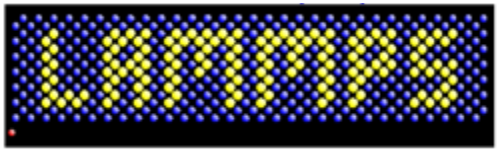
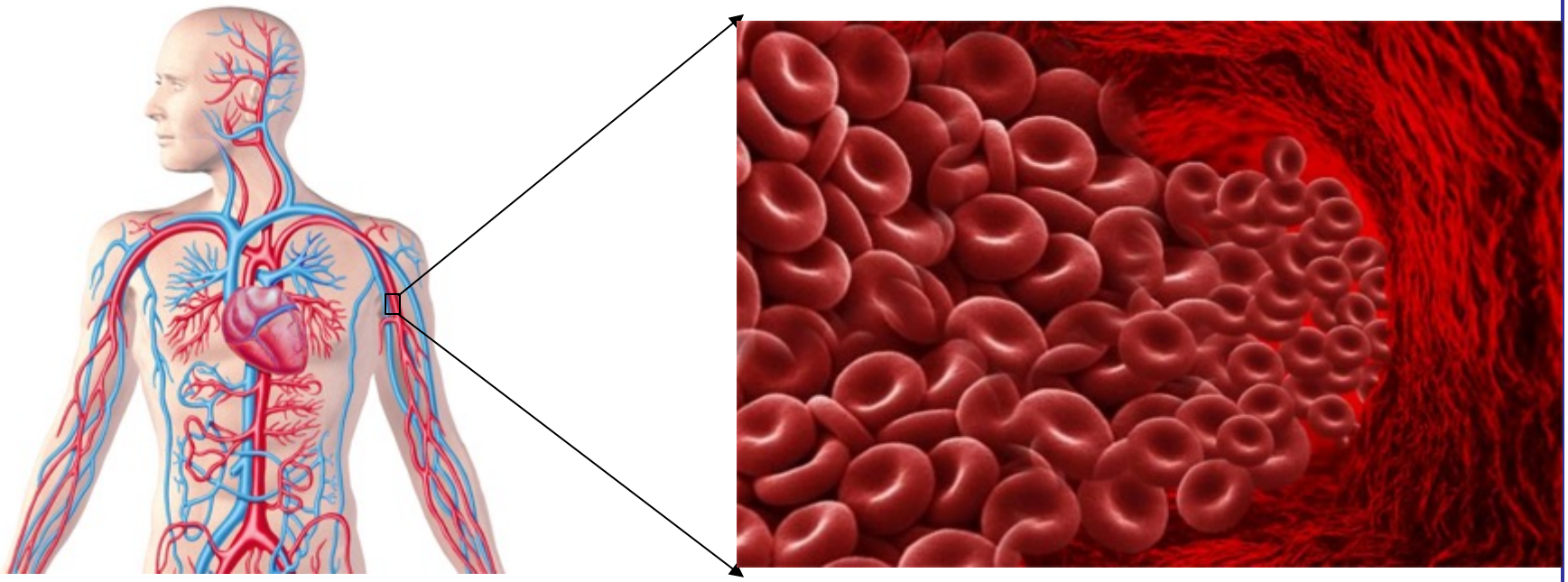


A highly efficient and portable fluid-structure simulation package implemented by LAMMPS

Huilin Ye
Advisor: Ying Li

Department of Mechanical Engineering, University of Connecticut

Background



Issues to address:

- Structure motion (blood cells, ~45% highly deformable Red blood cells)
- Plasma dynamics (fluid flow)
- Interaction

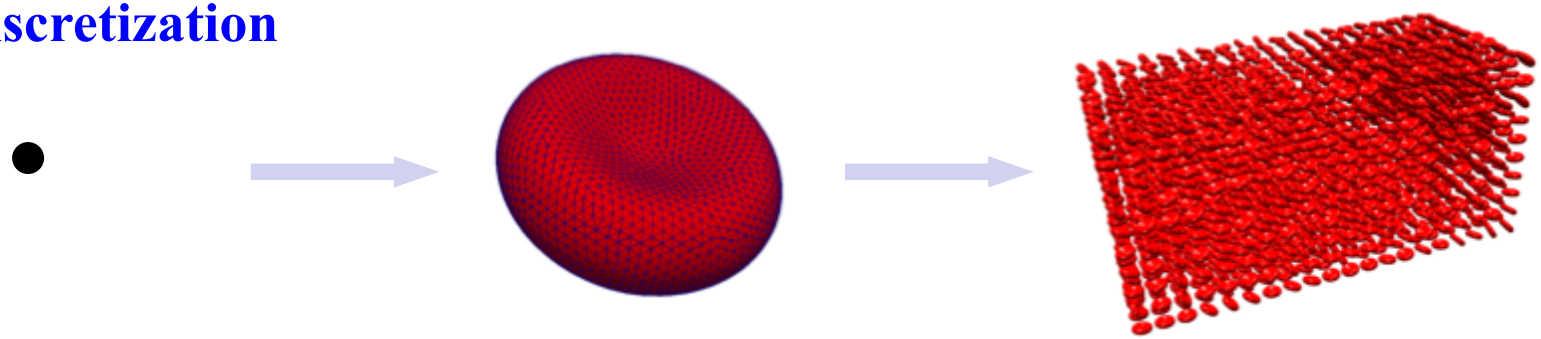
http://www.westfloridaveincenter.com/2015/12/interesting-facts circulatory-system/
https://sites.jmu.edu/bio103shook

Solid solver

LAMMPS is good at:

- **Spatial decomposition**
- **Parallel computing (Message Passing technique)**
- **Particle-based method (neighbor list and ghost atom schemes)**

❑ Solid discretization



Coarse-grained particle Single RBC RBC Suspension

Coarse-grained model

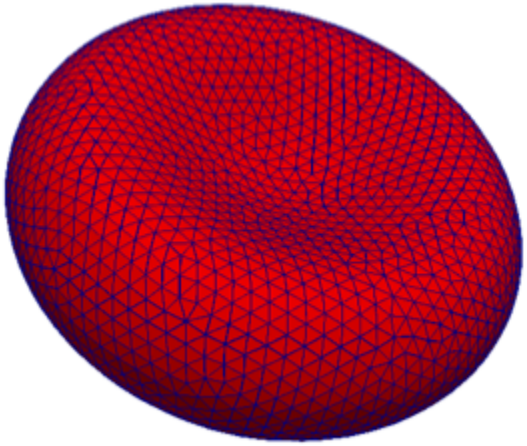
$$U_{WLC} = \frac{k_B T l_m}{4p}\frac{3x^2 - 2x^3}{1-x}, \quad U_{POW} = \frac{k_p}{l}$$ **Bond**

