Tutorial on the smooth particle-mesh Ewald algorithm

These notes explain the smooth particle-mesh Ewald algorithm (SPME) in detail. The accompanying library `libpme6` is a fully-featured implementation of SPME that can be used for experimentation and reference. This content can also be found in PDF format here.

Introduction

Motivation and overview of the SPME algorithm

Consider two atoms, labeled 1 and 2, contained in a parallelepiped with sides determined by the (positively oriented) vectors $\ell_1, \ell_2, \ell_3 \in \mathbb{R}^3$ (see Figure). Then the matrix $\mathtt{L} = [\ell_1, \ell_2, \ell_3] \in \mathbb{R}^{3\times 3}$ is such

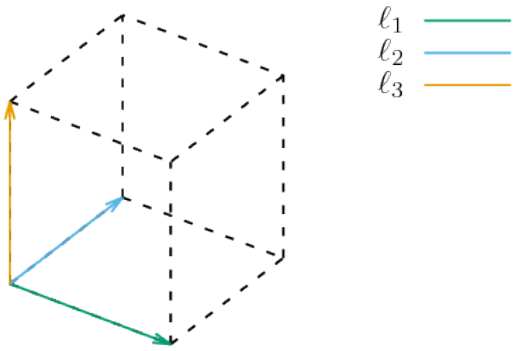

Figure 1: Simulation box spanned by three vectors.

that $V = \det \mathtt{L} > 0$. Now suppose that atom i is at a position $\mathbf{r}_i = \mathtt{L}\,\mathbf{x}_i$ where $\mathbf{x}_i \in [0,1)^3$ for $i = 1,2$ and that $r_{ij} = \|\mathbf{r}_i - \mathbf{r}_j\|$ (see Figure). Between these two atoms there is a force that depends on

Figure 2: Two atoms at a distance r_{ij}.

their distance and whose corresponding potential energy, $U_{ij} = U_{ij}(r_{ij})$, is shown in Figure . If instead of just two atoms we had a total of $N > 2$ atoms (see Figure), then the total potential energy would be equal to

$$H = \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\ i\neq j}}^{N} U_{ij}(r_{ij}). \tag{1}$$

By solving Newton's second law[1] we would be able to simulate the

[1] Force equals mass times acceleration.

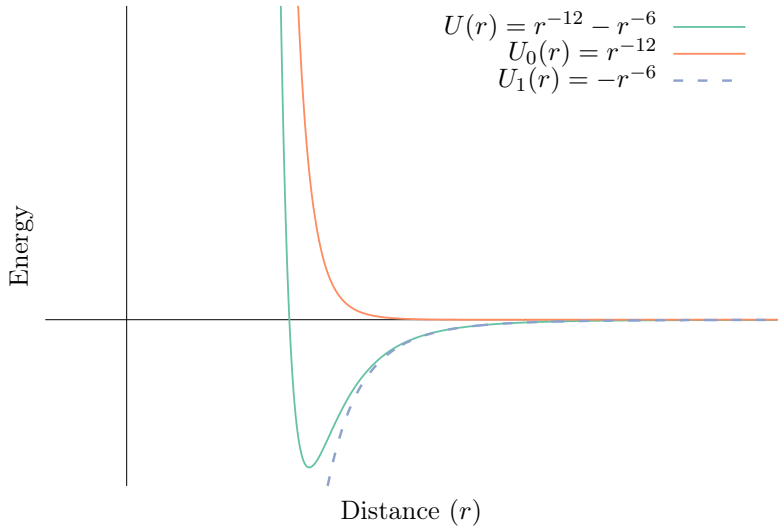

Figure 3: Decomposition of the Lennard Jones 12-6 potential into repulsive (powers of -12) and dispersive (powers of -6) contributions.

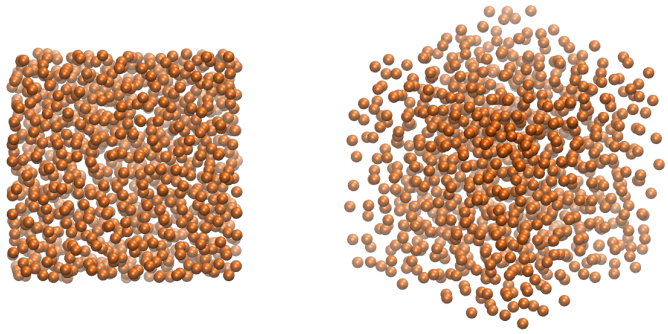

Figure 4: Argon gas ($N = 10^3$ atoms).

molecular system of N atoms that interact according to the (pairwise) forces given by $F = -\nabla U$. In practice, whatever value of N that can be tractable with current computers is still far away from the more realistic figure of $N_A = 6.022 \times 10^{23}$ (Avogadro's number) which would capture the real physics of the system.

