MC Methods in Natural Sciences, Engineering and Economics

Book of Abstracts

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MC generators based on GPUs

Gergely Barnaföldi, Wigner Institute

Monte Carlo-based particle generators widely used in particle and detector simulations require enormous number of Central Processing Units (CPU) and huge calculational time. Using a faster computing method might give a unique capability for collaborations to speed up their data analysis or simulations. Recently, programming frameworks of fast General Purpose Graphical Processing Units (GPGPU) reached the level to optimize some programming sub-processes running on GPUs. This is a challenging task, but might result 10 ? 100 times faster calculation theoretically.

As a first step on this way, an inclusion of a GPU implemented pseudo-random generators (PRNG) into a Monte Carlo-based particle generator (MC) is presented here. We performed the diehard-algorithms tests of PRNGs: a Mersenne Twister-based PRNG on CPU, a SIMD-oriented Mersenne Twister PRNG on GPU, and a linear-congruent MWC64X PRNG on GPU. Comparison of PRNGs were done within the AliROOT MC generator framework for both by CPU and GPU runs. Hadron production in proton-proton (pp) and lead-lead (PbPb) collisions were generated using GPU generated numbers.

Current methods for lattice QCD

Stefan Schäfer, CERN

Algorithms for lattice QCD have become much faster during the last decade. This is mainly because of a better understanding of the system which we simulate. After a short introduction to the concepts and the general algorithmic approach of lattice QCD calculations, the talk will highlight some of the ideas which have driven recent developments. A particular focus will be given to decompositions of the physical system and their interplay with the algorithms used for its simulation.

An introduction to particle filtering and sequential Monte Carlo methods

Hans-Rudolf Künsch, ETH Zurich

Fifty Years Later, Are Those Random Numbers Finally Good Enough?

Fred James, CERN

As a grad student in 1962, I discovered that the funny MC results I was getting were caused by a poor random number generator. Thirty years after that, the Phys Rev Letters paper of Ferrenberg et al showed that things had not yet improved, relative to the increased complexity of problems we were trying to solve. Then suddenly, due to the work of theoretical physicists, the situation changed dramatically, both with respect to pseudorandom numbers (the kind most of us use) and quasirandom points (the kind that are supposed to give convergence faster than $1/\sqrt{N}$). But very few MC users seem to be aware of the recent results in this field traditionally reserved for number theorists.

Iterated transport microsimulations

Gunnar Flötteröd, KTH Royal Institute of Technology, Stockholm

Urban transportation simulations typically iterate between a demand simulator (describing how humans plan their travel given the transportation network's state) and a supply simulator (describing how the transportation network performs given a certain travel behavior). If these iterations attain stationarity, the model is considered to be solved, in that mutually consistent demand and supply are found. We discuss this type of model system from a MCMC perspective.

Uncertainty management in traffic modelling

Vincenzo Punzo, University of Napoli and European Commission Joint Research Centre, and Biagio Ciuffo, European Commission Joint Research Centre

In the last century, contributions from engineers, physicists, mathematicians, and behavioural psychologists have lad to a better understanding of driver behaviour and vehicular traffic flow. The focus is the ability to forecast the effect on real systems of different applications ranging from novel driver-assistance systems, to intelligent approaches to optimizing traffic flow, to the precise detection of traffic jams and the short-term forecasting of traffic for dynamic navigation aids.

Increasingly sophisticated models have been therefore developed in the attempt of reproducing the intrinsic complexity of traffic behavior (and that of its components). The challenge and anxiety of providing certain answers has however diverted the attention from a basic consideration: "What makes modeling and scientific inquiry in general so painful is uncertainty. Uncertainty is not an accident of the scientific method, but its substance" (Saltelli et al., 2008).

As a matter of fact, (commercially) available traffic simulation models are fancy tools of (almost) non-demonstrated utility. In addition, the scientific community is only marginally contributing to identify correct ways to use what is available dealing in a proper manner with the underlying uncertainties of our tools. This is leading to the paradoxical situation in which the outputs of a traffic simulation are likely to be more affected by the assumptions made to define proper distributions for the model inputs than from the model itself.

