Invited Talks

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TITLE

From Monte Carlo to Quantum Computation

ABSTRACT

One of the most challenging questions of today, in the overlap of computer science, mathematics, and physics, is the exploration of potential capabilities of quantum computers. Milestones which intensified and enlarged research considerably were the algorithm of Shor [1], who showed that quantum computers could factor large integers efficiently (which is widely believed to be infeasible on classical computers) and the quantum search algorithm of Grover [2], which provides a quadratic speedup over deterministic and randomized classical algorithms of searching a database.

So far research was mainly concentrated on discrete problems like the above and many others one encounters in computer science. Much less is known about computational problems of analysis, including such typical field of application of Monte Carlo methods as high dimensional integration. We seek to understand how well these problems can be solved in the quantum model of computation (that is, on a – hypothetical – quantum computer) and how the outcome compares to the efficiency of deterministic or Monte Carlo algorithms on a classical (i. e. non-quantum) computer.

First steps were made by Novak [3], who considered integration of functions from Hölder spaces. This line of research was continued by the author [4], where quantum algorithms for the integration of L_p-functions and, as a key prerequisite, for the computation of the mean of p-summable sequences were constructed. In [4] a rigorous model of quantum computation for numerical problems was developed, as well. The case of integration of functions from Sobolev spaces is considered in [5], and more on the computation of the mean will be presented in [6]. These papers also established matching lower bounds. A short survey of first results can be found in [7].

Combining these results with previous ones of information-based complexity theory about the best possible ways of solving the respective problems deterministically or by Monte Carlo on classical computers, we are now in a position to fairly well answer the question where quantum computation can provide a speedup in high dimensional integration and where not. We know cases among the above where quantum algorithms yield an exponential speedup over deterministic algorithms and a quadratic speedup over randomized ones (on classical computers). In the present talk I will give an overview about the state of the art in this field.

Moreover, there is a close connection of quantum algorithms with Monte Carlo: While computations are carried out on superpositions of classical states of qubit systems, and thus in high parallelism, the result can only be accessed through a measurement, which destroys the superposition and outputs any one of the superposed states - with a certain probability. Thus, these algorithms are probabilistic, Monte Carlo, while, on the other hand, completely different laws govern the computation. Nevertheless various Monte Carlo techniques can be put into use to construct quantum algorithms (which then, combined with genuine quantum techniques, outperform their classical counterparts). In the talk I will describe and discuss some of these connections.

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Title

Quasi-Regression for Computer Experiments

Abstract

Computer experiments are used for approximating, optimizing and visualizing functions over moderate to high dimensional spaces. The planes we fly in, cars we drive, and the computers we use are designed with extensive computer experimentation, that usually precedes physical experimentation. These functions are usually deterministic, but their complexity and moderately high dimension, invite the use of statistical methods.

The standard methods are based on kriging. They are well suited to settings where the function is expensive to compute and only a few observations may be obtained. But the cost of kriging grows proportionally to the cube of the sample size. For large samples, one spends more computer time processing the data values than generating them.

We propose regression based methods that fit an approximation to the function and interpret the coefficients. In these regressions we can control the distribution of the predictor variables. This allows us to sample in such a way that the X'X matrix in regression has expected value proportional to the identity matrix. The method of quasi-regression (patterned after Chui and Diamond's quasi-interpolation) exploits the known expected value of X'X. Quasi-regression reduces the time and space required for regression on p variables by a factor of p each.

Some example functions are presented. One example is a function of 1,000,000 variables. Using quasi-regression it is possible to investigate the extent to which such a function is nearly linear, with only 90,000 function evaluations.

[1] joint work with Jian An

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Title

The Hartree-Fock Based Diagonalization - an Efficient Algorithm for the Exact Treatment of Many Interacting Disordered Electrons in Solid State Physics

Abstract

The numerical simulation of disordered many-electron systems is one of the most complicated problems in computational solid state physics, because the size of the Hilbert space grows exponentially with the system size. Moreover, due to the presence of disorder the calculation of expectation values or distribution functions of physical quantities requires the simulation of many samples with different disorder configurations. A standard method to treat these systems is the Hartree-Fock (HF) approach reducing the problem to an effective single-particle system, so that rather large systems (> 1000 sites) can be treated. However, the involved approximations are severe and it is difficult to improve them systematically. On the other hand, the application of exact diagonalization schemes to this problem of disordered interacting electrons can provide exact information, but it is feasible only for very small system sizes of, say, up to 20 sites at half filling.

Therefore we have developed an alternative method, the Hartree-Fock based diagonalization (HFD). It is an adaptation of the configuration interaction (CI) approach from quantum chemistry to disordered lattice models. The main idea is to limit the diagonalization of the secular matrix to a restricted Hilbert space which is spanned by the energetically low-lying eigenstates of the HF approximation to the Hamiltonian.

The HFD method proceeds as follows: After solving the HF approximation for, e.g., 32 electrons on 64 sites which is still a non-trivial task, one can easily construct the many-particle states as Slater determinants. However, in contrast to the CI method in quantum chemistry, it is now a difficult task to find (almost) all low-energy many-particles eigenstates. For this purpose we need the most effective combinatorial optimization schemes discussed below. It is then straightforward to transform the Hamiltonian to this basis. The diagonalization of the exact Hamiltonian within this basis is relatively easy, because a system size of a few 1000 basis states has turned out to be sufficient for our purposes. Finally one has to transform the observables to the HF basis and to calculate their values.

[1]joint work with **Thomas Vojta** (Theoretical Physics, Oxford University, Oxford OX3 1NP, U.K., vojta@thphys.ox.ac.uk) and **Arnulf Möbius** (Institut für Festkörper- und Werkstoffforschung Dresden, D-01171 Dresden, Germany, A.Moebius@ifw-dresden.de)

The Monte-Carlo method that we use to find the low-energy states is based on a local search for the minimal energy in the configuration space. In contrast to the usual simulated-annealing method in which it becomes more and more difficult with decreasing temperature to reach different local minima, we apply a thermal cycling, i.e. repeatedly heat and quench with decreasing amplitude, thus considerably improving the performance. An additional performance gain can be achieved using a multi-start local-search algorithm, in which we simultaneously start the search from several local minima on parallel computer architectures. We have further improved the optimization scheme by a so-called iterative partial transcription, merging pairs of solutions by systematically searching in the respective two configurations for corresponding clusters which can be exchanged between the configurations in order to optimize the energy of one of the configurations. We shall demonstrate the efficiency of our combinatorial optimization by an application to a standard example of the traveling salesman problem.

As an example for the application of the HFD method to physical problems, we investigate the quantum Coulomb glass, which models electrons with random potential energies on the sites of a regular lattice, interacting via the long-range Coulomb interaction. We demonstrate the efficiency of the method and the convergence of the calculation in dependence on the basis size. We study the density of states and its decrease near the Fermi energy, the so-called Coulomb gap. We determine the specific heat and investigate, how non-ergodic effects are reflected in the specific heat. We calculate the conductance and analyze its dependence on the strength of the Coulomb interaction for various values of the kinetic energy, i.e. the hopping strength between nearest neighbour sites. In this way we are able to treat a topical problem in mesoscopic physics, namely whether the Coulomb interaction increases or decreases the dc conductance of electrons in disordered systems.

A second example for the application of the HFD method to a problem in condensed matter physics concerns parabolic quantum dots, for which single-electron capacitance-spectroscopy experiments have revealed a peculiar bunching of energy levels in the electron addition spectrum. This means that at certain energies two or more electrons can enter the dot simultaneously which corresponds to a negative chemical potential in contradiction to the picture of single-particle energy levels spread by a homogeneous charging energy. We model the experimental situation by considering a system of up to 50 electrons in two dimensions in a parabolic confinement interacting via a screened Coulomb potential. For the HFD method here it is sufficient to use a basis of 4000 Slater determinants. If the screening is sufficiently strong, we find - in qualitative agreement with the experiment - bunching of energy levels due to an interplay of kinetic and interaction energies, well before reaching the limit of a Wigner crystal. It is interesting to note that the shell structure of classical and quantum-mechanical spatial charge distributions is quite similar.

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Title

Stochastic, Analytic and Numerical Aspects of Coagulation Processes

Abstract

Coagulation of particles (merging of components of different sizes) is a phenomenon observed in many areas of natural science and technology. Examples arise in meteorology (aerosols), chemistry (polymerization) and astrophysics (formation of planets). Mathematically the time evolution of such systems is described by nonlinear integrodifferential equations. In this talk we will address stochastic, analytic and numerical issues related to coagulation processes.

After discussing some applications we introduce the deterministic equations describing the time evolution of average characteristics of coagulating systems. The basic interest of the talk is on Monte Carlo algorithms for the numerical treatment of those equations. First we consider some Markovian stochastic interacting particle system and address the topic of its limiting behaviour for an increasing number of particles. Relative compactness of the sequence of empirical measures of the stochastic system is established, and weak accumulation points are characterized in terms of solutions. Then we discuss the issue of analytic implications of these results. It turns out that the probabilistic limit theorems imply new existence results for the deterministic equations.

Next we address a typical problem of Monte Carlo algorithms, namely variance reduction. The particle system introduced before serves as a direct simulation algorithm for comparison. Alternatively, using a transformation of the basic equation, we derive another stochastic particle system. Numerical investigations show that the new process has better approximation properties, i.e. smaller systematic and statistical error, compared with the direct simulation process. In particular, it allows us to study numerically the gelation (loss of mass) phenomenon.

Honorary Lecture

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TITLE

On the Range Test

ABSTRACT

1. Introduction. The range that was introduced in [1] as a quantitative measure of irregularity of distribution can be used for testing random points [2]. However, many questions related to the range remain unanswered.

2. Definition. Let I denote the interval $0 \le x \le 1$ and I^s — the s-dimensional unit hypercube. Dividing I into 2^m equal parts ($m = 0, 1, 2, \ldots$) we obtain dyadic intervals. A dyadic box Π in I^s is the Cartesian product of s dyadic intervals.

Given a fixed set of points $x^{(1)}, \ldots, x^{(N)}$ in I^s, denote by $S_N(G)$ the number of points $x^{(i)} \in G$ as $1 \le i \le N$. For an arbitrary dyadic partition of I^s into equal dyadic boxes Π_α, $1 \le \alpha \le 2^M$, the numbers $S_N(\Pi_\alpha)$ can be computed. The difference $\max\limits_\alpha S_N(\Pi_\alpha)$ — $\min\limits_\alpha S_N(\Pi_\alpha)$ is a measure of nonuniformity for this partition.

The range $\psi = \psi(x^{(1)}, \ldots, x^{(N)})$ is the upper bound

$$\psi = \sup \left[\max_\alpha S_N(\Pi_\alpha) - \min_\alpha S_N(\Pi_\alpha) \right] \tag{1}$$

extended over all dyadic partitions of I^s.

It can be easily proved that in (1) only a finite number of partitious must be taken into consideration. Clearly, ψ is an integer, $1 \le \psi \le N$.

A very fast subroutine for computing ψ was written by B.V.Shukhman.

3. Ranges in the theory of uniform distribution (u.d.). The range is similar to the classical discrepancy but more crude. An infinite sequence of points $x^{(1)}, x^{(2)}, \ldots$, is u.d. in I^s if and only if at $N \to \infty$

$$\psi(x^{(1)}, \ldots, x^{(N)}) = o(N).$$

In particular, if $x^{(1)}, \ldots, x^{(N)}$ are initial points of an LP_τ - sequence in I^s (also called (τ, s) - sequence in base 2) then

$$\psi(x^{(1)}, \ldots, x^{(N)}) \le 2^\tau.$$

This is the best possible order of growth for all u.d. sequences: $\psi = O(1)$. However, exact minimal values of ψ in I^s are not known.

4. Random ranges. Random variables $\psi_N = \psi(x^{(1)}, \ldots, x^{(N)})$ are called random ranges if $x^{(1)}, \ldots, x^{(N)}$ are independent random points u.d. in I^s. Rather unexpectedly, the probability distributions $P\{\psi_N = i\}$ are not monotone and even cogged.

Table 1. Example: Ten one-dimensional points. $y_i = -\log_{10} P\{\psi_{10} = i\}$.

i	1	2	3	4	5	6	7	8	9	10
y_i	2.47	0.86	0.50	0.49	1.08	0.98	2.19	1.70	4.12	2.71

An explanation for this phenomenon is suggested in [2] but there are no proofs.

A deterministic algotithm for computing $P\{\psi_N = i\}$ was set up but it proved efficient only at $s = 1$ and $N \leq 50$. In all other cases Monte Carlo simulation was applied.

5. Reduced random ranges. Random variables $\xi_N = \psi_N/\sqrt{N}$ are called reduced random ranges. Their possible values are $i/\sqrt{N}$ where $1 \leq i \leq N$. There is much evidence that their probability distributions converge and a limiting probability density $p_s(x)$ exists:

$$\lim_{N\to\infty} P\{\xi_N < x\} = \int_0^x p_s(x)dx.$$

However, this assertion remains unproved. There is only one theorem in this direction.

Theorem. Let G and G' be nonoverlapping regions inside I^s with equal volumes $Vol(G) = Vol(G') = v$. Then as $N \to \infty$ the expectation

$$E\,|S_N(G) - S_N(G')| \sim \sqrt{\frac{4}{\pi} vN}.$$

6. Empirical estimation of $p_s(x)$. Large samples containing millions of ξ_N values were used for constructing histograms. Cogged histograms were avoided by introducing doubled intervals $\Delta x = 2/\sqrt{N}$.

For N exceeding 1000, these histograms were visually indistinguishable. The ones for $N = 50000$ provided approximations for $p_s(x)$. From these approximations percentage points were computed.

7. The range test for pseudorandom numbers. Given a sequence of pseudorandom numbers $\gamma_1, \gamma_2, \ldots$ one can define s-dimensional points $(\gamma_1, \ldots, \gamma_s)$, $(\gamma_{s+1}, \ldots, \gamma_{2s}), \ldots$ and compute ξ_N for increasing sets of N points. The computed ξ_N should be compared with the available percentage points.

Of course, the test should be carried out for dimensions $s = 1, 2, \ldots$. However, the quantiles in [2] are only for $s \leq 4$.

Numerical example. The infamous RANDU generator whose failure in dimension $s = 3$ was already known, was tested.

