FINAL REPORT TO DOE

This is the final report to the Department of Energy concerning the grant DE-FG03-97ER25338 in support of the **Third International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing (MCQMC98)**. The Conference was held in Claremont, California from June 22, 1998 through June 26, 1998. The original grant period of September 1, 1997 through September 1, 1998 was extended at no cost (Amendment M001) to February 28, 1999 in a letter dated August 28, 1998 from Amy Lee to (then) Dean Murray Schwartz.

As reported in my letter of August 13, 1998 to Joyce Taylor requesting the no-cost extension, the Conference was regarded by all that participated as a great success. By any measure - the number of registrants, the number of presented papers, total financial support received, number of papers submitted for consideration in the Conference Proceedings - MCQMC98 surpassed the previous two international conferences (one held in Las Vegas in 1994 and the other in Salzburg, Austria in 1996) in every way. The attendees were lavish in their praise for the overall organization of the Conference. They were not only impressed with the technical programming, but commended us on the special events we had arranged for MCQMC98.

More than 90 persons from 21 countries registered for the Conference. A total of 74 papers (ten of these invited, hour-long addresses) were listed on the final program (see enclosed Program Book), although several were not given because of illness and

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unanticipated travel difficulties at the last moment. As evidence of the robustness of the technical program, 42 manuscripts were submitted for consideration in the Proceedings of the Conference, to be published by Springer-Verlag. These manuscripts are all under review at this writing. Although it is undoubtedly the case that not all of these manuscripts will appear in the published Proceedings, the final volume will represent an exceptionally strong contribution to the literature in this rapidly expanding area that spans many subdisciplines of both pure and applied mathematics.

As further evidence of the enthusiasm and support of the international mathematical community for the Claremont Conference:

1. All ten invited speakers promptly accepted their invitations. The list of invited speakers, and their affiliations, is:

1. *Harald Niederreiter, Austrian Academy of Sciences*
2. *Makoto Matsumoto, Keio University*
3. *Jerome Spanier, Claremont Research Institute of Applied
Mathematical Sciences*
4. *Thomas E. Booth, Los Alamos National Laboratory*
5. *Ahmed Badruzzaman, Chevron Petroleum Technology Company*
6. *George Fishman, University of North Carolina*
7. *Art Owen, Stanford University*
8. *Fred J. Hickernell, Hong Kong Baptist University*
9. *Henryk Wozniakowski, University of Warsaw and Columbia University*
10. *M. H. Kalós, Cornell University*

2. Thirteen of fourteen persons asked to serve on the International Program Committee accepted and served. The list of the members of the Program Committee, and their affiliations, is:

1. *Harald Niederreiter, Austrian Academy of Sciences*
2. *Pierre L'Ecuyer, Université de Montréal*
3. *Henryk Wozniakowski, University of Warsaw and Columbia University*
4. *Fred J. Hickernell, Hong Kong Baptist University*
5. *Gerhard Larcher, University of Salzburg*
6. *Jerome Spanier, Claremont Research Institute of Applied Mathematical Sciences*
7. *Ahmed Badruzzaman, Chevron Petroleum Technology Company*
8. *Kurt Binder, University of Mainz*
9. *Bennett Fox, SIM-OPT Consulting*
10. *Ely Gelbard, Argonne National Laboratory*
11. *Peter Glynn, Stanford University*
12. *John Halton, University of North Carolina*
13. *P. Shiue, University of Las Vegas*

3. Four federal grant proposals were submitted requesting total support of \$42,142.00; all four agencies responded with grants totaling \$38,792.00. The agencies, and the amounts requested and granted, are:

1. *Department of Energy*
Requested \$10,000
Received \$10,000
2. *National Security Agency*
Requested \$9,725
Received \$9,725
3. *National Science Foundation*
Requested \$12,267
Received \$12,267
4. *Army Research Office*

Requested \$10,150

Received \$6,800

4. An electronic database of Monte Carlo and quasi-Monte Carlo expertise, developed with the help of a NSF grant, was implemented in advance of the Claremont Conference. Beginning with its first entry on October 28, 1997, the database now has 96 persons listed in it, together with key information on how these individuals may be contacted, their areas of expertise/interest, etc. It was expected that this database would serve for the international community as a permanent repository of information. With the successful recent transfer of the database to Hong Kong (site of the Fourth International Conference on Monte Carlo & Quasi-Monte Carlo Methods in Scientific Computing in the year 2000), that permanence is now assured.

Department of Energy financial support contributed in a major way to the success of the Claremont Conference. For example, \$6,050.06 (\$6,000 was allocated) was awarded to 11 conference participants in support of travel and other conference-related expenses. These awards ranged from \$130 for the reimbursement of registration fees to \$1,250 in support of travel and local expenses incurred by one of our invited speakers.

A total of \$1,711.33 (out of \$2,000 allocated) was spent on printing and other costs associated mainly with advance advertisement of the Claremont conference and to pay the major costs associated with the preparation and distribution of registration materials.

A total of an additional \$1,957.19 (out of \$2,000 allocated) was spent on a large number of items – including \$1,264.57 for 125 registration tote bags - and costs associated with copying, faxing, and mailing conference materials.

~~A detailed financial report follows:~~

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CONFERENCE PROGRAM BOOK

**June 22-26, 1998
Claremont, California USA**

**CONFERENCE
PROGRAM**

MCQMC98 Technical Program Monday, June 22 1998		
8:15	Plenary Opening Session Galileo Hall - McAlister Auditorium Welcome: Jerome Spanier, Conference Co-Chair and John D. Maguire, President of Claremont Graduate University	
9:00	Invited Session 1 Chair: Jerome Spanier Galileo Hall - McAlister Auditorium Invited Speaker: Harald Niederreiter Constructions of (t,m,s)-Nets	
10:00	Break	
	Technical Sessions 1A Chair: H. Niederreiter Galileo/Pryne	Technical Sessions 1B Chair: J. Spanier Galileo/Edwards
10:30	Michael Mascagni Testing Parallel Random Number Generators	Eric Veach Metropolis Particle Transport: a New Approach to Transport Problems
10:55	Hannes Leeb The Higher-Dimensional Properties of Pseudo-Random Variates	Herbert Rief A Method for the Exact Solution of Linear Systems based on Monte Carlo Gradient Estimation
11:20	Sibylle Strandt New Results for the Quadratic Congruential Pseudorandom Number Generator	Hedley Morris Active Walk Models in Biological Evolution
12:00	Lunch	
1:30	Invited Session 2 Chair: P. L'Ecuyer Galileo Hall - McAlister Auditorium Invited Speaker: M. Matsumoto Dynamic Creation of Pseudorandom Number Generators for Distributed Systems	
	Technical Sessions 2A Chair: P. L'Ecuyer Galileo/Pryne	Technical Sessions 2B Chair: J. P. Lambert Galileo/Edwards
2:30	Ken Umeno Permutable Ergodic Transformations with Non-Uniform Densities and their Applications to Monte Carlo Methods	G. Paulmier Monte Carlo Simulation of Photometric Measurements in Fog
2:55	C-R Hwang On the Average-Case Analysis of Dynamic Monte Carlo Schemes	Eric Dumont Quasi-Monte Carlo Light Tracing Applied to the Problem of Road Visibility in Fog
3:20		Alexander Keller Photorealistic Rendering using the Method of Dependent Tests
3:45	Break	
	Technical Sessions 3A Chair: J-P. Shiue Galileo/Pryne	Technical Sessions 3B Chair: TBA Galileo/Edwards
4:00	Michael Mascagni SPRNG: A Scalable Library for Monte Carlo Applications	Henry Schellhorn Variance Reduction Techniques for Large Scale Risk Management
4:25	U. Dieter Pseudorandom Numbers: The Discrepancy in Dimension Two	Genevieve Gauthier Evaluation of the Variance of Derivative Securities Prices Obtained with an Empirical Martingale Simulation
5:30	Welcome Reception and Barbeque Dinner Hixon Court Wine/Beer: 5:30-6:30 Dinner: 6:30 - 7:30	

MCQMC98 Technical Program

Tuesday, June 23 1998

8:30	Invited Session 3 Chair: Harald Niederreiter Galileo Hall - McAlister Auditorium Invited Speaker: J. Spanier Geometrically Convergent Learning Algorithms for Global Solutions of Transport Problems	
	Technical Sessions 4A Chair: H. Faure Galileo/Pryne	Technical Sessions 4B Chair: H. Rief Galileo/Edwards
9:30	Yijun Xiao The Diaphony and the Star-Diaphony of some Two-Dimensional Sequences	Rong Kong and Jerome Spanier Sequential Correlated Sampling Methods for some Transport Problems
9:55	Wolfgang Schmid Improvements & Extensions of the "Salzburg Tables" by using Irreducible Polynomials	Yongzeng Lai and Jerome Spanier Adaptive Importance Sampling Algorithms for Transport Problems
10:20	Gang Wei Best Representative Points in the Square	Carole Hayakawa and Jerome Spanier Comparison of Monte Carlo Algorithms for Obtaining Geometric Convergence for Model Transport Problems
10:45	Break	
	Technical Sessions 5A Chair: M. Mascagni Galileo/Pryne	Technical Sessions 5B, Chair: C. Lecot Galileo/Edwards
11:00	Stefan Weggenkittl Structures in the Scatterplots of Inversive Generators	Giray Ökten Mixed (s,d) Sequences: Theory & Applications
11:25	Hannes Leeb The Limit Laws of the Spectral Test and Related Variants	Liming Li Quasi-Monte Carlo Simulation Methods for Measurement Uncertainty
12:00	Lunch	
1:30	Invited Session 4 B. Fox, Chair Galileo - McAlister Auditorium Invited Speaker: T. E. Booth Adaptively Learning an Importance Function using Transport Constrained Monte Carlo	
	Technical Sessions 6A Chair: M. Matsumoto Galileo/Pryne	Technical Sessions 6B Chair: A. Badruzzaman Galileo/Edwards
2:30	Pierre L'Ecuyer and Richard Simard Systematic Tests of RNG Families	S. Heinrich Wavelet Monte Carlo Methods for the Global Solution of Integral Equations
2:55	Jürgen Eichenauer-Herrmann and Eva Herrmann New Results and Recent Improvements in the Analysis of Modified Inversive Congruential Pseudorandom Numbers with Power of Two Modulus	Rong Kong and Jerome Spanier Error Analysis of Sequential Monte Carlo Methods for Transport Problems
3:20	Hozumi Morohoshi and Masanori Fushimi Designing Asymptotically Random GFSR Sequences	Y. Z. Kandiev and G. N. Malyshev The Importance Biasing Scheme Implemented in PRIZMA Code
3:45	Break	
	Technical Sessions 7A Chair: F. Su Galileo/Pryne	Technical Sessions 7B Chair: T. E. Booth Galileo/Edwards
4:00	J.P. Lambert Perspectives on a Dyadic 2-Dimensional Van der Corput Sequence	Henry J. Alme, Garry H Rodrigue and George B. Zimmerman Domain Decomposition for Parallel Fluid Models with Monte Carlo Transport
4:25	Henri Faure An Equidistribution Property in Relation with Lower Bounds for Discrepancy	Aldo H. Romero, David Rapson and Ivan K. Schuller Resistance Exponential Dependence on Thickness of Thin Films: a Classical Monte Carlo Study
5:00	Conference Photo Hixon Court	
8:00	Free Concert Albrecht Auditorium, CGU	

MCQMC98 Technical Program Wednesday, June 24 1998		
8:30	Invited Session 5 Chair: T. E. Booth Galileo Hall - McAlister Auditorium Invited Speaker: A. Badruzzaman Transport Theory Methods for Geophysical Problems	
	Technical Sessions 8A Chair: H. Wozniakowski Galileo/Pryne	Technical Sessions 8B Chair: G. Fishman Galileo/Edwards
9:30	P. Baldi, L. Caramellino and M. Iovino Pricing Barrier Options with General Features: a Large Deviation Approach	Sven-Ake Gustafson Monte Carlo Approaches to Linear Semi-Infinite Optimization
9:55	A. Kreinin, L. Merkoullovitch, D. Rosen and M. Zerbs Application of Quasi-Monte Carlo and Stratified Sampling Methods to Measure Portfolio Risk	William Martin Linear Programming Bounds for Ordered Orthogonal Arrays and (t,m,s)-Nets
10:20	Yongzeng Lai and Jerome Spanier Applications of Monte Carlo and Quasi-Monte Carlo Methods in Finance: Option Pricing	Kaiqi Xiong and Jerome Spanier Monte Carlo Methods and Importance Sampling Algorithms for Nonlinear Filtering Problems
10:45	Break	
11:00	Invited Session 6 Chair: P. Glynn Galileo Hall - McAlister Auditorium Invited Speaker: G. Fishman Making it Easier to Assess the Accuracy of Time Averages in Discrete-Event Simulation and Markov Chain Monte Carlo Experiments	
12:00	Lunch	
1:00 to 8:00	Getty Center Trip Buses Depart 1:15 pm Arrive at Getty Center 2:30 pm Buses Return 7:00 pm Arrive Claremont 8:30 - 9:00 pm	

