

PROJECT INTRODUCTION

Objectives

To create various DPD models for DNA molecules, blood cells and micro vessels and to explore in particular bio-fluid flows in micro channels and simulate micro cell trapping and micro filtration.

Project Investigator / Manager

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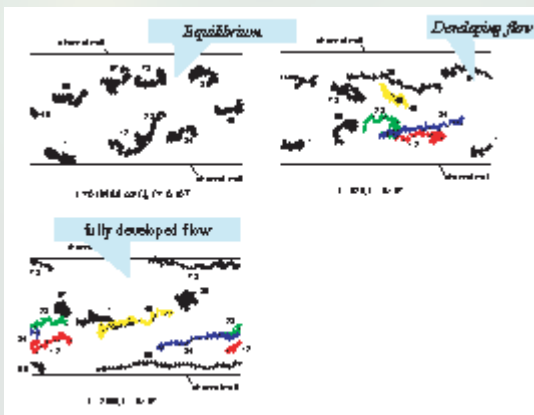
Abstract

Dissipative Particle Dynamics (DPD) is a relatively new mesoscale simulation technique; its mean quantities satisfy the conservation laws exactly. It can cope with complex-structured fluids, such as colloids, polymer solutions, especially bio-fluids. In BioMEMS devices and micro vessels, the size of the channels is in the same order of magnitude as that of DNA molecules and blood cells. The validity of continuum mechanics may be in doubt in these cases, while molecular dynamics is too inefficient for these mesoscale flows. This project uses DPD Simulation to create the various DPD models required.

PROJECT DETAILS

Description

In our study, the flow of molecules through a slit (see figure) has been examined using DPD. The suspending fluid is treated as an ensemble of interacting particles. Molecules are treated as particles that are connected by spring like forces (FENE model). Molecule-fluid particle interaction forces are the same those for fluid-fluid particle interactions. There are approximately 90,000 particles in the system.



Bio-fluid flows in micro channels

The results of the project would have a direct benefit to the following:

- BioMEMS design;
- Research institute on blood micro circulation; and
- Industries dealing with suspensions, colloids and emulsions.

DPD simulation is a compute-intensive process. Grid Computing in this process enables each flow domain to be divided into several subdomains which is then assigned to compute resources in the Grid environment where the simulations of particle flows are executed concurrently – tapping unused resources over the Grid to provide the speed-up in simulation and accelerate analytical and decision making process.

Collaborating Organization:

Institute of High Performance Computing