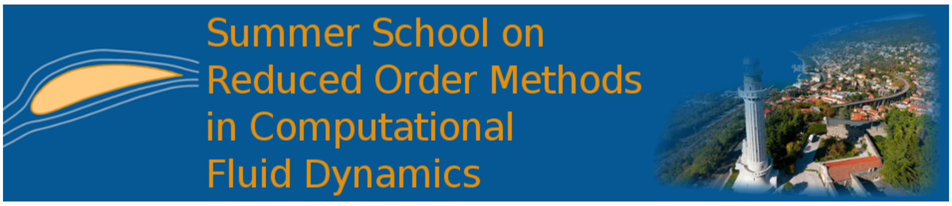

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Multi-scale numerical modeling of sorption kinetics

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The trapping of diffusing particles by either a single or a distribution of moving traps is an interesting topic that has been employed to model a variety of different real problems in chemistry, physics and biology. Here we study the dynamics of diffusing particles in a domain with an oscillating bubble. Laboratory experiments provide evidence of a non monotone behavior in time of the concentration of particles by a detector located behind the bubble, under suitable experimental condition. A comprehensive explanation of the phenomenon is not yet fully available.
The particles are attracted and trapped near the surface of the bubble. The basic mathematical model is a drift-diffusion model, where the particles diffuse and feel the potential of the bubble when they are near its surface. The numerical simulation of the system presents two multi-scale challenges. One is spatial: the range of the bubble potential is confined within a few microns at the bubble surface, while the bubble radius is of the order of a millimeter, so a fully resolved solution would be too expensive. The second challenge is on the time scale: the bubble oscillates with a frequency of the order of 100 Hz, while the diffusion time scale is of the order of 103 seconds, this requiring at least 106 time steps to fully resolve the problem in time.
A reduced model is derived to solve the multi-scale problem it space: the interaction with the bubble is modeled as a very thin layer, with a particle surface density proportional to the local density in the bulk, near the bubble. In the rest of the domain the particle density satisfies just a diffusion equation, with suitable boundary conditions on the bubble, deduced from conservation properties.
The model is carefully tested on problems in 1D, 2D planar and 3D axis-symmetric geometry. The equation is discretized on a regular Cartesian mesh, using a ghost-point approach, and solved by Crank-Nicolson scheme. The implicit step is efficiently solved by a suitably adapted multi-grid method.
The amplitude of the bubble oscillations is small compared to the bubble radius. We take advantage of this fact by replacing the time dependent position by imposing a suitable time dependent velocity at the bubble surface. Because of the low Reynolds number, the velocity distribution is computed by Stokes approximation. The multi-scale challenge in time is still under investigation.

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