Table 2. Reduced range values ξ_N for RANDU points

0.01 N	2^{12}	2^{13}	2^{14}	2^{15}	2^{16}	10^5
s=1	1.46	1.35	0.92	1.15	1.24	0.96
s=2	1.98	1.88	1.37	1.71	1.23	1.17
s=3	1.84	2.48	3.18	4.39	6.08	7.37

The 99 % quantiles for these dimensions are 2.60, 2.82 and 2.94.

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Special Sessions

Special Session
Monte Carlo Methods for Linear Algebra and Applications

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V. Alexandrov
Coarse Grained Parallel Monte Carlo Algorithms for Matrix Computations

V. Alexandrov, I. T. Dimov, A. Karaivanova, and C. J. K. Tan
Parallel Monte Carlo Algorithms for Information Retrieval

B. Fathi, B. Liu, and V. Alaxandrov
On the Preconditioned Monte Carlo Methods for Solving Systems of Linear Equations

C. J. K. Tan
Parallel Pseudo-Random Number Generators and Monte Carlo Linear Solvers — Cancelled

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Title

Coarse Grained Parallel Monte Carlo Algorithms for Matrix Computations

Abstract

The problems of solving System of Linear Algebraic Equations (SLAE) and Inverting Matrices (MI) by parallel Monte Carlo numerical methods is considered.

During the past decade this has been an active area of research. We consider Monte Carlo methods for solving SLAE and MI since: **firstly,** only $O(NT)$ steps are required to find an element of the inverse matrix (MI) or component of the solution vector of SLAE (N is a number of chains and T is a measure on the chains length in the stochastic process, which are independent of matrix size n) and **secondly,** the sampling process for stochastic methods is inherently parallel [1, 2, 3, 4].

The method(s) require $O(nNT)$ steps to find the full solution vector or full inverted matrix. Considered Monte Carlo methods for matrix computations can be parallelized efficiently due to the inherent parallelism of the method, e.g. provided that the data are localized through a proper partition of the matrix, all the sampling and computations can be done in parallel [4, 2].

We will consider several Monte Carlo methods: Almost Optimal Monte Carlo method (MAO), Uniform (UM), Monte Carlo with column and row reduction and the Resolvent Monte Carlo method [2]. It will be shown that the execution time for solving SLAE or for MI by Monte Carlo on p processors is bounded by $O(nNT/p)$ (excluding the initial loading of the data). Comparative study of the efficiency of the above methods has been made and the results are reported in this paper. Numerical tests are performed for a number of dense and sparse test matrices using PVM and MPI on a cluster of workstations.

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Title

Parallel Monte Carlo Algorithms for Information Retrieval

Abstract

In any data mining applications, automated text and text and image retrieval of information is needed. This becomes essential with the growth of the Internet and digital libraries. Our approach is based on the Latent Semantic Indexing and the corresponding term-by-document matrix suggested by Berry and his co-authors. Instead of using deterministic methods to find the required number of first "k" singular triplets, we propose a stochastic approach. First we use Monte Carlo method to sample and to build much smaller size term-by-document matrix (e.g. we build $k \times k$ matrix) from where we then find the first "k" triplets using standard deterministic methods. Second we investigate how we can reduce the problem to finding the "k" largest eigenvalues using parallel Monte Carlo methods. We apply these methods to the initial matrix and also to the reduced one.

The algorithms are running on a cluster of workstations under MPI and results of the experiments arising in textual retrieval of Web documents as well as comparison of the stochastic methods proposed will be presented.

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Title

On the Preconditioned Monte Carlo Methods for Solving Systems of Linear Equations

Abstract

A solution of system of linear algebraic equation using Markov Chain Monte Carlo method is considered. It is well known that Monte Carlo methods are efficient for solving large linear system due to the inherent parallelism of the methods and their time complexity. In this paper we investigate how the efficiency of these methods can be improved for more general case of linear system with matrix norm greater than one by suitable decompositions of coefficient matrix A of $Ax = b$, where $A_{n\times n}$ is a nonsingular matrix. First the original system is transferred to an equivalent system in an iterative form $x = Tx + f$, where T satisfies the criteria for convergence of Monte Carlo method. We consider a regular splitting $A = T - C$, where T is lower (upper triangular) or diagonal and $C = T - A$. We then further apply different methods to compress the matrix and annihilate some non-zero elements of the matrix. We consider also two cases when A is diagonally dominant or M-matrix, and we employ either uniform Monte Carlo (UM) or almost optimal Monte Carlo (MAO) methods.

The relevant experiments with dense and sparse matrices are carried out. Comparison of the efficiency of different methods is made.

Special Session
Monte Carlo in Particle Transport

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E. Atanassov, I. Dimov and A. Dubus
A New Weighted Monte Carlo Algorithm for Elastic Electron Backscattering from Surfaces

O. Smidts and M. Magolu monga Made
Transport of Radionuclides in Porous Media: A Double Randomization Technique for the Uncertainty Analysis

M. Marseguerra, E. Padovani, and Sara Pozzi
Simulating the Wrong Physics Can Yield Correct Results

F. Giacobbo, M. Marseguerra, E. Patelli, and E. Zio
Monte Carlo Simulation of the Effects of Different Engineered Barriers on the Diffusion of Radioactive Contaminant

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Title

A New Weighted Monte Carlo Algorithm for Elastic Electron Backscattering from Surfaces

Abstract

When a monoenergetic electron beam is bombarding a solid target, some electrons are emitted from the target with the energy of the incident beam. These electrons are called "elastically backscattered electrons". This elastic electron backscattering effect plays an important role in many experimental techniques, like low-energy electron diffraction, scanning electron microscopy and others. The acronym EPES (Elastic Peak Electron Spectroscopy) corresponds the surface analytical technique based on the measurement of the characteristics of these elastically reflected electrons. Recently, this acronym has been used to denote the particular use of the elastic peak for the experimental determination of electron Inelastic Mean Free Paths (IMFPs) in the solid (these IMFPs are fundamental data for surface analytical techniques like Auger Electron Spectroscopy of X-Ray Photoelectron Spectroscopy). This experimental determination (which is now considered as the most reliable [1]) consists in comparing the measurement to a model calculation in which the IMFP is a parameter. In most cases, for the model calculation, a simple nonanalog Monte Carlo simulation (where the inelastic events are considered as absorptions and taken into account by a weight) is used. In many cases, long computational times are needed (especially when the solid angle of the electron detector is small). In this work we investigate weighted Monte Carlo algorithm with decreased variance. The introduction of additional artificial absorption and the use of randomized quadrature lead to substantially faster computation, especially in the above case. The results of extensive numerical tests are presented and discussed.

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Title

Transport of Radionuclides in Porous Media: A Double Randomization Technique for the Uncertainty Analysis

Abstract

An adjoint Monte Carlo (MC) method for the simulation of radionuclide chain migration in porous media has been recently developed in the context of the performance assessment of HLW repositories in deep geological formation. In this kind of application where uncertainty is omnipresent, the PRA methodology is widely used to estimate the effects of parameters uncertainty through the transport models of radionuclide migration. When a random walk method is used for the transport simulation, it is convenient to use the double randomization technique (DRT) which in essence allows us to optimize computational costs between parameter sampling and transport simulation. The key variable in this optimization is the batch size , the number of random walk per sampling of a parameter set. It has been shown in previous transport simulations with the adjoint MC method that M is moderate and therefore the DRT is efficient for the evaluation of mean concentration of radionuclides. The DRT is however not able to assess with accuracy the higher moments of the concentration distribution and a priori the estimation of distribution tails within accessible computing times. We propose in this paper an improvement of the DRT in which different batch size values (M_T and M_P) are used for the estimations of concentrations in the tail and everywhere else in the distribution. A first MC run and a semi-analytical formula derived from statistical considerations are used to evaluate optimal values of M_T and M_P. The method is applied for the accurate assessment of the probabilities of exceeding given concentration thresholds. The knowledge of these probabilities may be of great importance when regulatory requirements (critical concentration over the geosphere-biosphere interface, or dose in the environment, for instance) are imposed. The generalized DRT will be described and numerical results will be presented.

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Title

Simulating the Wrong Physics Can Yield Correct Results

Abstract

In the Monte Carlo simulation of the transport of particles such as neutrons and photons, the various interactions are generally simulated by considering first the probability of interaction, and then the resulting collision kernel. This approach can be purposely not followed in some large codes, in which, for efficiency reasons, the simulated physics of the single interaction is unphysical. For example, the multiplicity of generated particles can be incorrectly described and certain laws, such as the conservation of energy, can be disregarded. The codes nevertheless provide correct results, but it should be understood that the correctness does not refer to the single history but instead to the average output of a large number of histories. A drawback of such a formulation is that the sequence of the events occurring in a single history is not correctly simulated, and the code cannot be utilized for correlation studies. On the other hand, this approach allows an easy implementation of a biased Monte Carlo simulation. In the present paper one example of this kind is analyzed in detail and the correctness of the results obtained when considering average values is verified.

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Title

Monte Carlo Simulation of the Effects of Different Engineered Barriers on the Diffusion of Radioactive Contaminant

Abstract

In the current conception of permanent deposits for radioactive wastes, the wastes after proper conditioning are trapped within cement matrices placed in special drums. These drums in turn are placed in a concrete container called module in which the space between the drums is back-filled with grout. Through this multiple barrier defense-in-depth design, typical of the nuclear industry, the disposal facility is expected to control the radiological impacts of the wastes by meeting various functional objectives which aim at avoiding the leakage of radionuclides to the environment. Since one of the principal vectors of radioactivity release is water infiltration into the various constituents of the deposit and successive percolation into the groundwater system, it is of utmost importance to study the phenomena of diffusion of radionuclides in the artificial porous matrices hosting the waste and subsequently in the natural rock matrix of the hosting geosphere.

This paper addresses the problem of radionuclides dispersion through the different porous matrices constituting the engineered barriers of the repository. The complexity of the phenomena involved, augmented by the heterogeneity and stochasticity of the media constituting the different layers in which transport occurs, render the classical analytical-numerical approaches scarcely adequate for a close-to-reality modeling. Hence, we propound the use of a Monte Carlo simulation method based on the Kolmogorov and Dmitriev theory of branching stochastic processes. This approach is well suited for treating the transport process though a sequence of different engineered barriers constituted by stochastic porous media.

Special Session
Random Numbers in Monte Carlo and Cryptography

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Pierre L'Ecuyer
What's Up with Uniform Random Number Generation?

Luc Devroye
Recent Trends in Non-Uniform Random Variate Generation

Ueli Maurer
Randomness and Pseudo-Randomness in Cryptography

Karl Entacher
Monte Carlo or Quasi-Monte Carlo? A Strategy to Use Both Methods in a Simultaneous Way

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TITLE

What's Up with Uniform Random Number Generation?

ABSTRACT

This talk gives a brief overview of design principles and some recent developments on uniform random number generators for simulation.

We first recall the main requirements for a good generator (good multidimensional uniformity, high speed, etc.) and theoretical figures of merit that are widely used for certain classes of linear-type generators. As it turns out, small instances of these linear generators, selected on the basis of the same figures of merit, can be used as well as low-discrepancy point sets for quasi-Monte Carlo integration in an arbitrary number of dimensions. We explain this strong connection between RNGs and QMC.

We then examine examples of generators recently proposed in the scientific literature or used in very popular software products such as Excel, Visual Basic, Java standard libraries, etc., and find out, perhaps not surprisingly, that unsafe generators still abound. n particular, the latter generators fail very simple statistical tests with small sample sizes.

The last part of the talk summarizes some recent ideas for constructing fast and reliable generators. We discuss: (a) combined multiple recursive generators with coefficients that are a sum or a difference of a few powers of 2; (b) combined generators whose components are based on linear recurrences modulo 2 (such as Tausworthe, twisted GFSR, etc.); (c) polynomial linear congruential generators with tempering; (d) mixted linear/nonlinear combined generators; (e) and other ideas. Specific examples are given.

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TITLE

Recent Trends in Non-Uniform Random Variate Generation

ABSTRACT

We review some recent results in non-uniform random variate generation, and highlight some remaining open problems. We will discuss in particular random variate generation when the distributions are specified indirectly, e.g., as solutions of distributionsl identities, or when the distributions cannot be computed in finite time, e.g., when densities are given as infinite sums or indefinite integrals.

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Title

Randomness and Pseudo-Randomness in Cryptography

Abstract

Randomness is of crucial importance in cryptography, in particular for the generation of cryptographic keys and system parameters. Moreover, many cryptographic protocols are probabilistic, involving freshly generated random values. The requirement for a cryptographic random generator is that its output should be highly unpredictable. Unpredictability can be captured using information-theoretic concepts like entropy. This should be reflected in the statistical tests used for testing cryptographic random generators.

Like in many other applications, in cryptography random values are often generated in a pseudo-random manner, derived from a short secret seed. Pseudo-randomness and indistinguishability are central concept in cryptography, where one considers not only pseudo-random number generators, but also pseudo-random functions and other pseudo-random systems. A system is pseudo-random if it cannot efficiently be distinguished from a corresponding random system, i.e., roughly speaking, if there exists no efficient algorithm, interacting with the system, such that the algorithm behaves noticeably differently if the pseudo-random is replaced by a truly random system.

After a brief introduction to cryptography and its applications, we discuss statistical randomness tests for cryptography and the definitions of pseudo-randomness and indistinguishability, contrasting the cryptographic view with that taken in the Monte Carlo simulation community. A few constructions of cryptographic pseudo-random generators and pseudo-random functions are discussed, together with some techniques used in security proofs.

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Title

Monte Carlo or Quasi-Monte Carlo? A Strategy to Use Both Methods in a Simultaneous Way.

Abstract

Among many other applications, Monte Carlo (MC) methods provide a very efficient and reliable technique for numerical quadrature of high-dimensional integrals by computing the average of the integrand over some point set P.

For randomly chosen point sets, consisting of N points in the standard domain $[0,1[^s$ for instance, we may expect the classical Monte Carlo error $O(1/\sqrt{N})$ for the approximation.

A modern approach, the so-called Quasi-Monte Carlo (QMC) method tries to decrease this error by choosing the point sets more evenly distributed than pseudo-random numbers used in MC. Such *quasi*-random points[1], in general, provide an improved integration error bound $O((\log N)^{s-1}/N)$.

But for explicit applications, the real error obviously depends on several additional factors such as the regularity of the integrand, the constants in the $O()$ term, the the dimension s or the maximally computable sample size N. For more detailed discussions and references see the monographs [1, 2, 3, 4].

Our presentation is directed to users which do not have any knowledge about the structural behavior or regularity of their integrands and simply want to try both methods in comparison.

