Investigating the Use of Low-Discrepancy Sequences in Particle Simulations for Rarefied Gas Flows

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Overview

- Examples of fluidic MEMS
- Simulation challenges of rarefied gas flows
- Theoretical improvements offered by low-discrepancy (LD) sequences
- Sample problem: collisionless flow in a 2D duct
- Success in low dimensions (< 100 dimensions)
- Physical explanation of poor convergence in high dimensions – particle move correlation
- Conclusions and future work

Fluidic MEMS

Fluidic Micro-Electro-Mechanical-Systems

- Air friction in non-vacuum sealed micro-machines*
- Micro-sensors: chemical detectors, fluid monitors
- Micro patterned explosives – on chip gas generation
- Micro-thrusters – very precise satellite attitude control
- Micro-fliers – “ultimate” fly on the wall spy, and biomedical applications

* Image courtesy of Sandia National Laboratories, SUMMiT™ Technologies, www.mems.sandia.gov

Simulation Challenges

- Fluidic MEMS often operate in the transition region between continuum and collisionless flow (0.1 < Kn < 10)

$$Kn = \frac{\text{mean free path between gas molecules}}{\text{length scale}}$$

- Traditional continuum and near-continuum solutions (Euler, Navier-Stokes) lose physical accuracy.
- There are insufficient molecular collisions occurring in the volume of interest for the gas to reach local thermodynamic equilibrium (LTE).
- Need to include non-equilibrium effects for an accurate simulation.

Simulation Challenges

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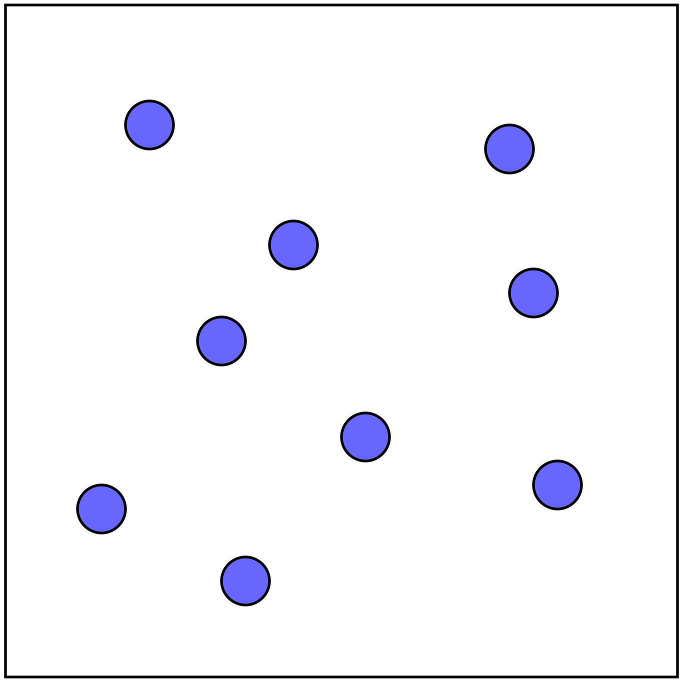
- Boltzmann equation: 7-dimensions $f(x_1,x_2,x_3,v_1,v_2,v_3,t)$ non-linear, integro-differential equation.

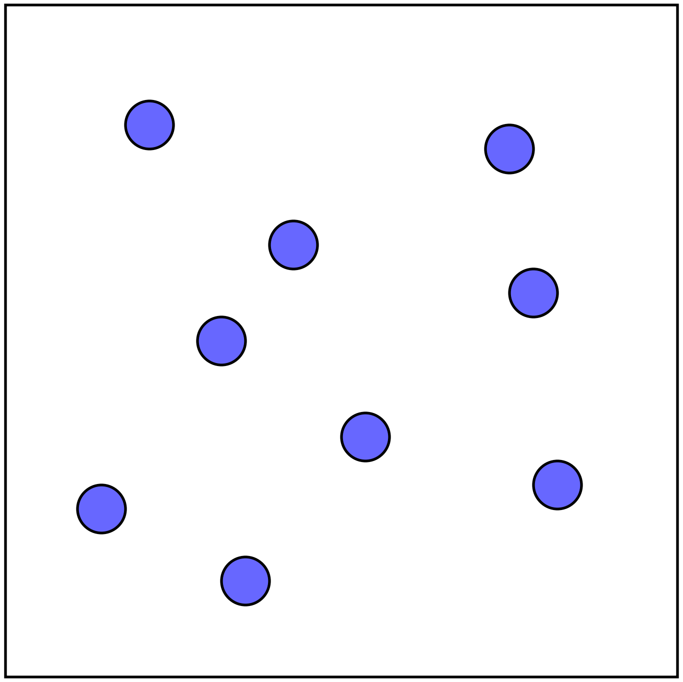
$$\frac{\partial(nf)}{\partial t}+\mathbf{v}\cdot\nabla_{\mathbf{x}}(nf)+\mathbf{g}\cdot\nabla_{\mathbf{v}}(nf)=\int_{-\infty}^{\infty}\int_{0}^{4\pi}n^2(f^*f_1^*-ff_1)\mathbf{v_r}S\mathrm{d}\Omega\mathrm{d}\mathbf{v_1}$$

- Simulation via a direct discretization of the equation is difficult because of the memory requirements, even the simplest 1D spatial geometries require a 3D grid.
- The velocity domain is infinite.
- Direct Simulation Monte Carlo (DSMC) allows for a physically accurate non-equilibrium solution by tracking the local behavior of the gas molecules.



