MODELING THE VASCULAR TRANSPORT AND ADHESION MECHANICS OF DEFORMABLE NANOCONSTRUCTS

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ABSTRACT

Nanoconstructs are small, man-made objects that can load and systemically deliver multiple therapeutic and imaging agents. Enhancing the vascular transport and adhesion of nanoconstructs is crucial in the development of more effective therapeutic strategies against cancer and other diseases. The *size*, *shape*, *surface* properties and mechanical *stiffness* (*4S design parameters*) of nanoconstructs can be precisely and independently tailored providing numerous paths towards optimization [1,2]. This work focuses on the role of nanoconstruct stiffness in modulating vascular transport and adhesion mechanics.

Lattice Boltzmann (LB) and Immersed boundary (IB) methods are combined together for predicting the dynamics of deformable nanoconstructs in a linear, laminar flow. For the LB modeling, the lattice equation is derived using a Gauss-Hermite projection, wall boundary conditions are imposed through the Zou-He framework[3], and a moving least square algorithm is used to reconstruct the forcing term accounting for the immersed boundaries [4]. Nanoconstructs are modeled as a collection of mass-spring elements (elastic membrane) responding to a bending potential, a worm-like chain potential and the area conservation constraint. Furthermore, the nanoconstruct surface is decorated with adhesive molecules, ligands, interacting specifically with counter-molecules, receptors, distributed over the vascular walls. The molecular adhesive forces are computed through a probabilistic approach determining binding and unbinding over the entire surface as a function of local forces.

Vascular transport and adhesion can be characterized in terms of hydrodynamic conditions (Reynolds number and blockage ratio), initial configuration and 4S design parameters of the nanoconstruct.

REFERENCES

[1] G. Bao, Y. Bazilevs, J.-H. Chung, P. Decuzzi, H. Espinosa, M. Ferrari, H. Gao, S. Hossain, T. Hughes, R. Kamm, W. Liu, A. Marsden, B. Schrefler, Usnctam perspectives on mechanics in medicine, Journal of the Royal Society Interface 11 (97).O.C. Zienkiewicz and R.C. Taylor, *The finite element method*, 4th Edition, Vol. 1, McGraw Hill, 1989.

[2] S.-Y. Lee, M. Ferrari, P. Decuzzi, Shaping nano- micro-particles for enhanced vascular interaction in laminar flows, Nanotechnology 20 (49) (2009) 495101.

[3] Q. Zou, X. He, On pressure and velocity boundary conditions for the lattice boltzmann bgk model, Physics of Fluids 9 (6) (1997) 1591–1598.

[4] M. Vanella, E. Balaras, A moving-least-squares reconstruction for embedded-boundary formulations, Journal of Computational Physics 228 (18) (2009) 6617 – 6628.