PRACE Autumn School 2018
HPC for engineering and Chemistry
HANDS-ON
Molecular Dynamics and Computational Fluid Dynamics for Nanofluidics
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Problem

Use the commercial CFD package STAR-CCM+ to study the nanofluidic flow past a sphere at a Reynolds numbers $\mathrm{Re} = \rho U R \mu^{-1} = 0.1$. Here R denotes the radius of the sphere, U the free stream velocity, and ρ and μ the density and viscosity of the fluid, respectively. Assume the flow is steady, laminar and potentially subject to some fluid slip at the fluid-solid interface. The slip is model by the Navier slip boundary condition

$$v_s = l_s \left[\frac{\partial u_t}{\partial n} - \frac{v_t}{\kappa} \right], \tag{1}$$

where v_s denotes the slip velocity at the surface, l_s is the slip length, n is the surface normal, and κ the radius of curvature cf. Fig. 1.

Perform simulations imposing the no-slip and perfect slip boundary conditions available without special modeling. Compare the drag forces with the Stokes-Oseen drag taking into account partial slip cf. [1]

$$D \approx 6\pi\mu R U \left(1 + \frac{3}{8}\mathrm{Re}\right) \frac{R + 2l_s}{R + 3l_s}. \tag{2}$$

We note that Eq. (2) recovers the classical Stoke drag $D = 6\pi\mu R U$ for the no-slip condition as $\mathrm{Re} \to 0$, and $D = 4\pi\mu R U$ for the perfect slip ($l_s \to \infty$).

Setting up the simulation

Create a cylindrical mesh around the sphere extending sufficiently far away to allow us to impose a uniform velocity at the inflow boundaries:

1. When starting STAR-CCM+ use the `Power On-Demand` license and enter the key: `OMFPuuG67LGBsdiie2ZkfA`. If you use a local/personal installation, then set the environment variable: `CDLMD_LICENSE_FILE=1999@flex.cd-adapco.com`.

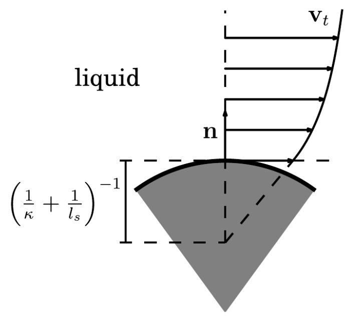

Figure 1: Schematic of the Navier boundary condition. The shaded region represents the solid and the region above it the liquid [1].

2. On the ULFME cluster set the environment variables using the console command:

   `module add star-ccm+/13.04.011`.

3. On linux systems add the `CDLMD_LICENSE_FILE` to the file `~/.flexlmrc`, and consider defining the license key in an environment variable, fx. in `~/.bashrc` add `export KEY=OMFPuuG67LGBsdiie2ZkfA`. Now, to launch STAR-CCM+ on linux systems using 4 cores on the local host write:

   `starccm+ -np 4 on localhost -power -podkey $KEY exercise01.sim`

   provided the file `exercise01.sim` exist; otherwise replace this file name with the option `-new`:

   `starccm+ -np 4 on localhost -power -podkey $KEY -new`.

4. Create the mesh directly using the build-in CAD tool: `3D-CAD Models`:

   - `Geometry` → right click on `3D-CAD Models` and select `New`.
   - Select `Features` → `XY` and right click and select `Create Sketch`.
   - Draw a half-circle centered at origo with a radius of 1 m.
   - Draw two lines: one upstream and one downstream coinciding with the axis of symmetry: both with a length of 19 m, placing the upstream and downstream faces at -20 m and 20 m. Draw the outer boundary placing the two corners at (-20 m; 40 m) and (20 m; 40 m) cf. Fig. 2.
   - Revolve the sketch to create the 3D body: right click on `Sketch 1` and select `Revolve`. Select 360 deg (`Body Type`: `Solid` and `Body Interaction`: `Merge`.

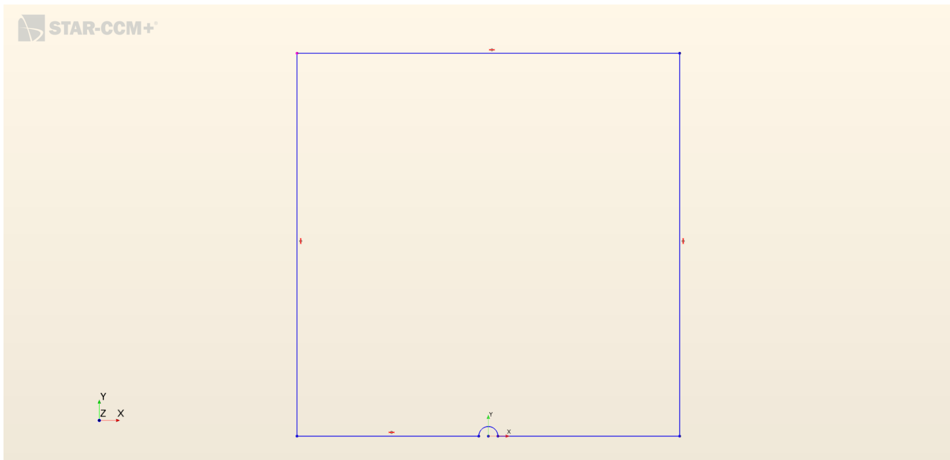

Figure 2: CAD drawing defining the geometry.