One trick to somehow get closer to N_A is to use a tractable value of N and impose periodic boundary conditions (PBCs). This means that we now have an infinite lattice of simulation boxes with identical copies of the particles in each box. By computing the interactions between the atoms in the original box and their copies (only the copies in the neighboring simulation boxes are typically taken into account —this is called the *minimum image convention*—), we can make our simulations more realistic.

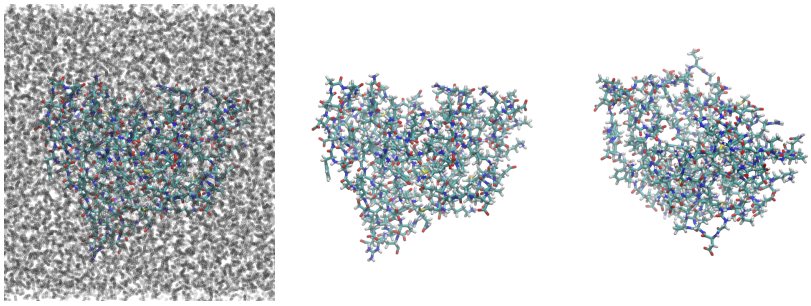

Figure 5: The protein DHFR solvated in water (left) and two views (center, right) without solvent. This system has $N = 23536$ atoms, so $N^2 \approx 10^8$ and $N \log_2 N \approx 10^5$.

The total potential energy (1) then becomes

$$H = \frac{1}{2} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ i \neq j}}^{N} U_{ij}(\|\mathbf{r}_i - \mathbf{r}_j\|) + \frac{1}{2} \sum_{\substack{\mathbf{n} \in \mathbb{Z}^3 \\ \mathbf{n} \neq 0}} \sum_{i=1}^{N} \sum_{j=1}^{N} U_{ij}(\|\mathbf{r}_i - \mathbf{r}_j + \mathrm{L}\mathbf{n}\|).$$

The naive approach to PBCs requires $\mathcal{O}(N^2)$ calculations and is unfeasible, hence the interest of finding efficient ways of carrying out this task. Ewald summation [2] takes advantage of ideas from Harmonic analysis to reduce the complexity to $\mathcal{O}(N^{3/2})$ operations, which is still impractical if we want to solve the equations of motion of a large system. The Particle-Mesh Ewald (PME) method [3] uses the Fast Fourier Transform to bring the complexity down to $\mathcal{O}(N \log N)$, and this algorithm has been a staple of Molecular Simulation since its appearance. The Smooth Particle-Mesh Ewald (SPME) improves on PME by giving a sufficiently smooth energy function whose derivative can be obtained analytically, which results in more realistic simulations due to improved energy conservation.

Some of the people involved in the development of the SPME algorithm appear in Figure .

[2] P. P. Ewald. Die Berechnung optischer und elektrostatischer Gitterpotentiale. *Annalen der Physik*, 369(3):253–287, 1921

[3] T. Darden, D. York, and L. Pedersen. Particle mesh Ewald: An $N \log(N)$ method for Ewald sums in large systems. *The Journal of Chemical Physics*, 98(12):10089, 1993

Smooth Particle-Mesh Ewald

We derive the formulas for Ewald summation following [4] and then we introduce the smooth Particle-Mesh Ewald method from [5].

[4] D. E. Williams. Accelerated convergence treatment of R^{-n} lattice sums. In Uri Shmueli, editor, *International Tables for Crystallography*, volume B, pages 385–397. Kluwer Academic Publishers, 2006

[5] U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee, and L. G. Pedersen. A smooth particle mesh Ewald method. *The Journal of Chemical Physics*, 103(19):8577, 1995

Decomposition of the potential energy function

Ewald summation can be applied whenever the pairwise potential energy $U = U(r)$ is proportional to r^{-n} for some $n \in \mathbb{N}$ (a concrete instance of U appears in Figure). In that case, we can write U as a sum of the form

$$U(r) = U_0(r) + U_1(r), \tag{2}$$

(a) Paul Peter Ewald (1888-1985).

(b) Tom Darden and Lee Pedersen.

(c) Mike Crowley.