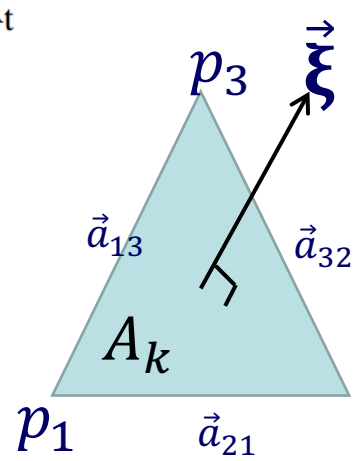
$$U_{bending} = \sum_{k\in 1\ldots N_s} k_b[1-\cos(\theta_k - \theta_0)]$$ **Dihedral**

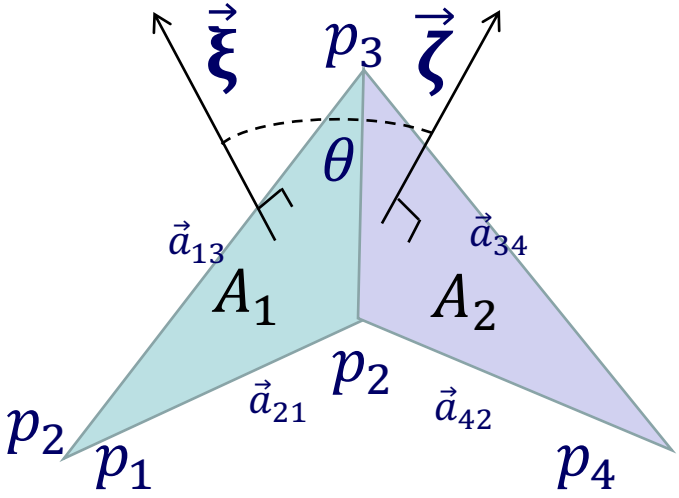
$$U_{area} = \sum_{k=1\ldots N_t} \frac{k_d(A_k - A_{k0})^2}{2A_{k0}} + \frac{k_a(A_t - A_{t0})^2}{2A_t}$$

Angle

$$U_{volume} = \frac{k_v(V - V_0)}{2V_0}$$







$$U(\{\mathbf{x}_i\}) = U_{stretching} + U_{bending} + U_{area} + U_{volume}$$

Fedosov et al. (2010)

Flow Solver

❑ Plasma dynamics

Incompressible Flow (CFD)

Palabos
CFD, COMPLEX PHYSICS

$$\nabla \cdot \boldsymbol{v} = 0$$

$$\rho\left(\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v}\right) = -\nabla p + \mu \nabla^2 \boldsymbol{v} + \boldsymbol{f}$$

- Particle-based model: Lattice Boltzmann Method
- Innovative matrix-based interface
- block-structured partitioning

Palabos offers a powerful environment of fluid flow simulations

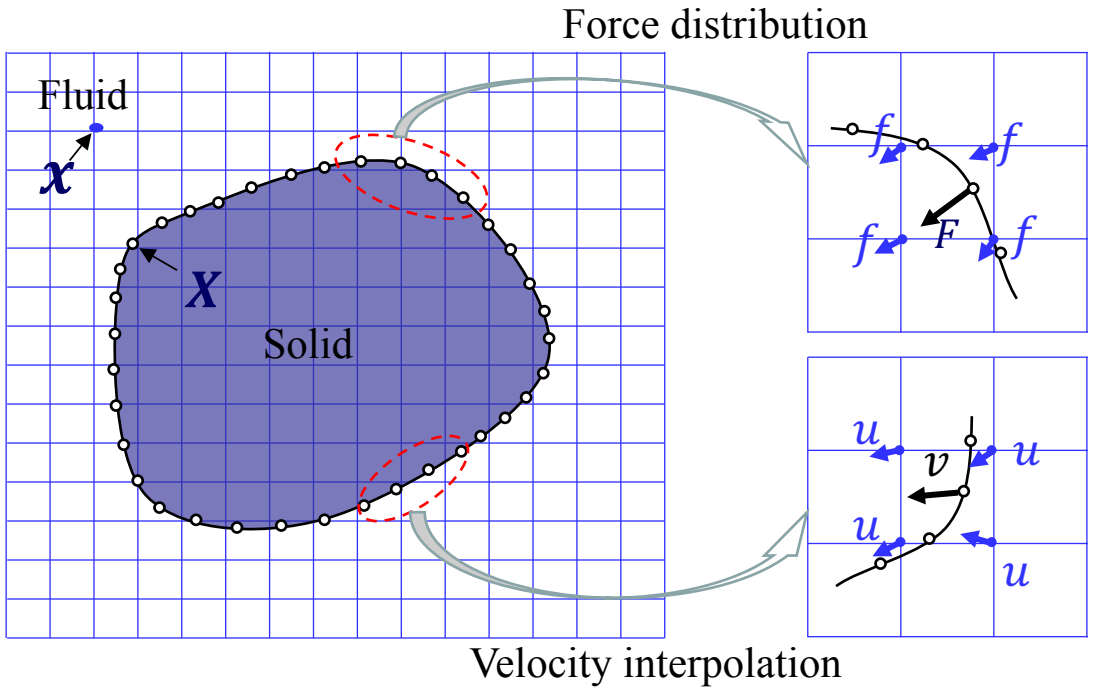
Interaction

❑ Interaction

Immersed boundary

$$u_i^s(\mathbf{X}^s,t) = \int_\Omega u_i(\mathbf{x},t)\delta(\mathbf{x}-\mathbf{x}^s(\mathbf{X}^s,t))\mathrm{d}\Omega$$

