Modelling of arbitrary shaped channels and obstacles by distance function

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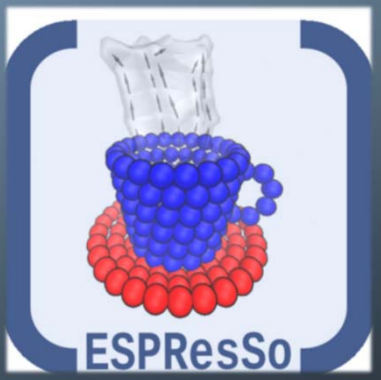
PURPOSE

- method of defining boundaries and obstacle objects with complex and non-trivial shapes in numerical simulations
- accuracy speed

- method of creation of a general obstacle and channel shape, with simulations run with ESPResSo
- Distance function

- will be used in further simulations of helical devices with non-circular cross-section, in order to sort the cells that flow through it, in a function of their size or elasticity

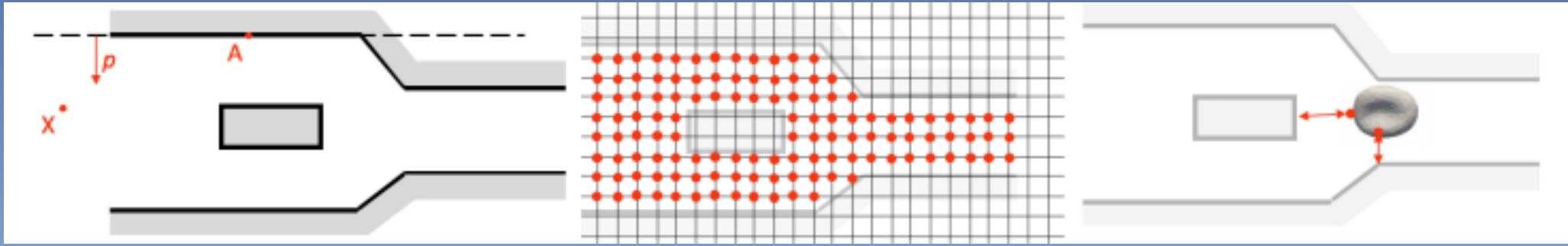
presented on a concrete examples involving several simulations performed within a simulation package ESPResSo



open-source simulation package

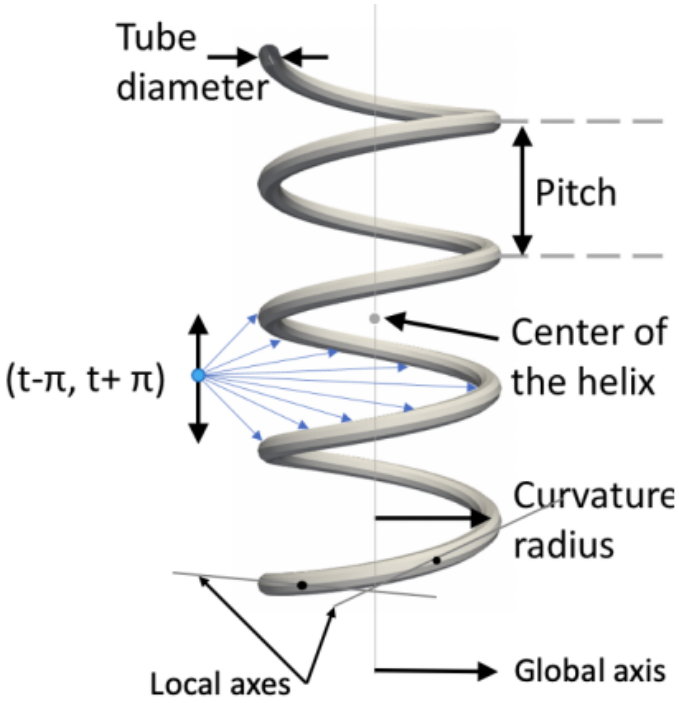
Numerical concept of a boundary

Interaction between boundaries and immersed particles

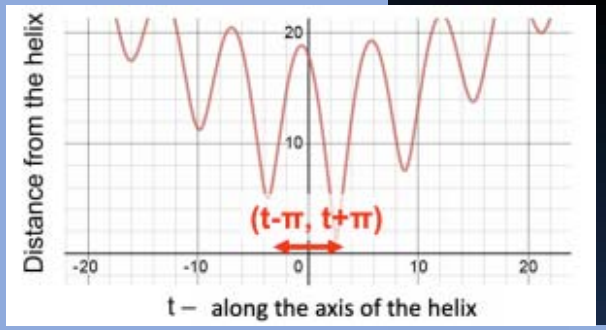


- example of a geometry depicting a narrowing channel with a rectangular obstacle
- fixed grid discretization of the fluid requires to identify the lattice points that are located inside the channel (in red).
- triangular discretization of an object requires to know the distance of its mesh points from nearest boundary (red arrows), for example to apply repelling force from the boundary