Figure 6: Some of the people behind SPME. Pictures reproduced from `http://journals.iucr.org/a/issues/2012/01/00/wx0006/` and `http://www.psc.edu/science/Darden/`.

where the *short-range term*, U_0, decays fast as r goes to infinity (so that it can be truncated) and the *long-range term*, U_1, is very spread out and smooth, so that its Fourier transform is concentrated (and can also be truncated).

There are many ways of splitting the potential energy but [6] establishes the optimality for a class of functions involving the (incomplete) Gamma function. If we define

$$\varphi_n(r) = 1 - \frac{\Gamma(n/2, \alpha^2 \pi r^2)}{\Gamma(n/2)},$$

where α^2 is a parameter to be discussed later, then we clearly have

$$\frac{1}{r^n} = \frac{1}{r^n} \left(\varphi_n(r) + (1 - \varphi_n(r))\right).$$

We are going to concern ourselves with the case $n = 6$ (see Figure), and to define $\psi(r) = r^{-6}\varphi_6(r)$.

The free parameter α is determined by numerically solving the equation

$$r^{-6}\left(1 - \varphi_6(r_{\text{cutoff}}; \alpha)\right) = \varepsilon$$

with prescribed values of r_{cutoff} and ε (the function $1 - \varphi_n$ must be decreasing for $r > r_{\text{cutoff}}$). This makes the short-range part of the computation involving effectively vanish for $r > r_{\text{cutoff}}$.

[6] B. R. A. Nijboer and F. W. De Wette. On the calculation of lattice sums. *Physica*, 23(1-5):309–321, 1957

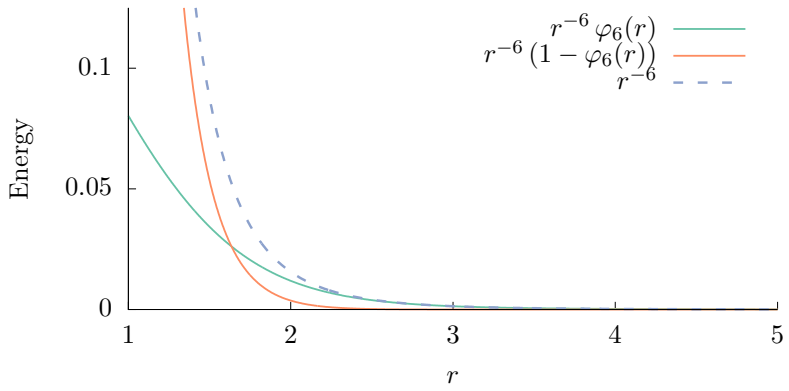

Figure 7: Decomposition of the function r^{-6} into short-range and long-range terms.

Recall that in the case of $N > 2$ particles, we have

$$H = \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\ i\neq j}}^{N} U_{ij}(\|\mathbf{r}_i - \mathbf{r}_j\|) + \frac{1}{2}\sum_{\substack{\mathbf{n}\in\mathbb{Z}^3\\ \mathbf{n}\neq 0}}\sum_{i=1}^{N}\sum_{j=1}^{N} U_{ij}(\|\mathbf{r}_i - \mathbf{r}_j + \mathrm{L}\mathbf{n}\|).$$

where r_{ij} is the distance between atoms i and j. We can split the pairwise potential U_{ij} above as in (2).

Ewald summation

The summation of the long-range terms (with $b_i > 0$),

$$U_1 = \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\ i\neq j}}^{N} b_i b_j\ \psi(\|\mathbf{r}_i - \mathbf{r}_j\|) + \frac{1}{2}\sum_{\substack{\mathbf{n}\in\mathbb{Z}^3\\ \mathbf{n}\neq 0}}\sum_{i=1}^{N}\sum_{j=1}^{N} b_i b_j\,\psi(\|\mathbf{r}_i - \mathbf{r}_j + \mathrm{L}\mathbf{n}\|) \tag{3}$$

can be rearranged as

$$U_1 = \frac{1}{2}\sum_{\mathbf{n}\in\mathbb{Z}^3}\sum_{i=1}^{N}\sum_{j=1}^{N} b_i b_j\,\psi(\|\mathbf{r}_i - \mathbf{r}_j + \mathrm{L}\mathbf{n}\|) - \frac{1}{2}\sum_{i=1}^{N} b_i^2\,\psi(0), \tag{4}$$

where $\psi(0) = \lim_{r\to 0^+}\psi(r)$.