MCQMC98 Technical Program

Thursday, June 25 1998

8:30	Invited Session 7 Chair: F. Hickernell Galileo Hall - McAlister Auditorium Invited Speaker: Art Owen Randomized Quasi-Monte Carlo Methods	
	Technical Sessions 9A Chair: J. Myhre Galileo/Pryne	Technical Sessions 9B Chair: H. Krieger Galileo/Edwards
9:30	Kai-Tai Fang and Peter Winker Uniformity and Orthogonality	Geon Choe, Chihurn Kim and Dong Han Kim Tests of Randomness using the First Return Time
9:55	M. Ostland and B. Yu Exploring Quasi-Monte Carlo for Marginal Density Approximation	Christian Lecot and Afiss Koudiraty Grid-free Simulation of Convection-Diffusion
10:20	Janet Myhre and Solly Sieberts Accuracy of Approximate Bounds for the Reliability of Coherent Systems	Christiane Lemieux and Pierre L'Ecuyer A Comparison of Monte Carlo, Lattice Rules and Other Low-Discrepancy Point Sets
10:45	Break	
11:00	Invited Session 8 Chair: H. Wozniakowski Galileo Hall - McAlister Auditorium Invited Speaker: F. Hickernell What Affects the Accuracy of Quasi-Monte Carlo Quadrature?	
12:00	Lunch	
1:30	Invited Session 9 Chair: A. Owen Galileo Hall - McAlister Auditorium Invited Speaker: H. Wozniakowski Efficiency of Quasi-Monte Carlo Algorithms for High Dimension	
	Technical Sessions 10A Chair: A. Owen Galileo/Pryne	Technical Sessions 10B Chair: K. Cooke Galileo/Edwards
2:30	T. Langtry A Discrepancy-Based Analysis of Figures of Merit for Lattice Rules	Francis Edward Su Random Walk Discrepancy Bounds
2:55	Thomas Gerstner and Michael Griebel Multivariate Sparse Grid Integration and its Applications	Nikolai A. Simonov Monte Carlo Conditional Estimator for Diffusion in a Random Field
3:20	Karl Entacher, Peter Hellekalek and Pierre L'Ecuyer Quasi-Monte Carlo Integration with Linear Congruential Generators	
3:45	Break	
	Technical Sessions 11A Chair: F. Hickernell Galileo/Pryne	Technical Sessions 11B Chair: A. Keller Galileo/Edwards
4:00	Alan Genz Methods for Generating Random and Quasi-Random Orthogonal Matrices	Francesc Castro and Mateu Sbert Application of Quasi-Monte Carlo Sampling to the Multi-Path Method for Radiosity
4:25	Hozumi Morohosi and Masanori Fushimi A Practical Approach to the Error Estimation of Quasi-Monte Carlo Integrations	Philippe Bekaert, Ronald Cools and Yves D. Willems The Effectiveness of Quasi-Monte Carlo Sampling for Solving the Radiosity Problem
4:50	John Halton A Rigorous Justification for Quasi-Monte Carlo Methods and Valid Statistical Estimates of their Accuracy	
	Closing Banquet Faculty House	
6:30	Reception	
7:00	Dinner	

MCQMC98 Technical Program**Friday, June 26 1998**

8:30	Invited Session 10 Chair: E. M. Gelbard Galileo Hall Invited Speaker: M. H. Kalos Fermion Monte Carlo	
	Technical Sessions 12A Chair: M. H. Kalos Galileo/Pryne	Technical Sessions 12B Chair: J. Cuzick Galileo/Edwards
9:30	Wolfgang Wagner Monte Carlo Methods for Nonlinear Equations	Zhongping Chen, Tore Lindmo, Derek J. Smithies, Thomas E. Milner and J. Stuart Nelson Monte Carlo Simulation of Optical Coherence Tomography and Optical Doppler Tomography
9:55	S. M. Prigarin Spectral Models of Random Fields: Theory and Applications	Habib Zaidi Design of Nuclear Medical Imaging Systems using the Monte Carlo Method
10:20	Boris A. Kargin, Ulrich G. Oppel and Sergei M. Prigarin Monte Carlo Methods in Stochastic Problems of the Atmosphere-Ocean Optics	
10:45	Break	
	Technical Sessions 13 Chair: W. Wagner Galileo/Pryne	
11:00	Victor Antyufeev Monte Carlo Solution of the Generalized Transport Equation with Highly Peaked Phase Function	
11:25	A. S. Rasulov Monte Carlo Method for Solution of Nonlinear Neyman's Problem	
12:00	Conference Concludes	

**PROGRAM
ABSTRACTS**

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Domain Decomposition for Parallel Laser-Tissue Models with Monte Carlo Transport²

Using parallelism in simulations that use Monte Carlo transport methods presents interesting problems. For problems that require domain decomposition, load balance can be harder to achieve. The Monte Carlo transport package may have to operate with other packages that have different optimal domain decompositions for a given problem. To examine some of these issues, we have developed a code that simulates the interaction of a laser with biological tissue; it uses a Monte Carlo method to simulate the laser and a finite element model to simulate the temperature field in the tissue. We will present speedup and load balance results obtained for a suite of problems decomposed using a few domain decomposition algorithms we have developed.

¹Speaker

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Monte Carlo Solution of the Generalized Transport Equation with Highly Peaked Phase Function

Radiation transfer in a deterministic medium may be described by the "standard transport equation". It can be written in two forms: integro-differential form and integral equation of the second kind. For a stochastic medium (broken clouds, for instance) we use an averaged transport equation in integral form. We shall call it "generalized equation". It looks like the standard transport equation in integral form, but there are two major differences:

1. it cannot be represented in integro-differential form;
2. the probability density for free path length has a different form.

When the phase function is highly peaked (looks like a delta-function) the statistical estimation has a large variance and the accuracy of the Monte Carlo computation is very low.

In case of the standard transport equation it is easy to get around this difficulty by a simple algebraic transformation in the integro-differential equation. But in the case of non-standard generalized equation we cannot use the same transform because it does not have integro-differential form.

In this work a special transformation is proposed, so that the phase function transforms into another phase function without a peak and the free path density takes another form.

Numerical experiments have shown large increase in efficiency of Monte Carlo computation.

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Transport Theory Methods for Geophysical Problems

Computational methods based on radiation transport theory are used to study the response characteristics of nuclear measuring devices that are used to probe geological media, primarily by the oil industry. Both Monte Carlo techniques and deterministic solutions of the linear Boltzmann Transport Equation have been utilized. Monte Carlo techniques can represent, almost exactly, the complex geometry and physics that arise in these problems and are thus the techniques of choice in these problems. However, Monte Carlo methods are handicapped by the statistical errors that make them computationally intensive to achieve a required precision in nuclear geophysical problems. Deterministic methods discretize the phase space variables. The resultant approximation of the non-orthogonal curved geometry can yield large errors in the solution. The paper discusses a number of applications of both methods to solve geophysical problems using nuclear sources.

There has been a considerable effort to advance the state-of-the-art in these methods for nuclear geophysical problems. Advances in Monte Carlo methods include the recent work to improve the efficiency by using quasi-random sampling, modified expected-value estimation, and perturbation theory techniques. Developments in deterministic methods include, finite moments techniques based on integrating the transport equation, a boundary-fitted coordinate transformation of the transport equation to address the difficulty of treating the non-orthogonal curved geometry in geophysical problems, and arbitrary non-orthogonal mesh techniques.

Finally, we discuss a Boltzmann Transport Equation formulation of a non-nuclear geophysical problem, namely hydrological transport in fractured rocks that includes possible transport of radionuclides in groundwater. A transport theory formulation will address the limitations of the current (diffusion theory) formulation of this highly forward-peaked problem in terms of Darcy's equation. With a transport theory formulation, we can readily utilize techniques that have been developed for the radiation transport problem. Finite moments transport techniques that possess the appropriate boundary, interface and asymptotic properties, and Monte Carlo methods will be of particular interest. Of course, the non-linear aspects of the flow problem will have to be addressed to make radiation transport theory methods compatible with it.

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The Effectiveness of Quasi-Monte Carlo Sampling for Solving the Radiosity Problem

We discuss the application of quasi-Monte Carlo simulation for computing the illumination in Lambertian (diffuse) environments, an important problem in computer graphics. Quasi-Monte Carlo techniques have been introduced for solving the radiosity problem by Alexander Keller (see e.g. [1, 2]) some years ago. In these papers however, quasi-Monte Carlo sampling appears to be only slightly more effective than pseudo-random sampling. Recently, other radiosity algorithms have appeared (e.g. [3]) in which quasi-Monte Carlo sampling leads to much faster convergence.

Depending on the equations that are being solved, two classes of quasi-Monte Carlo algorithms can be distinguished:

- Some algorithms, such as those in [1, 2], directly solve the second kind Fredholm integral equation that describes the light transport without discretisation;
- Other quasi-Monte Carlo radiosity algorithms, such as [3], assume that the surfaces in the environment are discretised into patches. On each patch, the radiance is approximated by a low-order polynomial approximation.

An empirical comparison of quasi-Monte Carlo radiosity algorithms suggests that quasi-Monte Carlo sampling is significantly more effective when applied to the latter class of algorithms.

References

- [1] A. Keller, *A Quasi-Monte Carlo Algorithm for the Global Illumination Problem in the Radiosity Setting*, Lecture Notes in Statistics, 106 (ed. by H. Niederreiter and P. Shiue), pp. 239-251.
- [2] A. Keller, *Quasi-Monte Carlo Radiosity*, Rendering Techniques '96, (ed. by X. Pueyo and P. Schröder), Springer, 1996, pp. 101-110. Also in Proceedings of the 6th Eurographics Workshop on Rendering, Porto, Portugal, June 1996.
- [3] A. Neumann, L. Neumann, Ph. Bekaert, *Radiosity with Well Distributed Ray Sets*, Computer Graphics Forum, Vol 16 nr 3, August 1997, (Proceedings of Eurographics '97, Budapest, Hungary), pp. 261-270.

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Pricing Barrier Options with General Features: A Large Deviation Approach

In the past few years barrier options have become increasingly popular in the financial markets. These derivatives allow practitioners to hedge their exposures without paying for states they believe are unlikely to occur.

Since Merton's seminal paper in 1973, closed-form solutions have been provided for options with constant barriers (see [5]), as well as for time-varying barriers (see [6]), under the Black and Scholes model. However, the hypothesis of lognormal rate of returns for the underlying asset prices carries well known biases. This has led recent literature to focus on the pricing of barrier options under more general models. In 1997, Boyle and Tian (see [4]) offered a numerical solution to the pricing of barrier options with constant barriers, under the Constant Elasticity Variance (CEV) process.

As it stands, one is forced to use Monte Carlo simulations for handling the pricing of options with general curved barriers when the underlying asset price evolves as a diffusion process. As it has been already pointed out by several authors, such a method does not provide good results.

In this work, we propose a numerical procedure which improves the standard Monte Carlo by introducing a correction involving Sharp Large Deviation estimates. For this purpose, we determine a reasonable approximation of the conditional probability that the underlying price process hits the barriers without being detected by the standard Monte Carlo procedure.

In conclusion, our method is very general and can include several Markovian models (for which the corresponding bridges are independent). Moreover, numerical comparisons with frameworks where pricing formulas are available have shown the accuracy of the procedure proposed with respect to the standard Monte Carlo (which could achieve the same accuracy only by reducing drastically the step-size). Finally, the correction probability shows a very simple form and the complexity of the standard simulation algorithm is not changed by introducing the correction.

References

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- [2] Baldi, P., Caramellino L., M.G. Iovino: Pricing Single and Double Barrier Options via Large Sharp Deviations Techniques. Working paper, (1997)

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Adaptively Learning an Importance Function using Transport Constrained Monte Carlo

It is well known that a Monte Carlo estimate can be obtained with zero-variance if an exact importance function for the estimate is known. There are many ways that one might iteratively seek to obtain an ever more exact importance function. This paper describes two methods that have obtained ever more exact importance functions that empirically produce an error that is dropping exponentially with computer time. A common feature of these two methods is that the importance function is constrained in some way by the (adjoint) Boltzmann transport equation. These constrained methods will be contrasted with one or two unconstrained methods.

Figure 1 shows exponential convergence for transport on a line and Figure 2 shows exponential convergence for transport through a slab.

1mfp c=.5 1000 particles/iteration fsdma=1.e8

(mmx=0 for 0-th iteration) xza14.f

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Application of Quasi-Monte Carlo Sampling to the Multi-Path Method for Radiosity

The multi-path method [5, 6] is a Monte Carlo technique that solves the radiosity problem, i.e. the illumination in a scene with diffuse (also called lambertian) surfaces. This technique uses random global lines for the transport of energy, contrary to classic techniques, in which the lines used are local to the surface where they exited from. The global lines are drawn taking pairs of points on the surface of a sphere surrounding the scene, obtaining thus a uniform density [4, 5]. The multi-path technique borrows results from Integral Geometry [3, 4] to predict the correct transfer of energy, and can be shown to be a random walk method, in which a physical path transports many logical paths, similar to the covering paths described in Rubinstein [2].

We will study in this paper the application of quasi-Monte Carlo sequences to the generation of the global lines. It will be shown that we have to use 4-dimensional sequences, as with 2-dimensional ones there is a high correlation between the points in a pair, and this would result in a non uniform distribution of lines. Important improvements in the efficiency of the multi-path method for certain sequences will be demonstrated. Alternative ways of generating global lines will also be studied in the context of quasi-Monte Carlo. The generation of uniform densities of lines has become a key issue in the new field of Image-based Rendering [1].

