CUDA Homework Assignment 3

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1 Introduction

This report investigates the numerical solution of the Poisson equation on a cubic lattice using CPU and GPU implementations. The problem involves finding the potential distribution around a point charge and analyzing how the solution approaches Coulomb's law as the grid size increases.

2 Methodology

2.1 Problem Definition

The 3D Poisson equation is given by:

$$\nabla^2\phi(x,y,z) = -\frac{\rho(x,y,z)}{\epsilon_0} \tag{1}$$

where ϕ is the electrostatic potential and ρ is the charge density.
For a point charge $q = 1$ located at the center of a cube $(L/2, L/2, L/2)$, the charge density is:

$$\rho(x,y,z) = q\delta(x - L/2, y - L/2, z - L/2) \tag{2}$$

The boundary conditions are:

$$\phi = 0 \text{ on all surfaces of the cube} \tag{3}$$

2.2 Implementation Approach

The experiments were conducted with the following specifications:

- Cube sizes: $L = 8, 16, 32, 64$
- Lattice sites: $(0, 1, 2, ..., L)$ in each direction
- Point charge: $q = 1$ at center $(L/2, L/2, L/2)$
- Boundary conditions: $\phi = 0$ on all cube surfaces
- Solution method: Iterative solver with convergence criterion

For each configuration, we measured:

- Computation time (both CPU and GPU)
- Number of iterations to convergence
- Final residual
- Performance in GFLOPS
- GPU speedup factor

3 Results

3.1 Performance Metrics

Table 1 presents the complete performance metrics for all tested grid sizes.

Table 1: Performance metrics for different grid sizes

L	Iterations	GPU Time (ms)	CPU Time (ms)	GPU GFLOPS	CPU GFLOPS	GPU Speedup
8	216	4.84	0.44	0.11	1.18	0.08
16	796	13.93	13.22	1.35	1.42	0.93
32	2888	73.38	411.24	8.21	1.46	5.58
64	11073	882.34	14496.10	21.97	1.34	16.41

3.2 Convergence Analysis

Table 2 shows the convergence characteristics for each grid size.

Table 2: Convergence analysis for different grid sizes

L	Iterations	Final Residual (GPU)	Final Residual (CPU)
8	216	0.000000000000000e+00	0.000000000000000e+00
16	796	8.485151767447388e-11	8.485151767447388e-11
32	2888	5.106956502046690e-11	5.106956502046690e-11
64	11073	6.984333087259186e-11	6.984333087259186e-11