We demonstrate an easy way to use MC and QMC *simultaneously* by using classical linear random number generators (LCGs). Our strategy is based on the basic property of LCGs; namely, that all overlapping s-dimensional vectors, generated from certain LCGs, provide classical QMC point sets, so-called *integration lattices*. Therefore, one easily may apply LCGs with *varying* periods in order to get a steady transition from MC point sets to QMC points.

We apply the latter approach to different types of integrands and demonstrate the behavior of the resulting integration error. Our results provide interesting insights concerning differences between MC and QMC integration, and additional information on the maximal sample size

[1]The term quasi-random is misleading, since such point sets show absolutely no "random" behavior. They are deterministically constructed in order to get low measures of uniform distribution such as *discrepancy*. Therefore the term low-discrepancy point sets or - sequences is used and deems us more appropriate.

which can be used from a LCG in order to get reliable MC simulations. A sophisticated method to obtain the necessary parameters for the LCGs implementation used in our strategy will be presented as well.

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Special Session
Monte Carlo Methods in Computer Graphics

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Philippe Bekaert
Stochastic Relaxation Methods for Radiosity

Francesc Castro and Mateu Sbert
Distributed Multi Path using Transmittances

Ferenc Csonka, György Antal and László Szirmay-Kalos
Cost-driven Multiple Importance Sampling in Monte-Carlo Rendering

Dirk Ormoneit, Christiane Lemieux and David J. Fleet
Lattice Particle Filters

Alexander Keller
Consequences of Interleaved Sampling

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Title

Stochastic Relaxation Methods for Radiosity

Abstract

The radiosity method in computer graphics is a finite element method for computing the diffuse illumination in a scene. It leads to very large systems of linear equations, with coefficients that contain non-trivial 4-dimensional integrals called form factors. The resulting linear systems are generally solved using relaxation algorithms, such as Jacobi, Gauss-Seidel or Southwell iterations.

Each iteration of such a relaxation algorithm basically consists of a matrix-vector product, or in other words, a number of sums. Monte Carlo estimation of these matrix-vector products then yields a corresponding stochastic relaxation algorithm. In the context of radiosity, the form factors form a probability distribution which can be sampled easily and so are a natural choice.

Stochastic relaxation methods for radiosity have been proposed by different authors in the last 10 years. In this talk, an overview of these methods will be presented and their time complexity analyzed. They will be compared with random walk methods for linear systems. Finally, variance reduction techniques will be discussed.

Francesc Castro
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Title

Distributed Multi Path using Transmittances

Abstract

The Multipath method is a Monte Carlo technique that solves the radiosity problem, i.e. the illumination in a scene with diffuse surfaces. Uniformly distributed "global" lines intersect the scene and the so created intersection lists are used to simulate simultaneous random paths.

The new approach we propose here is based on the subdivision of a complex scene in a hierarchy of subscenes. It allows the execution of the Multipath algorithm not only in the context of the whole scene (it will be called external Multipath) but also in the context of the subscenes (internal Multipath). This distribution could allow the parallelization of the method.

Each subscene will be bounded by a box where each face will be subdivided in a grid of virtual patches and hemispherical regions that will act as accumulators of undistributed incoming and outgoing power. We will be able to establish an alternance of internal and external executions that will iterate until the undistributed power is low enough.

The cost of this method will be dramatically reduced by computing only once the intersections for each subscene. These intersections will be saved in external files and so they will be used once and again by simply reading these files.

Finally, the obtained intersections for each subscene allow the easy computation of the transmittance for each virtual region, that is, the fraction of power that will be able to cross the subscene in this direction. Transmittances will be used to accelerate the first shot, i.e. direct illumination from the sources, and also the external Multipath.

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Title

Cost-driven Multiple Importance Sampling in Monte Carlo Rendering

Abstract

The global illumination problem results in a Fredholm type integral equation that can be solved by Monte Carlo techniques. The variance of the Monte Carlo estimator can be significantly reduced by drawing samples from several distributions and combining them according to predefined weights. This variance reduction technique is called *multiple importance sampling*. In the rendering literature several strategies were proposed for optimally combining different sampling techniques, but the costs of individual methods were neglected. In this paper we develop a more general approach that takes into account the costs of the methods to be combined as well. The approach is used to combine very different global illumination techniques: bidirectional path tracing and ray-bundle iteration. We conclude that our methods offer manageable error control for multi-pass algorithms.

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Title

Lattice Particle Filters

Abstract

A promising approach to approximate inference in state-space models is particle filtering. However, the performance of particle filters often varies significantly due to their stochastic nature. We present a class of algorithms, called lattice particle filters, that circumvent this difficulty by placing the particles deterministically according to a quasi-Monte Carlo integration rule. We describe a practical realization of this idea, discuss its theoretical properties, and its efficiency. Experimental results with a synthetic 2D tracking problem show that the lattice particle filter is equivalent to a conventional particle filter that has between 10 and 60% more particles, depending on their "sparsity" in the state-space. We also present results on inferring 3D human motion from moving light displays.

Alexander Keller
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Title

Consequences of Interleaved Sampling

Abstract

Interleaved sampling is a special case of the method of dependent tests. It interleaves regular grids by using low-discrepancy points as offsets. While the global grid structures allow for highly efficient implementations, the local low discrepancy guarantees for fast convergence.

Applied to classical rendering algorithms, interleaved sampling improves the local spectral properties by spreading out aliasing artifacts so that they become imperceptible.

We present how the application of $(0, m, s)$-nets and $(0, s)$-sequences to interleaved sampling and dependent splitting increases the efficiency of the rendering algorithms ray tracing, ray casting, and hardware rasterization and how it improves the visual quality as compared to previous approaches. A highly coherent parallel implementation in soft- and hardware is intrinsic to the approach.

Special Session
Monte Carlo Simulation of Semiconductor Structures and Devices

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P. Bordone, A. Bertoni, R. Brunetti, and C. Jacoboni
Monte Carlo Simulation of Quantum Electron Transport Based on Wigner Paths

M. Fischetti and S. Laux
Semiclassical Monte Carlo Simulation of Long-Range Coulomb Interactions in Semiconductors: Performance Degradation of Small Silicon Devices — Cancelled

C. Jungemann and B. Meinerzhagen
Modeling of the Stochastic Noise of Monte Carlo Device Simulations

M. Nedjalkov, H. Kosina and S. Selberherr
Monte Carlo Algorithms for Stationary Device Simulation

C. Pennetta and L. Reggiani
Monte Carlo Simulation of Electromigration Phenomena in Metallic Lines

U. Ravaioli
Monte Carlo Simulation of Charge Transport in Nanostructures — Shifted to Special Session on Quantum Monte Carlo Methods

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Title

Monte Carlo Simulation of Quantum Electron Transport Based on Wigner Paths

Abstract

Advancements and improvements in the Wigner-function approach to quantum electron transport are presented.

The Wigner formulation of quantum mechanics based on the concept of Wigner function (WF) is particularly suitable for the study of quantum transport in mesoscopic systems since it allows to describe quantum mechanical effects using a function defined in a (**r**,**p**) "phase space", in analogy with what is done for classical systems. Furthermore Wigner paths (WP's) in this phase space can be defined that provide a pictorial representation of the quantum evolution of the system of interest and constitute a useful tool for numerical solutions of the quantum transport equation [1].

The dynamical equation for the WF f_w for an electron subject to a constant or harmonic force **F**, to a potential profile $V(\mathbf{r})$ and to the interaction with phonons, is

$$\frac{\partial}{\partial t} f_w + \frac{\mathbf{p}}{m} \nabla f_w + \mathbf{F} \nabla_p f_w = \frac{1}{(2\pi\hbar)^3} \int d\mathbf{p}' \, \mathcal{V}_w(\mathbf{r}, \mathbf{p} - \mathbf{p}') f_w(\mathbf{r}, \mathbf{p}') + \Xi\left(f_w, \mathbf{r}, \mathbf{p}, \{n_q\}, t\right) \tag{1}$$

where

$$\mathcal{V}_w(\mathbf{r}, \mathbf{p}) = \frac{1}{i\hbar} \int d\mathbf{r}' e^{-i\mathbf{p}\cdot\mathbf{r}'/\hbar} \left[V\left(\mathbf{r} + \frac{\mathbf{r}'}{2}\right) - V\left(\mathbf{r} - \frac{\mathbf{r}'}{2}\right) \right], \tag{2}$$

$\Xi\left(\mathbf{r}, \mathbf{p}, \{n_q\}, t\right)$ is the term including the electron-phonon scattering, depending linearly on f_w, and $\{n_q\}$ is the set of phonon occupation numbers [1].

WP's are based on the linearity of such evolution equation with respect to f_w, and are defined as the path followed by a "simulative particle" carrying a δ-contribution of the Wigner

function through the Wigner phase-space, and are formed by ballistic free flights separated by scattering processes (both scattering with phonons and with an arbitrary potential profile can be included), as for the case of semiclassical particles. Thus, the integral transport equation (1) can be solved by a Monte Carlo (MC) technique by means of simulative particles following classical trajectories, in complete analogy to the "Weighted Monte Carlo" solution of the Boltzmann equation in the integral form. More precisely, the solution of the Wigner equation is obtained as a sum of contributions calculated along WP's formed by ballistic fragments, described by classical dynamics, separated by interaction vertices due to electron-phonon or potential interaction. The absorption or emission of a phonon corresponds to two interaction vertices. Each of them transfers half of the phonon momentum to the electron. The energy conservation of the semiclassical theory is recovered when sufficient interference among the contributions to the Wigner function coming from all possible paths is established. This interference is disturbed by the occurrence of other scattering vertices between the two vertices of a given phonon scattering (collisional broadening). The authors have developed a MC code based on the above described concepts, in strict analogy with the traditional MC simulation technique used to study semiclassical transport phenomena. So far such a code has been used to simulate quantum transport in homogeneous semiconductors including carrier-phonon scattering. Our rigorous quantum approach allows to analyze in detail real scatterings, virtual scatterings, multiple scatterings, and the so called "intra-collision" field effect. Up to now, due to computational time problems, results have been obtained for times of the order of 100 fs, for which only paths including two phonon scatterings at most can contribute. Comparison have been performed with the outcomes of a code based on a traditional weighted MC algorithm. In particular the effect on transport phenomena of the relaxation of the semiclassical assumption of energy conservation and point-like nature in space time of the scattering processes has been analyzed [2].

Since the above mentioned MC approach is based on the simulation of a number of WP's, where the larger is the number of paths accounted for, the better is the statistical precision achieved, the main limitation to an extensive application of the method has been, so far, the simulation times required to obtain reliable results. To improve the efficiency of the code we are developing a numerical algorithm that includes the quantum self-scattering mechanism [3]. This method is based on the introduction of an appropriate imaginary part of the self-energy $\Gamma = 1/\tau_\circ$ which plays a role analogous to that of the maximum scattering rate in the traditional MC method. At each perturbative order the exact correction to Γ is evaluated. Let us define

$$\tilde{f}_w\left(\boldsymbol{r}, \boldsymbol{p}, \{n_q\}, t\right) = e^{\Gamma(t-t_\circ)} f_w\left(\boldsymbol{r}, \boldsymbol{p}, \{n_q\}, t\right), \tag{3}$$

performing the derivative with respect to time we get

$$\frac{\partial}{\partial t} f_w = -\Gamma e^{-\Gamma(t-t_\circ)} \tilde{f}_w + e^{-\Gamma(t-t_\circ)} \frac{\partial}{\partial t} \tilde{f}_w \,. \tag{4}$$

Substituting Eq.(4) into Eq.(1) and using Eq.(3) leads to

$$\frac{\partial}{\partial t} \tilde{f}_w + \frac{\boldsymbol{p}}{m} \nabla \tilde{f}_w + \mathbf{F} \nabla_p \tilde{f}_w = \frac{1}{(2\pi\hbar)^3} \int d\boldsymbol{p}' \mathcal{V}_w(\boldsymbol{r}, \boldsymbol{p} - \boldsymbol{p}') \tilde{f}_w(\boldsymbol{r}, \boldsymbol{p}') + \Xi\left(\tilde{f}_w\right) + \Gamma \tilde{f}_w \tag{5}$$

where the introduction of the exponential factor brings about an additional interaction mechanism, with a constant coupling Γ. The WP's method is then applied to Eq.(3). This new

algorithm makes possible the inclusion in the simulation of a higher number of electron-phonon scattering events, thus allowing to reach longer and physically more significant simulation times.

The treatment of the scattering of the carriers with the potential profile has proved to be another crucial point of our approach. In fact, simply considering the potential as an additional scattering mechanism to be tackled with a full perturbative approach leads to such a computational burden that it has been impossible, so far, to simulate realistic potential profile. To simplify this problem we have developed a method that allows to separate the effect of the classical force from quantum corrections. It is well known that the effect of a potential $V(\mathbf{r})$ in the Wigner equation, given by the integral term of the type in Eq.(1), reduces to the classical-force term on the left hand side of the Wigner equation for potentials up to quadratic. In the general case, it is possible to separate the effect of the classical force from quantum corrections by defining the quantity

$$\tilde{V}(\mathbf{r}, \mathbf{r}') = V\left(\mathbf{r} + \mathbf{r}'\right) - \nabla V(\mathbf{r}) \cdot \mathbf{r}' \,.$$

Now the dynamical equation for the Wigner function becomes

$$\frac{\partial f_w}{\partial t} + \frac{\mathbf{p}}{m}\nabla f_w + \mathbf{F}\nabla_p f_w(\mathbf{r}, \mathbf{p}) = \frac{1}{(2\pi\hbar)^3}\int d\mathbf{p}'\, \tilde{\mathcal{V}}_w(\mathbf{r}, \mathbf{p} - \mathbf{p}') f_w(\mathbf{r}, \mathbf{p}') + \Xi\left(\mathbf{r}, \mathbf{p}, \{n_q\}, t\right) \,, \tag{6}$$

where $\mathbf{F} = -\nabla V(\mathbf{r})$ is the classical force, and $\tilde{\mathcal{V}}_w(\mathbf{r}, \mathbf{p})$, the usual integral kernel with $\tilde{V}$ in place of V, is a term including only quantum corrections to the classical orbits. The inclusion of Eq.(6) in the above described MC algorithm is at present under development.

