Accurate and efficient computation of nonlocal potentials using NUFFT and Gaussian-Sum Method

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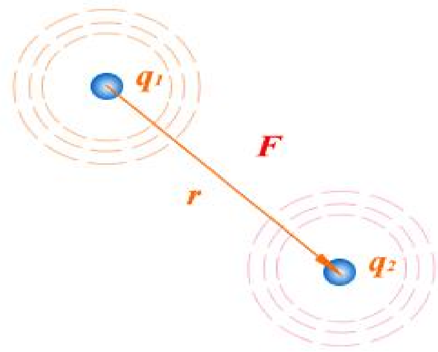
Introduction

Nonlocal potential of interest

Some physical non-local long-range interaction examples

- Coulomb interaction, isotropic
- Dipole-Dipole interaction, anisotropic, including Polar molecules, Rydberg atoms, Light-induced dipoles and Magnetic dipoles[a]

[a] Rep. Prog. Phys. 72 (2009) 126401



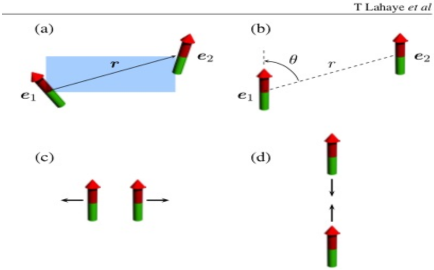


Figure 2. Two particles interacting via the dipole–dipole interaction. (*a*) Non-polarized case; (*b*) polarized case; (*c*) two polarized dipoles side by side repel each other (black arrows); (*d*) two polarized dipoles in a 'head-to-tail' configuration attract each other (black arrows).

Nonlocal potential of interest

Direct summation method for particles

- Assume N particle (source) with charge/momentum q_j located at x_j
- Target: Potential at x_i (excluding the singular contribution)
- Direct summation

$$\Phi(x_i) = \sum_{j=1}^{N} q_j U(x_i - x_j), \quad i = 1, \dots, N.$$

here, $U(x)$ is the fundamental interaction, it requires N^2 operations

Nonlocal potential of interest

We consider the following convolution form

$$u(\mathbf{x}) = \int_{\mathbb{R}^d} U(\mathbf{x}-\mathbf{y})\rho(\mathbf{y})d\mathbf{y}, \quad \mathbf{x} \in \mathbb{R}^d \tag{1}$$

where

$$U(\mathbf{x}) = \begin{cases} \frac{1}{4\pi|\mathbf{x}|}, & 3D \text{ Coulomb}, \\ -(\mathbf{m}\cdot\mathbf{n})\delta(\mathbf{x}) - 3\,\partial_{\mathbf{nm}}\left(\frac{1}{4\pi|\mathbf{x}|}\right), & 3D \text{ Dipolar}, \\ \frac{1}{2\pi|\mathbf{x}|}, & 2D \text{ Coulomb}, \\ -\frac{1}{2\pi}\ln|\mathbf{x}|, & 2D \text{ Poisson}. \end{cases} \tag{2}$$

Common in Fields as follows:

- Bose-Einstein Condensates (Dipolar) , Many-body system (Coulomb, Poisson)
- Computational chemistry, Density function theory, Surface physics etc.

Discussion

- Assumptions: Density: smooth and fast decaying
- Density well approximated on uniform mesh by finite FFT series

Nonlocal potential with free boundary condition

Existing solvers

- PDE/pseudo differential equation approach: boundary condition [a]
- Fast multipole method: adaptive density distribution, Greengard and Rokhlin [b]
- Wavelet-based method: Convolution, Genovese etc [c]
- Nonuniform FFT method: Fourier space [d]
- Gaussian-Sum method: Convolution (physical), spectral representation [e]
- Truncated Kernel method: kernel truncation, fast Fourier transform [f]

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[a] Bao CMS 03'; Bao JCP 10'; Zhang JCP 11'; Zhang CiCP, 14'

[b] J. Comput. Phys. 87'; Acta Numer,97' etc

[c] J. Chem. Phys. 06'; J. Comput. Chem. 07' etc

[d] Jiang, Greengard and Bao, SISC 14'; Bao, Jiang,Tang and Zhang, JCP 15', Bao,Tang and Zhang, CiCP 16'

[e] Zhang, Exl and Mauser, JCP 16'; Antoine, Tang and Zhang, JCP,16', Zhang, Tang and Mauser,16'

[f] Vico, Greengard and Ferrando, JCP 16'

Numerical method: NUFFT

NUFFT method:Jiang, Greengard and Bao, SISC, 14'

