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On the Efficient Evaluation of Coalescence Integrals in Population Balance Models

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Abstract

The solution of population balance equations is a function $f(t,r,x)$ describing a population density of particles of the property x at time t and space r. For instance, the additional independent variable x may denote the particle size. The describing partial differential equation contains additional sink and source terms involving integral operators. Since the coordinate x adds at least one further dimension to the spatial directions and time coordinate, an efficient numerical treatment of the integral terms is crucial. One of the more involved integral terms appearing in population balance models is the *coalescence integral*, which is of the form $\int_0^x \kappa(x-y,y)f(y)f(x-y)\mathrm{d}y$. In this paper we describe an evaluation method of this integral which needs only $\mathcal{O}(n\log n)$ operations, where n is the number of degrees of freedom with respect to the variable x. This cost can also be obtained in the case of a grid geometrically refined towards $x=0$.

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1 Introduction

Populations of many (small) particles of different size are described by a function $f(t,r,x)$ which indicates the density of particles of size x at time t and space r. In general, x might denote also other properties than size and may also be vector valued describing several properties. As a standard reference to population balance models, we refer to Ramkrishna [10]. While the flow with respect to t,r,x is described by a pde of the form $\frac{\partial}{\partial t}f+\mathrm{div}_r A_r(f)+\mathrm{div}_x B_x(f)=Q(f)$ (cf. [10, (2.7.9)]), additional sink and source terms appear due to the interaction of particles. Since the coordinate x adds at least one further dimension to the 1-3 spatial directions and time coordinate, an efficient numerical treatment is crucial in computational engineering.

One of the more involved integral terms appearing in population balance models is the *aggregation integral*, which we consider in this paper. It describes the effect that two particles say of mass x' and x'' combine to a new particle of mass $x=x'+x''$. As can be seen from [10, §3.3.2] or [2, p. 208], the source part of the aggregation integral takes the form

$$Q(f)(x)=\int_0^x \kappa(x-y,y)f(y)f(x-y)\mathrm{d}y \tag{1.1}$$

(the space/time variables r,t of f are not written, but note that such integrals appear for all grid points in space and time). The integral term is quadratic with respect to f and is of convolution type (at least, concerning the part $f(y)f(x-y)$). The kernel function $\kappa(\cdot,\cdot)$ describes the aggregation rate and depends on the particular model. In the case of crystallisation or emulsion processes, κ is also called agglomeration or coalescence rate, however, the form (1.1) of the integral is the same.

Usually, $\kappa(\cdot,\cdot)$ is analytic for positive arguments. For instance, for Brownian motion in a continuum regime, i.e., particles in liquid, the agglomeration coefficient is

$$\kappa(x,y)=C\left(\frac{1}{x}+\frac{1}{y}\right)(x+y) \tag{1.2}$$

with some constant C (cf. [10, p.99]).

Often, the kernel function is to be fitted to the experiment. For instance,

$$\kappa(x,y) = C \cdot (x+y)^a \,/\, (xy)^b \tag{1.3}$$

is an approach proposed by Kapur [5]. For a concrete example discussed in [9, §4.4], the optimal parameters are $a = 0.71053$ and $b = 0.06211$.

A much more complicated example of κ is

$$\kappa(x,y) = \left(\frac{1}{x} + \frac{1}{y}\right) / \int_{x+y}^{\infty} t^{-2} \exp\left(E(x,y,t)\right) \mathrm{d}t \tag{1.4}$$

with

$$E(x,y,t) := \frac{xy}{x+y} e^{-t} + 1 - \left(\frac{xy}{t^2 - (x+y)^2} + \frac{xy}{t^2 - (x-y)^2} + \log \frac{t^2 - (x+y)^2}{t^2 - (x-y)^2} \right),$$

which is taken from [4, Eqs. (11)-(16)], where for the sake of readability we have replaced all constants by 1.

Usually, the function f is approximated by a piecewise constant ansatz function. Let n be the number of degrees of freedom. Then the integral (1.1) has to be evaluated for $\mathcal{O}(n)$ different values of x. The naive approach would be to divide each integral (1.1) into $\mathcal{O}(n)$ subintervals where $f(y)f(x-y)$ is constant. This leads to at least $\mathcal{O}(n^2)$ arithmetical operations for the evaluation at one space/time grid point. This is much too costly unless n is rather small.

We shall describe an evaluation method with the cost $\mathcal{O}(n \log n)$. The algorithm combines a separable approximation of $\kappa(\cdot,\cdot)$ with the fast Fourier transform for the arising convolution integrals. Accordingly, the separable approximation of κ is explained in the next Section §2. In §3 the kind of ansatz functions and the properties of $Q(f)$ are addressed. Since the fast Fourier transform requires a uniform mesh, we start in §5 with a uniform grid discretisation. However, the nature of aggregation / agglomeration / coalescence processes is much better described by a grid which is refined at zero. For this purpose, in §6, we introduce a wavelet representation as a third algorithmic component. Wavelets yield not only an excellent representation of such grids but also lead to simple integral evaluations. Again, $\mathcal{O}(N \log N)$ bounds the cost, where N is the number of intervals of the graded mesh. More precisely, all estimates $\mathcal{O}(\ldots)$ of this paper contain a factor k, which is the separation rank introduced below.

2 Separable Approximation of the Kernel function

The function $\kappa(x,y)$ is called *separable* (with separation rank k), if it is of the form

$$\kappa(x,y) = \sum_{\nu=1}^{k} \alpha_\nu(x)\beta_\nu(y). \tag{2.1}$$

The essential fact is that the variables x and y are separated. α_ν, β_ν may be any kind of functions[1], in particular, no special basis functions (like certain polynomials) are prescribed.

We notice that the Brownian kernel from (1.2) is of separation rank $k = 3$ with $\alpha_1 = \beta_1 = \sqrt{2C}$, $\alpha_2(x) = C/x$, $\beta_2(y) = y$, $\alpha_3(x) = x$, $\beta_3(y) = C/y$.

