Realtime Computational Fluid Dynamics Simulations using the Lattice Boltzmann Method TJHSST Senior Research Project Computer Systems Lab 2009-2010

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Abstract

Fluid simulations are useful in many different areas ranging from weather modeling to microscopic physics. Using the conventional method of solving the districtized Navier-Stokes equations is very computationally intensive and relatively hard to parallelize. The lattice boltzmann method instead uses the discrete Boltzmann equation to simulate Newtonian fluids using various collision models.

Keywords: computational fluid dynamics, lattice boltzmann methods, parallel computing

1 Introduction

Fluid dynamics are useful in a broad range of fields including meteorology, computer graphics, aerodynamics, and microscopic physics. The purpose of this project is to accelerate relatively new methods in the field of computational fluid dynamics in order to be able to run realtime simulations. This includes using new methods that can be parallelized more effectively and vectorizing these methods and running them on new hardware using GPGPU techniques.

2 Background

2.1 Boltzmann Equation

The Boltzmann equation

$$f(x + vdt, v, t + dt) = f(x, v, t) + \Omega(x, v, t)$$

describes the time evolution of system of particles that interact with each other via the collision operator Ω . It consists of two parts, streaming and collisions. During streaming, particles are moved according to their velocities. During the collision stage, the distribution functions (DFs) at each lattice point undergo a collision operator, which is left as a choice.

2.2 The BGK collision operator

$$\Omega_{BGK} = \frac{f - f_e q}{\tau}$$

Collisions tend to push the system towards local equilibrium. This model is computationally simple, yet accurate, making it ideal, and thus very popular, for use in lattice Boltzmann Simulations. It is the one that I am using for my project.

2.3 Lattice Gas Cellular Automata

One approach to fluid dynamics modelling is to make a hexagonal grid, with every grid point having a set of 7 possible velocities, each pointing to the neighboring lattice point, or staying still. No two particles can occupy the same point with the same velocity. At each time step, particles move to the next point dictated by their velocity. If another particle is also moving to the same space, a collision model is used to determine where each particle settles. From this microscopic model, macroscopic behavior consistent with the Navier-Stokes equations emerges.

2.4 Discretization of Phase Space

In order to solve Boltzmann equation numerically, the domain must be districtized in phase space, consisting of time, configuration space, and velocity space. Time is split up by time step. Configuration space is split apart into a lattice with a discrete set of velocities connecting neighboring nodes. Lattices are classified by a DnQm scheme where n is the number of dimensions and m is the number of velocities. For example, D2Q9 is a two dimensional lattice with 9 velocities connecting neighboring nodes (4 to each corner, 4 to each midpoint, and 1 stationary).



Figure 1: Various lattice and velocity configurations

3 Procedure

The first steps of this project are learning the physics behind the boltzmann equation and various collision operators. Then, I have to learn how the boltzmann equation is districtized into a lattice. Then, I will code a 2 dimensional simulation in order to get a basic simulation working. Then, I will expand it into 3 dimensions and start work on parallelizing and making sure it is working correctly.

4 Implementation Details

Currently, my simulation is a D2Q9 simulation using the BGK collision operator. It is programmed in the C programming language as this is a very performance intensive project and I am more comfortable in C than in Fortran. OpenGL is used to provide visualization display and input. For visualization, a grayscale image is presented with each pixel taking on the value proportional to the amount of fluid present at a lattice point. Mouse presses currently add stationary fluid at the pointer location. OpenMP is used for intra-node parallelism and MPI is used for inter-node parallelism.

Two steps are performed at each time step: the stream step and the collision step.

4.1 The Stream Step

In the stream step, the first part of the Boltzmann equation is computed. The distribution functions for each velocity at each lattice point are moved to neighboring lattice points based on their velocity.

$$f(x + e_i, e_i, t + dt) = f(x, e_i, t)$$

If a distribution function is hitting a boundary, then it undergoes the noslip boundary condition and stays at the same lattice point, except with the inverse velocity.

$$f(x, e_{\overline{i}}, t + dt) = f(x, e_i, t)$$

This step is parallelized very easily. At each time step, the only communication that needs to occur between nodes is the transfer of the status of neighboring nodes.

4.1.1 Streaming Code

```
#pragma omp parallel for
for (int x = 0; x < SIZEX; x++) {
     for (int y = 0; y < SIZEY; y++) {
   if (flags[x][y] = OBSTACLE) {
        continue;
   }
   for (int d = 0; d < DIRS; d++) {
        int nx = x + dx[d];
        int ny = y + dy[d];
        if (flags[nx][ny] = OBSTACLE) {
      //no slip boundary condition
     domain [new] [x] [y] [I(d)] += domain [old] [x] [y] [d];
        } else {
     \operatorname{domain}[\operatorname{new}][\operatorname{nx}][\operatorname{ny}][d] = \operatorname{domain}[\operatorname{old}][\operatorname{x}][\operatorname{y}][d];
        }
   }
     }
}
```

4.2 The Collision Step

In the collision step, the second part of the Boltzmann equation is computed. The interactions that particles have with each other. The collision operator is based off the fact that collisions tend to make the particles approach equilibrium, governed by the Maxwell-Boltzmann distribution. At each time step, a finite number of collisions occur, so the particles are only pushed partway towards equilibrium. So the particle distribution functions after collisions are a mixture of the pre-collision distribution functions and equilibrium distribution functions.

