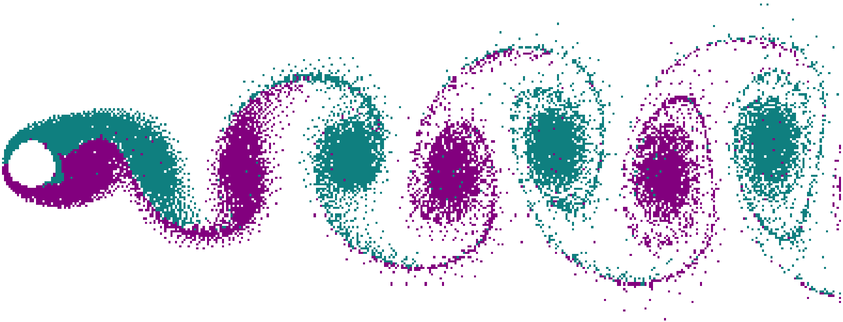
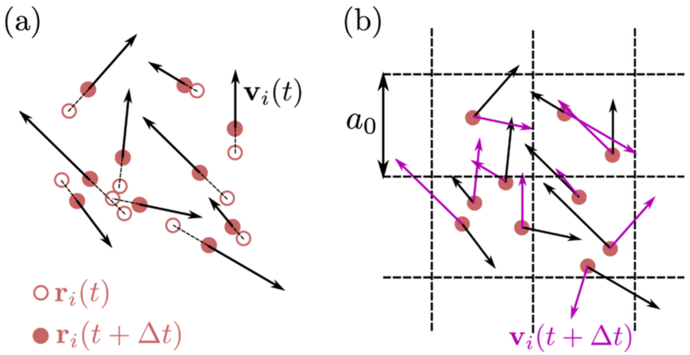
Multi-particle collision dynamics



Algorithm



(a) $\mathbf{r}_i(t+\Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t)\Delta t$

(b) $\mathbf{v}_i(t+\Delta t) = \mathbf{u}(t) + \Omega(\mathbf{v}_i(t) - \mathbf{u}(t))$

Thermostats

The resulting velocity distribution is of the Maxwell type. Thermostatting is required for non-equilibrium simulation due to viscous heating.

Various technique have been proposed:

- Velocity rescaling
- Andersen thermostat (1)
- External forces

$$\mathbf{v}_i(t+\Delta t) = \mathbf{u}(t) + \delta\mathbf{v}_i^{\mathsf{ran}} = \mathbf{u}(t) + \mathbf{v}_i^{\mathsf{ran}} - \sum_{j\in\mathsf{cell}} \frac{\mathbf{v}_i^{\mathsf{ran}}}{N_c} \tag{1}$$

Galilean Invariance

It was shown that for small mean-free path correlations in the velocities appears.

Random shift of the lattice cells before any collision steps: break correlations and Galilean invariance is restored.

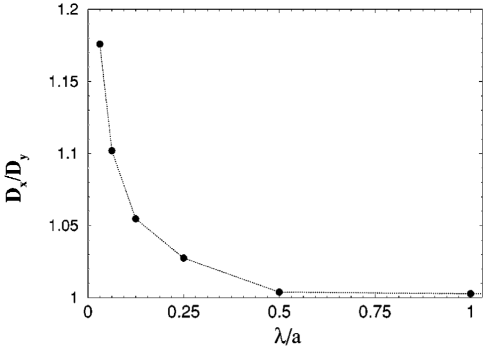
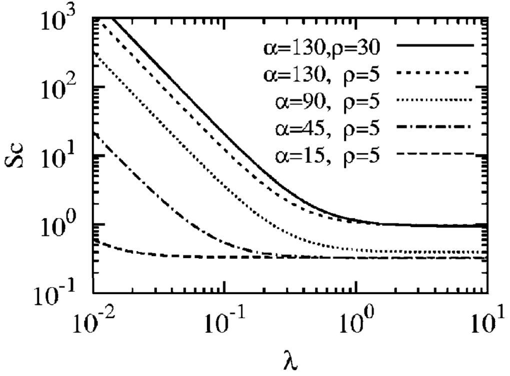


FIG. 1. Test of Galilean invariance. The ratio of the self-diffusion coefficients D_x and D_y in x and y directions plotted as a function of the ratio of the mean free path λ to the cell size a.

Transport coefficients

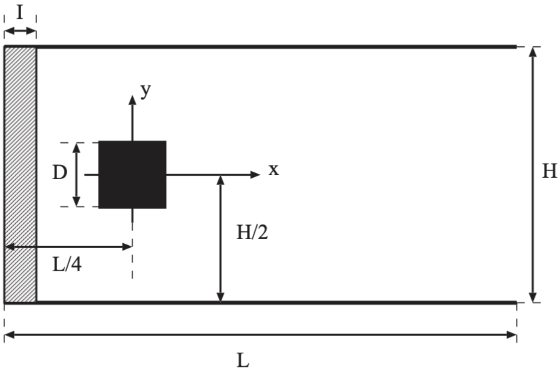


Schimdt number as a function of Δt and α

Changing Δt and α allows to change the Schmidt number and the interval of S_c that can be reproduced is big.

Accurate theoretical prediction of transport coefficients allows to easily setup simulation for different fluids.

