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Fast Monte Carlo simulation for particle coagulation in population balance

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ABSTRACT

The Monte Carlo (MC) method for population balance modeling (PBM) has become increasingly popular because the discrete and stochastic nature of the MC method is especially suited for particle dynamics. However, for the two-particle events (typically, particle coagulation), the double looping over all simulation particles is required in normal MC methods, and the computational cost is $O(N_s^2)$, where N_s is the simulation particle number. This paper proposes a fast random simulation scheme based on the differentially-weighted Monte Carlo (DWMC) method. The majorant of coagulation kernel was introduced to estimate the maximum coagulation rate by a single looping over all particles rather than the double looping. The acceptance–rejection process then proceeded to select successful coagulation particle pairs randomly, and meanwhile the waiting time (time-step) for a coagulation event was estimated by summing the coagulation kernels of rejected and accepted particle pairs. In such a way, the double looping is avoided and computational efficiency is greatly improved as expected. Five coagulation cases for which analytical solutions or benchmark solutions exist were simulated by the fast and normal DWMC, respectively. It is found the CPU time required is orders of magnitude lower and only increases linearly with N_s; at the same time the computational accuracy is guaranteed very favorably.

1. Introduction

Coagulation between particles (or bubbles, droplets) is ubiquitous in many different fields of nature and engineering (Friedlander, 2000), including atmospheric physics (aerosol dynamics), combustion (the growth of particulate matter, soot and PAH), chemical engineering (e.g., polymerization, granulation, crystallization, and precipitation), catalytic chemical processes, food processes, nanoparticle synthesis, and so on. The particle coagulation refers to two particles collide and adhere together, leading to the increase of average particle size and the decrease of particle number concentration, i.e., the dynamic evolution of particle size distribution (PSD). Among the various particle dynamic events, coagulation is the most demanding event for modeling, as it always involves two discrete particles. The population balance equitation (PBE) for particle coagulation, which characterizes coagulation dynamics in term of the time evolution of PSD, is represented by the following mathematical equation:

$$\frac{\partial n(v,t)}{\partial t}=\frac{1}{2}\int_{v_{\min}}^{v}\beta(v-u,u,t)n(v-u,t)n(u,t)\mathrm{d}u-n(v,t)\int_{v_{\min}}^{v_{\max}}\beta(v,u,t)n(u,t)\mathrm{d}u. \tag{1}$$

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where $n(v, t)$ with dimension $m^{-3}\,m^{-3}$ is the particle size distribution function (PSDF) at time t, so that $n(v, t)dv$ is the number concentration of particles with size range between v and $v+dv$ at time t; $\beta(v, u, t)$ is the coagulation kernel for two particles of volumes v and u at time t, $m^3\,s^{-1}$.

Because of the partial integro-differential nature of the PBE, it is difficult to solve it directly. Only for a few ideal cases can we get analytic solutions, otherwise we can only get approximate solutions by numerical methods. The deterministic scheme such as sectional method and method of moments (Frenklach & Harris, 1987; Gelbard et al., 1980) is capable of solving Eq. (1) either through an appropriate discretization scheme or by quadrature. However, there exist some difficulties such as complicated mathematical models (especially for multivariate population balance) and discrete errors for the deterministic methods. The stochastic (Monte Carlo) scheme, which describes directly the dynamic evolution of particle population in dispersed systems, approximates the PBE solution through a large amount of random sampling from the system. The discrete nature of the MC method adapts itself naturally to the discrete process (i.e., the discrete particle population and the discrete dynamic events). The population balance-Monte Carlo (PBMC) can obtain the details of the dynamic evolution of multi-dimensional, multi-component, and polydispersed particle population (Zhao & Zheng, 2011, 2013; Zhao et al., 2011). Furthermore, the MC algorithm is comparatively easy to program. Owing to these advantages, MC constitutes an important class of methods for the numerical solution of the population balance modeling (PBM).