The WP's method has also been extended to the case of a two-time Wigner function. A MC approach based on the generation of WP's (analogous to the one realized for the single-time Wigner function) has been developed. The only difference with the algorithm discussed above is that, in the sequence of random choices and operations which define a particular path, at each electron-phonon interaction vertex half of the phonon frequency (besides half of the phonon momentum) is either added or subtracted to the electron energy. Since energy is not exactly conserved in the scattering process, momentum and energy are now independent variables. Results have been obtained for electrons subject to the action of an external field and in presence of scattering with optical phonons.

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Title

Modeling of the Stochastic Noise of Monte Carlo Device Simulations

Abstract

Device modeling by the comprehensive Monte Carlo (MC) method becomes more and more important due to the increasing impact of hot-electron effects caused by the aggressive scaling of microelectronics. On the other hand, application of the MC method in a TCAD framework is difficult because of the stochastic nature of the MC results and an automatic error control is required. In addition, the MC method is very CPU intensive and more efficient simulation methods should be developed. This necessitates a thoroughgoing analysis of the properties of the stochastic noise of the MC method, because otherwise misleading or even erroneous results might be obtained as shown below.

The methods required for the modeling of stochastic noise are similar to the methods used for electronic noise modeling and in this work it will be shown how these methods can be utilized to analyze the stochastic noise of stationary MC device simulations. A CPU efficient Langevin-type drift-diffusion (LDD) model is derived from the Boltzmann-Langevin equation on which the analysis will be based. The accuracy of this approach is checked by a comparison with MC device simulations. The result of an LDD simulation is the spectral intensity of the stochastic variables and the relationship between the spectral intensities and the stochastic error (variance of the time average) of the corresponding MC variables is outlined allowing to develop guidelines for automatic error control.

Based on the above methods the efficiency of two different terminal current estimators, the Ramo-Shockley theorem and the so-called variance-minimizing estimator by Yoder et al., is analyzed. It turns out that the variance-minimizing estimator is not more efficient than the Ramo-Shockley theorem, although apparently the current fluctuations are reduced. Moreover, it is shown that the intuitive concept of high and low noise regions in a device with respect to current is wrong. In the same sense spatially smooth results do not necessarily imply a low variance.

Previously it has been shown by MC simulations that nonself-consistent device simulations with respect to the electric field are not as efficient as self-consistent ones. An analysis based on the LDD model shows that the efficiency of both methods is the same, while the frequency dependencies of the spectral intensities strongly differ. These different frequency dependencies indicate that certain characteristic relaxation times in the nonself-consistent case are orders

of magnitude larger than in the self-consistent case necessitating orders of magnitude longer simulations. The reason for the deviating MC results seems to be a too short simulation time during which the low-frequency limit was not reached, resulting in a spurious overestimation of the current noise. In the case of the particle density the unexpected result is found that the self-consistent method is more efficient.

In the case of the particle density also the impact of statistical enhancement is investigated. The simulation particle density is modified by a population control method in such a way that the number of simulation particles in a region with a low real particle density is increased. This effect is modeled in the LDD model by adjusting the relative particle weight in the local noise source. This does not account for the noise and correlation introduced by the particle splitting procedure of the population control method. Comparison of the LDD and MC model reveals that the efficiency of the population control method is degraded by the correlation after the particle splitting and the reduction in the variance is less than the increase in the number of simulation particles.

These results clearly demonstrate the need for a proper noise analysis in order to avoid misleading results.

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Title

Monte Carlo Algorithms for Stationary Device Simulation

Abstract

The Monte Carlo (MC) method for simulation of semi-classical transport in semiconductors evolved for more than three decades to meet the challenges in the research and development of new semiconductor devices. The main MC algorithms used to date were initially devised from merely physical considerations, viewing the method as a direct emulation of the elementary events underlying the transport process. Later it has been proved that these algorithms implicitly solve the equation governing semi-classical transport, namely the Boltzmann equation (BE). The ensemble MC algorithm (EMC) simulates an ensemble of test particles assuming physically-based probability distributions. The ensemble is simulated starting from a given initial distribution until some final distribution is reached at the selected evolution time. The physical quantities are obtained as ensemble averages taken at the end of the simulation so that the algorithm is appropriate for transient phenomena.

Especially designed for stationary simulations is the single-particle MC algorithm (SPMC), which is the subject this work. The algorithm relies on the ergodicity of the stationary process allowing to replace the ensemble average by a time average. Then a single test particle can be followed and the averages are recorded during the whole time of simulation. The time recording technique estimates the distribution in a phase space domain Ω by the relative time spent by the particle in Ω. Using the before-scattering technique, averages are formed by sampling the trajectory at the end of each free flight.

The alternative way to use the BE explicitly and to formulate stochastic algorithms for its solution initiated one decade ago [1][2]. The integral form of the transient BE and its conjugate equation have been approached by numerical MC methods for solving integrals and integral equations. As applied to the BE, the approach yields a MC backward algorithm. The simulation follows the natural evolution back in time until the initial time is reached. The conjugate equation gives rise to the EMC and the weighted EMC algorithms. In the latter the probabilities of the natural events are biased to guide the particles towards the region of interest, making numerical trajectories differ from the natural ones [2]. Each test

[1]This work has been partly supported by the IST program, project NANOTCAD, IST-1999-10828.

particle gives a single realization of the random variable θ which samples a desired physical quantity.

This work addresses the extension of the approach to stationary transport, formulated as a stationary boundary value problem [3]. The boundary conditions provide not only the free term of the integral form of the BE, but also affect the kernel. It is proved that the boundary conditions guarantee a unique solution. A backward stationary MC algorithm is derived in analogy with its transient counterpart, with the difference being that the backward simulation continues in a variable time interval, until the boundary is reached. The forward stationary MC algorithm offers more peculiar results. The derivation of the conjugate equation gives an additional time integration in the iteration terms as compared to the transient case. The extra time integral allows to derive both the before-scattering and time integration methods for average recording. Moreover, it proves the ergodicity of the stationary transport process. In the iteration terms a velocity weighted boundary distribution appears. Injection from the boundaries must be chosen according the product of the velocity and the distribution function imposed on the boundaries.

An independent realization of the random variable θ is related to a complete numerical trajectory that starts and terminates at the boundary. Therefore, the SPMC algorithm can interpreted to simulate a regenerative stationary process [5]. A new variance estimation method is proposed [4], which avoids the commonly assumed separation of the particle's history into sub-histories with artificially predefined duration.

A weighted SPMC algorithm has been developed, which biases the probabilities for phonon emission and absorption to create artificial carrier heating and the scattering angle to introduce artificial carrier diffusion. The experiments show that event biasing is a competitive statistical enhancement technique. It can be applied by its own or in combination with other variance reduction techniques.

Finally, an application of the approach to small signal analysis is discussed. Both existing and a variety of new stationary MC algorithms are obtained in a unified way and the physical explanation of the algorithms is supported [6].

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Title

Monte Carlo Simulation of Electromigration Phenomena in Metallic Lines

Abstract

Electromigration (EM) arises in a metallic line from the transport of matter at an atomic level due to the flow of a stressing electronic current (electron wind) [1]. The consequent growth of voids and hillocks is responsible for the electrical degradation and the final breakdown of the line, i.e. an irreversible modification of its electrical resistance. In to-date micro and nanoelectronics, the importance of EM is associated with the issue of device reliability. Indeed, EM is a relevant source of degradation towards electrical breakdown of metallic interconnects and in turn of the whole device.

The theoretical approaches of EM phenomena in interconnects are mostly based on microscopic deterministic models describing the transport of ions due to the combined action of electrical, thermal, and mechanical forces. These models require a detailed knowledge of the physical mechanisms responsible for the transport of matter. However, in doing so the stochastic character of macroscopic measurements, such as the sample to sample difference of the resistance evolution under current stress of a set of identical specimens and the associated time to failure distribution are missed. Alternatively, the use of stochastic models, like Monte Carlo simulators at a kinetic level, or of other statistical approaches, was proven to reproduce the statistical features associated with the distribution of the times to failure, one of the crucial quantity to be understood.

Actually, the final failure is reached by adding the effects of many different parameters, including temperature, current density, mechanical stress, compositional and geometrical variations, which can hardly be taken in full account at the same time in a deterministic model. Moreover, to assess the reliability of a device one is more interested in the time to failure rather than in the variation of a specific parameter, for instance the line resistance. Therefore, the relation between the smooth evolution of the resistance occurring on a long time scale and the abrupt failure occurring within a very short time scale is a key point that remains largely an unsolved problem.

The aim of this paper is to address this issue by presenting a stochastic approach which simulates EM damages in metallic interconnects in terms of a percolative process in a random

[1]The research is developed within the STATE project supported by the INFM.

resistor network [2][3]. Making use of Monte Carlo simulations, the effects associated with the transport of mass are accounted for by the stochastic generation and recovery of voids driven by a stressing current. As a consequence, we succeed in providing simultaneously the smooth and catastrophic behaviors of a typical resistance evolution. This approach has the inherent novelty of exhibiting specific stochastic features during both degradation and recovery processes associated with a current stress. Accordingly, most of the experimental features are naturally explained. These include the phenomenological laws used to interpret the median time to failure, and the existence of a threshold current for the onset of EM. Furthermore, most of the compositional effects acting during the early stages of EM in Al alloys [1] are reproduced. The importance of recovery processes is emphasized for the two relevant cases of defect healing during EM damage and transient compositional effects associated with Joule heating. The reproduction of the general features exhibited by the resistance evolution of Al-0.5%Cu and Al-1%Si lines supports the physical background of the proposed approach. The simulations enable us to investigate within a unified theoretical framework a variety of relevant aspects of EM degradation as: damage patterns, the distribution of the time to failures, early stage resistance degradations in the presence of compositional effects, peculiarities related to Black's laws, geometrical effects etc. Remarkably, the approach enables one to look for the existence of scaling relations which would open the possibility of predicting the failure time of a metallic line from the knowledge of the early time evolution of its resistance.

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Title

Monte Carlo Simulation of Charge Transport in Nanostructures

Abstract

The size of semiconductor devices has been scaled down to nanoscale dimensions, where ballistic and quantum effects start to appear. As MOSFET approach the end of the industry roadmap, it is likely that standard integrated devices will present a mixture of semi-classical and quantum transport at normal operation temperatures. Full quantum approaches are computationally expensive, and in many cases still too immature to provide a sufficiently complete physical model for practical applications as needed in the near term. Monte Carlo particle simulation, on the other hand, is based on semi-classical models, but it has a number distinct advantages over any other type of approach. Because of its particle nature, a Monte Carlo simulation can naturally include doping granularity and fluctuations when appropriate techniques for charge-charge interaction are applied. In addition, the particle behavior can be corrected to follow the overall quantum effects in the system, providing in certain regions an ensemble average of classical trajectories that overall approach the quantum behavior.

Detailed charge-charge (carrier-carrier, carrier-ion) interaction can be evaluated following a number of approaches. In our 3-D code development we have chosen to implement the particle-particle particle-mesh (P3M) approach, because it seems to offer a good trade-off between computational efficiency and accuracy. Solution of Poisson equation provides the "long-range" part of interaction, down to mesh resolution. Within a certain radius around each particles, direct "short-range" coulomb interaction is also evaluated. Since the interaction radius has to be chosen necessarily to span several meshes in each direction, there is an overlap between the particle-mesh and the particle-particle domains, where double counting of the interaction takes place. The so-called reference force is introduced to remove the double counting and this force can be calculated in practice by assuming that the charge of the particle under examination extends like a cloud over the short-range spherical domain. This approach allows one to introduce granular doping by placing individual ion in arbitrary positions, and dealing with force evaluation as it they were mobile particles. Tests have shown that in this way it is possible to evaluate properly the ionized-impurity interaction giving correct mobilities in silicon, which is somewhat problematic when scattering rates are used, particularly at high dopings. The effects of carrier-carrier interaction on the high-energy tail on the distribution function can also be evaluated with this procedure.

In very small silicon structures at normal temperatures it is appealing to deal with quantum effects by introducing quantum correction that modify the potential seen by the carrier. In

this way it is possible to deal with size quantization and with tunneling through single barriers, without changing the semi-classical nature of the simulation. This is important from a practical point of view, since it is always problematic to accomplish coupling between regions where semi-classical (e.g. contacts) or quantum simulation (e.g. channel) are conducted separately. Test simulations have been conducted for a number of cases. We obtained a basic hierarchy of quantum corrections directly from the Wigner transport equation, by truncating the interaction expansion to first order, yielding a transport equation which closely resembles the Boltzmann equation. In this form, certain features of the complete quantum model are lost. For instance, the distribution function is always positive, while it is well known that under interference conditions the Wigner distribution function may assume negative values. The quantum correction consists in an additional force that modifies the electrostatic potential. To test this approach, the model was applied to the case of a 1-D MOS capacitor structure. The MOS capacitor is the basic building block of MOSFET devices, where size quantization takes place in the quantum well created by the gate potential at the silicon dioxide interface. A classical solution of the MOS capacitor in inversion results in a maximum of the charge concentration at the oxide interface. The quantum correction applied to a semiclassical simulation modifies the potential energy, so that on the average the particles are not as close to the interface. Simulations clearly show that the quantum correction prevents the otherwise classical particles from falling to energy states forbidden by the quantization, thus reshaping the potential energy so that the particle ensemble mimic the overall quantum behavior. The maximum of the charge density is now shifted from the interface. Similar simulations applied to MOS structures in accumulation regime give also good results that can fit well quantum solutions obtained with self-consistent Schrdinger equation. The approach has been carried over to a 2-D MOS Monte Carlo simulator. Here, other issues are at play. First, there are problems with noise in the potential averaging to obtain the correction. Second, one has to take into account interface roughness scattering in a manner consistent with the quantum correction model. The talk will deal with these issues and present an approach that should provide a reasonable solution. Other computational experiments will also be shown for tunneling through barriers in III-V compound heterojunction systems. Here, the quantum correction lowers and smoothes out the potential barrier, to allow more particles to traverse the heterointerface. Typically, simulation of these systems also present size quantization effects in the well formed before the barrier by self-consistency under a bias. The quantum corrected Monte Carlo approach gives a satisfactory and practical representation of this effect.

Monte Carlo simulation has also potential application for transport in molecular nanostructures. For instance, ionic channels are being actively investigated because they behave as nanotube devices and could be used for a variety of sensing applications. One of the goals is to implant ionic channels on the gate of MOS structures, to create hybrid semiconductor/molecular sensors. In this case, the actual medium is the water solution in which the channel is immersed, and the transport of ions can be treated with very similar Monte Carlo procedure as used in semiconductor devices. An active area of investigation is the inclusion of effects of finite ion size in the transport, since the radius of the ion may be comparable with the size of the channel opening. The talk will give a glimpse on future applications and if time allows recent developments will be discussed.