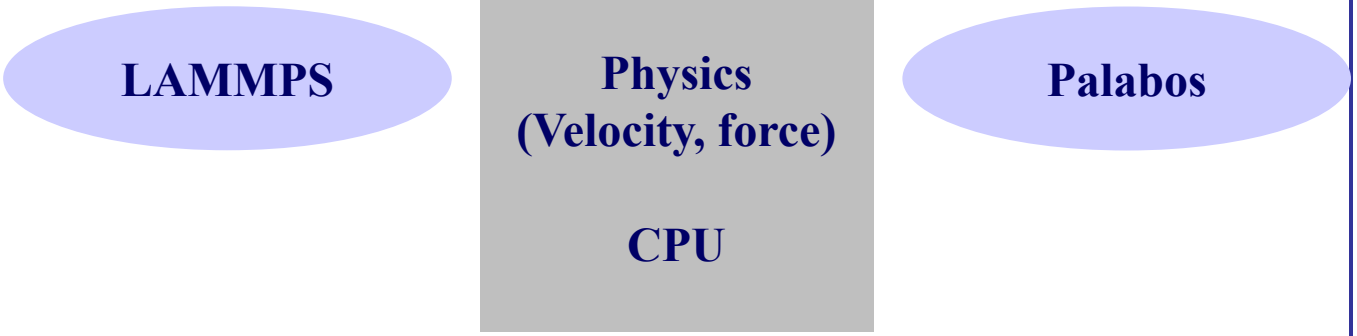
$$f_i^{FSI,s}(\mathbf{x},t) = \int_{\Omega^s} F_i^{FSI,s}(\mathbf{X}^s,t)\delta(\mathbf{x}-\mathbf{x}^s(\mathbf{X}^s,t))d\Omega$$



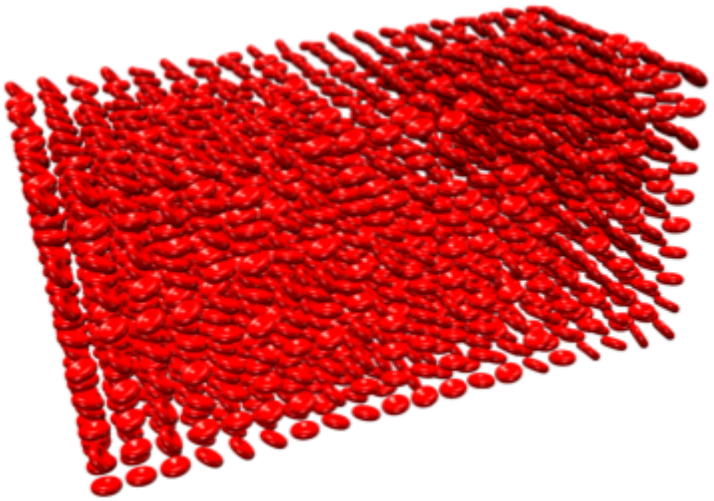
❑ CPU mapping

LAMMPS: solid nodes

Palabos: fluid nodes



Results: Large scale blood flow



System: 2,000 RBCs

Grid

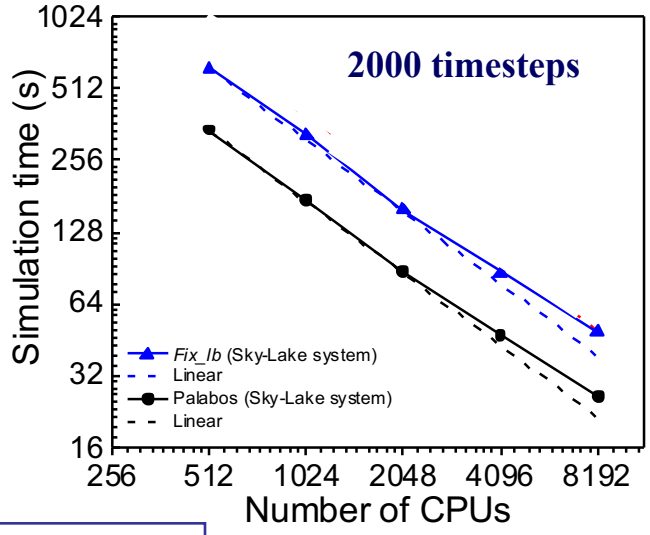
Solid : $3264 * 2000 = 6{,}528{,}000$

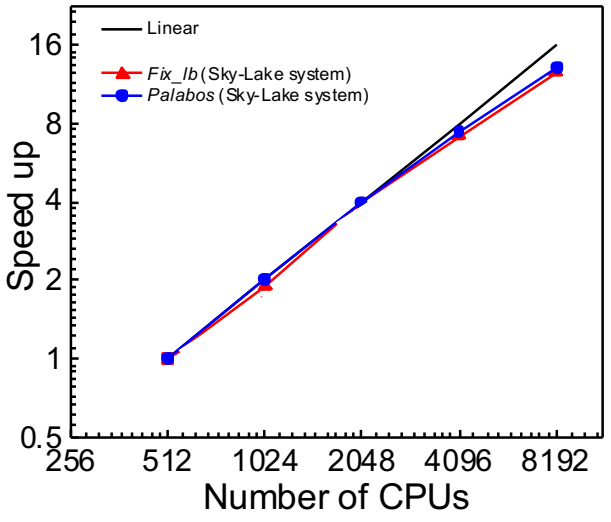
Fluid : $360 \times 720 \times 360 = 93{,}312{,}000$

