µLatte3D: Tool for Lattice-Boltzmann Phase Analysis

In this effort, user-interface capabilities were added to existing lattice-Boltzmann (LB) capabilities, which include analysis for filtration, collection, separation, and sample preparation processes. They also enable analysis of both viscous and gaseous fluid phases, particulates, and sieving media. The packaged capability integrates interfaces, analysis tools, and physics modules into a single software package that facilitates ease of use and hybrid analysis with other computational capabilities.

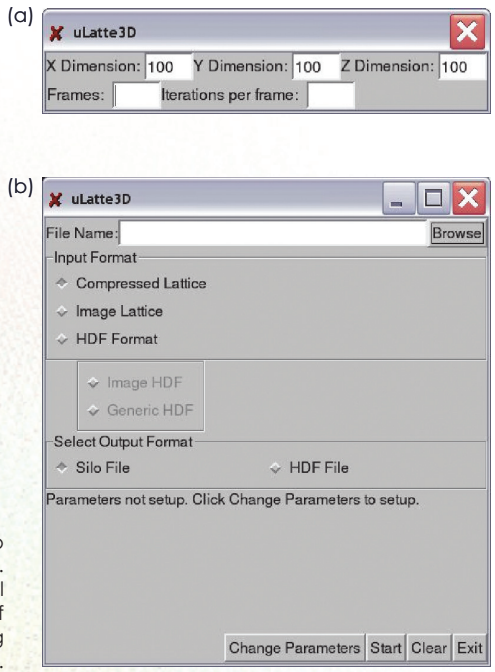

Figure 1. User interface to set up and launch µLatte3D simulations. (a) Set-up of the computational domain and duration of simulation "time;" (b) importing the lattice structure.

Project Goals

The package framework incorporates all of the scripts for problem set-up, job control, data analysis and visualization, and a user-friendly interface to enable pedestrian use of this capability. Now known as µLatte3D, the tool handles both gaseous and viscous fluids. It is a 3-D and parallel analysis tool that currently runs on Linux, AIX, and DEC/Compaq platforms.

Relevance to LLNL Mission

The LLNL programs that will benefit directly are Homeland Security, Medical Technologies (Bioengineering), programs related to Earth and Environmental Sciences, and bio-computations (Genomes To Life and fundamental biology). µLatte3D enables predictive analysis of complex fluids in complex micro- and nano- environments.

FY2005 Accomplishments and Results

In FY2005, the existing LB capabilities, both viscous and gaseous phase, were packaged into a single capability, now known as µLatte3D. To facilitate ease of use, a user interface,

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for both input and output/visualization, was also integrated with the overall μLatte3D package. The input facilities were enabled by leveraging the geometry infrastructure from CASC's Overture framework (www.llnl.gov/CASC/Overture/). The framework was modified to include a new lattice generation module. This tool can be used to interactively create new problem definitions (geometry) or to import geometry from CAD via the industry standard IGES file format. Overture's fast geometry query tools are then used to generate the computational domain and boundary information required by μLatte3D.

To facilitate easy problem set-up, all flags, physics, and lattice parameters are now integrated into a single input file. This single input file can be accessed and modified directly or through an easy-to-use interface, as shown in Fig. 1.

All input, run time, and output data structures are stored in Silo and/or HDF5 formats, and the output data structures are directly accessible to visualization tools. Figure 2 shows an example: VisIt visualization output for the velocity field around a suspension of spherical particles.

A variety of data will be written to the graphics files and viewable with VisIt, including materials (walls and channels); and particle data, to include position, velocity, and bulk suspension behavior. Additionally, fluid velocity, shear, and temperature fields can be displayed. The capability enables characterization of particle and fluid transport in complex micro- and nano-environments, both gas and liquid phases, with parallel restarts.

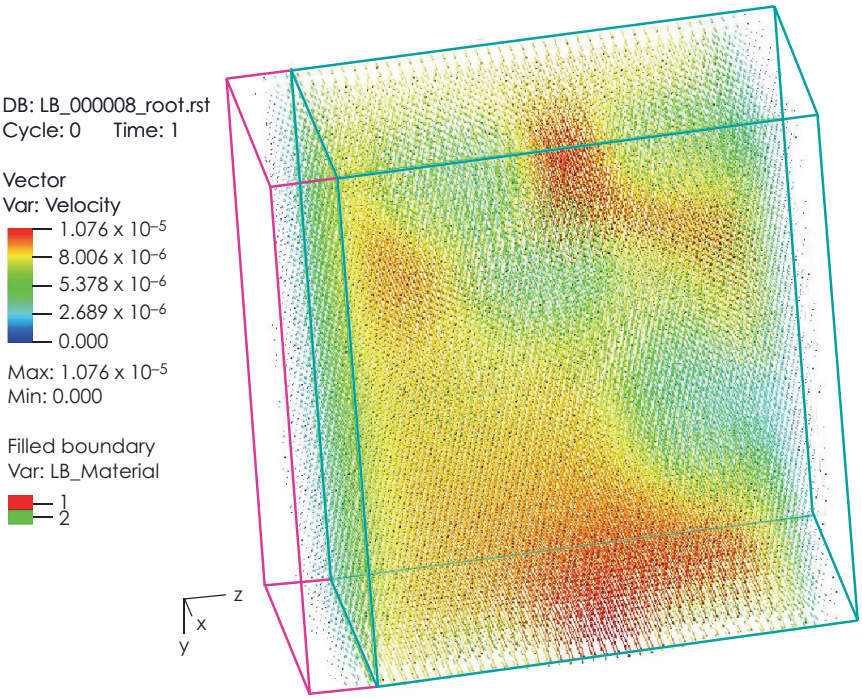

Figure 2. Frame from a movie of particles in channel flow. Velocity field is produced by μLatte3D viewed using VisIt.