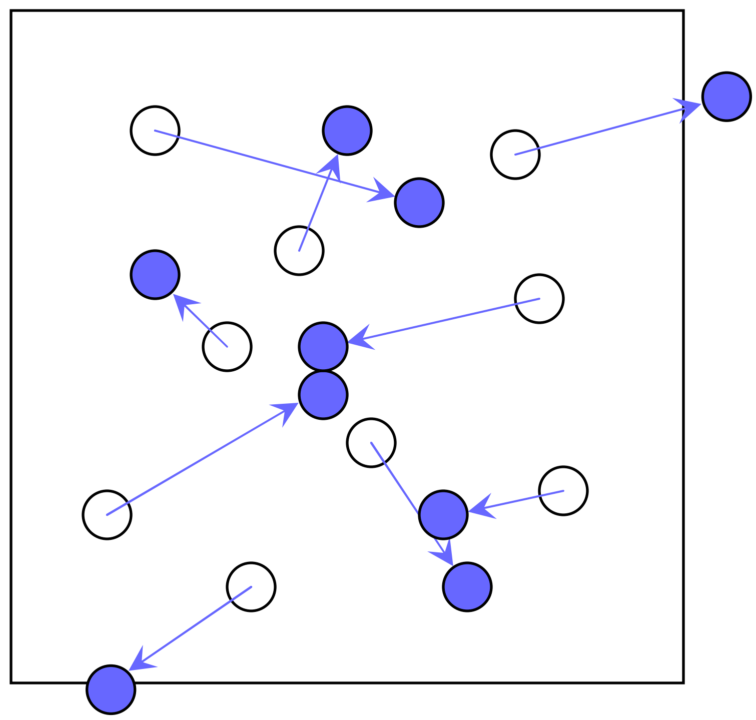
1. Choose a particle weight – in most cases there are too many physical particles (10^{20}) in the simulation domain, instead simulate a statistically valid number of sample particles.

DSMC



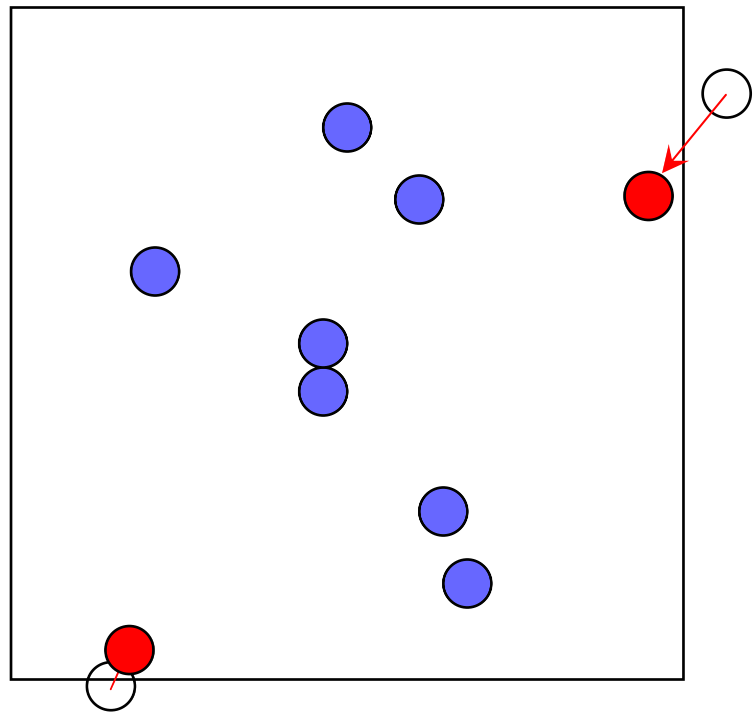
2. Choose a time step small enough so that on average only a fraction of particles undergo a collision (physics-splitting).