Lemma 1 (Poisson's summation formula)**.** *If* $D(\mathbf{r}) = \sum_{\mathbf{n}\in\mathbb{Z}^3}\delta(\mathbf{r} - \mathrm{L}\mathbf{n})$, *then* $\widehat{D}(\mathbf{h}) = \frac{1}{V}\sum_{\mathbf{d}\in\mathbb{Z}^3}\delta(\mathbf{h} - \mathrm{L}^{-\mathrm{T}}\mathbf{d})$.

Lemma 2. *Consider the distributions* $\rho(\mathbf{r}) = \sum_{i=1}^{N} b_i\,\delta(\mathbf{r} - \mathbf{r}_i)$, $\eta(\mathbf{r}) = \rho(-\mathbf{r})$, *and* $D(\mathbf{r}) = \sum_{\mathbf{n}\in\mathbb{Z}^3}\delta(\mathbf{r} - \mathrm{L}\mathbf{n})$. *The following identity holds:*

$$\sum_{\mathbf{n}\in\mathbb{Z}^3}\sum_{i=1}^{N}\sum_{j=1}^{N} b_i b_j\,\psi(\|\mathbf{r}_i - \mathbf{r}_j + \mathrm{L}\mathbf{n}\|) = \int \psi(r)\ (\rho\star\eta\star D)\,(\mathbf{r})\,\mathrm{d}\mathbf{r},$$

where $r = \|\mathbf{r}\|$.

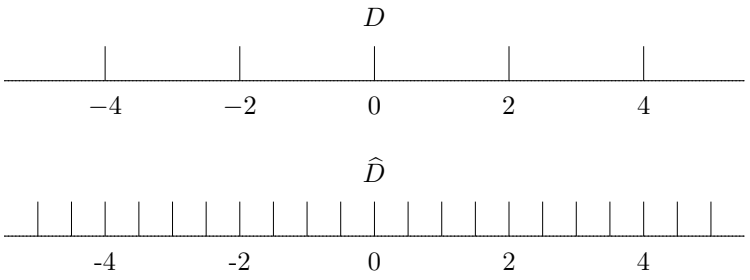

Figure 8: Example of Poisson's summation formula.

Proof. First,

$$\begin{aligned}\rho \star \eta\,(\mathbf{r}) &= \int \rho(\mathbf{s})\,\eta(\mathbf{r}-\mathbf{s})\,\mathrm{d}\mathbf{s}\\ &= \int \rho(\mathbf{s})\,\rho(\mathbf{s}-\mathbf{r})\,\mathrm{d}\mathbf{s}\\ &= \sum_{i=1}^{N}\sum_{j=1}^{N} b_i b_j \int \delta(\mathbf{s}-\mathbf{r}_i)\,\delta(\mathbf{r}-\mathbf{s}-\mathbf{r}_j)\,\mathrm{d}\mathbf{s}\\ &= \sum_{i=1}^{N}\sum_{j=1}^{N} b_i b_j\,\delta(\mathbf{r}-(\mathbf{r}_i-\mathbf{r}_j)).\end{aligned}$$

By the associative property of the convolution, we have

$$\rho \star \eta \star D = (\rho \star \eta) \star D,$$

so

$$\begin{aligned}\rho \star \eta \star D\,(\mathbf{r}) &= \int \rho \star \eta\,(\mathbf{s})\,D(\mathbf{s}-\mathbf{r})\,\mathrm{d}\mathbf{s}\\ &= \sum_{i=1}^{N}\sum_{j=1}^{N} b_i b_j \int \delta(\mathbf{s}-(\mathbf{r}_i-\mathbf{r}_j))\,D(\mathbf{s}-\mathbf{r})\,\mathrm{d}\mathbf{s}\\ &= \sum_{i=1}^{N}\sum_{j=1}^{N} b_i b_j\,D(\mathbf{s}-(\mathbf{r}_i-\mathbf{r}_j))\\ &= \sum_{\mathbf{n}\in\mathbb{Z}^3}\sum_{i=1}^{N}\sum_{j=1}^{N} b_i b_j\,\delta(\mathbf{s}-(\mathbf{r}_i-\mathbf{r}_j+\mathrm{L}\mathbf{n})).\end{aligned}$$

