Probabilistic Modeling for Mega-Bangs and Mini-Bangs

Participants :	R. Soltz, N. Schunck, V. Bulaevskaya, R. Vogt, C. Mattoon, 2 Postdocs
LLNL Collaborators:	M. Buchoff, J. Wasem, A. Kupresanin
Ext. Collaborators:	Prof. A. Majumder (WSU), Prof. B. Sanso (UCSC), Prof. W. Nazarewicz (MSU), Dr. N. Dubray (CEA, France)
Focus Areas :	Nuclear Science, Stockpile Science, High Performance Computing
Budget :	\$600k/yr

Abstract

We propose a fundamental advance in the treatment of probabilistic modeling as it applies to nuclear fission calculations of nuclear database inputs and produced particle distributions in heavy ion collisions. This proposal begins with precise calculations of covariant uncertainty distributions in fission outputs using density functional theory, and propagates all correlated errors in neutron distributions. These correlations are then entered into the nuclear databases using the GND format. State of the art tools in uncertainty quantification can propagate errors but the need to track covariant aleatoric (random) and epistemic (systematic) errors for fission product distributions requires the development of new statistical and computational tools. Identical challenges exist in heavy ion collision where uncertainty quantification techniques are used to determine transport and equation of state properties of the quark gluon plasma, a state of matter formed one micro-second after the big bang and recreated in high statistics events at the Relativistic Heavy Ion and Large Hadron Colliders (RHIC & LHC). Advances are needed to understand the properties of high energy collimated streams of particles known as jets. Determining the mechanism by which these jets lose energy as they traverse the plasma will address one of the last unanswered questions in this field, and will elucidate the nature of the substructure that makes this plasma so strongly coupled. This project will enable LLNL to play significant and leading roles in important topics specified in the NACS 2016 Strategic Plan and the 2015 Nuclear Science Long Range Plan while strengthening our understanding of uncertainties for stockpile science.

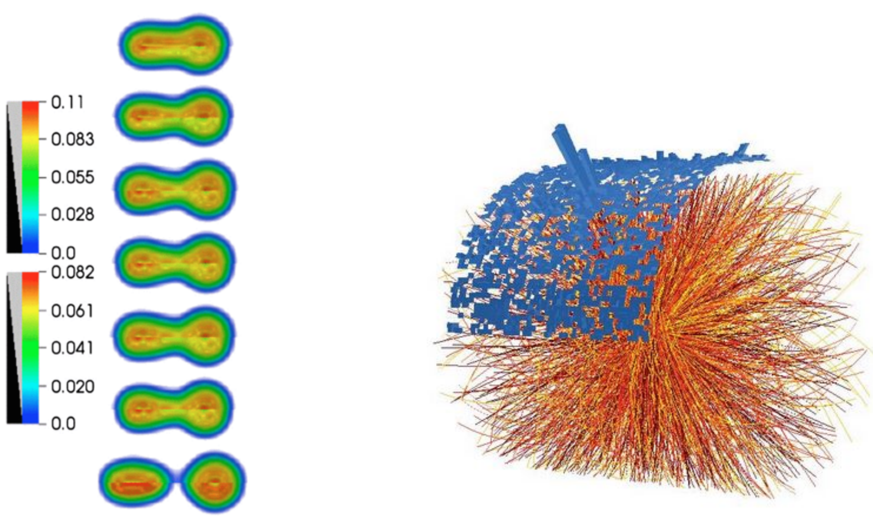

Figure 1: Left panel shows time slices of neutron (proton) density distributions on the top (bottom) for ^{240}Pu spontaneous fission from [1]. Right panel shows event display for a single jet protruding from the background in a 2.76 TeV Pb+Pb collision observed by the ALICE experiment.

Contents

1 Previous LDRD support **3**

2 Introduction **4**

3 Project Plan **5**
3.1 Fission Theory 5
3.2 Jet quenching 6
3.3 Uncertainty Quantification 7

4 Management Plan **10**
4.1 Roles and Responsibilities 10
4.2 Deliverables and Milestones 10
4.3 Communication and Coordination 11

5 Risk Mitigation **11**

6 Strategic Alignment **11**

7 Dissemination **12**

8 Summary **12**

9 References **13**

10 Biographical Sketches **16**

1 Previous LDRD support

Tracking Code	Title and Impact
10-ERD-029	*Modeling and Measuring the Quark-Gluon Plasma Shock Waves* Initiated a modeling effort within the heavy ion group to search for the possible presence of shock waves heavy ion collisions and seeded LLNL participation in heavy ion collisions at the Large Hadron Collider (LHC). These results were reported in publications [2, 3], and enabled related publications that followed [4, 5]. This LDRD also led to a $570k investment by DOE-SC/NP to procure a grid-computing cluster sited at LLNL to fulfill the U.S. fair-share computing obligations to the ALICE heavy ion experiment at the LHC.
10-SI-013	*The Advance of Uncertainty Quantification Science* Initiated an effort to streamline uncertainty quantification (UQ) methodology across the laboratory, with a particular emphasis on climate, weapons and NIF applications, and implemented this methodology in the UQ Pipeline scheduling system. Results on aggregation of adaptive sampling criteria led to an ongoing research effort, and a manuscript describing the work is currently being prepared [6].
12-ER-069	*Forecasting and UQ of Power from Intermittent Renewable Energy Sources* Initiated an effort to introduce statistical methodology into the field of wind power forecasting. Results led to a publication in a renewable energy journal [7], as well as ongoing collaborations with several wind industry partners.

2 Introduction

According to current estimates, our universe began with the Big Bang 13.80 ± 0.21 billion years ago [8]. Approximately one microsecond later, when the temperature had cooled to 1.79 ± 0.10 trillion degrees [4], the standard model constituents of the strong nuclear force known as quarks coalesced into stable light nuclei: H, He, and Li, whcih formed the first population III stars around 560 million years later. These light metal stars were the pre-requisites for the collapsing supernovae and merging neutron star furnaces that produced the heavy elements, the heaviest of which are unstable and break apart spontaneously or under the slightest provocation (i.e. neutron bombardment) in a process called nuclear fission.

It was only 77 years ago that this process was discovered experimentally by Hahn and Strassman when they observed Barium elements after bombarding Uranium with neutrons [9]. Soon after, the first theoretical calculations were published by Bohr and Wheeler [10]. Global events led to the extremely rapid application of this new fundamental knowledge (Mega-Bangs), but a complete microscopic theory of fission remains elusive due to the challenge of obtaining complete experimental data sets and the shear complexity of the nuclear fission process. Mastering this complexity requires the development of new time-dependent methods in nuclear density functional theory (DFT) [11], combined with many orders of magnitude improvements in computational capabilities and the application of Bayesian methods to scientific modeling [12]. Initial success in applying these tools to fission calculations has set the stage for further advances that will enable accurate predictions of fission observables. However, the quality of these predictions will ultimately depend on our fundamental understanding of nuclear forces inside the nucleus. These forces are derived from the theory of the strong interaction for quarks and gluons, quantum chromodynamics (QCD). Although the basic equations of QCD are well known, full calculations with QCD are limited to high energy interactions that produce energetic collimated streams of particles called jets, and high temperatures of the early universe described above, in which the quarks become de-confined to form a quark gluon plasma (QGP). Both of these phenomena are generated in high energy nuclear collisions, an experimental program first suggested by LLNL scientists in 1973 [13] even before the implications of QCD were fully understood. Because of the tremendous amount of data generated in such collisions, the growth of this field has paralleled the development of advanced scientific computing tools and methods. In particular, the application of Bayesian methods was an essential development in extracting the bulk physics properties of the QGP, including its behavior as a strongly-coupled (low viscosity to entropy) plasma [14]. A similar approach is now needed to understand the microscopic properties of the QGP through the study of jet quenching, the process by which jets loose energy as they traverse the QGP. This is the goal of a new dedicated jet experiment at RHIC as described in the 2015 Nuclear Science Long Range Plan.

We now stand at a point where Bayesian methods have become an accepted means for determining physics parameters for understanding nuclear structure (nuclear properties at zero temperature) and bulk properties of the quark gluon plasma (nuclear matter near the QCD phase transition). Yet, they cannot yet be readily applied to the development of a predictive model of fission or the description of the underlying substructure that gives the quark-gluon plasma its unique properties. Indeed, existing Bayesian methods are designed to compare model predictions to a set of *discrete* measurements with associated errors. New uncertainty quantification methods are needed to generate *functional* distributions, such as the mass distribution of fission product yields or the magnitude and shape of jets as they are quenched by the QGP. This proposal brings together a statistician, a heavy ion experimentalist, and a nuclear theorist to develop a novel UQ framework that will lead to 1) a new DFT fission theory capable of predicting prompt neutron distributions with correlated uncertainties, and 2) a new method for probing the microscopic properties of the QGP in a new dedicated jet experiment at RHIC.