Special Session
Monte Carlo and Quasi-Monte Carlo Methods in Finance

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Michael Fu
Pricing American-Style Options: A Comparison of Monte Carlo Approaches.

Martin Predota
Quasi-Monte Carlo Methods for Option Pricing in the Hyperbolic Model

Jin-Chuan Duan, Genevive Gauthier and Jean-Guy Simonato
Numerical Pricing of Contingent Claims on Multiple Assets and/or Factors: A Low-Discrepancy Markov Chain Approach

Giray Oekten
A Numerical Comparison of Some Randomized Quasi-Monte Carlo Methods in Pricing Complex Securities — Cancelled

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TITLE

Pricing American-Style Options: A Comparison of Monte Carlo Approaches.

ABSTRACT

A number of Monte Carlo simulation-based approaches have been proposed within the past decade to address the problem of pricing American-style derivatives. We report some results from empirically testing some of these algorithms on a common set of problems in order to be able to assess the strengths and weaknesses of each approach as a function of the problem characteristics. The algorithms considered include the simulated trees method and stochastic mesh method of Broadie/Glasserman, the least-squares regression approach of Longstaff/Schwartz, the dynamic-programming approaches of Grants/
Vora/Weeks and Tilley, and our method, which parameterizes the early exercise curve and casts the valuation problem as an optimization problem of maximizing the expected payoff (under the martingale measure) with respect to the associated parameters. Derivatives considered include various American/Bermudan options on a single asset and on multiple assets (max option) and Asian-American options

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Title

Quasi-Monte Carlo Methods for Option Pricing in the Hyperbolic Model

Abstract

Asian options, i.e. options whose payoff is based on the average of daily stock prices, play an important role in financial markets. Since the payoff is path-dependent, it is not possible to evaluate their prices analytically in most cases. Thus one has to use numerical simulation methods. Empirical analysis of stock prices (see Eberlein and Keller 1995) shows that hyperbolic distributions, a subclass of generalized hyperbolic distributions, which were introduced by Barndorff-Nielsen (1977), allow a more realistic description of log-returns than the classical Gaussian model. The hyperbolic is an incomplete market model, hence option prices are not unique. One possibility is to calculate prices via the so-called Esscher-measure (see Gerber and Shiu, 1994). Using Monte Carlo and quasi-Monte Carlo methods we simulate Asian option prices based on the hyperbolic model and compare our results with the classical normal model (see e.g. Kemna and Vorst, 1990). The talk is based on joint work with Gerhard Larcher and Robert Tichy.

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Title

Numerical Pricing of Contingent Claims on Multiple Assets and/or Factors: A Low-Discrepancy Markov Chain Approach

Abstract

We develop a Markov chain pricing method capable of handling several state variables. The Markov chain construction of Duan and Simonato (2000) is modified so that higher-dimensional valuation problems can be dealt with. Their design relied on a Cartesian product, which grows in a power fashion as the number of assets/factors increases. We use a multi-dimensional low-discrepancy sequence as the building block for constructing the Markov chain in order to take advantage of the high degree of uniformity inherent in such sequences. Our design contains two critical components. First, we have devised a way of computing analytically the entries of the transition probability matrix and then shown that such a Markov chain converges weakly to the target Markov process. Second, we have utilized an elliptical restriction as a way of removing non-critical components of the Markov chain to enhance the computational efficiency. Numerical examples are provided.

Tractability of Integration

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On Tractability of Weighted Integration over $\mathbf{R}^d$

Leszek Plaskota
Exponent of Tractability for Sparse Grid Quadratures

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When are Integration and Discrepancy Tractable?

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Using Ergodic Markov Chains for Numerical Integration

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Title

On Tractability of Weighted Integration over $\mathbf{R}^d$

Abstract

We present recent results on the tractability of weighted integration problems over unbounded domains. More specifically, we consider special weighted tensor product spaces of d-variate functions of regularity r; the weights defining the spaces are denoted by γ_d. The weight function defining the integral is a tensor product of a univariate probability density with different variances σ_d. The main results are necessary and sufficient conditions (in terms of the sequences γ_d and σ) for the strong tractability or tractability of the corresponding integration problems.

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TITLE

Exponent of Tractability for Sparse Grid Quadratures

ABSTRACT

Sparse grid quadratures, *SGQ*, are tensor product methods for computing multiple integrals. They use a part of a grid as sample points. We study the power of SGQ in the average case setting, with respect to the Wiener sheet. It is known that, for fixed dimension d, the error of appropriately chosen SGQ (*Smolyak*'s quadratures) decreases at least as $n^{-1}(\ln n)^{3(d-1)/2}$, as the number of samples $n \to \infty$. Hence SGQ seem to be a good alternative to Monte Carlo and quasi-Monte Carlo methods when dimension is small. It turns out, however, that SGQ do not do so well for large dimensions.

Specifically, for a class of quadratures, define the *exponent of tractability* α^* as the infimum of α for which at most $C\varepsilon^{-\alpha}$ samples are needed to calulate the integral with error ε, where C is independent of d. Then, for SGQ we have $2.1933 \le \alpha^* \le 2.4526$. Thus the exponent of SGQ is rather poor since the exponent of (non-deterministic) Monte Carlo is 2, and it is known that there exist deterministic quadratures with the exponent at most 1.4778. Still, 2.4526 attained by Smolyak's quadratures is the best exponent obtained constructively.

We also study the exponent of SGQ with respect to "weighted" distributions where the covariance kernel $K(\vec{x},\vec{y}) = \prod_{j=1}^{d}(1+\gamma_j \min\{x_j, y_j\})$, with $\gamma_1 \ge \gamma_2 \ge \cdots > 0$ and $\sum_{j=1}^{\infty}\gamma_j < \infty$. In this case, for SGQ we have $\alpha^* = \max\{1, 2(p^*-1)^{-1}\}$ where p^* is the supremum over p such that $\gamma_j = O(j^{-p})$. This implies that the exponent is optimal if $\gamma_j = O(j^{-3}$, and far away from being optimal if γ_j decreases "very slowly".

The results obtained are related to the discrepancy of sparse grid points.

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Title

When are Integration and Discrepancy Tractable?

Abstract

We explain and discuss two results from two recent papers:

- "The (normalized) L_2-discrepancy is *not* tractable." This is a joint result with H. Woźniakowski, J. Complexity, June 2001.
- "The inverse of the star-discrepancy depends linearly on the dimension." This is a joint result with S. Heinrich, G. W. Wasilkowski, and H. Woźniakowski, Acta Arithmetica, 2001.

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TITLE

Using Ergodic Markov Chains for Numerical Integration

ABSTRACT

Numerical integration over high-dimensional domains is typically carried out by means of Monte Carlo methods. In many situations direct sampling of the desired target distribution is not feasible and asymptotic methods (Markov Chain Monte Carlo) have to be applied; that is, N independent samples are replaced by N steps of an appropriate Markov chain. The error is considered uniformly over some class of input functions.
The efficiency of MCMC depends on

- ergodic properties of the Markov chain,
- the initial distribution and
- the class of input functions.

First we recall results [1] for *uniformly ergodic Markov chains*, where the error bounds are valid for any bounded class of square integrable functions, but restrict the admissible initial distributions, unless the state space is finite.

For general state space it is unlikely to design a uniformly ergodic Markov chain. However, in many situations it is possible to construct Markov chains which satisfy a relaxed ergodicity property, *V-uniform ergodicity* [2].

We analyze the error behavior for this generalized case. In particular we discuss the interplay between relaxed ergodicity, feasible initial distribution and restriction on the class of input functions.

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Special Session
Dynamical Systems and QMCM in Numerical Solution of Differential Equations

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Makoto Mori
Brownian Motion Generated by One–Dimensional Dynamical Systems

Syoiti Ninomiya
A New Simulation Scheme: Application of the Kusuoka Approximation to Finance Problems

Hiroshi Sugita
Random Weyl Sampling for Drastic Reduction of Randomness in Monte-Carlo Method

Christian Lécot and Shigeyoshi Ogawa
Random Walk Methods Using Quasirandom Numbers

Christian Lécot
Quasi-Monte Carlo Methods for Ordinary Differential Equations

Tomoaki Takemi and Shigeyoshi Ogawa
Report on the Numerical Experiments of the Haselgrove's Method Applied to the Numerical Solution of PDEs

Makoto Mori
Construction of Higher Dimensional Low Discrepancy Sequences

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Title

Brownian Motion Generated by One–Dimensional Dynamical Systems

Abstract

In recent days, as represented by mathematical finance, the role of stochastic differential equations becomes more and more important to analyze random phenomena. The aim of this paper is to construct a thoretical foundation to get a numerical solution of stocahstic differential equation by reliable Monte Carlo method (cf. Ogawa[3]). For this purpose, we will give an algorithm to construct pathes of Brownian motion from the view point of dynamical system.

The most famous and simplest way to construct pathes of Brownian motion is to use random walk. Let (Ω, P) be a probability space, and $X_1, X_2, \dots$ be independent and identically distributed random variables such that

$$P\{\omega \in \Omega \colon X_n(\omega) = +1\} = \frac{1}{2},$$
$$P\{\omega \in \Omega \colon X_n(\omega) = -1\} = \frac{1}{2}.$$

Then for any $t \geq 0$

$$\frac{X_1(\omega) + \cdots + X_{[nt](\omega)}}{\sqrt{n}}$$

converges to a path of Brownian motion as n tends to infinity. Here $[x]$ expresses the largest integer which does not exceed x.

We can express these random variables as a dynamical system on the unit interval with transformation

$$F(x) = 2x \pmod 1.$$

This dynamical system is Bernoulli and, by this reason, it is not at all difficult to show the above assertion.

In this article, we will consider more general piecewise linear expanding and topologically transitive transformations F on the unit interval and, using these transformations, we will construct pathes of Brownian motion.

Calculating the spectra of the Perron–Frobenius operator concretely, we got in [1], the invariant probability measure μ and its decay rate of correlation. Expanding this idea, we

constructed a renewal equation on functional spaces and determined the order of convergence for higher order mixing property ([2]).

Then, we will show that a random walk given by dynamical system:

$$\sum_{k=0}^{n-1} \frac{h(F^k(x)) - \int h\, d\mu}{\sqrt{n}}$$

converges to Brownian path in law, using Taylor expansion of the characteristic function of the random walk. Moreover, we will show the tightness, we prove that the random walk coverges to Brownian motion in measure.

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Title

A New Simulation Scheme: Application of the Kusuoka Approximation to Finance Problems

Abstract

Numerical calculation of E[f(X(t,x))], where X(t,x) denotes a diffusion process that is a solution of some SDE and f is a function with some regularity, is practically very important in many fields. There are two major ways to solve this problem. The PDE approach and the simulation approach. When we face finance problems, it is often that there are obstacles to the former approach and we are forced to take the latter. When we do the "simulation", we usually do Euler- Maruyama approximation of the diffusion process. It is well known that under some regularity condition, Euler-Maruyama approximation gives accuracy proportional to the width of discretization unit. This means that if we want to make the error caused by the discretization smaller, we have to increase the number of discretizing points, and at last, we find that we are facing the famous formidable problem "numerical integration in a huge dimensional space". Quasi-Monte Carlo methods and many variance reduction techniques are proposed to break this situation by conquering the "huge dimension" problems.

In 1999, S. Kusuoka[K] introduced a new simulation scheme based on Malliavin calculus and higher order stochastic expansion with discrete random variables. We call this scheme Kusuoka approximation. He also showed that by using Kusuoka approximation, we can achieve more accurate approximation than Euler-Maruyama approximation provided that the calculation workloads are equal. In Kusuoka approximation, we do not discretize the time interval into equally separated intervals but into various sized intervals according to the given function f and we use a set of discrete random variables called m-moment similar family.

In this talk, we apply the Kusuoka-approximation to simulate finance problems. We also try Quasi-Monte Carlo methods to the simulation scheme.

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Title

Random Weyl Sampling for Drastic Reduction of Randomness in Monte-Carlo Method

Abstract

When we have to integrate numerically a very complicated function, to which it is impossible to apply even any QMC method, we usually apply the i.i.d.-sampling, i.e., the sampling by means of *i*ndependently *i*dentically *d*istributed (i.i.d.) random variables. Although the i.i.d.-sampling converges rather slowly, we should remark that it is applicable for a very wide class of integrands, say, L^2-functions.

However, in implementing the i.i.d.-sampling with large sample size, we must be careful about the quality of pseudo-random numbers. That is, if their quality is not sufficiently high, it is likely that their statistical bias will be amplified to a big error.

Therefore we are reassured by the existence of a sampling method with very little randomness which nevertheless has a similar error estimate as the i.i.d.-sampling for all L^2-functions. Indeed, the *random Weyl sampling*, introduced by [1, 2], is such a sampling method.

By the random Weyl sampling, we can drastically reduce pseudo-random numbers, for instance, in the following way: Let a random variable X be calculated by 500 tosses of a coin. For the i.i.d.-sampling to integrate X with 10^7 samples, we need $500 \times 10^7 = 5 \times 10^9$ pseudo-random bits, while for the random Weyl sampling with the same sample size, we only need $\lceil 500 + \log_2 10^7 \rceil \times 2 = 1048$ pseudo-random bits. In addition, both sampling methods have the same error estimate in variance for all X as long as they are calculated by 500 tosses of a coin.

The drastic reduction of pseudo-random numbers brings the following benefits: (1)The random Weyl sampling is much less sensitive to the quality of pseudo-random numbers. So pseudo-random numbers of low quality can be used for precise numerical integration. (2)A slow but very precise pseudo-random generator, such as a cryptographically secure one, can be used for a large scale random Weyl sampling. Then the numerical integration will be most reliable.

In addition, the random Weyl sampling is very fitted to parallel computation. As a result, we strongly recommend the random Weyl sampling for large scale complicated numerical integration.

We note that the random Weyl sampling is a kind of pseudo-random generation in the sense that it lets little randomness look big randomness. But its usage is limited: only for numerical integration.

Definition. The pair $(x, \alpha) \in [0,1)^s \times [0,1)^s$ being independent and both uniformly distrubuted random variables, the sampling method by means of $\{f((x+n\alpha) \bmod \mathbf{1})\}_n$ is called the random Weyl sampling.