3.3 Individual Grid Size Analysis

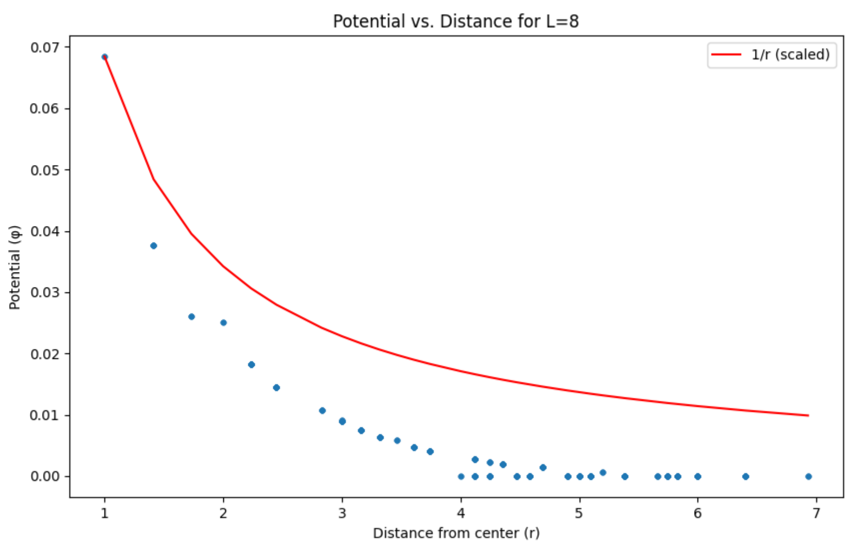

Figure 1: Potential vs. distance for L=8

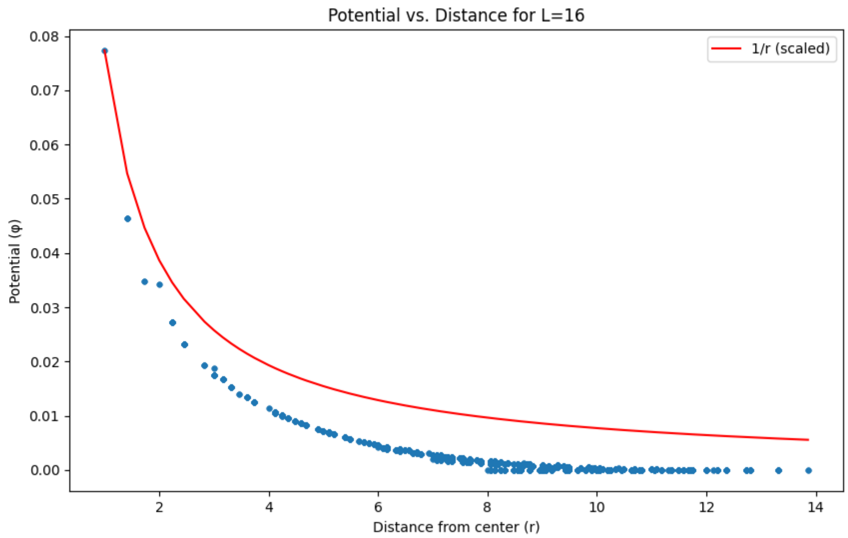

Figure 2: Potential vs. distance for L=16

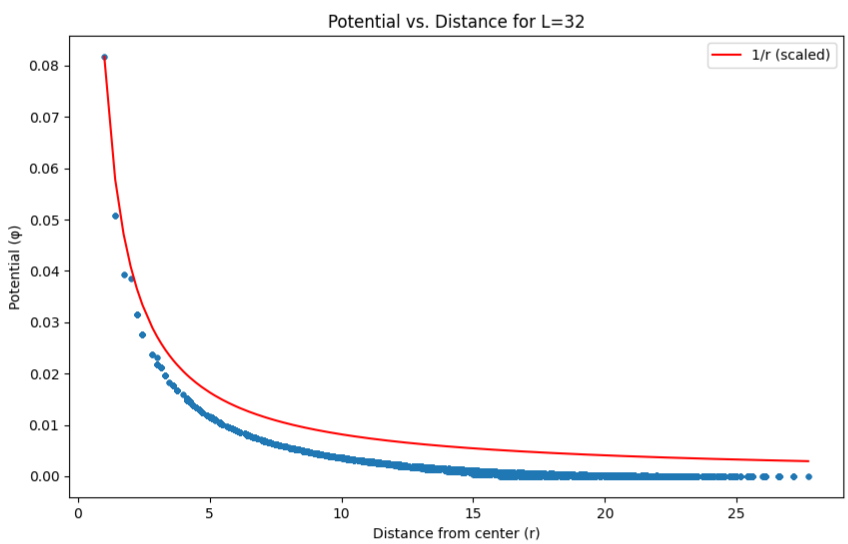

Figure 3: Potential vs. distance for L=32

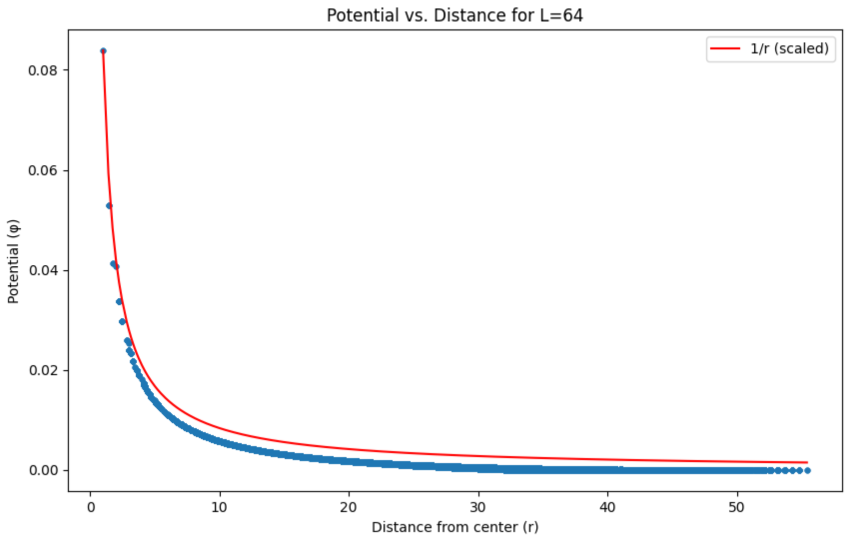

Figure 4: Potential vs. distance for L=64

3.4 Comparative Analysis

