BROOKHAVEN NATIONAL LABORATORY
PROPOSAL INFORMATION QUESTIONNAIRE
LABORATORY DIRECTED RESEARCH AND DEVELOPMENT PROGRAM

PRINCIPAL INVESTIGATOR	**Robert Szafron**	**PHONE**	
DEPARTMENT/DIVISION	**Physics**	**DATE**	**29 May 2022**
OTHER INVESTIGATORS	**Peter Boyle, Taku Izubuchi, Tobias Neumann, Sally Dawson**		
TITLE OF PROPOSAL **TYPE A**	**Towards a Brookhaven integrator for precision physics on GPUs**		
PROPOSAL TERM (month/year)	From **9/1/2022**	Through **8/31/2025**	

SUMMARY OF PROPOSAL

Description of Project:

Precise theoretical predictions for future colliders are hindered by the speed of numerical integrators. This proposal aims to apply methods used in lattice gauge theory (to importance sample the Feynman path integral) to numerical integration in precision physics.

A key limiting factor in numerical integrators such as the popular VEGAS package are the constraints in parametrizing the probabilistic sampling of the integral. These are structured to use a weighting function that is easy to sample but does well describe sharply peaked functions of up to 20 variables. Metropolis MCMC methods, originally developed within theoretical physics by scientists on the Manhattan project, are currently used in lattice gauge theory to importance sample up to 1 billion variables the distribution of QCD.

We will combine these methods with more powerful adaptive sample probability distributions that can better match the Feynman amplitudes being integrated.

We will also combine lattice techniques for programming modern GPU computers with the problem of numerical integration to pave the way towards a Brookhaven integrator.

Expected Results:
Improved precision of high order numerical integration approaches to precision physics that will enable inclusion of higher order and thus more precise calculations in event generators for current and future colliders. This may lead to funding opportunities and a unique Brookhaven scientific software capability.

PROPOSAL

Precise theoretical predictions for future colliders are hindered by the speed of numerical integrators. These have two roles. Firstly high order numerical loop integration involves integration over up to twenty degrees of freedom depending on the order. Secondly, final state phase space integration. (Tobias, Robert physics case?)

For precision theoretical results to be useful to the HEP experimental program, they must be practical to include in event generation for the experimental events to be statistically compared to the theoretically predicted distribution of any experimentally measured process.

Monte Carlo Integration:

Numerical integration is performed using random sampling Monte Carlo methods, Figure 1. Popular numerical integrators, such as the VEGAS package[1] use an ideal strategy called importance sampling to draw more samples in the regions of integration that dominate the integral, and fewer samples where the integrand is small. This implies distributing the samples for integration according to a designed probability distribution that accurately weights the important parts of the integral, while giving less numerical effort on the less important parts to be efficient.

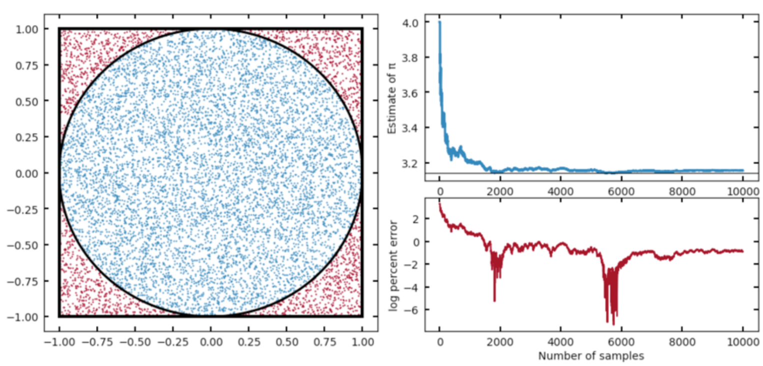


Figure 1: *one can integrate the area of a circle, or any other shape, by throwing darts randomly at a circle. The area of the square is 4 while the area of the circle is π. The fraction of darts that fall inside the circle is $\pi/4$.*

