gLBM: A GPU enabled Lattice Boltzmann Method Library

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Software

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Summary

Lattice Boltzmann Methods (LBM) are a class of computational fluid dynamics (CFD) for simulation. Unlike traditional formulations of the Navier-Stokes equations that simulate fluid dynamics on a macroscopic level, the LBM characterizes the problem on a mesoscopic level applied to a grid discretization. LBM solves the fluid density problem with collide and stream (relaxation) processes. This approach has several advantages, including its adaptability to numerous fluid domains (i.e., vapours, liquid droplets), complex boundaries, and parallelization. Traditional CFD methods are limited in the ability to parallelize the algorithm; however, the LBM algorithm discretization can be easily parallelized both for CPUs and GPUs. This enables fast fluid solutions for complex fluid domains. There are limitations associated with the LBM, including high mach number applications. However, active research is addressing these limitations.

Statement of need

The `gLBM` library is the Lattice Boltzmann algorithm implemented using GPUs for a fast fluid solver. The library is implemented in C++ and Cuda and is validated using a robust suite of custom verification and validation tools for sustainable community-based use and development. `gLBM` leverages an easy to use API that is well-documented to import geometries for analysis using formats supported by ITK (McCormick et al., 2014), the open source Insight Toolkit, and configuration files that define the fluid parameters, grid discretization properites, and simulation parameters. An Apache 2.0 license was selected to support the widest distribution and use of the `gLBM` library.

The LBM algorithm builds on established work by (Krüger et al., 2017)(He & Luo, 1997)(Latt et al., 2008)(Succi, 2001)(Ubertini et al., 2010) to solve for the pressure and flow in the fluid domain. `gLBM` expands on this work to integrate solutions for wall shear stress and temperature. Initial work using this library has been published as pertains to analysis of the upper airways (Quammen et al., 2016)(R. B. Clipp et al., 2018)(R. B. P. Clipp et al., 2019). The combination of speed (GPU implementation), flexibility, permissive licensing, and integrated verification and validation make this library unique when compared to other available libraries of the LBM ("Palabos," 2020)("OpenLB – Open Source Lattice Boltzmann Code," 2020)("Lattice Boltzmann (LBM) Simulation Package for GPUs (CUDA, OpenCL)," 2020). This library is ideal for students, researchers, and industry users looking to expand their use of the LBM and will be supported and maintained by Kitware, Inc., leaders in open source software development.

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gLBM in Action

Numerical Benchmarking

We benchmarked the LBM implemented in `gLBM` by comparing the solution in cylindrical and rectangular channels with the analytic solutions. The cylindrical channel of length 0.1 meters and diameter of 0.01 meters was executed for a grid spacing (Δx) of 0.0004, 0.0005, 0.0006, and 0.0007 meters. A rectangular channel with dimensions of 0.08 meters in the x-direction, 0.02 meters in y-direction, and 0.01 meters in the z-direction was analyzed with the same grid spacings. The solutions were executed for 10,000 iterations under an imposed constant pressure gradient. The results for numerical and grid convergence were similar for both geometries, with the results showing an iteration convergence occurring at less than 3,000 iterations and grid convergence evident. The analytical solutions are implemented in the `gLBM` library for future verification and validation efforts. The comparison between the analytical and the computed solutions for the rectangular channel are shown in **Figure 1**. For both geometries, we observed an entrance effect and a fast convergence to a fully developed parabolic profile with less than 1% error. This is clearer when investigating the results slice by slice through both channels, as shown in **Figure 2**.

