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Badr Kaoui

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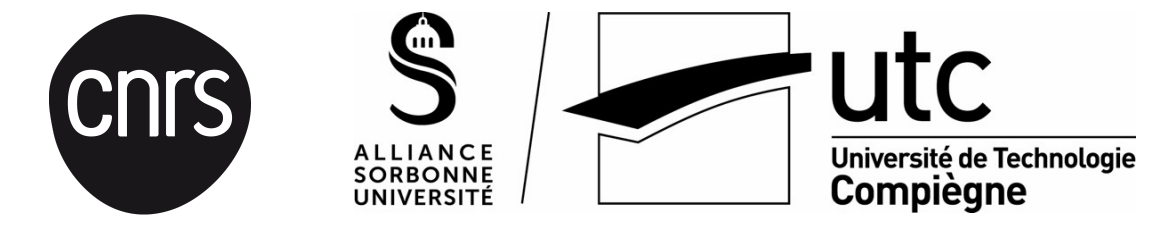
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HPC in Biomedical Engineering: Drug Release and Deformation of Microcapsules



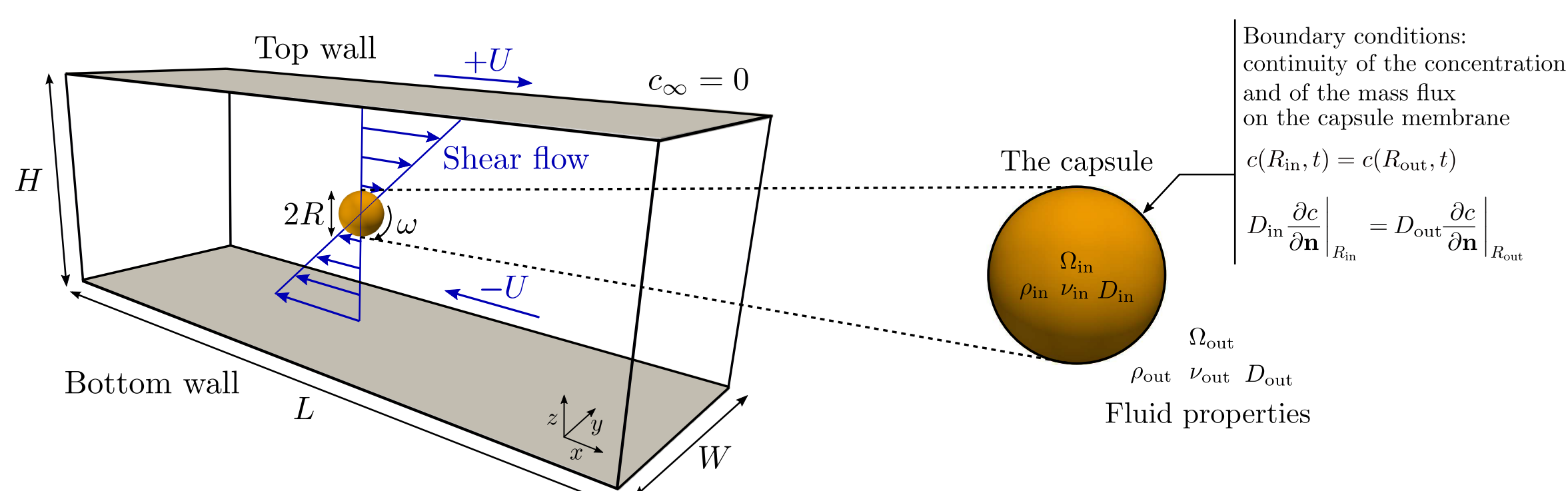
Badr Kaoui, Biomechanics and Bioengineering, CNRS, Université de Technologie de Compiègne, Compiègne, France

We use advanced numerical methods to model fluid-structure coupling with transport phenomena (fluid flow and mass transfer) involved in biomedical systems, such as controlled drug delivery and transport of deformable microcapsules into microfluidic chips. The simulations require high grid resolution to predict and to capture the details of each particle deformation and the released drug spatial distribution. The computer code solver that is based on the lattice-Boltzmann method, which is a state-of-the-art computational fluid dynamics method, is parallelized using both the MPI (Message Passing Interface) and the CAF (Co-Array Fortran 2008). We present the performance of the code on different machines when using either MPI or CAF. We show original results and data obtained with our computer codes. The drug release rate as a function of the flow around a capsule, and the clog and no-clog states of multiple capsules when squeezed into a microfluidic constriction. The HPC has allowed us to speed up the simulation run time, and therefore, to explore a wide range of the key control parameters. These studies are used to guide experimental studies with the hope to be used in the near future as a computer-aided design tool in pharmaceuticals and biomedical industry.

