

— PROJECT NARRATIVE —
Cover Page

Application for Funding Opportunity #DE-FOA-0001414
U.S. Department of Energy

— Project Title —

**NON-CLASSICAL TRANSPORT THEORY WITH MULTISCALE PATH
DISTRIBUTIONS IN REAL-WORLD APPLICATIONS**

- Applicant: **The Regents of the University of California, Berkeley**
Street Address: **2150 Shattuck Avenue, Suite 300**
City: **Berkeley**
State: **California**
Zip: **94704-5940**
- Postal Address: **The Regents of the University of California, Berkeley**
c/o Sponsored Projects Office
2150 Shattuck Avenue, Suite 300
University of California, Berkeley, CA 94704-5940
- Lead PI name: **Rachel N. Slaybaugh**
Telephone Number: **570-850-3385**
Email: **slaybaugh@berkeley.edu**
- Administrative Point of Contact Name: **Joy Ayson-Yu**
Telephone Number: **510-664-4458**
Email: **laysonyu@berkeley.edu**
- Funding Opportunity FOA Number: **DE-FOA-0001414**
- DOE/Office of Science Program Office: **ASCR - Adv. Sci. Comp. Research**
Topic Area: **Applied Mathematics**
Topic Area Program Manager: **Steven Lee**
- PAMS Preproposal Tracking Number: **PRE-0000008821**

1 Introduction

We propose to establish and formalize the mathematical foundation of a novel homogenization approach known as *non-classical transport* [1–4], which will enable better mathematical and computational modeling of particle and radiation transport calculations in heterogeneous random media. The main impact of this work will be on improving the modeling of transport processes in general three-dimensional (3D) stochastic systems. We will develop a methodology that will allow us to accurately solve coupled multiscale transport problems in highly heterogeneous systems. We will also develop an approach to quantify uncertainty with respect to the particular homogenization of the medium.

Accurate modeling of transport processes in optical media is integral to several real-world applications that are in line with the goals of the Department of Energy (DOE) and the Advanced Scientific Computing Research (ASCR) program. These include neutron transport in certain types of nuclear reactors (see [5, 6], and references therein), radiative transfer in the Earth’s cloudy atmosphere (see [2, 4], and references therein), and computational graphics (CG) rendering (see [7, 8], and references therein). Due to the complexity of these systems, spatial variations are often represented with stochastic models.

There are many ways to address stochastic spatial variability in a transport medium; a widely-used and natural approach is *homogenization* [9, 10]. In this approach, the solution of the transport problem in the heterogeneous stochastic medium is predicted by solving a transport problem in an uniform medium. The accuracy with which this *homogenized* uniform medium mimics the physics of the random system will depend on the homogenization approach.

Current homogenization techniques fail to accurately represent the true behavior of the transport process taking place in certain types of random and heterogeneous systems. Situations in which classical homogenization performs poorly include anomalous diffusion, Lèvy flights, long-range correlations, and non-exponential decay, to name a few. In this work, we propose to homogenize and model particle transport in these applications using a *non-classical theory*, which can properly capture and preserve important physical aspects of the system [1, 2, 4, 6, 11].

In this project, we will focus in particular on improving predictive capabilities and increasing spatial resolution of neutron transport calculations in Pebble Bed Reactor (PBR) cores. The PBR is a graphite-moderated, helium- or liquid salt-cooled, very-high-temperature (generation IV) reactor

concept with highly desirable characteristics. These include convenient long-term waste storage, meltdown-proof passive safety, modular construction, on-line refueling, and means to hydrogen production and desalination [12–14].

We will also address the challenges involved in modeling the transport of solar and thermal radiation in atmospheric clouds. The ability to do that accurately in the cloudy atmosphere is crucial to climate modeling research. This has been pointed out in a recent report [15] by the Intergovernmental Panel on Climate Change (IPCC), which states (p. 53) that

“The uncertainty in the WMGHG RF¹ is due in part to its radiative properties but mostly to the full accounting of atmospheric radiative transfer including clouds”.

Moreover, this has been identified by the Exascale Mathematics Working Group as a key area of interest for ASCR research [16]. On the subject of developing new mathematical tools to address climate models, their report says that (p. 6)

“... models based on a Markovian assumption will not be adequate. Models that can represent the physics across a range of scales are likely to be stochastic and include memory effects”.

This is exactly what our proposed work does: it includes a memory variable (the free-path of the particle) to preserve important physical aspects of the stochastic system.

In addition, we will establish a cross-disciplinary collaboration in the field of computer graphics, as computing the light transport equations is central to many rendering algorithms. Incorporating non-classical free-paths in volume-rendering algorithms will produce more realistic images, as deep penetration of photons is a key feature of high albedo media. We will study the parallels and lessons from research done in nuclear physics, among other areas, and how that connects, mirrors, and informs CG rendering. Specifically, we will make use of the synergy between these two applications to develop novel approaches, which will provide many insights to both communities.

Finally, we point out that the work we propose will open new research avenues in vital areas of interest for the Applied Mathematics topic area of the ASCR program. These include, but are not limited to, the implementation of novel computational methods for solving the differential, integral, and integro-differential equations involved; studies in uncertainty quantification; innovations in computing large systems of linear equations; and the development of coupled multiscale models. In short, this work supports the Applied Mathematics goal to solve problems of interest with greater accuracy by more accurately capturing the physics.

¹Well-mixed greenhouse gas radiative forcing

In the following sections we will describe the work we will undertake, why it will contribute to advancing the knowledge and understanding of transport problems in stochastic media, and how we will complete the objectives of the proposal. We start with a discussion on the classical approach used by current tools and why it is insufficient to accurately model non-classical particle transport in relevant applications. This will be followed by a description of the non-classical theory and a discussion of how it will improve our ability to accurately model these problems. Finally, a detailed research plan describing project execution, milestones, deliverables, and responsibilities is described.

2 The Challenge

We define the free-path s as the distance traveled by a particle (neutron or photon) since its previous interaction (birth or scattering event). In this definition, the instant after a particle is born or scatters, its value of s is 0. In the classical theory of linear particle transport, the incremental probability dp that a particle at point $\vec{r} = (x, y, z)$ with energy E will experience an interaction while traveling an incremental distance ds is given by $\Sigma_t(\vec{r}, E)ds$. Here, the total cross section Σ_t is independent of the free-path s and of the direction of flight $\hat{\Omega} = (\Omega_x, \Omega_y, \Omega_z)$, where $|\hat{\Omega}| = 1$.

Let us consider a single volume of Poisson-distributed (spatially uncorrelated) scattering centers (Fig. 1). Particles that enter such a volume will undergo many collisions before exiting from it.

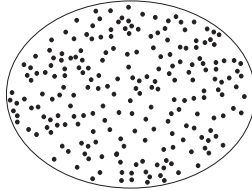


Figure 1: Sketch of a volume region containing Poisson-distributed scattering centers.

The probability density function describing the distribution of free-paths within this volume obeys the Beer-Lambert law, and is represented by the exponential

$$p(s) = \Sigma_t e^{-\Sigma_t s}. \quad (1)$$

Note that the scattering centers in this system can be viewed as water droplets in an idealized homogeneous cloud where the transported particles are (e.g., solar) photons.

Now consider a much larger system formed by randomly placing many of these volumes in a background “void”, as sketched in Fig. 2. This type of clumpy medium is present in PBRs [5, 6], where the volume regions represent the fuel pebbles in the reactor core, with thousands of them

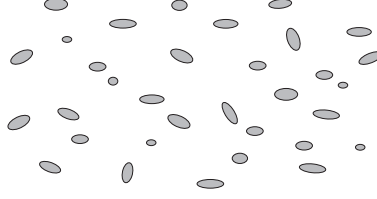


Figure 2: Heterogeneous random system formed by many volumes suspended in a void.

piled on top of one another in a random manner. Real clouds in planetary atmospheres, starting with the Earth's, are constantly churned by turbulent motion, and this generates strong spatial heterogeneity in their local microphysical and hence optical properties.

