—— 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**

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

# 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 computer 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 safety and efficiency 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 RF*[1] *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.

[1] Well-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 $\Sigma_t$ 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.

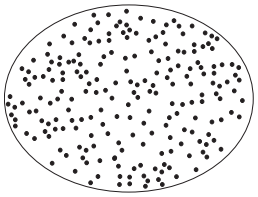

Figure 1: Sketch of a volume region containing Poisson-distributed scattering centers.

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

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

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 backround "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

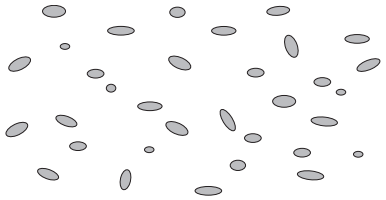

Figure 2: Heterogeneous random system formed by many volumes suspended in a void.

piled on top of one another in a random manner. Further, 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 $\Sigma_t$ 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 to this type of transport process as *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. The homogenization approach therefore leads to unreliable estimates of the particle flux in these applications because important physical quantities are 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

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

where $\psi$ 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

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

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

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

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]

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

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 modeling 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.

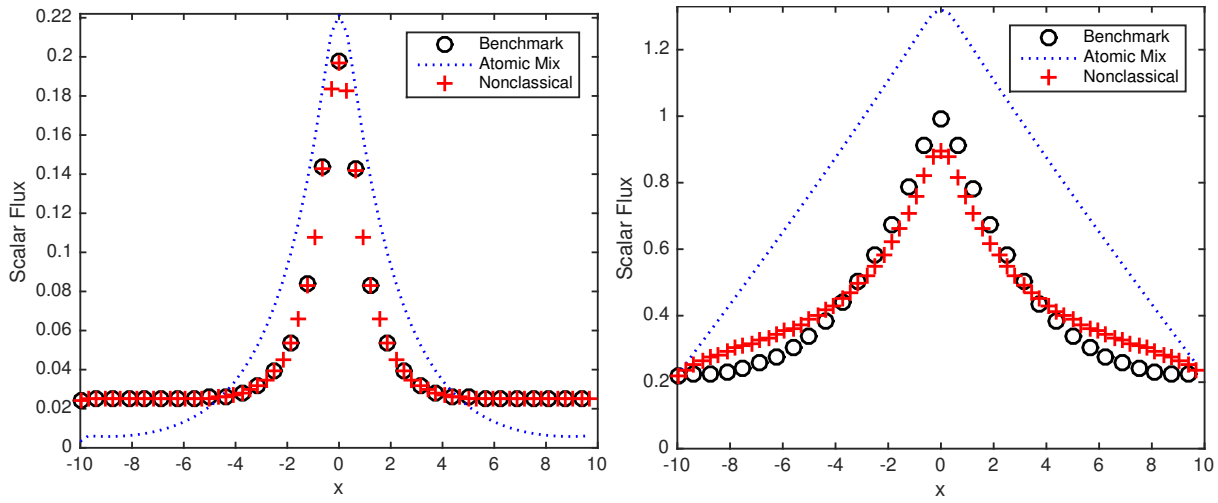


Figure 3: Ensemble-averaged scalar fluxes in a 1D random periodic system with parameters as defined in [26]. The scattering ratio $c$ of the solid material is defined as 0 (**left**) and 0.99 (**right**).

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 $p_a(s) = \langle\Sigma_t\rangle / \left(1 + \langle\Sigma_t\rangle s/a\right)^{1+a}$, 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 $\infty$ 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.