DSMC

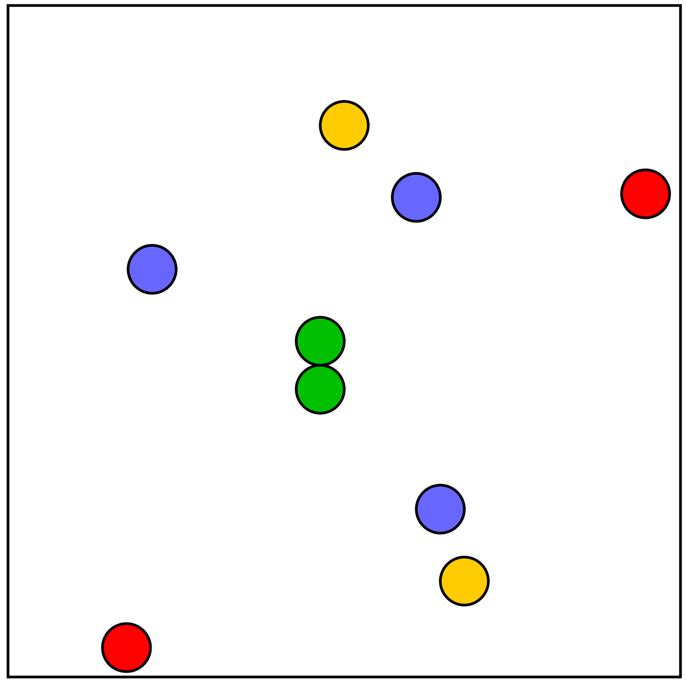


3. Move the particles based on current velocity.

DSMC

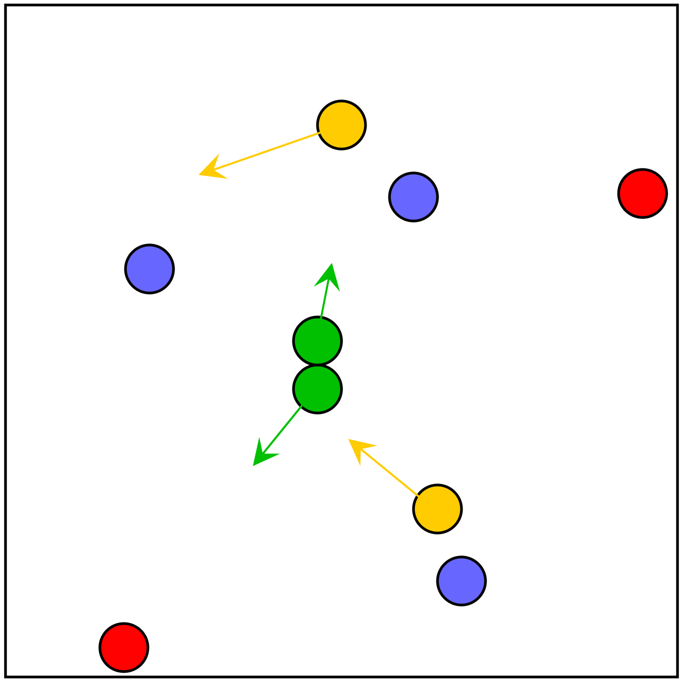


4. Find the particle-boundary interactions and select the new trajectory using the probabilistic boundary conditions and a pseudo-random number (PRN) generator.



5. Calculate the number of collisions that should occur on average in the region of interest, based on the local particle density and randomly (PRN) select the collision pairs.

DSMC



6. Sample the post collision trajectories using the PRN generator from the appropriate probabilistic description of the interaction.
7. Repeat until there are sufficient independent samples.

DSMC

- DSMC generates sample particle behavior consistent with the Boltzmann equation without directly solving it.
- The collection of all the sample particles approximates the velocity distribution function $f(x_1,x_2,x_3,v_1,v_2,v_3,t)$ and can be used to calculate the flow properties.
- The probabilistic error bound on the method is $\sigma/N^{-1/2}$.
- For air at room temperature: V_{avg} = 470 m/s, σ = 300 m/s.
- The problem with fluidic MEMS simulations is that the bulk flow is often very much less than the standard deviation.
- For example: 100 mm/s accuracy requires 9M samples
  10 mm/s accuracy requires 900M samples

Low Discrepancy

- Koksma-Hlawka inequality bounds the error sampling the integrand.

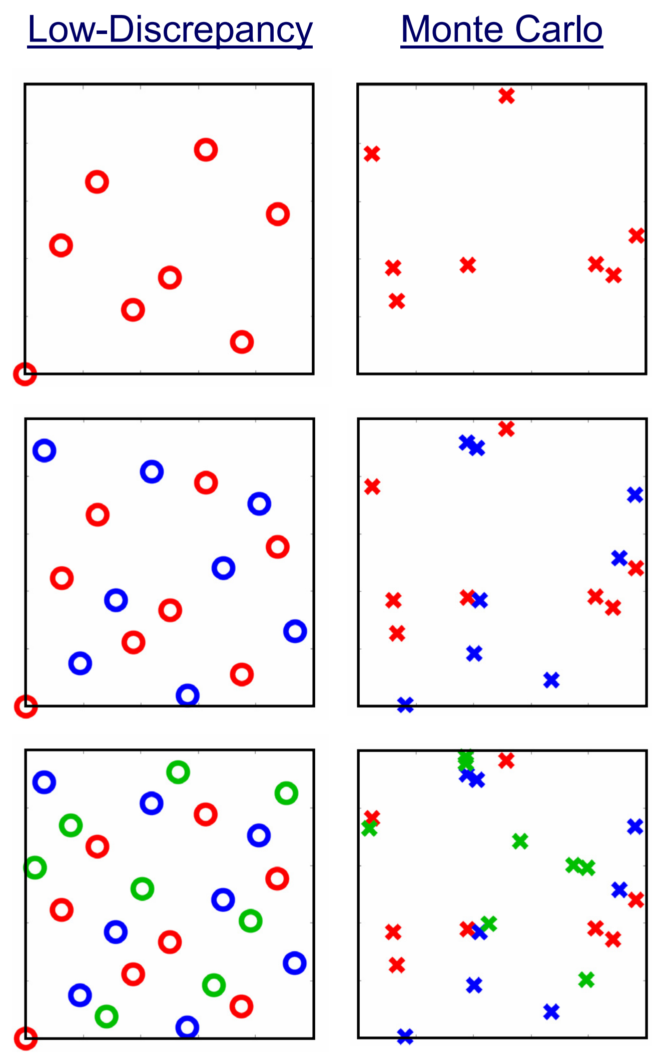
$$\left| \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{x}_n) - \int_{[0,1)^s} f(\mathbf{u}) d\mathbf{u} \right| \le V(f) D^*(N)$$