It is common to use a homogenization model to address transport problems in this kind of random system. This type of approach seeks to develop effective material properties that can be used in the solution of a transport problem for a uniform medium, while achieving an accurate prediction of the flux behavior in the heterogeneous stochastic medium. Nevertheless, standard homogenization techniques inherently assume that Eq. (1) holds in the homogenized material; that is, they assume that the free-path distribution in the uniform medium is given by an exponential (classical transport).

However, the assumption that Σ_t is independent of s is not valid when the locations of the volume regions in the system are correlated. This correlation leads to a *non-exponential* free-path distribution $p(s)$; we refer this type of transport processes *non-classical*. The classical homogenization approaches used to address these problems are not capable of preserving the true non-exponential attenuation law that arises in these heterogeneous systems. This leads to unreliable estimates of the particle flux in these applications, due to important physical quantities being poorly approximated.

The challenge is to develop and implement a methodology that (i) determines the true free-path distribution in these systems, and (ii) uses that information in a model that preserves the physics of these stochastic processes. To do that, we will use a novel theory specifically developed to address non-classical transport.

3 The Non-classical Theory

To address the challenges of modeling systems with non-exponential particle attenuation, a generalization of the linear Boltzmann equation has been developed [1–4]. The generalized equation assumes that the positions of the scattering centers are correlated but independent of direction $\hat{\Omega}$. For the sake of simplicity, let us consider monoenergetic transport with isotropic scattering; in this

case, the *non-classical transport equation* can be written as

$$\begin{aligned} \frac{\partial \psi}{\partial s}(\vec{r}, \hat{\Omega}, s) + \hat{\Omega} \cdot \nabla \psi(\vec{r}, \hat{\Omega}, s) + \Sigma_t(s) \psi(\vec{r}, \hat{\Omega}, s) \\ = \frac{\delta(s)}{4\pi} \left[c \int_{4\pi} \int_0^\infty \Sigma_t(s') \psi(\vec{r}, \hat{\Omega}', s') ds' d\Omega' + Q(\vec{r}) \right], \end{aligned} \quad (2)$$

where ψ is the non-classical angular flux, c is the scattering ratio (such that the scattering cross section $\Sigma_s = c\Sigma_t$), and Q is an isotropic source. Here, the non-classical homogenized total cross section $\Sigma_t(s)$ is defined such that

the probability that a particle that has traveled a distance s since its previous
 $\Sigma_t(s)ds =$ interaction (birth as a source particle or scattering event) will experience its
 next interaction while traveling a further distance ds ,

and we can obtain the angular flux $\Psi(\vec{r}, \hat{\Omega})$ by computing

$$\Psi(\vec{r}, \hat{\Omega}) = \int_0^\infty \psi(\vec{r}, \hat{\Omega}, s) ds. \quad (3)$$

The generalized model described by Eq. (2) effectively homogenizes the heterogeneous media by including the memory variable s and by incorporating its *true* (non-exponential) free-path distribution $p(s)$, which is related to the non-classical cross-section by [1]

$$p(s) = \Sigma_t(s) \exp \left[- \int_0^s \Sigma_t(s') ds' \right]. \quad (4)$$

Notice that, if $\Sigma_t(s) \equiv \Sigma_t$, independent of s , then Eq. (4) reduces to Eq. (1), and Eq. (2) reduces to the classical transport equation

$$\hat{\Omega} \cdot \nabla \Psi(\vec{r}, \hat{\Omega}) + \Sigma_t \Psi(\vec{r}, \hat{\Omega}) = \frac{1}{4\pi} \left[c \int_{4\pi} \Sigma_t \Psi(\vec{r}, \hat{\Omega}') d\Omega' + Q(\vec{r}) \right].$$

Existence and uniqueness of solutions have been rigorously discussed in [17]. The non-classical theory was extended in [3] to include angular-dependent free-path distributions in order to investigate anisotropic diffusion of neutrons in 3D PBR cores. A similar kinetic equation with free-path as an independent variable has been rigorously derived for the periodic Lorentz gas in a series of papers by Golse and colleagues (cf. [18] for a review), and by Marklof & Strömbergsson (cf. [19,20]).

4 Related Preliminary Results

We have already shown that the simplified P_1 (SP_1 , or classical diffusion), SP_2 , and SP_3 approximations to the *classical* linear Boltzmann equation can be represented exactly by a non-classical transport equation for an infinite, homogeneous medium [21]. Similarly, the non-classical transport equation can also exactly represent the *non-classical diffusion equation* [22]. Moreover, one can combine moment methods and the Fourier transform to derive fractional diffusion equations from the non-classical transport equation [23]. This is key to model radiative transfer problems in atmospheric clouds, where generalized (a.k.a. anomalous) diffusion arises due to long-tailed free-path distributions [24, 25].

With respect to nuclear reactor applications, the non-classical theory has been shown to be more accurate than classical approaches in certain types of one-dimensional (1D) transport problems [26]. Figure 3 depicts the ensemble-averaged scalar fluxes obtained with non-classical and classical (atomic mix) approaches in a 1D random periodic system consisting of alternating layers of solid and void materials.

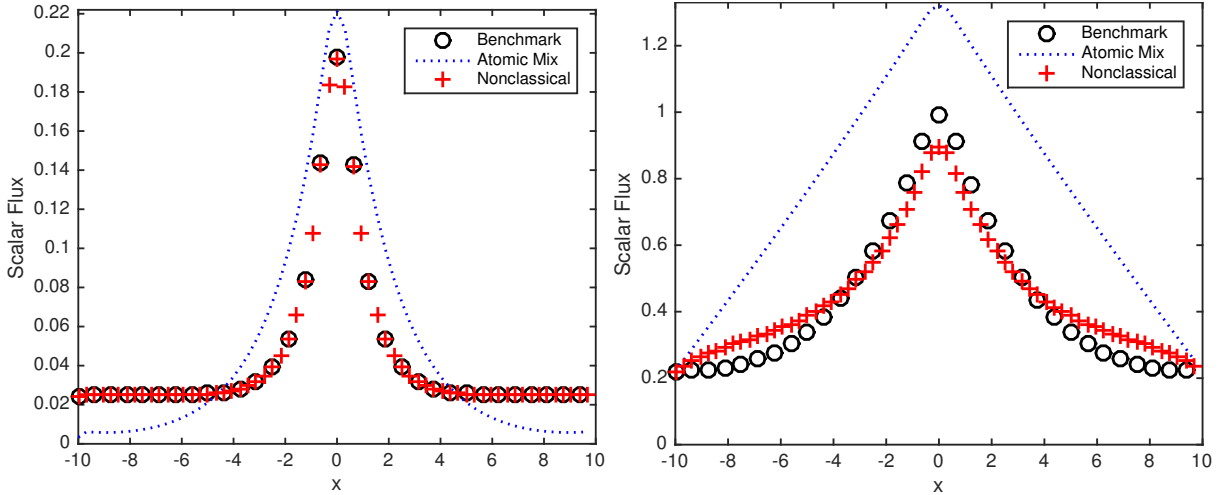


Figure 3: Ensemble-averaged scalar fluxes in a 1D random periodic system with parameters as defined in [26]. The scattering ratio c of the solid material is defined as 0 (**left**) and 0.99 (**right**).

Non-classical methods also outperform current homogenization techniques in PBR diffusive systems [1, 6, 11]. Table 1 shows the gain in accuracy attained with the non-classical theory in estimating diffusion coefficients for transport problems in PBR random structures. It displays isotropic (*iso*) and anisotropic (*gt*) diffusion coefficients obtained with the non-classical theory, and compares these results with those obtained by classical approaches: atomic mix (*am*), Behrens correction (*B*), and Lieberoth correction (*L*). Relative errors are calculated with respect to benchmark Monte Carlo (*mc*) results.