Supercomputer (XSEDE, Stampede2):
Sky-Lake system

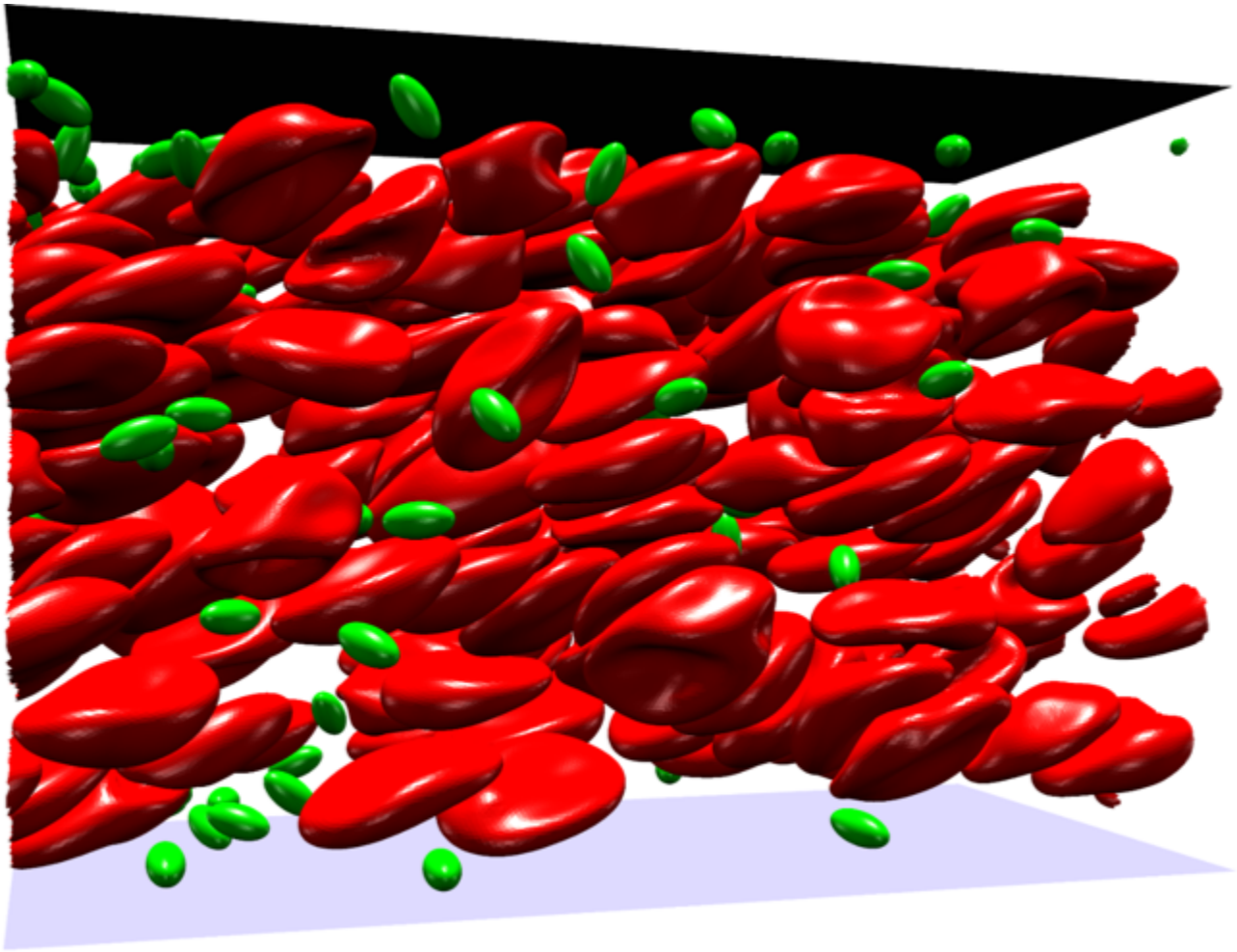
Fluid solver

- USER_LB package in LAMMPS
- Palabos (open source)

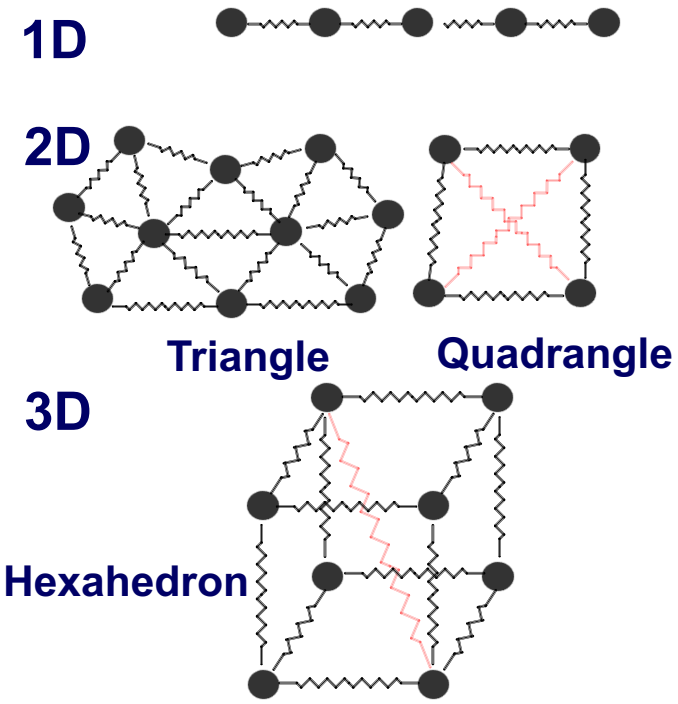




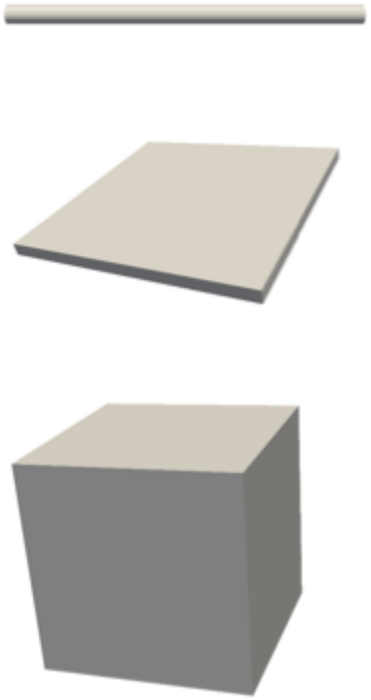
Applications: drug delivery system



General FSI



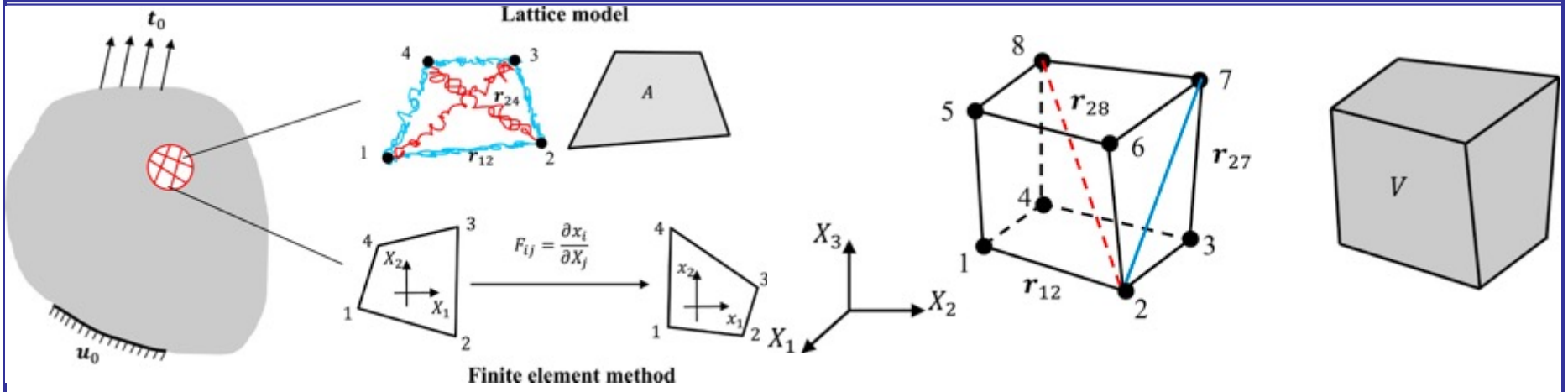
?