- V(f) is the bounded variation of the integrand – “smoothness”
- D*(N) is the star-discrepancy of the N-point sequence – “uniformity”
- For a Monte Carlo sequence:

$$D^*(N) = O(N^{-1/2})$$

- For a Low-Discrepancy sequence:

$$D^*(N) = O(N^{-1} (\log N)^s)$$



Low Discrepancy

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- We replace the pseudo-random number (PRN) generator of the Monte Carlo method with a low-discrepancy (LD) sequence.
- The hope is that the resulting method will maintain the non-equilibrium accuracy of a particle method while achieving a near-linear convergence rate.
- Many LD sequences available:

Van der Corput, Halton, Faure	prime numbers
Richtmyer, Ramshaw	irrational fractions
Niederreiter	irreducible polynomials
Sobol’	primitive polynomials

Problem Description

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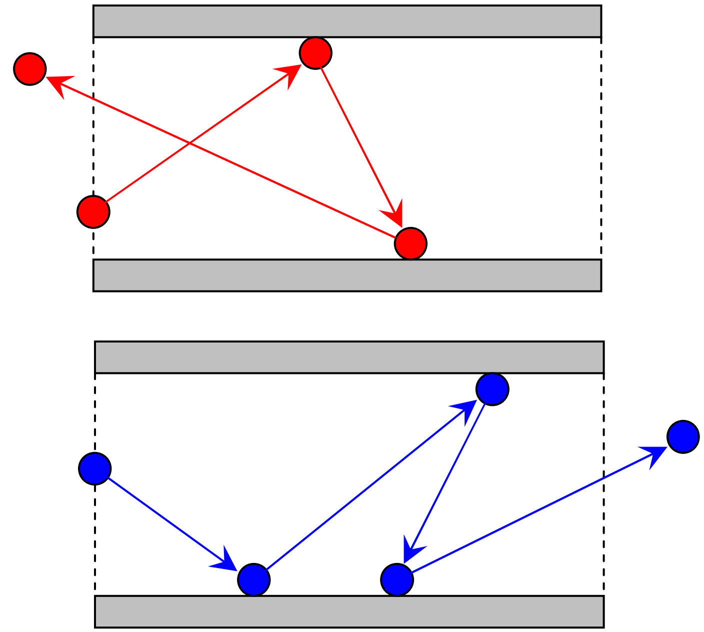
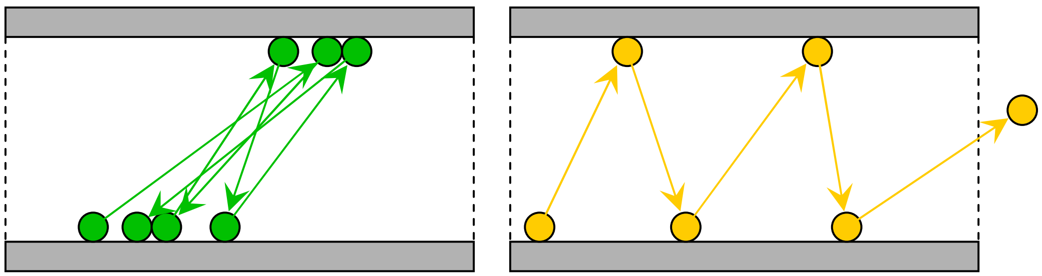
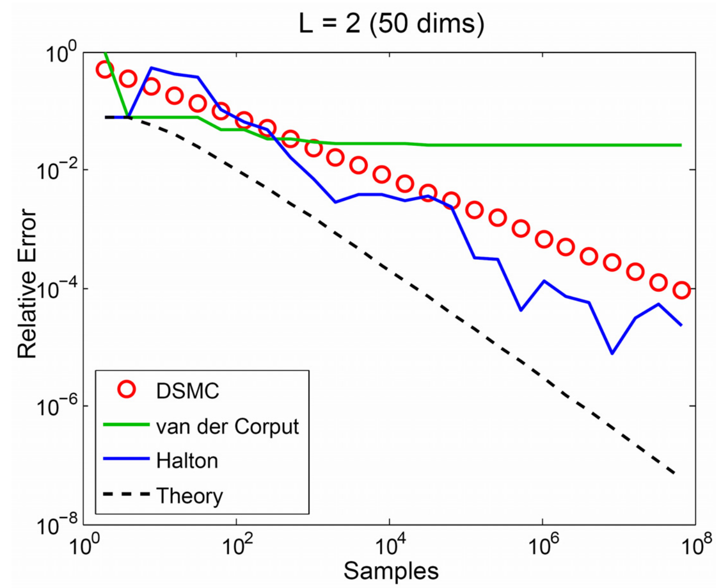
- Collisionless gas flow in a 2D duct (L = length to height ratio).
- Only tracking particle-boundary interactions.
- Inlet – gas at equilibrium.
- Outlet – vacuum.
- Wall assumed to be fully diffuse (typical > 90%) – wall reflection independent of incoming trajectory.



- Simulated quantity is the particle flow conductance which equals the fraction of particles that eventually escape the outlet from the inlet.

