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An Unsplit Monte-Carlo solver for the resolution of the linear Boltzmann equation coupled to (stiff) Bateman equations

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ABSTRACT

In this paper, we are interested in the resolution of the time-dependent problem of particle transport in a medium whose composition evolves with time due to interactions. As a constraint, we want to use of Monte-Carlo (MC) scheme for the transport phase. A common resolution strategy consists in a splitting between the MC/transport phase and the time discretization scheme/medium evolution phase. After going over and illustrating the main drawbacks of split solvers in a simplified configuration (monokinetic, scalar Bateman problem), we build a new Unsplit MC (UMC) solver improving the accuracy of the solutions, avoiding numerical instabilities, and less sensitive to time discretization. The new solver is essentially based on a Monte Carlo scheme with time dependent cross sections implying the on-the-fly resolution of a reduced model for each MC particle describing the time evolution of the matter along their flight path.

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1. Introduction

In this paper, we are interested in the resolution of the time-dependent problem of particle transport in a medium whose composition evolves with time due to interactions (reactions) with particles. We suppose transport to be driven by the linear Boltzmann equation (1a) for particles having position $x \in \mathcal{D} \subset \mathbb{R}^3$, velocity $v \in \mathbb{R}^+$, direction $\omega \in [0, 2\pi] \times [0, \pi]$, at time $t \in [0, T] \subset \mathbb{R}^+$ and where the quantity $n(x, t, v, \omega)$ is the density of presence of the particles at (x, t, v, ω). We assume the time variation of the medium composition (vector $\boldsymbol{N}$) can be accurately modeled by Bateman equations (1b) (see [10]) where $\boldsymbol{r}(x, t, v) = (r_1(x, t, v), ..., r_M(x, t, v))^t$ is the vector of reaction rates (depending on particle velocity/energy). In this paper, we consider the vector of reaction rates is stiff. By stiff, we mean the characteristic time for the reactions is much smaller than the transport one, at least for some medium components, in some subsets of the computational domain $\mathcal{D}$. As a result, problem (1) is stiff, non-linear and strongly coupled:

$$\begin{cases} \partial_t n(x,t,v,\omega) + v\omega\nabla_x n(x,t,v,\omega) + \Sigma_t(\boldsymbol{N}(x,t),v)vn(x,t,v,\omega) \\ \quad = \iint \Sigma_c(\boldsymbol{N}(x,t),\omega',\omega,v',v)v'n(x,t,v',\omega')\,\mathrm{d}\omega'\,\mathrm{d}v', & \text{(a)} \\ \partial_t \boldsymbol{N}(x,t) = \iint \boldsymbol{r}(\boldsymbol{N}(x,t),v)vn(x,t,v,\omega)\,\mathrm{d}\omega\,\mathrm{d}v. & \text{(b)} \end{cases} \tag{1}$$

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The interaction of particles with the medium is described through total interaction probability $\Sigma_t(x,t,v)$ and a collision term $\Sigma_c(x,t,\omega,\omega',v,v')$. Macroscopic interaction properties depend on both microscopic ones designated by $(\sigma_{\alpha,m})_{\alpha\in\{t,c\}}$ and the medium composition vector $\boldsymbol{N}(x,t)=(N_1(x,t),...,N_M(x,t))^t$:

$$\Sigma_t(\boldsymbol{N}(x,t),v)=\sum_{m=1}^{M}\sigma_{t,m}(v)N_m(x,t),\qquad \Sigma_c(\boldsymbol{N}(x,t),\omega',\omega,v',v)=\sum_{m=1}^{M}\sigma_{c,m}(\omega',\omega,v',v)N_m(x,t). \tag{2}$$