In general, $\kappa(x,y)$ has no finite separation rank but can be approximated by an rank k expression:

$$\kappa(x,y) \approx \sum_{\nu=1}^{k} \alpha_\nu(x)\beta_\nu(y), \tag{2.2}$$

where the error should be under control. Then the right-hand side in (2.2) is called a *separable approximation* (of separation rank k).

In the case of (1.3) we can easily derive such a separable approximation. The following value of a corresponds to the value from [9, §4.4].

[1] The only mathematical requirement is that the functions are integrable.

Remark 2.1 *Assume $x, y \in [0, 1/2]$ and $a = 0.71053$ in the kernel function (1.3). Approximate the function $\gamma(s) = s^a$ in $[0, 1]$ by the exponential ansatz*[2] *$\tilde{\gamma}(s) \approx \omega_1 + \sum_{\nu=2}^{k} \omega_\nu \exp(-\theta_\nu s)$. The best approximation (with respect to the maximum norm) yields, e.g., the accuracy $\varepsilon < 0.0004$ for $k = 5$. Inserting $s = x + y \in [0, 1]$, we obtain the approximation*

$$\kappa(x, y) = (x + y)^a / (xy)^b \approx \frac{\omega_1}{x^b y^b} + \sum_{\nu=2}^{k} \omega_\nu \frac{\exp(-\theta_\nu x)}{x^b} \frac{\exp(-\theta_\nu y)}{y^b}$$

of separation rank k.

Also the complicated kernel (1.4) has a separable approximation due to its analyticity in the interior. In the following, we assume that instead of κ we may use a separable expression with a rank k which is small. In particular, in the complexity estimates k is considered as a constant.[3]

Replacing the kernel $\kappa(x, y)$ by a separable expression $\sum_{\nu=1}^{k} \alpha_\nu(x)\beta_\nu(y)$, the integral (1.1) becomes

$$Q(f)(x) \approx \int_0^x \left(\sum_{\nu=1}^{k} \alpha_\nu(x - y)\beta_\nu(y) \right) f(y) f(x - y) \mathrm{d}y = \sum_{\nu=1}^{k} \int_0^x \alpha_\nu(x - y)\beta_\nu(y) f(y) f(x - y) \mathrm{d}y.$$

In the following, it suffices to consider one of the k terms. Hence, we may replace the notation α_ν, β_ν by α, β. The resulting problem is formulated in

Problem 2.2 *Instead of treating $Q(f)$ from (1.1) we have to provide an efficient evaluation method for integrals of the form*

$$\int_0^x \alpha(x - y)\beta(y) f(y) f(x - y) \mathrm{d}y, \tag{2.3}$$

where f belongs to the ansatz space, while α, β are functions arising from the separable approximation.

3 Ansatz Functions and Properties of Q

The variable[4] x in (2.3) is bounded from above, while zero is a natural lower bound. Therefore, we may assume without loss of generality that

$$x \in [0, 1]. \tag{3.1}$$

We assume a grid $0 = x_0 < x_1 < \ldots < x_n = 1$ and start with a *piecewise constant* ansatz space $\mathcal{S}$, i.e., $f \in \mathcal{S}$ is constant in each subinterval[5] (x_{i-1}, x_i).

An inspection of the integrand in (2.3) shows that one should combine $\beta(y)$ and $f(y)$ on the one hand side and $\alpha(x - y)$ and $f(x - y)$ on the other hand, to obtain a standard *convolution integral*

$$\int_0^x \varphi(y)\psi(x - y) \mathrm{d}y \qquad \text{with } \varphi := \beta f,\ \psi := \alpha f.$$

It is inconvenient to form $\beta f,\ \alpha f$ exactly, since they do not belong to the ansatz space $\mathcal{S}$ of piecewise constant functions. Instead one should use a projection of $\beta f,\ \alpha f$ onto $\mathcal{S}$. The L^2 orthogonal projection would be

$$\varphi(x) = f(x) \cdot \frac{1}{x_i - x_{i-1}} \int_{x_{i-1}}^{x_i} \beta(s) \mathrm{d}s \qquad \text{for } x \in (x_{i-1}, x_i). \tag{3.2}$$

A simpler (non-orthogonal) projection is

$$\varphi(x) = f(x) \cdot \beta\left(\frac{x_{i-1} + x_i}{2} \right) \qquad \text{for } x \in (x_{i-1}, x_i). \tag{3.3}$$

$\psi \approx \alpha f$ is treated similarly. Since the approximation errors $\varphi - \beta f,\ \psi - \alpha f$ of the projected φ, ψ are similar to the already introduced discretisation error, the approximation of $\beta f, \alpha f$ is no serious drawback.

[2] For approximations by best exponential sums see [3], and for a special case [1].

[3] To be precise, k depends on the accuracy requirement and often $k = \mathcal{O}(\log^2 \frac{1}{\varepsilon})$ holds (cf. [1]).

[4] Most of the population balance models in engineering applications restrict to one variable $x = x_1$. Nevertheless, there is strong interest to treat more than one particle property. A two-dimensional case is considered in [8].

[5] For this kind of application, these intervals are also called *compartments* in the language of engineering sciences.

Problem 3.1 *After the projection, the new problem to be solved is the evaluation of integrals of the type*

$$\int_0^x \varphi(y)\psi(x-y)\mathrm{d}y \tag{3.4}$$

for piecewise constant functions $\varphi, \psi \in \mathcal{S}$.

The precise goal of evaluation depends on the kind of discretisation scheme. In the case of a collocation method, one might be interested in $\int_0^{\xi_i} \varphi(y)\psi(\xi_i - y)\mathrm{d}y$ at the collocation points $\xi_i = \frac{x_{i-1}+x_i}{2}$. The Galerkin discretisation uses the weighted means

$$\int_{x_{i-1}}^{x_i} \left(\int_0^{\xi} \varphi(y)\psi(\xi - y)\mathrm{d}y \right) d\xi \qquad \text{for } i = 1, \ldots, n. \tag{3.5}$$

In Section 4 we will introduce a third functional (see (4.3)).