3 Project Plan

3.1 Fission Theory

Understanding the fundamental mechanisms of nuclear fission is essential for science-based stockpile stewardship, one of the primary missions of LLNL. For the past 10 years, LLNL has been leading the development of a microscopic theory of induced fission [11, 15–22]. Our theoretical framework combines advanced many-body methods of quantum mechanics with our best knowledge of nuclear forces and highly optimized computer programs running on leadership class computers. The left panel in Figure 2 illustrates the state of the art of calculations of fission product yields (FPY) in the benchmark case of the neutron-induced fission of ^{239}Pu. Without the adjustment of a single parameter to fission data, the theory can predict FPY to within about 30%. However, the determination and impact of several key input parameters on the FPY remain poorly understood as illustrated in the right panel of Figure 2. In addition, early calculations by Younes and Gogny in [18] point to large uncertainties in the prediction of the distribution of total kinetic energy (TKE) and total excitation energy (TXE) released during fission. The goal of this part of the project is to quantify the uncertainties associated with each component of the theoretical model on the charge, mass, TKE and TXE distribution of the fission fragments (sensitivity analysis), and calculate the Bayesian joint posterior distribution of these components based on existing data, accounting for experimental uncertainties.

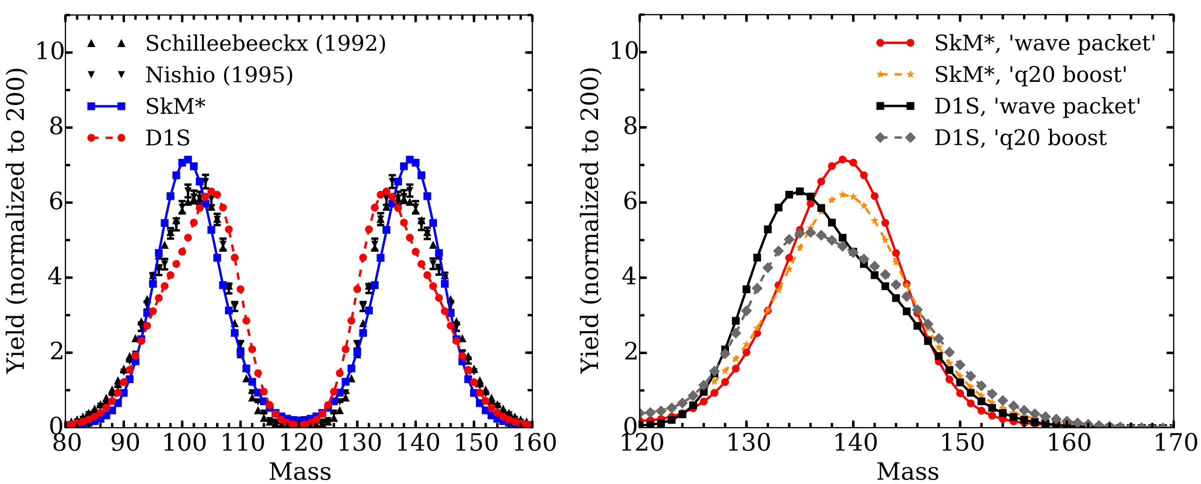

Figure 2: Left: Mass distribution of fission fragments in the neutron-induced fission of ^{239}Pu for thermal neutron (with kinetic energy of a few meV). Calculations with two standard energy functionals, SkM* of [23] and D1S of [24], are compared with two experimental datasets from [25, 26]. Right: influence of two different prescriptions for the initial state on the heavy fragment peak. Both figures from [22].

Our theoretical approach is based on nuclear density functional theory (DFT) with effective energy density functionals (EDF) and the adiabatic approximation to large amplitude collective motion. In this approach, fission is controlled by only a few "collective variables" such as deformations of the nuclear shape. FPY are computed in a two-step process: first, the DFT equations are solved numerically by our DFT solver suite (LLNL-CODE-470611, LLNL-CODE-573953) on a grid for the two collective variables q and q' deemed most relevant for fission ($q \equiv$ elongation and $q' \equiv$ mass asymmetry). This step of the calculation gives potential energy surfaces (PES), that is, the function $E(q, q')$ where E is the energy of the fissioning nucleus. It requires supercomputers, as the number of points on the grid is currently of the order of 5,000 and each point takes about half a day on a single node. A time-dependent generator coordinate method (TDGCM) solver is used to compute the time evolution of the probability distribution of the nucleus having collective variable values (q, q'), that is, $f(q, q'; t)$ where t is time. Knowing these probability distributions for any combination of q and q' as a function of time t allows the determination of FPY. This step is done with our code FELIX [22].

The overall calculation depends on several key ingredients: (i) the form and parameters $\boldsymbol{p}$ of the EDF, (ii) the collective inertia tensor $\mathsf{B}(q, q')$ (= the equivalent of the mass of the nucleus in the collective space), (iii) the initial state for the time-evolution in the TDGCM solver, i.e., the function $f(q, q'; t_0)$, (iv) the final states in the PES (scission configurations). In addition, the mechanism by which the total excitation energy of the fissioning nucleus is distributed to the fragments is largely unknown. Our estimate of the distribution of TXE in the fragment will thus depend on a model for the energy sharing distribution of the fragments. Finally, fission fragment distributions, which are the output of the DFT modeling of fission, are inputs to reaction codes such as FREYA [27], which simulate the characteristics of the neutrons emitted during fission. In the first phase, we will use the new methods discussed in Section 3.3 to determine the joint Bayesian posterior distributions for the parameters of the initial TDGCM state, scission configuration and energy sharing model. This will require the development of an emulator for the FPY as a function of these parameters and large number of TDGCM runs to train the model. In the second phase, we will explore the uncertainties of the parameters $\boldsymbol{p}$ of the EDF itself and study how they propagate into the FPY outputs.

3.2 Jet quenching

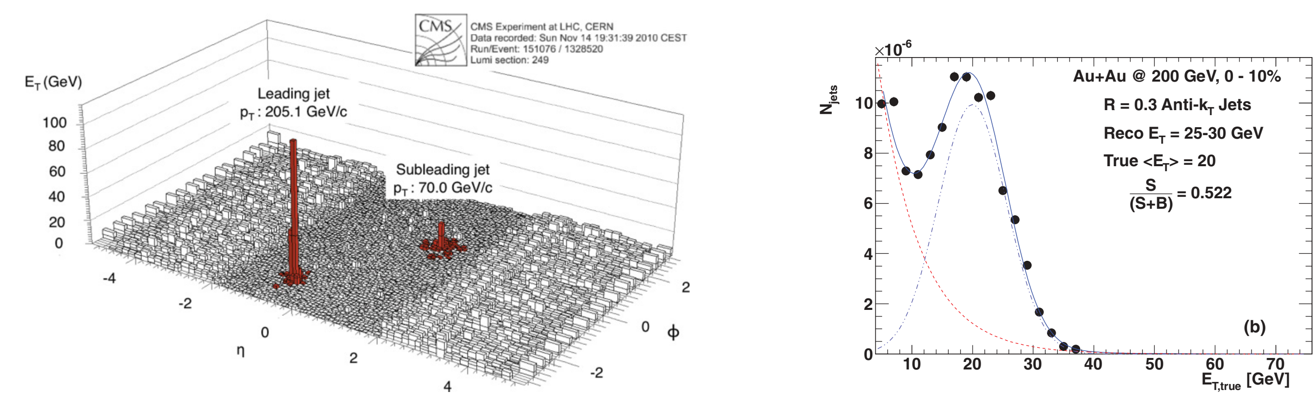

Figure 3: Left panel shows lego plot of leading and quenched jet event for 2.76 TeV Pb+Pb collisions reported by CMS [28], and right panel shows the results of applying a standard jet-finding algorithm to a simulation for 100 GeV Au+Au collisions at RHIC [29]. The red dashed line shows the significant contribution from fake jets that must be subtracted to recover an estimate of the input jet energy of 20 GeV.

The plan to study jet quenching in heavy ion collisions can be divided into two parts. The first part involves working with simple models to develop new methods to measure jet quenching within in fluctuating background of produced particles. Analogous to the way in which Rutherford used alpha particles to probe the structure of the atom, high energy jets probe the structure of the QGP, except that these probes are produced from within and during the early stages of the heavy ion collisions. The jet production rates are extremely well understood, and there exists a well calibrated model, PYTHIA, developed over

35 years of continuous validation with experimental data from high energy proton-proton collisions and electron-positron annihilations. The information on the QGP substructure is obtained by measuring the reduced energy or quenched jets that emerge from the plasma, but for experiments at RHIC, where the initial collision energy is lower than the LHC, the quenched jets can be overwhelmed by the stochastic background. This is evident in Figure 3, which shows on the left a lego plot of the angular distribution of transverse energy (E_T) in the special relativity polar angle coordinate $\eta = -\ln(\tan(\theta/2))$ and azimuthal angle ϕ. One jet escapes the plasma with 200 GeV of energy while its partner retains only 70 GeV and is closer to the level of the background [28]. The right panel is a simulation of jets at RHIC, where a standard jet finding algorithm (anti-k_T) reconstructed a significant portion of fake jets (dashed-red line) that arise from fluctuations in the background [29]. In the past few years experimentalists have made limited progress reconstructing jets at RHIC energies, but all methods continue to follow [29], in pursuing an iterative method of jet-finding and background subtraction. These methods are unable to reach the lowest and most interesting jet energies, nor are they able to provide quantitative information on the jet shapes, a crucial element in determining the energy loss mechanisms. The same probabilistic Bayesian approach needed for fission theory is extremely well suited to the challenge of finding and understanding the modification of jets in heavy ion collisions. Instead of the fission fragment mass distributions in Section 3.1 we will model the energy and angular distributions of opposing pairs of high energy jets within a complex background. The idea is thus to create initial jets in PYTHIA and calculate the joint Bayesian posterior distribution of jet drag and diffusion parameters by comparing to experimental data. Because the collision background is understood, we will begin by developing and testing the Bayesian tools entirely within a simulation framework, in which the heavy ion background is characterized by four parameters: a temperature scale T, and three azimuthal moments, v_1, v_2, v_3, and the jet quenching is governed by three energy-loss parameters, $\hat{e}$, $\hat{e_2}$, $\hat{q}$. For the purposes of this proposal, the 40 input parameters of PYTHIA ("PYTHIA tunes") are regarded as fixed, although we may work with more than one "tune" as a means of estimating systematic errors. Initially we will demonstrate that meaningful posterior distributions can be obtained for the scale and shape parameterizations, first for simulations, and then for proton-proton and heavy ion collision data. The proton-proton data will serve as a calibration, given that no shape modifications are expected.