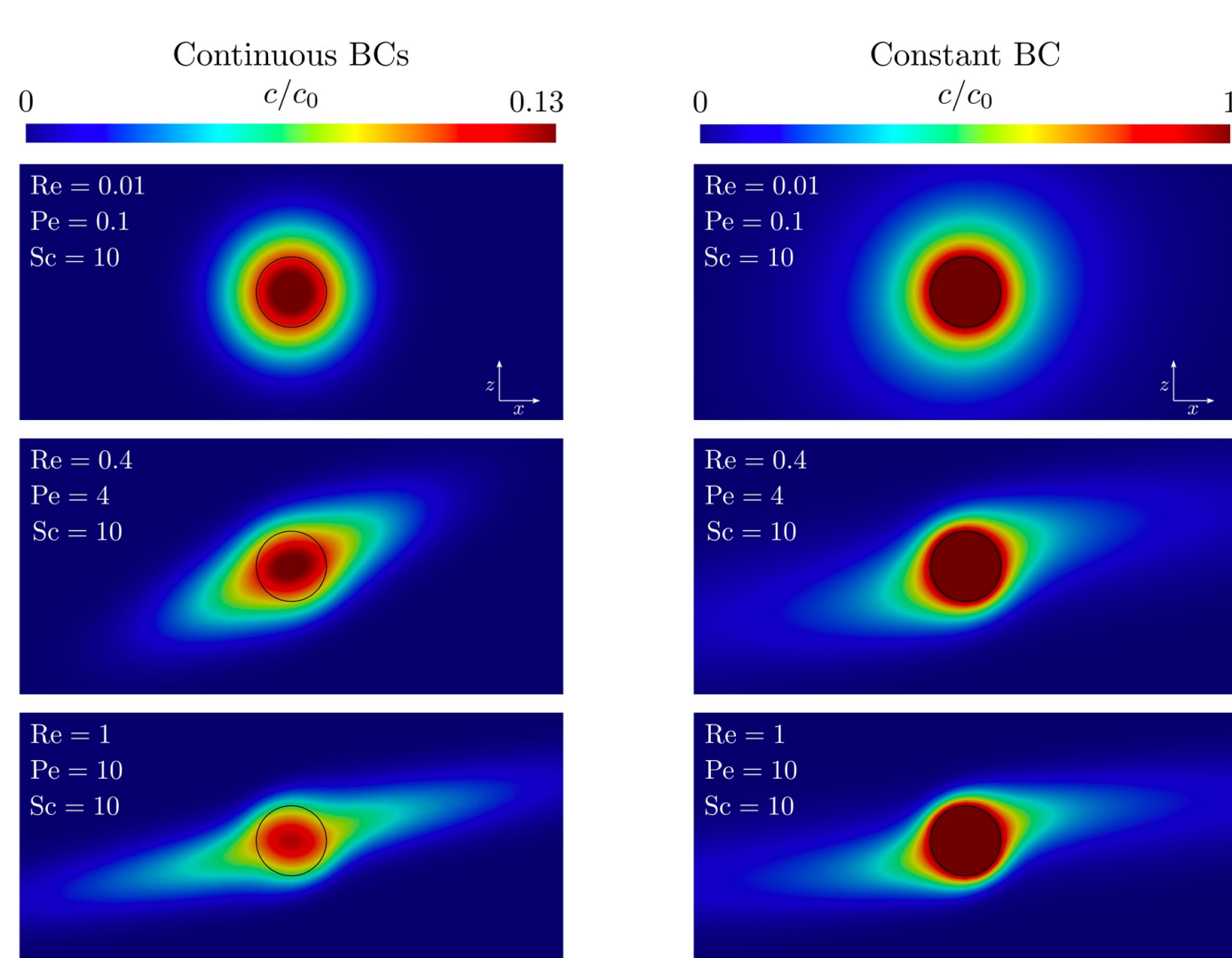
Mass transfer from a sheared spherical rigid capsule