Basic algorithm (Coulomb potential as an example)

$$
\begin{aligned}
u(\mathbf{x}) &= \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} e^{i\,\mathbf{k}\cdot\mathbf{x}}\ \widehat{U}_{\mathrm{Cou}}(\mathbf{k})\,\widehat{\rho}(\mathbf{k})\,d\mathbf{k} = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \frac{1}{|\mathbf{k}|^{d-1}}\,e^{i\,\mathbf{k}\cdot\mathbf{x}}\,\widehat{\rho}(\mathbf{k})\,d\mathbf{k} \\
&\approx \frac{1}{(2\pi)^d}\int_{|\mathbf{k}|\le P} \frac{1}{|\mathbf{k}|^{d-1}}\,e^{i\mathbf{k}\cdot\mathbf{x}}\,\widehat{\rho}(\mathbf{k})\,d\mathbf{k} \\
&= \frac{1}{(2\pi)^d}\begin{cases} \displaystyle\int_0^P\int_0^\pi\int_0^{2\pi} e^{i\mathbf{k}\cdot\mathbf{x}}\,\widehat{\rho}(\mathbf{k})\,\sin\theta\ d|\mathbf{k}|d\theta d\phi, & d=3, \\ \displaystyle\int_0^P\int_0^{2\pi} e^{i\mathbf{k}\cdot\mathbf{x}}\,\widehat{\rho}(\mathbf{k})\,d|\mathbf{k}|d\phi, & d=2, \end{cases}
\end{aligned} \tag{3}
$$

NUFFT method

Improved version

$$
\begin{aligned}
u(\mathbf{x}) &\approx \frac{1}{(2\pi)^d}\int_{|\mathbf{k}|\le P}\frac{1}{|\mathbf{k}|^{d-1}}\,e^{i\mathbf{k}\cdot\mathbf{x}}\,\widehat{\rho}(\mathbf{k})\,d\mathbf{k} \\
&= \frac{1}{(2\pi)^d}\int_{|\mathbf{k}|\le P} e^{i\mathbf{k}\cdot\mathbf{x}}\,\frac{1-p_d(\mathbf{k})}{|\mathbf{k}|^{d-1}}\,\widehat{\rho}(\mathbf{k})\,d\mathbf{k} + \frac{1}{(2\pi)^d}\int_{|\mathbf{k}|\le P} e^{i\mathbf{k}\cdot\mathbf{x}}\,\frac{p_d(\mathbf{k})}{|\mathbf{k}|^{d-1}}\,\widehat{\rho}(\mathbf{k})\,d\mathbf{k} \\
&\approx \frac{1}{(2\pi)^d}\int_{\mathcal{D}} e^{i\mathbf{k}\cdot\mathbf{x}}\,w_d(\mathbf{k})\,\widehat{\rho}(\mathbf{k})\,d\mathbf{k} + \frac{1}{(2\pi)^d}\int_{|\mathbf{k}|\le P} e^{i\mathbf{k}\cdot\mathbf{x}}\,\frac{p_d(\mathbf{k})}{|\mathbf{k}|^{d-1}}\,\widehat{\rho}(\mathbf{k})\,d\mathbf{k} \qquad (4)
\end{aligned}
$$

Choice of $p_d(\mathbf{x})$ and quadrature

1. C^∞ function that decays exponentially fast as $|\mathbf{k}| \to \infty$
2. $w_d(\mathbf{k}) := \frac{1-p_d(\mathbf{k})}{|\mathbf{k}|^{d-1}}$ is smooth for $\mathbf{k} \in \mathbb{R}^d$.

The first regular integral is well-resolved by FFT (zero-padding of density)
The second integral is done quadrature in spherical domain, using NUFFT.

NUFFT method: brief review

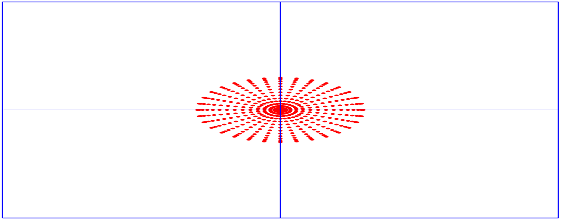
NUFFT algorithm: pure acceleration

Type 1: nonuniform $\mathbf{k}_n$ to $\mathbf{x}_j$ uniform

$$f(\mathbf{x}_j) = \sum_{n=0}^{M-1} F_n e^{i\,\mathbf{k}_n \cdot \mathbf{x}_j} \tag{5}$$

Type 2: uniform source $f(\mathbf{x}_j)$ to nonuniform targets $\mathbf{k}_n$

$$F(\mathbf{k}_n) = \sum_{j=1}^{M} f(\mathbf{x}_j) e^{-i\,\mathbf{k}_n \cdot \mathbf{x}_j} \tag{6}$$



NUFFT method: Bao, Jiang, Tang and Zhang, JCP,15'

2D Poisson

$$u(\mathbf{x}) \quad \approx \quad \frac{1}{(2\pi)^2} \int_{|\mathbf{k}|\le P} \frac{1}{|\mathbf{k}|^2}\, e^{i\mathbf{k}\cdot\mathbf{x}}\, \widehat{\rho}(\mathbf{k})\, d\mathbf{k}, \qquad \mathbf{x} \in \mathbb{R}^2 \tag{7}$$