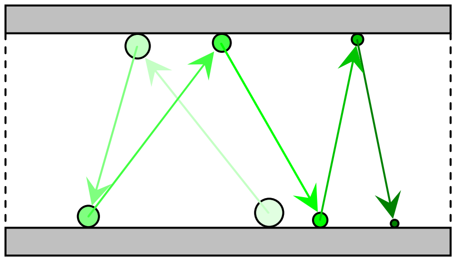
Direct Replacement

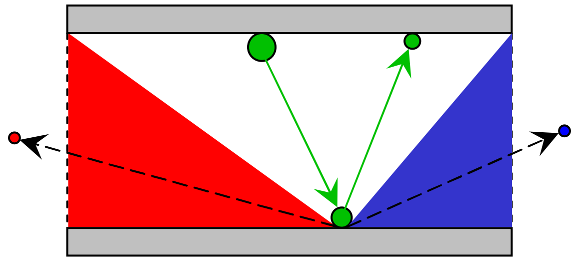


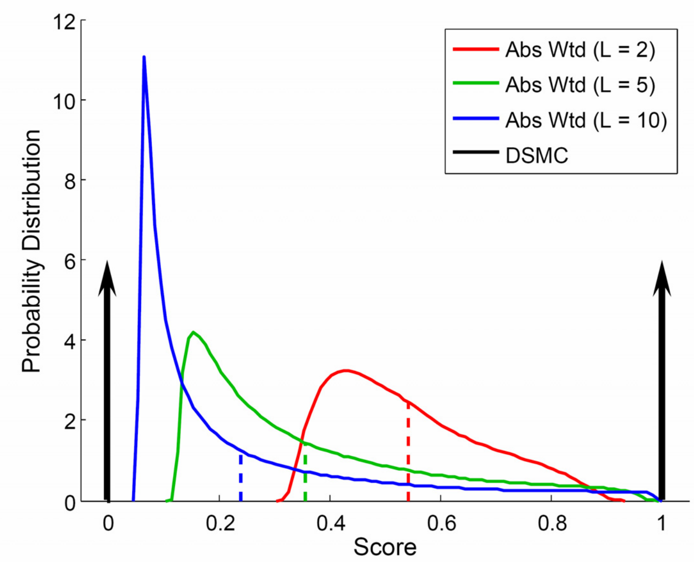


- Replacing PRN generator with a 1D low-discrepancy sequence (van der Corput) does not converge.
- Particles move in highly correlated patterns: RLRLRLRL or RRRRLLLL.
- Instead use a multi-D, low-discrepancy sequence (Halton) with each dimension representing a particle move.
- Faster than DSMC, but does not reach theoretical rate.

