Journal of Computational Physics 322 (2016) 21–32

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Accelerated simulation of stochastic particle removal processes in particle-resolved aerosol models

J.H. Curtis [a], M.D. Michelotti [b], N. Riemer [a], M.T. Heath [b], M. West [c,*]

[a] Department of Atmospheric Sciences, University of Illinois at Urbana–Champaign, 105 S. Gregory St., Urbana, IL 61801, USA
[b] Department of Computer Science, University of Illinois at Urbana–Champaign, 201 North Goodwin Avenue, Urbana, IL 61801, USA
[c] Department of Mechanical Science and Engineering, University of Illinois at Urbana–Champaign, 1206 W. Green St., Urbana, IL 61801, USA

ARTICLE INFO

Article history:
Received 27 December 2015
Received in revised form 13 June 2016
Accepted 16 June 2016
Available online 21 June 2016

Keywords:
Aerosol modeling
Stochastic simulations
Particle methods
Aerosol removal

ABSTRACT

Stochastic particle-resolved methods have proven useful for simulating multi-dimensional systems such as composition-resolved aerosol size distributions. While particle-resolved methods have substantial benefits for highly detailed simulations, these techniques suffer from high computational cost, motivating efforts to improve their algorithmic efficiency. Here we formulate an algorithm for accelerating particle removal processes by aggregating particles of similar size into bins. We present the Binned Algorithm for particle removal processes and analyze its performance with application to the atmospherically relevant process of aerosol dry deposition. We show that the Binned Algorithm can dramatically improve the efficiency of particle removals, particularly for low removal rates, and that computational cost is reduced without introducing additional error. In simulations of aerosol particle removal by dry deposition in atmospherically relevant conditions, we demonstrate about 50-times increase in algorithm efficiency.

1. Introduction

Monte Carlo particle techniques are used in various disciplines to solve population balance equations numerically. Particle methods have been applied to cloud physics [1–3], polymer science [4–6], and aerosol physics [7–15], the focus of this paper. Particle-resolved techniques are particularly advantageous for simulating multidimensional systems and do not suffer from artificial numerical diffusion found in implementations of finite difference methods. Unfortunately, the computational expense of these techniques remains a substantial drawback.

An atmospheric aerosol population is a multidimensional system in the space of aerosol composition. Aerosol particles consist of a complex mixture of chemical species, such as soluble inorganic salts and acids, insoluble crustal materials (dust), trace metals, and carbonaceous materials [16–19]. The aerosol life-cycle consists of three stages: formation, transformation, and removal. Atmospheric aerosols can originate from primary emission sources or may be formed by nucleation. The composition of aerosol particles evolves over time due to coagulation with other particles and to mass transfer to and from gas-phase species. Ultimately, aerosol particles are removed from the atmosphere by precipitation (“wet deposition”) or by deposition to the ground or other surfaces in the absence of precipitation (“dry deposition”).

* Corresponding author.
E-mail address: mwest@illinois.edu (M. West).

http://dx.doi.org/10.1016/j.jcp.2016.06.029
0021-9991/

To model the multidimensional aerosol size distribution, particle-resolved models [10] explicitly resolve the evolution of individual aerosol particles within a representative volume of air. These processes can include coagulation, gas-particle mass transfer, emission, dilution with background air, and wet or dry deposition.

In this paper we use the particle-resolved model PartMC-MOSAIC (Particle Monte Carlo—Model for Simulating Aerosol Interactions and Chemistry) [20] as a testbed. While particle-based models have the advantage of avoiding *a priori* assumptions regarding particle composition, they can be very expensive computationally, resulting in the need for highly efficient algorithms [10,21–23]. Efficient implementations, such as the PartMC-MOSAIC code, have storage cost proportional to the number of particles, computational cost for evaporation/condensation proportional to the number of particles, and computational cost for coagulation proportional to the number of coagulation events.

In this paper, we focus on the simulation of dry deposition as an important representative of aerosol removal processes, however our method applies to single-event particle removal processes in general. Dry deposition—the removal of particles in absence of precipitation—determines the particles' residence time in the atmosphere. Calculating the dry deposition rate is highly complex due to its dependence on physical and chemical properties of the aerosol, land surface characteristics, and meteorological conditions. As dry deposition is a size-dependent process, it also shapes the aerosol size distribution.