References

- [1] M. Levoy and P. Hanrahan. Light-field rendering. In *Computer Graphics, Annual Conference Series, 1996 (SIGGRAPH '96 Proceedings)*.
- [2] Reuven Y. Rubinstein, *Simulation and the Monte Carlo method*. John Wiley & Sons, New York, 1981.
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On the Average-Case Analysis of Dynamic Monte Carlo Schemes

In many situations the evaluation of expectations in large sample spaces has to resort to approximation by Monte Carlo methods. Moreover a direct sampling from the very large underlying space is not feasible, hence, dynamic Monte Carlo methods are often used. Mathematically the following setup is considered. Let π be a fixed probability measure on a finite set S . Let $X_0, X_1, \dots, X_n, \dots$ be a Markov chain with transition matrix P and the equilibrium probability π . Under suitable condition on P , it is known that $\frac{1}{n} \sum_{k=0}^{n-1} f(X_k)$ converges to $\sum_{s \in S} f(s)\pi(s)$, denoted by $\pi(f)$, for any real-valued function f defined on S . Moreover the corresponding asymptotic variance, denoted by $v(f, P)$, depends only on f and P . Regarding P as a theoretical algorithm, it is natural to consider $v_a(P)$, defined by averaging $v(f, P)$ over f with $\sum_{s \in S} f(s)^2 \pi(s) = 1$ and $\pi(f) = 0$, as a quantity to evaluate the average performance of P without exploiting any prior knowledge on any specific f . This quantity is related to $\text{trace}(I - P)^{-1}$ where the inverse is taken in the space with $\pi(f) = 0$. The minimizer of $v_a(P)$ for P in some general classes is still open. Special case and worst-case analysis will also be discussed.

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Monte Carlo Simulation of Optical Coherence Tomography and Optical Doppler Tomography

Optical coherence tomography (OCT) and optical Doppler tomography (ODT) are promising non-invasive optical technology for high-resolution biomedical imaging of static tissue structures as well as blood flow. Imaging depth and imaging resolution are, however, strongly influenced by the optical properties of the imaging medium. Multiple scattering effects not only cause loss of localized signal but may also cause artifacts such as flow shadowing underneath vessels containing flowing blood. A better understanding of the OCT and ODT imaging process in highly turbid media would facilitate instrument development and identification of promising application areas for OCT/ODT.

A Monte Carlo simulation model has been developed to study how OCT and ODT imaging results are influenced by multiple scattering effects. The OCT/ODT simulation is designed such that different device parameters can be investigated from a photon history file generated from a single Monte Carlo simulation. The simulation can be divided into four modules: launching of photons, generation of photon histories, detection of photons with coherence gating, and processing and visualization. The physical model comprises a blood vessel surrounded by a scattering medium, which consists of intralipid for in vitro studies and epidermal and dermal layers for human skin. A parabolic velocity profile is assumed for blood flow in small vessels. Simulated depth profiles of average Doppler frequency shift demonstrated good accuracy in absolute velocity values and localization of flow boundaries (3-4 % deviation). Doppler frequency noise was observed in backscattering from regions underneath the vessel. The effects of multiple scattering and coherence gating, as well as probing parameters such as confocality and numerical aperture, on OCT/ODT images in turbid fluid flow media will be reported.

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Tests of Randomness using the First Return Time

Entropy is the limit of $-\frac{1}{n} \sum_i p_i \log p_i$ as $n \rightarrow \infty$, where the p_i 's are the relative frequencies of blocks of length n in a binary sequence. It measures the amount of randomness.

In the conventional entropy test one has to estimate the value p_i of the i -th block of length n and investigate the behavior of $-\frac{1}{n} \sum_{i=1}^{2^n} p_i \log p_i$. In this paper we use a different definition of entropy: For each sample sequence $x = (x_1, x_2, \dots)$ of an ergodic finite valued stationary source define the first return time by $R_n(x) = \min\{j \geq n : x_1 \dots x_n = x_{j+1} \dots x_{j+n}\}$. It is known that $\frac{\log R_n(x)}{n}$ converges to the entropy for almost every sequence x . We employ $\log R_n$ as a test random variable for randomness of prng's.

The method of using the expectation of R_n itself is so weak that even the rng RANDU does not fail the test. We find the exact discrete probability distribution for the random variable R_n and apply the Kolmogorov-Smirnov test, which forces RANDU, Microsoft C and ANSI C to fail the test. Or we use the expectation of $\log R_n$, which performs as well as the K-S test using the exact distribution of R_n .

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Pseudo Random Numbers: The Discrepancy in Dimension 2

For each sequence $\{u_i\}$ of $[0, 1)$ - uniformly distributed random numbers the quantity

$$\Delta_n(s_j, t_j) = \frac{\#\{U_i = (u_{i+1}, \dots, u_{i+n}) \mid s_j < u_{i+j} < t_j\}}{\#\{U_i = (u_{i+1}, \dots, u_{i+n})\}} - \prod_{j=1}^n (t_j - s_j) \quad (1)$$

is called the local deviation, and its supremum

$$\Delta_n = \sup \{|\Delta_n(s_j, t_j)| \mid 0 \leq s_j \leq t_j \leq 1, j = 1 \dots n\} \quad (2)$$

is called the "discrepancy" of the sequence. Most computer programs generate uniform random numbers by the "Linear Congruential Method", for which some results are known.

For $n = 2$ U. Dieter [1971] showed that the local deviation is an alternating sum of four generalized Dedekind sums. For its supremum the greatest and smallest values of these sums have to be known. These values were calculated by D.E. Knuth in his paper of 1977. Hence the discrepancy can be calculated by simple computer programs. A different method of Afflerbach and Weilbacher [1988] needs large computer times. The exact values are close to the upper bounds which were published by U. Dieter in 1971. The lowerbounds of U. Dieter and H. Niederreiter [1978] are far away from the exact values. For $n > 2$ only bounds are known, which are difficult to calculate.

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Evaluation of the Variance of Derivative Securities Prices Obtained with an Empirical Martingale Simulation

Monte Carlo simulation is now a widely used tool in finance. The method is especially useful for estimating theoretical prices of derivatives securities model for which there is no analytical solution. Recently, because rapidity plays a key role in option pricing estimation, new variance reduction methods have been introduced in this field. These techniques, known as moment matching techniques (Boyle, Broadie and Glasserman 1997), are easy to apply and demand very little computing effort. One drawback of these techniques is that we usually lose the standard error estimator of the price estimate. Furthermore, it is not clear if the modified estimator obtained with this method is still asymptotically normal. Studying a particular moment matching method known as the empirical martingale simulation (Duan and Simonato 1998), we use the dependency structure between the generated observations to evaluate the variance of the price estimate. It is then possible to measure the gain in precision obtained from this variance reduction method. A numerical study follows, showing the efficiency of the method.

¹Speaker

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Quasi-Monte Carlo Light Tracing Applied to the Study of Road Visibility in Fog

Simulation is a valuable tool as a complement to experiments for the network of Laboratoires des Ponts et Chaussées in its research on road safety in fog. A quasi-Monte Carlo simulation code has been implemented in order to study the influence of fog microphysical characteristics on visibility.

A pure Monte Carlo method proved to be quite inefficient when dealing with small detectors like photometers or cameras. A review of existing computer graphic methods to render anisotropic scattering media like fog showed that stochastic methods are still more versatile and closer to physical reality, compared to finite element based methods. So we implemented a quasi-Monte Carlo light tracing technique, which simulates multiple scattering of light by fog in an intuitive way, and allows us to collect photometrical data.

This paper describes this quasi-Monte Carlo light tracing technique and how we get accurate photometrical values. The photometer calibration procedure is modeled and used as a test. Then we give an example of application which compares the effect of various types of fog (with different particle size distributions) on the visibility of a speed limit sign. Finally, possible improvements are presented which could increase speed of convergence and reduce noise.

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New Results and Recent Improvements in the Analysis of Modified Inversive Congruential Pseudorandom Numbers with Power of Two Modulus

Nonlinear methods for the generation of uniform pseudorandom numbers for stochastic simulations provide promising alternatives to classical linear generators. Their theoretical and empirical analysis is currently a particularly active field of research. The results that have been obtained so far clearly indicate that inversive congruential methods play an outstanding role in this area. These pseudorandom number generators achieve nonlinearity by multiplicative inversion in modular arithmetic. The talk will concentrate on the important case of a power of two modulus $m = 2^\omega$ and the modified inversive congruential method, which was introduced and studied in [1]. This computationally interesting approach is based on a generalized multiplicative inverse modulo m defined by $(0)^- = 0$ and $(2^\alpha z)^- \equiv 2^\alpha z^{-1} \pmod{m}$ for $\alpha \geq 0$ and odd integers z , where z^{-1} denotes the usual multiplicative inverse modulo m satisfying $zz^{-1} \equiv 1 \pmod{m}$. In the talk, improved versions of the main results in [1] and several new results on the theoretical properties and the empirical behavior of the generated pseudorandom numbers will be presented and discussed.

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Quasi-Monte Carlo Integration with Linear Congruential Generators

In this paper we present a new approach to finding good lattice points. We use a well-known figure of merit for uniform random number generators, the so-called spectral test. This concept leads to an assessment of lattice points $\mathbf{g}$ that is closely related to the classical quantity $\rho(\mathbf{g}, \mathbf{N})$. The spectral test can be implemented very efficiently. We present tables of good lattice points for sample sizes up to 2^{31} and dimensions up to 30. Further, we compare the performance of our integration nodes to the best available (t, m, s) nets and show how the spectral test quantity is related to $\rho(\mathbf{g}, \mathbf{N})$ by general inequalities.

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Uniformity and Orthogonality

An $n \times s$ matrix with entries $1, \dots, q$ is called an orthogonal design (OD) if it satisfies: 1) each entry in each column occurs the same number of times and 2) in any two columns each pair $(1, 1), \dots, (1, q), (2, 1), \dots, (2, q), \dots, (q, q)$ occurs the same number of times. The OD is one major kind of fractional factorial designs with good properties and has been widely used. Most of existing ODs are obtained by orthogonal Latin squares, Hadamard matrices, group theory and finite fields during the past decades.

In this talk we propose alternative approach on construction of the ODs. We treat each OD as a uniform design, i.e., a U-type design with the best uniformity under a certain sense. An $n \times s$ matrix U with entries $1, \dots, q$ is called a U-type design if each entry in each column occurs the same number of times. Each OD is a U-type design, but the inverse is not true. The induced matrix $X = (x_{ij})$ of U is defined by $x_{ij} = (u_{ij} - 0.5)/q$ and represents n points in $C^s = [0, 1]^s$. Let D be a measure of uniformity defined on C^s , for example, the symmetric L_2 -discrepancy or the centered L_2 -discrepancy suggested by Hickernell (1995). For given n, s, q and the discrepancy D , we find that most ODs can be obtained by minimizing D of the induced matrix over all U-type designs of size $n \times s$. The threshold accepting algorithm, one of global optimization algorithms, plays an important role in minimizing the discrepancy D .

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An Equidistribution Property in Relation with Lower Bounds for Discrepancy

In this communication, we present improved lower bounds for the discrepancy of special infinite sequences in two dimensions; these lower bounds are based on an equidistribution property for the sums of binomial coefficients modulo a prime number; we think the proof of this property is interesting in itself, in particular because the method for the proof of the well known result on the equidistribution of non-zero binomial coefficients does not apply in this case.

We are interested in the following two-dimensional sequences, denoted S_b^f with b prime, which have the smallest discrepancy presently known:

given integers $b \geq 2$ and $n \geq 1$, let $n - 1 = \sum_{r=0}^{\infty} a_r(n) b^r$ be the expansion of $(n - 1)$ in base b ; the van der Corput sequence in base b is $\phi_b(n) = \sum_{r=0}^{\infty} a_r(n) b^{-r-1}$;

for f integer, $1 \leq f \leq b - 1$, let $\binom{h}{l}_f = \binom{h}{l} f^{h-l}$ be the generalized " f -binomial" coefficient;

given a prime base b , we denote by S_b^f the sequence $(\phi_b, C^f \phi_b)$ in which

$$C^f \phi_b(n) = \sum_{j=0}^{\infty} y_j^f(n) b^{-j-1} \text{ with } y_j^f(n) = \sum_{r \geq j} \binom{r}{j}_f a_r(n) \bmod b;$$

with the notation $d_2(X) = \limsup_{N \rightarrow \infty} (D^*(N, X) / (\log N)^2)$, in which D^* is the usual star discrepancy, we have the following lower bound for any prime base b :

$$d_2(S_b^1) \geq \frac{\max\left(\frac{1}{4}, \frac{1}{2} - \frac{1}{b-1}\right)}{(b^2 \log b)^2};$$

we conjecture the same result holds for all S_b^f ; at the present, we have only the property for special cases.

The equidistribution property reads as follows:

let $\sigma(c, l) = \sum_{h=0}^l \binom{c}{h}$ modulo b ; then the $\sigma(c, l)$, for $0 \leq l \leq c < b^n$, are equidistributed in the residue classes modulo b , as n tends to infinity. The method, using the Perron-Frobenius theorem, applies also to $\binom{c}{l}$ and gives a new proof of the result for the non-zero binomial coefficients modulo b .

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Making it Easier to Assess the Accuracy of Time Averages in Discrete-Event Simulation and Markov Chain Monte Carlo Experiments

While regularly mentioned in many courses in simulation, the statistical analysis of sample path output data is rarely performed; and if performed, rarely supported by rigorous statistical theory. Why is this so?