- Convert the CAD drawing to `Parts`: close the CAD tool and right click on `3D-CAD Model 1` and press `New Geometry Part`. Select `Tesselation Density` as `Very Fine`.
- Split the surface into separate entities to enable different boundary conditions, select: `Parts` → `Body 1` → `Surfaces` and divide the surface using `Split by Angle`. Rename the surface to give them meaningful names (right click and select `Rename`).
- To create a domain that can be meshed, convert the `Parts` to a `Region` by right clicking on `Body 1` and select `Assign Parts to Regions`; to ensure the renamed boundaries are transferred, choose `Create a Boundary for Each Part Surface`.
- Setup the mesh generator in `Geometry` → `Operations` → `New` → `Mesh` → `Automated Mesh`. Right click on `Automated Mesh` and select `Surface Remesher`, `Polyhedral Mesher` and `Prism Layer Mesher`.
- Select as `Input Parts` the `Body 1`.
- Select the parameters for the meshers in `Automated Mesh` → `Default Controls` and select
  - A typical mesh size in `Base Size` — in this case 4 m.
  - Set `Minimum Surface Size` to 0.1 % corresponding to 4 mm.
  - In `Surface Curvature` set `Pts/circle` to 100.
  - Select a `Surface Growth Rate` of 1.3
  - Set `Number of Prism Layers` to 10.
  - Set `Prism Layer Stretch` to 1.3.
  - Set `Prism Layer Thickness` to 5 % of Base.

- Add a `Custom Controls`: right click `Surface Control` and select as `Part Surface` the solid surface of the sphere. Set the target surface size in `Surface Controls` → `Controls` → `Target Surface Size` and select `Custom` and add the value in `Values` and select here `Percentage of Base` and choose 2.0.

5. In `Continua` right click and select `New` → `Physics Continuum`. Right click on `Physics 1` and `Select Models`:

   - `Three Dimensional`.
   - `Steady`.
   - `Gas`.
   - `Segregated Flow`.
   - `Constant Density`.
   - `Laminar`.
   - `Maxwell Slip`.

6. In `Physics 1`: change the fluid properties from the default values for water to match the required Reynolds number (in `Models` → `Liquid Air` → `Material Properties`). Suggestion: select a unit value (1.0) for density, velocity, and length, and modify the dynamic viscosity to give the desired Reynolds number.

7. Define the boundary conditions: (in `Regions` → `Boundaries`)

   - Set the free stream velocity on the front and side surfaces In `Properties` (lower left window) set the `Type` to `Velocity Inlet`. and define the velocity specification to `Components` in `Physics Conditions` → `Velocity Specification` and define the components in `Physics Values` and set `[1.0, 0.0, 0.0] m/s`.
   - For the outlet condition choose `Pressure Outlet`.
   - For the solid wall of the sphere keep the default `Wall` and select the no-slip, slip or partial slip in `Physics Conditions` → `Shear Stress Specification`. The slip length is defined in `Continua` → `Physics 1` → `Models` → `Gas` → `Air` → `Material Properties` → `Mean Free Path`.

8. Create the mesh by pressing the: `Generate Volume Mesh` .

9. Before running the calculations, instrument the code to output the drag on the sphere: `Reports` right click `New Report` and select `Force`. In the `Properties` window select the `Direction` and `Parts` on which you wish to record the forces; here choose `Regions` and select the solid surface. To ensure this report is executed at every iteration create a

monitor (and plot) from the report: `Create Monitor and Plot from Report`.

10. Change the initial conditions from the default stagnant flow to a parallel flow: `Continua` → `Physics 1` → `Initial Conditions`.

11. Run the simulation by pressing the: `Run (Ctrl+R)` 

12. Make sure the number of iterations are sufficient to reach a steady state ie., monitor the residuals (the convergence error of the simulation during iterations) and the drag forces. The default stopping criteria are defined in `Stopping Criteria`.

Post-processing

If the simulation is launched interactively, the residuals are automatically plotted as a Scene. To create more scenes select the scenes symbol in the top bar or right click on the `Scenes` on the left: `New Scene` and select

- `Geometry`: for plotting the CAD or Part geometry.
- `Mesh`: for plotting the finite-volume mesh.
- `Scalar`: produces a surface or contour plot of any scalar.
- `Vector`: produces a vector field.

Notice, that you need to select the `Part` to visualize: fx. in `Scene/Plot` (upper left panel) for a `Vector` scene, expand `Vector 1` and click on `Parts` and in the bottom `Parts - Properties` window select the desired `Parts`: often the entire fluid `Region`; but it is also useful to define a plane cutting through the domain: `Derived Parts` right click `New Part` → `Section` → `Plane`.

Flow Simulations

Simulate the steady state flow and consider slip lengths of $l_s = 0\,\mathrm{m}$ (no-slip), $l_s = \infty$ (full slip), and $l_s = 0.2\,\mathrm{m}$.

1. Run on 1, 2, 4, 8, and 12 cores and measure the elapse time per time step: `Report` → `New Report` → `Solver Iteration Elapse Time`. What (strong) scaling do you observe ? Note, that the mesh has approximately 230.000 cells (a small problem size) and that the current recommended minimum number of cells per core 30.000 for STAR-CCM+.

2. Compare the drag with the analytical model (Eq. 2).

3. Plot the velocity and pressure fields on a plane cutting through the domain.

4. Describe the flow field — is the flow "adequately" resolved (based on the smoothness of the pressure and flow fields) ?

5. How many iterations are needed and which value(s) do the residuals level off to when the drag force has converged ?

References

[1] A. Popadić, M. Praprotnik, Koumoutsakos P., and J. H. Walther. Continuum simulations of water flow past fullerene molecules. *Eur. Phys. J. Special Topics*, 224:2321–2330, 2015.