Lattice model

Continuum model

Lattice model



$$U_{neo} = \mu^s (I_1 - 3)/2 - \mu^s \ln J + \lambda (\ln J)^2/2$$

$$F_{ij} = \frac{\partial x_i}{\partial X_j} = x_i^a \frac{\partial N^a}{\partial X_j}$$

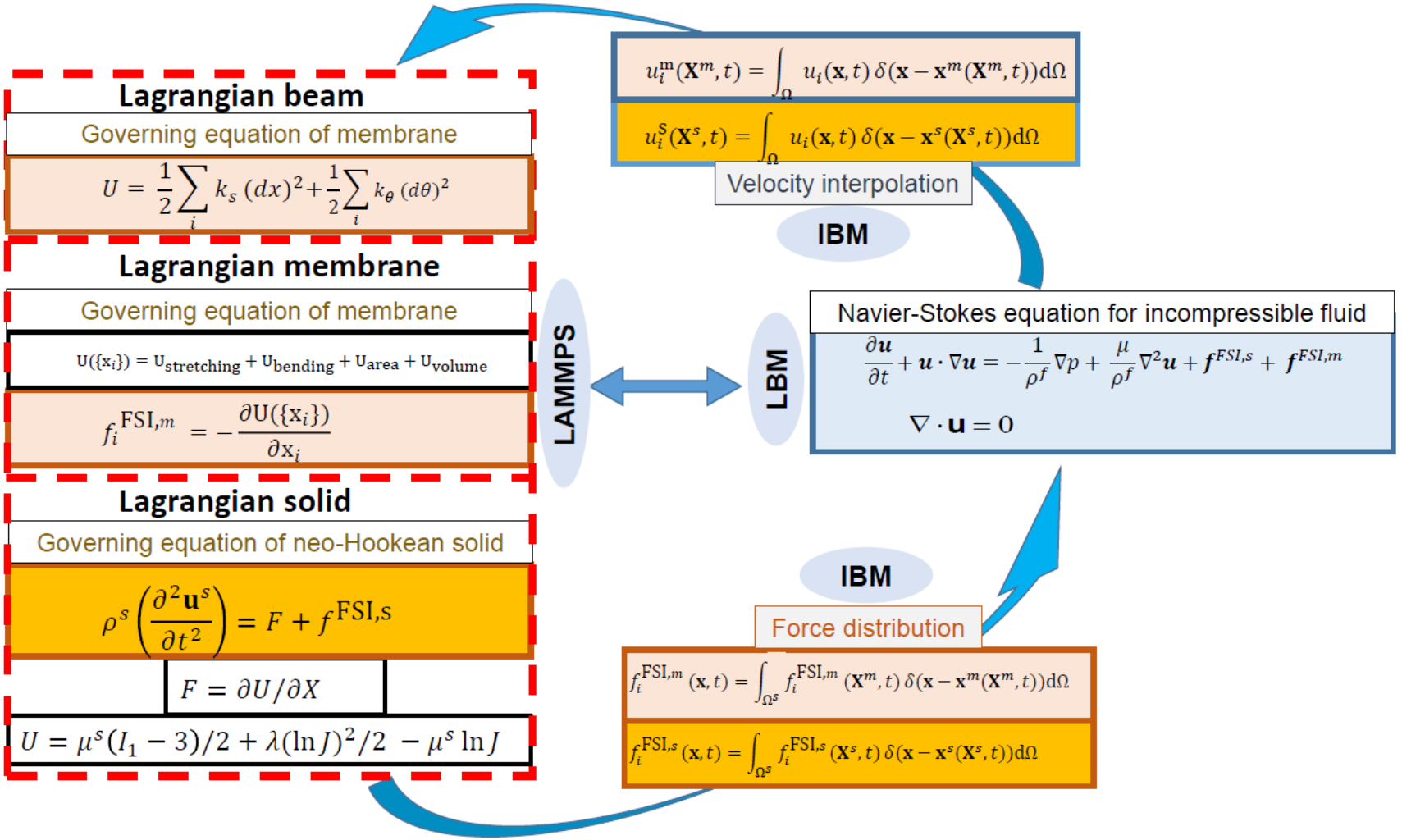
Harmonic bonds!

$$I_1 = F_{ij} F_{ij} + 1$$

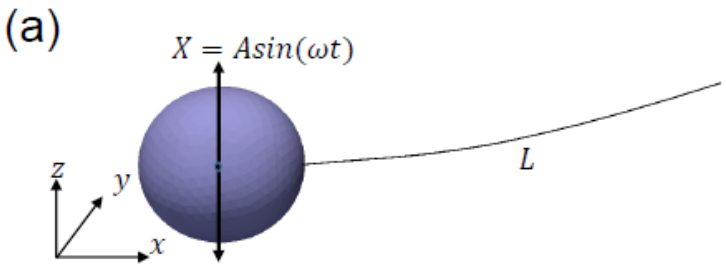
$$A_0 U_{I_1} = \int \frac{1}{2} \mu^s (x_i^a x_i^b \frac{\partial N^a}{\partial X_j} \frac{\partial N^b}{\partial X_j} - 2) dA_0 = -\frac{1}{2} k_{ab} x_i^a x_i^b - \mu^s A_0$$

