Numerical computation of Coulomb potential

Konrad Kobuszewski

March 28, 2017

1 Naive method. Accurancy problems.

We consider continuous distribution of charge $\rho(\boldsymbol{r}) = qn(\boldsymbol{r})$, where $n(\boldsymbol{r}) = \sum_{k=1}^{N} |\psi_k|^2(\boldsymbol{r})$ ($\psi_k \in \mathbb{C}$ for $N = 1$ is assumed to be the input of the program). Coulomb potential of such a distribution is given by (we used $\varepsilon_0 = 1$):

$$V_{coulomb}(\boldsymbol{r}) = \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{q^2}{|\boldsymbol{r}-\boldsymbol{r'}|} n(\boldsymbol{r'})\, d^3r' = \mathcal{F}^{-1}\left[\frac{q^2}{k^2}\mathcal{F}\left[n(\boldsymbol{r})\right](\boldsymbol{k})\right](\boldsymbol{r})$$

This is general solution of Poisson equation in an integral form.
We used Borel's convolution theorem for conversion in equation above.

In case of testing accurancy of algorithm $n(\boldsymbol{r}) = \frac{1}{(2\pi\sigma^2)^{3/2}} e^{-\frac{r^2}{2\sigma^2}} = \frac{1}{\left(\pi a_{ho}^2\right)^{3/2}} e^{-\frac{r^2}{a_{ho}^2}}$ will be used, because analitic solution is known (wiki):

$$V_{coulomb}(\boldsymbol{r}) = \frac{1}{4\pi}\frac{q^2}{r}\,\mathrm{erf}\left(\frac{r}{\sqrt{2}\sigma}\right) = \frac{1}{4\pi}\frac{q^2}{r}\,\mathrm{erf}\left(\frac{r}{a_{ho}}\right)$$

$a_{ho} = \sqrt{\frac{\hbar}{m\omega}}$ is characteristic length of harmonic oscilator (groundstate wavefunction is a kind of gaussian).

Advantages:

- Straight forward implementation

Disadvantages:

- Due to long range behaviour of Coulomb potential poor accurancy is expected.

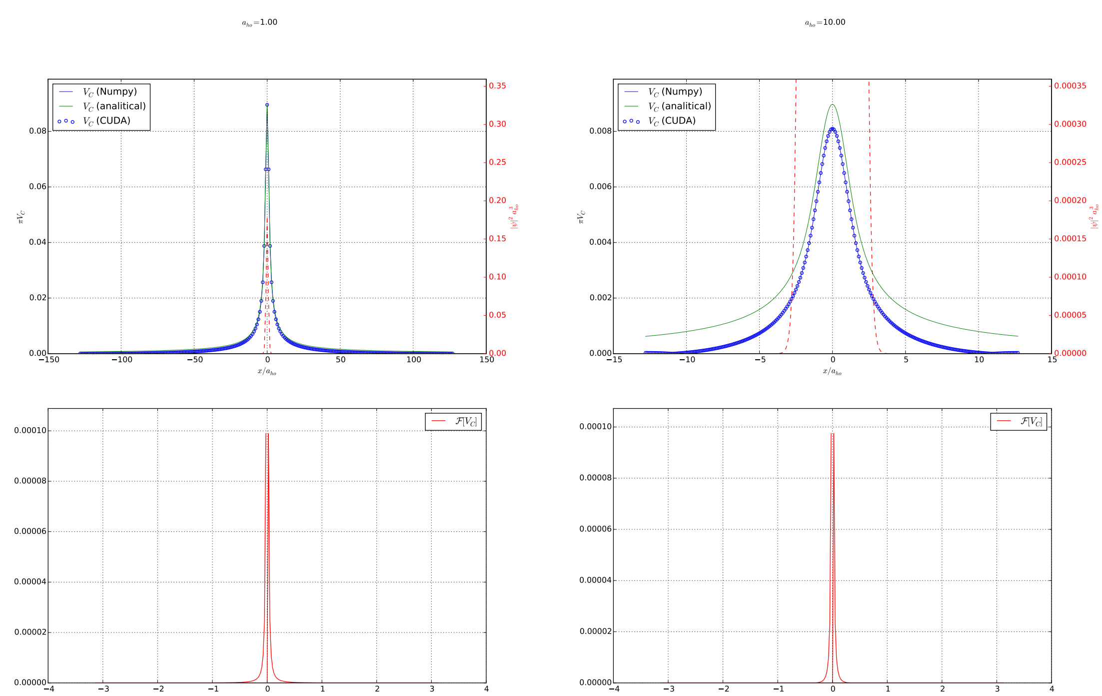

Figure 1: Ilustration of misaccurancy of computing Coulomb potential with naive method.

2 Methods of increasing accuracy of Coulomb potential computation

2.1 Performing computation on larger lattice

First conclusion from analysis of fig. 1 suggests just to perform computation on bigger grid.
We need to get values from smaller lattice and copy to „centre" of bigger array and also fill other entries of bigger array with zeros.