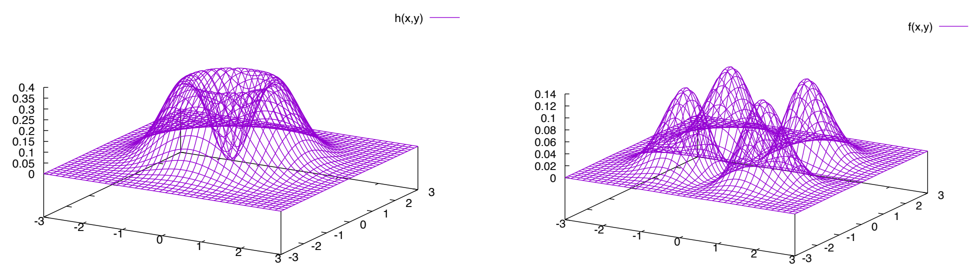
For the process to be efficient, the integrator should automatically learn something about the integrand, and model its shape. Numerical integrators construct a probability distribution on the domain of integration, and sample from this. The probability distribution is factored into the integration weight and the probability density and the value of the integrand combined in the integration result. VEGAS constructs its probability distribution an approximation to the modulus of the integrand.

In order for the VEGAS probability distribution to be easy to sample from, as factorized form is assumed. In two variables, x and y, the probability takes the form P(x,y) = X(x) Y(y).
The functions X(x) and Y(y) are piecewise linear and learned in a training phase. This make x and y possible to independently sample and the distribution easy to normalize, however this has drawback

that complex integrand shapes cannot all be well described. This is particularly troublesome as the number of integration variables becomes large and the target problem space is now reaching up to twenty dimensional integrals.

As an illustration, Figure 2 displays a non-factorized probability distribution and an obvious factorized 'close' representation which fails to match this. The failure to match will result in more Monte Carlo samples being required for the same statistical precision, and consequently long computer run times.

Figure 2: *A non-trivial probability distribution, $P(x,y) = (x^2+y^2) e^{-x^2+y^2}$ in two dimensions and the obvious closest factorization $P(x,y) = x^2 e^{-x^2} y^2 e^{-y^2}$. The assumptions made in setting up a probability function in VEGAS that is simple to sample lead to constraints in the Monte Carlo sampling that can be inefficient, particularly in high dimensional integrals.*



In recent years, due to the deficiencies of popular numerical integrators, precision theoretical physics has looked at Machine Learning and neural networks to generate the modelled probabilistic sampling. The expense of the neural network training however has left this unsuccessful in generating a compelling class of numerical integration algorithms and workhorse tools like VEGAS remain state of the art.

Monte Carlo simulation, or random sampling algorithms, have a rich Department of Energy heritage. Monte Carlo as a name invented by Nicholas Metropolis, a member of the Manhattan project, and the idea connects back to John von Neumann and Stanislaw Ulam.

This proposal is to replace conventional Monte Carlo numerical integrator algorithms used in precision theoretical calculation with a specific type of Monte Carlo method, most commonly known as a Metropolis algorithm (or in computer science known as a Metropolis-Hastings algorithm). These were developed by members of the DOE in Los Alamos in the 1950's, applied to statistical mechanical systems but also used to simulate neutron populations in nuclear reactors. Although given the single name Metropolis, coauthors of the original paper played strong roles and include Edward and Augusta Teller and Marshall and Arianna Rosenbluth, with A. Teller and A. Rosenbluth developing the simulation codes and performing the simulations on the Los Alamos built MANIAC computer.

The methods essentially perform a random walk in the variable space of a target multivariate probability distribution and show that with an update rule satisfying certain simple constraints (the Metropolis conditions) the distribution of these coordinates in the walk will asymptotically converge on desired distribution. This is a powerful method that lets any designed probability distribution be sampled, but at the expense that enough walking steps must be performed to decorrelate consecutive samples.