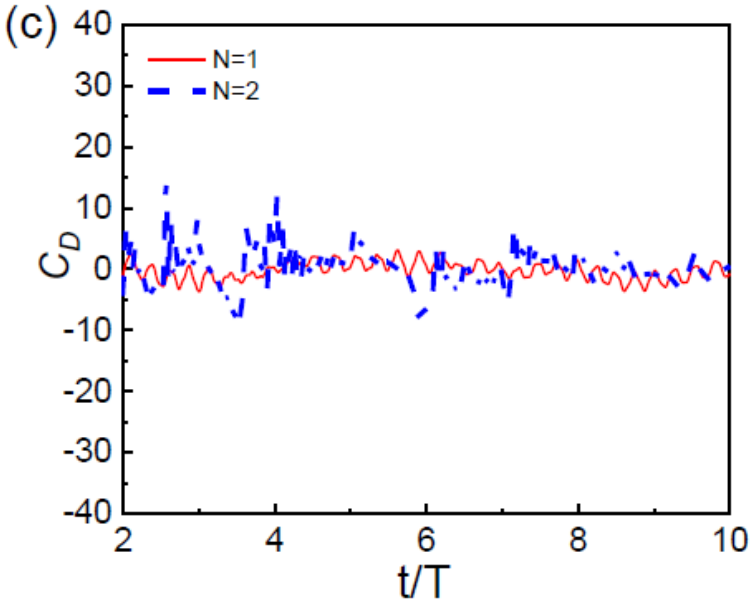
$$k_{ab} = -\int \mu^s \frac{\partial N^a}{\partial X_j} \frac{\partial N^b}{\partial X_j} dA_0$$

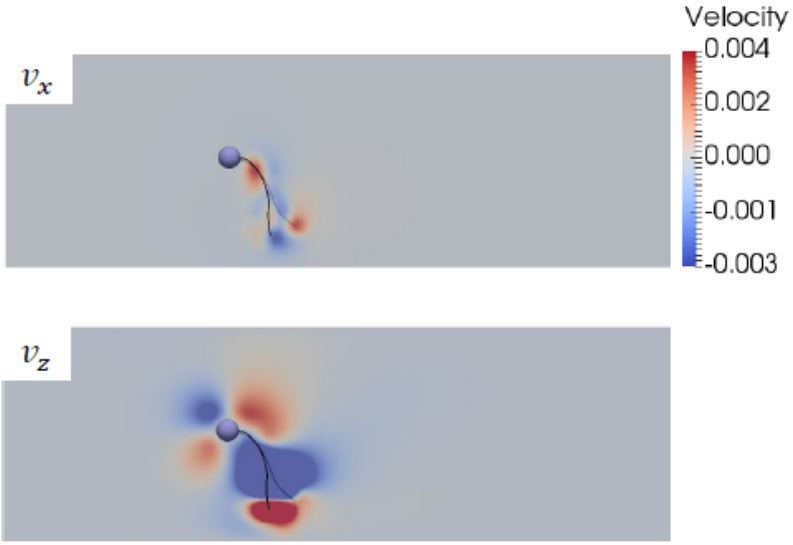
Package Framework



Results: Swimming of micro-organism

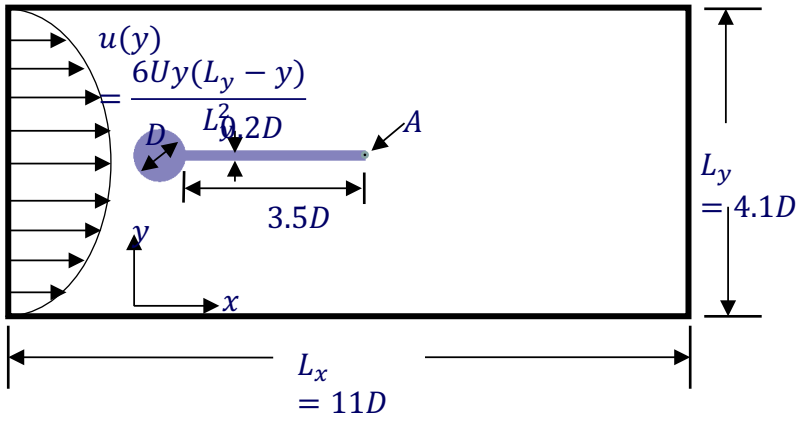




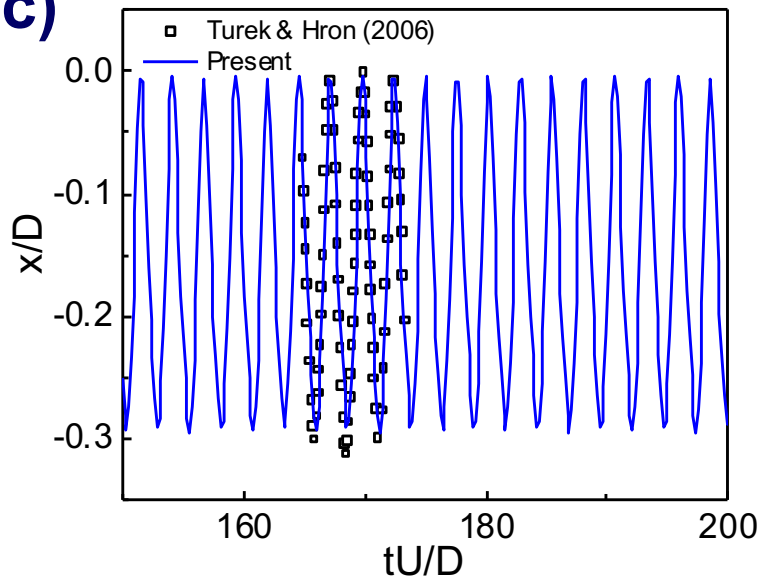


Results: Flapping of an elastic 2D beam

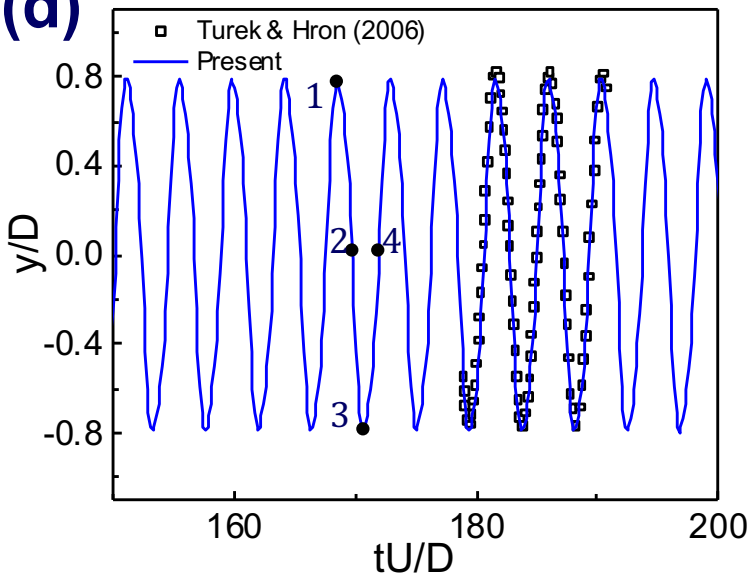
(a)