Unlike sample sequences of i.i.d. data on which so much of elementary statistics focuses, sample paths generated in discrete-event simulations and Markov Chain Monte Carlo experiments usually contains correlated data. As a consequence, assessing how well a time average, based on a finite sample path length, approximates a long-run system time average calls for more than elementary statistical methods. Although techniques for performing this assessment are well known, they have traditionally been cumbersome to apply in practice, thus limiting their use.

This presentation aims at overcoming these impediments by describing newly available software, LABATCH.2, a collection of computer programs available in C, FORTRAN, and SIMSCRIPT II.5, that perform statistical analyses on multiple sample sequences collected on strictly stationary stochastic processes. It may be invoked in-line by a single statement each time a data vector is generated within an executing program (e.g., simulation), or it may take its input from a stored data file. For sample path length t , LABATCH.2 takes $O(t)$ computing time and $O(\log_2 t)$ space. LABATCH.2, offers an interactive option, is available by anonymous ftp, and is considerably more user friendly than an earlier package called LABATCH.

LABATCH.2 contains decision rules that automatically lead to the computation of a strongly consistent estimator of the asymptotic variance of the time average for each series and to an assessment of the quality of each variance estimate. This assessment is critical if the ensuing confidence interval for the long-run average is to be asymptotically valid. Once path length, significance level, and number of series are specified, the built-in decision rules relieve the user of the burden of estimation.

To illustrate how LABATCH.2 works, the presentation relies on its automatically generated tableaux and on graphs computed from these tableaux. The tableaux contain data that allow a user to assess the quality of variance estimates and the extent to which the sample average for each series is free of the initial conditions that prevailed at the beginning of the simulation.

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Methods of Generating Random and Quasi-Random Orthogonal Matrices

Random orthogonal matrices are used to randomize integration methods for m -dimensional integrals over spherically symmetric integration regions. Currently available methods for the generation of random orthogonal matrices will be reviewed, and methods for the generation of quasi-random orthogonal matrices will be described and analyzed. These methods all have $O(m^3)$ time complexity. Some new methods to generate both random and quasi-random orthogonal matrices will be described and analyzed. The new methods use products of butterfly matrices, and have time complexity $O(\log(m)m^2)$. The use of these methods will be illustrated with results from the numerical computation of high-dimensional integrals from computational finance applications.

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Multivariate Sparse Grid Integration and its Applications

Algorithms for the numerical integration of multivariate integrals are often limited by the "curse of dimension", meaning that the computing cost grows exponentially with the dimension of the problem. Moreover, theoretical complexity investigations reveal that also the minimal computing cost grows exponentially with the dimension for many integration problems.

However, for special function classes, such as spaces of functions which have bounded mixed derivatives, Smolyak's construction can overcome this curse of dimension to a certain extent. In this approach, multivariate quadrature formulas are constructed using combinations of tensor products of suited one-dimensional formulas. In this way, the number of function evaluations and the numerical accuracy gets independent of the dimension of the problem up to logarithmic factors. The abscissas of the resulting quadrature formula form a so-called sparse grid.

We review several methods based on Smolyak's construction and introduce additional constructions based on univariate extended Gauss formulas which achieve the highest possible polynomial exactness among all nested quadrature formulas which use the same number of function evaluations.

The so created quadrature formulas are tested in a variety of applications in physics and financial mathematics which require e.g. the numerical solution of multivariate integral equations of the numerical computation of path integrals.

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Monte Carlo Approaches to Linear Semi-Infinite Optimization

Let S be a compact subset of R^k , and let $u_1, \dots, u_n$ and f be functions that are continuous on S . We consider the problem of approximating f with a linear combination of $u_1, \dots, u_n$ and assume that these functions may be evaluated at any point $s \in S$. We will discuss the problems:

$$\text{Minimize over } y \in R^n, \ c^T y \text{ when } \sum_{r=1}^n y_r u_r(s) \geq f(s), s \in S,$$

and

$$\min \|y^T u - f\|_\infty \text{ over } y.$$

If S is a finite subset of R^k , then these problems may be solved by means of linear programming, which can be done as a finite process. Using simplex exchange steps we may, also for general S , construct a sequence of vectors y , such that the preference functions of the corresponding dual problems increase monotonically. In each simplex step we need to treat a global problem of the form

$$\text{Minimize } y^T u(s) - f(s), \ s \in S.$$

We propose to use random sequences of points, both to construct new points for simplex steps and to estimate the value of the global minimum with statistical tests. We note, that in semi-infinite programming one needs to verify functional inequalities over S , which may be difficult, since infinitely many inequalities must be checked. If S has a low dimension k , one may contemplate approximating S with a finite set T and use numerical values on T combined with assumptions on the derivatives of $u_1, \dots, u_n$ and f to conclude that the inequalities are satisfied within a certain tolerance. Here we propose instead a verification, where we accept a certain low probability that the calculated solution is not optimal. However, we have always that the accepted solution is better than the one used to start the calculation. Further, from the dual problem one gets a bound for the optimal value sought, and hence the possible improvement one at most has foregone, when a "good" but not proven optimal solution is accepted.

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A Rigorous Justification for Quasi-Monte Carlo Methods and Valid Statistical Estimates of their Accuracy

Quasi-random sequences are extremely useful, relatively new tools for performing accurate, efficient Monte Carlo computations. However, two major problems arise in their use. First, how can statistical and probabilistic concepts be applied to what are patently deterministic quantities? Secondly, how can we accurately estimate the errors generated by quasi-Monte Carlo calculations? By demonstrating that these sequences can be viewed, in an appropriate and precisely defined sense, as representative of random samples drawn from truly random processes, their use in a statistical setting is rigorously justified. By further pointing out that a multi-dimensional quasi-random sequence can be decomposed into mutually statistically independent sequences (of one or more dimensions), we can apply the Central Limit Theorem to generate valid statistical estimates of the errors generated by computations depending on such sequences.

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Comparison of Monte Carlo Algorithms for Obtaining Geometric Convergence for Model Transport Problems

Two quite different methods for accelerating the convergence of Monte Carlo solutions of continuous transport problems have been developed recently in Claremont. One of these is based on a sequential form of correlated sampling, first proposed for matrix problems by Halton (1962). The second method makes use of importance sampling transformations applied adaptively. These two methods are contrasted and compared for a family of model transport problems in one dimension.

Both methods collect information in groups of histories, called stages, and use the information from a given stage to improve the solution for the next stage. The sequential correlated sampling algorithm uses the current stage information to reduce the source for the next stage. The adaptive importance sampling method uses the solution from the current stage to modify both the source and kernel operator which describes how particles move from point to point in the next stage. In our numerical study, an attempt is made to describe a parametrized family of model problems to serve as a testbed for the comparison. Comparative results are then averaged over a representative set of problems selected randomly from the family. The intent is to draw conclusions about the rates of convergence of the two methods, one depending on the predominantly additive nature of the sequential correlated method and the other on the predominantly multiplicative nature of the adaptive importance sampling.

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Wavelet Monte Carlo Methods for the Global Solution of Integral Equations

We study the global solution of Fredholm integral equations of the second kind

$$u(s) - \int_G k(s,t)u(t)dt = f(s)$$

by the help of Monte Carlo methods. Global solution means that we seek to approximate the full solution function u . This is opposed to the usual applications of Monte Carlo, where one only wants to approximate a functional of u such as the value $u(t_0)$ in a fixed point t_0 or a mean $(u, g) = \int_G u(t)g(t)dt$ with a given g . In recent years several researchers developed Monte Carlo methods also for the global problem. These algorithms usually fix a grid and combine standard estimators for the values in the grid nodes in various ways.

In this talk we present a new Monte Carlo algorithm for the global solution of integral equations. We use multiwavelet expansions to approximate the solution. We study the behavior of variance on increasing levels, and based on this, develop a new variance reduction technique. It is shown that this algorithm has a higher convergence rate than previously developed algorithm for the global problem. Moreover, for a model class of smooth kernels and right-hand sides an information-based complexity analysis shows that this algorithm is optimal among all stochastic algorithms of the same computational cost and that no deterministic algorithms of the same cost can reach its convergence rate.

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What Affects the Accuracy of Quasi-Monte Carlo Quadrature?

Quasi-Monte Carlo methods for multidimensional quadrature can work very well in practice. Two well-known error bounds are the Koksma-Hlawka inequality and an inequality involving $\mathcal{P}_\alpha$ for lattice rules. However, these bounds are often too pessimistic. This talk presents new worst-case and average-case error analyses that are extensions of the traditional ones. These analyses suggest how to measure the effective dimension of an integrand, which may or may not correspond to the nominal dimension. It is also found that for sufficiently smooth integrands and good quasi-random points one can expect the quasi-Monte Carlo quadrature error to be $O(N^{-1.5+\epsilon})$ for N points. The consequences of these results for the generation of quasi-random points are discussed. Finally, several open problems are raised.

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Fermion Monte Carlo

We will review the fundamental challenge of fermion Monte Carlo for continuous systems, the "sign problem," and some of the proposals that have been made for its solution. The issue is to find not the fundamental eigenmode of the partial differential equation in many dimensions, but one that has a special inversion of sign- antisymmetry in the exchange of pairs of coordinates. Thus the function sought is not everywhere positive. In particular, we describe methods that depend upon the use of correlated dynamics of ensembles of correlated walkers that carry opposite signs. We discuss the algorithmic symmetry between such walkers that must be broken to create a method that is both exact and as effective as for symmetric functions. We explain the concept of marginally correct dynamics. Stable overlaps with an antisymmetric trial function given by such dynamics correspond to the lowest antisymmetric mode. Many-body harmonic oscillator problems are particularly tractable: their stochastic dynamics permit the use of regular geometric structures for the ensembles, structures that are stable when appropriate correlations are introduced, and that avoid the decay of signal-to-noise that is a normal characteristic of the sign problem. Finally, we outline a generalization of the method for arbitrary potentials and describe the progress in treating some model problems and few-electron systems.

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The Importance Biasing Scheme Implemented in PRIZMA Code

The presentation gives the general approach to applying the importance biasing scheme to complicated transport problems and its implementation in the three-dimensional code PRIZMA intended for Monte Carlo simulation of linear coupled transport of neutrons, photons, electrons, positrons, and heavy charged particles.

The scheme was developed employing an idea of step-by-step calculation of complicated problems according to which initial problem is split into several subproblems which are solvable and are solved successively (results of the first subproblem become input data for the second and so on). Main drawbacks of this way of solving are, first, error emerging due to data conversion at the moment of transit from one subproblem to another and, second, uncertainty in estimating statistical error of the final result.

The scheme implemented in the PRIZMA code enables the final result to be obtained by splitting the problem into subproblems in order to use methods of non-analog modeling at different steps.

For this purpose we defined four classes of subproblems with simple relations between source and detector so that the majority of conventional problems of linear transport theory can be reduced to some combinations of them. Schemes of non-analog modeling and principles of building approximate importance function and appropriate non-analog distributions were selected for each class of problem. A special tool for "calculation control" was created allowing to switch from one subproblem to another while simulating history of a particle.

The capabilities of the code are demonstrated by several problems including simulation of deep penetration and detection at up to 100 optical distances from source. Calculated results are compared with known exact solution of this problem.

Proposed is a formula for assessing the benefit of non-analog modeling against analog one, when the values to be estimated are so small that their analogous simulation cannot be performed in reasonable time.

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Monte Carlo Methods in Stochastic Problems of the Atmosphere-Ocean Optics

The paper deals with the simulation of stochastic structure of clouds fields and sea surface undulation for solving problems of the atmosphere-ocean optics by Monte Carlo method.

1. The experimental data of statistical properties of the wind-driven undulation of the water surface testifies that it may be described with high precision by a homogeneous Gaussian random field of surface deviations with respect to mean level. A time-spatial model of the sea surface was constructed on the basis of the spectral methods for approximate modeling of Gaussian homogeneous fields.

It was shown that simulation of the sea surface elevations makes possible to determine more precisely (as compared to the conventional facet model) the optical properties of the swell taking into account multiple reflection effects and radiation shading by the surface elements. The model was also used for solving problems of laser remote sensing of the swell.

2. The spectral methods were used also for simulating stochastic fields of cumulus and broken clouds for studying the processes of the solar radiation transfer in the cloudy atmosphere. A technique of adjustment of the models and results of Monte Carlo simulation are presented.

Moreover, we used the spectral models of random fields to simulate stochastic structure of stratus clouds. The numerical algorithms for stratus clouds based on spectral models have essential advantages in comparison with the so-called cascade models.

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Photorealistic Rendering using the Method of Dependent Tests

Photorealistic rendering consists of projecting the solution of a second kind Fredholm integral equation onto the screen in order to synthesize images in very short times. We present an algorithm using the method of dependent tests, which solves the global illumination problem of computer graphics. First we approximate the solution of the integral equation using elements of low discrepancy sequences for discrete density approximation of the radiance in the scene. Then this density is used for illuminating the scene by the method of dependent tests. Nowadays graphics hardware can be efficiently used to implement this procedure, yielding rendering times of a few seconds. As compared to finite element approaches, the presented algorithm consumes only little memory, is very general and one of the fastest radiosity renderers.

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Sequential Correlated Sampling Methods for some Transport Problems

In this paper, we will describe how to extend to the solution of certain simple particle transport problems a sequential correlated sampling method introduced by Halton in 1962 for the efficient solution of certain matrix problems. Although the methods apply quite generally, we have so far studied in detail only problems involving planar geometry.