Table 1: Diffusion coefficients in PBR random systems [6]

Problem		Monte Carlo		Atomic Mix and Corrections			Non-classical Theory		
		D_{xy}^{mc}	D_z^{mc}	D^{am}	D^B	D^L	D^{iso}	D_{xy}^{gt}	D_z^{gt}
1	Diffusion								
	Coeff.	0.6144	0.6157	0.5617	0.6009	0.5990	0.6147	0.6146	0.6150
	error _{xy} (%)	-	-	8.580	2.201	2.506	0.049	0.029	-
	error _z (%)	-	-	8.776	2.411	2.716	0.166	-	0.126
2	Diffusion								
	Coeff.	0.3286	0.3295	0.2809	0.3200	0.3214	0.3326	0.3324	0.3329
	error _{xy} (%)	-	-	14.542	2.617	2.214	1.204	1.154	-
	error _z (%)	-	-	14.771	2.877	2.475	0.934	-	1.034

With respect to atmospheric clouds, co-I Davis and co-workers have used the explicit parameterization $p_a(s) = \langle \Sigma_t \rangle / (1 + \langle \Sigma_t \rangle s/a)^{1+a}$, where $\langle \Sigma_t \rangle$ is the average cross-section and a is the spatial variability parameter. It ranges from unity (excluded) to infinity (included). In the later limit, the classic exponential law in Eq. (1) is recovered. In the former one, the mean-free-path diverges and this is not seen in the observations [25]. This choice of $p(s)$ defines the generalized radiative transfer (GRT) model [2, 4] (previously called “anomalous” or “Lévy” transport [24]). Figure 4 shows a series of GRT particle random walks in a medium with a common $\langle \Sigma_t \rangle$ but a decreasing from ∞ to 1.2. We notice the similarity of the clusters of small steps that would occur in localized opaque regions, i.e., isolated clouds, and the increasingly large jumps between these clusters/clouds as the tail of the selected $p(s)$ distributions becomes longer.

These preliminary numerical results offer a strong case for the non-classical theory, and justify the efforts to develop and improve related tools. However, results for transport problems in higher dimensions have not yet been performed. The reason is that, in order to solve the non-classical transport equation, one must know the true (ensemble-averaged) free-path distribution function of the system. Although there are a few particular cases in which an analytical expression for $p(s)$ can be obtained [26, 27], doing so for general 3D random systems is still far from being achieved.

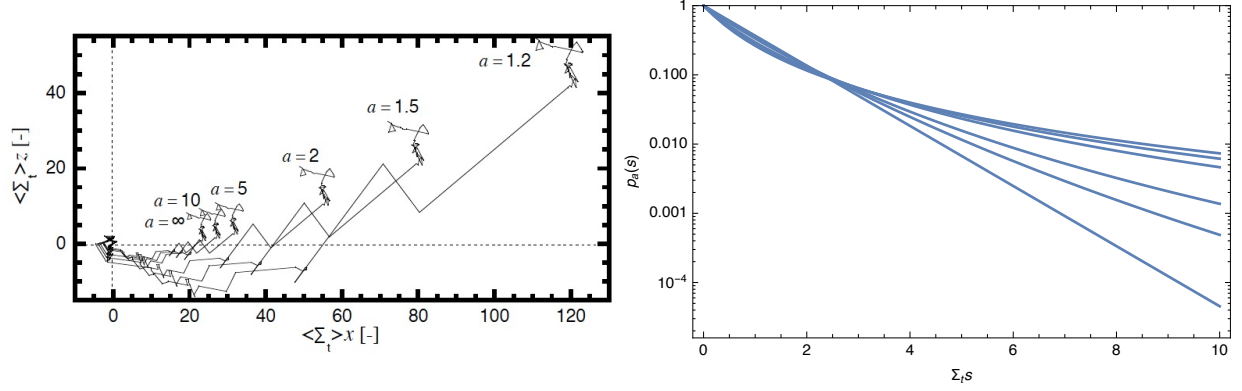


Figure 4: **Left:** 2D unbounded random walks, 100 steps each, all starting in the same direction at the origin of the axes, by isotropically scattered particles following $p_a(s)$ with the choices of a called out in the text. **Right:** Log plots of $p(s)$ for the traces plotted in the left panel.

5 Description of Proposed Research

5.1 Objectives

This project will focus on advancing the mathematical aspects of the non-classical theory, and on developing a set of computational tools to solve general, 3D non-classical transport problems in real-world applications. To achieve that, we will build upon the results presented in the last section to expand and improve the mathematical and computational aspects of the non-classical theory. Moreover, the interdisciplinary scope of the project combined to the different areas of expertise of the team will create perfect conditions to perform cutting-edge research, fostering ideas and driving innovations.

We will leverage computational techniques currently used in CG rendering (cloud modeling) to create a tool that will allow us to numerically estimate the $p(s)$ in general 3D stochastic and heterogeneous systems. This will enable us to solve the full non-classical transport equation and study its performance in different scenarios, while addressing a number of current challenges in the areas of applied mathematics and engineering.

One of the main features of this approach will be the ability to refine the resolution of the free-path distribution in different regions of interest, allowing us to accurately solve coupled multiscale transport problems in highly heterogeneous systems. The expectation is that the non-classical approach will be less costly and more accurate than existing methods once it is fully implemented since it preserves important elements of physics that are not captured by the current models.

5.2 Path to Success

We identify *five* key tasks that need to be completed in order to successfully accomplish the proposed work: numerically determining $p(s)$; choosing the transport solver; implementing and validating the method; extending the method to multiscale problems; and measuring the impact. These are the major steps in the project; the work involved to achieve them will fill gaps in science and engineering research that further DOE-ASCR goals. We will now describe the approach we will use to fulfill each of these tasks.

- Numerically Determining $p(s)$:

The initial phase of this work will focus on the development and analysis of the numerical approach to obtain the homogenized free-path distribution $p(s)$ in general, 3D, stochastic and heterogeneous systems. This will be accomplished by taking full advantage of the team's expert in graphics research. Tapping into this expertise, we will apply cutting-edge techniques used in volume-rendering algorithms to efficiently tally an accurate numerical estimate of the ensemble-averaged $p(s)$ in these random systems.

This algorithm will first be implemented in a scoping code for method characterization and investigation. Determining the best way to obtain the ensemble-averaged $p(s)$ for any stochastic mixture will be the primary challenge of this task; the lessons learned in doing so will be a valuable contribution to the wider scientific community. We will carry on the mathematical formalization of the methodology, and will quantify the uncertainty arising from the choice of $p(s)$. This will be done by performing a sensitivity analysis of the non-classical transport equation with respect to $p(s)$ using adjoint calculus [28, 29].

- Choosing the Transport Solver

Once we have developed the algorithm to attain $p(s)$, we need to introduce it into a code to solve the 3D non-classical transport equation. The choice of solver to use—deterministic or Monte Carlo—is of vital importance for the success of the project; thus, we will thoroughly weigh the pros and cons of each approach.

To do that, we will write preliminary versions of the codes for each solver and apply them to simple transport problems. We will evaluate the results and carry out a technical assessment, taking into account the accuracy, cost-efficiency, and potential pitfalls identified for each solver, as well as other foreseen issues as we move forward.

First, we will test the non-classical codes by solving *classical* transport problems in homogeneous and heterogeneous systems; this will allow us to validate the methods using standard (classical)

solution techniques. Next, we will solve non-classical problems in specific “toy” models, for which either analytical or benchmark solutions exist for a reliable comparison. We will then have enough the data to make an informed decision. If early in this process it becomes clear that one of the models strongly outperforms the other, we shall pick that method without having to complete this evaluation.

- Implementing and Validating the Method

Having chosen the transport solver, we can proceed to implement the full computational model. As we move from the basic transport problems addressed in the previous task to more complex non-classical problems, we need to use different approaches to validate the proposed method. These will depend on the type of applications/systems being addressed, and will include any combination of benchmark solutions, Monte Carlo simulations of the random system (not homogenized), and experimental results.