Lemma 3.2 *Piecewise constant functions* $\varphi, \psi \in \mathcal{S}$ *yield a convolution result* $\omega(x) := \int_0^x \varphi(y)\psi(x-y)\mathrm{d}y$, *which is piecewise linear. Hence,* ω *is completely known, if* ω *is evaluated at all points where* ω' *is discontinuous. The set of discontinuity points is* $\{x_i : 1 \le i \le n\} \cup \{x_j + x_i \le 1 : 1 \le i, j \le n\}$.

Proof. The derivative of ω is $\varphi(x)\psi(0) + \sum_{x_i<x} \varphi(x - x_i)\,[\psi]\,(x_i)$, which is piecewise constant ($[\psi]$ denotes the jump of ψ). ∎

Although the derivative ω' is piecewise constant, it is in general not in the same space $\mathcal{S}$ as the ansatz functions, since the set of discontinuity points contains possibly more points $\{x_j + x_i \le 1 : 1 \le i, j \le n\}$. This is a strong reason to require a *uniform grid*:

$$x_i = ih \qquad \text{for } i = 0, 1, \ldots, n, \quad h = \frac{1}{n}. \tag{3.6}$$

Lemma 3.3 *Under condition (3.6),* $\varphi, \psi \in \mathcal{S}$ *lead to* ω *with* $\omega' \in \mathcal{S}$. *Therefore, is suffices to evaluate* ω *at* $x = x_i$ $(0 \le i \le n)$. *In particular, the Galerkin integral (3.5) equals* $\frac{x_i - x_{i-1}}{2}\left(\omega(x_i) + \omega(x_{i+1})\right)$.

In this new situation the actual problem takes the following form:

Problem 3.4 *Under condition (3.6), one has to compute* $\omega(x_i) := \int_0^{x_i} \varphi(y)\psi(x_i - y)\mathrm{d}y$ *with* $\varphi, \psi \in \mathcal{S}$ *for all* $x_i = ih$ $(0 \le i \le n)$.

The space of piecewise constant ansatz functions can be generalised to piecewise polynomials of degree p. If φ and ψ are piecewise of degree p, ω is piecewise of degree $2p + 1$.

4 Conservation of Mass

Before we continue with algorithmic details of the evaluation, we discuss a question concerning the discretisation scheme[6]. Since the pde is of conservation form, its discretisation is usually designed in such a way that important physical quantities like the mass are invariant, provided that there is no outer sink or source. A standard choice of the property coordinate x is the mass of a particle. Therefore one is interested that the treatment of the integral terms in $Q(f)$ is such that *mass conservation* is guaranteed. On the level of the undiscretised integro-differential equation, the condition $\int_0^\infty xQ(f(t,r,\cdot)(x)\mathrm{d}x = 0$ must be required, i.e., for all time and space points there is no mass entering and leaving the system. This condition does not hold for (1.1), since (1.1) only describes the source term Q_{source} due to aggregation. The aggregation process creates a second sink term $Q_{\text{sink}}(f)(x) = 2f(x)\int_0^\infty \kappa(x,y)f(y)\mathrm{d}y$, so that $Q = Q_{\text{source}} - Q_{\text{sink}}$ satisfies the zero balance condition (cf. [2, (7.67)], [11, Eq. (2)]). The second integral term Q_{sink} is not considered in this paper, since its numerical treatment is much easier.

[6] The author thanks the referees for putting forward the question of mass conservation. The present subsection is added to answer this question.

First, we have to consider the approximation of $\kappa(x,y)$ by the right-hand side $\tilde{\kappa}(x,y)$ of (2.2) together with the projection (3.2) or (3.3) applied to the factors α_ν, β_ν. This replacement of κ should be done *simultaneously* in Q_{source} and Q_{sink}. Then the resulting terms $\tilde{Q}_{\text{source}}$ and $\tilde{Q}_{\text{sink}}$ still are in balance.

Second, the discretisation using the uniform grid (3.6) is to be considered. The mass part in the interval $[x_{i-1}, x_i] = [(i-1)\,h, ih]$ is $M_i := \int_{x_{i-1}}^{x_i} x\tilde{Q}_{\text{source}}(f)(x)\mathrm{d}x$ so that $\sum_i M_i = \int_0^\infty \tilde{Q}_{\text{source}}(f)(x)\mathrm{d}x$ is the total mass, where now $f \in \mathcal{S}$ is an ansatz function. We recall that $\tilde{Q}_{\text{source}}(f)$ consists of convolutions $\omega := \varphi * \psi$. The critical question is how the piecewise *linear* function $\omega := \varphi * \psi$ ($\varphi, \psi \in \mathcal{S}$, see Lemma 3.2) is to be mapped into a piecewise *constant* function $\omega_c := \Pi\omega \in \mathcal{S}$ by means of some projection Π. It is to be checked whether the mass part $M_i = \int_{x_{i-1}}^{x_i} x\tilde{Q}_{\text{source}}(f)(x)\ \mathrm{d}x$ equals $\int_{x_{i-1}}^{x_i} x\left(\Pi\tilde{Q}_{\text{source}}(f)\right)(x)\ \mathrm{d}x$. Assuming that a similar identity holds for the discretisation of the simpler sink term $\tilde{Q}_{\text{sink}}$, we obtain exact mass conservation.