We will describe important features of the resulting algorithm in which random walks are processed in stages, each stage producing a small "correction" to the solution obtained from the previous stage. Issues encountered in the course of implementing such an algorithm for practical transport problems will be discussed and numerical evidence of the geometric convergence achieved will be presented for several model problems.

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Error Analysis of Sequential Monte Carlo Methods for Transport Problems

In 1962, Halton introduced a sequential correlated sampling algorithm for the efficient solution of certain matrix problems. We have extended Halton's method to the solution of certain simple transport problems and the resulting algorithm is capable of producing geometric convergence for these problems. That is, random walks are processed in groups called stages, and the error after the n th stage can be made strictly smaller than the error after $n-1$ stages. Of critical importance, then, is to determine conditions that guarantee such strict error reduction for various transport problems. Specifically, if $\Phi(x)$ is the true transport solution and $\tilde{\Phi}^{n-1}(x)$ and $\tilde{\Phi}^n(x)$ are the estimated solutions from the $(n-1)$ st and n th stages, respectively, we demonstrate the existence of a number λ , $0 < \lambda < 1$, which is independent of n , such that

$$\|\tilde{\Phi}^n(x) - \Phi(x)\| \leq \lambda \|\tilde{\Phi}^{n-1}(x) - \Phi(x)\| + \epsilon$$

in a certain probabilistic sense, where ϵ is an error term that tends to zero as both the number of terms representing the global solution and the number of random walks per stage tend to infinity.

We will indicate how to find such a λ , which is defined in terms of the number of random walks per stage and the coefficients of the transport problem in a rather natural way.

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Application of Quasi-Monte Carlo and Stratified Sampling Methods to Measure Portfolio Risk

Accurate and efficient risk management is at the core of an Enterprise Wide Risk Management strategy. However, it is not unusual for financial institutions, such as banks or insurance companies, to require a risk management engine that allows the computation of daily Value at Risk (VaR) estimates of their whole portfolio, which may contain several hundred thousand positions, including substantial volumes of complex derivative products such as swaps, caps and floors, swaptions, mortgage backed securities, etc. In particular, simulation methods may be unavoidable to get an accurate picture of risk when the portfolios contain substantial positions in instruments with optionality. However, full simulation of very large and complex portfolios is computationally expensive and may not even be achievable with the top of the line computers in a reasonable time.

In this paper, we explore the use of Low Discrepancy Sequences (LDS) and stratified sampling methods to measure portfolio distributions and VaR, and we contrast the results with standard Monte Carlo methods based on pseudo-random sampling. Although the application of LDS is currently a topic of much debate for derivatives pricing, they have not been generally applied to measure portfolio risk, where the interest is in the tails of the distributions and not on the average. We show that both stratified sampling and LDS methods result in substantial improvements in computational time for various problems. Furthermore we introduce a novel simulation technique that uses, in addition, portfolio sensitivities with principal components to reduce the effective dimensionality of the simulation.

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Systematic Tests of RNG Families

After a random number generator (RNG) has been designed and implemented, hopefully on the basis of a sound theoretical analysis of its structure, it is common practice to test it empirically. There is a list of more or less standard statistical tests for that purpose (e.g., proposed by Knuth, Marsaglia, and others). None of these tests can *prove* that a generator is fully reliable, and the question of which tests are most relevant has no general satisfactory answer. It is nevertheless interesting to understand what types of defects or structures in the generator's output are detected by the standard tests for specific families of generators.

This talk reports a systematic analysis of the interaction between certain tests and the structure of certain RNG families. For each pair [test, generator family], we estimate a function that predicts at which sample size the test will start to fail decisively as a function of the size (or period length) of the generator. We also look at how to choose the test parameters to make the tests most sensitive to certain types of structures, for a given sample size. The tests considered include most of the classical ones, some in a generalized form. The RNG families examined include linear congruential generators (LCGs) with a good lattice structure, LCGs with a bad lattice structure, explicit inversive generators, combined cubic generators, combined Tausworthe generators, and perhaps others if time permits.

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Adaptive Importance Sampling Algorithms for Transport Problems

In this talk we will describe how importance sampling methods may be applied adaptively to the solution of particle transport problems. While the methods apply quite generally, we have so far studied in detail only problems involving planar geometry.

The technique used is to represent the global solution of the transport equation as a linear combination of appropriately chosen basis functions and estimate a finite number of these coefficients in stages. Each stage processes a fixed number of random walks making use of an importance function that has been determined from the previous stage. Special methods have been developed for importance sampling the resulting source and kernel, and some of these will be described. Numerical results exhibiting geometric convergence for the resulting algorithm will be shown.

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Applications of Monte Carlo and Quasi-Monte Carlo Methods in Finance: Option Pricing

The pricing of options is a very important problem encountered in financial markets today. The famous Black-Scholes model provides explicit closed form solutions for the values of certain (European style) call and put options. But for many other options, either there are no closed form solutions, or if such closed form solutions exist, the formulas exhibiting them are complicated and difficult to evaluate accurately by conventional methods.

In this talk, we illustrate how Monte Carlo & quasi-Monte Carlo methods can be applied to the pricing of options in the following two ways:

1. The values of European style options, based on several assets, can be expressed in the form of multiple integrals. Monte Carlo & quasi-Monte Carlo methods can then be applied directly to evaluate such integrals.
2. The values of many options are believed to satisfy partial differential equations, most of them without closed form solutions. These equations become systems of linear equations when finite difference approximations are applied. Very efficient adaptive Monte Carlo methods, based either upon the use of correlated sampling or importance sampling, can then be used to solve these matrix equations.

Numerical results illustrate these techniques.

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Perspectives on a Dyadic Two-Dimensional Van Der Corput Sequence

A recursive dyadic point sequence in the unit square, with precisely known and notable low dispersion, was introduced in [1]. Here we reconsider this sequence, which can be viewed as an extension of the well-known one-dimensional van der Corput sequence, from certain geometric and computational perspectives. Specifically, we examine: (1) the Voronoi cell structure induced by this sequence; (2) a transformation of this sequence onto the surface of a sphere and use of the resulting spherical sequence in numerical optimization; and (3) the combined use of a pseudo-random number generator along with this sequence to construct "mixed sequences" in the sense of Ökten and of Spanier.

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A Discrepancy-Based Analysis of Figures of Merit for Lattice Rules

A classical figure of merit for choosing quasi-Monte Carlo methods for integration over the s -dimensional hypercube is the L^2 star discrepancy of the corresponding set of quadrature points. Another figure of merit commonly used when considering periodic integrands is P_α , usually with α an even positive integer. Hickernell (1996) introduced a generalised notion of discrepancy of which both these figures of merit are special cases. In this paper Hickernell's decomposition of generalised discrepancy into lower dimensional components is used to investigate certain numerical results concerning P_α and star discrepancy values. These results suggest a further generalisation with application in the context of rank 1 lattice rules and their n^s copies. Recent work by the author concerning a method for choosing a copy rule by comparing quadrature error estimates for related rank 1 rules is described.

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Grid-free Simulation of Convection-Diffusion

Accurate modelling of the interaction between convective and diffusive processes is a challenging task in the numerical approximation of partial differential equations. Particle-tracking models have been extensively used. Convection is simulated by a translation of each particle and diffusion is generally simulated using the random walk technique. The method suffers from the poor accuracy due to random fluctuations. Quasirandom methods are known to outperform their probabilistic versions.

This paper examines a particle numerical method for time-dependent convection-diffusion equations in d -dimensions. The solution is approximated as a linear combination of Dirac measures (particles). Particles are sampled from the initial data. The evolution of the system in a time interval Δt is obtained in two steps. In the first step the particles are transported under the action of the convective field. In the second step the diffusion is interpreted as a quasi-Monte Carlo approximation in the $2d$ -dimensional unit cube.

The most effective constructions of quasirandom point sets are obtained from the theory of (t, m, s) -nets and (t, s) -sequences. But quasirandom points cannot be blindly used in place of pseudorandom points for particle simulations. A reformulation is usually needed to insure that the resulting integrands are smooth. In the present paper we use the same renumbering technique as that used in applying quasirandom sequences for solving kinetic equations. In every time step, the number order of the particles is scrambled according to their positions before assigning a new quasirandom point to each particle.

We prove a convergence theorem for the particle method using a $(0, 2d)$ -sequence with this renumbering technique. Pseudorandom and quasirandom sequences are compared in computational experiments, for some simple model problems whose solutions can be found analytically. The results show that quasirandom points can produce more accurate results than pseudorandom points.

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The Limit Laws of the Spectral Test and Related Variants

We present the weak limits of the classical spectral test, of diaphony, and of several related variants in arbitrary dimension. Further, we show that certain weighted spectral tests are related to each other by a common empirical process; we give the strong and weak limits of this process, from which the corresponding limits of the respective weighted spectral tests follow immediately. Finally, we present techniques for calculating the cumulative distribution function of diaphony and its variants in higher dimensions.

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The Higher-Dimensional Properties of Pseudo-Random Variates

The literature on uniform random number generation contains a large number of papers dealing with the quality of different uniform pseudo-random number generators. Papers on the generation of non-uniform variates mainly deal with the speed and simplicity of the proposed algorithms. The methods generate non-uniform random numbers by transforming an independent sequence of (perfect) uniform random numbers. But investigations dealing with the effects that can occur when such an exact transformation method is combined with a pseudo-random sequence are very rare and are mainly discussing the quality of the one-dimensional distribution or the robustness of such transformations (e.g. [1]). The last author has studied the effects of uniform random number generators on the quality of transform methods. But his results (e.g. [2]) are restricted to the one-dimensional distribution and LCGs.

It is well known and accepted that the investigation of the distribution of n -tuples in several dimensions is necessary to assess the quality of a uniform random number generator. New proposals of high-dimensional tests for random number generators give us the possibility to assess the distribution of the n -tuples of non-uniform variates which was not done up to now. This means that we can investigate the quality of non-uniform pseudo-random variates by analyzing their multidimensional distribution in an empirical study.

We tested a variety of transformation methods (rejection, ratio of uniforms and patchwork-rejection) combined with different uniform pseudo-random number generators. The results do not only confirm the one-dimensional theoretical considerations for the combination of ratio of uniforms method and the rejection method in combination with LCGs but also have the power to distinguish between combinations (transformation method and uniform generator) of good and of poor quality.

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A Comparison of Monte Carlo, Lattice Rules and Other Low-Discrepancy Point Sets

Quasi-Monte Carlo methods have been proposed as a way of dealing with the general problem of multidimensional numerical integration. These methods can be classified in two families: Lattice rules and low-discrepancy sequences, such as those proposed by Sobol, Halton, Faure and Niederreiter.

In this presentation, we compare empirically these two families on practical problems arising in finance, such as the evaluation of asian options, which typically involve large dimensions. The comparisons are made for problems with different numbers of dimensions and for different sample sizes. For a given dimension and number of sample points, we use the connection between lattice rules and multiplicative linear congruential generator (MLCG) to choose appropriate rules. More precisely, we use the spectral test, a widely accepted figure of merit for MLCGs, to select the lattice rules.

Low-discrepancy sequences have already been used for this kind of practical problems, whereas lattice rules have been consistently overlooked in the financial literature. Our examples provide promising results indicating that simple lattice rules are competitive. In certain examples, we find that the estimator derived from a properly chosen lattice rule can be as much as 800 times more efficient than the one obtained from the naive Monte Carlo method. More generally, our results suggest that the class of functions for which lattice rules provide a good method for numerical integration is wider than what is usually expected.

The problems we will look at are the evaluation of asian, barrier and multiasset options in finance and the probability of ruin in risk theory. Following the idea in Ackworth, Broadie and Glasserman (1997), we will also examine if the principal components construction can improve the accuracy of the estimator generated by a lattice rule.

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Quasi-Monte Carlo Simulation Methods for Measurement Uncertainty

Modern dimensional metrology, which deals with the art and science of measuring manufactured parts in industry, is one current source of important problems involving geometric computations. From this viewpoint, the performance evaluation of software and hardware of the Coordinate Measuring Machine (CMM) system would be valuable for both the inspecting of parts and in the purchasing of a CMM system.

The estimation of the magnitude of the uncertainty sources and their effect on the measurement results is very important in all industrial measurements. Constructing a mathematical model for measurement uncertainty, this paper uses quasi-Monte Carlo methods to simulate the relationship between the measurement result and the sources of error in order to predict the measurement uncertainty. The approach also is applied to the testing of algorithms of a CMM software system.

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Linear Programming Bounds for Ordered Orthogonal Arrays and (T, M, S) -Nets

In recent years, a very important result - obtained by Schmid and Lawrence independently - established an equivalence between (T, M, S) -nets in base b and ordered orthogonal arrays (or, generalized orthogonal arrays) $OOA_{\lambda, T}(M - T, S, M - T, b)$. An *ordered orthogonal array* $OOA_{\lambda}(t, s, l, v)$ is a $\lambda v^t \times sl$ array over an alphabet of size v whose columns are partitioned into s groups, each of size l . This array must satisfy the following balance condition: if any t columns are chosen in such a way that the i chosen columns in any group constitute the first i columns of the group, then every possible t -tuple over the alphabet occurs exactly λ times in the subarray obtained by restricting to these t columns. This translation into combinatorial language opens the door to new constructions and new techniques for non-existence results.