Smooth Integrand

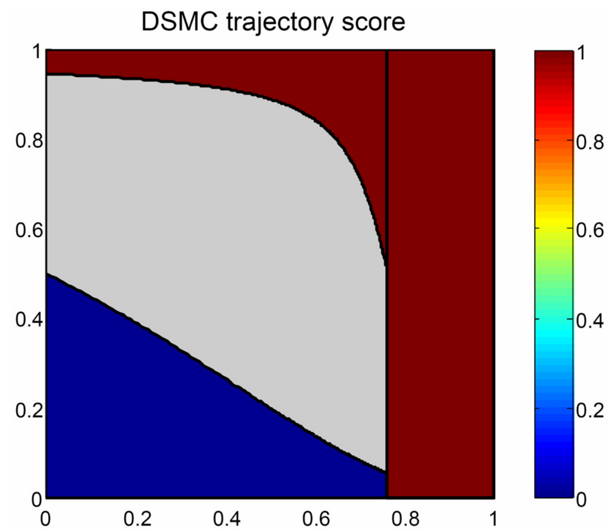


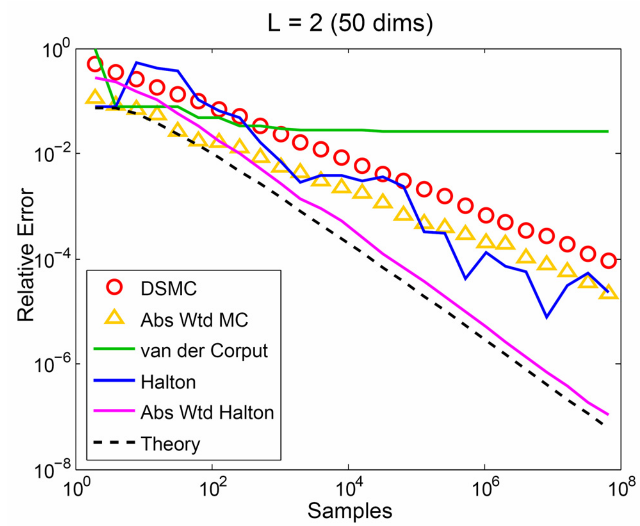


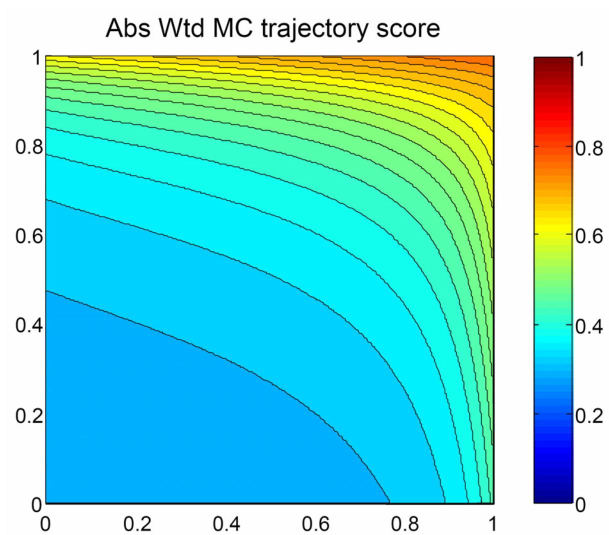


- The smoothness of an integrand generally affects the LD sequence performance.
- The discontinuous YES/NO decisions of the DSMC method can be avoided.
- Borrow the absorption weighting technique used for variance reduction in radiation transport problems.
- Particles no longer escape, instead the weight is reduced at each move by the fraction that should escape.

Absorption Weighting

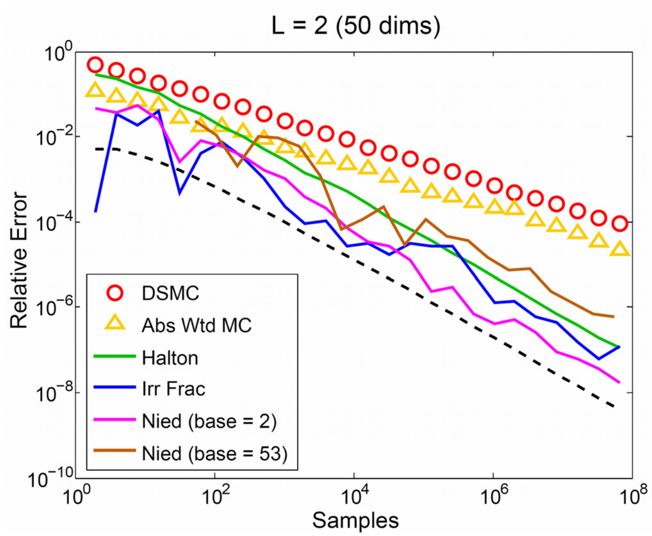


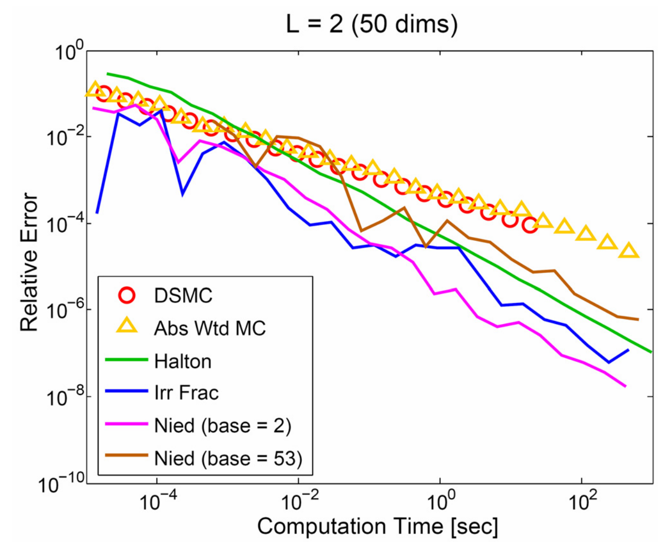




- LD performance degrades when discontinuities in the integrand are not aligned with the axes.
- The absorption weighted technique eliminates the discontinuities.
- LD sequence results in near-linear convergence.