$u = u_1 + u_2$

$$G(\mathbf{x}) = \frac{1}{2\pi\sigma^2} e^{-\frac{|\mathbf{x}|^2}{2\sigma^2}}, \qquad G_1(\mathbf{x}) = \widehat{\rho}(\mathbf{z})\, G(\mathbf{x}) - \widehat{(\mathbf{x}\rho)}(\mathbf{z}) \cdot \nabla_{\mathbf{x}} G(\mathbf{x}) \tag{8}$$

$$u_1(\mathbf{x}) = (U_{\mathrm{Lap}} * G_1)(\mathbf{x}) = \widehat{\rho}(\mathbf{z})\, u_{1,1}(\mathbf{x}) - \widehat{(\mathbf{x}\rho)}(\mathbf{z}) \cdot \mathbf{u}_{1,2}(\mathbf{x}) \tag{9}$$

with

$$u_{1,1}(\mathbf{x}) = (U_{\mathrm{Lap}} * G)(\mathbf{x}), \qquad \mathbf{u}_{1,2}(\mathbf{x}) = \nabla_{\mathbf{x}}\, u_{1,1}(\mathbf{x}) \tag{10}$$

u_2: remaining well-defined integral

$$\begin{aligned} u_2(\mathbf{x}) \quad &= \quad (U_{\mathrm{Lap}} * (\rho - G_1))(\mathbf{x}) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{\widehat{\rho}(\mathbf{k}) - \widehat{G}_1(\mathbf{k})}{|\mathbf{k}|^2}\; e^{i\,\mathbf{k}\cdot\mathbf{x}}\; d\mathbf{k} \\ &= \quad \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{W(\mathbf{k})}{|\mathbf{k}|}\; e^{i\,\mathbf{k}\cdot\mathbf{x}}\; d\mathbf{k} \approx \frac{1}{(2\pi)^2} \int_0^P \int_0^{2\pi} W(\mathbf{k})\; e^{i\,\mathbf{k}\cdot\mathbf{x}}\; d|\mathbf{k}|\, d\theta \end{aligned} \tag{11}$$

Numerical method : Truncated Kernel method

Truncated Kernel method

Kernel truncation and Fourier Transform

$$U_D(\mathbf{x}) = \frac{1}{4\pi|\mathbf{x}|}\mathbb{I}_{\mathcal{B}_D}(\mathbf{x}) \qquad \Longrightarrow \qquad \widehat{U_D}(\mathbf{k}) = \frac{1}{|\mathbf{k}|^2}(1 - \cos(|\mathbf{k}|D)) \tag{12}$$

$D = \sqrt{d}L$ where density is compactly supported in $[-L, L]^d$.

Truncated Kernel method

Kernel truncation and Fourier Transform

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$D = \sqrt{d}L$ where density is compactly supported in $[-L, L]^d$.

Advantages and adaptation

- Simple to implement in Fourier domain [a]
- Easy extensions to other kernel, including helmholtz, Yukawa potential etc
- Not easy adaptation for anisotropic density,e.g. $[-L, L]^2 \times \gamma[-L, L]$

[a] PRB 06', Greengard et al 16'

Numerical method : GS-based solver

Nonlocal potential with free boundary condition

Discussion

- Efficiency: NUFFT method is slow in 3D
- Accuracy: Wavelet-based method neglects the near field integral
- Anisotropic density: Computational cost increases with stronger anisotropy
- Observation:
  (1) Faithful FFT representation of the density
  (2) Smooth/separable approx. of kernel by Gaussians (+ for storage/accuracy)
  (3) Compute the correction integral for near field interaction

Rescaling to unit box $\mathbf{B}_1$

Assumptions on the density ρ

- smooth
- decays fast enough, compactly supported in bounded domain, e.g. $\mathbf{B}_L \in \mathbb{R}^d$

Target

- Given density ρ on uniform grid $\mathcal{M}$, discretisation of $\mathbf{B}_L$
- Aim to evaluate the potential u on the same uniform grid $\mathcal{M}$

Rescaling to unit box $\mathbf{B}_1$

- $\mathbf{x} = \widetilde{\mathbf{x}}\, L, \quad \rho(\mathbf{x}) = \widetilde{\rho}(\widetilde{\mathbf{x}}), \quad \Longrightarrow \quad \widetilde{\mathbf{x}} \in \mathbf{B}_1, \;\; \mathrm{supp}(\widetilde{\rho}) \subset \mathbf{B}_1$
-

$$u(\mathbf{x}) = \int_{\mathbb{R}^d} U(\mathbf{x}-\mathbf{y})\rho(\mathbf{y})d\mathbf{y} = \int_{\mathbf{B}_L} U(\mathbf{x}-\mathbf{y})\rho(\mathbf{y})d\mathbf{y} = L^d \int_{\mathbf{B}_1} \widetilde{U}(\widetilde{\mathbf{x}}-\widetilde{\mathbf{y}})\widetilde{\rho}(\widetilde{\mathbf{y}})d\widetilde{\mathbf{y}}. \quad (13)$$

with $\widetilde{U}(\widetilde{\mathbf{x}}) = U(\mathbf{x}) = U(\widetilde{\mathbf{x}}L) = L^{-1}U(\widetilde{\mathbf{x}})$.