The second part of this project will involve working with more complex jet quenching models in which the jets are fully coupled to the hydrodynamic evolution of the plasma created in a heavy ion collision. Such a model is currently under development within the scientific community, through the newly funded JETSCAPE collaboration of which LLNL is a member. Unlike this proposal, which seeks to develop new tools for the direct analysis of data, JETSCAPE is tasked with developing a freely distributable physics code for comparison to processed data, in which jet finding algorithms have already been applied. Therefore this project will gain from access to higher-fidelity physics codes and will benefit from interactions with theory as well as experimental collaborations. This higher-fidelity physics code will be used in place of the simpler modeling schemes developed for the first part. Because it will take time for JETSCAPE to develop this model, this phase of the LDRD will occur in the final year of this project.

3.3 Uncertainty Quantification

Both the fission theory and jet quenching research described in Sections 3.1 and 3.2 will make very heavy use of uncertainty quantification (UQ) methodology. This section will therefore discuss the various statistical tools that will be relevant for both of these research efforts.

Both areas call for a statistical emulator to be built to act as a surrogate to the computer models. Such emulation has a long history in the field of computer experiments since it offers a cheaper alternative when the computer model in question is computationally expensive [30, 31]. The computer model of interest is first run at a relatively few distinct input configurations. A statistical model is then trained on the output obtained so that it can emulate the computer model by predicting the value of the output for any new given input configuration. The emulator can thus estimate the entire response surface as a function of the inputs. Because the model is a statistical approximation to the computer model output, it produces both the prediction and the uncertainty associated with this prediction.

There are many possible statistical emulators, such as neural networks, support vector machines, multivariate adaptive regression splines, random forests and Gaussian process models, among many others. While each of these statistical models has its strengths and shortcomings, we will focus on the Gaussian process model (GPM). The particular appeal of the GPM is that its theoretical foundation is very clearly defined. As a result, this model allows for a very natural modeling of prediction uncertainty. In particular, as its name implies, the GPM models the error in the output prediction as a multivariate Gaussian random variable. This random variable has a mean of zero and a covariance function that is itself modeled in terms of the Euclidean distance between a pair of input value vectors. As a consequence of modeling the output in this way, the conditional distribution of the new prediction given all the output observed from the computer model is also Gaussian with a very well specified mean and covariance. This makes modeling the uncertainty associated with the predictions straightforward (for more on the GPM model, see [31–33]). Figure 4 shows an example of a GPM prediction for a 1-dimensional function. As can be seen from the figure, the uncertainty bands get wider for the input values that are further away from the values for which the output has been observed.

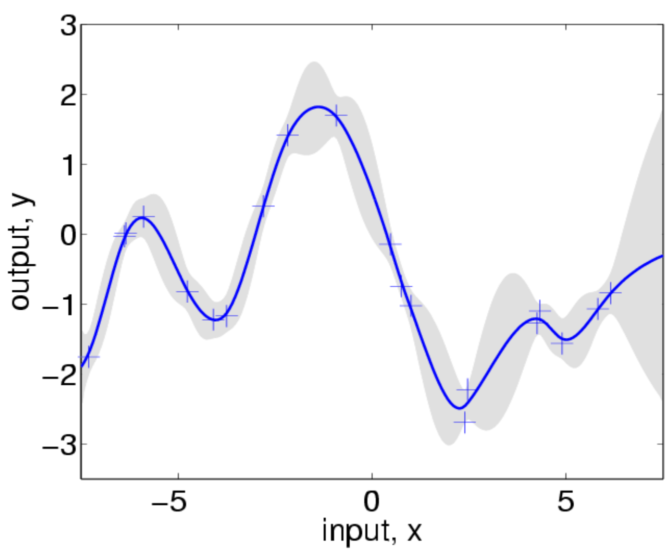

Figure 4: An example of a GPM prediction for a 1-dimensional function with an input x and an output y. The crosses represent the values that have been observed and that were used to train the GPM, the solid blue curve is the GPM prediction at x and the shaded grey area is the uncertainty band around each prediction.

As mentioned above, training the GPM requires samples from the computer model. Since the reason for using an emulator is that the computer model is computationally expensive, one can only sample it for a limited number of points (input configurations). These points must therefore be chosen strategically, in order to maximize the gain in the information about the response surface. This is done in a sequential fashion. An initial (typically relatively small) set of points is chosen at random for the computer model to sample, and this first sample is used to produce an initial estimate of the response surface with the emulator. This estimate is used to determine the next set of points, one that will provide the most value with respect to some user-defined criterion of information about the response surface. The recommended points are then sampled with a computer model, and the initial sample is augmented with these points. The whole process is then repeated again until a certain convergence criterion is met. This type of sampling is known as adaptive sampling (AS) [34].

Different criteria can be used to sample the model when using AS: one could sample points at which the least amount of information about the response surface is currently available (Active Learning MacKay criterion – ALM [35]). Alternatively, one could choose the points with the most amount of change in the response. Yet another option is to use a hybrid of these two criteria, either by weighing them equally and giving rise to a so-called Expected Improvement criterion [36, 37] or by choosing the weights of the two criteria adaptively. The latter option was investigated in a past LDRD project (described in Section 1) and is the subject of ongoing research by one of the authors of this proposal [6]. It has been shown to perform very well in many examples relative to both random sampling and each of the individual criteria mentioned above and is thus expected to be heavily leveraged in this effort.

With an emulator in hand, one can assess the relative impact of various input variables on the output. We will perform this sensitivity analysis (SA) both for fission theory and jet quenching models. The SA involves decomposing the total variance in the output into parts that can be attributed to each input individually, as well as in combination with other inputs. We will use the very established method of obtaining such a decomposition via Sobol indices [38].

Once the important inputs have been identified, we can focus on tuning their values so that the computer model output best matches experimental data (calibration). We will use a Bayesian approach to calibration by setting prior distributions on the input parameters of interest and obtaining their joint posterior distribution conditional on the experimental data. A summary statistic of this posterior distribution, such as the mean or the mode (this depends on the metric one uses to measure the agreement between the computer model output and the data), is then taken to be the optimal configuration of the inputs.

Bayesian methodology is particularly well suited for computer model calibration. This is because it allows a very natural incorporation of the prior knowledge about the input parameter constraints. This includes lack of knowledge about such constraints, in which case a very diffuse prior is specified. Moreover, in contrast to deterministic methods that produce point estimates for the input parameter values, the Bayesian framework produces a full posterior distribution of these values conditional on the experimental observations. Not only do such distributions convey the uncertainty in the input parameters more adequately than do point estimates, this uncertainty can be easily propagated further down the modeling chain. For these reasons, Bayesian calibration framework has been advocated and used by many statisticians and practitioners (see, for example, [30, 39, 40]), and we will make heavy use of it in both fission theory and jet quenching efforts.

While much of the UQ methodology described so far is well established for scalar and even multivariate output, it is much less straightforward for outputs with constraints. This is for instance the case for the FPY outputs, since it is a probability distribution that must integrate to 1. Emulation, sensitivity analysis and calibration all become more complicated as a result of this constraint. One approach to modeling this output is to omit one of the dimensions, thus leaving only the unconstrained values. This can be a workable solution, but the inference may depend heavily on which of the dimensions is omitted since different dimensions in the output vector may have a different amount of uncertainty associated with them. Another approach is to model the constraints directly in the covariance function. This is the approach taken in [41], but its computational burden may be too great in our context. Finding an optimal approach to this particular problem is an open problem in the UQ community and will be the subject of statistical research in the course of this project.

4 Management Plan

4.1 Roles and Responsibilities

Ron Soltz (PLS) is an expert in the physics of quark gluon plasmas and a principle investigator for the NuDet Detection System (NDS) V&V effort at LLNL. He will mentor a heavy-ion postdoc and serve as PI for this proposal.

Nicolas Schunck (PLS) is a leading expert in Density Functional Theory. He will oversee the fission modeling and will mentor a nuclear-theory postdoc.

Vera Bulaevskaya (ENG) is an expert in the development of statistical tools and will work within the LLNL statistics group to develop new methodology for probabilistic modeling and advise the application scientists.

Ramona Vogt (PLS) is an expert on neutron and photon distributions from fission, as well as heavy ion modeling. She will generate the fission output distributions and work on improved models for heavy ion collisions.