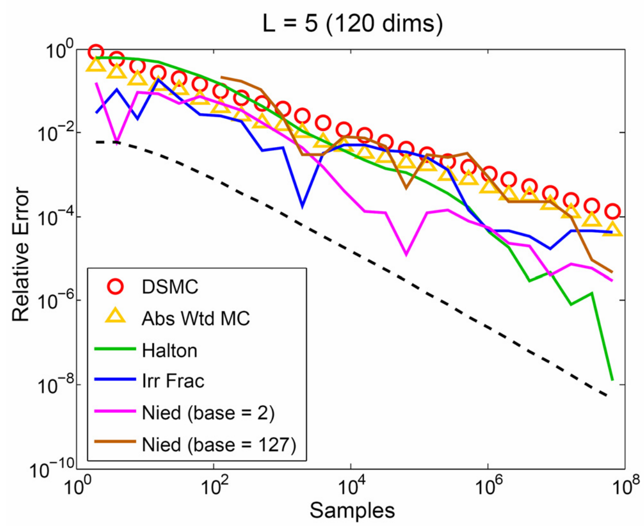
Performance

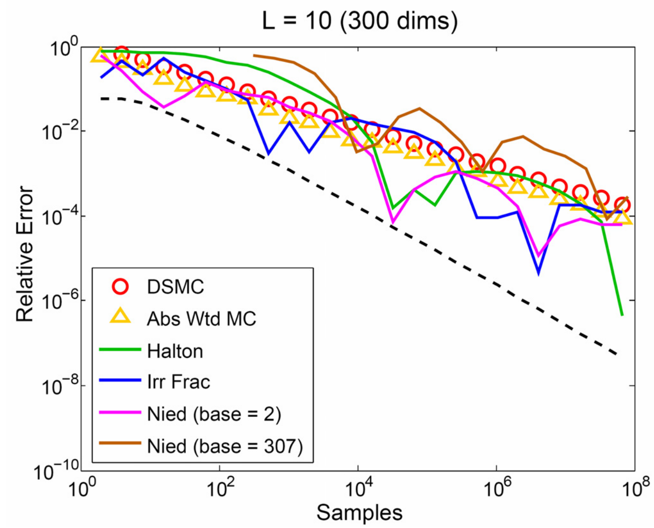




- All LD sequences eventually approach the theoretical convergence rate $O(N^{-1} (\log N)^s)$.
- Absorption weighting does lower variance but is not actually faster than direct simulation for Monte-Carlo.
- Niederreiter's sequence in base 2 consistently the fastest and most accurate.

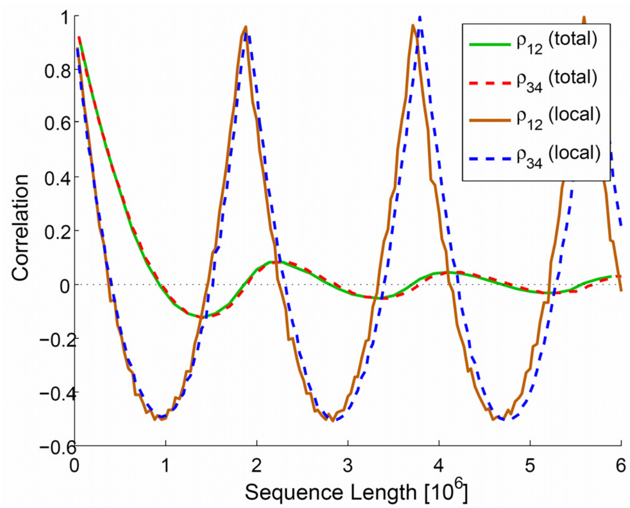
Performance

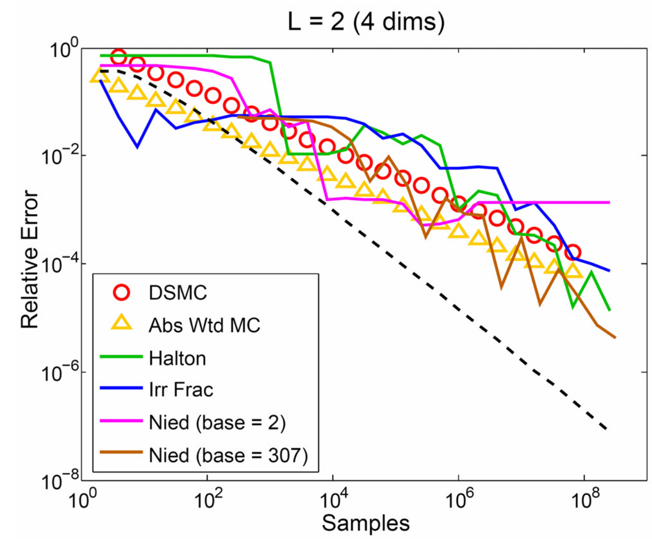




- For L = 5, only the Halton's and Niederreiter's sequence in base 2 show consistent gains over PRN generator.
- No sequence is clearly approaching the theoretical convergence rate.
- For L = 10, no sequence shows consistent improvement over PRN generator.

Correlation Problems





- In higher dimensions, the "independent" LD generators for each dimension become more similar.
- When 2D correlation between pairs of sequences ρ_{12} and ρ_{34} is similar the resulting 4D correlation persists longer.
- Four move simulation using the most "obvious" candidates from the 300 dimensional sequences shows similar convergence to the L = 10 case.

Conclusions

- It is possible to construct a simple particle simulation that achieves near linear convergence $O(N^{-1} (\log N)^s)$ using low-discrepancy sequences.
- You cannot simply replace the PRN generator in your DSMC code with a low-discrepancy one.
- When the dimension of the problem is sufficiently small ($D < 50$), significant performance gains can be achieved (350 times faster).
- In higher dimensions ($D < 120$), some low-discrepancy sequences still offer faster convergence than Monte-Carlo.
- Correlation between dimensions of the LD sequence causes the particle moves to have non-physical behavior.
- Offers potential for improving solutions for fluidic MEMS.

Future Work

- Reduce the problem dimension:
  - \+ use LD sequences only on “dominant” dimensions
  - \+ discretize the problem and try to smooth the grid interaction
- Coupling between two probabilistic processes.
- Other variance reduction techniques.

Acknowledgements

I would like to thank the Department of Energy and the Krell Institute for their financial support through the CSGF.

I would also like to thank Sandia National Laboratories, in particular, Michael Gallis, Wahid Hermina and the Engineering Sciences Center dept. 9113 for their support during my practicum.