Theorem. ([1]) *For each $f \in L^2([0,1)^s, P^s)$, we have*

$$\iint_{[0,1)^s \times [0,1)^s} \left| \frac{1}{N} \sum_{n=0}^{N-1} f\left((x+n\alpha) \bmod \mathbf{1}\right) - \int_{[0,1)^s} f(t)dt \right|^2 dxd\alpha = \frac{\mathbf{Var}(f)}{N},$$

where $\mathbf{Var}(f) := \int_{[0,1)^s} \left| f(t) - \int_{[0,1)^s} f(u)du \right|^2 dt$.

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Title

Random Walk Methods Using Quasirandom Numbers

Abstract

We are interested in mathematical models that involve a combination of convection, reaction and diffusion. In these settings, particle methods are useful computational tools for solving equations in which diffusion may be small. The attraction of such methods is that, unlike finite-difference, finite-element or finite-volume methods, they do not introduce numerical diffusion. The method of splitting consists of reducing the original evolutionary problem to a sequence of problems describing the convective, the reactive and the diffusive processes respectively. Convection is simulated by a translation of each particle, reaction is modeled as growth or decay of the particles masses, and diffusion is simulated by applying a random walk technique. The random particle method suffers from several drawbacks. The accuracy is poor because of the random fluctuations and the error is $\mathcal{O}(1/\sqrt{N})$, where N is the number of particles used. A step toward improving the accuracy is to have the density of diffusing elements represent the gradient of the solution, rather than the solution itself. We present here a quasi-Monte Carlo approach to the random walk technique. The idea is to replace the pseudorandom numbers in the random walk by quasirandom points, i.e., low discrepancy point sets.

Quasi-Monte Carlo methods can be described as deterministic versions of Monte Carlo methods. Instead of random samples as in Monte Carlo methods, one employs quasirandom numbers. In Monte Carlo integration with N random nodes, the absolute value of the error has the average order $\mathcal{O}(1/\sqrt{N})$. The quasi-Monte Carlo method yields a much better result, giving us a deterministic error bound of the form $\mathcal{O}((\log N)^{s-1}/N)$ for quasirandom points. There are quasi-Monte Carlo methods not only for numerical integration, but also for various other computational problems and it is found that in certain types of such problems they significantly outperform Monte Carlo methods. Quasirandom points cannot be blindly used in place of pseudorandom points for particle simulations. It is necessary to take special measures to ensure that correlations across time steps are controlled. This is achieved here through the additional step of sorting the particles by position.

In the first part of the talk, we study a random particle method for approximating solutions

of the KPP (Kolmogorov-Petrovskii-Piskounov) equation:

$$\frac{\partial u}{\partial t}(x,t) = \nu \frac{\partial^2 u}{\partial x^2}(x,t) + f(u)(x,t), \quad x \in \mathbf{R},\ t > 0,$$
$$u(x,0) = u_0(x), \quad x \in \mathbf{R},$$

which is a 1-D reaction-diffusion equation with a forcing term f. It finds applications in laminar combustion and in biological systems. Examples of such equations are the Fisher equation, where $f(u) = u(1-u)$ and the Nagumo equation without recovery, where $f(u) = u(u-a)(1-u)$. We use a fractional step method: in every time step the equation is split into two evolution equations, each of which is solved separately. The reaction equation is solved using an ordinary differential equation solver; the diffusion process is simulated by random walking the particles. We compare standard gradient random walk method using pseudorandom numbers, and gradient quasirandom walk method using low discrepancy sequences with renumbering of particles according to their positions in every time step. We are interested in the case where the equation has a travelling wave solution and we use both methods to compute this known exact solution. We measure the error in the L^∞ norm. The experiments allow us to estimate the rate of convergence of each method, at least for the model problem. The numerical results show the effectiveness of the quasirandom strategy, even though the problem is nonlinear: an improvement in both magnitude of error and convergence rate is obtained.

In the second part of the talk we present a gradient random walk method used to solve the quasilinear diffusion equation

$$\frac{\partial u}{\partial t}(x,t) + \left(u \frac{\partial u}{\partial x}\right)(x,t) = \nu \frac{\partial^2 u}{\partial x^2}(x,t), \quad x \in \mathbf{R},\ t > 0,$$
$$u(x,0) = u_0(x), \quad x \in \mathbf{R},$$

with viscosity $\nu > 0$. The equation is attributed to Burgers and arises in a number of applications where viscous and nonlinear effects are equally important. The algorithm is based on a viscous splitting: in each time step the advection and the diffusion equations are solved sequentially. The inviscid Burgers equation is approximated by solving separately the Riemann problems associated with each discontinuity of the approximated solution; the diffusion is simulated by randomly perturbing the positions of the particles. We study the effectiveness of gradient quasirandom walk using low discrepancy sequences with sorting of particles according to position in every time step, when compared with standard gradient random walk using pseudorandom numbers. We can use the Cole-Hopf transformation to solve exactly the equation. The error of the simulation is measured in the L^∞ norm. The numerical experiments allow us to estimate the rates of convergence, at least for the model problem we have studied, for which exact answers are available. We see that the gradient quasirandom walk method clearly outperforms the gradient pseudorandom walk method, although the problem being dealt with is more complicated than simple diffusion problem.

In both cases, the results of the examples demonstrate that random walk using quasirandom numbers is feasible, and can produce more accurate results than standard random walk using pseudorandom numbers. It is the technique of relabeling which make this possible. We show that the algorithm can be tailored to fit in a fractional step scheme when other mechanisms are active.

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TITLE

Quasi-Monte Carlo Methods for Ordinary Differential Equations

ABSTRACT

We describe a family of numerical schemes for solving systems of ordinary differential equations

$$\begin{aligned} y'(t) &= f(t, y(t)), \quad 0 < t < T, \\ y(0) &= y_0, \end{aligned}$$

where $y_0 \in \mathbf{R}^p$. We are interested in systems in which f is smooth in space (y) but lacks regularity in time (t). More specifically, we assume that f satisfies the following hypothesis.

Hypothesis 1 *There exist $\tau > 0$ and $\rho > 0$ such that*

- *The function $D_y^r f$ is measurable on*

$$E := \bigcup_{0 \le t \le T} [t, \min(t + \tau, T)] \times B(y(t), \rho),$$

  for $0 \le r \le s$.

- *For every $t \in [0, T]$ the function $y \to D_y^r f(t, y)$ is continuous on the open ball $B(y(t), \rho)$, for $0 \le r \le s$.*

- *There are $\|D_y^r f\|_E$ for $0 \le r \le s$ and $V_E(D_y^r f)$ for $0 \le r \le s - 1$, such that for every $t \in [0, T]$ and every $y \in B(y(t), \rho)$,*

  [1] the function $u \to D_y^r f(u, y)$ is defined on $[t, \min(t + \tau, T)]$ and is bounded by $\|D_y^r f\|_E$, for $0 \le r \le s$,

  [2] the variation of the function $u \to D_y^r f(u, y)$ on $[t, \min(t + \tau, T)]$ is bounded by $V_E(D_y^r f)$, for $0 \le r \le s - 1$.

This formulation can provide a model for problems in which f varies significantly faster in time than in space and the useful range of the methods proposed in this talk consists of problems in which the rapid time variations of f cannot be followed in detail.

We consider a partition $0 = t_0 < t_1 < \ldots < t_{n^*} = T$ of $[0,T]$ into n^* subintervals of length $h_n := t_{n+1} - t_n$ and we set $H := \max_{0\le n<n^*} h_n$. Since the problems do not allow reliance on smoothness in t, the dependence on t is retained only through mean properties. Understanding solution in the sense of functions satisfying

$$\forall t_0, t_0 + h \in [0,T] \quad y(t_0 + h) = y(t_0) + \int_{t_0}^{t_0+h} y'(u)du,$$

we may write

$$\begin{aligned} y(t_{n+1}) = y(t_n) &+ \int_{t_n}^{t_{n+1}} F_1(u_1; y(t_n))du_1 \\ &+ \int_{t_n}^{t_{n+1}} \int_{t_n}^{u_1} F_2(u_1, u_2; y(t_n))du_2 du_1 + \cdots \\ &+ \int_{t_n}^{t_{n+1}} \int_{t_n}^{u_1} \cdots \int_{t_n}^{u_{s-1}} F_s(u_1, \ldots, u_s; y(t_n))du_s \ldots du_1 + \mathcal{O}(h_n^{s+1}), \end{aligned}$$

where the functionals F_i are defined recursively and involve y-partial derivatives of f. We unite all integrals into a single integral over $(t_n, t_{n+1})^s$. Then we combine Taylor expansions in order to express the integrand without derivatives. Neglecting the $\mathcal{O}(h_n^{s+1})$ term, we obtain algorithms like Runge-Kutta methods. We then approximate the integral using a Monte Carlo estimate. The resulting numerical scheme is called the Runge-Kutta Monte Carlo (RKMC) method of order s. When the integral is estimated using a low discrepancy point set $X \subset I^s$, the scheme is called the Runge-Kutta Quasi Monte Carlo (RKQMC) method of order s. Quasi-Monte Carlo methods are deterministic versions of Monte Carlo methods. Invariably, the basic idea is to replace the pseudorandom numbers in the Monte Carlo method by deterministic points that are well suited for the problem at hand. It is well known that in certain types of computational problems, quasi-Monte Carlo methods are superior to Monte Carlo methods. In numerical integration the probabilistic Monte Carlo error bound is $\mathcal{O}(1/\sqrt{N})$ with N random samples. The quasi-Monte Carlo method gives the deterministic error bound $\mathcal{O}((\log N)^{s-1}/N)$ for suitably chosen sets of nodes.

The error analysis of the RKQMC methods follows the general outline of the error analysis of the Runge-Kutta methods: local truncation errors and other standard error terms are analyzed in the same way. The bound for the error of the quasi-Monte Carlo approximation is obtained by using techniques of the functions of bounded variation in the sense of Hardy and Krause: the Koksma-Hlawka inequality is the main tool. Let $\|\cdot\|$ denote a norm on $\mathbf{R}^p$ and let $e_n := y_n - y(t_n)$ be the global error of the scheme. If $D_N^\star(X)$ denotes the star discrepancy of the point set X, we obtain

Proposition 1 *There are positive constants c_1, c_2, c_3 and c^* such that, if $H \le \tau$ and*

$$\mathrm{e}^{c_2 T}\|e_0\| + \frac{\mathrm{e}^{c_2 T} - 1}{c_2}(c_1 H^s + c_3 D_N^\star(X)) + c^* H \|f\|_E < \rho,$$

then

$$\|e_n\| \leq \mathrm{e}^{c_2 t_n}\|e_0\| + \frac{\mathrm{e}^{c_2 t_n} - 1}{c_2}(c_1 H^s + c_3 D_N^\star(X)), \quad 0 \leq n \leq n^*.$$

It has become customary to speak of low-discrepancy point sets in the case where their star-discrepancy is $\mathcal{O}((\log N)^{s-1}/N)$ in dimension s, with N being the number of points considered. According to the estimate of Proposition 1 the RKQMC algorithm using a low-discrepancy point set is of order s if $N = \mathcal{O}(H^{-s})$.

In order to compare RKMC and RKQMC methods, we solve a model problem in which f undergoes rapid time variations. We compute the errors obtained in solving this problem using three different strategies:

[1] a Runge-Kutta scheme of order s

[2] a RKMC method of order s

[3] a RKQMC method of order s

The numerical results show that RKMC and RKQMC methods outperform standard Runge-Kutta schemes when f varies very rapidly in time. In addition, it is shown that by using a quasirandom numbers in place of pseudo-random samples, we are able to obtain reduced errors.

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Title

Report on the Numerical Experiments of the Haselgrove's Method Applied to the Numerical Solution of PDEs

Abstract

The Monte Carlo method is well known as an effective method for the estimation of the multi dimensional integration with large dimensionality n

$$I = \int_0^1 \int_0^1 \cdots \int_0^1 f(x_1, x_2 \cdots, x_n) dx_1 dx_2 \cdots dx_n$$

The principal advantage of the Monte Carlo method is that we can calculate I with the accuracy $O(1/\sqrt{N})$for any function $f(x)$ without assuming regularity but integrability. On the other hand, we have the quasi-Monte Carlo method in which we assume a little restrictive condition on the regularity of the integrand $f(x)$, so that we can calculate I with the accuracy $O(logN)^{n-1}/N)$.
Apart from these, we are concerned with the Haselgrove's method and its applications. The key of the method is in the following three points:

[1] Instead of the arithmetic mean, we adopt the method of other way of summation for the calculation of mean.

[2] The employment of a good set of irrational numbers for the generation of random numbers by means of Weyl transformation.

[3] The integrand $f(x)$ is supposed to satisfy a more restrictive condision on its regularity.

It is then possible to realize the computation with accuracy $0(N^{-r}), (r = 1, 2, 3, 4)$. For example, to get the scheme of accuracy $r = 2$, we approximate I by the following

$$s(N) = \frac{1}{(N+1)^2} S_2(N)$$

where

$$S_r(N) = \sum_{k=-N}^{N} \begin{pmatrix} N - |k| + r - 1 \\ r - 1 \end{pmatrix} f([k\alpha_1], [k\alpha_2], \cdots, [k\alpha_n]) \quad (r \geq 1)$$

and $[z]$ stands for the distance from z to the nearest integer. Here the integrand $f(x)$ satisfies a stronger condition as follows: for some positive fixed number s there exists a constant M_s such that if none of the $m_i = 0$,

$$|a_{m_1,m_2\cdots,m_n}| \leq M_s |m_1 m_2 \cdots m_n|^{-s} \quad (s > r)$$

where $a_{m_1,m_2\cdots,m_n}$ is the Fourier coefficients of $f(x)$.

