Highly-scalable simulations of turbulent and particle-laden flows

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Summary of work to date

- Direct numerical simulation of three dimensional decaying turbulent flow in a periodic box, using the lattice-Boltzmann method, is presented. See Fig. 1.
- Here we explore the parallel scalability of this approach by comparing the parallel efficiencies of the code using one, two, and three dimensional domain decompositions.
- The scalability of the lattice-Boltzmann method using up to 512 processors is discussed using both actual timing data and a complexity analysis.
- Finally, the lattice-Boltzmann method is then compared to the pseudo-spectral method for differences in scalability

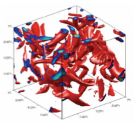


Fig. 1

Lattice-Boltzmann Method

- Lattice-Boltzmann method approximates solutions using a set of distribution functions. Eqn. 1
- Macroscopic variables can be easily recovered in this method. See eqns. 2 and 3 for the recovery of density and velocity respectively.
- In this model we use D3Q19 – 3 dimensions, with each lattice point having 19 vectors. Fig. 2
- The lattice-Boltzmann method is highly parallelizable because it requires only two steps; collision (computation), which involves only local variables on each processor, and streaming (communication).

$$\mathbf{f}(\mathbf{x}+\mathbf{e}_\alpha\delta t, t+\delta t) = \mathbf{f}(\mathbf{x},t) - \mathbf{M}^{-1}\cdot\mathbf{S}\cdot\left[\mathbf{m}-\mathbf{m}^{(\mathrm{eq})}\right]$$

Eqn. 1

$$\rho = \sum_i f_i$$

Eqn. 2

$$v = \sum_i f_i e_i / \rho$$

Eqn. 3

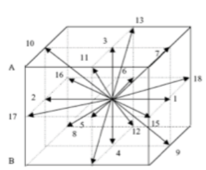


Fig. 2

Scalability: Data and Theory

- Tests were performed on both National Center for Atmospheric Research's (NCAR) Bluefire and the University of Delaware's Chimera machines.
- Complexity Analysis of lattice-Boltzmann for multiple domain decompositions developed by Orlando Ayala is presented in Fig.3. It includes time for computation, communication, transmission, and latency.
- Increasing resolution of lattice points increases computation removing communication noise from trials. For reference, see difference between 128^3 trials and 256^3 trials in Fig. 4
- Increasing resolution of lattice points also gives better convergence with complexity analysis. See Fig. 5 and Fig. 6 for comparison.

$$t_{LBM\,1D} = \underbrace{474\frac{N^3}{P}t_c}_{\text{Comp}} + \underbrace{\left(79\frac{N^3}{P}+20N^2\right)t_a}_{\text{Copy}} + \underbrace{20N^2 t_w}_{\text{Transm}} + \underbrace{20t_s}_{\text{Latency}}$$

$$t_{LBM\,2D} = 474\frac{N^3}{P}t_c + \left(79\frac{N^3}{P}+20N^2\left(\frac{1}{P_y}+\frac{1}{P_z}\right)\right)t_a + 20N^2\left(\frac{1}{P_y}+\frac{1}{P_z}\right)t_w + 40t_s$$

$$t_{LBM\,3D} = 474\frac{N^3}{P}t_c + \left(79\frac{N^3}{P}+20N^2\left(\frac{1}{P_yP_z}+\frac{1}{P_xP_z}+\frac{1}{P_xP_y}\right)\right)t_a + 20N^2\left(\frac{1}{P_yP_z}+\frac{1}{P_xP_z}+\frac{1}{P_xP_y}\right)t_w + 60t_s$$

Fig. 3

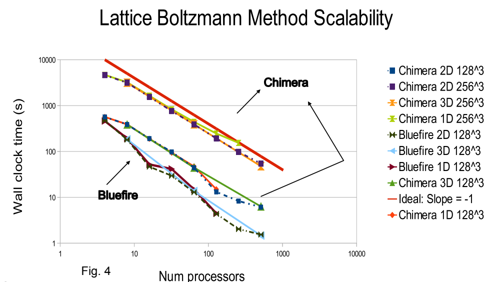


Fig. 4

1D,2D,3D decomposition results and theory

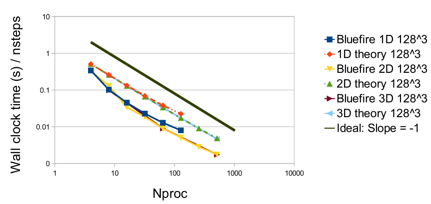


Fig. 5

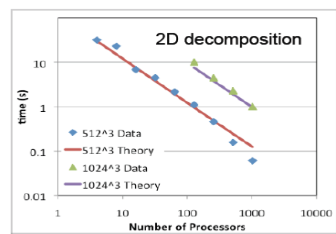
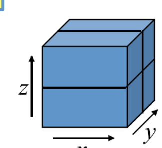


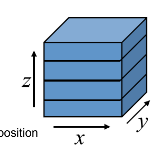
Fig. 6

Domain decomposition

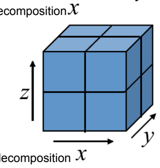
- Division of computational domain to reduce the amount of computation done by a single processor
- Each processor used handles one subdomain
- Efficient communication between processors very important



2D decomposition



1D decomposition



3D decomposition

	1D	2D	3D
LBM	$\sim\frac{P}{N}$	$\sim\frac{P^{1/2}}{N}$	$\sim\frac{P^{1/3}}{N}$
PS	$\sim\frac{1}{\log_2 N}$	$\sim\frac{1}{\log_2 N}$	$\sim\frac{1}{\log_2 N}$

Table 1

Motivation

- Particle-laden turbulent flows are found in many applications such as sediment transport, pollutant dispersion, interaction of cloud droplets, and chemical processing.
- The need for a highly scalable simulation of 3 dimensional flow grows with the availability of large clusters used for high performance parallel computing.
- A large range of length and time scales must be considered making problems in turbulence very computationally expensive.

Comparison of Lattice Boltzmann and Pseudo-spectral methods

- The Pseudo-spectral method is historically the most widely used approach for Direct Numerical Simulation (DNS). However, this approach may not scale well into a large number of processors due to the use of the Fast Fourier Transform (FFT)
- In our simulation the Pseudo-spectral method preforms better at a low number of processors while the lattice-Boltzmann method performs after using more than 64 processors. See Fig. 7.
- Through complexity analysis we show that the proportional ratio of communication to computation $\frac{t_{comm}}{t_{comp}}$ is steadily decreasing in the lattice-Boltzmann method but remains constant in the Pseudo-spectral method. See Table 1.
- Even though the lattice-Boltzmann method is second order accurate and the Pseudo-spectral method is exponentially accurate, the two methods are still comparable (see Y. Pend et.al. ,Comparison of the lattice Boltzmann and pseudo-

Comparison of Pseudo-spectral method and lattice-Boltzmann method

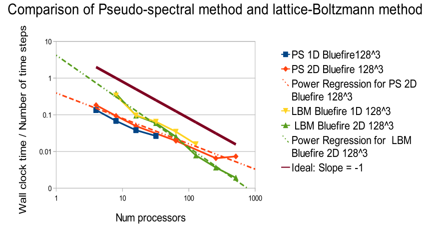


Fig. 7