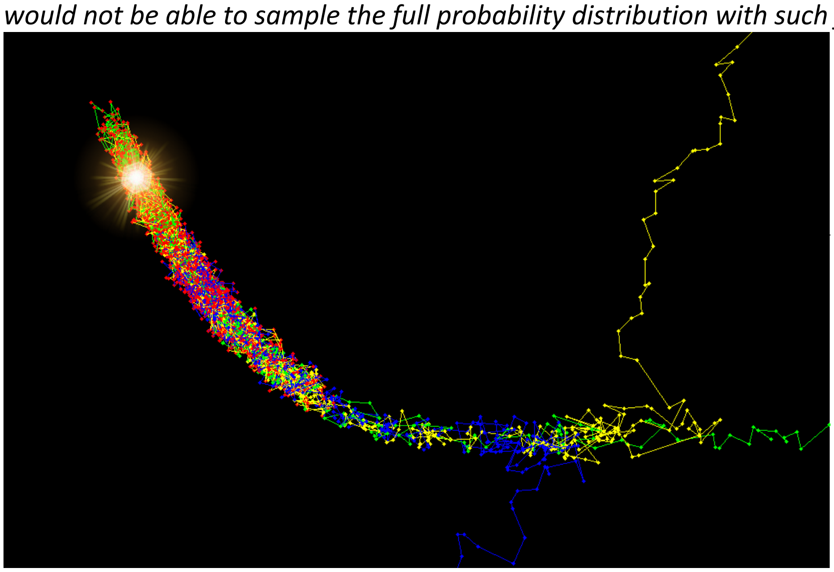
Lattice gauge theory among other scientific areas uses this completely different class of numerical integrator. The easy of producing independent samples is given up and traded for a rule-based update (called a Markov Chain) that performs a particular kind of random walk.

With any suitable (ergodic, reversible) proposal mechanism for a new sample x' given prior sample x, a new step in the walk is accepted absolutely if moving uphill in the target equilibrium distribution Peq(x'), and accepted with a probability determined by the loss in 'height' if downhill:

$$P_{acc}(X \to X') = \min(1, \frac{P_{eq}(X')}{P_{eq}(X)})$$

This simple rule leads to a class of method called Markov Chain Monte Carlo that can sample from an arbitrary target probability distribution, provided a large number of 'steps' in the random walk are taken in a Metropolis method. Indeed the 'gold standard' class of algorithm – Hybrid Monte Carlo or Hamiltonian Monte Carlo – were developed in High Energy Theory and are broadly used in a diverse range of fields including statistical inference, data science, condensed matter physics, computational biology and even linguistics. Lattice gauge theory regularly samples complex manifolds in 10^10 degrees of freedom, albeit with very significant numerical expense consuming cycles on many of the Department of Energy Leadership computing facilities.

Figure 3: *a complicated probability manifold can be explored with exact probability distribution sampling using an appropriate random walk in Markov Chain Monte Carlo. Here three initial starting positions are tracked and converged on the target probability distribution after sufficiently many steps are taken. In the example of figure 2, the Metropolis algorithms would have no problem at all in walking around the entire circular manifold, while a factorized approach as taken by more traditional numerical integrators would not be able to sample the full probability distribution with such fidelity.*



This LDRD proposal is to investigate the applicability of MCMC methods to the integrals that arise in precision perturbative calculations and to construct a new class of numerical integrator for this purpose.

Either the absolute value of the integrand, or a coarse grained 'tessellation' approximation to it will be used to define the sampled probability distribution. We aim develop GPU accelerated software that can run, in parallel, many MCMC sampling histories that draw from this distribution in parallel and generate the points in the integration domain with much greater fidelity to the integrand than is possible with tools like VEGAS. From a computational perspective, and particularly if a learned 'tessellation' is used to cover the space, the task would look like running many particles along trajectories in an approximate multi-dimensional potential (coupled with a Metropolis accept reject step). This is a task GPUs are very much ideal to perform.

The proposal is innovative and synergistic – it exploits expertise of both the perturbative and lattice researchers with HET in a highly complementary way. It attempts to take numerical integration for precision physics in a new direction. It blends expertise in a complementary way and has excitement and enthusiasm in a way that has the wholehearted support of the entire group. Further, the use of GPUs looks ideal and transfers know-how that has been built up with years of human effort. If successful it will pave the way develop a Brookhaven software project in a key area of theoretical physics. This will enable us to include higher order calculations in HEP event generators contributing to the discover potential of current and future colliders.