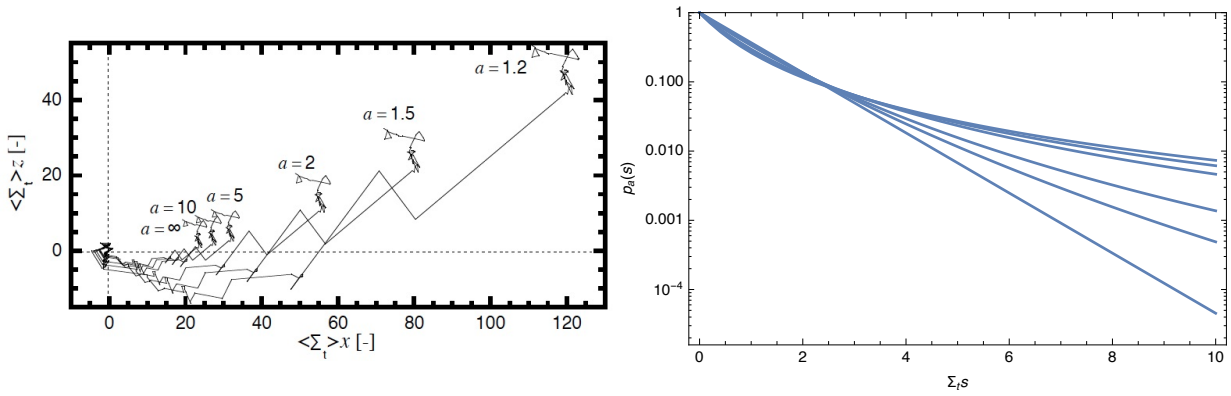


Figure 4: **Left**: 2D unbounded random walks of 100 steps each, all starting in the same direction at the origin of the axes, by isotropically scattered particles following $p_a(s)$ with the choices of $a$ called out in the text. **Right**: Log plots of $p(s)$ for the traces plotted in the left panel.

# 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 this, we will build upon the results presented in the last section– expanding and improving the mathematical and computational aspects of the non-classical theory. Moreover, the interdisciplinary scope of the project, combined with the different areas of expertise of the team, will create perfect conditions to perform cutting-edge research, fostering ideas and driving innovation.

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 will 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 method 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 it becomes clear early in this process that one of the models strongly outperforms the other, we shall pick that method without completing 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 a 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 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 having a 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 approaches other 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) computer 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 methods, high-quality software development and

reproducibility, and high-performance 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 and compliance with the Data Management Plan
- 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
  - Complete 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

**—— APPENDIX 2 ——**

CURRENT AND PENDING SUPPORT

## 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 particlev-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.

In case interim data storage or smaller computations are required, the group at UCB also has a server with two Intel Xeon Processor E52687W v3 3.10GHz 10-core processors (20 total cores), $16\times16$GB 2133 MHz Memory, and 1.6 TB of solid state memory.

For long term data storage and preservation, UC has the Merritt service, which provides a secure environment for long-term preservation of and access to digital assets of the university. Merritt uses redundancy to avoid potential single points of failure. The Merritt Storage service keeps two replicas of all content, stored in different data centers: the San Diego Supercomputer Center's Cloud Storage Service, and UCLA's Cloud Archival Storage Service. The Merritt service runs fixity checks continuously across the entire collection to monitor any possible corruption. Merritt

The work done at Zoox, and RWTH Aachen does not require special compute resources or other special facilities.

## 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 (numerically determining $p(s)$, choosing the transport solver, and implementing and validating the method), which will be conducted in Python.
2. Larger-scale method implementation, which will be conducted in a mix of Python and application-specific software.
3. Impact measurement, which will be done using the software developed in Step 2.

We will make all data generated in steps 1 and 2 publicly available by hosting our developed software (Python), test suite (Python), and problem sets (Python) 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 Python input files used to generate the data–all of which will be text-based data. For example, the 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 Doxgen-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.

We will archive our data in UC's Merritt system, which will generate a DOI for our data package, which we will include in publication references.

**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.

Part three code and results that are subject to export control restrictions will be stored in an archive or appropriate repository for the laboratory (resource depends on , and restrictions will be put in place that enable those to be accessed only by appropriate research partners.

**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 (papers and data) and the MIT license for software and scripts. 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, Zoox will modify their internal software.