C. Bielinski, L. Xia, G. Helbecque, B. Kaoui, *Physics of Fluids* 34, 031902 (2022)

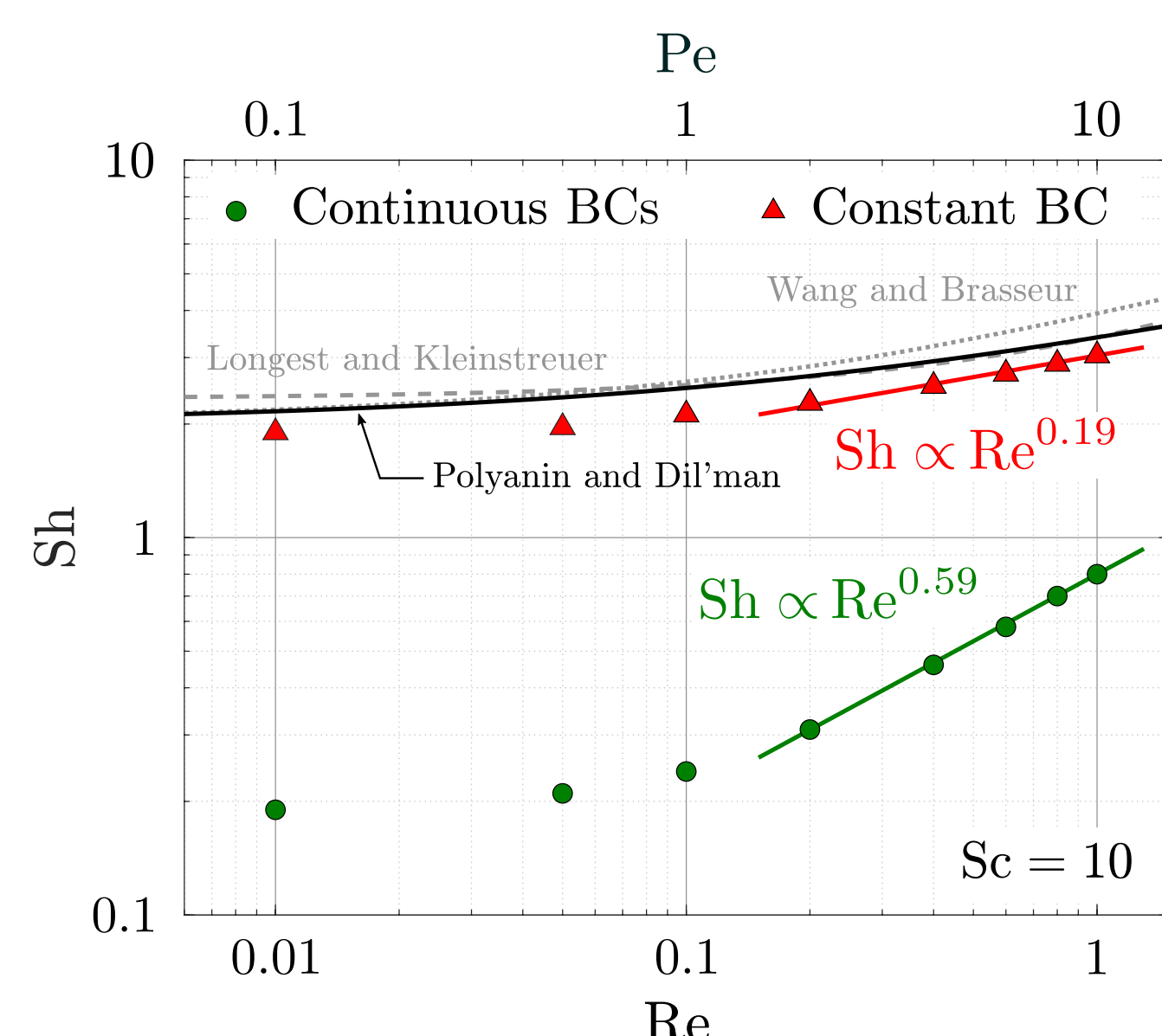
Solute mass transfer from a spherical fluid-filled rigid capsule subjected to shear flow is studied numerically, while considering unsteady, continuous, and nonuniform boundary conditions on its surface. Here, the capsule acts as a reservoir with its initially encapsulated solute concentration decaying over time. This scenario differs from the classical case study of either constant concentration or constant mass flux at the surface of the particle, and it is adapted to the case of drug release. The flow and the concentration field are computed using fully three-dimensional lattice Boltzmann simulations, where the fluid-structure two-way coupling is achieved by the immersed boundary method. The effects of the flow and the boundary conditions on mass transfer efficacy are quantified by the Sherwood number (the dimensionless mass transfer coefficient), which is found to increase due to the combined effects of forced convection and the rotation of the capsule. Having continuity of both the concentration and the mass flux on the capsule significantly decreases the Sherwood number as compared to the case with constant and uniform boundary condition.