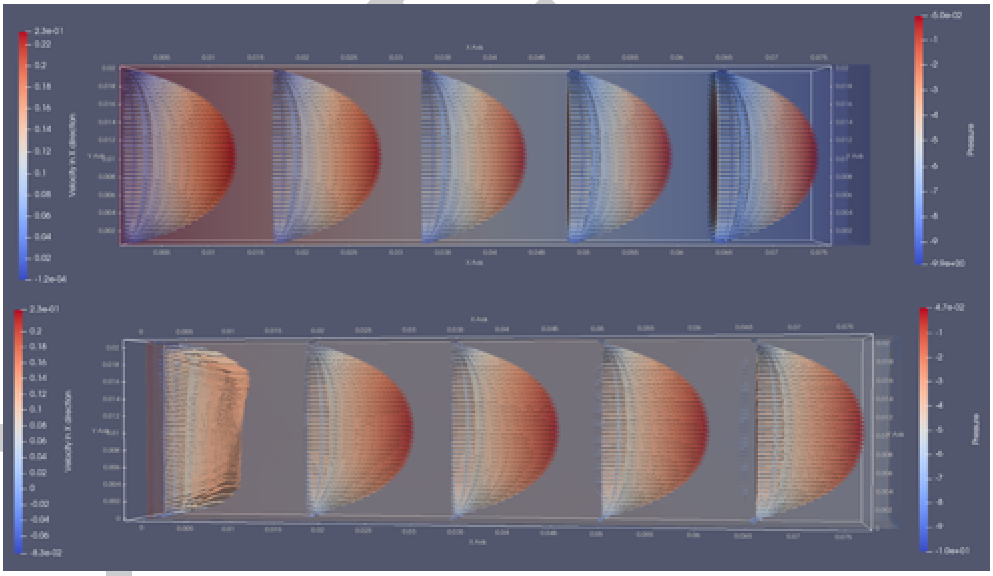

Figure 1: The analytical solution (top) is shown with the LBM computed solution (bottom) in ParaView for the axial velocity profile that varies along the channel width.

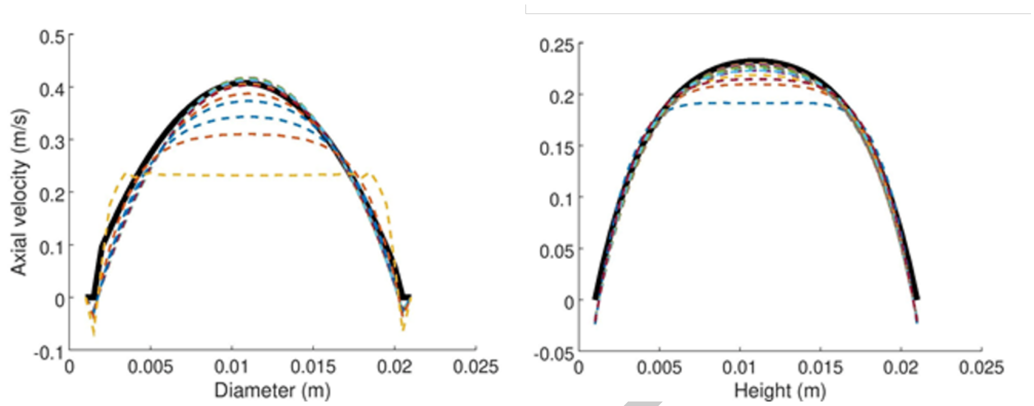

Figure 2: The solid black line depicts the exact solution (Poiseuille velocity profile) and the dashed lines represent the LBM solution at equally spaced locations along the length of the cylinder.

Automated Verification and Validation

To maintain its validity, we developed a verification and validation (V&V) suite to continually benchmark any algorithm changes and automatically execute multiple geometries. `gLBM` includes a verification execution library that is designed to simulate a list of geometries found in a configuration file. The analytical solutions for the cylindrical and rectangular channels are programmatically included in the V&V library. The dimensions, grid discretization, and fluid and simulations parameters can be set in the configuration file, which applies to both the LBM and analytical results. This allows for reproducible, easy simulation of the analytic cases with error reporting and plotting, which provides a method to continuously verify the numerical solution with the analytic solution. This is important when evaluating continual algorithm changes because it provides automatic error reporting and plotting of the solution vs numerical benchmarked data. We calculate the error at designated slices (axial locations) along the geometry and list these errors in a table for easy evaluation. We also plot the velocity profile in each dimension, overlaying the analytic solution, the baseline (the previously validated or best case results), and the computed solution for easy visual inspection, as shown in **Figure 3**. For more complex geometries, where the analytical solution is unavailable, only the baseline and current results are plotted for evaluation. As changes to the `gLBM` libary are made, it is easy to compare results to ensure results are moving closer to the analytic solution. We also plot the overall error at each iteration of the solution to evaluate convergence time for each solution.

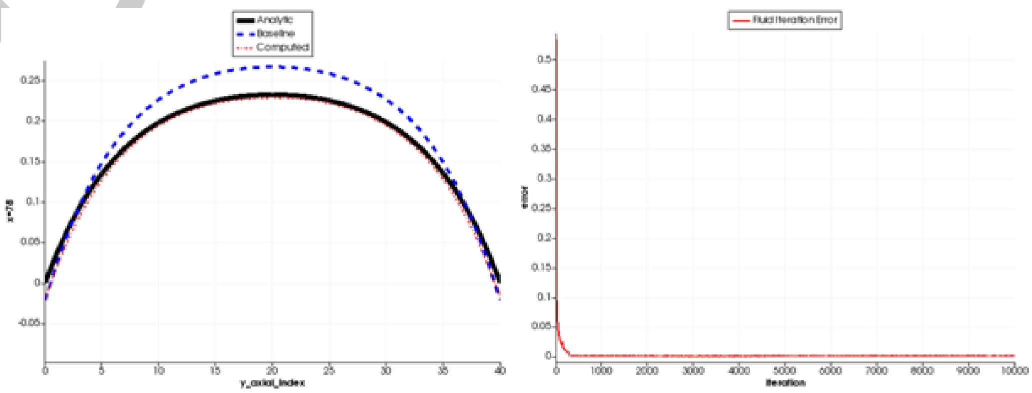

Figure 3: Example results from the verification and validation suite.