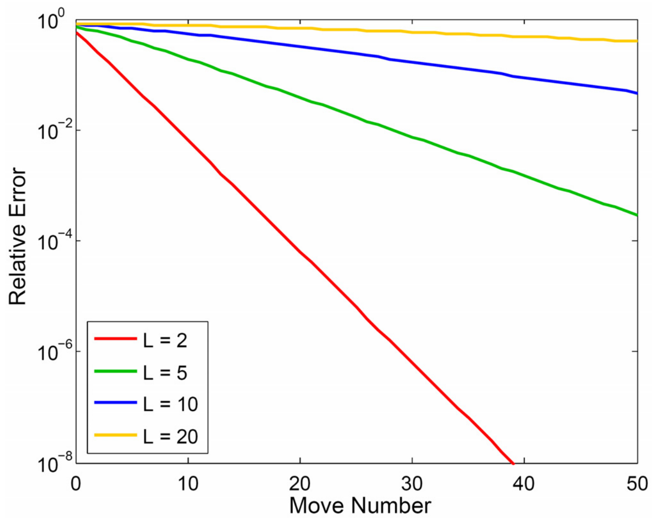
Questions?

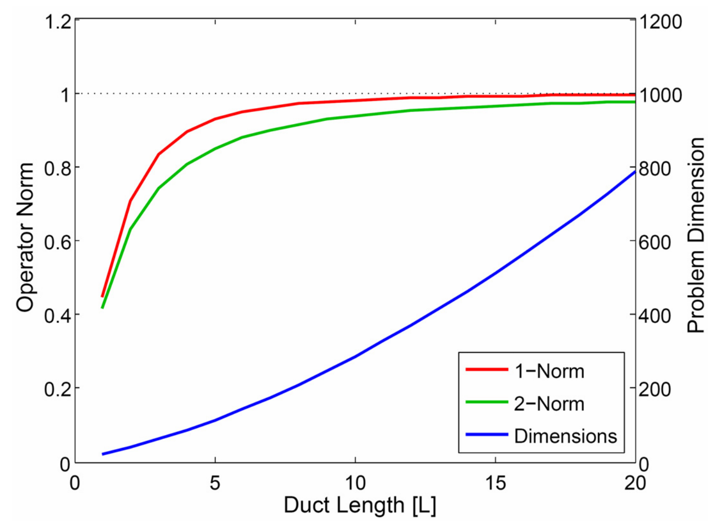
"Any one who considers arithmetical methods of producing random digits is, of course, in a state of sin."

- John von Neumann (1951)

J. Von Neumann, 'Various techniques used in connection with random digits.' *National Bureau of Standards Applied Mathematics Series*, vol. 12, 36-38, 1951.

Increasing Dimensions





- As duct length increases, so does the necessary number of particle moves (dimensions) to achieve a specific error.
- Physically, it means the particles are spending a longer time in the duct.
- Mathematically, the operator *K* governing the particle moves also governs the error $|e_{n+1}| < |K||e_n|$ and the norm approaches 1 as the duct length increases.

Correlation Patterns

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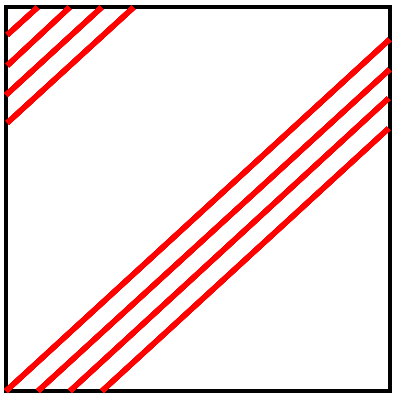
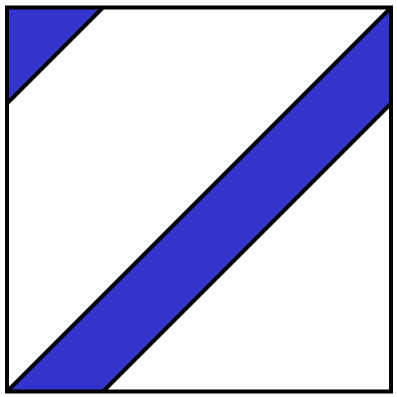
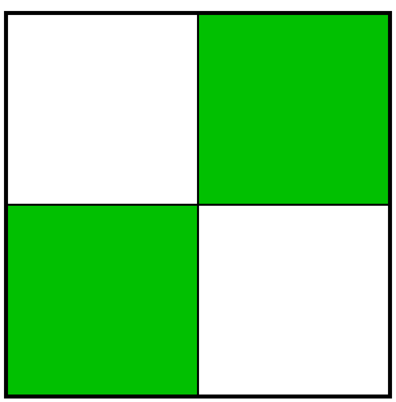
Halton
Max length: 1.8M



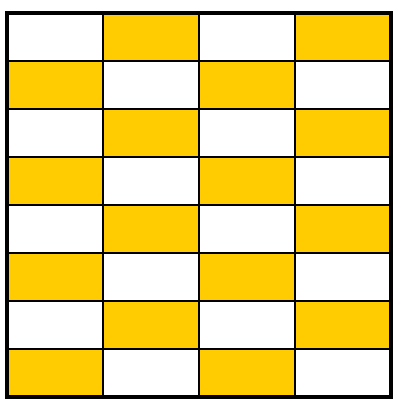
Irrational Fractions
Max length: 14M



Niederreiter (base 2)
Max length: 2.1M



Niederreiter (base 2)
Max length: >2.1M



- LD sequences in high dimension can show obvious correlation patterns between dimensions.
- The resulting correlation between moves is similar to the 1D sequence.
- Correlation is not bad provided that the correlated sequence length is smaller than the total simulation.
- The “curse of dimension.”