Rescaling to unit box $\mathbf{B}_1$

Coulomb potential, $d = 2, 3$

$$u(\mathbf{x}) = \widetilde{u}(\widetilde{\mathbf{x}}) = L^{d-1} \int_{\mathbf{B}_1} U(\widetilde{\mathbf{x}} - \widetilde{\mathbf{y}})\widetilde{\rho}(\widetilde{\mathbf{y}})d\widetilde{\mathbf{y}}, \qquad \widetilde{\mathbf{x}} \in \mathbf{B}_1, \quad d = 2, 3. \tag{14}$$

2d Poisson potential

$$u(\mathbf{x}) = \widetilde{u}(\widetilde{\mathbf{x}}) = -\frac{L^2}{2\pi} \int_{\mathbf{B}_1} \widetilde{\rho}(\widetilde{\mathbf{y}}) \ln|\widetilde{\mathbf{x}} - \widetilde{\mathbf{y}}| \, d\widetilde{\mathbf{y}} - \frac{L^2}{2\pi} \ln L \int_{\mathbf{B}_1} \widetilde{\rho}(\widetilde{\mathbf{y}}) \, d\widetilde{\mathbf{y}}, \quad \widetilde{\mathbf{x}} \in \mathbf{B}_1. \tag{15}$$

1. Reformulation

The key reformulation reads

$$
\begin{aligned}
u(\mathbf{x}) &= \int_{\mathbb{R}^d} U(\mathbf{y})\,\rho(\mathbf{x}-\mathbf{y})d\mathbf{y} \\
&= \int_{\mathbb{R}^d} U_{GS}(\mathbf{y})\rho(\mathbf{x}-\mathbf{y})d\mathbf{y} + \int_{\mathbb{R}^d} [U(\mathbf{y}) - U_{GS}(\mathbf{y})]\,\rho(\mathbf{x}-\mathbf{y})d\mathbf{y} \\
&:= I_1 + I_2,
\end{aligned}
$$

where Gaussian sum approximation

$$
U_{GS}(\mathbf{y}) = \sum_{j=0}^{S} w_j\, e^{-\tau_j^2|\mathbf{y}|^2}
$$

and I_1 and I_2 are the first (regular) and second integral (correction) , respectively.

2. Regular part

For $\mathbf{x} \in \mathbf{B}_1$, we have

$$I_1(\mathbf{x}) = \sum_{l=0}^{S} w_l \int_{\mathbf{B}_2} e^{-\tau_l^2 |\mathbf{y}|^2} \rho(\mathbf{x} - \mathbf{y}) d\mathbf{y} \tag{16}$$

Finite Fourier series approximation of the density:

$$\rho(\mathbf{z}) \approx \sum_{\mathbf{k}} \widehat{\rho}_{\mathbf{k}} \prod_{j=1}^{d} e^{\frac{2\pi i \ k_j}{b_j - a_j}(z^{(j)} - a_j)}, \qquad \mathbf{z} = (z^{(1)}, \ldots, z^{(d)}) \in \mathbf{B}_3, \tag{17}$$

$$\widehat{\rho}_{\mathbf{k}} = \frac{1}{|\mathbf{B}_3|} \int_{\mathbf{B}_3} \rho(\mathbf{z}) \prod_{j=1}^{d} e^{\frac{-2\pi i \ k_j}{b_j - a_j}(z^{(j)} - a_j)} d\mathbf{z}.$$

2. Regular part (cont'd)

Plugging (17) into (16), we shall have

$$I_1(\mathbf{x}) = \sum_{l=0}^{S} w_l \int_{\mathbf{B}_2} e^{-\tau_l^2|\mathbf{y}|^2} \rho(\mathbf{x}-\mathbf{y}) d\mathbf{y}$$
$$= \sum_{\mathbf{k}} \widehat{\rho}_{\mathbf{k}} \left(\sum_{l=0}^{S} w_l G_{\mathbf{k}}^l \right) \prod_{j=1}^{d} e^{\frac{2\pi i \ k_j}{b_j - a_j}(x^{(j)} - a_j)},$$

where

$$G_{\mathbf{k}}^l = \prod_{j=1}^{d} \int_{-2}^{2} e^{-\tau_l^2|y^{(j)}|^2} e^{\frac{-2\pi i k_j \ y^{(j)}}{b_j - a_j}} dy^{(j)}. \quad (18)$$

3. Correction Integral

I_2 is split into two integrals as

$$I_2(\mathbf{x}) = \int_{\mathbb{R}^d} \left(U(\mathbf{y}) - \sum_{k=0}^{S} w_k \, e^{-\tau_k^2 |\mathbf{y}|^2} \right) \rho(\mathbf{x}-\mathbf{y}) d\mathbf{y} \quad (19)$$

$$= \left(\int_{\mathcal{B}_\delta} + \int_{\mathcal{B}_\delta^c} \right) \left(U(\mathbf{y}) - \sum_{k=0}^{S} w_k \, e^{-\tau_k^2 |\mathbf{y}|^2} \right) \rho(\mathbf{x}-\mathbf{y}) d\mathbf{y} \quad (20)$$

$$= I_{2,1}(\mathbf{x}) + I_{2,2}(\mathbf{x}), \; \mathcal{B}_\delta = \{\mathbf{x} \in \mathbb{R}^d | \; |\mathbf{x}| < \delta\}, \; \mathcal{B}_\delta^c = \mathbb{R}^d \backslash \mathcal{B}_\delta. \quad (21)$$