It turns out that the collocation at $x_{i-1/2} := (i-1/2)\,h$ or the Galerkin evaluation (3.5) does *not* imply $\int_{x_{i-1}}^{x_i} x\omega(x)\mathrm{d}x = \int_{x_{i-1}}^{x_i} x\omega_c(x)\mathrm{d}x$. In order to ensure this identity, we need a special definition of ω_c. The exact value of $\int_{x_{i-1}}^{x_i} x\omega(x)\mathrm{d}x$ is given by Simpson's formula, since $x\omega(x)$ is quadratic in $[x_{i-1}, x_i]$:

$$\begin{aligned}\int_{x_{i-1}}^{x_i} x\omega(x)\mathrm{d}x &= \frac{h}{6}\left[x_i\omega_i + 4x_{i-1/2}\frac{\omega_{i-1}+\omega_i}{2} + x_{i-1}\omega_{i-1}\right] \\ &= \frac{h}{2}\left[\left(x_{i-1/2}+\frac{h}{6}\right)\omega_i + \left(x_{i-1/2}-\frac{h}{6}\right)\omega_{i-1}\right],\end{aligned} \tag{4.1}$$

where $\omega_i := \omega(x_i)$. On the other hand, the exact value of $\int_{x_{i-1}}^{x_i} x\omega_c\mathrm{d}x$ (ω_c constant in $[x_{i-1}, x_i]$) is

$$\int_{x_{i-1}}^{x_i} x\omega_c\mathrm{d}x = hx_{i-1/2}\omega_c\,. \tag{4.2}$$

Both expressions (4.1) and (4.2) become equal for the choice

$$\omega_c := \frac{\left(x_{i-1/2}+\frac{h}{6}\right)\omega_i + \left(x_{i-1/2}-\frac{h}{6}\right)\omega_{i-1}}{2x_{i-1/2}} \qquad \text{in } [x_{i-1}, x_i]\,. \tag{4.3}$$

Since the values ω_i will be determined exactly (see Problem 3.4), the computation of $\omega_c \in \mathcal{S}$ by (4.3) leads to exact mass conservation in the sense that $M_i = \int_{x_{i-1}}^{x_i} x\tilde{Q}_{\text{source}}(f)(x)\mathrm{d}x = \int_{x_{i-1}}^{x_i} x\left(\Pi\tilde{Q}_{\text{source}}(f)\right)(x)\mathrm{d}x$ and therefore $\int_0^1 x\tilde{Q}_{\text{source}}(f)(x)\mathrm{d}x = \int_0^1 x\left(\Pi\tilde{Q}_{\text{source}}(f)\right)(x)\mathrm{d}x$.

5 Convolution by FFT

Assumption (3.6) paves the way to the fast Fourier transform application. The functions $\varphi, \psi \in \mathcal{S}$ are given by their values φ_μ, ψ_μ ($1 \le \mu \le n$) in the intervals $(x_{\mu-1}, x_\mu)$. The values of ω are

$$\omega(x_\nu) =: \omega_\nu = h\sum_{\mu=1}^{\nu} \varphi_\mu\psi_{\nu-\mu+1} \qquad (1 \le \nu \le n)\,. \tag{5.1}$$

This formula includes $\omega(x_0) = 0$ because of the empty sum, but since this value is known it need not be computed.

We extend the vectors $(\varphi_\mu)_{\mu=1}^n$ and $(\psi_\mu)_{\mu=1}^n$ to $(\varphi_\mu)_{\mu\in\mathbb{Z}}$ and $(\psi_\mu)_{\mu\in\mathbb{Z}}$ by defining all further coefficients by zero. Then (5.1) can be equivalently written as

$$\omega_\nu = h\sum_{\mu=1-n}^{n} \varphi_\mu\psi_{\nu-\mu+1} \qquad (1 \le \nu \le n)\,. \tag{5.2}$$

Remark 5.1 *In (5.2) we may replace n by some integer $n' > n$. The newly defined ω_ν ($n < \nu \le n'$) cannot be interpreted as values of $\omega(x)$, but the equations for $1 \le \nu \le n$ are identical to (5.2). This is of interest, if one wants to replace n by the next power of two: $n' = 2^p$, to simplify the fast Fourier transform.*

By fast Fourier transform we can find coefficients $\hat{\varphi}_\mu$ and $\hat{\psi}_\mu$ $(1-n \le \mu \le n)$ so that

$$\varphi_\mu = \sum_{\nu=1-n}^{n} \hat{\varphi}_\nu e^{i\nu\mu\pi/n}, \quad \psi_\mu = \sum_{\nu=1-n}^{n} \hat{\psi}_\nu e^{i\nu\mu\pi/n} \qquad (1-n \le \mu \le n)\,.$$

Insertion of these representations into (5.2) yields

$$\begin{aligned}
\omega_\nu &= h \sum_{\mu=1-n}^{n} \sum_{\gamma=1-n}^{n} \hat{\varphi}_\gamma e^{i\gamma\mu\pi/n} \sum_{\lambda=1-n}^{n} \hat{\psi}_\lambda e^{i\lambda(\nu-\mu+1)\pi/n} \\
&= h \sum_{\gamma=1-n}^{n} \hat{\varphi}_\gamma \sum_{\lambda=1-n}^{n} \hat{\psi}_\lambda e^{i\lambda(\nu+1)\pi/n} \sum_{\mu=1-n}^{n} e^{i(\gamma-\lambda)\mu\pi/n} \\
&= h \sum_{\gamma=1-n}^{n} \hat{\varphi}_\gamma \sum_{\lambda=1-n}^{n} \hat{\psi}_\lambda e^{i\lambda(\nu+1)\pi/n} 2n\delta_{\gamma,\lambda} \qquad (\delta_{\gamma,\lambda}\text{: Kronecker delta}) \\
&= 2nh \sum_{\gamma=1-n}^{n} \hat{\varphi}_\gamma \hat{\psi}_\gamma e^{i\gamma(\nu+1)\pi/n} \qquad (1 \le \nu \le n)\,.
\end{aligned}$$

Setting $\hat{\omega}_\gamma := \hat{\varphi}_\gamma \hat{\psi}_\gamma e^{i\gamma\pi/n}$ $(1-n \le \gamma \le n)$, we obtain

$$\omega_\nu = 2nh \sum_{\gamma=1-n}^{n} \hat{\omega}_\gamma e^{i\gamma\nu\pi/n}.$$

The evaluation of ω_ν for $1-n \le \gamma \le n$ can again be performed by FFT. Only the values in the range $1 \le \nu \le n$ are the desired values $\omega(x_\nu)$.