Caleb Mattoon (PLS) is the primary scientist responsible for development of the Generalized Nuclear Data format. He will help the team translate fission outputs into the appropriate nuclear data formats.

4.2 Deliverables and Milestones

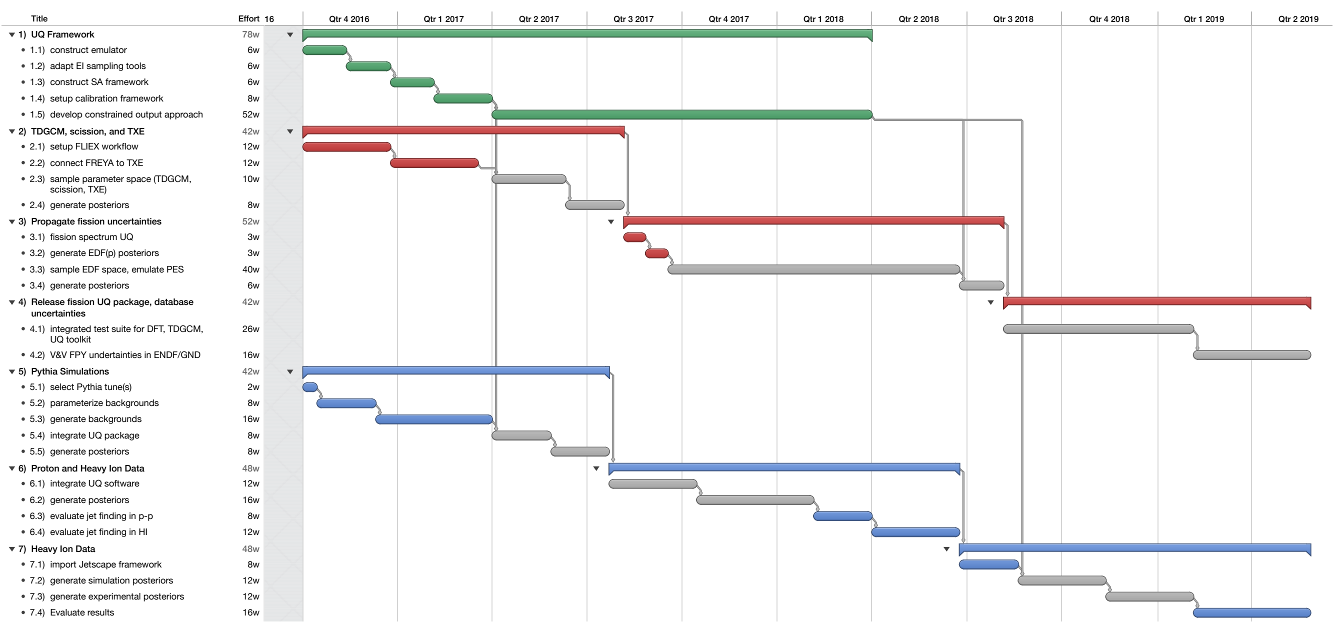

Figure 5: Project tasks and timeline. Silver tasks indicate collaborative effort among statisticians and application scientists.

4.3 Communication and Coordination

Coordination among the two applications will be achieved through bi-weekly meetings among the main participants, with R. Vogt and C. Mattoon joining. Independent communication within each application and the statistics group will occur as often as needed. Formal documentation and code will be developed on LC using Stash (a web-based implementation of github already in use for this proposal) and we will use cz-confluence for all meeting agendas, minutes, and other informal documentation. The PI and several team members have considerable experience managing diverse teams and working on large scale coding projects that extend well beyond the range of this proposal.

5 Risk Mitigation

We identify the following risks for this proposal: resource allocation among the two science applications and competition from external groups. The former will be mitigated through the communication and coordination strategies identified above. Because the two applications have very similar needs in probabilistic modeling, there are considerable benefits from combining these two applications in a single proposal:

1. The statistician will develop a single code base to be dynamically linked for each application.
2. The applications are sufficiently similar to enable cross-fertilization of ideas during the design phase.
3. Developing a common statistics library to be shared by two applications will improve modularity and increase the likelihood that future applications will benefit.
4. The heavy ion data sets will provide contact with very high statistics data sets to test the approach.
5. Improved communication with the statistics group and fission will benefit other program areas (e.g. stockpile science and the NDS V&V project).

These science applications are of significant interest to others in the nuclear physics community, but we are able to mitigate the risk of competition by forming strong collaborations. The role of the JETSCAPE collaboration has already been described previously. At this time, this is the only other funded effort that is applying Bayesian methods to study energy loss in heavy ion collisions. In the field of microscopic fission theory LLNL is the world leader, but also benefits from a strong collaboration with Prof. Witek Nazarewicz at Michigan State University through the NNSA Stockpile Science Academic Alliance (SSAA) program, which has been developing an improved theory for collective inertia that will ultimately be incorporated in our simulation suite. Part of the recent work on FPY was also performed within a NNSA/CEA agreement on fundamental science supporting stockpile stewardship. This collaboration will continue and will explore the impact of the dimensionality of the PES on FPY. Finally, support from the DOE SciDAC program was used to fund some of the code development, in particular with respect to their scaling to petascale computing facilities. These ties to external collaborations are highly beneficial to this proposal and serve to strengthen the overall scientific impact within the broader fields of nuclear physics and statistics.

6 Strategic Alignment

This work directly impacts and benefits the laboratory core competency in Nuclear, Chemical, and Isotopic Science and Technology through advances in nuclear theory and experiment. Work on a microscopic theory of fission and understanding jets are called for in the Nuclear and Chemical Sciences 2016 Strategic Plan, and the topic of uncertainty quantification is mentioned no fewer than eight times in the LLNL Investment

Strategy, under topics that span several mission focus areas and core competencies. We anticipate that UQ tools developed in this proposal will be applied to other laboratory mission areas.

This work will deliver for the first time an estimate of FPY uncertainties in the microscopic approach, information will help set priorities for future programmatic measurements. This project also has two side benefits: it will integrate in a single software suite the codes used for FPY calculations (DFT solver and FELIX) and the ones used for the calculation of the neutron and photon spectrum (FREYA). It will also deliver a framework for large-scale calculations of FPY which will accelerate future developments. Work on jet finding will be used to assess performance and improve the design of a new jet detector for RHIC. This detector, called for in the Nuclear Science Long Range Plan, will undergo construction during the time of this project in preparation for data taking in 2022-23, and is also intended to serve as a baseline detector for the Electron Ion Collider, identified as the top new construction priority for the US Nuclear Physics Community. This is an area that is projected to train nearly 40% of Ph.D.s in experimental nuclear physics in the near future, and as such is a vital component to maintaining a vibrant nuclear physics workforce at LLNL. Both the EIC and the need to develop a predictive theory of fission are specifically mentioned in the LLNL 2016 Investment Strategy.

7 Dissemination

This proposal will result in three or more journal publications:

1. New Methods in Probabilistic Modeling, Journal of Uncertainty Quantification
2. DFT calculations of fission distributions, Phys. Rev. C / Phys. Rev. Lett.
3. New methods in the study of jet energy loss in heavy ion collisions, Phys. Rev. C / Phys. Rev. Lett.

In addition, research performed within this project will be presented at many of the following conferences:

1. International Conference on nuclear reactions at near barrier energies (FUSION), February, 2017
2. Meeting of the Division of Nuclear Physics, Annual North American Conference, October 2017, 2018
3. International Conference on Hard and EM Probes in Heavy Ion Collisions, fall 2017, 2018
4. Conference on Data Analysis (CoDA), biannual conference, March 2018
5. SIAM UQ, biannual international conference, April 2018
6. Joint Statistical Meeting (JSM), annual conference in North America, August 2018
7. International Conference on Ultra-relativistic Heavy Ion Collisions, (Quark Matter), spring 2019

We plan for a minimum of one conference presentation for each staff, and two or more conference presentations for each of the two postdocs hired for this LDRD. At this time we have identified two potential postdoc candidates: Bastian Schuetrumpf from MSU for fission and Scott Moreland from Duke for jet quenching.

8 Summary

This project will develop new probabilistic methods to two important problems in nuclear physics: developing a microscopic theory of nuclear fission using nuclear density functional theory (DFT) and extracting physics from jet quenching in heavy ion collisions. The first is a necessary and crucial step to build a truly predictive theory of nuclear fission, whereas the second is essential to understanding the microscopic structure of the quark gluon plasma. Both science applications have similar needs for developing new Bayesian methods and will benefit by coordinating work with the statistics group and developing a common code base. Rigorous treatment of errors and Bayesian methods is key feature for making progress in each application. For the DFT, the accuracy in simulations of quantities like the fission product yields in actinide nuclei is limited by the low dimensionality of DFT calculations and the lack of control on uncertainties in DFT parameters. Also, for heavy ion collisions, a probabilistic approach to jet finding is needed to achieve an unbiased estimate of the jet quenching physics parameters. The UQ tools developed for these applications require methodological advances in the treatment of constrained outputs, and the results of this research will be of significant interest to the UQ community and the statistical community at large. Furthermore, the advances in the science applications have strategic impact for LLNL. The generation of covariant errors in DFT outputs will be incorporated into fission product yields and neutron distributions in the GND nuclear data formats. Advances in jet quenching will benefit the construction of a new dedicated jet detector at the RHIC, which is intended to provide a path to the Electron Ion Collider (EIC), the top new construction priority within the US nuclear physics community.

