To: Professor Paul McCudden 9/3/15
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From: Tannaz Oskui

Subject: Final Report
-Supercomputer Numerical Simulation of Astrophysical Processes
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My 2015 summer CURE project was to gain experience in the mathematics of Monte Carlo Analysis and the physics of stellar formation processes. These two research fields are both in pure research and in particular in pure mathematics. As such they are part of a multi-year, long term effort, to improve the computational capability via advanced Monte Carlo methods to model complex astrophysical processes.

One of the primary research directions for JPL and NASA is to understand, in as complete detail as possible, the stellar and planetary formation process. This involves the construction of theoretical models for the contraction process and the radiations that would be expected from such an occurrence. These radiations in turn should be observable from Earth with large ground based telescopes, the Hubble Space Telescope and the future James Webb Space Telescope. This would allow a comparison between the predicted and observed radiation fluxes, to see how well they matched and any differences can be used to refine the theoretical models. Once the models are deemed sufficiently accurate further research could then be done purely *numerically,* as is done in Numerical General Relativity, greatly improving the productivity and cost effectiveness of the space telescopes.

Unfortunately, classical closed form solutions of radiative transport problems are usually only possible with extremely simplified representations of real physical systems. To gain the type of clarity to do modern astrophysical research requires doing numerical integrations of high dimension. While in principle this is always possible and indeed it is the assumption of classical continuity which allows a Riemann sum to converge, that convergence rate will decrease rapidly with dimension.

To illustrate this consider modeling a single particle of mass m moving in a fixed volume V and elastically scattering off the walls. It would take 7 real numbers to specify the state of this particle classically. Three for the x, y, z classical Cartesian coordinates, three more for the classical velocity components v_x, v_y, v_z and one for time. To perform a numerical integration

$$\iiint \dots \int f(x_1 \dots x_7)\, d\, x_1 \dots dx_7$$

over these quantities to say, estimate the pressure of the system, would result in an error converging to zero at the rate of

$$error\ \alpha\ \frac{1}{\sqrt[7]{n}}$$

where n is the number of sample used in the integration estimate.

This is deduced by the fact that for each dimension in a problem it requires m sample *points for that dimension* to insure that the accuracy of that dimension is no more that $\frac{1}{m}$. And since the accuracy for the numerical integration over a hypercube of dimension s can be no more accurate that of an individual dimension it would require $n = m^s$ number of points to guarantee that no dimension was sampled less then m times. Thus for the entire integral to be guaranteed to have an error of less than $\frac{1}{m}$ would be achieved

$$if \;\; n = m^s$$

$$\Longrightarrow \frac{1}{m} = \frac{1}{\sqrt[s]{n}}$$

and thus the convergence rate is $\frac{1}{\sqrt[s]{n}}$ up to a multiplicative constant.

One of the immediate consequence for this in the case of the simple seven dimensional problem is that to improve the accuracy of a previous calculation by just two decimal points would require about 10^{14} more functional evaluations, not just floating point operations. Give typical computer speeds this could take on the order of a few hundred thousand years. The problem only gets worse with ever higher dimension.

This difficulty with dimension has been labeled, "The curse of dimensionality" and seemed be an impenetrable barrier until the 1940's when amazing minds of Stanislaw Ulam, Richard Feynman and Jon von Neumann, came up with a new paradigm to consider the question. Instead of doing such problems directly consider their solutions as the expectation values of probabilistic problems. The advantage would be that the problem would now have a guaranteed solution by one of the most famous and strongest theorem in probability theory, the central limit theorem. Thus the computation would converge at the rate of

$$\frac{1}{\sqrt[2]{n}}$$

and would be independent of the dimension!

Of course a drawback would be that the answer would only probabilistic and could be wrong, it was simply not *likely* if n was sufficiently large. As Ulam, Feynman and von Neuman were applying these methods to atomic weapon design computing only a high probability engineering estimates would normally not be acceptable for obvious reasons, but as these were the *only* methods that could give reasonable engineering answers is a short time they were quite a revolution.

As the methods were related to the analysis of games of chance and Ulam and other European scientist refugees were working on the Manhattan project had family or friends who went to Monte Carlo to gamble. The name Monte Carlo Method came to become common terminology for the method. To illustrate how the method works visually, consider the simple question of how you determine the area of a circle. Of course the standard formula could be used, but in the Monte Carlo method would ask you to consider throwing *random* darts at a square board of unit area. Then, *in the limit*, the ratio of the darts that fall into the circular area divided by the total number of darts would converge to the area of the circle and the error would converge at the rate of $\frac{1}{\sqrt[2]{n}}$ as guaranteed by the central limit theorem.

This approach can be easily tried on an ordinary computer and at first does not seem so impressive. However, it can also be used when the area is very arbitrary and would be a nightmare to do by classical methods even in two dimensions and starts to provide an overwhelming computational advantage even for dimensions as low as 3.

Thus success of the Monte Carlo methods led a number of researchers to explore more deeply why these methods worked so well. Over the next few decades it started to be appreciated that it was not the randomness *per se* of the random numbers but their ability to uniformly cover the space they sample that was important. This lead to a new branch of the method now called Quasi-Monte Carlo Methods which where deterministically constructed sequences and could be used in place of the purely pseudo random numbers. These sequences can be used to construct Quasi-Random vectors and can converge in quadrature problems with an error rate of proportional to

$$\frac{1}{n}$$

which is a fundamental qualitative improvement. Further, since these sequences are deterministic their errors also will have absolute bounds which are guaranteed by an analog of the central limit theorem called the Koskma Inequality to converge at the 1/n rate. In one dimension it has the form

- $\left|\int_{I^1} f(x)dx - \frac{1}{N}\sum_{k=1}^{N} f(x_k)\right| \leq \mathrm{V(f)}\, D^*(\mathrm{P})$

Here the quantity V(f) is the fixed variation of the function which for functions of bounded variation will be a fixed constant. The discrepancy, $D^*(P)$, for the point set P is figure of merit to measure how "good" a sequence is. This is the factor which has the 1/n convergence rate.

The discovery of improved Quasi-Random point's sets is at the frontier of the research in this field and something that I may wish to continue on in the future.

I wish to thank JPL and my mentors Dr. John Sepikas, Dr. Neal Turner, Professor Paul McCudden for this wonderful opportunity.