We will start by focusing on simple (but important) non-classical problems in real-world climate modeling/remote sensing applications, relying on the team’s expertise in this area to choose the best validation technique. We will then test and validate the proposed model in an expanded set of applications, including other areas in science and engineering where transport in 3D stochastic spatial structures is important.

Finally, we will use the proposed computational model to validate some mathematical aspects of the non-classical theory. The asymptotic convergence of the non-classical transport equation to simpler representations of the transport process will be examined, and original asymptotic analyses for selected models (e.g. simplified P_N equations) will be performed. We will use the set of tools developed to numerically validate these new results as well as other—already established—asymptotic limits of the non-classical theory (e.g. fractional diffusion).

- Extending the Method to Multiscale Problems

After the successful implementation and validation of the proposed model, we will extend the capabilities developed up to this point to create free-path distributions that can accurately capture highly-resolved heterogeneities in small length scales. This will enable us to “fine-tune” the $p(s)$ at different regions of the system, allowing us to effectively describe the non-classical transport process as a multiscale problem.

This gives us a set of coupled multiscale transport equations in the larger system that can be solved without the cost of fine resolution for the $p(s)$ everywhere, while still preserving significant information where needed. We will perform a thorough sensitivity analysis and will broaden the

uncertainty quantification approach used in the first task to include this extended, multiscale homogenization of $p(s)$.

- Measuring Impact

We will measure the impact of the proposed model by analyzing its performance (accuracy, time, etc.) compared to current homogenization techniques and other approaches than homogenization. We will investigate how the choice of the system affects its performance, and what kind of real-world applications are best suited to the non-classical theory. We will also determine how efficiently this approach models multiscale and multiresolution problems.

5.3 Deliverables

The first deliverable from this project will be a high-quality set of mathematical and computational tools to address non-classical transport problems in general 3D random systems. These tools will have the capability to accurately and efficiently solve coupled multiscale transport problems in systems with very strong heterogeneities. They will also contain an approach to quantify the uncertainties that emerge from the non-classical homogenization.

The second deliverable will consist of a series of impact studies on relevant application problems, which will become a powerful demonstration platform for our innovative methods in theoretical and computational transport. At a minimum, we will pursue: (1) transport physics in certain nuclear reactor cores, (2) solar radiative transfer in atmospheric clouds, and (3) computational graphics. We will provide a set of results and corresponding analysis from these impact studies using realistic problems; these will be the first examples of the impact that this new approach can have by incorporating non-classical transport characteristics.

These two deliverables will include an informative and robust test suite and version control of the source code as part of a transparent development process. Furthermore, we will focus in identifying how the improvements obtained with this new methodology will impact exascale-resolution problems.

6 Team Capabilities and Experience

This research is accomplishable because of the technical quality of the proposed work and the deep experience and strong capability of the applicant team. Our project team is strongly interdisciplinary, formed by experts in the different areas of the proposed scope:

- Slaybaugh is an Assistant Professor of Nuclear Engineering at UC Berkeley, with experience in deterministic and Monte Carlo radiation transport codes, high-quality software development, and

supercomputing. Her research program is based in computational methods applied to existing and advanced nuclear reactors, nuclear non-proliferation and security, and shielding applications.

- Vasques is a Project Scientist at UC Berkeley, with experience in mathematical and computational modeling of transport and diffusion processes, homogenization methods, variance reduction techniques, and stochastic processes. His main area of research is based on modeling transport processes in stochastic mixtures, focusing on non-classical particle transport.

- Davis is a Caltech Research Scientist working for NASA’s Jet Propulsion Laboratory. He is a leading expert in 3D radiative transfer (RT) in atmospheric clouds and cloud fields, covering theoretical, computational and observational aspects. His current interests are in the application of the “generalized” RT model to practical problems posed by unresolved fine-scale spatial and spectral variabilities. In parallel, he is involved in collaborative efforts in 3D cloud reconstruction based on multi-angle/multi-pixel data, efficient numerical 3D RT modeling and recent advances in inverse problem theory.

- Wrenninge is a film industry veteran working on synthetic imagery for training and testing of neural networks at Zoox, a Menlo Park start-up developing Level 4 autonomous vehicles. He is an expert in computer graphics for film and photorealistic image production, with a specialization in rendering of participating media. Before joining Zoox, he was a Principal Engineer at Pixar Animation Studios, where he focused on Monte Carlo-based methods for multiple scattering solutions in highly detailed heterogeneous media.

- Frank is a Professor for Computational Nuclear Engineering at RWTH Aachen University, Germany. He leads a group of two postdoctoral researchers and eight Ph.D. students. His research focuses on radiation transport, at the interface of analysis, numerical methods, and related inverse problems. Furthermore, the group is involved in several application-oriented projects with engineering groups and companies.

7 Timeline and Responsibilities

The PI will be responsible for

- Mentoring and directing the graduate students conducting research
- Ensuring good coding practices
- Helping students identify information and venues for presentation and publication of results
- Meeting all requirements for reports and deliverables to the sponsor
- Managing and administering awarded funds, assisted by the PI’s institution

The co-Investigators and collaborators will be responsible for

- Providing support and input throughout the project
- Contributing their time and expertise to specific tasks as applicable
- Providing additional student guidance and mentorship as applicable

The following is the project's timeline, identifying the major activities and indicating the responsible personnel:

- *Year 1*
 - Numerically determine $p(s)$: Vasques, Wrenninge
 - Begin quantifying uncertainty associated with $p(s)$: Frank, Vasques
 - Choose the transport solver: Davis, Slaybaugh, Vasques
 - Begin method implementation: Slaybaugh, Vasques
 - Begin identifying impact problem set: Davis, Slaybaugh, Wrenninge
- *Year 2*
 - Continue quantifying uncertainty associated with $p(s)$: Frank, Vasques
 - Complete method implementation, conduct associated validation: Slaybaugh, Vasques
 - Finish identifying impact problem set: Davis, Slaybaugh, Wrenninge
 - Begin extending the method to multiscale: Slaybaugh, Vasques, Wrenninge
- *Year 3*
 - Complete quantifying uncertainty associated with $p(s)$: Frank, Vasques
 - Complete extending the method to multiscale: All
 - Conduct impact tests: Davis, Slaybaugh, Vasques

— **APPENDIX 1** —
BIOGRAPHICAL SKETCH

RACHEL N. SLAYBAUGH

slaybaugh@berkeley.edu ◊ (570) · 850 · 3385

Department of Nuclear Engineering ◊ University of California, Berkeley
4173 Etcheverry Hall MC 1730 ◊ Berkeley, CA 94720

EDUCATION

Ph.D.	University of Wisconsin–Madison Nuclear Engineering and Engineering Physics, with a certificate in Energy Analysis and Policy	2011
M.S.	University of Wisconsin–Madison Nuclear Engineering and Engineering Physics	2008
B.S.	Pennsylvania State University Nuclear Engineering	2006