This proposal will build on LLNL expertise and leadership in nuclear theory, heavy ion physics and uncertainty quantification in order to develop new UQ tools that will lead to advances in nuclear theory and the interpretation of heavy ion data. The team has formed strong external collaborations to mitigate risk and to help disseminate results that are of great interest to the community while simultaneously providing important strategic benefits to LLNL.

9 References

[1] Aurel Bulgac, Piotr Magierski, Kenneth J Roche, and Ionel Stetcu. Induced fission of 240-Pu within a real-time microscopic framework. *Phys. Rev. Lett.*, 116(12):122504, 2016.

[2] Betty Abelev. Modeling quark gluon plasma using CHIMERA. *J. Phys.: Conf. Ser.*, 316:012030, September 2011.

[3] R A Soltz, I Garishvili, M Cheng, B Abelev, A Glenn, and others. Constraining the initial temperature and shear viscosity in a hybrid hydrodynamic model of $\sqrt{s}_{NN}$=200 GeV Au+Au collisions using pion spectra, elliptic flow, and femtoscopic radii. *Phys.Rev.*, C87(issue):044901, 2013.

[4] R A Soltz, C DeTar, F Karsch, Swagato Mukherjee, and P Vranas. Lattice QCD thermodynamics with physical quark masses. *Ann. Rev. Nucl. Part. Sci.*, 65(1):379–402, October 2015.

[5] J Scott Moreland and Ron A Soltz. Hydrodynamic simulations of relativistic heavy-ion collisions with different lattice QCD calculations of the equation of state. *arxiv.org*, December 2015.

[6] V. Bulaevskaya, G. Johannesson, and D. Domyancic. Aggregation of multiple adaptive sampling criteria in computer experiments. In progress.

[7] V. Bulaevskaya, S. Wharton, A. Clifton, G. Qualley, and W. Miller. Wind power curve modeling in complex terrain using statistical models. *Journal of Renewable and Sustainable Energy*, 7 103103, 2015.

[8] Planck Collaboration. Planck 2015 results. XIII. Cosmological parameters. 2015.

[9] O. Hahn and F. Strassmann. Über die Entstehung von Radiumisotopen aus Uran durch Bestrahlen mit schnellen und verlangsamten Neutronen. *Naturwiss.*, 26(46):755, 1938.

[10] Niels Bohr and John Archibald Wheeler. The mechanism of nuclear fission. *Phys. Rev.*, 56(5):426, 1939.

[11] N. Schunck and L.M. Robledo. Microscopic theory of nuclear fission: A review. *arxiv:1511.07517*, 2016.

[12] GEP Box. Sampling and Bayes' inference in scientific modelling and robustness. *Journal of the Royal Statistical Society Series A*, 143(4):383, 1980.

[13] G Chapline, M Johnson, E Teller, and M Weiss. Highly excited nuclear matter. *Phys. Rev. D*, 8(12):4302–4308, December 1973.

[14] J Novak, K Novak, S Pratt, J Vredevoogd, C E Coleman-Smith, and R L Wolpert. Determining fundamental properties of matter created in ultrarelativistic heavy-ion collisions. *Phys. Rev. C*, 89(3):034917–23, March 2014.

[15] W. Younes and D. Gogny. The microscopic theory of fission. In *AIP Conference Proceedings*, volume 1175, page 3. AIP Publishing, 2009.

[16] W. Younes and D. Gogny. Nuclear Scission and Quantum Localization. *Phys. Rev. Lett.*, 107(13):132501, 2011.

[17] W. Younes and D. Gogny. Collective Dissipation from Saddle to Scission in a Microscopic Approach. Technical Report LLNL-TR-586694, Lawrence Livermore National Laboratory (LLNL), Livermore, CA, 2012.

[18] W. Younes and D. Gogny. Fragment Yields Calculated in a Time-Dependent Microscopic Theory of Fission. Technical Report LLNL-TR-586678, Lawrence Livermore National Laboratory (LLNL), Livermore, CA, 2012.

[19] N. Schunck, D. Duke, H. Carr, and A. Knoll. Description of induced nuclear fission with Skyrme energy functionals: Static potential energy surfaces and fission fragment properties. *Phys. Rev. C*, 90(5):054305, 2014.

[20] N. Schunck, D. Duke, and H. Carr. Description of induced nuclear fission with Skyrme energy functionals. II. Finite temperature effects. *Phys. Rev. C*, 91(3):034327, 2015.

[21] D. Regnier, M. Verrière, N. Dubray, and N. Schunck. FELIX-1.0: A finite element solver for the time dependent generator coordinate method with the Gaussian overlap approximation. *Comput. Phys. Comm.*, 200:350, 2016.

[22] D. Regnier, N. Dubray, N. Schunck, and M. Verrière. Fission fragment charge and mass distributions in ^{239}Pu(n,f) in the adiabatic nuclear energy density functional theory. *arXiv:1603.08824*, 2016.

[23] J. Bartel, P. Quentin, M. Brack, C. Guet, and H.-B. Håkansson. Towards a better parametrisation of Skyrme-like effective forces: A critical study of the SkM force. *Nucl. Phys. A*, 386(1):79, 1982.

[24] J. F. Berger, M. Girod, and D. Gogny. Time-dependent quantum collective dynamics applied to nuclear fission. *Comput. Phys. Comm.*, 63(1):365, 1991.

[25] P. Schillebeeck, C. Wagemans, A. J. Deruytter, and R. Barthélémy. Comparative study of the fragments' mass and energy characteristics in the spontaneous fussion of 238Pu, 240Pu and 242Pu and in the thermal-neutron-induced fission of 239Pu. *Nucl. Phys. A*, 545(3):623, 1992.

[26] Katsuhisa Nishio, Yoshihiro Nakagome, Ikuo Kanno, and Itsuro Kimura. Measurement of Fragment Mass Dependent Kinetic Energy and Neutron Multiplicity for Thermal Neutron Induced Fission of Plutonium-239. *J. Nuc. Sci. Tech.*, 32(5):404, 1995.

[27] J.M. Verbeke, J. Randrup, and R. Vogt. Fission Reaction Event Yield Algorithm, FREYA — For event-by-event simulation of fission. *Comput. Phys. Comm.*, 191:178, 2015.

[28] S Chatrchyan et al. Observation and studies of jet quenching in PbPb collisions at $\sqrt{s}_{NN}$=2.76TeV. *Phys. Rev. C*, 84(2):024906, 2011.

[29] J Hanks, A Sickles, B Cole, A Franz, M McCumber, D Morrison, J Nagle, C Pinkenburg, B Sahlmueller, P Steinberg, M von Steinkirch, and M STONE. Method for separating jets and the underlying event in heavy ion collisions at the BNL Relativistic Heavy Ion Collider. *Phys. Rev. C*, 86(2):024908, 2012.

[30] M.C. Kennedy and A. O'Hagan. Bayesian calibration of computer models. *Journal of the Royal Statistical Society: Series B*, 63:425–464, 2002.

[31] T. J. Santner, B. J. Williams, and W. I. Notz. *The Design and Analysis of Computer Experiments*. Springer, 2003.

[32] J. Sacks, W. J. Welch, T. J Mitchell, and H. P. Wynn. Design and analysis of computer experiments. *Statistical Science*, 4:409–423, 1989.

[33] C. E. Rasmussen and C. K. I. Williams. *Gaussian Processes for Machine Learning*. The MIT Press, 2005.

[34] R. B. Gramacy and H. K. H. Lee. Adaptive design and analysis of supercomputer experiments. *Technometrics*, 51:130–145, 2009.

[35] D. MacKay. Information-based objective functions for active data selection. *Computation and Neural Systems*, 4:589–603, 1992.

[36] D. Jones, M. Schonlau, and W. Welch. Efficient global optimization of expensive black-box functions. *Journal of Global Optimization*, 13:455–492, 1998.

[37] C.Q. Lam. *Sequential Adaptive Designs in Computer Experiments for Response Surface Model Fit*. PhD thesis, Ohio State University, Columbus, OH, 2008.

[38] I. Sobol. Sensitivity estimates for nonlinear mathematical models. *Mathematical Modeling and Computational Experiment (Engl. Transl. from Russian)*, 1:407–414, 1993.

[39] M. J. Bayarri, J. O. Berger, R. Paulo, J. Sacks, J. A. Cafeo, J. Cavendish, C-H Lin, and J. Tu. A framework for validation of computer models. *Technometrics*, 49:138–154, 2007.

[40] D. Higdon, J. Gattiker, B. Williams, and M. Rightley. Computer model calibration using high-dimensional output. *Journal of the American Statistical Association*, 103:570–583, 2008.

[41] E.M. Constantinescu and M. Anitescu. Physics-based covariance models for Gaussian processes with multiple outputs. *International Journal for Uncertainty Quantification*, 3:47–71, 2013.