HELIX
boundary definition



helix boundary point with minimal distance from the space point is within interval (t−π, t+π).



HELIX boundary definition:

- center (point situated at the global axis of helix)
- tube radius
- pitch
- tube curvature radius

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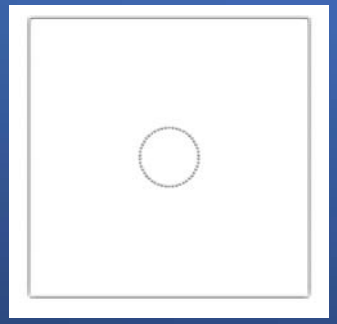
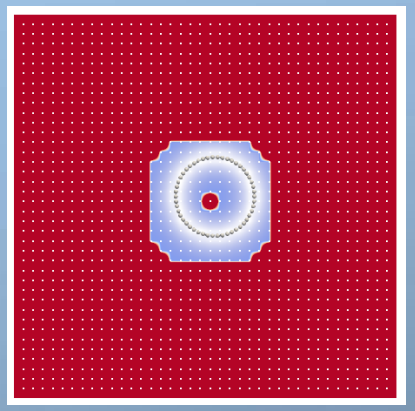
Generic boundary



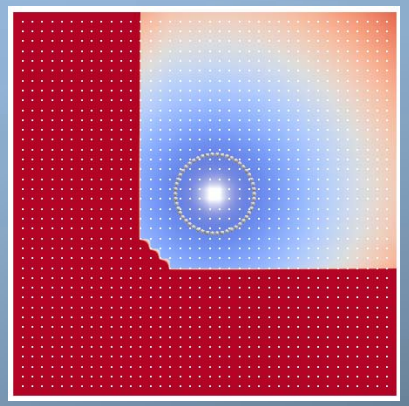
No a k tomuto třeba určitě obrázek, co je to vlastně source?

Vector Distance Transform algorithm

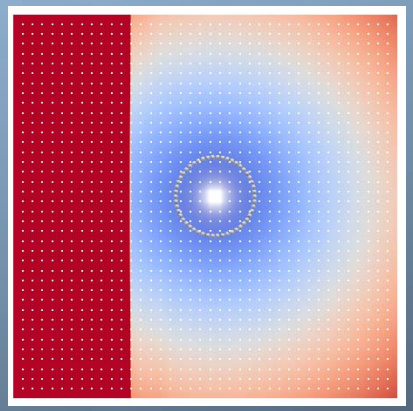
- Choose the source of the neighbors to calculate the smallest possible exact Euclidean distance at the current grid point (for this reason, we need to keep track of the sources, and every time we calculate a smaller distance value we update this information)



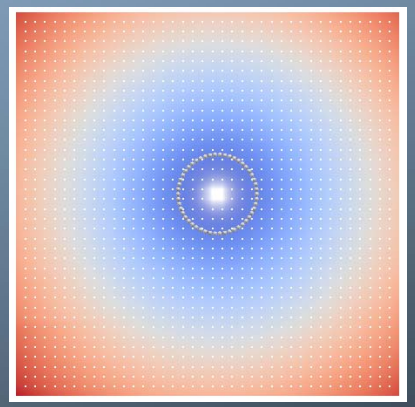
Initialisation: definition of distance function in proximity of cloud points



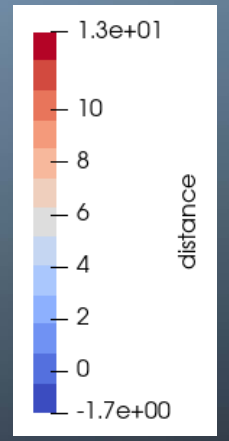
1st iteration: sweeping from the 1st corner