(c)

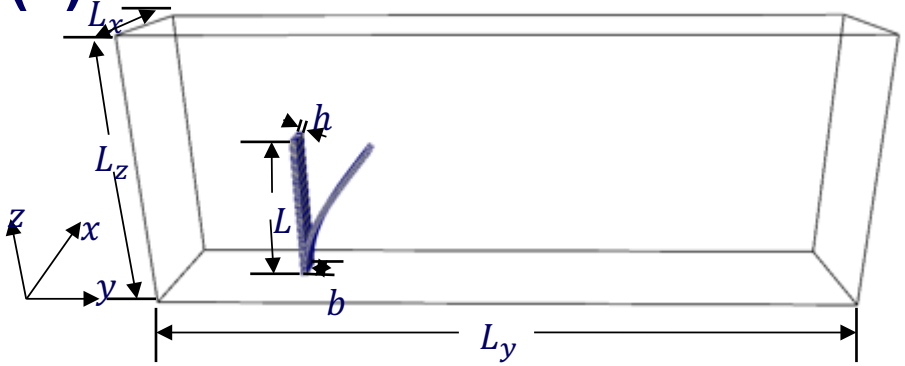


(d)

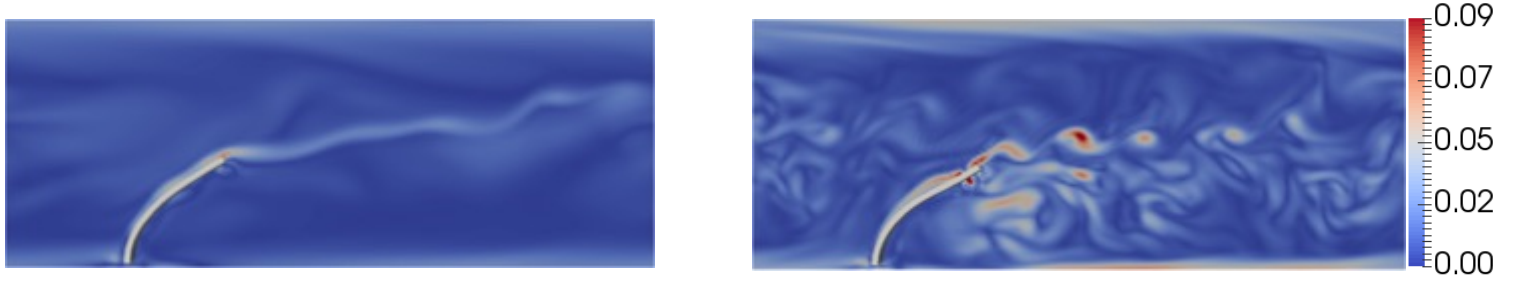


Results: Flow passing 3D flexible plate

(a)



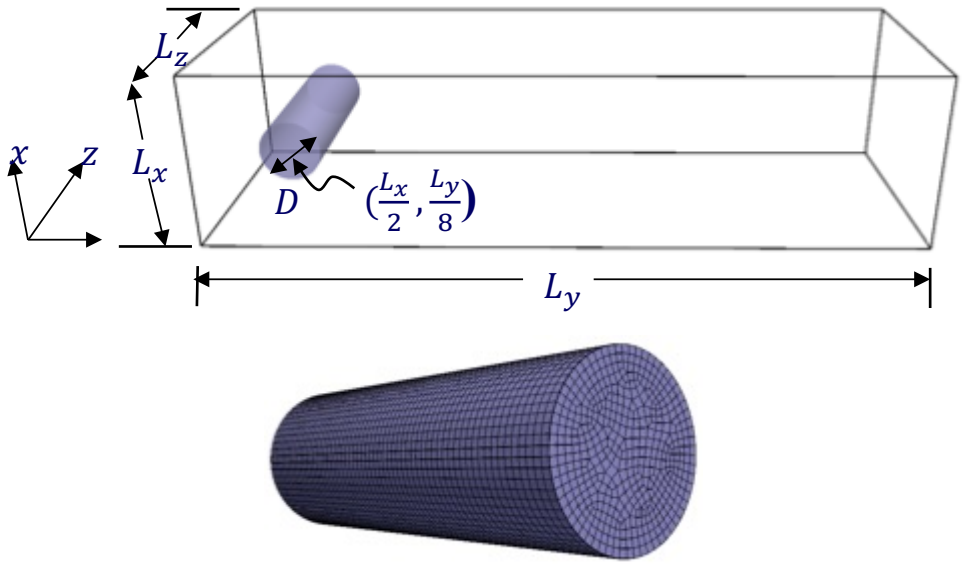
(b)