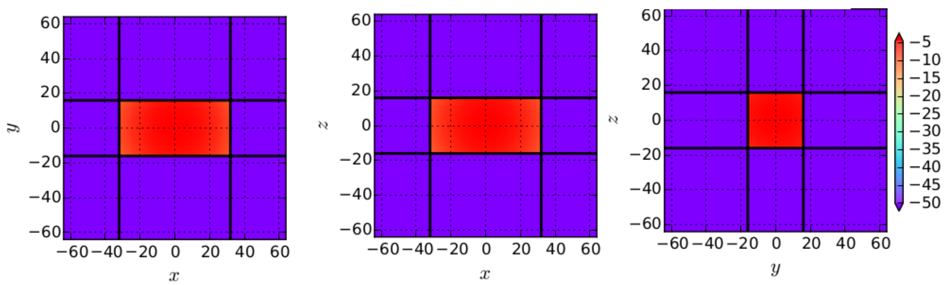

Figure 2: Example of resizing array in 3D. Colors correspond to density in logscale (orginal array was filled with constant).

Increase of lattice size in fact gives no more information about charge distribution, so there could exists better way for increasing accuracy without unnecessary increase of lattice and computation time, nevermore little more math have to be used. Two different cutoff methods dealing with this issue will be presented in next sections.

2.2 Spherical cutoff method

Given a cubic lattice of size $\left(1+\sqrt{3}\right)L_c$

$$\mathcal{F}^{-1}\left[\frac{q^2}{k^2}\left(1-\cos\left(\sqrt{3}L_c k\right)\right)\mathcal{F}\left[n\left(\boldsymbol{r}\right)\right]\left(\boldsymbol{k}\right)\right]\left(\boldsymbol{r}\right)$$

To deal with division by 0 we can use$\lim_{k\to 0}\frac{q^2}{k^2}\left(1-\cos\left(\sqrt{3}L_c k\right)\right)=\frac{3}{2}q^2 L_c$.

Advantages:

- Accurate.

Disadvantages:

- The lattice is much bigger, performing cuFFT and vector-vector multiplication is getting slower.

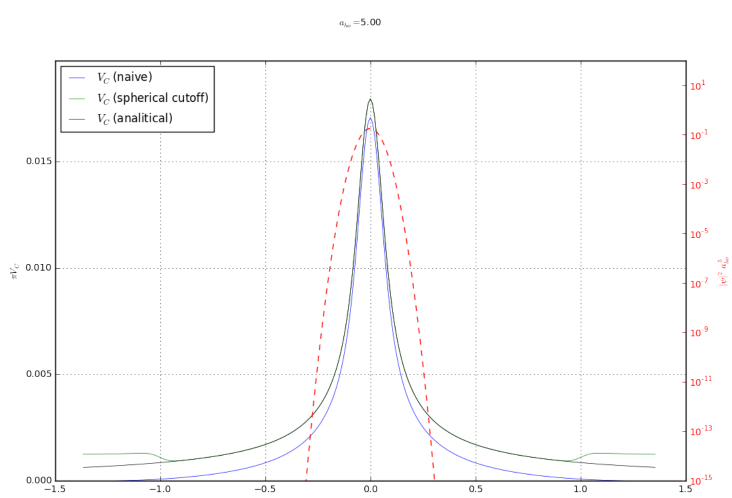

Figure 3: Spherical cutoff method is expected to give accurate results except edges of the lattice, so bigger box for computation and truncation of results is needed. (the red plot is density of charge in log-scale)

2.3 Cubic cutoff method

(not done yet...)

Appendix

Coulomb integral

$$\mathcal{F}\left[\frac{1}{4\pi}\frac{q^2}{|\boldsymbol{r}|}\right] = \frac{q^2}{4\pi}\lim_{\alpha\to 0}\int_0^{2\pi} d\phi \int_0^\infty dr \int_{-1}^{1} e^{ikr\cos\theta} e^{-\alpha r}\frac{1}{r}r^2 d\left(cos\theta\right) = \lim_{\alpha\to 0}\frac{q^2}{2ik}\int_0^\infty \left[\frac{1}{r}e^{ikrx}\right]_{x=-1}^{x=\ 1} e^{-\alpha r} r dr = \lim_{\alpha\to 0}\frac{q^2}{2ik}\int_0^\infty \left[e^{(ik-\alpha)r} - \right.$$

$$= \lim_{\alpha\to 0}\frac{q^2}{2ik}\left[\frac{1}{(ik-\alpha)}e^{(ik-\alpha)r} + \frac{1}{(ik+\alpha)}e^{-(ik+\alpha)r}\right]_{r=0}^{r=\infty} = \lim_{\alpha\to 0}\frac{q^2}{2ik}\left[\frac{(ik-\alpha)\,e^{ikr} + (ik+\alpha)\,e^{-ikr}}{(ik-\alpha)\,(ik+\alpha)}|_{r=\infty} - \frac{(ik-\alpha)+(ik+\alpha)}{(ik-\alpha)\,(ik+\alpha)}\right] =$$

$$= \frac{q^2}{2ik}\left[\frac{ik\left(e^{ikr}+e^{-ikr}\right)}{-k^2}|_{r=\infty} - \lim_{\alpha\to 0}\frac{2ik}{-k^2-\alpha^2}\right] = \lim_{R\to\infty}\frac{q^2}{2}\frac{2\cos\left(kr\right)}{-k^2}|_{r=R} + \lim_{\alpha\to 0}\frac{q^2}{k^2+\alpha^2}$$

$$= \lim_{R\to\infty} q^2\frac{1-\cos\left(kR\right)}{k^2}$$

See also:
http://physics.stackexchange.com/questions/7462/fourier-transform-of-the-coulomb-potential