

October 8⁸, 2026
Announcements

- HW1 graded
- HW3 due tonight
- Project proposals!
(due next week!)

Goals

- Enclad
- DMK
- Direct solvers.

Review

- Fourier
- NUFFT

Preliminaries: Convolution

$$(f * g)(x) = \int_{\mathbb{R}} f(\xi)g(x - \xi)d\xi.$$

- Convolution with a shifted δ is the same as shifting the function:

$$[f * (\xi \mapsto \delta(\xi - a))](x) = f(x - a).$$

- Convolution is linear (in both arguments) and commutative.

Preliminaries: Fourier Transform

$$\mathcal{F}(f)(\omega) = \int_{\mathbb{R}} f(x) e^{-2\pi i \omega x} dx.$$

- ▶ Convolution turns into multiplication: $\mathcal{F}\{f * g\} = \mathcal{F}f \cdot \mathcal{F}g$.
- ▶ A single shifted δ transforms as (as a distribution!)

$$\mathcal{F}\{\delta(x - a)\}(\omega) = e^{-2\pi i a \omega}.$$

- ▶ A unit-periodic “train” of δ s is its own $\mathcal{F}$ [Décoret '04]:

$$\mathcal{F}\left\{\sum_{\ell \in \mathbb{Z}} \delta(x - \ell)\right\}(\omega) = \sum_{k \in \mathbb{Z}} \delta(\omega - k).$$

What is $\mathcal{F}\{f(x - a)\}$?

Simple and Periodic: Ewald Summation

We want to evaluate the potential generated by an infinite periodic array of sources (self-interactions 0 by convention):

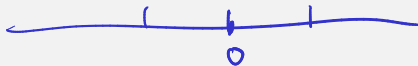
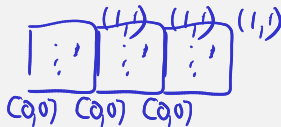


$$\psi(\mathbf{x}) = \sum_{\mathbf{m} \in \mathbb{Z}^d} \sum_{j=1}^{N_{\text{src}}} G(\mathbf{x}, \mathbf{y}_j + \mathbf{m}) \varphi(\mathbf{y}_j).$$


Assume the kernel is translation invariant: $G(\mathbf{x}, \mathbf{y}) = G(\mathbf{x} - \mathbf{y})$.

'Lattice sum'

$$\sum_n \frac{1}{n}$$



Lattice Sums: Convergence

Q: When is the lattice sum guaranteed to converge?

$\sum \frac{1}{i^\alpha}$ conv. if $\alpha > 1$

$$G(\vec{x}) = O(\|\vec{x}\|_2^{-p}) \quad (\text{as } \|\vec{x}\|_2 \rightarrow \infty)$$

$$\sum_{\vec{m} \in \mathbb{Z}^d} |G(\vec{m})| \lesssim \sum_i i^{d-1} \frac{1}{i^p}$$

$$d-1-p < -1 \Leftrightarrow p > d$$

Lattice Sums: More Kernels

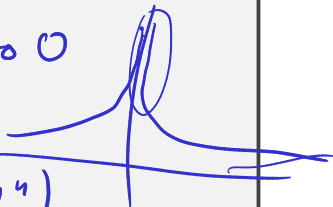
$p > d$ is mighty restrictive. What can we do to allow the Coulomb kernel?

- "charge neutrality"

$$\sum \varphi(\vec{r}_j) = 0$$

- Pole $\omega=0$ mode to 0

(aka "impose BCs
on finite-but-
-growing crystal")



Ewald Summation: Dealing with Smoothness

$$\psi(\mathbf{x}) = \sum_{\mathbf{i} \in \mathbb{Z}^d} \sum_{j=1}^{N_{\text{src}}} G(\mathbf{x}, \mathbf{y}_j + \mathbf{i}) \varphi(\mathbf{y}_j)$$

This is the convolution of G with a periodic discrete source distribution. We would like to use the fact that the Fourier transform turns convolutions into products. How?

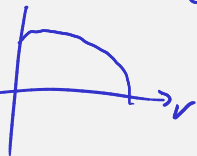
G non smooth
 $\rightarrow \mathcal{F}\{G\}?$

Ewald Summation: Screens

$$G(\vec{x}) = \underbrace{\sigma(\|\vec{x}\|_2) G(\vec{x})}_{\text{long-range}} + \underbrace{(1 - \sigma(\|\vec{x}\|_2)) G(\vec{x})}_{\text{short-range}}$$
$$G(\vec{x}) = \frac{1}{\|\vec{x}\|^2}$$

- σ smooth
- $\sigma(\|\vec{x}\|_2) = O(\|\vec{x}\|_2^4)$ as $\vec{x} \rightarrow 0$
• σ & G need σ to have derivatives at 0.

• $1 - \sigma$ should have bounded support.



Ewald Summation: Field Splitting

We can split the computation (from the perspective of a unit cell target) as follows:

	G_{SR}	G_{LR}
Close source	sum directly ↳ ⊕ periodic images	smooth
Far source	0	Fourier

Ewald Summation: Summation (1D for simplicity)

Interesting part: summing G_{LR} . Define the periodic source distribution

$$\rho(x) = \sum_{m \in \mathbb{Z}} \sum_{j=1}^{N_{src}} \varphi(y_j) \delta(x - y_j - m).$$

$$\begin{aligned} \mathcal{F}\{\rho\}(\omega) &= \sum_{j=1}^{N_{src}} \varphi(y_j) e^{-2\pi i y_j \omega} \sum_n \delta(\omega - n) \\ \mathcal{F}\{\psi_{LR}\}(\omega) &= \mathcal{F}\{G_{LR} * \rho\}(\omega) = \mathcal{F}\{G_{LR}\}(\omega) \mathcal{F}\{\rho\}(\omega) \end{aligned}$$

Provide an algorithmic outline for Ewald:

Pick $\mathcal{F}$ grid, Evaluate $\mathcal{F}(\rho)$ (NFFT), multiply by $\mathcal{F}(G_{LR})$ from G_{LR}
FFT $\rightarrow$ real space, add G_{SR} , subtract self-contrib

Ewald Summation: Summation (1D for simplicity), cont'd.

$$\mathcal{F}\{\psi_{\text{LR}}\}(\omega) = \mathcal{F}\{G_{\text{LR}}\}(\omega)\mathcal{F}\{\rho\}(\omega).$$



Ewald Summation: Remarks

In practice: Fourier transforms are carried out discretely using the FFT.

- ▶ Need to choose evaluation grid ('mesh')
 - ▶ In that case: Particle-Mesh Ewald ('PME').
- ▶ Additional error contributions from interpolation
(small if screen smooth enough to be well-sampled by mesh)
- ▶ $O(N \log N)$ cost (from FFT, assuming number of particles $N \sim$ mesh resolution)

Ewald vs FMMs

How does Ewald compare to an FMM?

- non-adaptive
- periodic BCs
- Neg. approaches
 - FMM by distance
 - Ewald by σ