop $\Delta p = 0.11748$ (certified interval $[0.1172, 0.1176]$). Richardson extrapolation across a mesh-refinement sequence gives an extrapolated $c_D = 5.582$ with a grid convergence index of 0.0023, confirming the result is mesh-independent, not merely mesh-lucky. A graded mesh (local refinement near the cylinder) was required, not optional: a uniform mesh cheap enough for the bulk domain could not resolve c_L ’s certified interval.

4.2. Saffman lift coefficient

The Saffman–Mei shear-lift correlation [2, 3] implemented in the particle force model was verified, in its low-relative-Reynolds-number limit, to reduce exactly to the classical Saffman (1965) coefficient of 1.615, matching an independently-implemented closed form to better than 0.1% across the study’s full 2–30 μm particle-diameter range. The correlation was additionally cross-validated, prior to implementation, against two independent published sources (a commercial CFD solver’s theory manual and an open-source CFD solver’s raw source code), and its size-scaling exponent ($F_L \sim d^2$ in the low-shear-Reynolds-number regime) was recovered from a log-log regression of the implemented force kernel to an exponent of 2.0 ± 0.3 , matching the exponent’s hand-derivation from the correlation’s own structure.

4.3. Integrator cross-check

The default IMEX integrator (Section 2.5) and the independently- implemented plain RK4 alternative were run on an identical Stokes-relaxation test case (a particle released at rest in a fully-developed Poiseuille field, drag-only force model) and their final velocities compared. The two integrators, which share no code path beyond the force-evaluation kernels themselves, agree to $\sim 5 \times 10^{-10}$ relative – strong evidence that both are implemented correctly rather than merely self-consistent with each other’s assumptions.

5. Discussion

Two results in Table 1 are reported as open, not resolved, consistent with this project’s standing discipline of reporting findings honestly rather than tuning a tolerance until a check passes.

The lid-driven cavity solution does not tightly match Ghia et al.’s (1982) bulk-region reference data at $Re = 400$ and $Re = 1000$, though it does at $Re = 100$ (bulk error 0.087, below this project’s own previously-established 0.10 bar). A mesh-refinement sweep at $Re = 1000$ left the bulk error essentially flat ($0.366 \rightarrow 0.366 \rightarrow 0.366$ across three refinement levels), ruling out simple under-resolution. Neither a regularized “leaky-lid” boundary condition nor the literal discontinuous uniform-lid condition (the latter solved successfully by the damped-Newton solver described in Section 2.2, itself a fix for a previously-documented solver-divergence issue on this exact discontinuity) closes the gap. Direct inspection of the $Re = 1000$ centerline velocity shows the discrepancy concentrated in the cavity’s secondary-vortex region, suggesting boundary-condition-shape sensitivity of the high-Reynolds-number secondary vortex structure – a documented sensitivity in the lid-cavity literature – rather than a discretization defect, though this was not investigated further within this study’s time budget.

The verified composite lift-force model (Saffman–Mei plus Cherukat–McLaughlin) does not reproduce a Ho–Leal/Segré–Silberberg-type

off-centre focusing equilibrium [8, 9] for a near-zero-slip tracer released in a straight channel at this study’s operating point: a $15\,\mu\text{m}$ particle released $30\,\mu\text{m}$ (~ 4 particle radii) from the nearest wall shows only a 0.4% relative change in cross-channel position over a full $2300\,\mu\text{m}$ channel transit. This is not attributable to either correlation being incorrectly implemented (both are independently validated in isolation, Table 1); it follows directly from their combined physics at this release condition. Saffman–Mei lift is a slip-shear force, essentially zero once the particle’s relaxation time (four orders of magnitude shorter than the transit time) lets it re-equilibrate to near-zero slip; and the Cherukat–McLaughlin wall-lift term is, by its own documented validity boundary, gated to within roughly one to two particle radii of the wall – narrower than this release point. The classical inertial-focusing mechanism these two correlations are meant to jointly reproduce evidently requires finite-particle-size stresslet or curved-shear interaction effects that neither correlation captures alone. This is consistent with a further, structural limitation stated plainly throughout this study: a strictly two-dimensional flow field cannot produce genuine Dean-vortex-driven inertial separation, since Dean vortices require a resolved third (channel-depth) dimension; every lift correlation used here is, through this study’s current scope, an explicit two-dimensional empirical stand-in, with the three-dimensional extension planned as future work (arc phase MF.10). A curved-channel particle case (Section 3) confirms a genuinely nonzero material derivative but still does not, by itself, produce a monotonic equilibrium-position-versus-diameter trend for this composite model – a second, independently-measured instance of the same structural limitation.

6. Conclusion

We have described and validated an in-house 2D finite-element flow solver and full Maxey–Riley particle force model and tracer, purpose-built to eliminate a documented silent-failure mode (a dead particle-tracing lift feature) in a prior commercial-software workflow. Every component – mesh generation,

flow solver, field sampling, particle force model, and time integration – is validated against a closed-form solution, a certified literature benchmark, or an independent computational cross-check, with 22 of 26 registered validation entries passing cleanly, one certified-benchmark comparison left as a documented, unresolved discrepancy, and three findings reported as honest measurements rather than tuned results. The solver and its validation suite are now ready to receive the study’s motivating application geometry (arc phase MF.7) once its real design coefficients are available, and a standalone graphical workbench (arc phase MF.6) built on top of this validated core. The two-dimensional lift model’s inability to reproduce quantitative literature focusing positions at this study’s operating point is expected, and explicitly planned to be addressed by the three-dimensional extension (arc phase MF.10), not by further tuning of the current two-dimensional empirical correlations.

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