Numerical setup of the problem. A spherical rigid capsule is suspended in the center of a channel. The upper and lower walls translate with the same velocity, but in opposite directions to generate a simple shear flow. This triggers the rotation of the capsule.



Solute concentration fields computed under various Reynolds numbers when considering continuous boundary conditions (left column). The steady concentration fields computed under the same Reynolds numbers, but with constant boundary condition (right column).

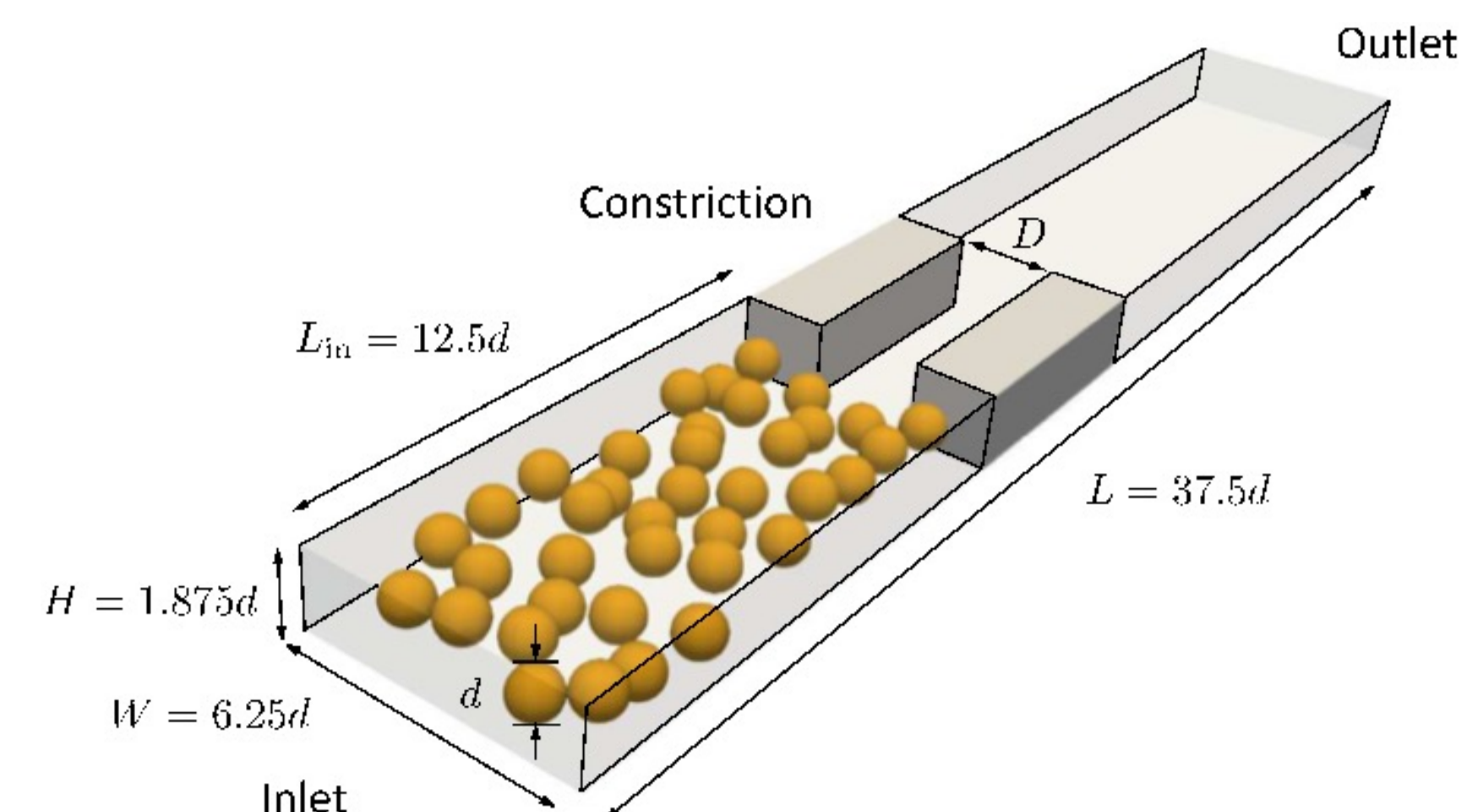


Steady average Sherwood number vs Reynolds number (Péclet number) computed at a given Schmidt number, while considering either unsteady continuous (circles) or constant (triangles) boundary conditions at the surface of the capsule.

