CUDA Simulation of Rayleigh-Taylor Instability

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1 Introduction

This report presents the implementation of a numerical simulation of the Rayleigh-Taylor instability using CUDA for GPU computing. The Rayleigh-Taylor instability occurs when a heavy fluid is placed above a lighter fluid in a gravitational field, creating an unstable interface that evolves over time. Our implementation solves the compressible fluid dynamics equations on a 2D grid, leveraging GPU parallelism for efficient computation.

2 Mathematical Model

2.1 Variables and Equations

Our simulation tracks four conserved variables: density (ρ), x-momentum (ρu), y-momentum (ρv), and total energy (e). From these, we derive primitive variables: velocities (u, v), pressure (p), and sound speed (c).

The governing equations are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = k_1 \left(\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2} \right) \tag{1}$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho uu)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial p}{\partial x} = k_2 \frac{\partial^2(\rho u)}{\partial x^2} \tag{2}$$

$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho uv)}{\partial x} + \frac{\partial(\rho vv)}{\partial y} + \frac{\partial p}{\partial y} = -g_a \rho + k_2 \frac{\partial^2(\rho v)}{\partial y^2} \tag{3}$$

$$\frac{\partial e}{\partial t} + \frac{\partial(u(e+p))}{\partial x} + \frac{\partial(v(e+p))}{\partial y} = -g_a \rho v + k_3 \left(\frac{\partial^2 e}{\partial x^2} + \frac{\partial^2 e}{\partial y^2} \right) \tag{4}$$

where $g_a = -10$ is gravitational acceleration, and k_1, k_2, k_3 are artificial diffusion coefficients.

2.2 Initial and Boundary Conditions

Initial conditions include a density discontinuity at $y = L_y/2$ ($\rho = 2.0$ above, $\rho = 1.0$ below), zero velocity except for a small perturbation near the interface, and hydrostatic pressure $p = 40 + \rho g_a (y - L_y/2)$. Boundary conditions are periodic in x and rigid walls (with $v = 0$) in y.

3 CUDA Implementation

Our code is structured around several key components:

- Main time-stepping loop in **main.cu**
- Initial condition setup in **init.cu**
- Boundary condition handling in **boundary.cu**
- Conservative-to-primitive variable conversion in **primitive.cu**
- Right-hand side terms computation in **rhs.cu**
- Time integration in **update.cu**
- CFL condition for time step calculation in **cfl.cu**

The simulation uses a 2D grid with ghost cells, typically sized 1024×512. Each CUDA thread processes one cell, with thread blocks of 16×16.

```
__host__ __device__ inline int idx(int i, int j, int Nx, int Ny) {
    return (i+1) + (j+1)*(Nx+2);  // +1 offset for ghost cells
}

__device__ inline float diffX(float f_ip1, float f_im1, float dx) {
    return (f_ip1 - f_im1) / (2.0f * dx);
}
```

Listing 1: Indexing and basic derivative computation

Performance optimizations include efficient derivatives computation and parallel reduction for CFL condition calculation, with local computations in shared memory before global reduction using Thrust.

4 Physical Analysis

4.1 Role of Density Discontinuity

The density discontinuity is fundamental to the Rayleigh-Taylor instability. The heavier fluid ($\rho = 2.0$) above the lighter fluid ($\rho = 1.0$) creates an inherently unstable configuration. Gravity pushes the dense fluid downward with twice the force of the light fluid, creating a force imbalance that drives the instability. This configuration allows the system to lower its center of mass, reducing potential energy as the instability develops.

4.2 Necessity of Initial Perturbation

An initial velocity perturbation is essential because the system would otherwise remain in metastable hydrostatic equilibrium. Our implementation uses a controlled bell-shaped perturbation:

```
if (fabsf(y - params.Ly/2.0f) <= 0.05f) {
    float width = 0.2f * params.Lx;
    if (distance_from_center < width) {
        float amplitude = 0.002f * expf(-8.0f * distance_from_center / params.Lx);
        v = -amplitude;
    }
}
```

This promotes coherent growth rather than random development from numerical noise, allowing controlled study of the instability.

4.3 The $-g_a \rho v$ Term in Energy Equation

The term $-g_a \rho v$ represents gravitational work. When fluid moves downward ($v < 0$), potential energy converts to internal/kinetic energy, increasing temperature and pressure. When fluid moves upward ($v > 0$), internal energy converts to potential energy. This term is crucial for energy conservation and correctly capturing thermodynamics in gravitational fields.

5 Numerical Exploration

5.1 Time Integration Schemes

We implemented the explicit Euler method: $q^{n+1} = q^n + \Delta t \cdot RHS(q^n)$. A Runge-Kutta 2 method would offer second-order accuracy and better stability but requires two RHS evaluations per time step, increasing computational cost.