Future Directions

Our team is working towards a fast fluid solution for the upper airways. Our initial studies have successfully executed the `gLBM` library for this domain with mixed results. An example of this geometry is included in the open source repository. Though initial results show promise, more work is required. Our future work will expand on the initial results shown in **Figure 4** and advancements will be committed to the `gLBM` repository.

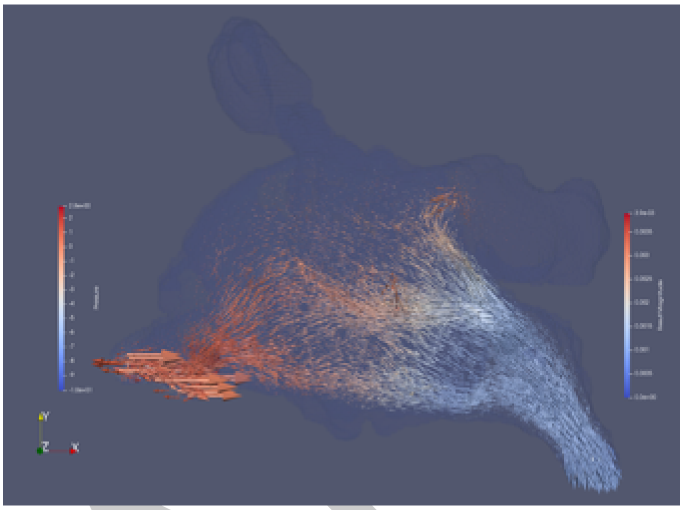

Figure 4: Initial results for the LBM simulation in the upper airways.

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References

Clipp, R. B. P., Vicory, J. P., Mitran, S. P., Kimball, J. S. P., Rhee, John S. MD, M., & Enquobahrie, A. P. (2019). Towards a Real-Time Solution for Virtual Surgical Planning of Upper Airway Procedures, Including Computational Fluid Dynamics. *Computer Methods in Biomechanics and Biomedical Engineering*.

Clipp, R. B., Vicory, J., Horvath, S., Mitran, S., Kimbell, J. S., Rhee, J. S., & Enquobahrie, A. (2018). An interactive, patient-specific virtual surgical planning system for upper airway obstruction treatments. *2018 40th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC)*, 5802–5805.

He, X., & Luo, L.-S. (1997). Lattice boltzmann model for the incompressible navier–stokes equation. *Journal of Statistical Physics*, *88*(3-4), 927–944.

Krüger, T., Kusumaatmaja, H., Kuzmin, A., Shardt, O., Silva, G., & Viggen, E. M. (2017). The lattice boltzmann method. *Springer International Publishing*, *10*(978-3), 4–15.

Latt, J., Chopard, B., Malaspinas, O., Deville, M., & Michler, A. (2008). Straight velocity boundaries in the lattice boltzmann method. *Physical Review E*, *77*(5), 056703.

Lattice boltzmann (LBM) simulation package for GPUs (CUDA, OpenCL). (2020). In *GitHub repository*. GitHub. https://github.com/sailfish-team/sailfish

McCormick, M. M., Liu, X., Ibanez, L., Jomier, J., & Marion, C. (2014). ITK: Enabling reproducible research and open science. *Frontiers in Neuroinformatics*, *8*, 13.

OpenLB – open source lattice boltzmann code. (2020). In *Website*. OpenLB. https://www.openlb.net/download/

Palabos: Parallel lattice boltzmann solver. (2020). In *GitHub repository*. GitHub. https://gitlab.com/unigespc/palabos

Quammen, C. W., Taylor, R. M., II, P. K., Mitran, S., Enquobahrie, A., Superfine, R., Davis, B., Davis, S., & Zdanski, C. (2016). The virtual pediatric airways workbench. *Studies in Health Technology and Informatics*, *220*, 295.

Succi, S. (2001). *The lattice boltzmann equation: For fluid dynamics and beyond*. Oxford university press.

Ubertini, S., Asinari, P., & Succi, S. (2010). Three ways to lattice boltzmann: A unified time-marching picture. *Physical Review E*, *81*(1), 016311.