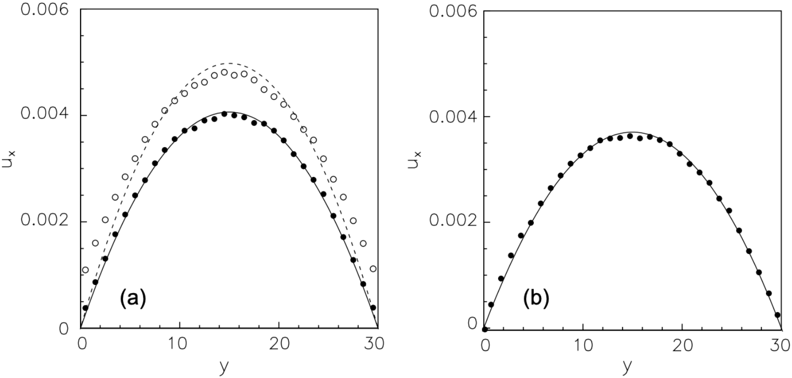
Implementation



Simulation of a square cylinder in a flow in a planar channel, to compare results with different implementation of boundary conditions.

Boundary conditions

Need to impose no-slip boundary condition. With cell-shifting the *bounce-back rule* gives a wrong velocity distribution.



Velocities distributions with different boundary conditions

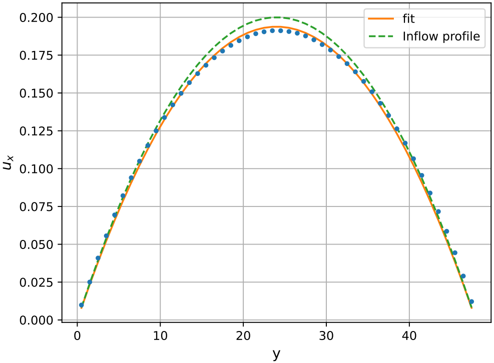
Viscosity calculation

In the planar Pouisille flow

$$u_x(y) = \frac{G}{2\mu}(H - y)y \quad (2)$$

Computing G and fitting the velocity profile we obtain

$$\nu = (0.108 \pm 0.002)\ a/\Delta t^2$$



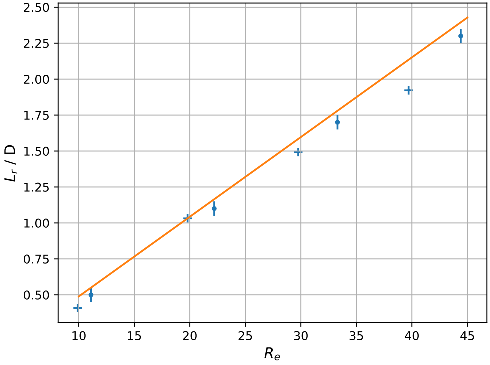
Compatible with the reference value of

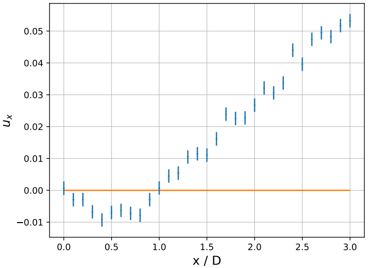
$$\nu_{\text{ref}} = (0.110 \pm 0.004)\ a/\Delta t^2$$

$$R_e \equiv \frac{v_{\text{max}} D}{\nu}$$

Recirculation length

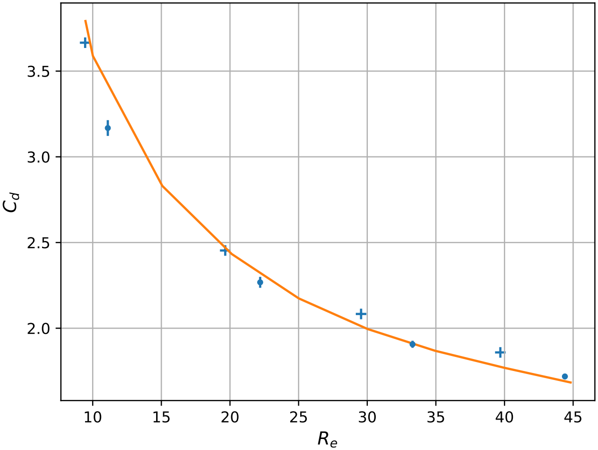
It's a measure of the size of the wake behind the object in the flow.





Example of velocity distribution behind the cylinder at $D = 12$

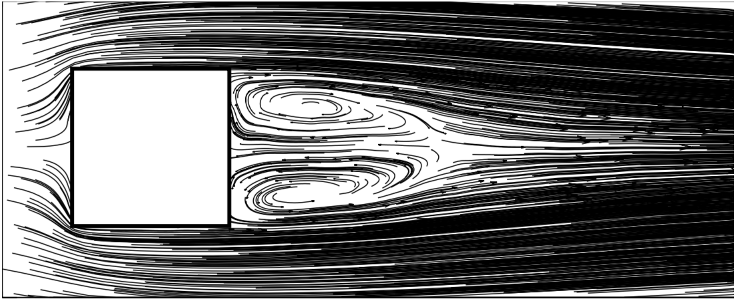
Drag coefficient



Wall effects for small D are less evident with the cell-shifting procedure.

Conclusion

The adaptability and the efficiency of the algorithms allow for accurate simulations of very different systems, in a wide spectrum of regimes.



Example of flow pattern at $R_e = 30$