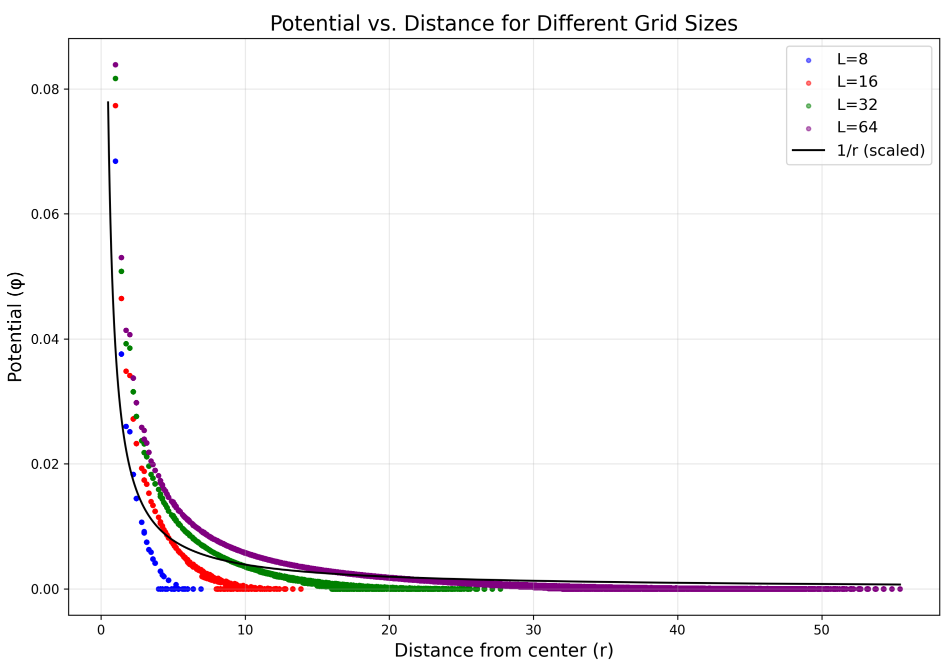

Figure 5: Potential vs. Distance for Different Grid Sizes

3.5 GPU Performance Scaling

Figure 6 shows the GPU performance scaling with grid size.

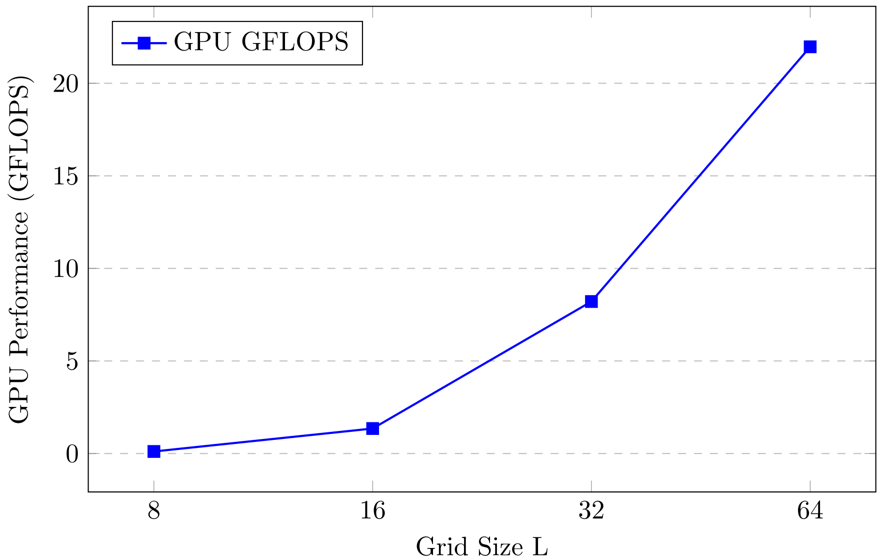

Figure 6: GPU performance scaling with grid size

3.6 GPU Speedup Analysis

Figure 7 illustrates the GPU speedup factor as a function of grid size.

