ISTITUTO ITALIANO DI TECNOLOGIA
DRUG DISCOVERY AND DEVELOPMENT

Nanoparticles transport for cancer therapy

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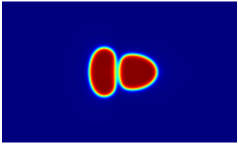
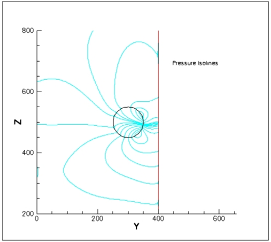
Few words about my interest areas...

Conservation laws

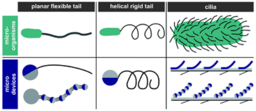
$$\partial_t u + \nabla \cdot f(u) = g(t, x),$$

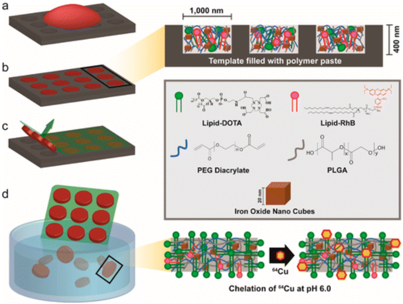
Turbulent Flames | Interacting Bubbles | Micro- and Nano-transport

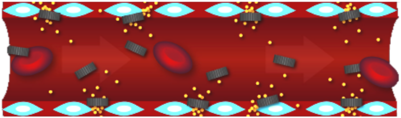




Micro- and Nano-transport

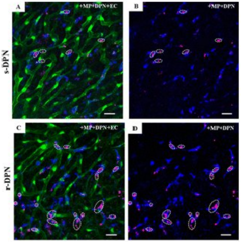




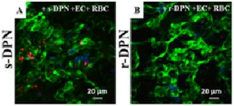


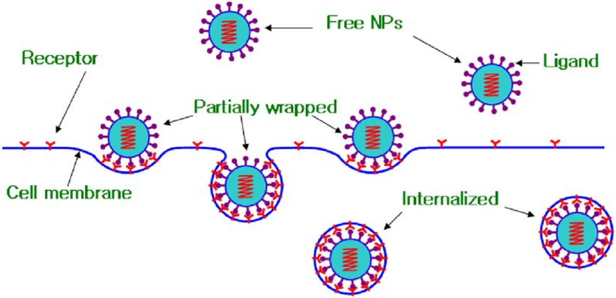
How a nanoparticle works?

DPNs in healthy liver

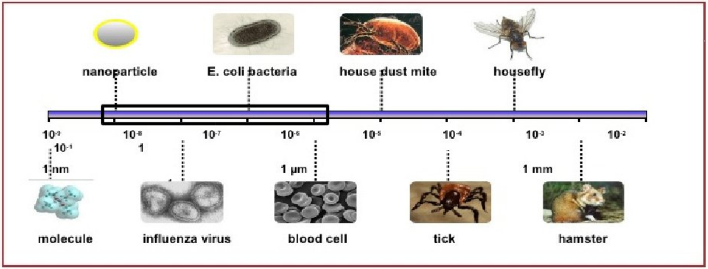


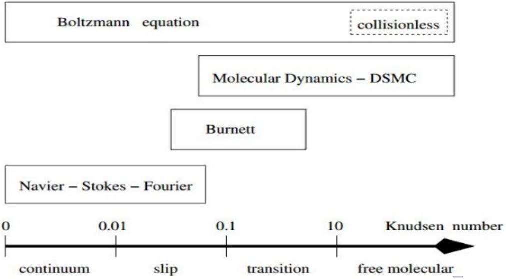
DPNs trapped in cancer





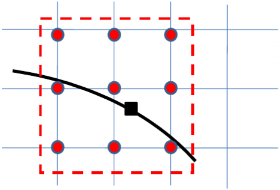
Why do we solve Boltzmann's equation?





Immersed-Boundary Technique

- Compute the intermediate velocity (non-solenoidal) in all of the Eulerian point through the Moving Least Squares (MLS) approximation
- Compute forcing at the Lagrangian markers
- Transfer the forcing at the Eulerian grid points
- The scaling factor, c_l, is such that the total forcing is not altered by the transferring process



$$\hat{\boldsymbol{U}}(\boldsymbol{x}) = \sum_{k=1}^{ne} \phi_k^l(\boldsymbol{x})\, \hat{\boldsymbol{u}}_k$$