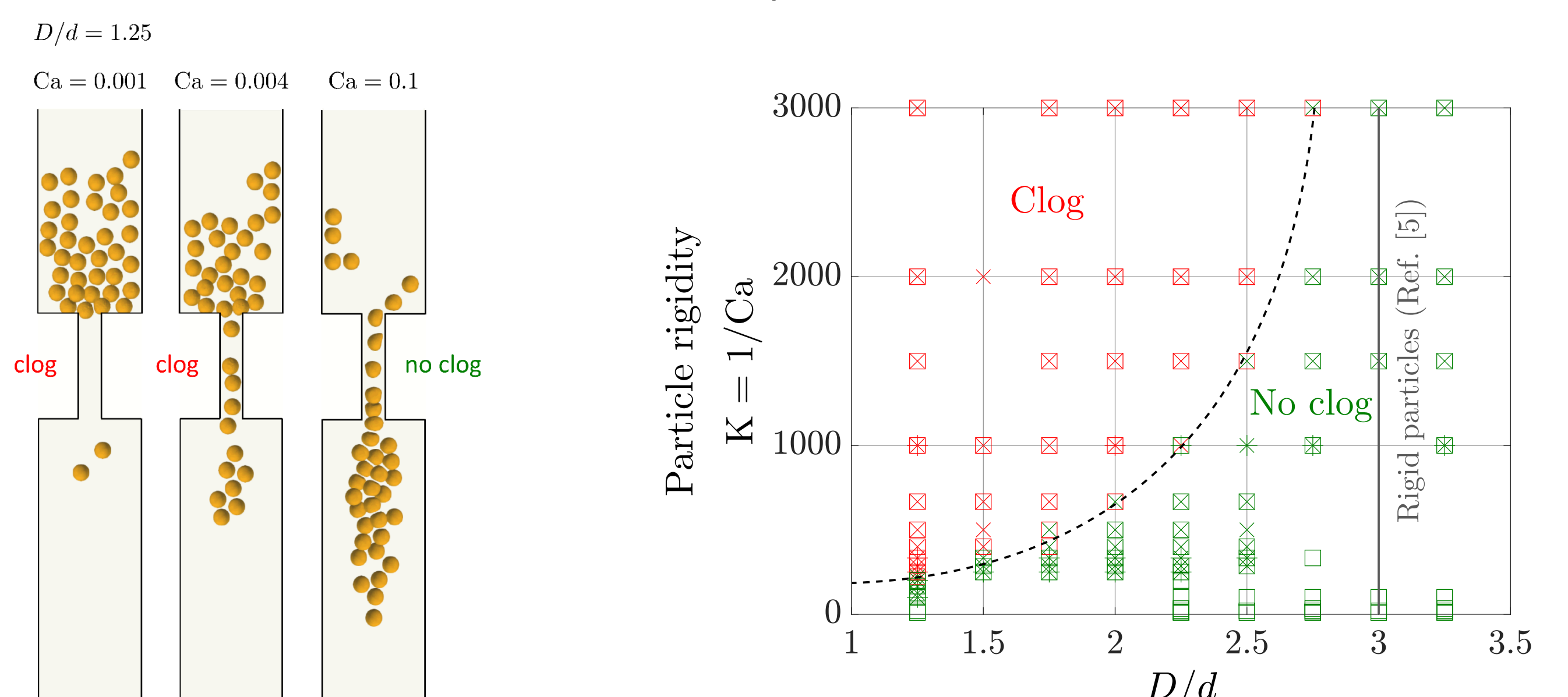
Squeezing multiple soft particles into a constriction: Transition to clogging

C. Bielinski, O. Aouane, J. Harting, B. Kaoui, *Physical Review E* 104, 065101 (2021)

We study numerically how multiple deformable capsules squeeze into a constriction. This situation is largely encountered in microfluidic chips designed to manipulate living cells, which are soft entities. We use fully three-dimensional simulations based on the lattice Boltzmann method to compute the flow of the suspending fluid and on the immersed boundary method to achieve the two-way fluid-structure interaction. The mechanics of the capsule membrane elasticity is computed with the finite-element method. We obtain two main states: continuous passage of the particles and their blockage that leads to clogging the constriction. The transition from one state to another is dictated by the ratio between the size of the capsules and the constriction width and by the capsule membrane deformability. The latter is found to enhance particle passage through narrower constrictions, where rigid particles with similar diameter are blocked and lead to clogging.



