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Numerical techniques for Particle Aggregation

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A variety of production processes in chemistry and biotechnology are concerned with particles dispersed in an environmental phase. The particle distribution is mathematically described by the solution of population balance equations of integro-differential type. These equations include terms to model processes like nucleation, growth, aggregation and breakage of particles. In this presentation, we will focus on the aggregation term which models the collision of two particles, resulting in the formation of a single new particle in exchange for the original two particles. Mathematically, it is described in terms of a convolution integral that is numerically expensive to evaluate and often dominates the total simulation cost.

We begin with the univariate case, i.e. only a single particle property, often its mass, is considered. Starting with the popular fixed pivot method, we describe various discretization schemes and their subsequent numerical evaluation. We will discuss aspects such as grid refinement (e.g., uniform, locally refined, structured or unstructured grids), order of discretization, and fast Fourier transformation (FFT) based fast evaluation methods which, if the aggregation kernel can be represented or approximated in separable form, allow to reduce the computational complexity from quadratic $\mathcal{O}(n^2)$ to almost linear $\mathcal{O}(n \log n)$ order where n denotes the number of unknowns (i.e., the number of considered particle size classes).

Next, we proceed to the multivariate case in which a particle may be characterized by multiple properties, e.g. mass, porosity, concentration of some substance, etc. In our model, we assume all considered properties to be additive, i.e., all properties can be measured by some positive real number, and aggregation of two particles leads to the addition of their respective values for the resulting particle.

Many of the methods for the univariate case can be (and have been) generalized to the multivariate case where they suffer from the so-called curse of dimensionality - their numerical complexity grows exponentially and quickly reaches the limits of modern machines both with respect to the required storage and computational time. We introduce some modern approaches that address and even may resolve these difficulties, including the application of multidimensional FFT methods (again requiring a separable aggregation kernel), parallelization, and modern tensor formats for the multivariate density functions.

We will provide numerical illustrations for many of the introduced methods with our focus on their numerical performance.