RESEARCH EXPERIENCE

University of California, Berkeley <i>Assistant Professor of Nuclear Engineering</i>	Jan. 2014 - Present <i>Berkeley, CA</i>
<ul style="list-style-type: none">• Researching numerical methods for neutral particle transport with an emphasis on supercomputing and advanced architectures; specialization in deterministic, Monte Carlo, and Hybrid methods• Applications in reactor design, shielding, and nuclear security and nonproliferation• Design Emphasis in Computational Science and Engineering Affiliated Faculty member	
Bettis Laboratory <i>Senior Engineer in the Shield Design and Development group</i>	Mar. 2012 - Aug. 2014 <i>West Mifflin, PA</i>
<ul style="list-style-type: none">• Implemented the Forward-Weighted Consistent Adjoint Driven Importance Sampling (FW-CADIS) method for variance reduction in Monte Carlo; accredited method for use in shield design• Developed new Resonance Factor variance reduction method for streaming through materials with space and energy self-shielding	
University of Wisconsin–Madison <i>Research Assistant / Rickover Fellow</i>	Sept. 2006 - Nov. 2011 <i>Madison, WI</i>
<ul style="list-style-type: none">• Researched Acceleration Methods for Massively Parallel Deterministic Transport: added parallelization in the energy domain, an advanced eigenvalue solver, and a new multigrid in energy preconditioner to Denovo, developed at Oak Ridge National Lab• Developed two Monte Carlo source sampling methods for arbitrarily shaped plasma sources; the sources are generated directly from plasma physics data	
Forschungszentrum Karlsruhe (KIT) <i>Visiting Researcher</i>	May 2008 - Dec. 2008 <i>Karlsruhe, Germany</i>
<ul style="list-style-type: none">• Learned about the Rigorous 2 Step method for Monte Carlo geometry conversion while working in the Reactor Safety group• Helped group incorporate DAGMC library into MCNP workflow	

SELECTED PUBLICATIONS

- R. Vasques and K. Krycki and R. N. Slaybaugh. “Nonclassical Particle Transport in 1-D Random Periodic Media,” *Nuclear Science and Engineering*. (accepted 2016)

- M. Munk, R.N. Slaybaugh, “An Angle-Informed Hybrid Method for CADIS and FW-CADIS.” Proceedings of the PHYSOR 2016 Meeting in Sun Valley, ID, May 2016. (accepted)
- J. Bevins, R. Slaybaugh, “Application of Metaheuristic Optimization Methods for Neutron Spectral Shaping Applications.” Proceedings of the Conference on Data Analysis 2016 in Santa Fe, NM, March 2016. (accepted)
- L. Bernstein, D. Brown, et al. “Nuclear Data Needs and Capabilities for Applications.” White Paper. Lawrence Berkeley National Laboratory, May 27-29 2015.
- R.N. Slaybaugh, T.M. Evans, G.G. Davidson, and P.P.H. Wilson, “Rayleigh Quotient Iteration with a Multigrid in Energy Preconditioner for Massively Parallel Neutron Transport,” Proceedings of Joint International Conference on Mathematics and Computation, Supercomputing in Nuclear Applications, and the Monte Carlo Method in Nashville, TN, April 2015.
- S.C. Wilson and R.N. Slaybaugh. “Improved Monte Carlo Variance Reduction for Space and Energy Self-Shielding,” *Nuclear Science and Engineering*. **179** (2015) 22-41.
- R.N. Slaybaugh, T.M. Evans, G.G. Davidson, and P.P.H. Wilson. “Multigrid in energy preconditioner for Krylov solvers,” *Journal of Computational Physics*. **242** (2013) 405-419.
- R.N. Slaybaugh, T.M. Evans, G.G. Davidson, and P.P.H. Wilson. “Rayleigh Quotient Iteration in 3D, Deterministic Neutron Transport,” Proceedings of the PHYSOR 2012 Meeting in Knoxville, TN, April 2012.
- T.M. Evans, A.S. Stafford, R.N. Slaybaugh, and K.T. Clarno. “Denovo—A new three-dimensional parallel discrete ordinates code in SCALE.” *Nuc. Tech.* **171** (2010) 171-200.
- R.N. Slaybaugh, P.P.H. Wilson, L.A. El-Guebaly, and E.P. Marriott. “Three-Dimensional Neutron Source Models for Toroidal Fusion Energy Systems.” *Fusion Engineering and Design*. **84** (2009) 1774-1778.

SYNERGISTIC ACTIVITIES

Nuclear Energy Advisory Committee	U.S. Secretary of Energy appointed 2016
Berkeley Institute for Data Science	Senior Fellow
The Hacker Within, UCB and UW	Faculty Advisor 2014-present; Founding member 2009
American Nuclear Society Math and Comp. Division,	Chair rotation 2016-present
Society of Industrial and Applied Mathematics (SIAM)	member since 2009

CONFLICT OF INTEREST

Collaborators	· Bates, C. (<i>LANL</i>)	· Bergmann, R. (<i>PSI</i>)
and Co-editors	· Bernstein, L. (<i>LLNL</i>)	· Biondo, E. (<i>Univ. Wisc.</i>)
· Brown, D. (<i>BNL</i>)	· Davidson, G. (<i>ORNL</i>)	· Dunlop, W. (<i>LLNL</i>)
· Evans, T. (<i>ORNL</i>)	· Fratoni, M. (<i>UCB</i>)	· Gidden, M. (<i>IIASA</i>)
· Hamilton, S. (<i>ORNL</i>)	· Henry, E. (<i>LLNL</i>)	· Hosemann, P. (<i>UCB</i>)
· Huff, K. (<i>UIUC</i>)	· Jarrell, J. (<i>ORNL</i>)	· Krykci, K. (<i>AINT, Germany</i>)
· Morgan, L. (<i>USGS</i>)	· Mosher, S. (<i>ORNL</i>)	· Pandya, T. (<i>ORNL</i>)
· Peplow, D. (<i>ORNL</i>)	· Radnović, N. (<i>UCB</i>)	· Scpoatz, A. (<i>U South Car.</i>)
· Vujić, J. (<i>UC Berkeley</i>)	· Wilson, P. (<i>Univ. Wisc.</i>)	· Wilson, S. (<i>ORNL</i>)
Graduate and	· Bevins, J. (<i>UC Berkeley</i>)	· Boado, E. (<i>UC Berkeley</i>)
Postdoctoral	· Munk, M. (<i>UC Berkeley</i>)	· Negus, M. (<i>UC Berkeley</i>)
Advisors(ees)	· Ortega, M. (<i>UC Berkeley</i>)	· Rehak, J. (<i>UC Berkeley</i>)
· Rowland, K. (<i>UC Berkeley</i>)	· Schunert, S. (<i>INL</i>)	· Zweiger, M. (<i>UC Berkeley</i>)

RICHARD VASQUES

rvasques@berkeley.edu \diamond (510) \cdot 340 \cdot 0930

Department of Nuclear Engineering \diamond University of California, Berkeley
4103 Etcheverry Hall MC 1730 \diamond Berkeley, CA 94720

EDUCATION

Ph.D.	University of Michigan–Ann Arbor Applied & Interdisciplinary Mathematics Partner Discipline: Nuclear Engineering & Radiological Sciences	2009
M.S.	Federal Univ. of Rio Grande do Sul (UFRGS)–Porto Alegre, Brazil Applied Mathematics	2005
B.S.	Federal Univ. of Rio Grande do Sul (UFRGS)–Porto Alegre, Brazil Applied & Computational Mathematics	2002

RESEARCH EXPERIENCE

University of California, Berkeley <i>Assistant Project Scientist</i>	Jun. 2015 - Present <i>Berkeley, CA</i>
<ul style="list-style-type: none">• Mathematical and computational modeling of transport and diffusion processes• Focus in non-classical transport, random mixtures, generalized diffusion, and angle-informed variance reduction techniques	
Federal Univ. of Rio Grande do Sul (UFRGS) <i>Research Fellow</i>	Jul. 2014 - May 2015 <i>Porto Alegre, Brazil</i>
<ul style="list-style-type: none">• Developed a semi-analytical representation of a nonstiff solution for the point kinetics equations with stochastic fluctuations• Demonstrated the accuracy of the non-classical Boltzmann equation in model 1-D systems, and proved that diffusion-based approximations to the Boltzmann equation can be exactly represented by the non-classical transport equation	
RWTH Aachen University <i>Research Assistant–Computational Nuclear Engineering Group</i>	Aug. 2012 - Jul. 2014 <i>Aachen, Germany</i>
<ul style="list-style-type: none">• Developed image reconstruction algorithms to correct diverging beams for a compact neutron radiography system for radioactive waste analysis• Generalized the non-classical transport theory to include angular-dependent path-length distributions, with applications in Pebble Bed reactors	
EAESP–Fundação Getulio Vargas <i>Assistant Professor of Mathematics</i>	Mar. 2011 - Jul. 2012 <i>São Paulo, Brazil</i>
<ul style="list-style-type: none">• Projects related to business strategy	
McKinsey & Company <i>Associate Consultant</i>	Oct. 2009 - Feb. 2011 <i>São Paulo, Brazil</i>
<ul style="list-style-type: none">• Several projects in Energy Distribution and business strategy	

SELECTED PUBLICATIONS

- R. Vasques, K. Krycki, R.N. Slaybaugh. “Nonclassical particle transport in 1-D random periodic media.” To appear in *Nuclear Science and Engineering* **184** (2016).
arxiv:1602.00825 [nucl-th]

MAGNUS WRENNINGE

magnus.wrenninge@gmail.com ♦ (310) · 795 · 3772

Zoox, Inc.