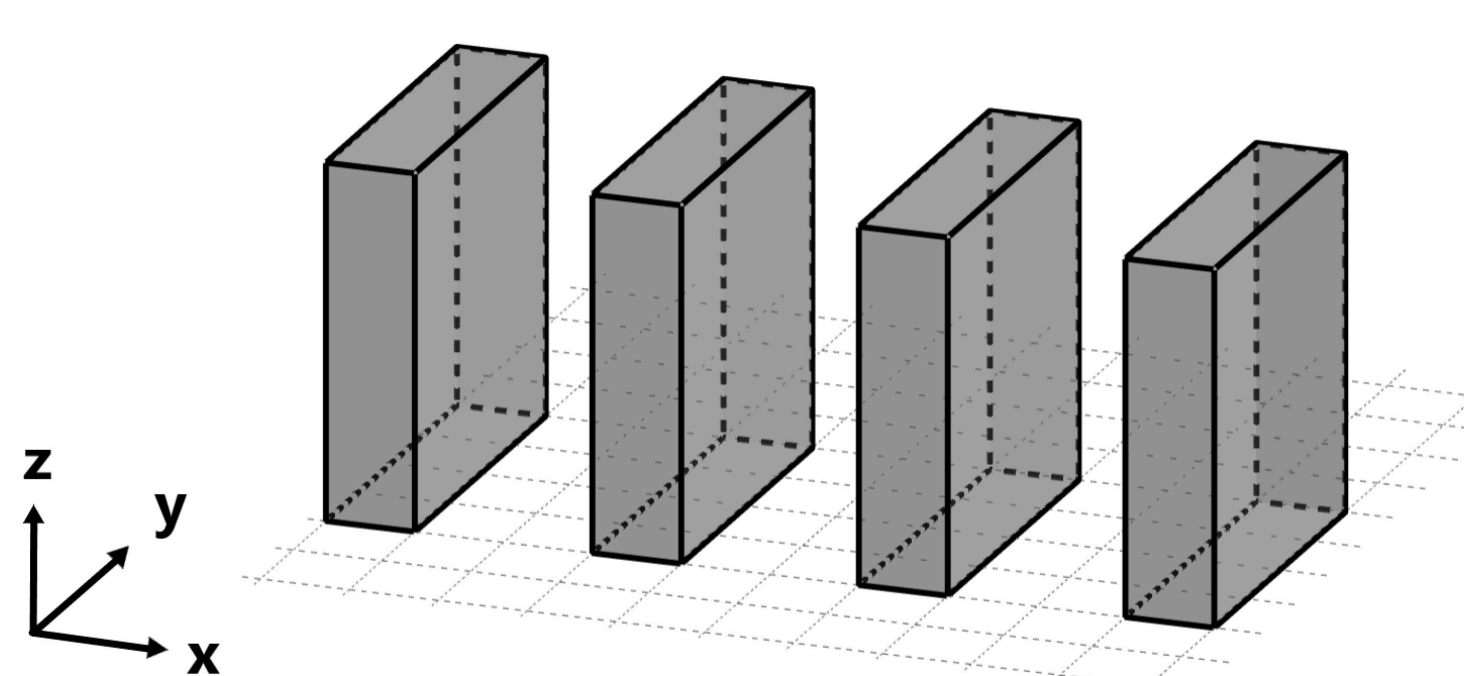
Numerical setup used to study the flow of capsules. The flow direction is from the left lower preconstriction chamber to the right upper postconstriction chamber. The main geometrical parameter is the ratio of the channel width D to the capsule diameter d, D/d.



Motion of multiple capsules at a microfluidic constriction for a given flow strength with the effect of particle deformability Ca. Easy passage of the particles is achieved at large Ca. Arch structures form at the entrance of the constriction for rigid particles.