Neglect this part:

$$|I_{2,2}(\mathbf{x})| \leq \varepsilon \int_{\mathbf{B}_3} |\rho(\mathbf{y})| d\mathbf{y} \leq \varepsilon \int_{\mathbb{R}^d} |\rho(\mathbf{y})| d\mathbf{y} = \varepsilon \|\rho\|_{L^1(\mathbb{R}^d)}. \quad (22)$$

3. Correction Integral (cont'd)

Taylor expansion of density within $\mathcal{B}_\delta$:

$$\rho_{\mathbf{x}}(\mathbf{y}) = \mathrm{T}_{\mathbf{x}}(\mathbf{y}) + \mathrm{R}_{\mathbf{x}}(\mathbf{y}), \quad \mathbf{y} \in \mathcal{B}_\delta, \tag{23}$$

where $\mathrm{T}_{\mathbf{x}}(\mathbf{y})$ is the third order Taylor expansion and the remainder $\mathrm{R}_{\mathbf{x}}(\mathbf{y}) = C(\rho, \mathbf{x})|\mathbf{y}|^4$ with the constant $C(\rho, \mathbf{x})$ depending on the density ρ and $\mathbf{x}$.

The accuracy of the approximation $\widetilde{I_{2,1}}$ of $I_{2,1}$ is estimated as follows:

$$|(I_{2,1} - \widetilde{I_{2,1}})(\mathbf{x})| \quad \leq \quad C(\rho, \mathbf{x})\,|S^{d-1}|\,C_S \begin{cases} \delta^{d+3}, & \text{Coulomb kernel} \\ \delta^6\,|\log\delta|, & \text{Poisson kernel in 2d} \end{cases} \tag{24}$$

where

$$\widetilde{I_{2,1}} = \int_{\mathcal{B}_\delta} \left(U(\mathbf{y}) - \sum_{l=0}^{S} w_l\, e^{-\tau_l^2 |\mathbf{y}|^2} \right) \mathrm{T}_{\mathbf{x}}(\mathbf{y}) d\mathbf{y}. \tag{25}$$

4. Sinc-quadrature

Proposition (Hackbusch/Khoromskij 2006)

Let $f \in H^1(D_\lambda)$ *with some* $\lambda < \pi/2$. *If* f *satisfies the condition*

$$|f(t)| \le C\,\exp(-be^{a|t|}) \quad \forall t \in \mathbb{R} \text{ with } a, b, C > 0, \tag{26}$$

then the quadrature error for the special choice $\vartheta = \ln(\frac{2\pi aS}{b})/(aS)$ *satisifies*

$$\left| \int_{\mathbb{R}} f(t)\,dt - \vartheta \sum_{|k|\le S} f(k\vartheta) \right| \le C\,N(f, D_\lambda)\,\exp\left(\frac{-2\pi\lambda aS}{\ln(2\pi aS/b)} \right). \tag{27}$$

4. Sinc-quadrature

Gaussian approximation of $1/r$ and $\ln r$ over $[\delta, 2]$

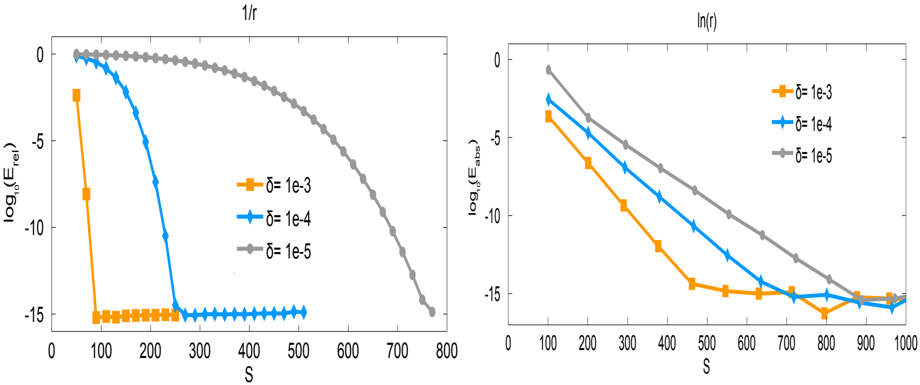

Figure: Number of terms S versus E_{rel} for the kernel $1/r$ (left) and E_{abs} for $\ln r$ (right) on $[\delta, 2]$.