Generally speaking, MC methods can be classified either by time discretization scheme into event-driven MC and time-driven MC, or by simulation particle weighting scheme into equally-weighted MC and differentially-weighted MC. Event-driven MC (Garcia et al., 1987) first calculates time interval (or waiting time) Δt_{ED} between two successive events based on the average rate of event processes and then uses the stochastic game to choose the event that happens after this waiting time. Time-driven MC (Liffman, 1992) considers all possible events that may happen within a pre-specified time step Δt_{TD} to be decoupled; Δt_{TD} is constrained to be less than or equal to the minimum time scale within which each simulation particle participates in one coagulation event at most. Most of the MC methods (Garcia et al., 1987; Liffman, 1992; Lin et al., 2002; Maisels et al., 2004) belong to the equally-weighted method, in which all simulation particles have the same weight. Usually a subsystem of the total system is simulated either explicitly or implicitly, in which the common weight is equal to the ratio of the volume of the total system to that of the subsystem. However, the equally weighting scheme leads to a great deal of statistical noise for particles in those less-populated sections such as at the edges of log-normal distributed size spectrum. In the differentially weighting scheme, these sections where the number density is low can be represented by simulation particles with appropriate number and relatively small weight. Keeping track of differentially weighted simulation particles of different sizes will thus help to improve the accuracy of MC. We have proposed the differentially-weighted Monte Carlo (DWMC) method for particle coagulation for univariate population balance (Zhao et al., 2005a, 2005b) and multivariate population balance (e.g., two-component aggregation) (Zhao et al., 2010, 2011). The key ideas are to establish the coagulation rules that describe how to deal with coagulation between differentially-weighted simulation particles, and to specify how the simulation particles should be homogeneously distributed over the size spectrum (rather than to let them evolve freely). The DWMC can evolve in either event-driven mode (Zhao & Zheng, 2009b) or time-driven mode (Zhao et al., 2010), and keeps the total number of simulation particles constant in simulation. It was validated that the DWMC methods perform better statistical accuracy than other equally-weighted MC.

It is worth emphasizing that an optimal combination of high accuracy and high efficiency are essential for PBMC, because with the increase in simulation particle number its numerical accuracy increases while its computational efficiency decreases. For the two-particle events such as coagulation (or aggregation, agglomeration), the normal PBMC simulation has to calculate/update the interaction probability of any particle pair each time step to obtain probability distribution of random events and the waiting time between two successive events. The double looping over all simulation particles is thus required in the normal PBMC methods, so the computational cost reaches $O(N_s^2)$, where N_s is the simulation particle number. Although there is dramatic increase in computational power over the past decade, it is still very necessary to improve the computational efficiency for fast prediction of particle dynamics. There are two kinds of ways to accelerate MC simulation: one is parallel computing (Kruis et al., 2010), including CPU parallel computing based on Message Passing Interface (MPI) and Open Multi-Processing (OpenMP), and Graphitic Processing Unit (GPU) parallel computing based on Open Computing Language (OpenCL) and Compute Unified Device Architecture (CUDA) (Wei & Kruis, 2013). Factually the parallel computing of MC simulation uses more computer source simultaneously to reduce computational time. Another is to improve the scheme of PBMC itself to accelerate simulation. Kruis et al. (2000) proposed the smart bookkeeping technology to avoid a large number of re-calculations of the coagulation rates of particles not participating in coagulation, in such a way that the CPU time is greatly saved without loss in accuracy. Wagner et al. (Eibeck & Wagner, 2000, 2001) and Kraft et al. (Goodson & Kraft, 2002) developed a new efficient MC which utilized the majorant of coagulation kernel to calculate the coagulation probability of all particle pairs by a single looping over all particles rather than the double looping. A Markov model with fictitious jumps was then constructed to simulate particle dynamics with high accuracy. The CPU time increases linearly with N_s, rather than as N_s^2 (as with the conventional MC). Recently, Wei (2013) proposed a fast acceptance–rejection scheme that can boost the performance of Monte Carlo methods for particle coagulation by establishing a connection between the information of particle pairs and the maximum coagulation rate. Lécot and Tarhini (2008) and Lécot and Wagner (2004) proposed the quasi-Monte Carlo to accelerate the convergence rate, in which pseudo-random numbers were replaced by quasi-random numbers or low-discrepancy point sets (which are “evenly distributed”). Similar idea in terms of good lattice point set was also used by Kruis et al. (2012) to estimate the maximum of coagulation kernel with a remarkable gain in efficiency. Another measure accelerating PBMC simulation is to simulate coagulation between particle species rather than