In a forthcoming paper, Stinson and the author used the theory of association schemes to obtain a linear programming approach to such non-existence results. For an $OOA(t, s, l, v)$, the linear program has $\binom{s+l}{l}$ variables and constraints. The application to (T, M, S) -nets follows from the Lawrence/Schmid Theorem: If there exist $s \leq S$, $t \leq M - T$, and $l \leq M - T$ such that the optimal objective value to the linear program for an $OOA(t, s, l, b)$ exceeds b^M , then no (T, M, S) -net exists in base b .

In this paper, we discuss implementation of this technique. We prove some results which simplify the system of linear inequalities. We describe an approach in which we compute the linear programming bound numerically and subsequently verify this bound in exact arithmetic. The core of the presentation is a new table of bounds for (T, M, S) -nets obtained via this approach which - in many cases - improve the lower bounds for T in terms of M and S given in the recent survey paper of Niederreiter, et al.

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SPRNG: A Scalable Library for Monte Carlo Applications,
<http://www.ncsa.uiuc.edu/Apps/SPRNG>

Over the past three years, we have developed a **Scalable Pseudo Random Number Generators (SPRNG)** library under the support of the DARPA Scalable Libraries Initiative.² SPRNG is a set of libraries for scalable and portable pseudorandom number generation that was developed with the requirements of the Monte Carlo applications community in mind.

At any given time, Monte Carlo calculations consume a large fraction of all supercomputing cycles. It is fair to say that a Monte Carlo computation can be viewed as a computational "black box", where random numbers are the input, and the quantities of interest are the output. Clearly, the fidelity of the output is highly dependent on properties of the input. Thus, it is equally clear that for parallel Monte Carlo applications to be accurate and robust, these applications must have high-quality pseudorandom numbers. While the issue of random number generation in sequential calculations has been well studied, albeit on less powerful computers, there has been considerably less work done in the context of parallel Monte Carlo applications. SPRNG was designed to be a comprehensive tool for parallel Monte Carlo applications by providing:

- Several, qualitatively distinct, well tested, scalable RNGs
- Initialization without interprocessor communication
- Reproducibility by using the parameters to index the streams
- A single "global" seed controls reproducibility
- Minimizes interprocessor correlation with the included generators
- A uniform C, C++, FORTRAN, and MPI interface
- Extensibility
- An integrated test suite including physical tests

¹Speaker

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Furthermore, the user can generate random numbers from more than one stream on each process. SPRNG also provides other facilities, such as for the checkpointing of the state of the random number streams and dynamic creation of new streams that are independent of the streams on other processes.

The generators currently implemented in SPRNG are:

- Additive lagged-Fibonacci: $x_n = x_{n-r} + x_{n-s} \pmod{2^m}$
- Prime modulus multiplicative congruential: $x_n = ax_{n-1} \pmod{m}$
- Power-of-two modulus linear congruential: $x_n = ax_{n-1} + b \pmod{2^m}$
- Combined multiple recursive generator: $z_n = x_n + y_n \times 2^{32}$, where x_n is a linear congruential generator modulo 2^{64} and y_n satisfies
 $y_n = 107374182y_{n-1} + 104480y_{n-5} \pmod{2147483647}$

Implementation of a multiplicative lagged-Fibonacci generator is in progress.

SPRNG has been ported to the CRAY T3E, HP/Convex Exemplar, IBM SP2, SGI-CRAY Origin 2000 and SGI Power Challenge parallel computers. It has also been ported to HP and SUN workstations, and also to PCs running Linux. It is hoped that SPRNG will become a *de facto* standard for parallel pseudorandom number generators.

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Dynamic Creation of Pseudorandom Number Generators for Distributed Systems¹

For a Monte Carlo simulation in a distributed system, usually each processor has the same pseudorandom number generator, with distinct initial values assigned. Here instead, we propose dynamic generation of pseudorandom number generators. For each processor, a distinct pseudorandom number generator is assigned. Each generator is a small Mersenne Twister, which we proposed previously.

¹Much of the work was performed jointly with Takuji Nishimura (nisimura@comb.math.keio.ac.jp)

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Designing Asymptotically Random GFSR Sequences

J.P.R. Tootill et al. (J. ACM, 1973) proposed the concept of an asymptotically random Tausworthe sequence, and gave an example of such sequence found by chance. However, no systematic way of finding such sequences has been proposed by now.

In this talk we will give an algorithm for designing GFSR sequences which satisfy the asymptotic randomness approximately. Our algorithm is based on repeated applications of the algorithm proposed by M. Fushimi (SIAM J. Comput., 1998). The sequences designed by the present algorithm have an added merit that their decimated sequences are also approximately asymptotically random. Some numerical examples will be shown.

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A Practical Approach to the Error Estimation of Quasi-Monte Carlo Integrations

There have been few studies on practical error estimation method of quasi-Monte Carlo integrations. Recently, Owen (SIAM J. Numer. Anal., 1997) proposed a scrambled net to analyze the quasi-Monte Carlo integration error. However his method is complicated to be implemented and needs huge computational efforts, so it would be of great interest to investigate a simple error estimation method. In this talk, we will propose a simple method, and report a numerical experiment of comparison between Owen's scrambling and our method. In our experiment, both methods have accurate error estimates. Some theoretical considerations on the relation between two methods will be also presented.

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Active Walk Models in Biological Evolution

The use of a walker in modeling physical and other phenomena has a long history. The most well known is a random walker, which has been used to mimick the Brownian motion of a particle suspended in a liquid and fluctuations in financial markets. A random walker does not change anything in its environment and is what we call a passive walker. In contrast an active walker is one who changes the landscape during its motion and is influenced by the landscape in choosing its next step [1].

Active Walk has been used to model many natural phenomena such as the formation of filamentary patterns in retinal neurons, surface reaction patterns in thin cells of fluid, anomalous ion transport in glasses and food collections by ant swarms. Active Walk has also been used in the social sciences to model urban growth and economic population games [2].

In this paper we briefly review Active Walk and show that it can be used to create models of Biological Evolution.

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Accuracy of Approximate Bounds for the Reliability of Coherent Systems

Computation of a lower confidence bound for the reliability of a multicomponent system is often based on techniques which use data from component tests rather than tests of the entire system.

For most types of component data (Bernoulli trials, exponential or Weibull time to failure) and system types (series, parallel, k out of n) the only viable methods available for computation of reliability bounds are those which produce approximate bounds.

For Binomial data the accuracy of these approximate bounds is usually evaluated by comparing their values to the values obtained for exact bounds in those limited cases where exact bounds are computable. Exact bounds are obtainable for systems of two or three components when the component data sets are of equal size.

Assessing the level of significance and expected length of approximate confidence bounds is best accomplished by using Monte Carlo simulation over selected subsets of the parameter space and the set of possible sample sizes.

The case discussed in this paper is that of determining which approximate bound technique is most applicable for determining a lower bound on the reliability, $h(p_1, \dots, p_m)$, for a coherent structure function ϕ of size m . In this case

$$p_i = P[i^{\text{th}} \text{ component in the structure } \phi \text{ works}] \quad i = 1, \dots, m$$

The data used are the number of successes X_i , in n_i independent Bernoulli trials: $X_i \sim B(n_i, p_i)$. The parameter space in this case is $\Omega = \{\mathbf{p} : 0 < p_i < 1\}$, and, for highly reliable systems, the subset of concern is $\omega = \{\mathbf{p} : p_i \geq \rho_i\}$ for ρ_i close to one.

It will be shown that Monte Carlo simulation can lead to conclusions concerning the desirability of one bound technique over another, which contradicts previously published results.

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Constructions of (t, m, s) -Nets

Low-discrepancy point sets play a crucial role in applications of quasi-Monte Carlo methods. In fact, the efficiency of a quasi-Monte Carlo method depends to a significant extent on the quality of the low-discrepancy point sets that are employed, i.e., on how small their discrepancy is. The most powerful known methods for the construction of low-discrepancy point sets utilize the theory of (t, m, s) -nets, which are sets of points in the s -dimensional unit cube $[0, 1]^s$ satisfying strong uniformity properties with respect to their distribution in $[0, 1]^s$. The quality parameter t measures these uniformity properties and should be as small as possible. The parameter m provides information on the size of the point set, e.g. in the most common base 2 a (t, m, s) -net consists of 2^m points.

Various methods for the construction of (t, m, s) -nets have been developed over the years. We present a survey of these techniques and describe also some new constructions that yield many improvements in the current tables of net parameters as well as (t, m, s) -nets in very high dimensions. The tools in these construction methods stem from a wide range of areas, such as number theory, algebra, combinatorics, coding theory, and algebraic geometry.

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Mixed (s,d) Sequences: Theory and Applications

The use of low-discrepancy sequences becomes problematic in high or infinite dimensional problems. In high dimensions, the number of vectors one has to generate to bring the discrepancy bound $O(\frac{(\log N)^s}{N})$ to a reasonable magnitude may not be feasible computationally, which may make the use of low-discrepancy sequences impractical in problems with "effective" dimension close to s . In addition, in infinite dimensional problems, i.e., in problems where random walks of arbitrary lengths need to be generated, some of the low-discrepancy sequences cannot be used because of theoretical reasons.

Different methods have been suggested to provide remedies for difficulties faced in high or infinite dimensional problems. One method that has been implemented successfully in several applications uses the mixed (s,d) sequences to generate the underlying random walks. A mixed (s,d) sequence is an s -dimensional sequence obtained by concatenating d -dimensional low-discrepancy vectors with $(s-d)$ -dimensional random vectors. These sequences have been used in problems from transport theory, computational finance and numerical integration, and numerical results have suggested that their use may become very advantageous in high dimensions where the low-discrepancy sequences start losing their effectiveness.

We will present probabilistic results on the discrepancy of mixed (s,d) sequences. Using numerical results, we will also illustrate the advantages of these sequences in comparison to pseudorandom and low-discrepancy sequences, as the dimension of the problem increases.

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Exploring Quasi-Monte Carlo for Marginal Density Approximation

We first review Quasi-Monte Carlo (QMC) integration for approximating integrals, which we believe is a useful tool often overlooked by statistics researchers. We then present a manually-adaptive extension of QMC for approximating marginal densities when the joint density is known up to a normalization constant. Randomization and a batch-wise approach involving $(0,s)$ -sequences are the cornerstones of our method. By incorporating a variety of graphical diagnostics the method allows the user to adaptively allocate points for joint density function evaluations. Through intelligent allocation of resources to different regions of the marginal space, the method can quickly produce reliable marginal density approximations in moderate dimensions. We demonstrate by examples that adaptive QMC can be a viable alternative to the Metropolis algorithm.

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Randomized Quasi-Monte Carlo Methods

This talk considers using randomization to improve upon quasi-Monte Carlo (QMC) methods. There is some irony in this because QMC methods arose from an attempt to improve upon Monte Carlo (MC) methods by derandomizing them.

The original motivation behind randomized quasi-Monte Carlo (RQMC) is to combine the superior accuracy of QMC methods with the data based estimates of accuracy available for MC. There are several ways of randomizing QMC points so that they maintain the properties that guarantee their accuracy while providing unbiased estimates. Standard statistical methods can be used to estimate error from independent replications of RQMC. One RQMC method, scrambled nets, has even been shown to improve upon the accuracy of the underlying QMC method.

A second use of randomization is to extend the reach of QMC methods into higher dimensions. In high enough dimensions it is difficult to construct a QMC point set with nontrivial equidistribution properties. The method of Latin supercube sampling (LSS) takes an s dimensional (R)QMC method and applies it to a d dimensional problem where $d > s$ or even $d \gg s$. The procedure works by partitioning the d input dimensions into k sets of s or fewer variables. An s dimensional (R)QMC method is applied within each set of inputs. The presentation order of these (R)QMC points is randomized separately within groups. Theory provides a guide on how to choose an effective partition of variables. At its best LSS estimates a d dimensional integral with an error usually seen in s dimensional methods.

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Monte Carlo Simulation of Photometrical Measurements in Fog

For their research activities on the visibility of road and vehicle equipments in fog, the network of Laboratoires des Ponts et Chaussées chose two complementary approaches: experiments on the one hand, carried out in the fog chambers of the Laboratoire de Clermont-Ferrand, and simulations on the other hand, using a Monte Carlo based code developed by the INSA de Rouen. The ambition is to validate simulation results for short distances and for some experimentally accessible artificial fogs. The Monte Carlo code can then be used for simulating traffic-like situations.

We proceed with photometrical measurements of illuminance and luminance of the fog due to a vehicle headlight. The geometry of these experiments is then modeled and the simulation code is run. Results of both methods are compared. The difficulty stands in the degree of concordance which can be reached between the real and modeled situations.

We lack full knowledge of some experimental elements, like the representativity of the particle size distribution or the uniformity of the fog, the photometrical characteristics of the walls of the chamber or the pavement, etc. Problems also come from the simulation: the degree of precision in the description of light sources, the oversize detectors compared to the real ones.

Nevertheless, illuminance comparisons show good agreement for the various directions that were tested. For the luminance however, the errors between measured and computed values have the same order of magnitude as experimental fluctuations, just like the influence of the two tested particle size distributions.

¹Paper presented by Eric Dumont

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Spectral Models of Random Fields: Theory and Applications

The paper deals with methods of numerical modeling of random processes and fields. The following algorithms are considered:

- (a) models of Gaussian homogeneous fields constructed on the basis of the spectral representation, dependent and conventional spectral models,
- (b) algorithms for modeling of isotropic fields in a space and on a sphere of an arbitrary dimension,
- (c) models of some classes of non-Gaussian fields.