Further, if successful it will lead to significant future funding opportunities. Firstly, the HEP FOA XXXX is an ideal target opportunity. Secondly, Robert Szafron is eligible for an early career award and this could be a contributory part of his case. Finally, as has been demonstrated to an extent in the lattice activity within HET, having a novel and innovative mathematical and algorithm and software direction with HET opens up additional income opportunities via the DOE's computation and ASCR budgets. We firmly believe the long term benefits of such a direction may include not just one off funding opportunities but if we develop a successful and world leading technology there could be recurring opportunities for Brookhaven.

BROOKHAVEN NATIONAL LABORATORY
PROPOSAL INFORMATION QUESTIONNAIRE
LABORATORY DIRECTED RESEARCH AND DEVELOPMENT PROGRAM

ONE-PAGE VITA FOR EACH PRINCIPAL INVESTIGATOR AND CO-PRINCIPAL INVESTIGATOR

1. ALIGNMENT WITH THE LABORATORY MISSION AND VISION

Please identify which area(s) the proposal supports.

This proposal supports area 5. High energy physics.

2. POTENTIAL FUTURE FUNDING

Identify below the Agencies and the specific program/office, which may be interested in supplying future funding. Give some indication of time frame. This information is required.

We hope this proposal can lead to

i) An early career award application by Szafron
ii) A submission to the expected DOE FOA
iii) If this direction is successful a unique BNL HET software capability in numerical integration could in future lead to diversification of HET funding to also have an ASCR element, which would be a large positive for the group.

3. BUDGET JUSTIFICATION

Include a description of all costs requested in your budget. You do not need to describe the Lab burdens.

4. NAME OF SUGGESTED BNL REVIEWERS

Provide the name of four BNL subject matter experts (SMEs). Two of the SMEs may be contacted as potential reviewers of your proposal. Their reviews will be in addition to those conducted by the Associate Lab Directors and their Deputies and the Directors of the Computational Science Initiative and Advanced Technology Research Office, Members of the Brookhaven Council, and Research Staff not associated with the research.

Peter Petreczky, Robert Pisarski, Nathan Urban, Kerstin Klees van Dam

5. EQUIPMENT (Reference: DOE Order 413.2C Chg. 1 (Min Chg) for guidance on equipment restrictions)

Will LDRD funding be used to purchase equipment? NO____

If "Yes," provide cost and description of equipment
Year 1 - $
Year 2 - $
Year 3 - $
Description:

6. HUMAN SUBJECTS (Reference: DOE Order 443.1C)

Are human subjects involved from BNL or a collaborating institution? Human Subjects is defined as "A living individual from whom an investigator obtains either (1) data about that individual through intervention or interaction with the individual, or (2) identifiable, private information about that individual".

If **yes**, attach copy of the current Institutional Review Board Approval and Informed Consent Form from BNL and/or NO _________ collaborating institution. ______

7. VERTEBRATE ANIMALS

Are live, vertebrate animals involved? NO ______

If **yes**, attach copy of approval from BNL's Institutional Animal Care and Use Committee.

8. NEPA REVIEW

Are the activities proposed similar to those now carried out in the Department/Division which have been previously reviewed for potential environmental impacts and compliance with federal, state, local rules and regulations, and BNL's Environment, Safety, and Health Standards? (Therefore, if funded, proposed activities would require no additional environmental evaluation.) YES ______

If **no**, has a NEPA review been completed in accordance with the National Environmental Policy Act (NEPA) and Cultural Resources Evaluations Subject Area and the results documented? N/A ______

(**Note:** If a NEPA review has not been completed, submit a copy of the work proposal to the BNL NEPA Coordinator for review. No work may commence until the review is completed and documented.)

9. ES&H CONSIDERATIONS

Does the proposal provide sufficient funding for appropriate decommissioning of the research space when the experiment is complete? YES ______

Is there an available waste disposal path for project wastes throughout the course of the experiment? N/A ______

Is funding available to properly dispose of project wastes throughout the course of the experiment? N/A ______

Are biohazards involved in the proposed work? If yes, attach a current copy of approval from the Institutional Biosafety Committee. N/A ______

Can the proposed work be carried out within the existing safety envelope of the facility (Facility Use Agreement, Nuclear Facility Authorization Agreement, Accelerator Safety Envelope, etc.) in which it will be performed? YES ______

If **no**, attach a statement indicating what has to be done and how modifications will be funded to prepare the facility to accept the work.

