HW3 Report

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1. Description

Under the ”b10505047_HW3” directory, my source code is in poisson.cu, and the input and output results that I tested are put under the “results” directory. The input files are Input_8, Input _16, Input_32, Input _64, and the output information of the CPU and GPU code execution are included in Output_8, Output_16, Output_32, Output_64. There are also some vr_result files which are the results of numerical potential and coulomb potential versus the distance r. To run the code, run “make” first and then run “condor_submit cmd” to submit the job. Go to the “cmd” file, then you can change “Initialdir” into your working directory and “Arguments” into different input and output files’ names.

2. Methods

Similar to 2D lattice case, now consider the Poisson equation $\nabla^2\phi = -\frac{\rho}{\varepsilon_0}$ on a 3D lattice with a point charge q=1 at center (x_0, y_0, z_0),

$$\nabla^2\phi = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial z^2} = -\frac{\rho(x,y,z)}{\varepsilon_0}$$

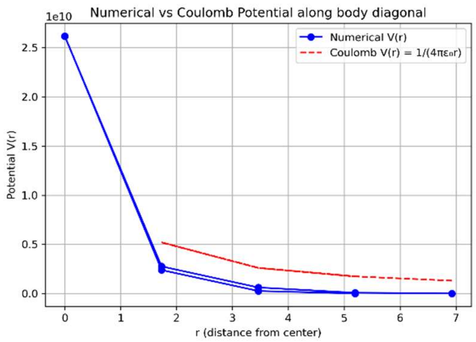
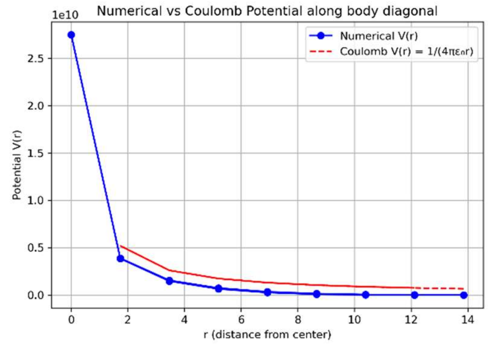
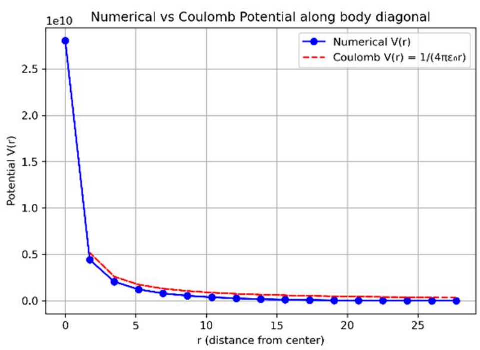
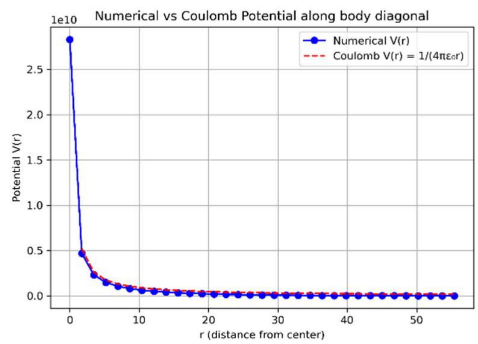
$$\Rightarrow \phi(x,y,z) = \frac{1}{6}\Big[\phi(x+a,y,z) + \phi(x-a,y,z) + \phi(x,y+a,z) + \phi(x,y-a,z)$$
$$+ \phi(x,y,z+a) + \phi(x,y,z-a) + \frac{q}{\varepsilon_0}\delta_{x,x_0}\delta_{y,y_0}\delta_{z,z_0}\Big]$$

(In the lattice unit a = 1)
On the other hand, the Coulomb’s law gives:

$\phi = \frac{q}{4\pi\varepsilon_0 r}$, where $r = \sqrt{(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2}$

3. Results

For L = 8, 16, 32, 64, I output the numerical potential (V_numerical) and the potential computed by the Coulomb’s law (V_coulomb) along the body diagonal x = y = z. Then I use these two potentials to plot the figure of V_numerical and V_coulomb versus the distance r (by plotV.py code), and the result is shown below (when r = 0, V_coulomb is infinite):

<table>
<tr><td>L=8</td><td>L=16</td></tr>
<tr><td>
</td><td>
</td></tr>
<tr><td>L=32</td><td>L=64</td></tr>
<tr><td>
</td><td>
</td></tr>
</table>

4. Discussion

According to the results, we can see that as L becomes larger, the curve of V_numerical versus r becomes more similar to the curve of V_coulomb versus r. Therefore, we can conclude that the potential approach the Coulomb's law in the limit L >> 1.