Clog and no-clog states of multiple capsules obtained when varying their deformability Ca (rigidity K) and the constriction width D/d, while holding the same applied flow strength. The deformability of the particles reduces the threshold of the transition to the no-clog state.

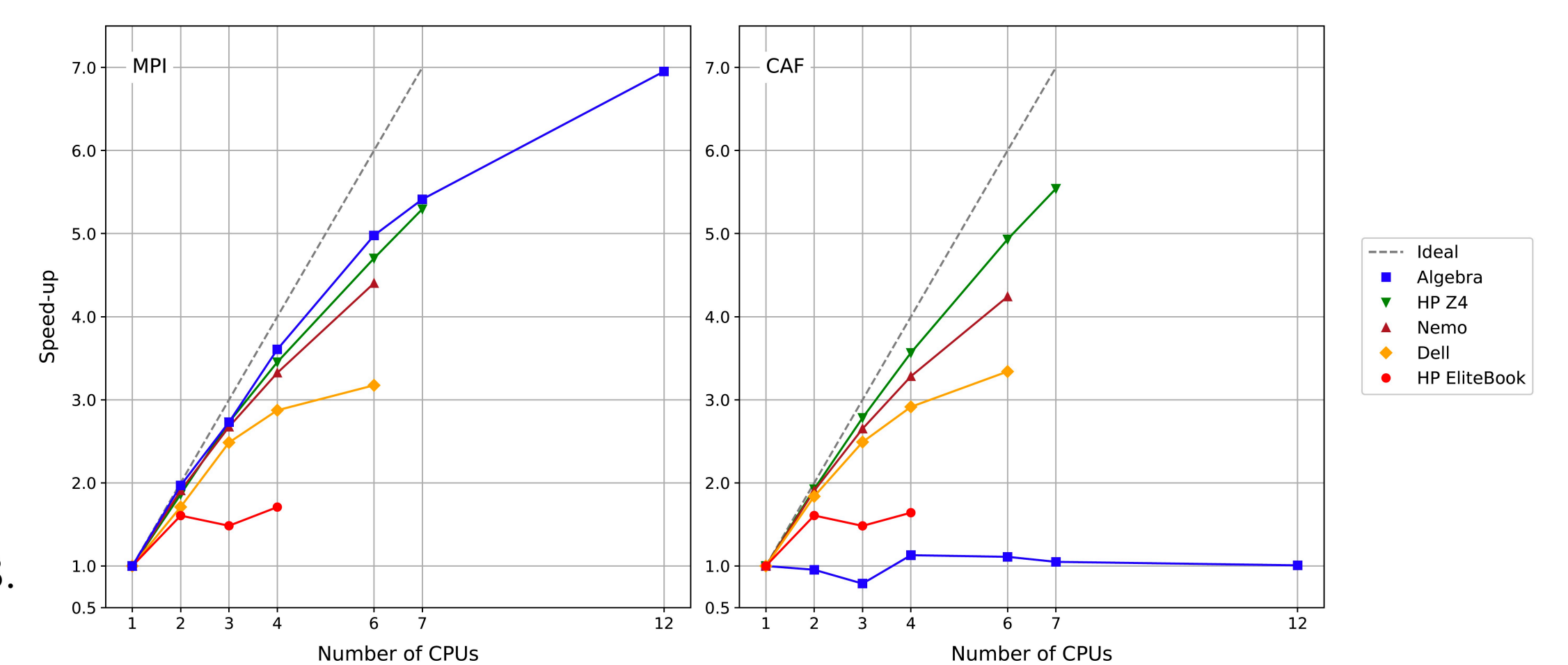
HPC performance of the "l3m3d" solver



Partition of the domain in the x-direction

- HP EliteBook: Intel® Core™ i5-5200U CPU @ 2.20 GHz × 4;
- Dell: Intel® Core™ i7-8750H @ 2.20 GHz × 6;
- Nemo: Intel® Xeon® CPU E5-1650 0 @ 3.20 GHz × 6;
- HP Z4: Intel® Xeon® W-2255 CPU @ 3.70 GHz × 10;
- Algebra: 2 Intel® Xeon® Platinum 8160 X7542 @ 2.10 GHz × 48.

CAF (Co-Array Fortran) and MPI (Message Passing Interface) speed-up performance on different computing machines. A cubic domain of size 84 is considered and 1000 time iterations are computed



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