2180 Sand Hill Rd. ♦ Menlo Park, CA 94025

EDUCATION

MS (Eng)	Linköping University, Sweden	2003
	Media Technology and Advanced Computer Graphics	

RESEARCH EXPERIENCE

Zoox, Inc.	May. 2016 - Present
<i>Rendering Architect</i>	<i>Menlo Park, CA</i>

- Research and development of rendering strategies for testing and training of neural networks
- Focus on rendering realism and architecture

Pixar Animation Studios	Mar. 2013 - May. 2016
<i>Principal Engineer</i>	<i>Emeryville, CA</i>

- Research and development of novel Monte Carlo-based rendering techniques for participating media in film production
- Focus on rendering of heterogeneous media, algorithms for multiple scattering and continuously-varying data sets

Sony Picture Imageworks	May. 2005 - Mar. 2013
<i>Lead Technical Director & Sr. Software Engineer</i>	<i>Culver City, CA</i>

- Research and development of construction and rendering techniques for participating media
- Focus on deployment of software for film production

Digital Domain	Jun. 2003 - May. 2005
<i>Sr. Software Engineer</i>	<i>Venice, CA</i>

- Research and development of rendering techniques for large synthetic environments
- Focus on deployment of software for film production

RELATED FILM EXPERIENCE

The Good Dinosaur	2015
<i>Volumetric Clouds Architect</i>	<i>Director: Peter Sohn</i>

- Developed and implemented Monte Carlo-based image rendering software for clouds, incorporating multi-path photon paths

Oz: The Great and Powerful	2013
<i>Lead Technical Director</i>	<i>Director: Sam Raimi</i>

- Led team of 20 engineers and artists in simulation efforts, with focus on simulation and rendering of participating media

Alice in Wonderland	2011
<i>Technical Director</i>	<i>Director: Tim Burton</i>

- Developed and implemented FLIP (fluid/implicit particle) method for tracking of highly detailed heterogeneous media

SELECTED PUBLICATIONS

- M. Webb, M. Wrenninge, J. Rempel, C. Harrington. “Making a Dinosaur Seem Small: Cloudscapes in The Good Dinosaur.” *SIGGRAPH Talks* (2016).
- M. Wrenninge, M. Rice. “Volume Modeling Techniques in The Good Dinosaur.” *SIGGRAPH Talks* (2016).
- M. Wrenninge “Efficient Rendering of Volumetric Motion Blur.” *Journal of Computer Graphics Tools* **Vol 5, No 1**: 1-34 (2016).
- M. Wrenninge “Art-Directable Multiple Volumetric Scattering.” *SIGGRAPH Talks* (2015).
- M. Wrenninge “Production Volume Rendering: Design and Implementation.” *CRC Press* (2012).
- M. Wrenninge, H. Fält, C. Allen, S. Marshall. “Capturing Thin Features in Smoke Simulations.” *SIGGRAPH Talks* (2011).
- M. Wrenninge, N. Bin Zafar “Production Volume Rendering: Fundamentals.” *SIGGRAPH Courses* (2011).
- M. Wrenninge, N. Bin Zafar, A. Bouthors, J. Tessendorf, V. Grant, A. Clinton, O. Harding, G. Graham “Production Volume Rendering: Systems.” *SIGGRAPH Courses* (2011).
- M. Wrenninge, N. Bin Zafar, J. Clifford, G. Graham, D. Penney, J. Kontkanen, J. Tessendorf, A. Clinton “Volumetric Methods in Visual Effects.” *SIGGRAPH Courses* (2010).

AWARDS

- | | |
|--|------|
| Technical Achievement Award: Field3D | 2015 |
| • Academy of Motion Picture Arts and Sciences | |
| Outstanding Achievement, Animated Effects · The Good Dinosaur | 2015 |
| • Annie Awards | |
| Outstanding Effects Simulations · The Good Dinosaur | 2015 |
| • Visual Effects Society | |

SYNERGISTIC ACTIVITIES

- | | | |
|-------------------------------|---|-----------------------------|
| Refereeing | · Academy of Motion Picture Arts and Sciences | |
| | · Digital Imaging Technology sub-committee | |
| | · SIGGRAPH Papers | |
| Professional Societies | · Visual Effects Society (VES) | <i>Member, 2007-Present</i> |
| | · ACM SIGGRAPH | <i>Member, 2003-Present</i> |

CONFLICT OF INTEREST

- Collaborators** · Unger, J. (*Linköping U., Sweden*) · Kronander, J. (*Linköping U., Sweden*)

MARTIN FRANK

frank@mathcces.rwth-aachen.de ♦ +49 241 80 98661
Department of Mathematics ♦ RWTH Aachen University
Schinkelstrasse 2 ♦ 52062 Aachen, Germany

EDUCATION

Ph.D.	TU Kaiserslautern, Germany	2005
	Mathematics	
Diploma	TU Darmstadt, Germany	2004
	Physics	
Diploma	TU Darmstadt, Germany	2001
	Mathematics	

RESEARCH EXPERIENCE

RWTH Aachen University	Oct. 2009 - Present
<i>Professor</i>	<i>Aachen, Germany</i>
<ul style="list-style-type: none">• Numerical methods for neutral and charged particle transport with emphasis on numerical analysis, inverse problems and sensitivity analysis• Foundations of radiation transport modeling, including non-classical transport and fractional diffusion limits• Applications in radiotherapy treatment planning, radioactive waste analysis and atmospheric sciences	
University Bordeaux, France	May 2013
<i>Visiting professor</i>	<i>Bordeaux, France</i>
<ul style="list-style-type: none">• Collaboration with CELIA (Centre Lasers Intenses et Applications) in plasma modeling	
TU Kaiserslautern, Germany	Oct. 2008 - Sep. 2009
<i>Assistant Professor</i>	<i>Kaiserslautern, Germany</i>
<ul style="list-style-type: none">• Investigated simulation and optimization methods for radiotherapy treatment planning	
TU Kaiserlautern	May 2005 - Sep. 2008
<i>Research Assistant</i>	<i>Kaiserslautern, Germany</i>
<ul style="list-style-type: none">• Developed models and numerical methods for radiation transport in industrial processes	

SELECTED PUBLICATIONS

- B. Seibold and M. Frank, *StaRMAP - A second order staggered grid method for spherical harmonics moment equations of radiative transfer*, ACM Trans. Math. Softw. 41 (2014).
- E. Olbrant, C. D. Hauck, and M. Frank, *A Realizability-Preserving Discontinuous Galerkin Method for the M1 Model of Radiative Transfer*, J. Comput. Phys. 231 (2012), 5612–5639.
- M. Schäfer, M. Frank, and C. D. Levermore, *Diffusive Corrections to Pn approximations*, Multiscale Model. Simul. 9 (2011), 1–28.
- M. Frank, M. Herty, and M. Schäfer, *Optimal treatment planning in radiotherapy based on Boltzmann transport equations*, Math. Mod. Meth. Appl. Sci. 18 (2008), 573–592.
- M. Frank, A. Klar, E. W. Larsen, and S. Yasuda, *Time-dependent Simplified Pn Approximation to the Equations of Radiative Transfer*, J. Comput. Phys. 226 (2007), 2289–2305.