Under this general form, model (1) can be relevant in many fields of applications. The Bateman counterpart (1b) may be considered as a particular case of the Lotka–Volterra system (see [24]) in which we only kept the strong coupling term. Amongst the applications (non exhaustive list), one can quote biology [24] with population dynamics, or physics with burn-up computations in neutronics [5,13,14,8]. In the following, we refer to publications dealing with burn-up applications as numerical studies have mainly been carried out in this context [5,13,14,8]. The particles are then neutrons, the medium is composed of nuclides and the description of the microscopic collision term $(\sigma_{c,m})_{m\in\{1,...,M\}}$ is usually explicitly decomposed into a scattering cross-section $(\sigma_{s,m})_{m\in\{1,...,M\}}$ and a fission cross-section (multiplicative reactions) $(\sigma_{f,m})_{m\in\{1,...,M\}}$. The macroscopic collision term is then:

$$\Sigma_c(\boldsymbol{N}(x,t),\omega,\omega',v,v')=\sum_{m=1}^{M}\sigma_{s,m}(\omega,\omega',v,v')N_m(x,t)+\nu_{f,m}(v)\sigma_{f,m}(\omega,\omega',v,v')N_m(x,t), \tag{3}$$

where $\nu_{f,m}(v)$ designates the fission multiplicity for material m and velocity v. Note that in the following, we will adopt the terminology commonly used in neutronics [3], except we gather scattering and fission under a unique collision term Σ_c for the sake of conciseness. Of course, the numerical methodology we develop in this paper is very general and can be broadened to a larger scope.

The most common resolution strategy consists in a splitting between the MC/transport phase and the time discretization scheme/Bateman phase. In particular, it implies freezing the nuclide concentrations during the transport phase. In section 2, we will examine several choices for the time discretization scheme.[1] To do so, we simplify system (1) (monokinetic transport and scalar Bateman equations) and build an analytical solution for the strongly coupled system under several general hypothesis. To our knowledge, such analytical solution has never been stated. It allows for a complete quantitative study of the numerical schemes at use in this paper and presents also an advantage in term of verification (as in Verification and Validation, V&V [1]). This study will help us conclude that whatever the time discretization scheme, the splitting strategy implies limitations, especially concerning the choice of the time step as soon as stiff regimes are at stakes.

In section 3 on page 217, we present a new MC solver aiming at addressing the aforementioned limitations. We rely on two ingredients: a Monte-Carlo scheme with time-dependent cross-sections (to alleviate the classical hypothesis of constant nuclide concentrations) and a way to approach nuclides concentration evolution during the Monte Carlo phase solving a reduced model which preserves the stiff regime. Combining these two elements, we build a new Unsplit Monte-Carlo (UMC) solver. The mathematical study of transport processes with time-dependent parameters (first ingredient mentioned above) is not new (see [20]), but is scarcely used and have never been applied in order to tackle coupled systems in stiff regimes to our knowledge.

Section 4 on page 227 is dedicated to the application of the general methodology of section 3 and benchmarks. The test problems are presented with increasing complexity. We first have a monokinetic-mononuclide configuration (section 4.1), then monokinetic-multinuclide (in section 4.2) and at last the most general case (section 4.3). With these three configurations we were able to highlight the different possibilities handled by the methodology relative to the type of reduced model (analytical or system of ODEs). Each test problem goes with performance considerations.

As a conclusion, in section 5 on page 233, we will briefly remind the main aspects of the paper, present future works, the expectations for our UMC solver in term of physical applications and concisely hint at some High Performance Computing (HPC) considerations.

Concerning the classical numerical methods used in the different phases (MC schemes for transport equation and time discretization schemes for the Bateman phase), we choose to detail their specifications in the Appendix A. Appendices also introduce some implementation details important for the sake of comparison and reproduction of the results presented in this paper.

2. Application and analysis of classical solvers on a simplified system

In this section, our aim is to pedagogically put forward the limitations of solvers involving a splitting between the transport equation (solved using MC method) and the Bateman system when the latter is stiff. To do so, we first make some simplifications allowing the construction of an analytical solution for a still strongly coupled system. We then perform some in-depth convergence studies with the common numerical solvers of the literature. Obviously, we do not test every existing solvers but only the ones we consider relevant to serve our purpose. For complementary studies, we refer to [5,13,8,7] with

[1] In a burn-up context, we refer to [5,13,8,7] and the reference therein for complete descriptions of the commonly used schemes.

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