The following two remarks describe two situations, where the computational cost can be still reduced.

Remark 5.2 *Let n determine the range of summation in (5.2), but assume that the ω_ν's are to be computed only for $1 \le \nu \le m$ with $m < n$. Then these ω_ν depend only on $\{\varphi_1, \ldots, \varphi_m\}$ and $\{\psi_1, \ldots, \psi_m\}$. Hence, the convolution problem reduces to a new problem of size m instead of n.*

The next remark is connected with the separable approximation mentioned in §2. In more complicated situations like for the kernel (1.4), it is hard to find a *global* separable approximation as in Remark 2.1. In such cases the domain $(0,1)^2$ of the kernel is subdivided into smaller squares. Then local separable approximations are constructed in smaller domains $(x', x'') \times (y', y'')$ (e.g., by polynomial interpolation). This is possible, since the functions $\alpha_\nu(x)$, $\beta_\nu(y)$ in (2.2) may also be discontinuous functions being zero outside of the respective intervals (x', x'') or (y', y'') (see Footnote 1). Of course, the total sum on the right-hand side of (2.2) contains the contributions of all subdomains. Then, also the products $\varphi := \beta f$ and $\psi := \alpha f$ (index ν omitted) vanish outside of (x', x'') or (y', y''), respectively. Therefore, the discrete values φ_μ and ψ_μ are non-zero only for a subset of indices μ. In the next remark, the number of non-zero φ_μ-values [ψ_μ-values] is at most $n''_\varphi - n'_\varphi$ [$n''_\psi - n'_\psi$].

Remark 5.3 *Assume that vectors $(\varphi_\mu)_{\mu=1}^n$ and $(\psi_\mu)_{\mu=1}^n$ are given with the property*

$$\begin{aligned}
\varphi_\mu &= 0 \qquad \text{for } 1 \le \mu \le n'_\varphi \text{ and } n''_\varphi + 1 \le \mu \le n, \\
\psi_\mu &= 0 \qquad \text{for } 1 \le \mu \le n'_\psi \text{ and } n''_\psi + 1 \le \mu \le n.
\end{aligned}$$

Then non-zero values of $(\omega_\nu)_{\nu=1}^n$ occur only for $n'_\varphi + n'_\psi + 1 \le \nu \le \min\{n, n''_\varphi + n''_\psi - 1\}$. Introducing the shifted values

$$\tilde{\varphi}_\mu = \varphi_{\mu+n'_\varphi}, \qquad \tilde{\psi}_\mu = \psi_{\mu+n'_\psi}, \qquad \tilde{\omega}_\nu = \omega_{\nu+n'_\varphi+n'_\psi},$$

equation (5.1) becomes

$$\tilde{\omega}_\nu = h \sum_{\mu=1}^{\nu} \tilde{\varphi}_\mu \tilde{\psi}_{\nu-\mu+1} \qquad \text{for } 1 \le \nu \le \min\{n - n'_\varphi - n'_\psi, n''_\varphi - n'_\varphi + n''_\psi - n'_\varphi - 1\}.$$

Denoting the length of the non-zero part of $\tilde{\varphi}_\mu$ and $\tilde{\psi}_\mu$ by $m_\varphi := n''_\varphi - n'_\varphi$ and $m_\psi := n''_\psi - n'_\psi$, one can bound the length of the $\tilde{\omega}_\nu$ sequence by $\min\{n-n'_\varphi-n'_\psi, m_\varphi+m_\psi-1\} \le m_\varphi+m_\psi-1$. Thus, separable approximations in small domains lead to small m_φ, m_ψ and therefore require proportionally less computational work.

6 Wavelets

Since the agglomeration of two particles of same mass yields a particle of double mass, an exponential grading of the grid is useful. Such a grid with exponential grading towards $x = 0$ will be constructed in §6.2. Our construction of the graded mesh uses a regular refinement of the starting uniform grid. Then the ratio of neighbouring intervals is either 1 or 2. Other approaches use a smooth transition of the step sizes by choosing grid points of the form $2^i const$ (see [11, §4.2]). However, for our efficient numerical treatment the following graded grid will be essential.

First we introduce the wavelets for a uniformly fine grid. Readers which are well acquainted with wavelets can skip the next subsection.

6.1 Wavelet Spaces

The space $\mathcal{S}$ of piecewise constant functions on the uniform grid of size h (see (3.6)) will now be renamed by $\mathcal{V}_0[0,1]$. The suffix $[0,1]$ has the following meaning. Let $\mathcal{V}_0[-\infty,\infty]$ be the set of functions being constant on each interval $(\nu h, (\nu+1)\,h)$ for $\nu \in \mathbb{Z}$. Then $\mathcal{V}_0[a,b]$ denotes the subset of $f \in \mathcal{V}_0[-\infty,\infty]$ with support contained in $[a,b]$.

More general, we introduce the spaces $\mathcal{V}_\ell[0,1]$ $(0 \le \ell \le L)$ of piecewise constant functions on the uniform grid of size $h_\ell := 2^{-\ell}h$. Obviously, the spaces are nested:

$$\mathcal{V}_L[0,1] \supset \mathcal{V}_{L-1}[0,1] \supset \ldots \supset \mathcal{V}_\ell[0,1] \supset \mathcal{V}_{\ell-1}[0,1] \supset \ldots \supset \mathcal{V}_0[0,1] = \mathcal{S}.$$

Because of $\mathcal{V}_\ell[0,1] \supset \mathcal{V}_{\ell-1}[0,1]$, one can decompose $\mathcal{V}_\ell[0,1]$ into $\mathcal{V}_{\ell-1}[0,1] \oplus \mathcal{W}_\ell[0,1]$, where $\mathcal{W}_\ell[0,1]$ is the orthogonal complement, i.e., $\mathcal{W}_\ell[0,1] = \{f \in \mathcal{V}_\ell[0,1] : \int_0^1 fg\mathrm{d}x = 0 \text{ for all } g \in \mathcal{V}_{\ell-1}[0,1]\}$. Inserting this decomposition recursively for $\mathcal{V}_{\ell-1}[0,1]$ etc., one obtains the representation

$$\mathcal{V}_L[0,1] = \mathcal{V}_0[0,1] \oplus \mathcal{W}_1[0,1] \oplus \mathcal{W}_2[0,1] \oplus \ldots \oplus \mathcal{W}_L[0,1]. \tag{6.1}$$

The index $\ell \in \{0,\ldots,L\}$ indicates the refinement level and is connected with the step size $h_\ell = 2^{-\ell}h$.