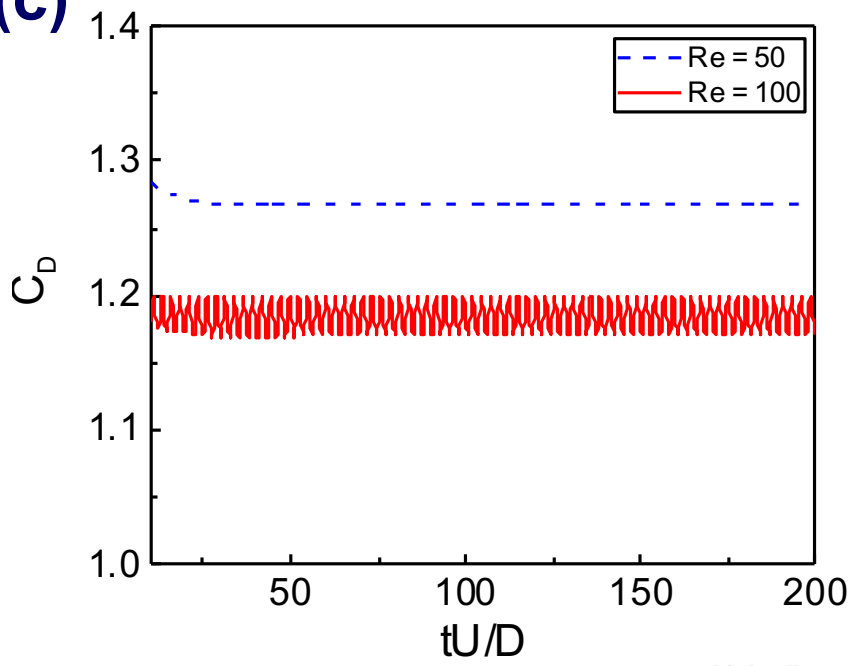
$Re = 60$ $Re = 100$

Results: Flow passing rigid cylinder

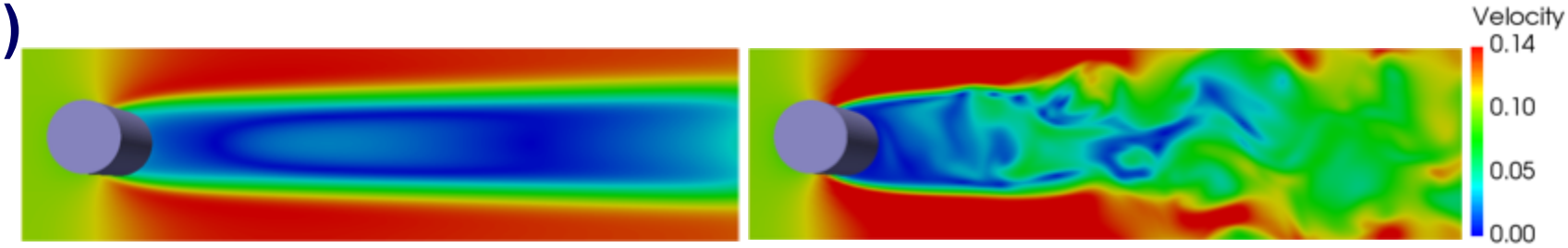
(a)



(c)

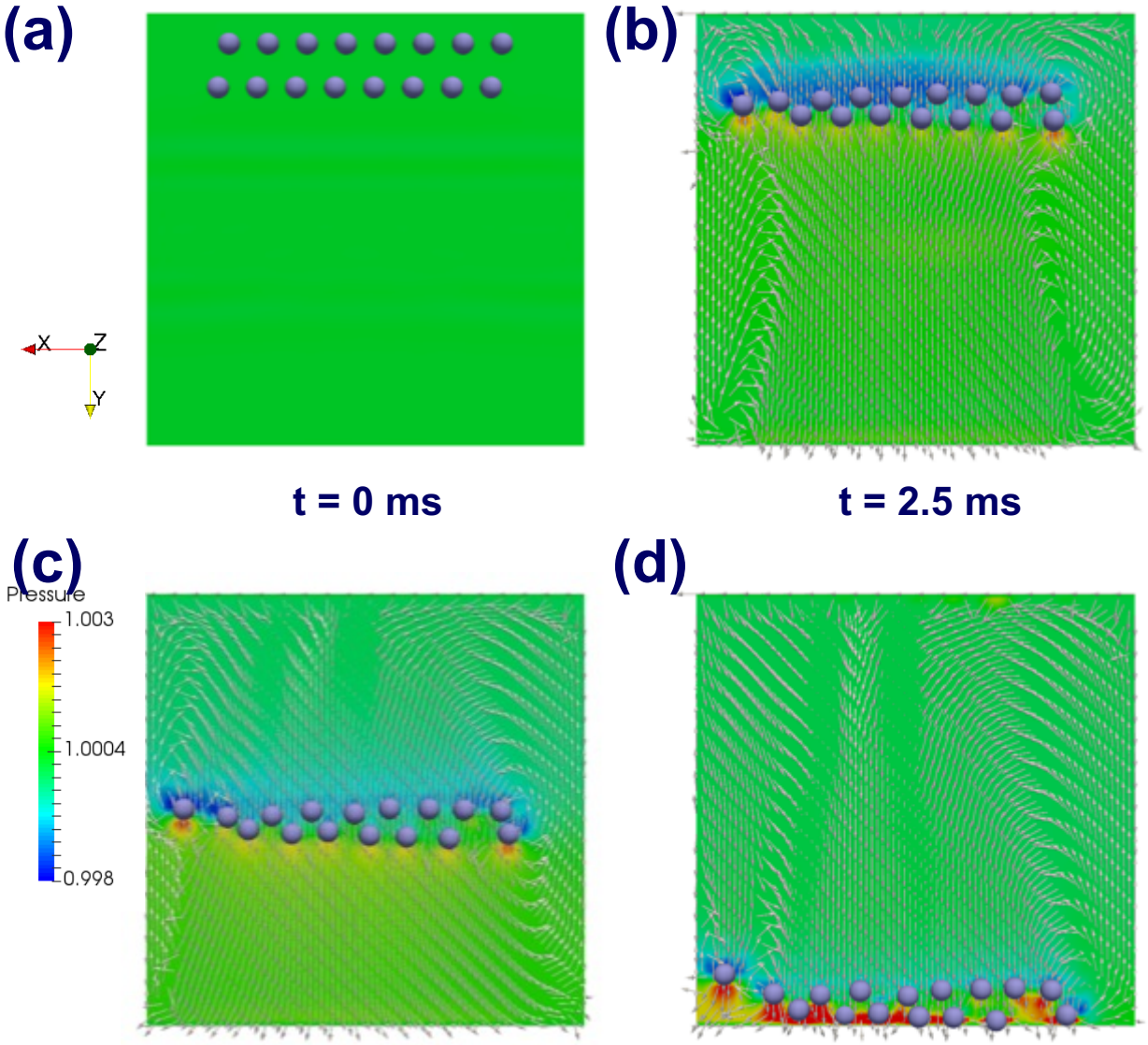


(b)



$Re = 50$ $Re = 100$

Results: Deposition of rigid spheres



Conclusion

- Coupling Palabos and LAMMPS
- Higher efficiency in application in blood flow
- Extending to general FSI problem

Funding Support

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GE Fellowship for Innovation