In this talk, we will also consider the application of the method to the numerical solution of the following Cauchy problem of heat equation

$$\frac{\partial u(t,x)}{\partial t} = c^2 \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_n^2} \right) u(t,x)$$

$$u(0,x) = u_0(x).$$

We will show the experimental results, and we will compare them with those by Monte Carlo method and those by quasi-Monte Carlo method. As another application, we will refer to the case of Burger's equation.

$$\frac{\partial u(t,x)}{\partial t} + u(t,x) \frac{\partial u(t,x)}{\partial x} = c^2 \frac{\partial^2 u(t,x)}{\partial x^2}$$

$$u(0,x) = u_0(x)$$

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Title

Construction of Higher Dimensional Low Discrepancy Sequences

Abstract

Looking van der Corput sequence from the view point of dynamical system, Ninomiya([6],[7]) has proved that the sequences constructed by Markov β-transformations are of low discrepancy. Applying the spectral theory of the Perron–Frobenius operator associated with dynamical systems (cf, [1],[2]), Mori gave the necessary and sufficient condition that the sequences constructed by one dimensional dynamical systems are of low discrepancy([4],[5]). For higher dimensional cases, as Mori showed in [3], in general no dynamical system has sufficently high mixing property to construct a sequence of low discrepancy. In this talk, for two dimensional cases, we will construct a dynamical system using symbolic dynamics which has high mixing property, and will show it generates a sequence of low discrepancy. We believe we can construct higher dimensional low discrepancy sequences using this idea.

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Special Session
Stochastic Models of Turbulent Transport

Organizer

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Karl Sabelfeld
Lagrangian Stochastic Models for Transport of Interacting and Diffusing Particles.

Michael Mascagni
First- and Last-Passage Diffusion: Key Concepts in the Study of Porous and Composite Media

Nikolai Simonov
On Random Vortex Method in Cylindrical Coordinates — Cancelled

Olivier Smidts
Lagrangian Stochastic Models for Transport in Statistically Homogeneous Porous Medium.

I.A. Shalimova
On a Variance Reduction Technique in the Particle Simulation Governed by SDEs.

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Title

Lagrangian Stochastic Models for Transport of Interacting and Diffusing Particles.

Abstract

In the presentation I deal with the following problem: construct the solution of a spatially inhomogeneous Smoluchowski equation governing coagulating and diffusing particles in a host gas, on the basis of solutions to homogeneous Smoluchowski equation. This problem can be solved by introducing Lagrangian variables in the case when there is no diffusion. The non-zero diffusion drastically complicates the situation. Under some general assumptions we give the interrelations between the homogeneous and inhomogeneous cases. This provides an effective numerical scheme especially when tye host gas is incompressible. We formulate some open problems related to the issue, in particlular, there is no evident way how to generalise the approach in the case when the molecular diffusion depends on the partiles size.

Michael Mascagni
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Title

**First- and Last-Passage Diffusion:
Key Concepts in the Study of Porous and Composite Media**

Abstract

We provide a review of a new method of addressing problems in diffusion Monte Carlo: the Green's function first-passage method (GFFP). In particular, we address four new strands of thought and their interaction

with the GFFP method: the use of angle-averaging methods to reduce vector or tensor Laplace equations to scalar Laplace equations; the use of the simulation-tabulation (ST) method to dramatically expand the range of the GFFP method; the use of the Feynman-Kac formula, combined with GFFP to actually perform path integrals, one patch at a time; and the development of last-passage diffusion methods; these drastically improve the efficiency of diffusion Monte Carlo methods. All of these claims are addressed in detail, with specific examples.

Olivier Smidts [1]

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Title

Lagrangian Stochastic Models for Transport in Statistically Homogeneous Porous Medium

Abstract

To simulate the transport of a scalar in a porous medium, we suggest a generalized Langevin equation in the phase-space (x, v), x being the spatial coordinates, and v is the groundwater velocity. In contrast to the commonly used random displacement models, where the random walk is constructed in the spatial coordinates only, we deal in our model with the simulation of the random process $(X(t), V(t))$ governed by Ito type stochastic differential equation. The main effort is made here in evaluation of the drift (deterministic) and dispersion (fluctuated) terms of this equation. These terms are obtained through a numerical solution of the stationary groundwater flow equation with a hydraulic conductivity assumed to be statistically homogeneous lognormally distributed random field.

[1] Joint work with O.Kurbanmuradov and K. Sabelfeld

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Title

On a Variance Reduction Technique in the Particle Simulation Governed by SDEs.

Abstract

When constructing a numerical method for evaluation of a functional on diffusion processes governed by stochastic differential equations, one of the most important practical issue is the variance reduction. Our experience has shown that the variances may vary drastically from an estimator to estimator, and there is no universal recommendation about the variance reduction strategy. A standard approach is based on the Girsanov transformation and a subsequent control variate technique. Another possibility is Thomson's well-mixed condition approach both for direct and backward trajectory simulations. In between, a set of different variance reduction technique can be suggested. In this presentation we analyse these approaches and suggest some comparisons.

Special Session
Monte Carlo Simulations in Solid State Physics and Material Sciences

Organizer

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James B. Anderson
Monte Carlo Methods in Electronic Structure for Large Systems

Alexandra Viel
Quantum Monte Carlo Study of Doped ^{4}He Clusters

Maziar Nekovee
Quantum Monte Carlo Studies of Density Functional Theory in the Strongly Inhomogeneous Electron Gas

Wolfram Strepp
Phase Transitions in Colloidal Systems in External Periodic Potentials

Andrzej Patrykiejew
The Interplay between Spreading of Adsorbed Films and their Wetting Behavior

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Title

Monte Carlo Methods in Electronic Structure for Large Systems

Abstract

Quantum Monte Carlo methods have recently made it possible to calculate with very high accuracy the electronic structures of relatively large collections of atoms in molecules, clusters, liquids, and solids. These large systems range from positron complexes [NH_2,Ps] with 9 electrons [1], to C_{20} isomers with 120 electrons [2], to silicon crystal structures of 250 atoms and 1000 valence electrons [3]. The techniques for such calculations and a sampling of applications will be discussed.

Typical of such calculations are those for the isomers of the carbon clusters C_{20} which may occur in the form of chains, rings, bowls, plates, cages, and combinations of these [4]. It is fairly well established that the C_{20} structures lowest in energy are the ring, bowl, and cage, but the relative energies for these three are predicted quite differently by different methods of quantum calculation. In general, Hartree-Fock (HF) methods favor the ring; Moller-Plesset (MP2) methods with small basis sets favor the cage and with large basis sets favor the bowl; coupled-cluster (CCSD and CCSD(T)) favor the bowl and cage; and density functional (LDA, BLYP, and B-PW91) calculations favor variously the ring, bowl, and cage. Quantum Monte Carlo (QMC) calculations – using procedures identical to those demonstrated to be accurate for C_8 and C_{10} isomers – favor the bowl [3,5].

The method used in QMC calculations for large systems is the diffusion QMC method (DQMC). It is based on the mathematical equivalence of the time-dependent Schrödinger equation and the diffusion equation with an added multiplication term. According to Metropolis and Ulam [6] it was Fermi who suggested in the 1940's that a collection of particles each executing a random walk along with occasional multiplication would eventually produce a spatial distribution corresponding to the ground-state wave function for the system. The successful extension of this initial concept has led to today's fixed-node diffusion Monte Carlo method (FN-DQMC) which is "already much more accurate than any competing method" [7].

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Title

Quantum Monte Carlo Study of Doped ^{4}He Clusters

Abstract

Over the last few years, spectroscopy of molecules attached and embedded in helium clusters has become a growing and significant field of quantum matrix spectroscopy. Clusters of ^{4}He appear to provide an ideal, cold quantum matrix characterized by weak interactions with guest molecules. This environment offers great potential for performing high resolution spectroscopy of embedded molecules and molecular aggregates.

Recent experiments from several groups show that rotational fine structure can be resolved in the infra-red spectra, and furthermore that these spectra are consistent with empirical Hamiltonian models of freely rotating molecules. The effect of the helium environment is in this case limited to the reduction of the effective rotational constants with respect to the corresponding gas phase values. Depending on the molecule, the effective rotational constant varies from $\sim 30\%$ to $\sim 80\%$ of the gas phase value.

Other experiments deal with vibrational spectra of the impurity embedded inside the clusters. In this case, the presence of surrounding helium atoms has also an effect which can be observed experimentally by the shift of the normal frequencies. This typical matrix effect is usually much smaller in helium than in other rare gas matrices. The primarily dispersive contribution of the helium-impurity interaction leads usually to red shifts, although at least one case of a strong blue-shifted vibrational frequency has been documented.

Diffusion Monte Carlo (DMC) is a powerful technique for solving the Schrödinger equation of these many-body systems. We present here DMC calculations of both ground and excited energy levels for two kinds of doped helium clusters: HCN ^{4}He$_n$ [1,2] and NH_3 ^{4}He$_n$ [3]. The aim of our HCN-doped helium cluster studies is to understand the observed small reduction of the rotational constant for this fast linear rotor. For the case of ammonia embedded in helium droplets, we are interested in understanding the unusually large blue shift observed for the inversion mode. The dynamics of this molecule also pose the question of how intramolecular tunneling motions are affected by the quantum environment provided by liquid helium.

The calculations are done using an importance sampled, rigid body DMC formalism [4]. In this approach the internal vibrational modes of the guest molecule are not explicitly taken into account, but all translational and rotational degrees of freedom are incorporated. An important characteristic of our approach is the use of importance sampling for all degrees of freedom, translations and rotations. This provides considerable flexibility and improved efficiency for all applications.

Although DMC is a ground state technique, it can also yield information about individual excited states. We can achieve this in two ways. The first method is the widely-used fixed node approximation. This involves making an approximation to the excited state nodal structure and then performing a DMC calculation for the state of interest, given these nodal constraints. However, the exact nodal structure of a given excited state for a general N-body system is not known in advance. To overcome this problem, one can use the exact Projection Operator Imaginary Time Spectral Evolution (POITSE) scheme developed in our group [5,6], which allows to compute excited state energies without any nodal approximation. The POITSE approach employs a DMC walk to evaluate an imaginary time correlation function of a projection operator chosen to project out excited states of interest. This decay is then subsequently inverted to yield to the energy spectrum.

In this talk I will describe these two methods and present applications of each to calculation of molecular excitations in the HCN- and NH_3-doped helium clusters. The relative merits and limitations of these two DMC-based approaches will be illustrated and discussed, together with the insight into the dynamics of molecules in bosonic clusters of ^{4}He that they have provided.

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TITLE

Quantum Monte Carlo Studies of Density Functional Theory in the Strongly Inhomogeneous Electron Gas

ABSTRACT

Density functional theory (DFT) is the most popular quantum-mechanical technique used to study atoms, molecules and solids. In this method the problem of finding the ground state properties of an interacting N-electron system ($N \approx 10^{23}$ in a small macroscopic piece of solid) is transformed into a problem for non-interacting electrons. This enormous simplification is exact in principle, but in practice it is necessary to approximate the unknown exchange-correlation energy functional E_{xc}, which expresses the many-body effects in terms of electron density $n(\mathbf{r})$. The most frequently used approximations to date are the local density approximation (LDA) and various generalized gradient approximations (GGA). The LDA works surprisingly well, but not well enough for many chemical and biological applications. Although better than the LDA in many situations, current GGAs are not able to consistently deliver the very high "chemical accuracy" which is often required in such applications and the quest for improved approximations of E_{xc} is the subject of much current research.

An entirely different approach to the ground-state many-body problem is the quantum Monte Carlo method (QMC). QMC calculations are computationally more demanding than density functional calculations. However, unlike the DFT approach, in which the ground-state density is the basic variable, QMC methods focus on sampling the full ground-state many-body wavefunction of the system under consideration and yield a more detailed description of many-body effects. QMC calculations can therefore be used to investigate DFT from "outside" and to test the performance of approximations to E_{xc}.

The exchange-correlation energy results from the interaction between electrons and the so-called exchange correlation hole n_{xc} which surrounds each electron as it moves in a many-electron system

$$E_{xc}(\mathbf{r},[n]) = \frac{1}{2}\int d\mathbf{r}\int d\mathbf{r}'\,\frac{n(\mathbf{r})n_{xc}(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} = \int d\mathbf{r} e_{xc}(\mathbf{r}) \tag{1}$$

where e_{xc} is the exchange-correlation energy density. The DFT exchange-correlation hole can be obtained via an adiabatic connection procedure in which one varies the electron-electron

interaction between 1 (corresponding to the fully interacting system) and 0 (corresponding to the non-interacting system) but maintains the electron density at $n(\mathbf{r})$ in this process:

$$n(\mathbf{r})n(\mathbf{r}') + n(\mathbf{r})n_{xc}(\mathbf{r},\mathbf{r}') = \int_0^1 d\lambda \, \langle \Psi^\lambda | \sum_i \sum_{j(\neq i)} \delta(\mathbf{r}-\mathbf{r}_i)\delta(\mathbf{r}'-\mathbf{r}_j) | \Psi^\lambda \rangle \qquad (2)$$

In the above equation Ψ^λ is the antisymmetric ground state of the Hamiltonian $\hat{H}^\lambda = \hat{T} + \lambda\hat{V}_{ee} + \hat{V}^\lambda$ associated with coupling constant λ. Here $\hat{T}$ and $\hat{V}_{ee}$ are the operators for the kinetic and electron-electron interaction energies, and $\hat{V}^\lambda = \Sigma V^\lambda(\mathbf{r}_i)$ is the one-electron potential needed to hold the electron density $n^\lambda(\mathbf{r})$ associated with Ψ^λ equal to $n(\mathbf{r})$ for all values of λ between 0 and 1.

We have developed a variational Monte Carlo (VMC) method for realizing the above adiabatic connection in DFT which allows us to perform accurate calculations of n_{xc}, e_{xc} and E_{xc} corresponding to a given electron density $n(\mathbf{r})$ [1].Our VMC method amounts to treating *both* Ψ^λ and V^λ variationally and determining the variational parameters by simultaneously minimizing the variance of the local energy and the deviation of n^λ from n. The multidimensional integrals involved in calculating the variance of local energy and n_{xc} are performed using the Monte Carlo Metropolis algorithm.

To open a new direction in the search for improved functionals we recently used our method to calculate n_{xc} and e_{xc} for several strongly inhomogeneous electron gases and analyzed the performance of the LDA and the GGA in these systems in detail [2]. In this talk I will describe our method together with the insight gained from its application to these system. The strong variation of $n(\mathbf{r})$ in our systems results in a strikingly nonlocal behavior of n_{xc} that cannot be described by semilocal corrections to the LDA (such as GGA). Our analysis shows, however, that the local density approximation of e_{xc} can be significantly improved by including a nonlinear dependence on the Laplacian of the electron density. The results also help to see why the GGA in fact worsens the LDA in a number of situations. [3]

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Title

Phase Transitions in Colloidal Systems in External Periodic Potentials

Abstract

One is often interested in long length scale and long time scale phenomena in solids. Such phenomena are usually described by continuum theories. Microscopic simulations [1] of finite systems, on the other hand, deal with microscopic variables like the positions and velocities of constituent particles. We present a new [2] coarse graining procedure for the computation of elastic constants of a crystalline solid in equilibrium. Fluctuations of the instantaneous local Lagrangian strain $\epsilon_{ij}(\mathbf{r}, \mathbf{t})$ are used to obtain accurate estimates of the elastic constants of model solids from atomistic computer simulations. The computed strains are systematically coarse-grained by averaging them within subsystems (of size L_b) of a system (of total size L). Using a simple finite size scaling theory we predict the behaviour of the fluctuations $< \epsilon_{ij}\epsilon_{kl} >$ as a function of L_b/L and extract elastic constants of the system *in the thermodynamic limit* at nonzero temperature. We illustrate the technique by computing isothermal elastic constants of the "soft" and the hard disk triangular solids in two dimensions from molecular dynamics and Monte Carlo simulations.