Finally,

$$\begin{aligned}&\int \psi(r)\ (\rho \star \eta \star D)\,(\mathbf{r})\,\mathrm{d}\mathbf{r}\\ &\quad= \int \psi(r) \sum_{\mathbf{n}\in\mathbb{Z}^3}\sum_{i=1}^{N}\sum_{j=1}^{N} b_i b_j\,\delta(\mathbf{s}-(\mathbf{r}_i-\mathbf{r}_j+\mathrm{L}\mathbf{n}))\,\mathrm{d}\mathbf{r}\\ &\quad= \sum_{\mathbf{n}\in\mathbb{Z}^3}\sum_{i=1}^{N}\sum_{j=1}^{N} b_i b_j\,\psi(\|\mathbf{r}_i-\mathbf{r}_j+\mathrm{L}\mathbf{n}\|).\end{aligned}$$

□

At this point we can go back to (4) and rewrite it as

$$U_1 = \frac{1}{2}\int \psi(r)\ (\rho \star \eta \star D)\,(\mathbf{r})\,\mathrm{d}\mathbf{r} - \frac{1}{2}\sum_{i=1}^{N} b_i^2\,\psi(0), \tag{5}$$

Furthermore, using Plancherel's Theorem [7] and the fact that $\rho \star \eta \star D$ is real-valued, we can write

$$\int \psi(r)\ (\rho \star \eta \star D)\,(\mathbf{r})\,\mathrm{d}\mathbf{r} = \int \widehat{\psi}(h)\,\widehat{(\rho \star \eta \star D)}(\mathbf{h})\,\mathrm{d}\mathbf{h}, \tag{6}$$

where $h = \|\mathbf{h}\|$. Consequently, equation (5) becomes

$$U_1 = \frac{1}{2}\int \widehat{\psi}(h)\,\widehat{(\rho \star \eta \star D)}(\mathbf{h})\,\mathrm{d}\mathbf{h} - \frac{1}{2}\sum_{i=1}^{N} b_i^2\,\psi(0), \tag{7}$$

By the properties of the Fourier transform of a convolution [8] and Poisson's summation formula 1,

$$\begin{aligned}\widehat{(\rho \star \eta \star D)}(\mathbf{h}) &= \widehat{\rho}(\mathbf{h})\,\widehat{\rho}(-\mathbf{h})\,\frac{1}{V}\sum_{\mathbf{d}\in\mathbb{Z}^3}\delta(\mathbf{h} - \mathtt{L}^{-\mathtt{T}}\mathbf{d}) \\ &= \left|\widehat{\rho}(\mathbf{h})\right|^2\frac{1}{V}\sum_{\mathbf{d}\in\mathbb{Z}^3}\delta(\mathbf{h} - \mathtt{L}^{-\mathtt{T}}\mathbf{d}).\end{aligned}$$

From the above and (6), we have

$$\begin{aligned}\int \widehat{\psi}\,\widehat{(\rho \star \eta \star D)} &= \int \widehat{\psi}(h)\left(\left|\widehat{\rho}(\mathbf{h})\right|^2\frac{1}{V}\sum_{\mathbf{d}\in\mathbb{Z}^3}\delta(\mathbf{h} - \mathtt{L}^{-\mathtt{T}}\mathbf{d})\right)\mathrm{d}\mathbf{h} \\ &= \frac{1}{V}\sum_{\mathbf{d}\in\mathbb{Z}^3}\widehat{\psi}(\|\mathtt{L}^{-\mathtt{T}}\mathbf{d}\|)\left|\widehat{\rho}(\mathtt{L}^{-\mathtt{T}}\mathbf{d})\right|^2 \\ &= \frac{1}{V}\sum_{\mathbf{m}}\widehat{\psi}(m)\left|\widehat{\rho}(\mathbf{m})\right|^2 \\ &= \frac{1}{V}\sum_{\mathbf{m}\neq 0}\widehat{\psi}(m)\left|\widehat{\rho}(\mathbf{m})\right|^2 + \frac{1}{V}\lim_{m\to 0}\widehat{\psi}(m)\left|\widehat{\rho}(0)\right|^2 \\ &= \frac{1}{V}\sum_{\mathbf{m}\neq 0}\widehat{\psi}(m)\left|\widehat{\rho}(\mathbf{m})\right|^2 + \frac{1}{V}\lim_{m\to 0}\widehat{\psi}(m)\left(\sum_{i=1}^{N} b_i\right)^2,\end{aligned}$$

where $\mathbf{m} = \mathtt{L}^{-\mathtt{T}}\mathbf{d}$ and $m = \|\mathbf{m}\|$. So, to sum up, we have arrived at the identity:

$$\begin{aligned}U_1 &= \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\ i\neq j}}^{N} b_i b_j\ \psi(\|\mathbf{r}_i - \mathbf{r}_j\|) + \frac{1}{2}\sum_{\substack{\mathbf{n}\in\mathbb{Z}^3\\ \mathbf{n}\neq 0}}\sum_{i=1}^{N}\sum_{j=1}^{N} b_i b_j\,\psi(\|\mathbf{r}_i - \mathbf{r}_j + \mathtt{L}\mathbf{n}\|) \\ &= \frac{1}{2V}\sum_{\mathbf{m}\neq 0}\widehat{\psi}(m)\left|\widehat{\rho}(\mathbf{m})\right|^2 + \frac{1}{2V}\widehat{\psi}(0)\left(\sum_{i=1}^{N} b_i\right)^2 - \frac{1}{2}\psi(0)\sum_{i=1}^{N} b_i^2,\end{aligned}$$

[7] T. H. Wolff. *Lectures on harmonic analysis*, volume 29 of *University Lecture Series*. American Mathematical Society, Providence, RI, 2003

[8] T. H. Wolff. *Lectures on harmonic analysis*, volume 29 of *University Lecture Series*. American Mathematical Society, Providence, RI, 2003

Fast Fourier Transform and Particle-Mesh method

Ewald summation using optimal parameters requires $\mathcal{O}(N^{3/2})$ operations [9] but it can be modified so that it involves only about $\mathcal{O}(N \log N)$ operations by using the Fast Fourier Transform [10].

We now concern ourselves with summing (and later taking derivatives of) the expression

$$\sum_{\mathbf{m}\neq 0} \widehat{\psi}(m) \left|\widehat{\rho}(\mathbf{m})\right|^2. \tag{8}$$

By the definition of the (inverse) Fourier Transform, we see that

$$\widehat{\rho}(\mathbf{m}) = \sum_{j=1}^{N} b_j \, \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{m}^{\mathrm{T}} \mathbf{r}_j},$$

where $\mathbf{r}_j = \mathrm{L}\,\mathbf{x}_j$ for some $\mathbf{x}_j \in [0,1)^3$. Moreover,

$$\widehat{\rho}(\mathbf{m}) = \sum_{j=1}^{N} b_j \, \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{m}^{\mathrm{T}} \mathbf{r}_j} = \sum_{j=1}^{N} b_j \, \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}} \mathrm{L}^{-1}\, \mathrm{L}\, \mathbf{x}_j} = \sum_{j=1}^{N} b_j \, \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}} \mathbf{x}_j}.$$

We are going to approximate the complex exponential terms above by means of Cardinal B-Splines [11]. An order p B-spline function is the p-fold convolution of the uniform density in the unit interval (see Figure). By construction, each order p B-spline is of class C^{p-1}, their integral equals 1, and they have compact support.

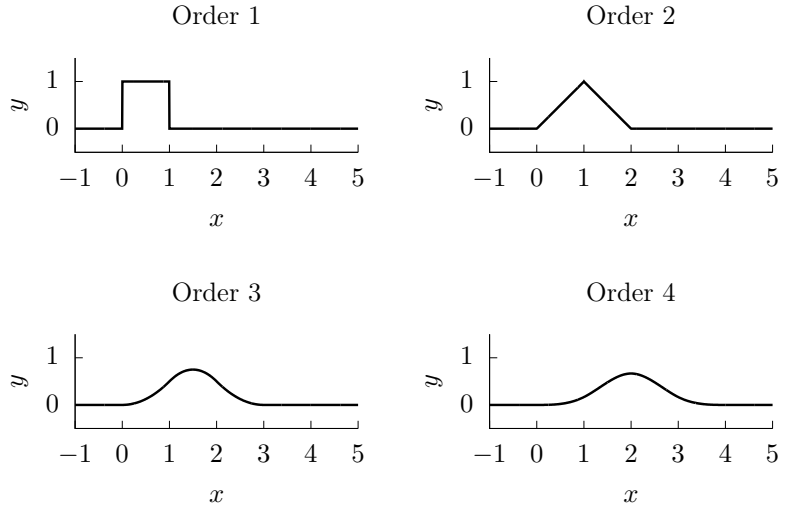

Figure 9: Basic B-splines

Remark. *Observe that these splines play the role of* approximations to the identity *when used in a meshing of the unit cell. It is in this sense that they play a role in approximating the Dirac delta functions in ρ.*

[9] S. W. de Leeuw, J. W. Perram, and E. R. Smith. Simulation of Electrostatic Systems in Periodic Boundary Conditions. I. Lattice Sums and Dielectric Constants. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 373(1752):27–56, October 1980