5.2 Impact of Diffusion Coefficients

Artificial diffusion coefficients are calculated as:

```
float k1 = 0.0125f * dx2 / (2.0f * dt);  // For density
float k2 = 0.125f * dx2 / (2.0f * dt);   // For momentum (10x stronger)
float k3 = 0.0125f * dx2 / (2.0f * dt);  // For energy
```

Increasing these coefficients improves stability but makes interfaces more diffuse and slows instability development. Decreasing them creates sharper interfaces but risks numerical instabilities. The momentum coefficient k_2 is 10 times larger because velocity gradients in turbulent flows require more stabilization.

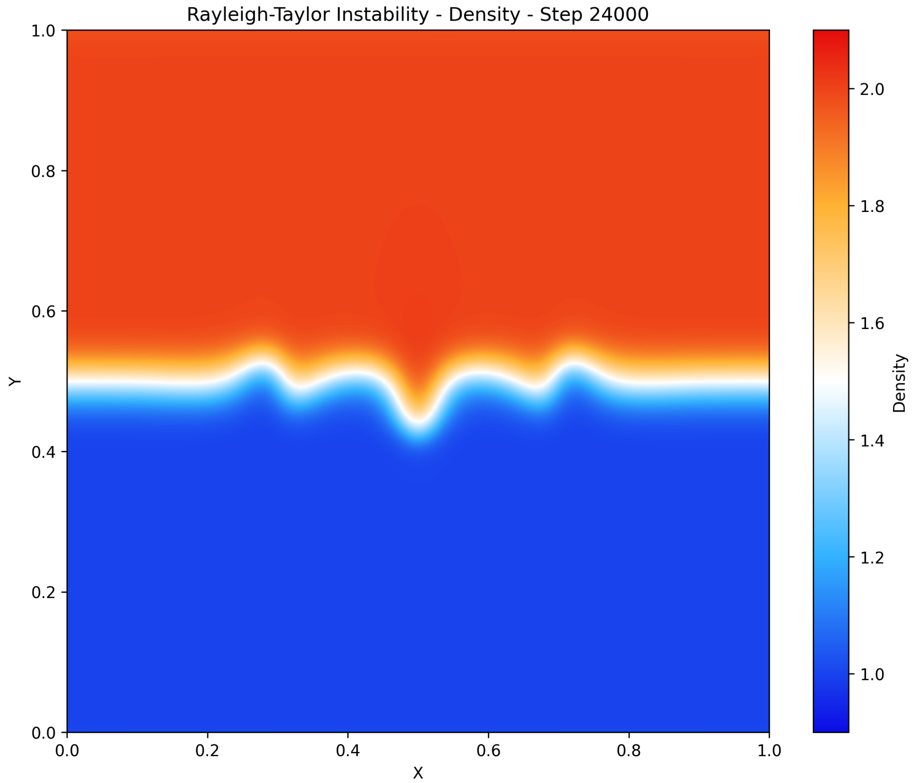

Figure 1: Early stage (Step 24000) showing small interface perturbations

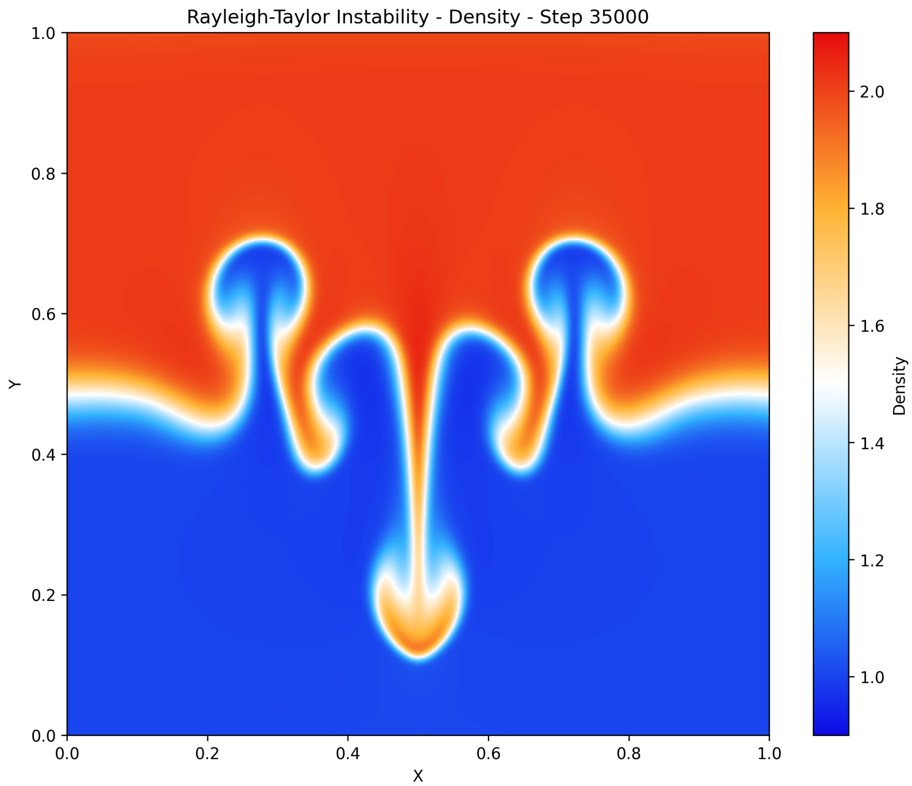

Figure 2: Intermediate stage (Step 35000) with mushroom structures

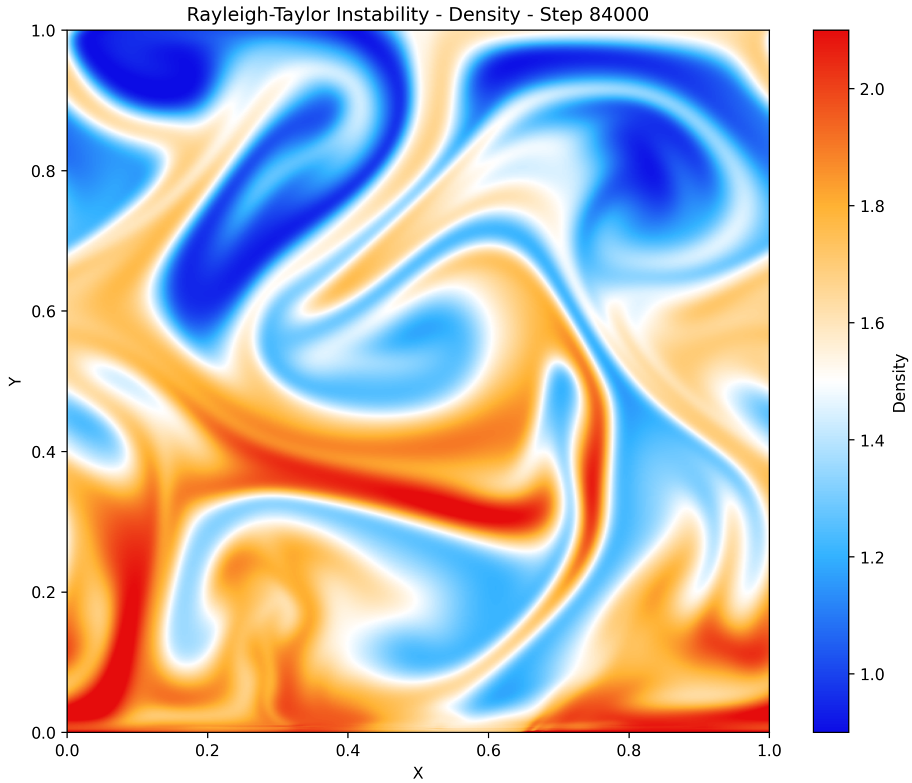

Figure 3: Advanced stage (Step 84000) with complex turbulent mixing

6 Results and Visualization

Our simulation captures the full evolution of the Rayleigh-Taylor instability:

Figure 1 (step 24000) shows the early development with small undulations at the initially flat interface between heavy fluid (red) and light fluid (blue). At this stage, the perturbation remains in its linear growth phase.

Figure 2 (step 35000) shows characteristic mushroom-shaped structures. Two symmetrical mushroom caps form where lighter fluid rises upward, while two central "fingers" of dense fluid penetrate downward. The central spike has developed a small mushroom cap at its tip.

Figure 3 (step 84000) reveals highly complex swirling patterns and extensive mixing. The clear structures have evolved into intricate vortices, demonstrating the transition to turbulent mixing. Periodic boundary conditions in the x-direction create interesting interactions between adjacent structures.

The color mapping shows density stratification, with heavier fluid (red) initially on top and lighter fluid (blue) on bottom. The interface sharpness diminishes over time, indicating increased mixing due to instability-driven turbulence.

7 Conclusion

We successfully implemented a CUDA simulation of the Rayleigh-Taylor instability, efficiently solving compressible fluid dynamics equations on a 2D grid. Our parallel GPU implementation captures the essential physical phenomena, from initial perturbation to turbulent mixing.

The simulation demonstrates the characteristic development patterns of the instability: initial perturbation growth, formation of density fingers and mushroom structures, and evolution into complex turbulent patterns. The numerical exploration provided insights into the effects of time-stepping schemes and diffusion parameters on simulation results.