Different kinds of convergence of numerical random models are investigated. The so-called weak convergence is important for Monte Carlo methods. Effective sufficient conditions of weak convergence are obtained for the spectral models of Gaussian fields and some classes of non-Gaussian fields.

Applications of spectral models of random fields are considered in brief for simulating such objects as the time-spatial structure of the undulated sea surface and stochastic fields of broken clouds. Models of these objects were used for solving problems of the atmosphere-ocean optics by Monte Carlo methods. In addition, the vector-valued spectral models were used for simulating turbulence. Demonstration programs for PC are presented.

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The Monte Carlo Method for Solution of Nonlinear Neyman's Problem

The purpose of this work is the construction of a stochastic algorithm for the solution at an arbitrary point of Neyman's problem for the Helmholtz's nonlinear equation. An algorithm making use of a construction of unbiased estimators based on a model of the corresponding stochastic processes is given. This algorithm differs from the usual one in its choice of transformation densities. Simple conditions for unbiasedness were obtained. The algorithm has been generalized to the case of variable coefficients. A method for constructing the estimators and for proving correctness of the result will be discussed.

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A Method for the Exact Solution of Linear Systems based upon Monte Carlo Gradient Estimation

In earlier work the author developed a powerful algorithm for calculating derivatives in systems of linear equations $\mathbf{x} = \mathbf{P}\mathbf{x} + \mathbf{a}$ describing random walk processes. The algorithm renders the first and higher-order derivatives of the unknowns x_i with respect to the matrix elements p_{ij} .

In this paper it is demonstrated how the derivatives constitute the essential information to determine an estimate of the inverse of the parameter matrix $\mathbf{R} = \mathbf{I} - \mathbf{P}$. It can be shown that the random walk procedure described here allows for the direct calculation of the inverse of the matrix characterizing the underlying system of linear equations. The inverse matrix is obtained directly from the derivatives of the unknowns with respect to the transition probabilities. The derivatives themselves are the result of a simple counting algorithm which can be considered to be an alternative to the Gaussian elimination technique.

The generation of the inverse of a large matrix by classical methods is usually a lengthy and cumbersome process. And indeed, the matrix inverse should be thought of as a useful algebraic concept rather than as an aid to numerical computation. Although the solution of simultaneous equations is rapid once the inverse has been found, the process of finding the inverse involves significantly more computation than is required for the direct solution of the original equations, and hence cannot be justified numerically.

This statement is, however, invalid if the Jacobian can be calculated by the simple and computationally inexpensive Monte Carlo sampling algorithm mentioned above. In this case the inverse can be calculated by straightforward matrix algebra.

Furthermore, it will be shown that $\mathbf{R}^{-1}$ can be used (by a short iterative process) to improve both, the inverse itself and the x_i 's, so that they converge to their exact numerical values (expectation), rendering a zero-variance result in an iteration procedure based upon statistical simulation.

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Resistance Exponential Dependence on Thickness in Thin Films: A Classical Monte Carlo Study

An exponential dependence on thickness has been treated as one of the tunneling signatures in Metal-Insulator-Metal systems. We argue, using classical Monte Carlo simulations, that in some experiments this exponential "law" could reflect not quantum effects but instead the role of roughness in classical physics. We present results from two different models. One is just a random deposition model. Analytical calculations are also discussed. The second, a modified molecular-beam-epitaxy model accounts for random deposition, surface relaxation and limited height difference (included in the Hamiltonian). The resistance is calculated assigning resistance values to the different conduction "channels". Another calculation will be also discussed, where electrons are allowed to diffuse in the "random media" and an estimation of the resistance is obtained from the Einstein relation.

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Variance Reduction Techniques for Large Scale Risk Management

In this paper we describe some of the most challenging issues associated with developing a Monte Carlo simulation system aimed at determining market value and Value-at-Risk of large financial institutions. This translates into computing solutions for a very large collection of Cauchy problems in high dimension on a non-parallel computer. All problems share the same underlying probability distribution, namely the probability distribution of interest rates. In order to achieve this goal in a realistic timeframe, the number of samples is kept low (less than 2000). Since most of the computing time is spent evaluating functions of the sample we carefully select samples by combining Low-Discrepancy sequences with measure transformation techniques.

Part of the approach was to evaluate various Low-Discrepancy Sequences and Brownian bridge constructions to generate Brownian motion. We also compared measure transformation techniques in discrete time and in continuous time, using Girsanov theorem for the latter. The implementation of an adaptive importance sampling scheme was achieved by an optimized aggregation of the Cauchy problems into "super-problems" characterized by the same importance function. In order to reduce the dimensionality of each "super-problem" we analyze the relative merit of two measures, namely the risk-neutral and the forward measure, and of various aggregated models of the path-dependency of the underlying financial instruments.

The paper concludes with our current work on estimating the histogram of Value-at-Risk.

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Improvements and Extensions of the "Salzburg Tables" by Using Irreducible Polynomials

The quality of quasi-Monte Carlo methods mainly depends on the distribution properties of the underlying (deterministic) point set. The theory of digital nets and sequences provides a method for the construction of extremely well distributed point sets in the s -dimensional unit cube.

In 1992, Niederreiter introduced a special family of digital (t, m, s) -nets which is based on rational functions over finite fields. To get suitable parameters for an explicit construction of these nets (especially in the binary case), one has to resort to a computer search. The first step in this direction was taken by Hansen, Mullen, and Niederreiter in 1993. Their search provided point sets of up to 2^{20} points in dimensions 3 and 4 and up to 2^{10} points in higher dimensions (therefore too small for applications).

By limiting the search domain we were able to extend this to sets of up to 2^{23} (and later 2^{25}) points in dimensions up to 15 ("Salzburg Tables" — joint work with Larcher, Lauß, and Niederreiter; SINUM, 1996). There are now several other (partially theoretical) methods yielding nets with better quality parameters t . Numerical experiments however have shown that the Salzburg Tables provide nets of a very high quality.

In the calculation of such binary (t, m, s) -nets we need Laurent series expansions of rational functions with a denominator $f(x) \in \mathbb{F}_2[x]$ of degree m . In all of the search procedures the most convenient choice $f(x) = x^m$ was used. Theoretical results however have shown slight improvements by using irreducible polynomials instead.

In practice it turned out that the change to irreducible polynomials, combined with a different algorithm for the computer search, exceeds all theoretical expectations by far.

We now are able to present an updated version of the Salzburg Tables with parameters for concrete digital (t, m, s) -nets of up to 2^{28} points in dimensions $3 \leq s \leq 50$. Many of them are equal or even better than the previously best available parameters.

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Monte Carlo Conditional Estimator for Diffusion in a Random Field

Consider the diffusion of a substance in a random velocity field. We suppose that it is described by a parabolic equation with random coefficients, spatial density of a substance being its solution. Let the random velocity vector satisfy conditions ensuring the mean square solution existence. In such a situation the (random) fundamental solution to the parabolic equation can be sought in the form of a mean square solution to the integral Volterra equation with the random kernel. Suppose that the initial value problem is set up. It can be reformulated in terms of the integral equation with the same integral operator (or the adjoint to it). The free term of this equation depends on the spatial source function which is also random. Mean square convergence of the Neumann series makes it possible to construct different Monte Carlo estimators. We define a Markov chain with the state space $\mathbb{R}^m \times (0, t]$, its transition density being consistent (in the mean square sense) with the kernel of the integral operator. Next the collision estimator is constructed, its conditional expectation is proved to be (almost sure) the mean square solution of the random parabolic equation. Hence, various functionals can be computed also, thus ensuring the possibility to clarify the intrinsically probabilistic features of the solution.

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Geometrically Convergent Learning Algorithms for Global Solutions of Transport Problems

In 1996 Los Alamos National Laboratory initiated an ambitious five year research program called "MCNP for the 21st Century" aimed at achieving geometric convergence for Monte Carlo solutions of difficult neutron and photon transport problems. Claremont students, working with the author in Mathematics Clinic projects that same year and subsequently, have been partners in this undertaking. This talk will summarize progress made at Claremont over the two year period.

The Claremont approach has been to maintain as much generality as possible, aiming ultimately at the Monte Carlo solution of quite general transport equations but studying various model transport problems - both discrete and continuous - to establish feasibility. As far as we are aware, only the discrete case had been seriously attacked by sequential sampling methods prior to this effort: by Halton beginning in 1962 and subsequently by Kollman in his 1993 Stanford dissertation. We have found that our adaptive importance sampling algorithm consistently outperforms a sequential correlated sampling algorithm developed here that is based on Halton's ideas for matrix problems. These findings are contrary to what Halton reported in 1962 and in subsequent papers.

These learning algorithms based on very different Monte Carlo strategies have recently been successfully extended to continuous problems. In this talk we will outline the methods and ideas employed, sketch the algorithms used and exhibit the geometric convergence obtained. We will also attempt to provide a rationale for the results obtained so far and indicate some of the remaining obstacles to achieving fully practical computation of general transport solutions by these means.

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Testing Parallel Random Number Generators

A parallel random number generator (PRNG) must be tested for two types of correlation, intra-stream correlation, as for any serial generator, and inter-stream correlation for correlations between random number streams on different processes. Unfortunately, important aspects of quality are very difficult to prove mathematically. Thus large empirical tests are crucial to understanding the effective randomness of a PRNG. As computational power increases, new generators will be proposed, and these will have to be tested using every larger sequences. Over the past three years, we have developed a Scalable Pseudo Random Number Generators (SPRNG) library under the support of the DARPA Scalable Libraries Initiative². SPRNG contains parallel test suite that we will describe.

The tests conducted by us on the SPRNG PRNGs can be broadly classified as being either purely statistical tests or physical model tests. The former compare the statistical property of a sample from the PRNG with the expected distribution for a random sample from a uniform distribution. The latter use random numbers in a "practical" application for which the solution is known, and verify if the results obtained are acceptable. The advantage of the former is that they are much faster; however, applications often use random numbers in a manner that is difficult to encapsulate in a statistical test, and thus physically based tests are essential.

We first perform "standard" tests proposed by Knuth, and those in Marsaglia's DIEHARD suite to test for intra-stream correlation, since any good PRNG must also be a good serial generator. In order to test for inter-stream correlation, we use a parallel version of the serial tests in which we interleave several streams to form a new stream. If the original streams are uncorrelated, then the resulting stream too should be uncorrelated, and this can be verified by serial tests on the new stream. We have also developed two inherently parallel tests based on the central limit theorem and the Fourier transform respectively.

In this talk, we shall also discuss the test results for our PRNGs, which have been tested with up to 10^{13} random numbers in certain tests, with larger tests in progress. In particular, we shall demonstrate the effectiveness of our parallel tests in detecting inter-stream correlation. We shall also discuss our proposed web-based test facility for the benefit of those developing new PRNGs.

¹Speaker

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New Results for the Quadratic Congruential Pseudorandom Number Generator

The generation of uniform pseudorandom numbers in the interval $[0,1)$ is a basic and crucial task in any stochastic simulation. The deficiencies and the intrinsic regularity of the linear congruential method show that it is very desirable to have other classes of generators available. The earliest nonlinear method is the quadratic congruential method proposed by D. E. Knuth in 1969. This method can also be seen as a simple alternative to inversive methods. In order to assess the usability of a pseudorandom number generator it is necessary to know as much as possible about its "random" behavior. Here, a survey of known and new results of a theoretical analysis of the quadratic congruential generator, based on the notion of discrepancy, will be given. The known results mostly refer to bounds for the discrepancy over the full period. Equidistribution and independence properties of the generated pseudorandom number sequences over parts of the period will be considered and upper bounds for the average value of these discrepancies will be established.

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Random Walk Discrepancy Bounds

The notion of discrepancy of sequences can be extended to measure the uniformity of probability distributions, which is useful for bounding rates of convergence of random walks on compact metric spaces. Discrepancy bounds derived in this context can also be applied to sequences. We exhibit such bounds on the circle, torus, and sphere, and give examples of the use of such bounds for both random walks and sequences.

In particular, on the circle we analyze the random walk generated by an irrational rotation. For quadratic irrationals we give a sharp rate of convergence, with lower and upper bounds of order $N^{-1/2}$, where N is the number of steps in the walk. (This contrasts with the case for the sequence $\{n\alpha\}_{n=1}^N$, which in addition to the doubled exponent has an extra $\log N$ term.) For arbitrary irrationals we establish bounds whose exponents are sharp up to an arbitrarily small epsilon. We also mention how the convergence of this walk may possibly be sped up by using more generators.

Similar bounds can be derived for sequences and random walks on the torus. We apply these bounds to Kronecker sequences and discrete walks on the torus. Random walks on the sphere generated by rotations can be analyzed by harmonic analysis on $SO(3)$, and we give an analysis for one such walk.

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Permutable Ergodic Transformations with Non-Uniform Densities and their Applications to Monte Carlo Methods

Recently, we have developed a systematic method for constructing an infinite number of ergodic transformations with explicit non-uniform invariant measures by addition theorems of elliptic functions [1, 2]. Interestingly, each pair of these mappings is permutable in the sense of J.F. Ritt [3, 4] and they can be seen as a generalization of the logistic map $Y = 4X(1 - X)$ given by Ulam and von Neumann [5] and Chebyshev maps given by Adler and Rivlin [6]. In this talk, I will report an algorithm for employing these kinds of chaotic mappings to perform numerical integrations. In comparison with most standard Monte Carlo methods, this method shows considerable reduction of errors because of the correlations of variables. A connection with the technique of antithetic variates [7] will be also discussed.