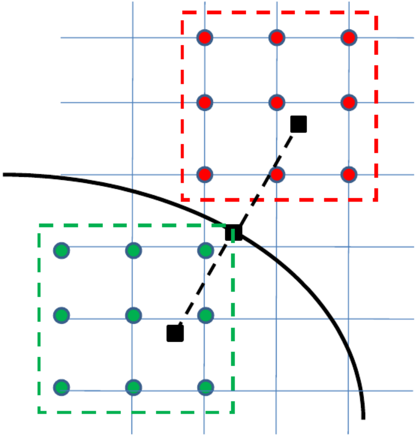
$$\boldsymbol{F} = \frac{\boldsymbol{U}_b - \hat{\boldsymbol{U}}}{\Delta t}$$

$$\boldsymbol{f}^k = \sum_{l=1}^{nl} c_l\, \phi_k^l \boldsymbol{F}_l$$

$$\frac{\partial \mathbf{u}_f}{\partial t} + \nabla \cdot (\mathbf{u}_f \mathbf{u}_f) = -\frac{\nabla p}{\rho_f} + \nu \nabla^2 \mathbf{u}_f + \boldsymbol{f}$$

Fluid-Structure Interaction

Using the same MLS formulation, the pressure and velocity derivatives are evaluated at the probe location.



$$p_l = p_l^p + \frac{D\boldsymbol{v}_l}{Dt} \cdot \boldsymbol{n}_l$$

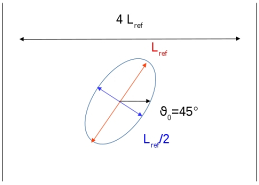
Velocity derivatives on the body are assumed to be equal to that on the probe location (linear velocity profile)

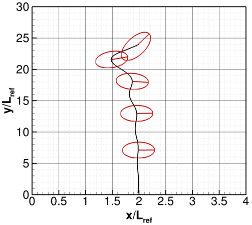
$$\boldsymbol{F}_{tot}(t) = \sum_{l=1} (\boldsymbol{\tau}_l \cdot \boldsymbol{n}_l - p_l \boldsymbol{n}_l)\, S_l$$

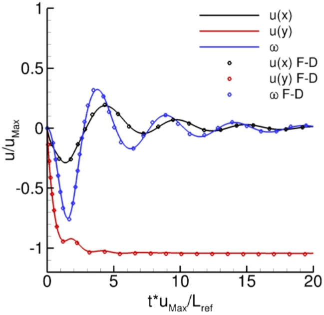
$$\boldsymbol{M}_{tot}(t) = \sum_{l=1}^{nl} [\boldsymbol{r}_l \times (\boldsymbol{\tau}_l \cdot \boldsymbol{n}_l - p_l \boldsymbol{n}_l)]\, S_l$$

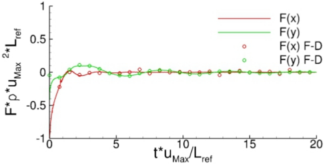
Zero-thickness bodies: two probes are created.

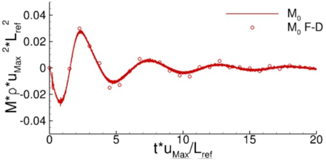
Sedimentation of an Elliptical particle



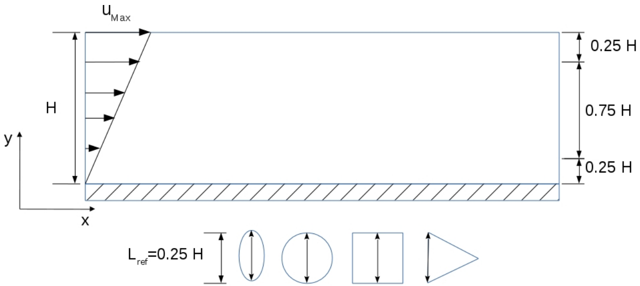


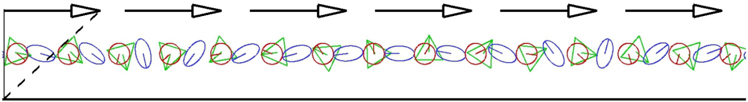




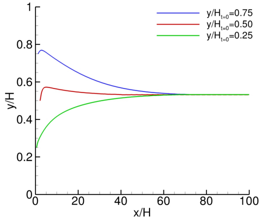


Particle transport in moderate and low Reynolds flows

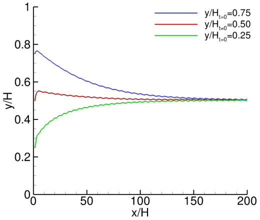




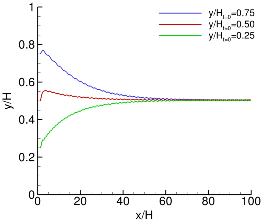
Particle transport in moderate Reynolds flows