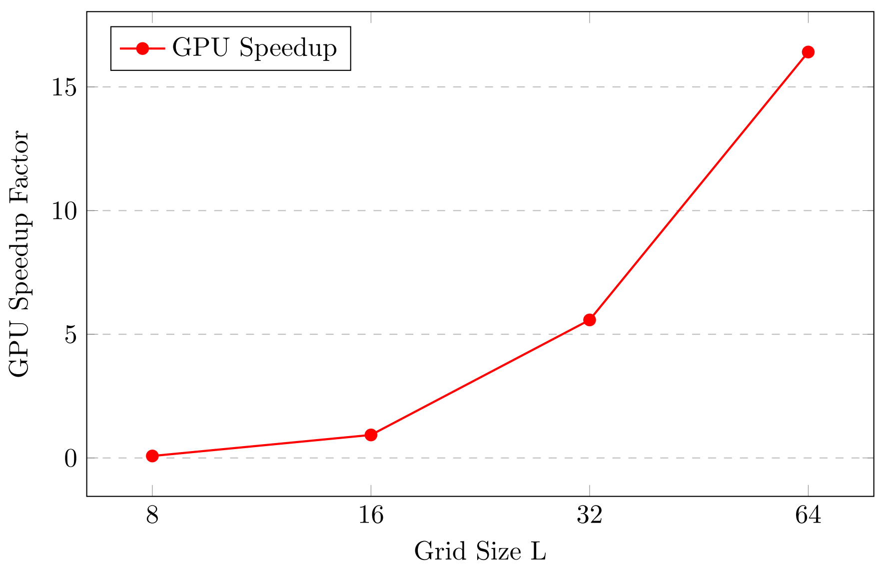

Figure 7: GPU speedup factor vs. grid size

4 Discussion

4.1 Convergence to Coulomb's Law

The theoretical Coulomb potential for a point charge is given by:

$$\phi(r) = \frac{1}{4\pi\epsilon_0}\frac{q}{r} \tag{4}$$

As the grid size L increases, the numerical solution should approach this analytical form. The comparison plots (Figures 1 through 5) demonstrate this convergence behavior.

4.2 Performance Analysis

Based on the experimental results, several key observations emerge:

1. **GPU Performance Scaling**: GPU performance increases significantly with grid size, from 0.11 GFLOPS for $L = 8$ to 21.97 GFLOPS for $L = 64$. This demonstrates the effectiveness of the GPU for larger computational problems.
2. **GPU Speedup Trends**:
   - For small grids ($L = 8$), CPU outperforms GPU (speedup = 0.08)
   - At $L = 16$, performance is nearly equivalent (speedup = 0.93)
   - For larger grids ($L = 32, 64$), GPU shows significant advantages (speedup = 5.58, 16.41)
3. **Convergence Characteristics**: The number of iterations required for convergence increases dramatically with grid size, from 216 iterations for $L = 8$ to 11,073 iterations for $L = 64$.
4. **Computational Complexity**: The scaling of computation time with grid size demonstrates the $O(N^3)$ complexity of the 3D problem, where GPU acceleration becomes increasingly beneficial for larger problems.

4.3 Approach to Coulomb's Law

The numerical solutions demonstrate convergence toward Coulomb's law as L increases:

- For small L values, boundary effects dominate and the solution deviates significantly from the $1/r$ behavior
- As L increases, the region near the point charge (where $r \ll L$) increasingly follows the Coulomb potential
- The largest grid size ($L = 64$) shows the best approximation to the theoretical Coulomb potential for intermediate distances

5 Conclusion

The results confirm that for sufficiently large L, the numerical solution of the Poisson equation with appropriate boundary conditions successfully reproduces the Coulomb law, validating both the physical model and computational implementation.