2nd iteration: sweeping from another corner



3rd iteration: sweeping from next corner

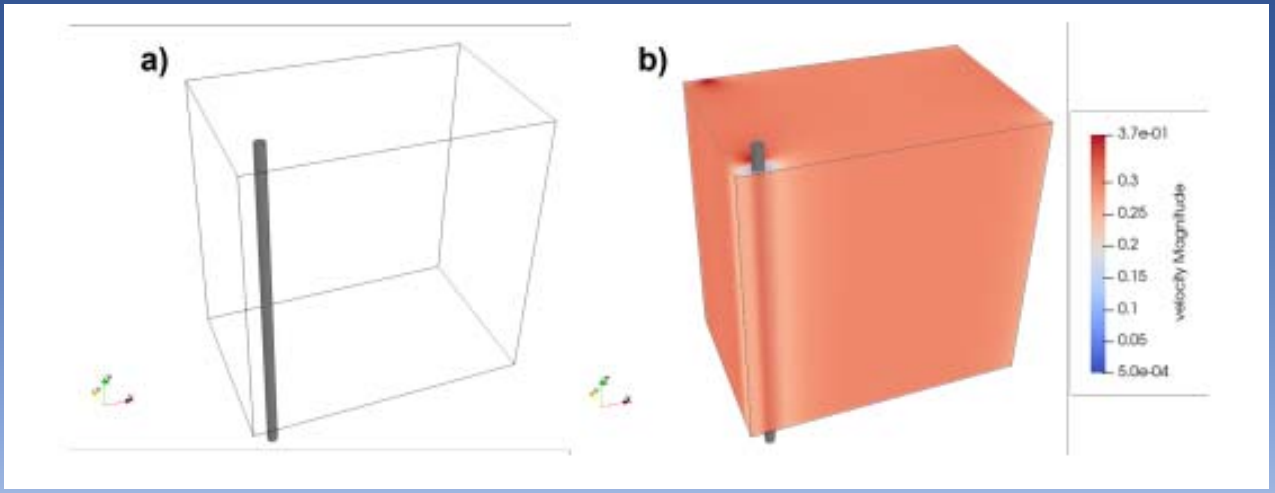


VERIFICATION

- comparing simulation with an existing basic obstacle, and an obstacle created with generic approach
  - contained a cylindrical obstacle
  - fluid was flowing around the cylindrical obstacle

Cylindrical obstacle in simulation box.

a) geometry of the numerical simulation
b) verification of the correctness of the fluid flow without particles



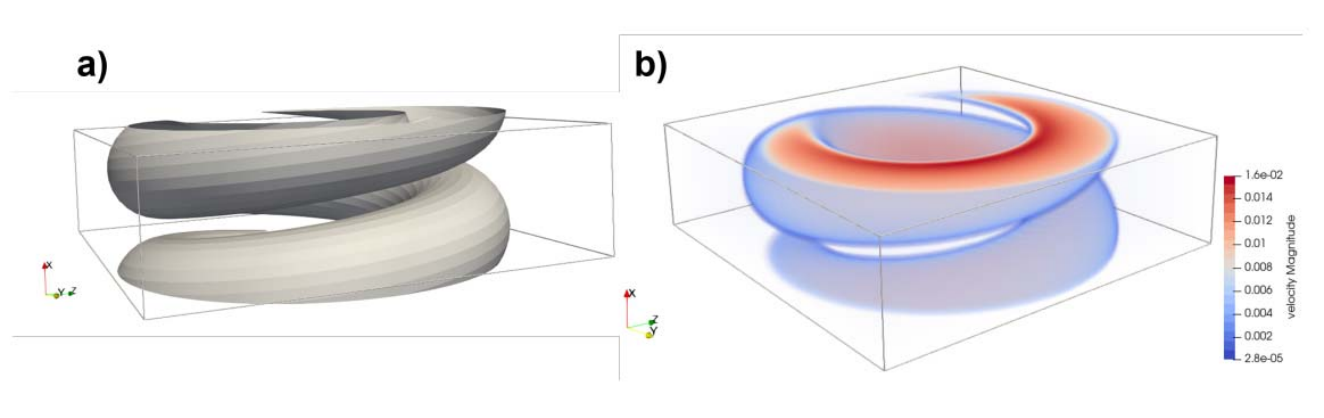
RESULT:

- there was no difference in the two compared flows, the difference in the fluid flow in each discretization point was literally 0 for all valid decimal places

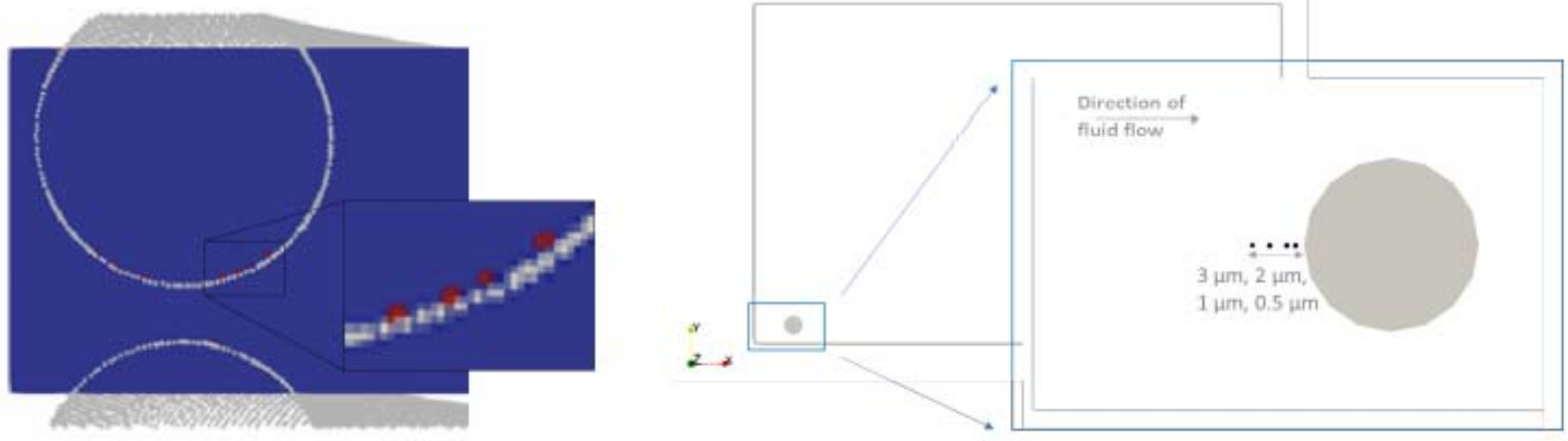
VERIFICATION

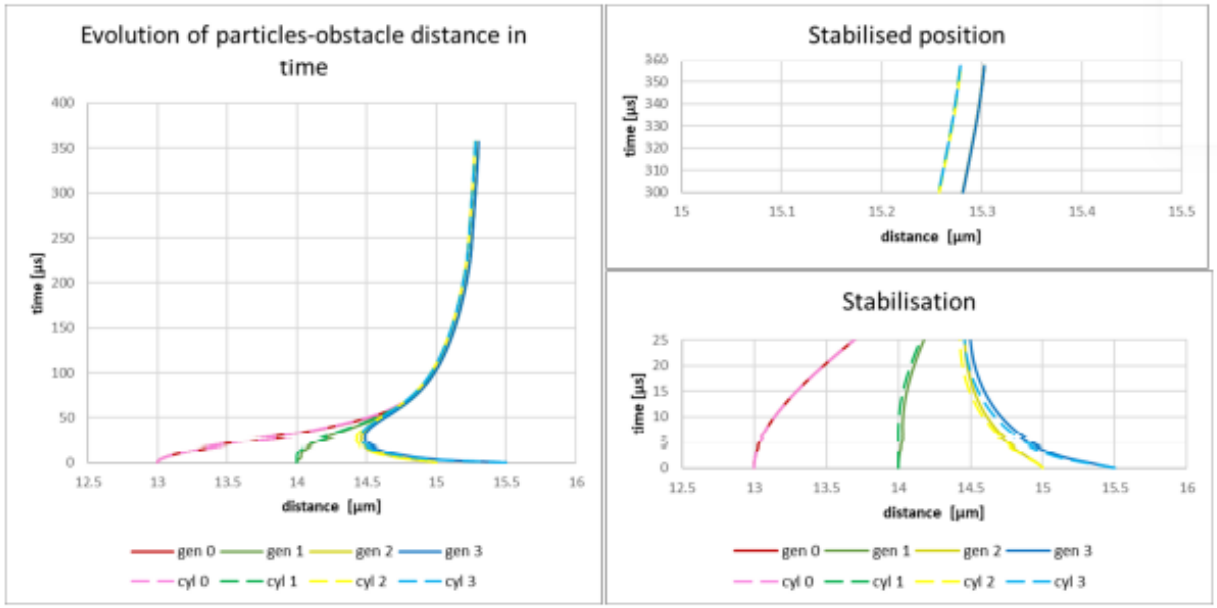
Helical channel in simulation box
a) geometry of the numerical simulation
b) verification of the correctness of the fluid flow without particles