For practical purpose, one needs basis functions of these subspaces. The basis functions of $\mathcal{V}_0[0,1]$ are $\left\{\Phi_j^0 : 0 \le j \le n-1\right\}$, which are given by

$$\Phi_0^\ell(x) = \left\{ \begin{array}{cl} 1/\sqrt{h_\ell} & \text{for } x \in [0,h_\ell) \\ 0 & \text{otherwise} \end{array} \right\}, \qquad \Phi_j^\ell(x) := \Phi_0^\ell(x - jh_\ell) \qquad \left(h_\ell = 2^{-\ell}h\right). \tag{6.2}$$

The scaling of Φ_j^0 is chosen such that the Φ_j^0 form an orthonormal basis.

The basis functions of $\mathcal{W}_\ell[0,1]$ are $\left\{\Psi_j^\ell : 0 \le j \le 2^{\ell-1}n-1\right\}$, where

$$\Psi_0^\ell(x) = \left\{ \begin{array}{cl} +1/\sqrt{2h_\ell} & \text{for } x \in [0,h_\ell) \\ -1/\sqrt{2h_\ell} & \text{for } x \in [h_\ell,2h_\ell) \\ 0 & \text{otherwise} \end{array} \right\}, \quad \Psi_j^\ell(x) = \Psi_0^\ell(x - 2jh_\ell) \qquad \left(h_\ell = 2^{-\ell}h\right) \tag{6.3}$$

describes the Haar wavelets (cf. [7]). One checks that these function span the space $\mathcal{W}_\ell[0,1]$ from (6.1). Furthermore, all functions $\Phi_j^0, \Psi_{j'}^\ell$ are pairwise orthonormal.

The dimension of $\mathcal{V}_L[0,1]$ is $2^L n$ corresponding to the fact that $\dim \mathcal{V}_0[0,1] = n$ and $\dim \mathcal{W}_\ell[0,1] = 2^{\ell-1}n$.

6.2 Wavelet Representation of the Graded Mesh

In the following we assume that n is an even number.

Since $\mathcal{V}_L[0,1]$ from (6.1) represents the piecewise constant functions on the uniform fine grid of size $h_L := 2^{-L}h$, it is much too costly for applications. Instead we define now a graded mesh as follows.

By $\mathcal{W}_\ell := \mathcal{W}_\ell[0, 2^{-\ell}]$ we denote the space spanned by the basis function with support in $[0, 2^{-\ell}]$, i.e.,

$$\mathcal{W}_\ell := \mathcal{W}_\ell[0, 2^{-\ell}] := \operatorname{span}\left\{\Psi_j^\ell : 0 \le j \le n/2 - 1\right\}.$$

Together with the unchanged space $\mathcal{V}_0 := \mathcal{V}_0[0, 1]$, we define the linear combination

$$\mathcal{S}_{\text{graded}} := \mathcal{V}_0 \oplus \mathcal{W}_1 \oplus \ldots \oplus \mathcal{W}_L. \tag{6.4}$$

Remark 6.1 *a) The dimension of $\mathcal{S}_{\text{graded}}$ is $N := (1 + L/2)\, n$. $\mathcal{S}_{\text{graded}}$ contains all piecewise constant functions on the grid*

$$\mathcal{G}_{\text{graded}} := \bigcup_{\ell=0}^{L} \mathcal{G}_\ell \quad \textit{with } \mathcal{G}_\ell := \left\{x_{\nu,\ell} = \nu 2^{-\ell} h : 0 \le \nu \le n\right\} \tag{6.5}$$

which is obtained by repeated halving of the intervals in the first half of the refined zone. It is depicted in Figure 6.1.

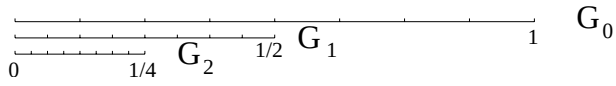

Figure 6.1: $\mathcal{G}_{\text{graded}}$ as union of $\mathcal{G}_0$, $\mathcal{G}_1$, $\mathcal{G}_2$

b) As before, all involved basis functions Φ_j^0, $\Psi_{j'}^\ell$, form an orthonormal basis.
c) Another way to describe $\mathcal{S}_{\text{graded}}$ is based on

$$\mathcal{S}_{\text{graded}} = \mathcal{V}_L[0, 2^{-L}] + \mathcal{V}_{L-1}[2^{-L}, 2^{1-L}] + \ldots + \mathcal{V}_1[1/4, 1/2] + \mathcal{V}_0[1/2, 1].$$

Functions $f \in \mathcal{S}_{\text{graded}}$ can be represented in two ways:

1. The traditional nodal basis in the graded grid $\mathcal{G}_{\text{graded}}$ uses the values of f in each interval of $\mathcal{G}_{\text{graded}}$ where f is constant. These are the coefficients $f_{j,\ell}$ of the representation

$$f = \sqrt{h_L} \sum_{j=0}^{n-1} f_{j,L} \Phi_j^L + \sum_{\ell=0}^{L-1} \sqrt{h_\ell} \sum_{j=n/2}^{n-1} f_{j,\ell} \Phi_j^\ell \tag{6.6}$$

   according to Remark 6.1c. Note that the factors $\sqrt{h_\ell}$ arise from the particular scaling in (6.2).