This deep quandary stems from two main factors: i) traffic dynamics are the results of the combination of several mutually correlated stochastic elements (drivers' behavior, environmental conditions, system performances, etc.), and any observation of the transportation system is just one of the possible occurrence generated by the same inputs.

These elements of intrinsic complexity call for the definition of suitable frameworks for the management of modeling uncertainties. Objective of the present work is to show how Monte Carlo methods can be fruitfully applied to make these frameworks operational.

Monte Carlo methods of electron kinetics in laser excited solids

Nikita Medvedev, CFEL

In this talk I will present a Monte Carlo based methods of modeling ultrafast electron kinetics in laser irradiated materials. I will briefly talk about the hierarchy of the statistical methods used in modeling electron excitation and relaxation processes in solids. It will be presented a standard Monte Carlo approach for electron kinetics and transport, most commonly used in studies of excited matter. It is based on the approach of individual particles and independent events. Some more advanced techniques, accounting for correlated events in electronic system, will be discussed. A combination of Monte Carlo methods with other approaches and techniques will be conclude the talk.

MC in Quantum Chemistry: Quantum Monte Carlo for Electronic Structure

William A. Lester, Berkeley

Background on the electronic structure of molecules will be presented leading to how QMC for molecules arose. Versions of the approach will be summarized including the algorithm that has dominated computations to date. Aspects that impact computational efficiency will be described and selected applications presented to provide insight on the capability of the method.

MC methods in pricing and risk assessment

Gabor Molnar-Saska, Morgan Stanley

Monte Carlo simulation is used extensively in financial mathematics since analytic solution for complex pricing problems does not exist. First, I will give some introduction on financial products and then the basic concept of pricing will be shown through a simple example. The advantages and challenges of Monte Carlo method will be presented in terms of valuation and risk calculations. A typical example of use of Monte Carlo methodology is the American type option, where the payout function of the product depends not only on the final value, rather the whole trajectory of the underlying products. In the presentation I will show some basic American type option problem, and show

how we can avoid generating bushy Monte Carlo paths based on a linear regression following the Longstaff-Schwartz methodology. Finally, I will present some possible extensions of this approach.

MCs in computational biology (protein folding and aggregation)

Sandipan Mohanty, FZ Jülich

Approximate Bayesian computation (ABC): advances and questions

Christian Robert

The lack of closed form likelihoods has been the bane of Bayesian computation for many years and, prior to the introduction of MCMC methods, a strong impediment to the propagation of the Bayesian paradigm. We are now facing models where an MCMC completion of the model towards closed-form likelihoods seems unachievable and where a further degree of approximation appears unavoidable. In this tutorial, I will present the motivation for approximative Bayesian computation (ABC) methods, the various implementations found in the current literature, as well as the inferential, rather than computational, challenges set by these methods.

MC event generators in high-energy physics and astro-particle physics

Leif Lönnblad, Lund

I will discuss the use of Monte Carlo methods in the simulation of high energy collisions between elementary particles. Such simulations, implemented in programs called Event Generators, have developed into indispensable tools for large-scale particle physics experiments such as the LHC at CERN. In particular, I will concentrate on the modeling of so-called parton showers, where a large number of particles are produced and described in an approximate way, and its interplay with the generation of few-particle states where more exact methods can be used.

Ensemble Kalman Methods for Inverse Problems

Andrew Stuart, Warwick

Many problems in the physical sciences require the determination of an unknown field from a finite set of indirect measurements. Examples include oceanography, oil recovery, water resource management and weather forecasting. This may be formulated as a least squares problem to match the model output to the data.

I will demonstrate that ideas from the Ensemble Kalman Filter can be adapted to solve such problems: by running multiple interacting copies of the model, and exposing their output to the (suitably randomized) data, a derivative-free minimization tool is constructed. A key theoretical result is described and this is used to motivate a series of experiments which demonstrate the efficacy of the algorithm.

Ensemble Methods in Atmospheric Data Assimilation

Harald Anlauf, DWD

In numerical weather prediction, data assimilation estimates the initial conditions for the forecast model by a statistical process that combines observational data with past information. In recent years, ensemble methods in data assimilation have matured to the extent that they are considered beneficial for operational numerical weather prediction. After a brief introduction to data assimilation, the presentation describes popular and efficient incarnations of Ensemble Kalman Filters and provides an outlook to Particle Filters for nonlinear data assimilation which is a subject of current research.