10 Biographical Sketches

Nicolas Schunck

Staff physicist

Nuclear Data and Theory Group, Nuclear and Chemical Science Division, Lawrence Livermore National Laboratory, P.O. 808, L-414, Livermore, CA-94551

Telephone: (925) 422-1621, Fax: (925) 422-8746; E-mail: schunck1@llnl.gov

Education and Training

- Ph.D., Theoretical Nuclear Physics, University of Strasbourg, France, 2001
- Engineer Degree, Physics, Ecole Nationale Supérieure de Physique, Strasbourg, France, 1997
- MS, Nuclear Physics, University of Strasbourg, 1997

Research and Professional Experience

- **2010-present**: Research Staff, Lawrence Livermore National Laboratory
- Previous appointments include: Research Associate 2001-2002 (University of Strasbourg); Postdoc 2002-2004 (University of Surrey), Visiting Professor 2004-2005 (Niels Bohr Institute, Copenhagen; Institute of Nuclear Physics, Kraków; University of Warsaw); Postdoc 2005-2007 (Universidad Autonoma de Madrid); Postdoc 2007-2010 (University of Tennessee)

Leadership Activities

- **2012-2017**: Co-PI for the SciDAC 3 collaboration "Computational Low Energy Nuclear Iniative"
- **2012-2017**: Co-PI for the INCITE project "Computational Nuclear Structure"
- **2014, 2015**: Reviewer for the 2014 DOE Early Career Program
- **2009**: Panel member on Forefront Questions in Nuclear Science and the Role of High Performance Computing, January 26-28, 2009 Washington D.C., USA
- **2008-2009**: Co-organizer of the joint meetings LACM-EFES-JUSTIPEN on theoretical nuclear structure and large amplitude collective motion, Jan. 23-25 2008 and Feb. 23-25 2009, Oak Ridge National Laboratory, USA

Synergistic Activities

- **2014, 2016**: Teacher at the TALENT summer school in "Nuclear Density Functional Theory and Self-Consistent Methods"
- **2012**: Teacher at the "Exotic Beam Summer School 2012", Argonne National Laboratory
- **2009**: Panel member on Forefront Questions in Nuclear Science and the Role of High Performance Computing, January 26-28, 2009 Washington D.C., USA
- Referee for Physical Review Letters, Physical Review C, Journal of Physics G, Computer Physics Communications, European Physical Journal A, Nuclear Physics A, International Journal of Quantum Chemistry, Acta Physica Polonica

Publications

- Author of **36 scientific publications**, 39 peer-reviewed conference proceedings, **h-index 19**.

- Delivered over 30 invited talks at international conferences and workshops, and departmental seminars and colloquia.

Selected Publications Most Relevant to This Proposal

1. D. Regnier, N. Dubray, N. Schunck, and M. Verrière, "FELIX-1.0: A finite element solver for the time dependent generator coordinate method with the Gaussian overlap approximation," Comp. Phys. Commun. **200**, 350 (2016)
2. N. Schunck, D. Duke, H. Carr, "Description of Induced Nuclear Fission with Skyrme Energy Functionals: II Finite Temperature Effects," Phys. Rev. C **91**, 034327 (2015)
3. J. McDonnell, N. Schunck, D. Higdon, J. Sarich, S. M. Wild, and W. Nazarewicz, "Uncertainty Quantification for Nuclear Density Functional Theory and Information Content of New Measurements," Phys. Rev. Lett. **114**, 122501 (2015)
4. N. Schunck, J. McDonnell, D. Higdon, J. Sarich, S. M. Wild, "Uncertainty quantification and propagation in nuclear density functional theory," Eur. Phys. J. A **51**, 12 (2015)
5. N. Schunck, D. Duke, H. Carr, A. Knoll, "Description of Induced Nuclear Fission with Skyrme Energy Functionals: Static Potential Energy Surfaces and Fission Fragment Properties," Phys. Rev. C **90**, 054305 (2014)
6. M. Kortelainen, J. McDonnell, W. Nazarewicz, E. Olsen, P.-G. Reinhard, J. Sarich, N. Schunck, S. M. Wild, D. Davesne, J. Erler, and A. Pastore, "Nuclear Energy Density Optimization: Shell Structure," Phys. Rev. C **89**, 054314 (2014)
7. M. V. Stoitsov, N. Schunck, M. Kortelainen, N. Michel, H. Nam, E. Olsen, J. Sarich, S. Wild, "Axially Deformed Solution of the Skyrme-Hartree-Fock-Bogolyubov Equations Using the Transformed Harmonic Oscillator Basis (II) HFBTHO v2.00d: A new version of the program," Comp. Phys. Comm. **184**, 1592 (2013)
8. M. Kortelainen, J. McDonnell, W. Nazarewicz, P.-G. Reinhard, J. Sarich, N. Schunck, M. V. Stoitsov, and S. M. Wild, "Nuclear Energy Density Optimization: Large deformations," Phys. Rev. C **85**, 024304 (2012)
9. N. Schunck, J. Dobaczewski, W. Satuła, J. A. Sheikh, A. Staszczak, M. Stoitsov and P. Toivanen, "Solution of the Skyrme-Hartree-Fock-Bogoliubov equations in the Cartesian deformed harmonic oscillator basis," Comp. Phys. Comm. **183**, 166 (2012)
10. M. Kortelainen, T. Lesinski, J. Moré, W. Nazarewicz, J. Sarich, N. Schunck, M. V. Stoitsov, and S. Wild, "Nuclear Energy Density Optimization," Phys. Rev. C **82**, 024313 (2010)

Collaborators and Co-editors

- M. Bender (IPN Lyon); H. Carr (University of Leeds); J. Dobaczewski (University of York); D. Duke (University of Leeds); J. Engel (University of North Carolina Chapell-Hill); D. Higdon (LANL); M. Kortelainen (University of Jyväskylä); T. Martinez (Stanford University); J. McDonnell (Francis Marion University); H.A. Nam (LANL); W. Nazarewicz (Michigan State University); P.-G. Reinhard (University of Erlangen); J. Sarich (ANL) W. Satula (University of Warsaw); J. Sheikh (Kashmir University); D. Sherrily (Georgia Institute of Technology); A. Staszczak (University Marie Curie-Sklodowska); S. Wild (ANL); W. Younes (LLNL)

Ron A. Soltz

7000 East Ave.	925 423-2647 (work)
LLNL, L-50	925 724-6463 (mobile)
Livermore, CA 94550	`soltz1@llnl.gov`

Education

Ph.D. Physics 1994
Massachusetts Institute of Technology, Cambridge, MA

M.A. Physics 1989
Columbia University, New York City, NY

B.S. Physics 1987
Massachusetts Institute of Technology, Cambridge, MA

Employment

Group Leader, Nuclear and Particle Physics 2015–present
Lawrence Livermore National Laboratory Livermore, CA 94450
- ◦ UDNDS PI for LLNL Verification and Validation (2014–present)
- ◦ DOE-NP PI for Heavy Ion Physics at LLNL (2000–present)
- ◦ Coordinator for HotQCD Lattice QCD Collaboration (2007–present)
- ◦ Lead Organizer: National Nuclear Physics Summer School, Tahoe, 2015

Group Leader, Nuclear and Particle Physics 2009–2014
Lawrence Livermore National Laboratory Livermore, CA 94450
- ◦ DNDO PI for DNDO Neutron Time Correlation SNM Detection (2011–2014)
- ◦ LDRD PI for Measuring and Modeling Shock Waves in QGP (2010–2012)
- ◦ ALICE-USA Computing Coordinator (2006–2012) Council Chair (2010-2012)

Staff Physicist 1997–2009
Lawrence Livermore National Laboratory Livermore, CA 94450
- ◦ LDRD PI for QCD Thermodynamics with LLNL supercomputers (2008–2009)
- ◦ DNDO PI for Global Security Passive-Aggressive Detection of Shielded SNM project (2006-2009)
- ◦ LDRD PI for Heavy Ion Physics, femtoscopy in heavy ion collisions on PHENIX (2000-2002)
- ◦ PHENIX Co-convenor Hadron Working Group (2004–2005)
- ◦ Co-Organizer: Quarks to Cosmos with Petaflops, Oakland, 2008
- ◦ Lead Organizer: Workshop on Particle Correlations and Femtoscopy Sonoma, 2007
- ◦ Lead Organizer: Modeling the QCD EoS at RHIC, Livermore 2006
- ◦ Co-Organizer: Quark Matter, Oakland 2004

Post Doctoral Fellow 1994–1997
Lawrence Livermore National Laboratory Livermore, CA 94450
- ◦ Deputy Spokesperson for AGS E910 Experiment.

Honors

Staff Mentor Award in Physics and Life Sciences, 2013.

Postdoc Mentor Award in Physics and Life Sciences, 2010.

Physics and Life Sciences Directorate Award for time correlated measurements of HEU, 2009.

Global Security Gold Award for contributions to Passive Detection of Shielded SNM, 2008.

Gordon Bell Prize for Special Achievement, “BlueGene/L Supercomputer and QCD”, 2006.

Physics Directorate Award for contributions to PHENIX analysis leading to QGP discovery, 2005.

Physics Directorate Award for Best Paper, “Formation of Dense Partonic Matter”, 2005.

Ron A. Soltz

Publications (selection of 20 from more than 280)

J. S. Moreland and R. A. Soltz, "Hydrodynamic simulations of relativistic heavy-ion collisions with different lattice QCD calculations of the equation of state", accepted by Phys. Rev. C., arxiv:1512.02189.

R.A. Soltz, C. DeTar, F. Karsch, S. Munkerjee, and P. Vranas, "Lattice QCD Thermodynamics with Physical Quark Masses", Ann. Rev. Nucl. and Part. Sci. 65, 379, 2015.