- M. Frank, B. Dubroca, and A. Klar, *Partial Moment Entropy Approximation to Radiative Heat Transfer*, J. Comput. Phys. 218 (2006), 1–18.
- R. Turpault, M. Frank, B. Dubroca, and A. Klar, *Multigroup half space moment approximations to the radiative heat transfer equations*, J. Comput. Phys. 198 (2004), 363–371.
- M. Seaïd, M. Frank, A. Klar, R. Pinnau, and G. Thömmes, *Efficient numerical methods for radiation in gas turbines*, J. Comput. Appl. Math. 170 (2004), 217–239.

SYNERGISTIC ACTIVITIES

Co-organizer of international conference International Conference on Hyperbolic Problems

Co-organizer of international conference Numerical Methods for Hyperbolic Equations with Source Terms and Applications

Founder and organizer of CAMMP Education Lab at RWTH Aachen University (Computational and Mathematical Modeling Program, cammp.rwth-aachen.de): projects and modeling weeks with high school students

Referee e.g. for DFG, Journal of Computational Physics, Numerical Methods for Partial Differential Equations, SIAM Journal of Scientific Computing, SIAM Journal of Applied Mathematics

CONFLICT OF INTEREST

Collaborators and Co-editors	· Barnard, R.C. (<i>ORNL</i>)	· Berthon, C. (<i>Nantes</i>)
	· Hauck, C.D. (<i>ORNL</i>)	· Herty, M. (<i>RWTH</i>)
	· Hinze, M. (<i>Hamburg</i>)	· Jin, S. (<i>Wisconsin</i>)
	· Larsen, E.W. (<i>Michigan</i>)	· Levermore, C.D. (<i>Maryland</i>)
	· Pinnau, R. (<i>Kaiserslautern</i>)	· Seibold, B. (<i>Temple</i>)
	· Sun, W. (<i>Simon Fraser</i>)	· Tervo, J. (<i>Kuopio</i>)
	· Turpault, R. (<i>Bordeaux</i>)	
Graduate and Postdoctoral Advisors(ees)	· Klar, A. (<i>TU Kaiserslautern</i>)	· Dubroca, B. (<i>Uni. Bordeaux</i>)
	· Krycki, K. (<i>AiNT, Germany</i>)	· Monreal, P. (<i>Trivago, Germany</i>)
	· Olbrant, E. (<i>Bosch, Germany</i>)	

— **APPENDIX 2** —
CURRENT AND PENDING SUPPORT

CURRENT & PENDING SUPPORT

Rachel Slaybaugh

Current

Principal Investigator

Project Title: University of California, Berkeley Department of Nuclear Engineering Graduate Fellowship Program

Source of Support: Nuclear Regulatory Commission

Total Award Amount: \$400,000

Total Period Covered: 08/01/14 – 07/31/18

Location of Project: University of California at Berkeley

Person-Months Per Year Committed to the Project: Cal: 0.00 Acad: 0.00 Sumr: 0.00

Principal Investigator

Project Title: Improved Hybrid Modeling of Used Fuel Storage Facilities

Source of Support: DOE

Total Award Amount: \$525,393

Total Period Covered: 01/01/15 to 12/31/17

Location of Project: University of California at Berkeley

Person-Months Per Year Committed to the Project: Cal: 0.00 Acad: 0.00 Sumr: 1.00

Principal Investigator

Project Title: MOOSE Application Collaboration Specifically Pronghorn and RELAP-7

Source of Support: Idaho National Laboratory

Total Award Amount: \$12,000

Total Period Covered: 01/27/16 to 09/30/17

Location of Project: University of California at Berkeley

Person-Months Per Year Committed to the Project: Cal: 0.00 Acad: 0.00 Sumr: 0.50

Co-Principal Investigator

Project Title: Nuclear Engineer Scholarships at the University of California, Berkeley to Support the Expansion and Diversity of the Undergraduate Program

Source of Support: NRC

Total Award Amount: \$200,000

Total Period Covered: 07/01/16 to 06/30/18

Location of Project: University of California at Berkeley

Person-Months Per Year Committed to the Project: Cal: 0.00 Acad: 0.00 Sumr: 0.00

Co-Principal Investigator

Project Title: Training the Next Generation of Nuclear Engineers: Graduate Fellowships at the University of California, Berkeley

Source of Support: NRC

Total Award Amount: \$400,000

Total Period Covered: 07/01/16 to 06/30/20

Location of Project: University of California at Berkeley

Person-Months Per Year Committed to the Project: Cal: 0.00 Acad: 0.00 Sumr: 0.00

Pending

Principal Investigator

Project Title: Nonclassical Transport Theory With Multiscale Path Distributions In Realworld Applications *[This Proposal]*

Source of Support: DOE

Total Award Amount: \$800,000

Total Period Covered: 01/01/17 to 12/31/19

Location of Project: University of California at Berkeley

Person-Months Per Year Committed to the Project: Cal: 0.00 Acad: 0.00 Sumr: 1.00

CURRENT & PENDING SUPPORT

Richard Vasques

Current

N/A

Pending

N/A

CURRENT & PENDING SUPPORT

Magnus Wrenninge

Current

N/A

Pending

N/A

CURRENT & PENDING SUPPORT

Martin Frank

Current

N/A

Pending

N/A

APPENDIX 3 – BIBLIOGRAPHY & REFERENCES CITED

- [1] E.W. Larsen and R. Vasques. “A generalized linear Boltzmann equation for non-classical particle transport.” *Journal of Quantitative Spectroscopy & Radiative Transfer* **112**: 619–631 (2011).
- [2] A.B. Davis and F. Xu. “A generalized linear transport model for spatially correlated stochastic media.” *Journal of Computational and Theoretical Transport* **43**: 474–514 (2014).
- [3] R. Vasques and E.W. Larsen. “Non-classical particle transport with angular-dependent path-length distributions. I: Theory.” *Annals of Nuclear Energy* **70**: 292–300 (2014).
- [4] F. Xu., A.B. Davis, and D.J. Diner. “Markov chain formalism for generalized radiative transfer in a plane-parallel medium, accounting for polarization.” *Journal of Quantitative Spectroscopy & Radiative Transfer* **184**: 14–26 (2016).
- [5] M. Fratoni and E. Greenspan. “Neutronic feasibility assessment of liquid salt-cooled pebble bed reactors.” *Nuclear Science and Engineering* **168**: 1–22 (2011).
- [6] R. Vasques and E.W. Larsen. “Non-classical particle transport with angular-dependent path-length distributions. II: Application to pebble bed reactor cores.” *Annals of Nuclear Energy* **70**: 301–311 (2014).
- [7] Y. Yue, K. Iwasaki, B-Y. Chen, Y. Dobashi, and T. Nishita. “Unbiased, adaptive stochastic sampling for rendering inhomogeneous participating media.” *ACM Transactions on Graphics* **29**: #177 (2010).
- [8] E. d’Eon. “Rigorous asymptotic and moment-preserving diffusion approximations for generalized linear Boltzmann transport in arbitrary dimension.” *Transport Theory and Statistical Physics* **42**: 237–297 (2014).
- [9] L. Dumas and F. Golse. “Homogenization of transport equations.” *SIAM Journal on Applied Mathematics* **60**: 1447–1470 (2000).
- [10] B. Cairns, A.A. Lacis, and B.E. Carlson. “Absorption within inhomogeneous clouds and its parameterization in general circulation models.” *Journal of the Atmospheric Sciences* **57**: 700–714 (2000).
- [11] R. Vasques. “Estimating anisotropic diffusion of neutrons near the boundary of a pebble bed random system.” *International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering*, May 5–9, Sun Valley, ID, U.S.A. (2013).
- [12] A. Koster, H.D. Matzner, and D.R. Nicholsi. “PBMR Design for the Future.” *Nuclear Engineering and Design* **222**: 231–245 (2003).