10. TYPE OF WORK Select Basic, Applied or Development BASIC

APPROVALS

Business Operations Manager

____
Print Name

Department Chair/Division Manager
To the Department Chair/Division Manager: Please indicate if this project is a sensitive technology under the S&T Risk Matrix. (Note: Red projects require an Access Management Plan.)

- ☐ Green
- ☐ Yellow
- ☐ Red
- ☐ Not Applicable

____
Print Name

Associate Laboratory Director
for Nuclear and Particle Physics

____
Haiyan Gao

BROOKHAVEN
NATIONAL LABORATORY

Project Type: -
Initiative:
Department: -
Directorate:
Principal Investigator: -

-

TERM #: mm/dd/yy - mm/dd/yy

This a sample of the budget template to be used.
Please consult with your Business Operations staff to develop your proposed budget using this template, which needs to then accompany the PIQ when it is submitted.

LABOR									
TYPE	YEAR 1		YEAR 2		YEAR 3		YEAR 4		TOTAL
	FTEs	COST	FTEs	COST	FTEs	COST	FTEs	COST	
SCIENTIFIC/SENIOR PERSONNEL	-	-	-	-	-	-	-	-	-
POST DOCTORAL ASSOCIATES	-	-	-	-	-	-	-	-	-
OTHER PROFESSIONAL	-	-	-	-	-	-	-	-	-
OTHER	-	-	-	-	-	-	-	-	-
TOTAL LABOR	-	$ -	-	$ -	-	$ -	-	$ -	$ -

OTHER LABOR						
TYPE		YEAR 1	YEAR 2	YEAR 3	YEAR 4	TOTAL
CONSULTANTS/COLLABORATORS		-	-	-	-	-
JOINT APPOINTMENTS		-	-	-	-	-
DISTRIBUTED LABOR		-	-	-	-	-
STUDENT CONTRACT		-	-	-	-	-
RECHARGES		-	-	-	-	-
TOTAL OTHER LABOR		$ -	$ -	$ -	$ -	$ -

MATERIALS, SUPPLIES & TRAVEL						
TYPE	CY RATE	YEAR 1	YEAR 2	YEAR 3	YEAR 4	TOTAL
MATERIALS & SUPPLIES		-	-	-	-	-
TRAVEL		-	-	-	-	-
EQUIPMENT (LOW/HIGH)		-	-	-	-	-
PURCHASE HIGH VALUE		-	-	-	-	-
TOTAL MATERIALS, SUPPLIES & TRAVEL		$ -	$ -	$ -	$ -	$ -

DEPARTMENTAL OVERHEADS						
TYPE	CY RATE	YEAR 1	YEAR 2	YEAR 3	YEAR 4	TOTAL
ELECTRIC	0.00%	-	-	-	-	-
SPACE	0.00%	-	-	-	-	-
WASTE MGMT	0.00%	-	-	-	-	-
ORG. BURDEN	0.00%	-	-	-	-	-
OTHER	0.00%	-	-	-	-	-
TOTAL DEPARTMENTAL OVERHEADS		$ -	$ -	$ -	$ -	$ -

GENERAL & ADMINISTRATIVE OVERHEADS						
TYPE	CY RATE	YEAR 1	YEAR 2	YEAR 3	YEAR 4	TOTAL
TRADITIONAL G&A		-	-	-	-	-
COMMON SUPPORT		-	-	-	-	-
TOTAL G&A OVERHEADS		$ -	$ -	$ -	$ -	$ -

TOTAL PROJECT COST	YEAR 1	YEAR 2	YEAR 3	YEAR 4	TOTAL
TOTAL DIRECT COSTS	-	-	-	-	-
TOTAL INDIRECT COSTS	-	-	-	-	-
TOTAL PROJECT COST	$ -	$ -	$ -	$ -	$ -

NOTE:	**ITEMIZE CAPITAL INDIVIDUALLY (include item and $ amount)**	
Post Doc Rate Exception:	1.	5.
No cost to be incurred on R/C 170 (Relocation Expense)	2.	6.
Funding for Program Development for more than 2 years is unlikely and	3.	7.
cannot exceed 3 years.	4.	8.