Wrap-up report of the CAPES Print Project on Computational modeling of non-classical neutral particle transport

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Outline for this wrap-up report

1. Motivation

2. Historial background

3. Challenging open questions

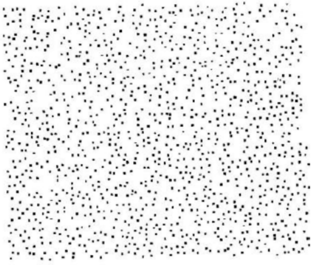
4. The CAPES Print Team Contributions

5. Future Work

Motivation

Motivation

- The transport phenomena of neutral particles can exhibit varied behavior depending on the spatial arrangement of the medium.

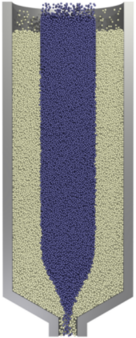


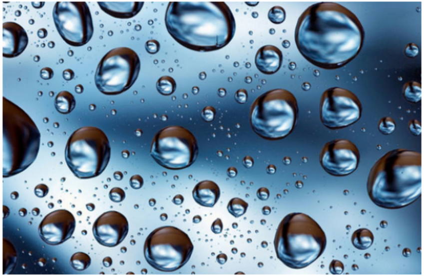
- Scattering centers are not spatially correlated;
- **Exponential attenuation.**

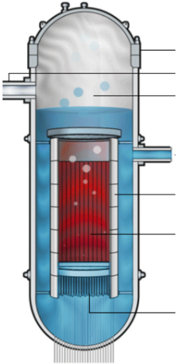
- Scattering centers are spatially correlated;
- **Non-exponential attenuation.**

Motivation

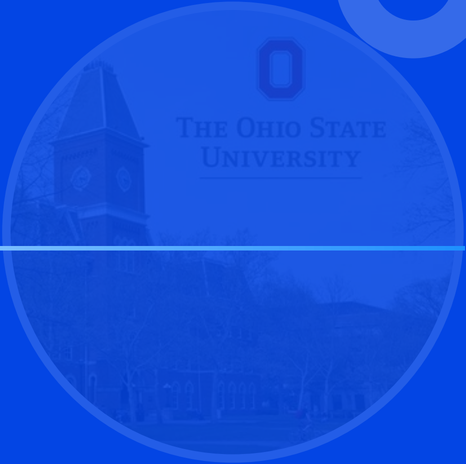
- Some applications of the non-classical transport models:







Historial background



Previous work

- **A generalized linear Boltzmann equation for non-classical particle transport**. Edward W. Larsen and Richard Vasques. Journal of Quantitative Spectroscopy & Radiative Transfer, vol. 112(4), 2011, pp. 619-631.
  - They present an initial study of a new generalized linear Boltzmann equation (GLBE), which mathematically models particle transport for random statistically homogeneous systems in which the distribution function for chord lengths between scattering centers is non-exponential, such as in the photon transport in atmospheric clouds.
  - This equation contains an additional independent variable as compared to the classical transport equation (the path length s).
  - This was a first attempt to develop a Boltzmann-like equation for non-classical neutral particle transport.
- **Non-classical particle transport with angular-dependent path-length distributions. I: Theory.** Richard Vasques and Edward W. Larsen. Annals of Nuclear Energy, vol. 70(-), 2014, pp. 292-300.
  - They relax the previous assumption that the non-exponential distribution function $p(s)$ does not depend on the direction of flight $\mathbf{\Omega}$.
  - This leads to a new GLBE that includes angular-dependent cross sections.

Previous work

- **Non-classical particle transport with angular-dependent path-length distributions. II: Application to pebble bed reactor cores.** Richard Vasques and Edward W. Larsen. Journal of Quantitative Spectroscopy & Radiative Transfer, vol. 112(4), 2011, pp. 619-631.
    - They describe an analysis of neutron transport in the pebble bed nuclear reactor (PBNR) cores, considering random pebble arrangements.
    - This new theory utilizes a non-classical form of the Boltzmann equation in which the locations of the collision centers in the system are correlated and the distance-to-collision is not exponentially distributed, thus using the GLBE, among other related mathematical models, such as the atomic mix model, the Behrens correction, the Lieberoth correction.
    - They conclude that the results predicted using the new GLBE theory are extremely accurate and greatly outperform the other models for the case of random PBNR systems.