- [13] Z. Zhang, Z. Wu, Y. Sun, and F. Li. “Design aspects of the Chinese modular high-temperature gas-cooled reactor HTR-PM.” *Nuclear Engineering and Design* **236**: 485–490 (2006).
- [14] A.C. Kadak. “MIT Pebble-Bed Reactor Project.” *Nuclear Engineering and Technology* **39**: 95–102 (2007).
- [15] IPCC, 2013: Summary for Policymakers. In: *Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change*; T.F. Stocker et al. (eds.). Cambridge University Press, Cambridge, United Kingdom and New York, NY, U.S.A. (2013).
- [16] J. Dongarra et al. “Applied Mathematics Research for Exascale Computing.” *Lawrence Livermore National Laboratory*, **LLNL-TR-651000** (2014).
<http://science.energy.gov/media/ascr/pdf/research/am/docs/EMWGREport.pdf>
- [17] M. Frank and T. Goudon. “On a generalized Boltzmann equation for non-classical particle transport.” *Kinetic and Related Models* **3**: 395–407 (2010).
- [18] F. Golse. “Recent results on the periodic Lorentz gas.” In: *Nonlinear Partial Differential Equations*; X. Cabré and J. Soler (eds.), pp. 39–99. Springer Basel, New York, NY (2012).
- [19] J. Marklof and A. Strömbergsson. “The Boltzmann-Grad limit of the periodic Lorentz gas.” *Annals of Mathematics* **174**: 225–298 (2011).
- [20] J. Marklof and A. Strömbergsson. “Generalized linear Boltzmann equations for particle-transport in polycrystals.” *Applied Mathematics Research eXpress* **2**: 274–295 (2015).
- [21] M. Frank, K. Krycki, E.W. Larsen, and R. Vasques. “The nonclassical Boltzmann equation, and diffusion-based approximations to the Boltzmann equation.” *SIAM Journal on Applied Mathematics* **75**: 1329–1345 (2015).
- [22] R. Vasques. “The nonclassical diffusion approximation to the nonclassical linear Boltzmann equation.” *Applied Mathematics Letters* **53**: 63–68 (2016).
- [23] M. Frank and W. Sun. “Fractional diffusion limits of non-classical transport equations.” (2016).
arXiv:1607.04028 [math.AP]
- [24] A. Davis and A. Marshak. “Lévy kinetics in slab geometry: Scaling of transmission probability.” In: *Fractal Frontiers*; M.M. Novak and T.G. Dewey (eds.). World Scientific, Singapore, pp. 63–72 (1997).
- [25] T. Scholl, K. Pfeilsticker, A.B. Davis, H. Klein Baltink, S. Crewell, U. Löhnert, C. Simmer, J. Meywerk, and M. Quante. “Path length distributions for solar photons under cloudy skies: Comparison of measured first and second moments with predictions from classical

- and anomalous diffusion theories.” *Journal of Geophysical Research* **111**: D12211–12226 (2006).
- [26] R. Vasques, K. Krycki, and R.N. Slaybaugh. “Nonclassical particle transport in 1-D random periodic media.” To appear in *Nuclear Science and Engineering* **184** (2016).
arxiv:1602.00825 [nucl-th]
- [27] R. Vasques, R.N. Slaybaugh, and K. Krycki. “Nonclassical particle transport in the 1-D diffusive limit.” *Transactions of the American Nuclear Society* **114**: 361–364 (2016).
- [28] R. Barnard, M. Frank, and K. Krycki. “Sensitivity analysis for dose deposition in radiotherapy via a Fokker-Planck model.” *Mathematical Medicine and Biology*, DOI:10.1093/imammb/dqv039 (2016).
- [29] D. G. Cacuci. *Sensitivity & Uncertainty Analysis, Volume 1: Theory*. London: Chapman & Hall (2003).

APPENDIX 4 – FACILITIES & OTHER RESOURCES

The proposed project will take advantage of the condo-model Savio computing cluster available at Berkeley (<http://research-it.berkeley.edu/services/high-performance-computing>). The Berkeley personnel in this proposal have 24 nodes, each consisting of Dual Ivybridge E5-2670v2 2.5Ghz 10-core processors (480 total cores), 64GB 1866 Mhz Memory, FDR Infiniband HCA, on this machine. They also have the ability to access the full machine, which has 331 compute nodes. These computing resources will facilitate the fast simulations required for this project. These resources will be available throughout the duration of this project and will be adequate for the computing to be conducted in this project.

APPENDIX 5 – EQUIPMENT

No equipment beyond the facilities listed in the **Appendix 4** (Facilities & Other Resources) is required.

APPENDIX 6 – DATA MANAGEMENT PLAN

Data types and sources

There are a few steps in our work:

1. method investigation and development
2. larger-scale method implementation
3. impact measurement

We will make all data generated in steps 1 and 2 publicly available by hosting our developed software, test suite, and problem sets on a public GitHub repository. Given the nature of the work, this is the easiest and least expensive way to not only share tools between collaborators at differing institutions, but also to make our work transparent and accessible to the wider community.

Part 3 may require using software or problem specifications that are not all publicly available because of export control issues (e.g. use of nuclear-specific software and reactor specifications). We will endeavor to use tools that are as open as possible. In the cases where software or materials must remain closed to at least some communities, we will manage our work in a private repository. We will make published data sets available on the public repository (see discussion of publications below). We will also make materials available to anyone who does have appropriate licenses.

We will post the preprints of all publications from this work on arXiv. Included in our publications will be a link to the portion of our repository containing (excepting the applicable limitations above) all of the data used to generate each plot, scripts to generate plots, and input files used to generate the data. We will also include a link to the software we used. With this information, it should be possible to reproduce the results in the paper. We will note versions of items used (e.g. Python 2.7.12 and repository commit index for our software) to facilitate reproducibility.

Content and format

In our software development we will use Doxygen-style code comments such that documentation can be easily generated.

Sharing and preservation To facilitate the accessibility of our work, we will do all investigatory development in Python and make our small problems available as Jupyter notebooks. We will make as much of our larger scale studies available as Jupyter notebooks as well. Hosting these on GitHub will facilitate accessibility and transparency. All software we use will be free.

Protection

As noted, we will refrain from publicly posting proprietary or export controlled information—we will only post relevant data that are publishable. We will not generate personally identifiable

information through this work. All of our work will be hosted with appropriate license information, as designated by our home institutions.

Rationale

Our plan is intended to serve several goals:

1. transparency of science: to the largest extent possible the data we publish in papers, along with the software and input files will be available so that anyone can check our work.
2. reproducibility: we will also include software version numbers, commit tags, and data processing/plotting scripts so that we or someone else can reproduce the work.
3. larger impact: by making our work publicly available anyone will be able to pick up our work and use it themselves, or build upon it to further knowledge or build ever more useful computational tools.

Software & Codes

The Open Source License to be used, if applicable: we will use the Creative Commons Attribution license for text documents and the MIT license for software. If executable versions of the software will also be released, and if so what format will be used: most development work will be in Python, which does not require an executable. We will not be able to generally distribute the application-specific software we will modify. In those cases the host institutions will distribute accepted code modifications through their own software release processes.

How software can be found and accessed and the length of time the software will be publicly available: as noted, we will link to repositories in our papers and that information will be available for as long as GitHub exists. If the data appears to be imperiled for some reason, we will move it and update the arXiv preprint with the new information.

How any proprietary 3rd party software or libraries are used in the creation of this software: we will use third party Python libraries such as NumPy and SciPy. We may also modify application-specific software with our new methods. For nuclear engineering, we will likely modify neutron transport software associated with the MOOSE project at Idaho National Laboratory. For atmospheric transport, JPL will modify either internal codes. For image rendering, Zoxx, Inc. will modify their internal software.