- fluid was flowing inside of the helical obstacle



RESULT:





gen – generic boundery
cyl – existing definition from ESPResSo

Comparison of trajectories

RESULT with particles:

No tu to bude treba povysvetľovať

BEGIN

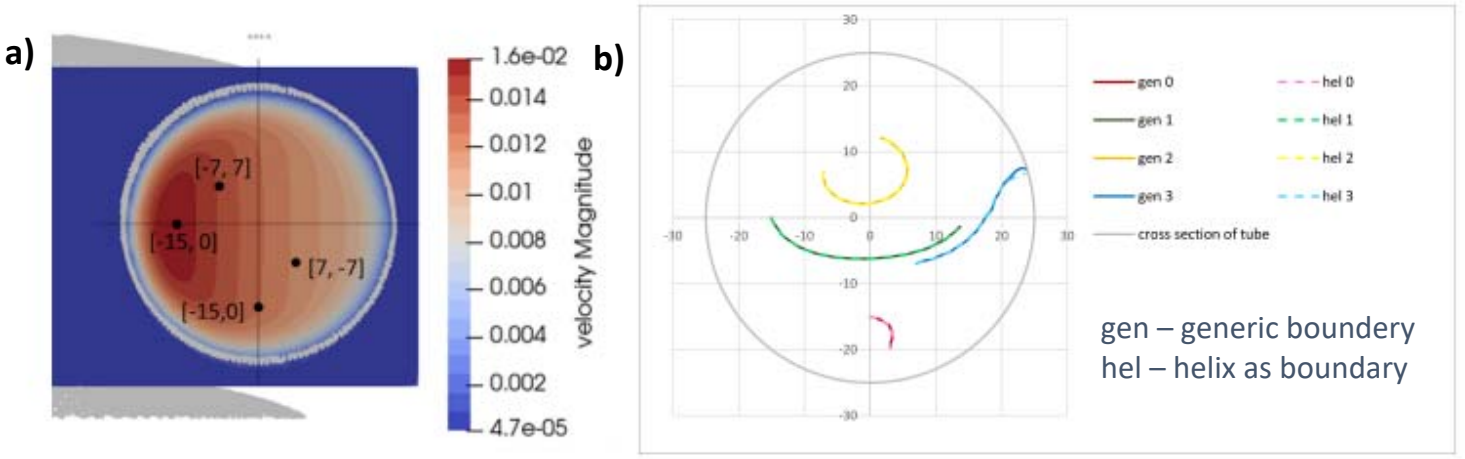
- 4 obstacles in positions 13 μm, 14 μm, 15 μm and 15.5 μm
- position on 16 μm – boundery
- Interaction = 2μm

END

- convergetion to the same position
- 0.025 μm deviation

Comparison of trajectories

RESULT with particles:



a) position of the four particles in flow with helical obstacle; the initial position of each particle is marked by a black dot

b) trajectories of particles in the helical microchannel, projected to the cross-section of the helical tube

CONCLUSION

- proposed and verified a numerical concept of a generic obstacle
  - concept was presented and verified within the simulation package ESPResSo
- in biological domain, the method can be used to model complicated shapes as blood vessels or multi-channel microfluidic devices.
  - to define the shape of a generic obstacle, we need to define a cloud of points that describe the surface of the object (the shape of the generic obstacle is thus limited only by our ability to create such cloud of points; after that, we use a VDT algorithm to find a distance function - a function that define for each simulation point a vector and a value that correspond to the distance to the closest boundary)
- will be used in further simulations of helical devices with non-circular cross-section, in order to sort the cells that flow through it, in a function of their size or elasticity.

THANK YOU

FOR YOUR ATTENTION

Pozn: ak to ma byt **AJ** ako PR k espresu, tak by som tu dala odkaz na www stranku espressa ☺