Path integral MC in real-time for open systems: challenges and applications

Joachim Ankerhold

Quantum systems interacting with surrounding reservoirs are of fundamental interest in atomic, molecular, and condensed matter physics. Due to the impressive experimental progress in tailoring and controlling quantum devices on nano- and microscales, theory is challenged to provide a detailed understanding of the nonequilibrum dynamics also in presence of external forces. A formally exact description is based on path integrals which can efficiently been evaluated with corresponding MC techniques. These have been substantially improved in the last decade to capture interactions with bosonic as well as fermionic reservoirs. In this talk I will describe the main challenges, numerical techniques, and typical applications.

Coupled CFD - Monte Carlo Transport Simulations for Magnetic Fusion Reactors

Detlev Reiter, FZ Jülich

With the first nuclear fusion reactor (ITER, Cadarche, France) currently being under construction, Monte Carlo particle transport simulations (radiation, atoms, molecules) in the plasma near high heat flux wall components of the burning chamber are challenged, because the interaction of these particles with the fusion plasma largely determine and control the macroscopic plasma flow and the response of exposed wall components of the reactor, and vice versa.

Linear multi-species Monte Carlo transport algorithms are integrated, iteratively, into specialised solvers for magnetised plasma flow equations (Navier Stokes type). Whereas each individual Monte Carlo part is fast and fully parallelised, the combined highly non-linear problem (plasma flow plus neutral particle transport) can be extremely CPU demanding, depending on convergence requirements. The current status of the numerical scheme as well as sample applications from the ongoing ITER design computations will be presented.

Plasma / fusion physics 2: EMC3 etc.

Yuhe Feng, Greifswald

The fluid model widely used for understanding plasma transport in the edge of magnetic confinement devices consists of a set of Braginskiis equations. Mathematically, they fall in the category of second-order partial differential equations of parabolic type. Numerical solutions of these equations for magnetically confined plasmas in realistic 3D geometry encounter the difficulty of dealing with highly anisotropic transport in rather complex magnetic field structures. Attempts of directly adopting conventional finite difference/element concepts can fail already when constructing a suitable computational mesh. The extremely high transport anisotropy necessitates field-aligned coordinates for a clean separation of the small cross-field transport from the much larger parallel one. In most of the practical 3D cases, where the fields usually exhibit a certain degree of stochastic behavior, it is very difficult to find a rule for ordering the stochastic field lines into a mesh acceptable by the conventional methods. This paper presents a Langevin approach to this problem, which is valid for arbitrarily complex magnetic field structures. First of all, the fluid equations are rearranged, not only for adapting them to the Langevin scheme but also for reasons of numerical stability of the strongly coupled, non-linear system. A Monte Carlo procedure for integrating the Langevin stochastic equations is formulated locally over a finite field line, following a generalized Stratonovich definition. The field-lines required for transport alignment are interpolated from the precalculated ones stored on a 3D mesh by employing a reversible field line mapping technique. The toroidal component of the 3D mesh carries the full magnetic field information, while the choice of the other two components is left free from magnetic fields. All these techniques/methods are integrated into the EMC3 (Edge Monte Carlo 3D) code. As there is no limitation in magnetic structures, the code has been widely applied to magnetic confinement fusion devices, including a wide variety of tokamaks and stellarators. The paper gives a brief introduction to the EMC3 code and shows examples of some applications.

MC simulations and radiation transport in medical physics

Ndimofor Chofor and Björn Poppe, Oldenburg

We shall describe typical applications of Monte Carlo (MC) methods in the computation of radiation transport specifically in the domain of radiotherapy and associated applications to derive quantities of interest such as the deposited energy per unit mass (otherwise known as the dose in Gray [J/Kg]). The suitability of MC in radiation physics is favoured by the stochastic nature of the underlying physical interaction mechanisms involved, thereby requiring the iterative sampling of multiple particle type-dependent variables the most important of which are the particle energy, its position and direction of travel. The complexity of the problem of radiation transport within matter renders analytical solutions to the Boltzmann transport equation very difficult, owed to the assumptions required to limit the transport problem to only a few independent variables. The implementation of sampling by using random numbers, alongside known probability distribution functions of the basic interaction mechanisms would finally lead to a convergence of the result to the true value of the macroscopic quantity of interest under investigation, if sampling is performed over a significantly large number of events.