The equilibrium distribution is found by taking the low Mach number expansion of the Maxwell-Boltzmann distribution

$$\sqrt{\frac{m}{2\pi kT}}e^{\frac{-mv^2}{2kT}}$$

yielding

$$f_i^{eq} = w_i(\rho + 3e_i \cdot u - \frac{3}{2}u^2 + \frac{9}{2}(e_i \cdot u)^2)$$

where

$$\rho = \sum f_i$$
$$u = \sum e_i f_i$$

After computing the equilibrium distribution, the distribution functions are then relaxed using the following relationship.

$$f(x, e_i, t + dt) = (1 - \omega)f(x, e_i, t + dt) + \omega f_i^{eq}$$

where ω is the parameter controlling the viscosity of the fluid. Values close to 0 represent very viscous flows.

4.2.1 Collision Code

```
#pragma omp parallel for
for (int x = 0; x < SIZEX; x++) {
   for (int y = 0; y < SIZEY; y++) {
      if (flags[x][y] == OBSTACLE)
          continue;
      float rho = 0.0;
      float ux = 0.0; float uy = 0.0;</pre>
```

```
for (int d = 0; d < DIRS; d++) {
    rho += domain [new] [x] [y] [d];
    ux += dx[d] * domain[new][x][y][d];
    uy += dy[d] * domain[new][x][y][d];
  if (flags[x][y] = VELOCITY)
    ux = 0.1 * rho;
  for (int d = 0; d < DIRS; d++) {
    float eq = 0.0;
    eq += rho;
    eq += 3*(dx[d]*ux+dy[d]*uy);
    eq = (ux * ux + uy * uy) * 3/2;
    eq += (dx [d] * ux + dy [d] * uy) * (dx [d] * ux + dy [d] * uy) * 9/2;
    eq *= weights [d];
    domain [new] [x] [y] [d] = (1 - omega) * domain [new] [x] [y] [d] +
        omega*eq;
  }
}
```

4.3 Different Cell Types

In order to handle the different cell types such as obstacles, fluid, constant velocity, gas, and interface cells, the type of each cell must be recorded. An array the size of the domain is used for this.

4.4 Visualization

}

There are many methods to visualize fluids on a computer screen showing different things from density to velocity to pressure to vorticity.

4.4.1 Density Plot

One way of visualization is to plot the density at each lattice point by setting pixels to a color proportional to the amount of fluid present. This shows fluid at each point, but fails to capture any other information such as velocity when density is constant as is the case in incompressible flows such as water.

4.4.2 Particles

Non-fluid particles may be placed in the fluid. These particles are then advected by the fluid at each timestep, using Euler's method or moving the particle by dt times the fluid velocity. The fluid velocity is computed by finding the moments and then dividing.

$$v = \frac{u}{\rho}$$

This shows how individual components of the fluid move and allows velocity to be gauaged even in incompressible flows.

4.4.3 Velocity Vector Field

Another way of showing velocity is to draw the velocity vector field. On an evenly spaced grid, vectors are drawn corresponding to the velocity at that grid point. One drawback to this is that it is hard to cover a wide range of velocities effectively.

5 Test Cases

5.1 Lid Driven Cavity

The lid driven cavity is a rectangular domain where the walls are non-slip except for the top wall, which is non-slip, but moving at a constant velocity. The simulation is setup to set the velocity of the fluid on the topmost row of pixels to 0.01 in the right direction, for all except the rightmost pixels.

6 Expected Results

The project will be expected to yield a CFD code that is able to simulate fluids in realtime. Physically correct results should be achieved, which will be measured using fundamental laws such as conservation of mass. This can be used in realtime predictions in various fields, for example control systems dealing with fluids. The speedup techniques used can also be applied to make larger simulations run faster.

7 Results

Current results consist of a simulation of a two dimensional fluid that can be conducted in realtime on a single processor on a 300x300 grid. The simulation

Figure 2: In process lid driven cavity simulations visualized using particles



is currently unoptimized since I copy the memory at each timestep, which while good for simplicity and getting a simulation up and running, is terrible for performance.

A CUDA version is also implemented. Running this on a GPU is very appealing because it is massively SIMD (single instruction multiple data). A GPU has many threads that can simultaneously process the same instructions on multiple data very efficiently. The Lattice Boltzmann method performs the same operations on every lattice point.

Physically, the simulation visually appears to model correct fluid dynamics behavior. However, using some code checks, I have found that mass in the simulation is not conserved. This is a problem, since mass should always be conserved. This is likely a result of the equilibrium distribution function I am using and so I will need to check this in the future.

Issues have been found with the simulation when velocities exceed approximately $\frac{1}{3}$. Under these conditions, the fluid tends to stop being incompressible and compress. The low mach number expansion of the Maxwell-Boltzmann distribution also tends to deterioate. In addition, the problem becomes ill-conditioned, yielding increased floating point error.

7.1 Performance

A widely used metric of Lattice Boltzmann codes is MLUPS or mega lattice updates per second, meaning how many millions of gridpoints can be updated in one second.

Single threaded performance:

Core 2 X9650	4.64 MLUPS
Xeon E5520	3.84 MLUPS

Multi threaded performance scales almost linearly under shared memory systems using OpenMP. Using 4 threads on a Core 2 Quad X9650, 16.26 MLUPS are acheived.

Figure 3: Visualization of an in progress fluid simulation



8 Conclusion

Lattice Boltzmann methods are a very attractive alternative to conventional fluid dynamics solvers since they exhibit accurate results and are much easier to parallelize. With the decline of Moore's law in serial performance, it has been realized in many-thread performance. Because of this, the Lattice Boltmzann method has become even more appealing as the future of fluid simulations.

Figure 4: Visualization of an in progress fluid simulation



Figure 5: Visualization of an in progress fluid simulation using a velocity field



8.1 Applications

One application would be to simulate dispersion of smoke or bio toxins inside a large city such as New York. Emergency management teams could use this information in order to more effectively control such outbreaks and prevent against terrorist attacks.

References

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