R.A. Soltz, [PHENIX], "PHENIX Beam Energy Scan Results", Nucl. Phys. A 931, 780, 2014.

T. Bhattacharya *et al.*, [HotQCD] "QCD Phase Transition with Chiral Quarks and Physical Quark Masses", Phys. Rev. Lett. 113, 082001, 2014.

A. Adare, *et al.*, [PHENIX] "Azimuthal-angle dependence of charged-pion-interferometry measurements with respect to 2nd and 3rd-order event plane in Au+Au collisions at $\sqrt{s_{NN}} = 200$ GeV", Phys. Rev. Lett. 112, 222301, 2014.

A. Bazavov, *et al.*, [HotQCD] "The equation of state in (2+1)-flavor QCD", Phys. Rev. D, 90, 094503, 2014.

R.A. Soltz *et al.*, "Constraining the initial temperature and shear viscosity in a hybrid hydrodynamic model of sNN=200 GeV Au+Au collisions using pion spectra, elliptic flow, and femtoscopic radii", Phys. Rev. C 87, 044901, 2013.

A. Bazavov, *et al.*, [HotQCD] "Fluctuations and Correlations of net baryon number, electric charge, and strangeness: A comparison of lattice QCD results with the hadron resonance gas model", Phys. Rev. D 86, 034509, 2012.

A. Bazavov, *et al.*, [HotQCD] "The chiral and deconfinement aspects of the QCD transition", Phys. Rev. D 85, 054503, 2012.

A. Bazavov, *et al.*, [HotQCD] "Equation of state and QCD transition at finite temperature", Phys. Rev. D 80, 014504, 2009.

A. Afanasiev, *et al.*, [PHENIX] "Kaon interferometric probes of space-time evolution in Au+Au collisions at $\sqrt{s_{NN}} = 200$ GeV", Phys. Rev. Lett. 103, 142301, 2009.

R.A. Soltz, *et al.*, [BNL-E910] "Centrality dependence of the thermal excitation-energy deposition in 8-15-GeV/c hadron-Au reactions", Phys. Rev. C 79, 034697, 2009.

S.S. Adler, *et al.*, [BNL-E910] "Centrality dependence of charged hadron production in d+Au and n+Au collisions at $\sqrt{s_{NN}}$=200 GeV", Phys. Rev. C 77, 014905, 2008.

D. Brown, R.A. Soltz, R.J. Newby, A. Kisiel, "Exploring lifetime effects in femtoscopy", Phys. Rev. C 76, 044906, 2007.

S. Adler, *et al.*, [PHENIX] "Evidence for a long-range component in the pion emission source in Au+Au Collisions at $\sqrt{s_{NN}}$=200 GeV", Phys. Rev. Lett. 98, 132301, 2007.

M. Lisa, S. Pratt, R.A. Soltz, U. Wiedemann, "Femtoscopy in Relativistic Heavy Ion Collisions", Ann. Rev. Nucl, and Part. Sci, 55,357, 2005.

K. Adcox, *et al.*, [PHENIX] "Formation of Dense Partonic Matter in Relativistic Nucleus-nucleus Collisions : Experimental evaluation by the PHENIX Collaboration", Nucl. Phys. A 757, 184, 2005.

S. Adler, *et al.*, "Bose-Einstein Correlations of Charged Pion Pairs in Au+Au Collisions at $\sqrt{s_{NN}}$=200 GeV", Phys. Rev. Lett. 93, 152302, 2004.

K. Adcox, *et al.*, [PHENIX] "Transverse Mass Dependence of the Two-Pion Correlations in Au+Au Collisions at $\sqrt{s_{NN}}$=130 GeV", Phys. Rev. Lett, 88, 192302, 2002.

L. Ahle, *et al.*, [BNL-E866] "System, centrality, and transverse mass dependence of two-pion correlation radii in heavy ion collisions at 11.6 and 14.6 A-GeV", Phys.. Rev. C. 66, 054906, 2002.

Vera L. Bulaevskaya, Ph.D.

Applied Statistician
Applied Statistics Group
Computational Engineering Division

7000 East Ave.
Lawrence Livermore National Laboratory, L-211
Email: verab@llnl.gov
Phone: (925) 423-8375

EDUCATION

Dec. 2002 Ph.D., Statistics, University of Minnesota

April 2001 M.S., Statistics, University of Minnesota

May 1997 B.S., Statistics, Iowa State University

PROFESSIONAL EXPERIENCE

Aug. 06 – present **Lawrence Livermore National Laboratory, Livermore, CA**
Applied Statistician, Applied Statistics Group

- Leading statistician on project teams in various areas, including uncertainty quantification, wind forecasting and modeling, energy and climate modeling, nuclear plant vulnerability assessment, nuclear reactor monitoring, detector modeling and pulse shape discrimination, X-ray imaging, blast effect modeling, radiation detection, seismic modeling
- Participated in the development of statistical tools, including computer code implementation, for general laboratory-wide and external use
- Principal statistical methods used: ensemble and particle filter methods, computer experiments, functional data analysis, classification and machine learning methods, advanced experimental design, Bayesian modeling, spatial modeling

Jan. 03 – July 06 **Carnegie Mellon University, Pittsburgh, PA**
Visiting Assistant Professor

- Conducted research on statistical applications in the areas of functional Magnetic Resonance Imaging and neuroscience
- Taught statistics and probability courses at undergraduate and graduate levels
- Advised graduate and undergraduate students

LEADERSHIP AND PROFESSIONAL ACTIVITIES

- LLNL Data Sciences Seminar Program Head (August 2014 – present)
- LLNL Data Heroes Summer Program Mentor (2015 – present)
- Member on a Ph.D. thesis committee of a student at UC Santa Cruz (2015 – present)
- Referee for several journals, including *Annals of Applied Statistics*, *Journal of Renewable and Sustainable Energy*, *Wind Energy*, *Journal of Agricultural, Biological and Environmental Statistics* and *American Society of Mechanical Engineers*

HONORS AND AWARDS

- Engineering Award for Outstanding Contribution to the Data Sciences Seminar Series (2016)
- Global Security Silver Award for work on Wind Energy Forecasting project (2014)
- Engineering Silver Award for work on California Energy Commission project (2013)
- Outstanding Presentation Award at the Joint Statistical Meetings in San Diego (2012)
- Global Security Gold Award for work on X-ray Baggage Screening project (2009)
- Global Security Gold Award for work on Transportation Security project (2009)

SELECTED AND RELEVANT PUBLICATIONS AND MANUSCRIPTS

Bulaevskaya, V., Wharton, S., Clifton, A., Qualley, G., Miller W. (2015). "Wind Power Curve Modeling in Complex Terrain Using Statistical Models", *Journal of Renewable and Sustainable Energy* 7, 103103, doi: 10.1063/1.4904430

Bulaevskaya, V.L., Bernstein, A. (2011). "Detection of Anomalous Activity Using Antineutrino Count Evolution Over a Course of a Reactor Cycle", *Journal of Applied Physics*. 109:11.

Bulaevskaya, V.L. and Oehlert, G.W. (2007). "A Penalized Likelihood Approach to Magnetic Resonance Image Reconstruction", *Statistics in Medicine* 26:2, 352-374.

Bulaevskaya, V., Lucas, D. "Objective Calibration of Model Parameters in CAM5 Across Different Spatial Resolutions", in progress.

Bulaevskaya, V., Johannesson, G., Domyancic, D. "Aggregation of Multiple Adaptive Sampling Criteria in Computer Experiments", in progress.

Ramona Vogt
Staff physicist *Nuclear Data and Theory Group, Nuclear and Chemical Sciences Divison, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551*
Office phone: (925) 423-8210; Mobile: (925) 724-7148; vogt2@llnl.gov

Education and Training:
A.S. Engineering, Kaskaskia College, Centralia, IL, USA, 1983
B.S. Physics, University of Illinois, Urbana, IL, USA 1985
M.S. Physics, SUNY at Stony Brook, Stony Brook, NY, USA, 1989
Ph.D. Physics, SUNY at Stony Brook, Stony Brook, NY, USA, 1989

Research and Professional Experience:
Staff Physicist, Nuclear and Chemical Sciences Division, Lawrence Livermore National Laboratory, Livermore, CA, USA, 2007-
Adjunct Professor, Physics Department, University of California at Davis, Davis, CA, USA, 1995-
Staff Scientist, Affiliate Scientist, Nuclear Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA, 1993-
Postdoc, Lawrence Livermore National Laboratory, Livermore, CA, 1989-1991
Postdoc, Gesellschaft für Schwerionenforschung, Darmstadt, Germany, 1991-1993
Other Appointments Guest Scientist, Physics Department, University of Jyväskylä, Jyväskylä, Finland, 2003; IN2P3 Exchange Visitor, Grand Accelerateur d'Ions Lourds, Caen, France, 2001; Rosenberg Fellow, Niels Bohr Institute, Copenhagen, Denmark, 2001; Guest Scientist, Gesellschaft für Schwerionenforschung, Darmstadt, Germany, 2001

Honors:
UC Davis Academic Federation Excellence in Research Award, 2001
Fellow of the American Physical Society, 2010
Physical and Life Sciences Directorate Award, LLNL, 2011