One of the first continuous systems to be studied by computer simulations [3] is the system of hard disks of diameter σ (=1). The nature of the phase transition at high densities ρ, however, is still being debated [3,4]. In Ref. [5] we investigated the melting transition of the solid phase. Elastic moduli and dislocation core energy of the triangular solid of hard disks are obtained in the limit of vanishing dislocation-antidislocation pair density, from Monte Carlo simulations which incorporate a constraint, namely that all moves altering the local connectivity away from that of the ideal triangular lattice are rejected. In this limit, we show that the solid is stable against all other fluctuations at least up to densities as low as $\rho\sigma^2 = 0.88$. We conclude that a KTHNY [6] transition from the solid to a hexatic phase preempts the solid to liquid first order transition in this system albeit by a very small margin, easily masked by crossover effects in unconstrained "brute-force" simulations with small number of particles. The scenario of a solid $\rightarrow$ hexatic transition is in accordance with recent experiments in colloidal systems [7].

The liquid-solid transition in systems of particles under the influence of external modulating potentials has recently attracted a fair amount of attention [8]. This is partly due to the fact that well controlled experiments can be performed using colloidal particles confined between glass plates subjected to a spatially periodic electromagnetic field generated by interfering crossed laser beams. One of the more surprising results of these studies, where a commensurate, one dimensional, modulating potential is imposed, is the fact that there exist regions in the phase diagram over which one observes re-entrant freezing/melting behaviour. Computer simulation results in this field have so far been controversial and inconclusive. Motivated, in part, by this controversy, we have investigated [9] the freezing/melting behaviour of a two dimensional hard disk system subjected to similar modulating external potentials. Detailed finite size scaling analyses of various thermodynamic quantities like the order parameter, its cumulants etc. are used to map the phase diagram of the system for various values of the density and the amplitude of the external potential. We find clear indication of a re-entrant liquid phase over a significant region of the parameter space. Our simulations therefore show that the system of hard disks behaves in a fashion similar to charge stabilized colloids which are known to undergo an initial freezing, followed by a re-melting transition as the amplitude of the imposed, modulating field produced by crossed laser beams is steadily increased. Detailed analysis of our data shows several features consistent with a recent dislocation unbinding theory of laser induced melting. Our simulations with DLVO- and $1/r^{12}$-pair potentials show these reentrance phenomena as well.

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Title

The Interplay between Spreading of Adsorbed Films and their Wetting Behavior

Abstract

It has long been recognized that the wetting behavior of adsorption systems is primarily dominated by a balance between the forces which define the adsorbate–adsorbate and the adsorbate–substrate interactions [1,2]. A detailed and systematic discussion of that problem, in the framework of a lattice gas model, was presented by Pandit, Schick and Wortis [1] and a more general discussion can be found in the review article by Dietrich [2]. When the potential generated by the solid substrate is sufficiently strong the adsorbate wets the surface at any temperature, down to $T = 0$. Such behavior has been found in many adsorption systems [2]. In the case of weakly attractive surfaces the regime of complete wetting terminates at a certain nonzero wetting temperature, T_w. As long as the temperature is lower than T_w the adsorbed layer remains microscopically thin up to the point of bulk vapor-liquid condensation. Only at the temperatures exceeding T_w the adsorbed film becomes infinitely thick when the pressure approaches the bulk coexistence point. In general, wetting transition at T_w can be of first order or continuous (critical wetting). When the wetting is a first-order transition, then at the temperatures above T_w and lower than a certain temperature T_{cpw} it is preceeded by another first-order (prewetting or thin-thick film) transition. The temperature T_{cpw} is the critical temperature of prewetting transition, so that at $T > T_{cpw}$ the film thickness increases smoothly with the gas pressure.

Nonwetting growth and the wetting transition have been experimentally observed in several adsorption systems [2]. Numerous theoretical [2,3] and computer simulation [4-6] studies have confirmed the above scenario.

Most of the experimental and computer simulation investigations of wetting transition in adsorption systems rest on the study of asymptotic behavior of adsorption isotherms when the gas pressure, or chemical potential, approaches the bulk gas–liquid coexistence. The main difficulty appearing in such study results from large fluctuations of density over a narrow range of gas pressure, near the bulk coexistence point. This problem is particularly troubling in the grand canonical Monte Carlo study. Near the wetting transition one often encounters metastabilities, in particular when the wetting temperature is close to the melting point.

One can also consider the transition from nonwetting to wetting regime as the problem of droplet spreading [2,6,7]. In our recent paper [6], we have proposed a method which allows to estimate the wetting temperature from canonical ensemble Monte Carlo simulation. The

method is based on the monitoring of temperature changes in the adsorbate–adsorbate and the adsorbate–substrate energies. At very low temperatures, well below the wetting transition and below the melting point of the adsorbate, the adsorbate forms small crystallites that cover only a fraction of the accessible surface. As the temperature increases to the melting point, the crystallites melt and sessile drops of liquid appear. As long as the temperature does not exceed the wetting temperature, the droplets retain stability. At still higher temperatures the droplets spread over the surface and form a more or less uniform layer.

In this talk I will present the results of canonical as well as grand canonical Monte Carlo simulations for a series of systems characterized by different strength of the surface potential and discuss the melting of 3D crystallites and the interplay between the spreading of small liquid droplets over the surface and the wetting behavior of adsorption systems. It will be also shown that the systems which exhibit complete wetting show rather peculiar changes in the properties of adsorbed films when the substrate potential stength is varied.

All the calculations have been performed assuming that the adsorbing surface is the (100) plane of a simple fcc crystal and that all interactions in the system are described by Lennard-Jones potential.

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Special Session
Quantum Monte Carlo Methods

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C.-O. Hwang and M. Mascagni
A Feynman-Kac Formula Implementation for the Linearized Poisson-Boltzmann Equation

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TITLE

Fermion Monte Carlo

ABSTRACT

We describe a new method for treating many-fermion systems by Quantum Monte Carlo[1,2]. The basic framework is that of Diffusion Monte Carlo, with significant algorithmic modifications. First, we use correlated pairs of random walkers that carry opposite signs so as to represent a wavefunction that is not everywhere positive. The "importance" or "guiding" functions for the walkers of different signs $\{R^+, R^-\}$ are different, and are defined by

$$\Psi_G^{\pm}(R^{\pm}) = \sqrt{\phi_S^2(R^{\pm}) + \phi_A^2(R^{\pm})} \pm \phi_A^2(R^{\pm})$$

where ϕ_S and ϕ_A are respectively a symmetric and antisymmetric trial solutions for the many–body Hamiltonian $\hat{H}$. The gaussian random variables associated with the random walks of the members of a pair are correlated, according to a reflected dynamics. The members of a pair cancel when close in a way that exactly conserves their expected future contributions. Branching is carried out keeping pairs to the largest extent possible. It includes the factors

$$\exp\left\{\delta\tau\left[E_T - \hat{H}\Psi_G^{\pm}(R^{\pm})/\Psi_G^{\pm}(R^{\pm})\right]\right\}$$

and is adjusted so that cancellation makes no change in the final answers. The correlations of the walkers have the property that such cancellation is not a rare event. A new fundamental ingredient for this algorithms is second stage importance sampling, which plays the role of the importance sampling but for pairs of walkers, and is intended to guide the pairs towards regions in which the signal to noise ratio in the energy average is maximized.

We have applied this method to two classes of many-body systems: fully-polarized systems of non-interacting fermions in a periodic box; and an unpolarized system of 14 ^{3}He atoms in a periodic box. Stability of the method is demonstrated for all three systems by the linear behavior of the denominator of the quotient used to calculate the energy. Normally, the "sign problem" makes this denominator asymptotically zero with statistical noise. The calculations of systems of free fermions give the analytic answer for the eigenvalue, and the atomic systems give eigenvalues in agreement with existing electronic structure results. The results for ^{3}He are reasonable based on comparison with variational and fixed nodes results for the same system. An extension of the calculation to 54 ^{3}He gives essentially the same stable results.

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TITLE

Thermodynamical Observables from the Quantum Hamiltonian

ABSTRACT

For the purpose to solve QFT on a space-time lattice, the Monte Carlo method has proven extremely useful. The enormous success of lattice gauge theory over the last two and half decades is due to the fact that the Monte Carlo method with importance sampling is an excellent technique to compute high (and even "infinite") dimensional integrals.

Despite this enormous success, lattice gauge theory, conventionally expressed by the action via the path integral, has brought only little computational progress in some areas, like (i) scattering amplitudes and cross sections, (ii) hadron structure functions, in particular for small Q^2, (iii) hadronic matter at finite density, (iv) spectrum of excited states and wave functions. For example, consider hadron spectra. Wave functions in conjunction with the energy spectrum contain more physical information than the energy spectrum alone. Although lattice QCD simulations in the Lagrangian formulation give good estimates of the hadron masses, one is yet far from a comprehensive understanding of hadrons. Let us take as example a new type of hardrons made of gluons, the so-called glueballs. Lattice QCD calculations[1] predict the mass of the lightest glueball with quantum number $J^{PC} = 0^{++}$, to be $1650 \pm 100 MeV$. Experimentally, there are at least two candidates: $f_0(1500)$ and $f_J(1710)$. The investigation of the glueball production and decays can certainly provide additional important information for experimental determination of a glueball. Therefore, it is important to be able to compute the glueball wave function.

In order to make progress on the above problems, the Hamiltonian formulation is a viable alternative, in our opinion. However, in the Hamiltonian formulation the genuine problem lies in the solution of the many-body problem. Recently, we made a new proposal in this direction [2, 3, 4, 5]. The idea is to construct an effective low energy Hamiltonian (in the sense of renormalisation à la Wilson-Kadanoff). This is done by taking over the virtues of the Monte Carlo method from the action to the Hamiltonian formulation. Via Monte Carlo we construct a so-called stochastic basis. From this basis we compute transition matrix elements again using Monte Carlo. Via algebraic diagonalisation we obtain the desired so-called **Quantum Hamiltonian**. The method has been tested and was found to work well in Q.M. for a number of potentials in D=1,2 and 3 dimensions. The quantum Hamiltonian has been computed and used for the calculation of spectra and thermodynamic observables, like average energy and specific heat [4, 5]. Here we want to report results of an application to a genuine many-body problem, the scalar ϕ^4 theory.

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Title

Investigation of the Sensitivity of the Monte Carlo Solution for the Barker-Ferry Equation Using Different Sequential and Parallel Pseudo-Random Number Generators

Abstract

Pseudo-random number generators (r.n.g.'s) are used in many algorithms for simulations in statistical physics, molecular dynamics and engineering. For many computational science applications, such as Monte Carlo simulation or stochastic optimization techniques, it is crucial that the r.n.g.'s have good randomness properties such as uniformly distributed, uncorrelated, have a large period of repetition and can be generated rapidly using limited computer memory. This is particularly true for large-scale simulations done on high-performance parallel computers. It is strongly recommended that all simulations be done with two or more different generators, and the results compared to check whether the r.n.g. is introducing a bias.

In this work we investigate the Monte Carlo (MC) solution for the Barker-Ferry equation [1] in the case of a zero electrical field, using various sequential and parallel r.n.g.'s. The quantum equation derived from the one-band model [6] for femtosecond relaxation of optically excited carriers accounts for the memory character of the electron-phonon interaction. The variance of the MC estimator for the electron energy distribution exponently increases with increasing evolution time [2]. We investigate the sensitiveness of the MC solution when various r.n.g's are used.

By definition, the constructive dimension (c.d.) of a Monte Carlo algorithm is the maximum number of uniformly distributed random numbers necessary for carrying out one trial [7]. In the case when an iterative MC algorithm computes the solution of the given problem using a terminated Markov chain the $c.d. = mE(l_\varepsilon)$, where $E(l_\varepsilon)$ is the mathematical expectation of the number of transitions in the Markov chain and m is the number of uniformly distributed random numbers in (0, 1) necessary to model one transition. Thus we can use random sequences from m parallel r.n.g's in order to compute every transition in the Markov chain.

The iterative MC algorithm presented in [2] is implemented using popular sequential r.n.g.'s and parallel pseudo-random number generator packages: CLCG (combined linear congruential generator) with parameters recommended by P. L'Ecuyer [4], the Scalable Parallel Random Number Generator (SPRNG) [5] Library and the shuffled nested Weyl sequences (SNWS) [3].

The Monte Carlo algorithm was tested using the material parameters for GaAs. Numerical results for the electron energy distribution at long evolution times are obtained. The computational cost of the algorithm, the accuracy and the discrepancy of the MC solution is investigated using the generators under consideration.

The numerical results show discrepancies in the MC solution when sequential r.n.g.'s are used; thus parallel r.n.g.'s are preferable to using sequential ones. Differences in behavior were also observed between the parallel pseudo-random number generators considered.

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Title

A Feynman-Kac Formula Implementation for the Linearized Poisson-Boltzmann Equation

Abstract

In this paper, we present a Feynman-Kac path-integral implementation for the Linearized Poisson-Boltzmann Equation (LPBE). This Feynman-Kac implementation is incorporated with the "Walks on Spheres" (WOS) method to provide a technique for estimating these path integrals without the need for simulating Brownian trajectories in detail. We interpret the exponential weighting in the Feynman-Kac implementation as a survival probability when we perform a WOS step. It is shown that this method is mathematically equivalent to the our previous modified WOS method for the LPBE. The effectiveness of this method is illustrated by computing the electrical potential in an electrolyte between two infinite charged parallel flat plates and is compared with our previous modified WOS method. While this method is somewhat slower than our previous method, this method holds the promise of extension to a method for the time-independent Schrödinger equation.