2. The wavelet representation uses the coefficients f_j^ℓ (denoted with ℓ as upper index) from

$$f = \sum_{j=0}^{n-1} f_j^0 \Phi_j^0 + \sum_{\ell=1}^{L} \sum_{j=0}^{n/2-1} f_j^\ell \Psi_j^\ell \tag{6.7}$$

   according to (6.4).

Remark 6.2 *a) Let $f \in \mathcal{S}_{\text{graded}}$. The transform of the nodal coefficients from (6.6) into the coefficients of the representation (6.7) as well as the back transform cost $\mathcal{O}(N)$ arithmetical operations*[7] *($N = (1 + L/2)\, n$).*
b) As a side product, we obtain the decomposition of $f \in \mathcal{S}_{\text{graded}}$ into

$$f = \sum_{\ell=0}^{L} f_\ell \quad \textit{with } f_0 = \sum_{j=0}^{n-1} f_j^0 \Phi_j^0 \in \mathcal{V}_0 \quad \textit{and } f_\ell = \sum_{j=0}^{n/2-1} f_j^\ell \Psi_j^\ell \in \mathcal{W}_\ell \quad (1 \le \ell \le L).$$

As pointed out in Lemma 3.2, the convolution of piecewise constant functions from $\mathcal{S}_{\text{graded}}$ are piecewise linear, but not with respect to the subintervals of $\mathcal{G}_{\text{graded}}$. Nevertheless, in the next subsection we only evaluate $\varphi * \psi$ at the nodal points x_i of $\mathcal{G}_{\text{graded}}$. In a forthcoming paper, we will describe another efficient procedure which computes the exact orthogonal projection onto each subinterval. To ensure conservation of mass (see §4) we need another kind of projection. Whether this mass conserving projection can be performed efficiently is presently under consideration.

[7] Because of the linear complexity, this transform is called the *fast wavelet transform* (cf. [7]).

6.3 Evaluation of the Convolution Integral

Now we reconsider the convolution integral $\int_0^{x_i} \varphi(y)\psi(x_i - y)\mathrm{d}y$ from Problem 3.4, where $\varphi, \psi \in \mathcal{S}_{\mathrm{graded}}$. Since φ and ψ are obtained by (3.2) or (3.3) on each subinterval, they are represented by their piecewise values, i.e., by (6.6). The wavelet transform gives us the decompositions $\varphi = \sum_{\ell=0}^{L} \varphi_\ell$ and $\psi = \sum_{\ell=0}^{L} \psi_\ell$ ($\varphi_0, \psi_0 \in \mathcal{V}_0$, $\varphi_\ell, \psi_\ell \in \mathcal{W}_\ell$, $1 \le \ell \le L$, cf. Remark 6.2b).

Next, it is essential that in our case the basis functions from (6.7) are symmetric in the sense that $\Phi_0^0(h_0 - x) = \Phi_0^0(x) \in \mathcal{V}_0$ and $\Psi_0^\ell(2h_\ell - x) = -\Psi_0^\ell(x) \in \mathcal{W}_\ell$. This fact ensures the implications

$$\begin{array}{lcll} \psi_0 \in \mathcal{V}_0 & \Rightarrow & \psi_0(x_i - \cdot) \in \mathcal{V}_0 & \text{for all } x_i \in \mathcal{G}_0 \quad (\mathcal{G}_0 \text{ from (6.5)}) \\ \psi_\ell \in \mathcal{W}_\ell & \Rightarrow & \psi_\ell(x_i - \cdot) \in \mathcal{W}_\ell[0,1] & \text{for all } x_i \in \tilde{\mathcal{G}}_{\ell-1} := \left\{\nu 2^{-\ell} h : 0 \le \nu \le 2^\ell n\right\},\ 1 \le \ell \le L. \end{array} \tag{6.8}$$

Hence, the terms in $\psi(x_i - \cdot) = \sum_{\ell=0}^{L} \psi_\ell(x_i - \cdot)$ describe a decomposition of $\psi(x_i - \cdot)$ into the components of $\mathcal{V}_0 \oplus \mathcal{W}_1[0,1] \oplus \ldots \oplus \mathcal{W}_L[0,1]$, provided that $x_i \in \mathcal{G}_0$. Note that we need $\mathcal{W}_\ell[0,1]$ instead of $\mathcal{W}_\ell = \mathcal{W}_\ell[0, 2^{-\ell}]$, since, e.g., for $x_i = 1$ $\psi_\ell \in \mathcal{W}_\ell[0, 2^{-\ell}]$ yields $\psi_\ell(1 - \cdot) \in \mathcal{W}_\ell[1 - 2^{-\ell}, 1] \subset \mathcal{W}_\ell[0,1]$.

The orthogonality of the subspaces in $\mathcal{V}_0 \oplus \mathcal{W}_1[0,1] \oplus \ldots \oplus \mathcal{W}_L[0,1]$ yields

$$\int_0^{x_i} \varphi(y)\psi(x_i - y)\mathrm{d}y = \sum_{\ell=0}^{L} \int_0^{x_i} \varphi_\ell(y)\psi_\ell(x_i - y)\mathrm{d}y \qquad \text{for } x_i \in \mathcal{G}_0. \tag{6.9}$$

Conclusion 6.3 *Let $x_i \in \mathcal{G}_0$. The evaluation of $\int_0^{x_i} \varphi(y)\psi(x_i - y)\mathrm{d}y$ can be reduced to the convolutions $\int_0^{x_i} \varphi_\ell(y)\psi_\ell(x_i - y)\mathrm{d}y$ involving the* uniform grids $\mathcal{G}_\ell$. *The latter integral can be computed as in §5.*

The practical performance simplifies further due to the following observation.

