ARGONNE **LEADERSHIP COMPUTING** FACILITY

Instrumenting Multiphysics Blood Flow Simulation Codes for In Situ Visualization and Analysis

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Abstract

Blood flow simulations have important applications in engineering and medicine, requiring visualization and analysis for both fluid (blood plasma) and solid (cells). Recent advances in blood flow simulations highlight the need of a more efficient analysis of large data sets. Traditionally, analysis is performed after a simulation is completed, and any changes of simulation settings require running the simulation again. With bi-directional in situ analysis we aim to solve this problem by allowing manipulation of simulation parameters in run time. In this project, we describe our early steps toward this goal and present the in situ instrumentation of two coupled codes for blood flow simulation using the SENSEI in situ framework.

Motivation

- Enabling faster analysis for large scale simulations without writing big data to files
- Leveraging in situ analysis and visualization frameworks for blood flow simulation
- Providing a next-generation interactive in situ simulation platform for medical training

Results

- LAMMPS and Palabos coupled simulation instrumented with SENSEI
- A workflow for creating an in situ pipeline was identified. Figure 1 describes our in situ pipeline and workflow
- Visual validation of the data with visualizations in ParaView. Figure 2 shows a visualization of LAMMPS (cells) and Palabos (background flow velocities) data with ParaView/Catalyst

Future Work

- Validation with large scale runs
- Bi-directional in situ in SENSEI will enable the user to change simulation properties in ParaView while the simulation runs
- Use this instrumentation to develop a platform for medical applications

References

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Methods

We integrate the SENSEI in situ framework with existing fluid/solid interaction code composed of the open-source fluid solver (Palabos) and solid solver (LAMMPS).

LAMMPS

- Large Scale Atomic/Molecular Massively Parallel Simulator
- Accepts user inputs such as bond type, number of particles, internal velocity, etc.
- Extended to model red blood cells with interactive membrane particles

Palabos

- Parallel Lattice Boltzmann Solver
- Solves fluid (blood plasma) properties using Lattice Boltzmann method [2].
- Fluid velocity, vorticity, and normalized velocity

In Situ Instrumentation

- We implement SENSEI Bridge and Data Adaptor in C++ code
- SENSEI Bridge is called from the simulation, initializes SENSEI, sends data to Data Adaptor, and calls SENSEI after every new simulation timestep
- SENSEI Data adaptor receives pointers to the arrays computed by LAMMPS and Palabos, creating VTK objects used by SENSEI analysis adaptors, and using zero-copy mechanisms when possible. It also provides data to the multiple SENSEI analysis adaptors available

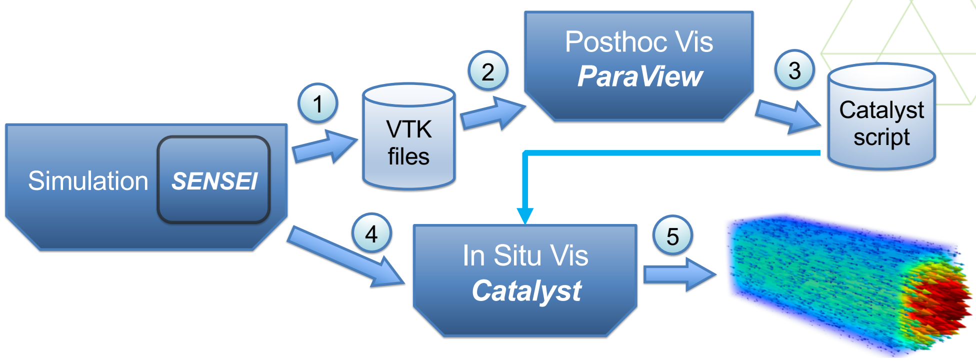

Figure 1: Workflow to create an in situ visualization pipeline.

Workflow

1. Run a small simulation with SENSEI and save a representative dataset;
2. Visualize interactively with ParaView and define parameters for the visualization pipeline;
3. Save the pipeline as a Catalyst script;
4. Run the simulation at scale with the SENSEI Catalyst adaptor, using the Catalyst script created in (3);
5. Visualize results in situ

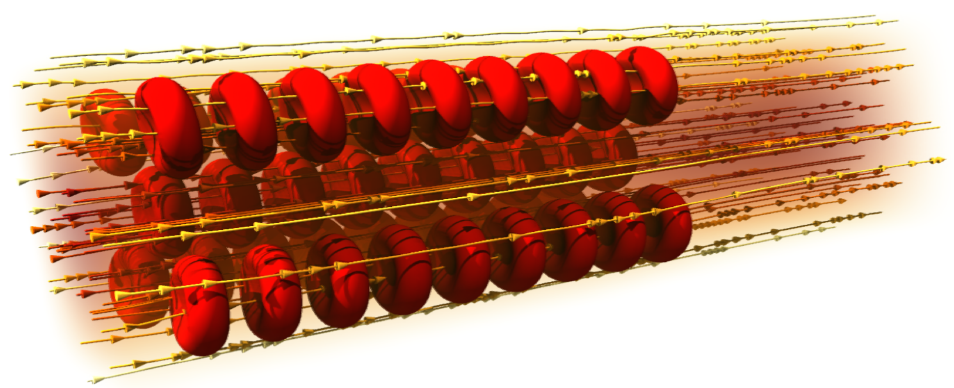

Figure 2: Visualization of blood cells and flow in ParaView. The data is extracted in situ with SENSEI

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