4. Sinc-quadrature

Coulomb kernel approximation

$$\frac{1}{|\mathbf{x}|} = \frac{2}{\sqrt{\pi}} \int_0^{\infty} e^{-|\mathbf{x}|^2 \tau^2} \, d\tau = \frac{2}{\sqrt{\pi}} \int_0^{\infty} \prod_{p=1}^{d} e^{-x^{(p)2} \tau^2} \, d\tau. \tag{28}$$

Applying some numerical quadrature to the integral $\int_0^{\infty} e^{\rho \tau^2} d\tau$ leads to a GS approximation

Coulomb kernel approximation

$$\frac{1}{|\mathbf{x}|} \approx \sum_q w_q \prod_{j=1}^{d} e^{-\tau_q^2 \, x^{(j)2}}. \tag{29}$$

4. Sinc-quadrature

2D Poisson kernel approximation: $\ln r$

$$\frac{1}{{x^{(1)}}^2 + {x^{(2)}}^2} = \int_0^\infty e^{-({x^{(1)}}^2 + {x^{(2)}}^2)\tau} \, d\tau. \tag{30}$$

Second

$$\ln \sqrt{{x^{(1)}}^2 + {x^{(2)}}^2} = \int_{\sqrt{1-{x^{(2)}}^2}}^{x^{(1)}} \frac{y}{y^2 + {x^{(2)}}^2} \, dy, \tag{31}$$

Apply the Sinc quadrature

$$\ln \sqrt{{x^{(1)}}^2 + {x^{(2)}}^2} \approx C_0 - \sum_{q=1}^{S} \widetilde{w}_q \, e^{-\widetilde{\tau_q}({x^{(1)}}^2 + {x^{(2)}}^2)} =: \sum_{q=0}^{S} w_q \, e^{-\tau_q^2({x^{(1)}}^2 + {x^{(2)}}^2)}, \tag{32}$$

Numerics of GS-based solver

3D Coulomb potential: $U(\mathbf{x}) = \frac{1}{4\pi|\mathbf{x}|}$

Exact solution for Gaussian density

For density $\rho(\mathbf{x}) := e^{-(x^2+y^2+\gamma^2 z^2)/\sigma^2}$, the potential is given exactly

$$u(\mathbf{x}) = \begin{cases} \frac{\sigma^3\sqrt{\pi}}{4\,|\mathbf{x}|}\,\mathrm{Erf}\left(\frac{|\mathbf{x}|}{\sigma}\right), & \gamma = 1, \\ \frac{\sigma^2}{4\gamma}\int_0^\infty \frac{e^{-\frac{x^2+y^2}{\sigma^2(t+1)}}\,e^{-\frac{z^2}{\sigma^2(t+\gamma^{-2})}}}{(t+1)\sqrt{t+\gamma^{-2}}}\,dt, & \gamma \neq 1, \end{cases} \qquad \mathbf{x} \in \mathbb{R}^3, \tag{33}$$

where $\mathrm{Erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt$ for $x \in \mathbb{R}$ is the error function.

Non symmetric density: Shifted density $\rho_{\mathbf{x}_0}(\mathbf{x}) := \rho(\mathbf{x} - \mathbf{x}_0)$, the potential is shifted correspondingly $u_{\mathbf{x}_0}(\mathbf{x}) = u(\mathbf{x} - \mathbf{x}_0)$.

3D Coulomb potential: $U(\mathbf{x}) = \frac{1}{4\pi|\mathbf{x}|}$

Table: Error E_h and timing of the 3D Coulomb potential with isotropic density with $\sigma = 1.2$ on $[-L, L]^3$.

$L = 8$	N	E_h	T_1	T_2	T_{total}
$h = 1$	16^3	1.096E-03	9.99E-04	1.00E-03	2.00E-03
h=1/2	32^3	1.130E-09	1.60E-02	2.00E-03	1.80E-02
h=1/4	64^3	6.169E-16	1.93E-01	1.90E-02	2.12E-01
h=1/8	128^3	6.187E-16	1.69	6.28E-01	2.31
h=1/16	256^3	7.725E-16	15.03	4.71	19.74
L=16	N	E_h	T_1	T_2	T_{total}
$h = 1$	32^3	1.113E-03	1.60E-02	2.00E-03	1.80E-02
h=1/2	64^3	1.191E-09	1.95E-01	2.10E-02	2.16E-01
h=1/4	128^3	9.259E-16	1.71	6.22E-01	2.33
h=1/8	256^3	9.271E-16	15.18	4.76	19.94

3D Coulomb potential: $U(\mathbf{x}) = \frac{1}{4\pi|\mathbf{x}|}$

Table: Error E_h and timing of the 3D Coulomb potential for shifted Gaussian density with $\sigma = 1.2$ and $\mathbf{x}_0 = (1, 2, 1)^T$ on $[-12, 12]^3$.

L=12	N	E_h	T_1	T_2	T_{total}
$h = 1$	24^3	1.108E-03	7.00E-03	4.00E-03	1.10E-02
h=1/2	48^3	1.175E-09	8.10E-02	1.20E-02	9.30E-02
h=1/4	96^3	6.182E-16	7.03E-01	1.08E-01	8.11E-01
h=1/8	192^3	7.717E-16	6.30	1.08	7.37

Table: Error E_h and timing of the 3D Coulomb potential for anisotropic densities with $\sigma = 2$ computed on $\Omega = [-12, 12]^2 \times \frac{1}{\gamma}[-12, 12]$ with $h_x = h_y = 1/8, h_z = h_x/\gamma$ and $N = 192^3$.