Leadership Activities: American Physical Society:
Member-at-Large, APS Topical Group in Hadronic Physics, 2008-2010
Vice-Chair, APS Topical Group in Hadronic Physics, 2010-2011
Chair-Elect, APS Topical Group in Hadronic Physics, 2011-2012
Program Committee Member, APS April Meeting, 2012
Chair, APS Topical Group in Hadronic Physics, 2012-2013
Past Chair, APS Topical Group in Hadronic Physics, 2013-2014
Secretary-Treasurer, APS Topical Group in Hadronic Physics, 2016-
Program Committee Member, APS Division of Nuclear Physics, 2016-

Leadership Activities: Selected Conference Organization:
In-Medium Convener, Quarkonium Working Group 2006-
Organizing committee of the APS Topical Group on Hadronic Physics Workshops, Denver, CO, 2009; Anaheim, CA, 2011 (co-chair); Denver, CO, 2013; Baltimore, MD, 2015
Lead Organizer, Heavy Flavor and Electromagnetic Probes in Heavy Ion Collisions, Institute for Nuclear Theory, Seattle, WA, September-October 2014
Member, Program Committee, PANIC 2008 (Eilat, Israel 2009)
Member, International Advisory Committee of CHARM conferences: CHARM 2015 (Detroit, May 2015); CHARM 2016 (Bologna, Italy, September 2016)
Member, International Advisory Committee of Hard Probes conferences: Hard Probes 2013 (Stellenbosch, South Africa, November 2013); Hard Probes 2015 (Montreal, Canada, June-July 2015);

Hard Probes 2016 (Wuhan, China, September 2016)

Leadership Activities: Grants:
NSF Nuclear Theory PI, UC Davis (2005-2010)
DOE-NP Heavy Ion Nuclear Theory PI, LLNL (2015-present)
NNSA PI for Event-by-Event Correlations in Fission (2011-2014)
NNSA Co-PI for Correlated Fission Data (2014-present)

Synergistic Activities:
Editorial Board Member for Physical Review C (2013-2016)
Grant proposal reviews for NSF, DOE-NP (including the Early Career Program), NNSA NA-22, and ANR (French Research Agency)
Referee for Physical Review Letters, Physical Review C, Physical Review D, Journal of Physics G, Computer Physics Communications, Nuclear Physics A, European Physical Journal A, European Physical Journal C
Member, Los Alamos Nuclear Science Center Program Advisory Committee, 2013-2014

Publications:
Heavy-Ion Physics
R. Vogt, J/ψ Production and Suppression, Phys. Rept. **310**, 197 (1998).
M. Cacciari, P. Nason and R. Vogt, QCD Predictions for Charm and Bottom Production at RHIC, Phys. Rev. Lett. **95**, 122001 (2005).
R. Vogt, Cold Nuclear Matter Effects on J/ψ and Υ Production at the LHC, Phys. Rev. C **81**, 044903 (2010).
N. Brambilla, S. Eidelman, B. K. Heltsley, R. Vogt, *et al.*, Heavy quarkonium: progress, puzzles, and opportunities, Eur. Phys. J. C **71**, 1534 (2011).
R. E. Nelson, R. Vogt and A. D. Frawley, Narrowing the uncertainty on the total charm cross section and its effect on the J/ψ cross section, Phys. Rev. C **87**, 014908 (2013).
J. L. Albacete, N. Armesto, R. Baier, R. Vogt *et al.*, Predictions for p+Pb Collisions at $\sqrt{s_{NN}} = 5$ TeV, Int. J. Mod. Phys. E **22**, 1330007 (2013).
N. Brambilla, S. Eidelman, P. Foka, R. Vogt *et al.*, QCD and Strongly Coupled Gauge Theories: Challenges and Perspectives, Eur. Phys. J. C **74**, 2981 (2014).
Nuclear Fission
Calculation of fission observables through event-by-event simulation, J. Randrup and R. Vogt, Phys. Rev. C **80**, 024601 (2009).
Event-by-event study of neutron observables in spontaneous and thermal fission, R. Vogt and J. Randrup, Phys. Rev. C **84**, 044621 (2011).
ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data, M. B. Chadwick, M. Herman, P. Oblozinsky, R. Vogt, *et al.* Nucl. Data Sheets **112**, 2887 (2011).
Nuclear Fission, R. Vogt and J. Randrup, in *100 Years of Subatomic Physics*, World Scientific, Singapore (2013).
Event-by-event study of photon observables in spontaneous and thermal fission, R. Vogt and J. Randrup, Phys. Rev. C **87**, 044602 (2013).
Neutron angular correlations in spontaneous and neutron-induced fission, R. Vogt and J. Randrup, Phys. Rev. C **90**, 064623 (2014).
Fission Reaction Event Yield Algorithm, `FREYA` – For event-by-event simulation of fission, J. M. Verbeke, J. Randrup and R. Vogt, Comp. Phys. Comm. **191** (2015) 178.
Prompt Fission Neutron Spectra of Actinides, R. Capote, R. Vogt *et al.*, Nucl. Data Sheets **131** (2016) 1.

Caleb M. Mattoon, Ph.D.

Lawrence Livermore National Lab
7000 East Ave, L-059
Livermore, CA 94550 USA

Office: (925) 423-9204
Mobile: (720) 220-9964
E-mail: mattoon1@llnl.gov

Education

Colorado School of Mines, Golden, Colorado USA

Ph.D., Applied Physics, December 2007

- Thesis title: *Beta-decay Studies of Neutron-rich ^{11}Li and ^{32}Na*
- Advisor: Professor Frederic Sarazin

Luther College, Decorah, Iowa USA

B.A., Mathematics and B.A., Physics, May, 2003

Professional Experience

Nuclear and Chemical Sciences Division, Lawrence Livermore National Lab, Livermore CA, USA

Staff Scientist September 2010 - Present

Modernizing infrastructure for storing and accessing nuclear reaction data in large-scale computer simulations, and working to improve the quality of evaluated nuclear reaction data including covariances.

Developing and maintaining 'kiwi', a computer code for applying covariance matrices to uncertainty quantification (UQ) studies.

Using machine learning to improve radiation detection capabilities when scanning traffic at US sea port facilities.

National Nuclear Data Center, Brookhaven National Lab, Upton NY, USA

Post-doctoral Research Associate June 2008 - August 2010

Developed the AFCI Covariance Library, which supplied evaluated or estimated covariances for 110 materials important to fast reactor design.

Developed the 'empy' module, designed to extend the capabilities of the nuclear reaction modeling code EMPIRE.

Academic Experience

Colorado School of Mines, Golden, Colorado USA

Research Assistant August, 2003 - December, 2007

Ph.D. work involved analyzing the results of two experiments performed with the 8π γ-ray spectrometer in Vancouver, BC.

- Used gamma-gamma coincidence techniques to explore the level schemes of neutron-rich nuclei, identify possible new transitions, and find γ-ray branching ratios.
- Simulated Doppler-broadened peaks in the ^{11}Li decay spectrum with Monte Carlo simulations written in C++, in order to measure branching ratios from the β-delayed neutron emission of ^{11}Li.

SKILLS

Communication

Experience working collaboratively in research, analysis, and publication

President, Brookhaven National Lab 'Association for Students and Postdocs', 2010

Treasurer, School of Mines Graduate Student Association, Spring 2006

DJ, Luther College campus radio, Fall 2000-Spring 2003

Analytic

Languages: Python, C, C++, Java, Fortran, unix shell scripts.

Data Analysis:

-extensive use of pandas (pandas.pydata.org) and root (www.root.cern.ch)

-experienced with tools producing and using nuclear data, including LLNL's processing codes, the ENDF and ENDL formats, and the nuclear reaction modeling code EMPIRE

Applications: numpy/scipy, Matlab, Mathematica, LaTeX, profiling and test coverage tools, version control systems

PUBLICATIONS

"Designing a new structure for storing nuclear data: Progress of the Working Party for Evaluation Cooperation subgroup #38" C.M. Mattoon, B.R. Beck, Eur. Phys. J. A **51** (2015)

"Covariances in the Generalized Nuclear Data (GND) Structure" C.M.Mattoon, Nuclear Data Sheets **123**, 36 (2015)

"Combined Use of Integral Experiments and Covariance Data" G. Palmiotti *et al.*, Nuclear Data Sheets **118**, 596 (2014)

"Determining the Np-239(n,f) cross section using the surrogate ratio method" A. Czeszumska *et al.*, Phys. Rev. C **87** (2013) 034613

"Generalized Nuclear Data: A New Structure (with Supporting Infrastructure) for Handling Nuclear Data" C.M.Mattoon *et al.*, Nuclear Data Sheets **113**, 3145 (2012)

"Covariance Applications with Kiwi" C.M.Mattoon *et al.*, EPJ Web of Conferences **27**, 00002 (2012)

"ENDF/B-VII.1: Nuclear Data for Nuclear Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data" M.B. Chadwick *et al.*, Nuclear Data Sheets **112**, 2887 (2011)

"Neutron Cross Section Covariances for Structural Materials and Fission Products" S. Hoblit *et al.*, Nuclear Data Sheets **112**, 3075 (2011)

"Issues in Neutron Cross Section Covariances" C.M.Mattoon and P.Obložinský, Jour. Kor. Phys. Soc. **59** (2011) 1242