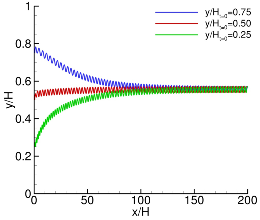
(a) Circle



(b) Ellipse

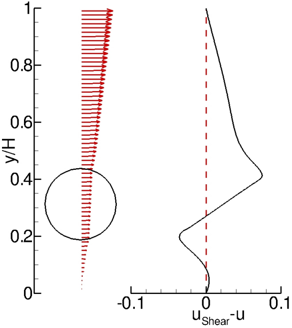


(c) Square

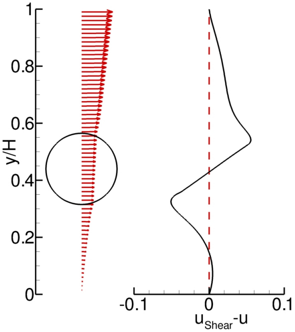


(d) Triangle

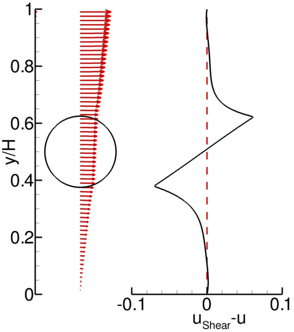
Particle transport in moderate Reynolds flows



(e) $t = 10$

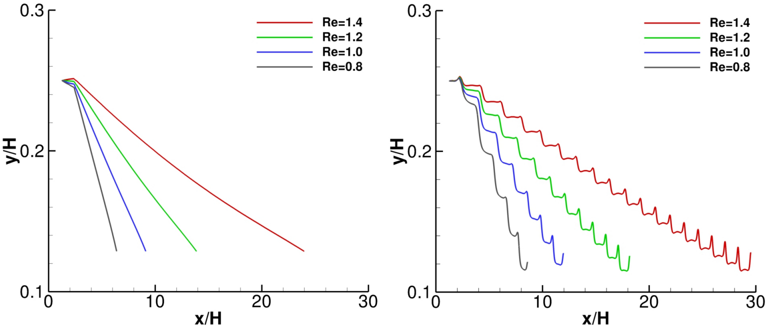


(f) $t = 50$



(g) $t = 500$

Particle transport in low-Reynolds flows: margination

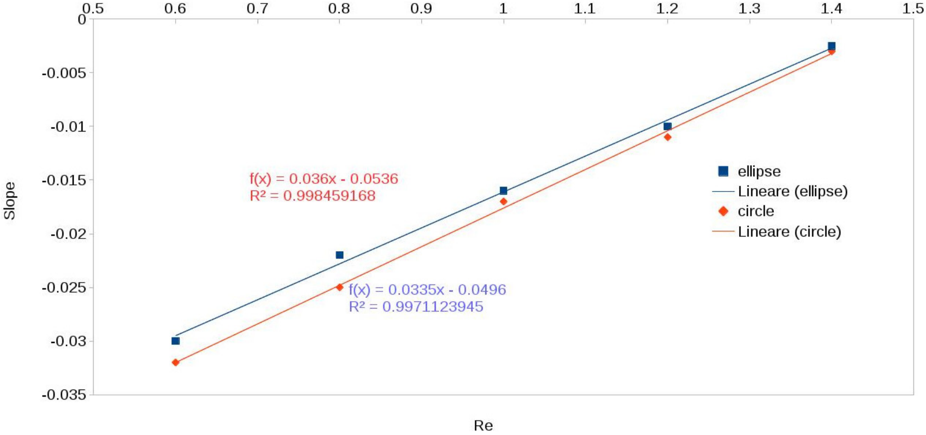


(h) Circle

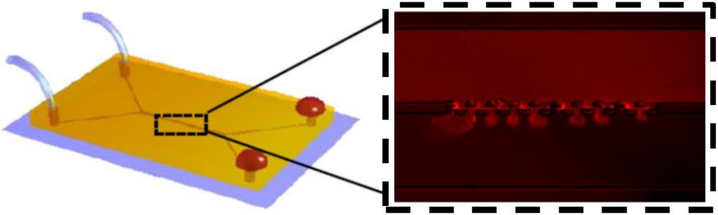
(i) Ellipse

Particle transport in low-Reynolds flows: margination

$\partial_x(y(x))$ linear in Re



Conclusions and Future works



- Rationally design polymeric nanoconstructs for multimodal imaging and combination therapy in cancer
- Fabricate microfluidic chips for rapid drug screening

Greetings from the Laboratory of Nanotechnology for Precision Medicine!!