[10] U. Essmann, L. Perera, M. L. Berkowitz, T. Darden, H. Lee, and L. G. Pedersen. A smooth particle mesh Ewald method. *The Journal of Chemical Physics*, 103(19):8577, 1995; and R. W. Hockney and J. J. W. Eastwood. *Computer Simulation Using Particles*. Adam Hilger, 1988

[11] I. J. Schoenberg. *Cardinal Spline Interpolation*. Society for Industrial and Applied Mathematics, 1973

Now, to discretize the simulation box we consider $K_1, K_2, K_3 \in \mathbb{N}$ and let

$$\mathtt{K} = \begin{bmatrix} K_1 & & \\ & K_2 & \\ & & K_3 \end{bmatrix}.$$

For each $\mathbf{r} = \mathtt{L}\mathbf{x}$, we set $\mathbf{u} = \mathtt{K}\mathbf{x}$ and we have

$$\begin{aligned} \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{m}^{\mathrm{T}}\mathbf{r}} = \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}}\mathbf{x}} = \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}}\mathtt{K}^{-1}\mathbf{u}} &\approx \sum_{\boldsymbol{\ell}\in\mathbb{Z}^3} W(\mathbf{u}-\boldsymbol{\ell})\, \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}}\mathtt{K}^{-1}\boldsymbol{\ell}} \\ &= \sum_{\mathbf{k}} \sum_{\mathbf{n}\in\mathbb{Z}^3} W(\mathbf{u}-(\mathbf{k}+\mathtt{K}\mathbf{n}))\, \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}}\mathtt{K}^{-1}(\mathbf{k}+\mathtt{K}\mathbf{n})} \\ &= \sum_{\mathbf{k}} \sum_{\mathbf{n}\in\mathbb{Z}^3} W(\mathbf{u}-(\mathbf{k}+\mathtt{K}\mathbf{n}))\, \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}}\mathtt{K}^{-1}\mathbf{k}} \underbrace{\mathrm{e}^{2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}}\mathbf{n}}}_{=1} \\ &= \sum_{\mathbf{k}} \sum_{\mathbf{n}\in\mathbb{Z}^3} W(\mathbf{u}-(\mathbf{k}+\mathtt{K}\mathbf{n}))\, \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}}\mathtt{K}^{-1}\mathbf{k}}, \end{aligned}$$

where we have used the *Euclidean algorithm* to write

$$\boldsymbol{\ell} = \mathbf{k} + \mathtt{K}\mathbf{n} \quad \text{with} \quad k_i \in \{0, 1, \ldots, K_i - 1\} \quad \text{and} \quad \mathbf{n} \in \mathbb{Z}^3.$$

We also define the forward (unnormalized) DFT of the 3D array $Q_{\mathbf{k}}$ as

$$\widehat{Q}_{\mathbf{d}} = \mathrm{DFT}[Q_{\mathbf{k}}]_{\mathbf{d}} = \sum_{k_1=0}^{K_1-1} \sum_{k_2=0}^{K_2-1} \sum_{k_3=0}^{K_3-1} Q_{\mathbf{k}}\, \mathrm{e}^{-2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}}\mathtt{K}^{-1}\mathbf{k}}.$$

And, likewise, the backward DFT is

$$\mathrm{IDFT}[\widehat{Q}_{\mathbf{d}}]_{\mathbf{k}} = \sum_{d_1=0}^{K_1-1} \sum_{d_2=0}^{K_2-1} \sum_{d_3=0}^{K_3-1} \widehat{Q}_{\mathbf{d}}\, \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}}\mathtt{K}^{-1}\mathbf{k}}.$$

Using the previous results, we write

$$\begin{aligned} \widehat{\rho}(\mathbf{m}) &= \sum_{j=1}^{N} b_j\, \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}}\mathbf{x}_j} \\ &\approx \sum_{\mathbf{k}} \underbrace{\sum_{j=1}^{N} b_j \sum_{\mathbf{n}\in\mathbb{Z}^3} W(\mathbf{u}-(\mathbf{k}+\mathtt{K}\mathbf{n}))}_{=Q_{\mathbf{k}}}\, \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}}\mathtt{K}^{-1}\mathbf{k}} \\ &= \sum_{\mathbf{k}} Q_{\mathbf{k}}\, \mathrm{e}^{2\pi \mathrm{i}\, \mathbf{d}^{\mathrm{T}}\mathtt{K}^{-1}\mathbf{k}} = \widehat{Q}_{\mathbf{d}}. \end{aligned}$$