γ	E_h	$\|u\|_{\max}$	T_1	T_2	T_{total}
1	8.894E-16	2	6.09	1.06	7.15
2	7.360E-16	1.209	6.14	1.05	7.19
4	1.664E-14	0.681	6.34	1.05	7.39
8	1.474E-12	0.364	6.94	1.34	8.29
16	2.226E-12	0.189	6.26	1.06	7.32

3D Dipolar potential

Dipolar potential definition

$$u(\mathbf{x}) = -(\mathbf{n}\cdot\mathbf{m})\,\rho(\mathbf{x}) - 3\,\partial_{\mathbf{nm}}\left(\frac{1}{4\pi|\mathbf{x}|} * \rho\right) \quad (34)$$

$$= -(\mathbf{n}\cdot\mathbf{m})\,\rho(\mathbf{x}) - 3\,\frac{1}{4\pi|\mathbf{x}|} * \left(\partial_{\mathbf{nm}}\,\rho\right), \quad (35)$$

Exact solution for $\rho(\mathbf{x}) = e^{-|\mathbf{x}|^2/\sigma^2}$

$$uviathe2DCoulombpotential(\mathbf{x}) = -(\mathbf{n}\cdot\mathbf{m})\,\rho(\mathbf{x}) - 3\,\partial_{\mathbf{nm}}\left(\frac{1}{4\pi|\mathbf{x}|} * \rho\right) = -(\mathbf{n}\cdot\mathbf{m})\,\rho(\mathbf{x})$$

$$= -(\mathbf{n}\cdot\mathbf{m})\,\rho(\mathbf{x}) - 3\,\mathbf{n}^T\mathbf{D}\,\mathbf{m},$$

where δ_{ij} is the Dirac delta function and the Hessian matrix $\mathbf{D}$ is given as follows

$$\mathbf{D}_{ij} = \delta_{ij}\left(\frac{\sigma^2}{2r^2}e^{-\frac{r^2}{\sigma^2}} - \frac{\sigma^3\sqrt{\pi}}{4r^3}\mathrm{Erf}\left(\frac{r}{\sigma}\right)\right) + \quad (37)$$

$$\mathbf{x}_i\mathbf{x}_j\left(-\frac{3\,\sigma^2}{2\,r^4}e^{-\frac{r^2}{\sigma^2}} - \frac{1}{r^2}e^{-\frac{r^2}{\sigma^2}} + \frac{3\,\sigma^3\sqrt{\pi}}{4\,r^5}\mathrm{Erf}\left(\frac{r}{\sigma}\right)\right), \qquad i,j = 1,2,3. \quad (38)$$

3D Dipolar potential

Table: Error E_h and timing of the 3D dipolar potential with $\sigma = 1.2, \mathbf{n} = (0.82778, 0.41505, -0.37751)^T, \mathbf{m} = (0.3118, 0.9378, -0.15214)^T$ on $[-8, 8]^3$.

$L = 8$	N	E_h	$T_{\rm pre}$	T_1	T_2	T_{total}
$h = 1$	16^3	1.380E-02	0	2.00E-03	0	2.00E-03
h=1/2	32^3	2.647E-07	2.00E-03	1.50E-02	2.00E-03	1.90E-02
h=1/4	64^3	1.430E-14	1.70E-02	2.00E-01	1.90E-02	2.35E-01
h=1/8	128^3	4.076E-14	1.96E-01	1.68	2.20E-01	2.10

2D Coulomb potential: $U(\mathbf{x}) = \frac{1}{2\pi|\mathbf{x}|}$

Exact solution for Gaussian density

For density $\rho(\mathbf{x}) = e^{-(x^2+\gamma^2 y^2)/\sigma^2}$ with $\sigma > 0$ and $\gamma \geq 1$, the 2D Coulomb potential, with kernel $U(\mathbf{x}) = \frac{1}{2\pi|\mathbf{x}|}$, can be obtained analytically as

$$u(\mathbf{x}) = \begin{cases} \frac{\sqrt{\pi}\,\sigma}{2}\,\mathrm{I}_0\left(\frac{|\mathbf{x}|^2}{2\sigma^2}\right)\,e^{-\frac{|\mathbf{x}|^2}{2\sigma^2}}, & \gamma = 1, \\ \frac{\sigma}{\gamma\sqrt{\pi}}\int_0^\infty \frac{e^{-\frac{x^2}{\sigma^2(t^2+1)}}\,e^{-\frac{y^2}{\sigma^2(t^2+\gamma^{-2})}}}{\sqrt{t^2+1}\,\sqrt{t^2+\gamma^{-2}}}\,dt, & \gamma \neq 1, \end{cases} \qquad \mathbf{x} \in \mathbb{R}^2, \tag{39}$$

where I_0 is the modified Bessel function of order zero.

2D Coulomb potential: $U(\mathbf{x}) = \frac{1}{2\pi|\mathbf{x}|}$

Table: Error E_h and timing of the 2D Coulomb potential on $[-L, L]^2$ with different mesh size h.