A naive approach to simulating dry deposition results in computational cost proportional to the number of particles. The naive approach becomes computationally expensive for simulations that involve a large number of particles and becomes computationally prohibitive for inclusion of particle-resolved aerosol representation within 3D regional weather models. Here we present an algorithm, based on the Stochastic Simulation Algorithm (SSA), to improve the performance of particle removal due to dry deposition. The contribution of this paper is (1) a new algorithm that uses one-dimensional binning and geometric sampling while maintaining exactness and (2) its application to the process of dry deposition where we showed a very significant reduction in the computational cost with no additional error incurred.

The Stochastic Simulation Algorithm (SSA) [24,25] is a Monte Carlo procedure for producing an exact realization of a continuous-time Markov chain. The original formulation of SSA was designed for Markov chains that involved pairwise interacting entities, such as coagulating aerosol particles. However, it can be modified easily to consider events that involve only a single entity, such as stochastic particle deposition.

The high computational cost of SSA has motivated the development of more efficient variants for specific applications. Some of these retain the exactness of SSA (e.g. [26–28]), while others sacrifice exactness to gain numerical efficiency. Popular examples of approximate methods are Tau Leaping [29] and later variants [30–34], which can achieve greater efficiency by simulating all events within a small time interval τ but which does not generate exact realizations of the stochastic process. In [22], binned versions of SSA and Tau Leaping were developed that are more efficient for particle processes. These binned variants have similar properties to the original methods, in that Binned SSA is exact while Binned Tau Leaping can be more efficient but is not exact, and they can both be adapted to single-particle processes such as deposition.

In this paper, we present a new binned algorithm (Algorithm 2) that combines the advantages of Binned Tau Leaping and Binned SSA when applied to single-particle non-interacting processes such as particle deposition. This new algorithm is at least as efficient as Binned Tau Leaping and follows it in using a discrete time step τ and being simple to implement. However, it retains the exactness of Binned SSA, making it both fast and exact. We demonstrate the performance of the new algorithm using numerical results from an implementation of this algorithm that we integrated with the PartMC software library [10,35,36,21].

2. Formulation

Consider a set of possible "particles" $\mathcal{P}$. In our model problem, we model atmospheric aerosol particles and represent each particle by the volume of d different chemical species, where $d = 20$ is typical. We will also impose minimum and maximum volumes $v_{\min}$ and $v_{\max}$. Thus, we will use the following set:

$$\mathcal{P} = \left\{ p \in \mathbb{R}^d : p \geq \mathbf{0}, v_{\min} \leq \|p\|_1 \leq v_{\max} \right\}. \tag{1}$$

Let $\pi \subset \mathcal{P}$ be the finite set of particles currently present in the simulation. There may be multiple identical particles, so π is a multiset in the sense of Knuth [37, p. 473]. Throughout a simulation, these particles may be affected by several processes. For atmospheric aerosol modeling, the set of particles π may be affected by emissions, coagulation, condensation, chemical reactions, etc.

Consider the process of particle deposition. Let $K : \mathcal{P} \to \mathbb{R}$ be a kernel denoting the rate of deposition. A particle $p \in \pi$ should be removed from the simulation at stochastic rate $K(p)$. If p and K are not affected by any other processes, the time at which p is removed from the simulation should be chosen from an exponential distribution with rate $K(p)$. However, p and K are likely to be affected by other processes, so it is better to take a time-stepping approach in which we must determine which particles should be removed from the simulation over a time step of size τ.

Algorithm 1 is a Naive Algorithm to simulate particle deposition over a time step of size τ, which checks each particle individually. The function randUnif() returns a uniform random number from $[0, 1)$. Note that Algorithm 1 requires $O(|\pi|)$ computation time, regardless of how many particles are actually removed. This is reasonable if we have many removals, but suppose the number of removals is much less than $|\pi|$. In this case, the algorithm is inefficient.