While the simulation of photon transport is less cumbersome, electron transport is very delicate especially at the boundaries between different media. Besides this, with regard to the multitude of catastrophic events involved in electron interactions, the computation time to achieve low statistical uncertainties may become very large. Typical techniques to circumvent lengthy tracking of electron events shall be described. An example is the condensed history technique entailing the grouping of a number of microscopic transport steps into one fictitious interaction step. To improve efficiency of calculations without compromising the results, typical variance reduction techniques such as range rejection, bremsstrahlung splitting and the Russian Roulette method shall be described. Furthermore, energy thresholds are set for both photons and electrons to values below which the particle is no longer tracked and its energy locally deposited. The proper choice of the cut-off energy significantly affects the simulation time and thereby the overall efficiency, keeping in mind that a significant interaction event may occur below this threshold, depending on the problem under consideration.

The roles of the afore-mentioned techniques shall be highlighted in typical applications in medical radiation physics such as in the simulation of medical linear electron accelerators and dosimetric detector systems. Other MC applications in treatment planning techniques shall also be described, alongside some examples of commercial MC-based systems.

State-of-the-art variance reduction methods for Monte Carlo radiative transfer in atmospheric remote sensing

Robert Buras, TU Mnchen

Remote sensing in a cloudy atmosphere is an inherently three-dimensional problem which is best solved using the Monte Carlo method as radiative transfer (RT) solver. Although generally much slower than analytic one-dimensional RT solvers, the results obtained by Monte Carlo solvers can help quantify the errors made by the 1D approximation, and can even be used to parameterize the 3D effects in retrieval algorithms.

However, scattering of radiation on water droplets and ice crystals is highly anisotropic, which leads to extremely slow convergence of the Monte Carlo results in the absence of variance reduction techniques (VRT).

I will present several VRTs which reduce the computational time of the Monte Carlo RT solver by several orders of magnitude, thereby making the simulation of passive and active remote sensing instruments feasible. Surprisingly, for some 1D applications the accelerated Monte Carlo method yields to be faster than analytic RT solvers.

On Linearisation, Importance Sampling and Adaptive Variance Reduction Techniques Applied to Solutions of Fredholm Integral Equations in Atmospheric Optics

Tim Deutschmann, Heidelberg

The Monte Carlo method in particle transport simulation stems from the context of nuclear reactor physics and was ported to atmospheric optics by G.I. Marchuk in the early 1980s. In comparison with analytical methods, the Monte Carlo method is conceptually simple and is able to describe the underlying physics with arbitrary accuracy.

Radiation transport (RT) in atmospheric optics is described by a Fredholm integral equation of the second kind. In applying the Monte Carlo method to solutions of the RT equation (RTE), sequential importance sampling in combination with the so called local estimate method established itself as the dominant technique. When calculation certain functionals of the RTE the importance sampling technique is applied.

I will show, how importance sampling is used in order to obtain 1st and 2nd derivatives and exact corrections for simulating certain physical details such as the so called vector Ring effect. Furthermore I will give a small outlook how the importance sampling weight fluctuations can be addressed by using a variance reduction technique, the so called weight window method recently developed in nuclear physics.

Uncertainty quantification and going beyond the independent particle approximation

Maria Grazia Pia, INFN Genova

Ultra-cold atom quantum simulators pass first key test

Lode Pollet, LMU Munich

Ultracold atoms trapped by laser beams make artificial materials which can be engineered with a remarkable level of control and tunability. They provide a unique toolbox for emulating the prototypical models of condensed matter physics. Before they can be trusted as quantum simulators, they need to be checked and validated against known results, for which quantum Monte Carlo simulations are ideally suited. I will give a brief overview of the state of the art of quantum simulation for both ultracold bosonic and fermionic systems, starting with time-of-flight interference patterns and single site resolution techniques. I will proceed with a discussion on recent lattice modulation experiments addressing the possible existence of a well-defined amplitude mode in a strongly-interacting two-dimensional superfluid. This mode is a direct analog of the Higgs boson in particle physics. I will conclude by giving a perspective on future directions in simulating strongly correlated fermionic systems.