$L = 8$	N	E_h	T_1	T_2	T_{total}
$h = 1$	16^2	9.426E-04	0	0	0
h=1/2	32^2	1.720E-09	0	0	0
h=1/4	64^2	4.190E-16	2.00E-03	1.01E-03	3.00E-03
h=1/8	128^2	5.229E-16	6.00E-03	2.00E-03	8.00E-03
h=1/16	256^2	5.229E-16	2.30E-02	7.01E-03	3.00E-02
L=16	N	E_h	T_1	T_2	T_{total}
$h = 1$	32^3	9.576E-04	1.00E-03	0	1.00E-03
h=1/2	64^3	1.815E-09	1.00E-03	0	1.00E-03
h=1/4	128^3	5.846E-15	5.00E-03	2.00E-03	7.00E-03
h=1/8	256^3	5.846E-15	2.60E-02	7.00E-03	3.30E-02
h=1/16	512^2	6.055E-15	2.47E-01	2.80E-02	2.75E-01

2D Coulomb potential: $U(\mathbf{x}) = \frac{1}{2\pi|\mathbf{x}|}$

Table: Error E_h and timing of the 2D Coulomb potential for anisotropic densities with $\sigma = 2$ computed on $\Omega = [-12, 12] \times \frac{1}{\gamma}[-12, 12]$ with $h_x = 1/8, h_y = h_x/\gamma$ and $N = 192^2$.

γ	E_h	$\|u\|_{\max}$	T_1	T_2	T_{total}
1	5.047E-16	1.773	1.00E-02	2.00E-03	1.20E-02
2	5.479E-16	1.217	1.20E-02	3.00E-03	1.50E-02
4	4.235E-16	7.902E-01	9.00E-03	2.00E-03	1.10E-02
8	1.402E-15	4.902E-01	1.20E-02	2.00E-03	1.40E-02
16	8.387E-15	2.935E-01	1.20E-02	2.00E-03	1.40E-02

2D Poisson potential: $U(\mathbf{x}) = -\frac{1}{2\pi} \ln |\mathbf{x}|$

Exact solution

For $\rho(\mathbf{x}) := e^{-|\mathbf{x}|^2/\sigma^2} = e^{-r^2/\sigma^2}$ with $r = |\mathbf{x}|$ and $\sigma > 0$, the 2D Poisson potential, with kernel $U(\mathbf{x}) = -\frac{1}{2\pi} \ln |\mathbf{x}|$, can be obtained analytically as

$$u(\mathbf{x}) = \begin{cases} -\frac{\sigma^2}{4} \left[\mathrm{E}_1\left(\frac{|\mathbf{x}|^2}{\sigma^2}\right) + 2\ln(|\mathbf{x}|)\right], & \mathbf{x} \neq 0, \\ \frac{\sigma^2}{4}\left(\gamma_e - \ln(\sigma^2)\right), & \mathbf{x} = \mathbf{0}, \end{cases} \tag{40}$$

where $\mathrm{E}_1(r) := \int_r^\infty t^{-1} e^{-t} dt$ for $r > 0$ is the exponential integral function and $\gamma_e \approx 0.5772156649015328606$ is the Euler-Mascheroni constant.

2D Poisson potential: $U(\mathbf{x}) = -\frac{1}{2\pi} \ln |\mathbf{x}|$

Table: Error E_h and timing of the 2D Poisson potential with $\sigma = 1.2$ on $[-L, L]^2$.

$L = 8$	N	E_h	T_1	T_2	T_{total}
$h = 1$	16^2	3.768E-04	0	0	0
h=1/2	32^2	3.331E-10	1.00E-03	0	1.00E-03
h=1/4	64^2	3.623E-15	2.00E-03	1.00E-03	3.00E-03
h=1/8	128^2	2.988E-15	6.00E-03	1.00E-03	7.00E-03
h=1/16	256^2	5.085E-15	2.30E-02	4.00E-03	2.70E-02

L=16	N	E_h	T_1	T_2	T_{total}
$h = 1$	32^2	2.966E-04	1.00E-04	0	1.00E-03
h=1/2	64^2	2.713E-10	2.00E-03	0	2.00E-03
h=1/4	128^2	3.856E-15	6.00E-03	2.00E-03	8.00E-03
h=1/8	256^2	3.164E-15	2.60E-02	6.00E-03	3.20E-02
h=1/16	512^2	6.921E-15	2.47E-01	3.00E-02	2.77E-01

Extension to other nonlocal potentials

- 2D Dipolar potential via the 2D Coulomb potential
- Davey-Stewartson nonlocal potential [1]
- KP-II nonlocal potential etc
- Yukawa potential $U(r) = \frac{e^{-\mu r}}{r}, \ \mu > 0$
- Helmholtz potential $U(r) = \frac{e^{ikr}}{r}$:difficult for high k
- Combination with Finite element method

[1] Stimming, Mauser and Zhang,14'

Conclusion and Discussion

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- efficient : implemented with FFTs, thus ideal for parallel computing, e.g. MPI, GPUs
- adaptable to other kernels

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Discussion

- Application to BECs involving dipolar, Coulomb interaction without truncation
- ability with anisotropic density without increasing cost in CPU and storage
- accurate energy evaluation can also benefit
- optimal GS approximation in terms of number of Gaussians

Thanks for all your attention !!