Remark 6.4 *Since the grid points $x_i \in \mathcal{G}_0 \cap [0, 1/2]$ are also elements of $\mathcal{G}_1$ and grid points $x_i \in \mathcal{G}_1$ will be treated later, the evaluation can be restricted to $x_i \in \mathcal{G}_0 \cap (1/2, 1]$. For $\ell \ge 2$ the support of φ_ℓ lies in $[0, 1/4]$, while the support of $\psi_\ell(x_i - \cdot)$ is contained in $[x_i - 1/4, x_i] \subset (1/4, 1]$. Hence the supports are disjoint and $\int_0^{x_i} \varphi_\ell(y)\psi_\ell(x_i - y)\mathrm{d}y = 0$ results for all $x_i \in \mathcal{G}_0 \cap (1/2, 1]$ and $2 \le \ell \le L$. Therefore, the FFT computation of the convolutions is to be performed only for the levels $\ell = 0, 1$.*

We have to evaluate $\int_0^{x_i} \varphi(y)\psi(x_i - y)\mathrm{d}y$ for each $x_i \in \mathcal{G}_{\mathrm{graded}}$ from (6.5). Since $\mathcal{G}_0$ is only a part of $\mathcal{G}_{\mathrm{graded}}$, we have next to consider the convolution integral for $x_i \in \mathcal{G}_1 = \{x_{\nu,1} = \nu h/2 : 0 \le \nu \le n\}$.

Let $\psi = \sum_{\ell=0}^{L} \psi_\ell$ be the decomposition from above and split ψ_0 into $\psi_{0,\mathrm{left}} + \psi_{0,\mathrm{right}}$ such that the support of $\psi_{0,\mathrm{left}}$ is in $[0, 1/2]$, while $\psi_{0,\mathrm{right}}$ has its support in $[1/2, 1]$. Since $x_i \in \mathcal{G}_1$ implies $x_i \le 1/2$, $\psi_{0,\mathrm{right}} \in \mathcal{V}_0[1/2, 1]$ leads to $\psi_{0,\mathrm{right}}(x_i - \cdot) \in \mathcal{V}_0[-\infty, 0]$. This means that $\psi_{0,\mathrm{right}}$ is irrelevant for the convolution integral and can be omitted[8] (this fact is equivalent to the statement in Remark 5.2).

It is still easier to see that the part $\varphi_{0,\mathrm{right}}$ of the corresponding splitting $\varphi = \sum_{\ell=0}^{L} \varphi_\ell$, $\varphi_0 = \varphi_{0,\mathrm{left}} + \varphi_{0,\mathrm{right}}$ can be omitted.[8]

Now we perform one partial step of the wavelet transform and replace the representation

$$\varphi_0 + \varphi_1 = \sum_{j=0}^{n/2-1} \varphi_j^0 \Phi_j^0 + \sum_{j=0}^{n/2-1} \varphi_j^1 \Psi_j^1 \in \mathcal{V}_0[0, 1/2] \oplus \mathcal{W}_1[0, 1/2]$$

(the terms φ_j^0 with $j > \frac{n}{2}$ are omitted!) by its representation in $\mathcal{V}_1[0, 1/2]$, i.e., $\varphi_1^{\mathrm{new}} = \varphi_0 + \varphi_1 = \sum_{j=0}^{n-1} \varphi_{1,j} \Phi_j^1$. The same is done for the ψ components. Hence, we end up in

$$\varphi, \psi \in \mathcal{V}_1[0, 1/2] \oplus \mathcal{W}_2[0, 1/4] \oplus \ldots \oplus \mathcal{W}_\ell[0, 2^{-\ell}] \oplus \ldots \oplus \mathcal{W}_L[0, 2^{-L}] = \mathcal{V}_1[0, 1/2] \oplus \mathcal{W}_2 \oplus \ldots \oplus \mathcal{W}_L.$$

This is the same situation as in (6.4), except that $h = h_0$ is replaced by h_1 and the interval $[0, 1]$ is replaced by $[0, 1/2]$. Obviously, Conclusion 6.3 and Remark 6.4 apply now to $x_i \in \mathcal{G}_1$ and to $x_i \in \mathcal{G}_1 \cap [1/4, 1/2]$, respectively.

[8] The function without these terms is denoted by the same name!

7 Complexity

First we consider the case of one uniform grid.

Problem 2.2 occurs k-times, where k is the separation rank in (2.2). Each of these problems is reduced to Problem 3.4. Its solution in §5 requires three FFT applications ($\varphi_\mu \mapsto \hat{\varphi}_\mu$, $\psi_\mu \mapsto \hat{\psi}_\mu$, $\hat{\omega}_\nu \mapsto \omega_\nu$), the evaluation of (3.2) or (3.3) in each interval and the computation of the products $\hat{\varphi}_\gamma \hat{\psi}_\gamma e^{i\gamma\pi/n}$ $(1-n \le \gamma \le n)$. Possibly, the convolution results at x_i are used to the compute the Galerkin integrals as in Lemma 3.3. Altogether, the cost is $\mathcal{O}(n \log n)$. With the factor k from above we get the following result.

Lemma 7.1 *Let (2.2) with separation rank k be the approximation of the kernel $\kappa(x,y)$ and let n be the number of intervals of the uniform grid. Then the cost is of order $\mathcal{O}(nk \log n)$.*

Next we consider the case of the graded mesh from §6, which is characterised by the numbers n and L. We recall that $N = (1 + L/2)\, n$ is the total number of subintervals.

Due to Remark 6.4, the calculations at level $\ell = 0$ consists of two convolution problems of the respective sizes n and $n/2$ in uniform grids. Hence, the cost is $\mathcal{O}(nk \log n)$. As described above, we have to solve similar problems of the same size at the levels $\ell = 1, \ldots, L$. This leads to the next lemma.

Lemma 7.2 *Let (2.2) with separation rank k be the approximation of the kernel $\kappa(x,y)$. Define the graded mesh as in §6 with the parameters n and L. Then the cost for evaluating the convolution integral is of order $\mathcal{O}(nkL \log n) \le \mathcal{O}(Nk \log N)$, where $N = (1 + L/2)\, n$ is the dimension of the space $\mathcal{S}_{\text{graded}}$.*

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