Explicit Invariant Densities of Rational Ergodic Mappings	
Rational Mappings on $[0,1]$	Algebraic Densities on $[0,1]$
$y = 4x(1 - x)$	$\rho(x) = \frac{1}{\pi\sqrt{x(1-x)}} \quad [5]$
$y = x(3 - 4x)^2$	$\rho(x) = \frac{1}{\pi\sqrt{x(1-x)}} \quad [6]$
$y = \frac{4x(1-x)(1-lx)(1-mx)}{1-2(l+rn+lm)x^2+8lmx^3+(l^2+m^2-2lm-2l^2m-2lm^2+l^2m^2)x^4}$	$\rho(x) = \frac{1}{K(l,m)\sqrt{x(1-x)(1-lx)(1-mx)}} \quad [1, 2]$

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Metropolis Particle Transport: A New Approach to Transport Problems

We propose a new Monte Carlo approach to particle transport problems, based on the well-known Metropolis sampling algorithm. We start by defining a special probability measure on the space of particle histories (i.e. the set of all possible paths that particles can follow). The probability density assigned to a given path is proportional to the contribution that the flux on that path makes to the desired set of measurements. The algorithm then proceeds by choosing a single initial particle history, and applying a series of random mutations to it (such as inserting a new collision point), thus generating a random walk through the path space. Each mutation has a chance of being accepted or rejected (according to the usual Metropolis rules), in order to ensure that paths are sampled according to the contribution they make to the desired set of measurements.

We show that the resulting algorithm is unbiased, uses little storage, and is fully general with respect to the geometric environments and scattering models that can be used. The key difference with previous approaches is that the path space is explored locally, by favoring mutations that make small changes to the current particle history. This has several advantages. First, the average cost per sample is small (since each mutation typically modifies only one or two collisions). Second, once an important path is found, the nearby paths are explored as well. This amortizes the cost of finding such paths over many samples. Finally, the path sampling automatically adapts to the desired set of measurements. This has great potential for the solution of difficult transport problems, for which a specialized sampling strategy would normally have to be designed and tuned by hand.

We have implemented this technique for the particular case of light transport (photons) between surfaces. The resulting algorithm has been useful in the field of computer graphics, for computing realistic images of virtual environments.

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Monte Carlo Methods for Nonlinear Equations

An important field of application of the Monte Carlo method is the numerical solution of nonlinear equations of high dimension. An example is the Boltzmann equation in rarefied gas dynamics, where the unknown function depends on three coordinates in the position space and on three coordinates in the velocity space. Stochastic particle methods for nonlinear equations are related to Markov systems of (many) interacting particles.

The purpose of the talk is to present some new results concerning the variance reduction problem for nonlinear kinetic equations. In recent years a new algorithm called the stochastic weighted particle method has been developed. The main idea is the introduction of a generalized interaction mechanism, which is based on the partial weight transfer during the interaction. This mechanism provides certain degrees of freedom, which are used for the purpose of variance reduction. The algorithm contains the standard DSMC (direct simulation Monte Carlo) method as a special case. However, the new interaction mechanism leads to an artificial blow-up of the simulation system.

In the talk various ideas for the reduction of the number of particles in the stochastic weighted particle method for the Boltzmann equation are discussed. It is shown that the reduction of the number of particles does not affect the accuracy of the numerical scheme. Corresponding error bounds are obtained. Numerical tests for the spatially homogeneous Boltzmann equation are presented.

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Structures in the Scatterplots of Inversive Generators

Given a scatterplot of a significant fraction (with respect to the period length) of the overlapping pairs (x_n, x_{n+1}) of pseudorandom numbers and the information that it stems from either a linear congruential or an explicit inversive congruential generator with small modulus, it is usually no problem to guess the type of the generator: points from a linear generator form a lattice or grid, whereas explicit inversive pseudorandom numbers contain hyperbola-like structures. In this talk we give an analytical description of this most eye-catching structural element of explicit inversive congruential generators. We also show that even well-visible hyperbolas are not detected by standard serial tests.

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Best Representative Points in the Square

Using the max-min distance as the uniformity measure, the most "natural" (in the sense of having the largest circular neighbourhood) representative points could be constructed with an optimization. We demonstrate that careful consideration of the boundaries should be taken so as to optimize the coverage efficiency by the neighbouring circles. In the same sense, the construction of the representative point set is equivalent to the best circle packing problem. Thus the hexagonal structure is dominant in the limit. Significant improvements of accuracy in numerical integration are observed and analyzed for the integrand with continuous first and second order derivatives. With additional boundary conditions, such that the unit square is topologically equivalent to the sphere/torus, the Euler Formula (in graph theory) takes effect upon the optimal point sets. I.e. most points are surrounded by hexagons while just a few ones are surrounded by pentagons.

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Efficiency of Quasi-Monte Carlo Algorithms for High Dimensions

Recently quasi-Monte Carlo algorithms have been successfully used for multivariate integration of high dimension d , and were significantly more efficient than Monte Carlo algorithms. The existing theory of the worst case error bounds of quasi-Monte Carlo algorithms does not explain this phenomenon.

In a paper with Ian H. Sloan we present a partial answer to why quasi-Monte Carlo algorithms can work well for arbitrarily large d . It is done by identifying classes of functions for which the effect of the dimension d is negligible. These are *weighted* classes in which the behavior in the successive dimensions is moderated by a sequence of weights γ_j . We prove that the minimal *worst case* error of quasi-Monte Carlo algorithms does not depend on the dimension d iff $\sum_{j=1}^{\infty} \gamma_j < \infty$. We also prove that the minimal number of function values in the worst case setting needed to reduce the initial error by ε is bounded by $C\varepsilon^{-p}$, where the exponent $p \in [1, 2]$, and C depends exponentially on the sum of weights. Hence, the relatively small sum of the weights makes some quasi-Monte Carlo algorithms efficient for all d .

We show in a non-constructive way that many quasi-Monte Carlo algorithms are strongly tractable. Even random selection of sample points (done once for the whole weighted class of functions and then the worst case error is established for the particular selection, in contrast to Monte Carlo where random selection of sample points is carried out for a fixed function) leads to efficient quasi-Monte Carlo algorithms. In this case the minimal number of function values in the *worst case* setting is of order ε^{-p} with the exponent $p = 2$.

We also present some results for more general algorithms than quasi-Monte Carlo algorithms. In a paper with F. J. Hickernell we prove in a *non-constructive* way that there exist algorithms for which the exponent $p = 1$ whenever $\sum_{j=1}^{\infty} \gamma_j^{1/2} < \infty$. In a paper with G. W. Wasilkowski we show in a *constructive* way that $p = 1$ whenever $\sum_{j=1}^{\infty} \gamma_j^{1/3} < \infty$. This is achieved by a *weighted tensor product* algorithm which can be also applied for more general linear problems than multivariate integration

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The Diaphony and the Star-Diaphony of some Two-Dimensional Sequences

Let $\sigma = (\xi_n)_{n \geq 0}$ be a finite or infinite sequence of points in the unit cube $I^s = [0, 1]^s$ and let it contain at least N terms. For each $\mathbf{x} = (x_1, \dots, x_s)$ in I^s , $A_N(\mathbf{x}, \sigma)$ denotes the number of indices n such that $0 \leq n \leq N-1$ and $\xi_n \in \prod_{i=1}^s [0, x_i)$ and $E_N(\mathbf{x}, \sigma)$ the remainder to ideal distribution:

$$E_N(\mathbf{x}, \sigma) = A_N(\mathbf{x}, \sigma) - x_1 \dots x_s N.$$

A classical measure for the irregularity of the distribution of a sequence σ in I^s is the L^2 -discrepancy $T_N(\sigma)$ which is defined for every positive integer N by

$$T_N(\sigma) = \frac{1}{N} \left(\int_{I^s} |E_N(\mathbf{x}, \sigma)|^2 d\mathbf{x} \right)^{\frac{1}{2}}.$$

Another measure for the irregularity of the distribution of a sequence σ in I^s is the diaphony $F_N(\sigma)$ which is defined for every positive integer N by,

$$F_N(\sigma) = \left(\sum_{\mathbf{h} \in \mathbb{Z}^s - \{0\}} \frac{1}{r(\mathbf{h})^2} \left| \frac{1}{N} \sum_{n=0}^{N-1} e^{2\pi i \mathbf{h} \cdot \xi_n} \right|^2 \right)^{\frac{1}{2}},$$

where $\mathbf{h} = (h_1, \dots, h_s)$, $\mathbf{h} \cdot \mathbf{x} = \sum_{i=1}^s h_i x_i$ and $r(\mathbf{h}) = \prod_{i=1}^s \max\{1, |h_i|\}$.

For the purpose of numerical integration, we have introduced in [1] a new version of diaphony, the so-called star-diaphony, which is defined for every positive integer N by

$$F_N^*(\sigma) = \frac{(2\pi)^s}{N} \left(\sum_{\mathbf{h} \in \mathbb{Z}^s - \{0\}} \left| \int_{I^s} E_N(\mathbf{x}, \sigma) e^{2\pi i \mathbf{h} \cdot \mathbf{x}} d\mathbf{x} \right|^2 \right)^{\frac{1}{2}}.$$

The F_N^* is related naturally to T_N by the so-called Koksma formula,

$$T_N^2(\sigma) = I_N^2(\sigma) + \frac{1}{(2\pi)^{2s}} (F_N^*(\sigma))^2$$

where

$$I_N(\sigma) = \frac{1}{N} \sum_{k=1}^N \prod_{j=1}^s (1 - \xi_k^j) - \frac{1}{2^s}.$$

In this communication, we give some estimates of the diaphony and the star-diaphony for some two-dimensional (finite) sequences, such as, the Roth sequence, the Zaremba sequence and the good lattice points.

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Monte Carlo Methods and Importance Sampling Algorithms for Nonlinear Filtering Problems

Nonlinear filtering problems involve estimating the state of a nonlinear stochastic system from noisy observation data. Here let us discuss the problem for the discrete-time signal system for R^n -valued process $x(k)$ (we can similarly study the continuous-time signal system):

$$x(k) = f(x(k-1)) + w(k) \quad (1)$$

and the observation process $y(k) \in R^p$ is given by

$$y(k) = h(x(k)) + v(k) \quad (2)$$

where $w(k)$ and $v(k)$ are white noise with covariances Q and R respectively. We assume that the initial condition $x(0)$ and $w(k), v(k)$ are independent random variables. The optimal nonlinear filtering problem is to find the conditional expectation $E(x(k)|Y_k)$ of the process $x(k)$ given the observation data $Y_k = \{y(j), 1 \leq j \leq k\}$. The probability density function $p_{k|k}$ of the conditional expectation $E[x(k)|Y_k]$ is given by Bayes' formula

$$p_{k|k-1}(x) = \int_{R^n} \left(\int_{R^n} \frac{1}{((2\pi)^n \det Q)^{1/2}} e^{\frac{1}{2}(x-f(t))^t Q^{-1}(x-f(t))} dx \right) p_{k-1|k-1}(t) dt \quad (3)$$

and

$$p_{k|k}(x) = c e^{\frac{1}{2}(y-h(x))^t R^{-1}(y-h(x))} p_{k|k-1}(x) \quad (4)$$

where $p_{k|k-1}$ is the one-step prediction and is the probability density function of $E[x(k)|Y_{k-1}]$. That is, the recursive filter (3)-(4) consists of the prediction step (3) and the correction step (4).

The filtering problem is an important theme in the area of applied statistics and probability. It has been the subject of considerable research interest during the past several decades because it has many significant applications in science and engineering such as data fusion, finance, and random media analysis, medical data processing, computer vision, target tracking, and air traffic control. As we know the most widely used filter is the extended Kalman filter for nonlinear filtering problems which is regarded as a mainstay of modern aerospace engineering. It is derived from the Kalman filter based on the successive linearization of signal process and observation map. The extended Kalman filter has been successfully applied to numerous nonlinear filtering problems. If nonlinearities are significant, however, its performance can be substantially improved. Such efforts have also been reported. New Gaussian and mixed Gaussian filtering algorithms have been recently proposed in Ito's and Xiong's paper. The filtering algorithms show superior performance against the extended Kalman filter.

In this paper our objective is to further develop and analyze real-time and accurate filtering algorithms for nonlinear filtering problems based on Monte Carlo methods and importance sampling algorithms. We present the systematic formulation of the Monte Carlo filters and importance sampling filters. Our numerical testing demonstrates that new filtering algorithms significantly improve the existing ones, especially the extended Kalman filter with no additional cost, and have a nearly optimal performance.

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Design of Nuclear Medical Imaging Systems using the Monte Carlo Method

There has been enormous increase and interest in the use of Monte Carlo techniques in all aspects of nuclear medical imaging, including planar imaging, Single-Photon Emission Computed Tomography (SPECT) and Positron Emission Tomography (PET). Especially they have been applied to simulate processes involving random behaviour such as emission and interaction of the radiation with matter and to quantify physical parameters that are difficult or even impossible to calculate by experimental measurements. This paper presents derivation and methodological basis for this approach. Potential applications in different areas of nuclear imaging such as detector modeling and systems design, image reconstruction and scatter correction techniques, and internal dosimetry are presented. An overview of existing simulation programs is provided and illustrated with examples of some useful features of such sophisticated tools in connection with common computing facilities available in hospital environments. Vectorized and parallel implementations of Monte Carlo codes and some strategies for future development in the field are also discussed.

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