Remark. *It is important to notice that since the splines have compact support, the infinite series above is actually a finite sum.*

Remark. *The following diagram depicts the relationships between the different objects involved in the SPME method:*

$$\begin{array}{ccc} \rho & \xrightarrow{\approx} & Q \\ {\scriptstyle IFT}\downarrow & & \downarrow{\scriptstyle IDFT} \\ \widehat{\rho} & \xrightarrow{\approx} & \widehat{Q} \end{array}$$

Going back to (8), we carry out the following approximation:

$$\sum_{\mathbf{m}\neq 0} \widehat{\psi}(m)\,\left|\widehat{\rho}(\mathbf{m})\right|^2 = \sum_{\mathbf{m}\neq 0} \widehat{\psi}(m)\,\widehat{\rho}(-\mathbf{m})\,\widehat{\rho}(\mathbf{m}) \approx \sum_{\mathbf{d}\neq 0} \widehat{\psi}(\|\mathtt{L}^{-\mathtt{T}}\,\mathbf{d}\|)\,\widehat{Q}_{-\mathbf{d}}\,\widehat{Q}_{\mathbf{d}}$$

Now define

$$A_{\mathbf{d}} = \begin{cases} \widehat{\varphi}(\|\mathtt{L}^{\mathtt{T}}\,\mathbf{h}\|), & \text{if } \mathbf{h}\neq 0,\\ 0, & \text{if } \mathbf{h}=0. \end{cases}$$

with

$$h_i(\mathbf{d}) = \begin{cases} d_i, & \text{if } 0\le d_i < \frac{1}{2}K_i,\\ K_i - d_i, & \text{if } \frac{1}{2}K_i \le d_i < K_i. \end{cases}$$

(note that $-\frac{K_i}{2} \le h_i < \frac{K_i}{2} - 1$). Then,

$$\sum_{d_1=-\frac{K_1}{2}}^{\frac{K_1}{2}-1}\sum_{d_2=-\frac{K_2}{2}}^{\frac{K_2}{2}-1}\sum_{d_3=-\frac{K_3}{2}}^{\frac{K_3}{2}-1} \widehat{\psi}(\|\mathtt{L}^{-\mathtt{T}}\,\mathbf{d}\|)\,\widehat{Q}_{-\mathbf{d}}\,\widehat{Q}_{\mathbf{d}} = \sum_{d_1=0}^{K_1-1}\sum_{d_2=0}^{K_2-1}\sum_{d_3=0}^{K_3-1} A_{\mathbf{d}}\,\widehat{Q}_{-\mathbf{d}}\,\widehat{Q}_{\mathbf{d}}.$$

Applying the following property of the Fourier transform (see [12]),

$$\int \widehat{f}\,\mathrm{d}g = \int \widehat{g}\,\mathrm{d}f,$$

we write (using the notation of the previous section and keeping in mind that the result works in the distributional sense too)

$$\int \widehat{\psi}\,\widehat{\eta}\,\widehat{\rho} = \int \widehat{\widehat{\psi}\,\widehat{\eta}}\,\rho = \int \left(\widehat{C}\star\rho\right)\,\rho$$

where we have used that $\widehat{fg} = \widehat{f}\star\widehat{g}$ and that, for $f = f(x)$, $\widehat{\widehat{f}}(x) = f(-x)$ (again, see [13]).

Therefore, the algorithm boils down to:

$$\begin{aligned} Q_{\mathbf{k}} &\to \widehat{Q}_{-\mathbf{d}} = \mathrm{DFT}(Q)_d\\ &\to A_{\mathbf{d}}\cdot \mathrm{DFT}(Q)_{\mathbf{d}}\\ &\to \mathrm{IDFT}(A\cdot\mathrm{DFT}(Q))_{\mathbf{k}} = (\mathrm{IDFT}(A)\star Q)_{\mathbf{k}}\\ &\to (\mathrm{IDFT}(A)\star Q)_{\mathbf{k}}\cdot Q_{\mathbf{k}}, \end{aligned}$$

Assorted results in Harmonic analysis

Theorem 3 (The convolution is commutative)**.**

Theorem 4 (The Fourier transform of a convolution is the product of the Fourier transforms)**.**

Theorem 5. [14] *For absolutely continuous measures μ, ν in $\mathbb{R}^n$. We have*

$$\int \hat{\mu}\,\mathrm{d}\nu = \int \hat{\nu}\,\mathrm{d}\mu$$

Theorem 6 (Plancherel's theorem)**.**

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