ESPResSo Summer School 2013
Immersed boundary – object-in-fluid (OIF) module
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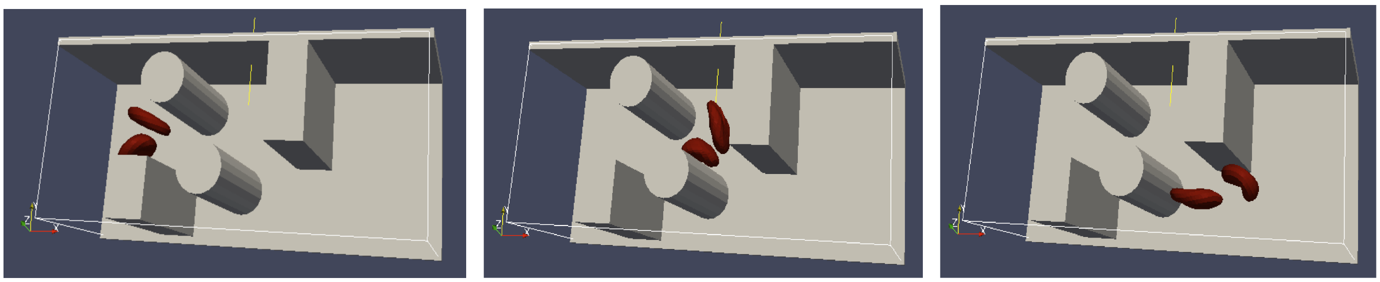
- developed primarily for simulations of blood flow in a microfluidic device, but can be used for other closed objects in a fluid flow
- suggested simulation for the hands-on session: two red blood cells moving in a channel with obstacles (cylinders, rhomboids)



Requirements:
- Espresso sources with correct myconfig-final.h and object_in_fluid.tcl
- Paraview or other software for visualization of .vtk files
- provided sample scripts and input data

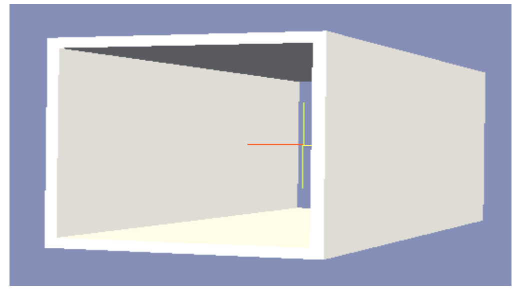
Following files are provided for this simulation:
- **cell_nodes.dat**, **cell_triangles.dat** – these input files contain triangulation data for the cell; no changes are necessary
- **boundaries.tcl** – this script specifies the boundaries and obstacles in your simulation. At the beginning of the file, there are two output procedures (one for rhomboid, one for cylinder) that do not need to be modified. After those comes the sample specification of individual walls and obstacles. Please, modify it using the suggestions below.
- **simulation.tcl** – this script contains the actual simulation including the specification of immersed objects. Please, modify it using the suggestions below.

OIF framework:
(optional parameters are [in brackets]; please, see oif_documentation.txt for more details)
- **oif_init** - initializes the OIF framework and must be used before any other OIF commands
- **oif_create_template** template-id *tid* nodes-file *nfile* triangles-file *tfile* [stretch *sx sy sz*] [ks *val*] [kb *val*] [kal *val*] [kag *val*] [kv *val*]
- **oif_add_object** object-id *oid* template-id *tid* origin *ox oy oz* part-type *ptype* [rotate *rx ry rz*] [mass *val*]
- **oif_object_output** object-id *oid* [vtk-pos *"file.vtk"*] [vtk-aff *"file.vtk"*] [mesh-nodes *"file.dat"*]

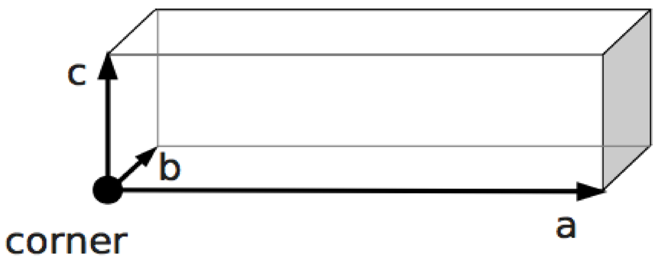
other available oif procedures (not needed for this simulation):
- **oif_info**
- **oif_mesh_analyze**
- **oif_object_set**
- **oif_object_analyze**

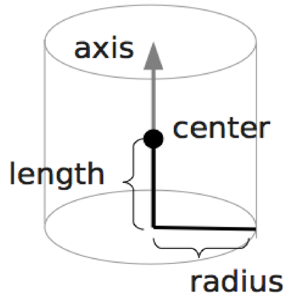
Steps:

1. **Create channel** (modify boundaries.tcl)
   design your geometry: create top, bottom and 2 side walls
   channel dimensions: around 50x20x20
   channel walls (for visualization): 4 rhomboids of thickness 1
   channel walls (for simulation): using lbboundary and constraint



2. **Create obstacles** (modify boundaries.tcl)
   Schematic pictures of rhomboid and cylinder obstacles:





   Examples:
   - rhomboid corner 30 10 1 a 5 0 0 b 0 11 0 c 0 0 18
   - cylinder center 16 17 10 axis 1 0 0 radius 3 length 9

   Note: Currently only cylinders with axis 1 0 0 are supported for proper visualization using Paraview

3. **Create objects** (modify simulation.tcl)
   first create templates, then add objects, such as
   cell 1: origin *o1_x o1_y o1_z* stretch 3.0 3.0 3.0 rotate 0 0 [expr $pi/2] ks 0.05 kb 0.01 kal 0.01 kag 0.01 kv 10.0 part-type 0 mass 1
   cell 2: origin *o2_x o2_y o2_z* stretch 1.0 2.0 3.0 ks 0.05 kb 0.01 kal 0.01 kag 0.01 kv 10.0 part-type 1 mass 1

4. **Create interactions** (modify simulation.tcl)
   suggested interactions:
   cell-cell: inter cell1_part-type cell2_ part-type soft-sphere 0.005 2.0 0.3 0.0
   cell-wall: inter cell_ part-type wall_type soft-sphere 0.0001 1.2 0.1 0.0

5. **Run simulation with only couple cycles**
   suggested fluid velocity: 0.01 0.0 0.0

6. **Visualize** .vtk data in Paraview and **check the geometry and objects**
   visualisation using Paraview:
   - open and load all .vtk files
   - press the Apply button
   - using the eye icon to the left of filenames, view the produced outputs in the individual time steps or all together
   - fluid can be visualized using Filters/Alphabetical/Glyph

7. Repeat previous steps if corrections are necessary

8. **Run the whole simulation and visualize results**
   suggested runtime for the parameters above:
   - whole simulation: 33000 cycles (about 15-20 min computation on personal laptop)
   - output: every 3000 cycles

   save the Paraview visualization as a movie

QUESTIONS? Please, ask Markus, Iveta or Renata.