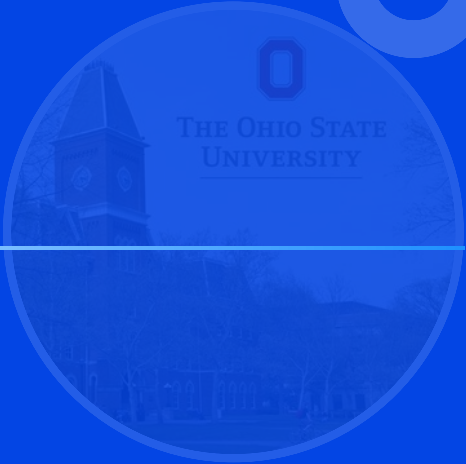
Previous work

- **The nonclassical Boltzmann equation and diffusion-based approximations to the Boltzmann equation.** Martin Frank, Kai Krycki, Edward W. Larsen and Richard Vasques. Siam Journal on Applied Mathematics, vol. 75(3), 2015, pp. 1329-1345.
  - They show that diffusion-based approximations (classical diffusion or SP_1, SP_2, SP_3) to the linear Boltzmann equation with isotropic scattering can (for an infinite, homogeneous medium) be represented exactly by a nonclassical transport equation.
  - Nonclassical versions of the SP_N equations are needed to model nonclassical transport in diffusive regimes.
- **The nonclassical diffusion approximation to the nonclassical linear Boltzmann equation**. Richard Vasques. Applied Mathematics Letters, vol. 53(-), 2016, pp. 63-68.
  - Richard shows that, by correctly selecting the probability distribution function $p(s)$ for a particle's distance-to-collision, the nonclassical diffusion equation can be represented exactly by the nonclassical linear Boltzmann equation for an infinite homogeneous medium.

Previous work

- **Nonclassical particle transport in one-dimensional random periodic media.** Richard Vasques, Kai Krycki and Rachel N. Slaybaugh. Nuclear Science and Engineering, vol. 185(1), 2017, pp. 78-106.
  - They consider a 1-D spatially periodic system consisting of alternating solid and void layers, randomly placed along the x-axis.
  - They obtain an analytical expression for $p(\mu, s)$ and use this result to compute the corresponding $\Sigma_t(\mu, s)$ to solve the nonclassical equation for different test problems numerically.
  - They conclude that the numerical results validate the nonclassical model.
- **Exact transport representations of the classical and nonclassical simplified P_N equations.** Ilker Makine, Richard Vasques and Rachel N. Slaybaugh. Journal of Computational and Theoretical Transport, vol. 47(4-6), 2018, pp. 326-349.
  - They show that the recently introduced nonclassical SP_N equations can be represented exactly by a nonclassical transport equation.

Challenging open questions



Challenging open questions

- How to numerically solve the nonclassical transport equation applying conventional numerical methods for classic transport? Are there strategies to mitigate the potential increase in mathematical and computational complexity?

- How can iterative schemes be improved through the use of efficient acceleration techniques?

- Are there specific methods that leverage the unique characteristics of the nonclassical framework to enhance solution efficiency?

- What specific challenges arise when applying conventional deterministic methods to the nonclassical transport equation?

The CAPES Print Team Contributions

The CAPES Print Team Contributions

- **Asymptotic derivation of the simplified P_N equations for nonclassical transport with anisotropic scattering**. Robert K. Palmer and Richard Vasques. Journal of Computational and Theoretical Transport, vol. 49(7), 2020, pp. 331-348.
  - As I mentioned, they had derived nonclassical SP_N equations to model isotropic scattering transport problems.
  - They present a new method for deriving all the nonclassical SP_N equations with anisotropic scattering.
- **A spectral approach for solving the nonclassical transport equation**. Richard Vasques, Leonardo R. C. Moraes, Ricardo C. Barros and Rachel N. Slaybaugh. Journal of Computational and Theoretical Transport, vol. 49(7), 2020, pp. 331-348.
  - The first contribution we have made towards answering the first challenging open question: we introduced in this paper a mathematical approach that allows one to solve the nonclassical transport equation using classical numerical methods numerically.
  - We used a spectral method to represent the nonclassical flux. The term Spectral is used to indicate that the nonclassical angular flux is approximated as a linear combination of spectral basis functions in the free-path variable s. In the spectral approach (SA) the basis functions are the Laguerre polynomials.
  - As a result, we obtained a nonclassical equation that has the form of a classical transport equation.

The CAPES Print Team Contributions

- **Transport synthetic acceleration for the solution of the one-speed nonclassical spectral S_N equations in slab geometry.** Japan K. Patel, Leonardo R. C. Moraes, Richard Vasques and Ricardo C. Barros. Journal of Computational and Applied Mathematics, vol. 401(-), 2022 , p. 113768.
  - The first contribution we have made towards answering the second challenging open question.
  - With the spectral approach to generate nonclassical spectral S_N equations, which can be numerically solved using classical numerical methods, this paper offers a transport synthetic acceleration procedure to speed up the conventional source iteration scheme for the solution of one-speed, slab-geometry nonclassical spectral S_N equations.
- **On the application of the analytical discrete ordinates method to the solution of nonclassical transport problems in slab geometry.** Leonardo R. C. Moraes, Liliane B. Barichello, Ricardo C. Barros and Richard Vasques. Journal of Computational Physics, vol. 455(-), 2022, p. 110982.
  - The first contribution we have made towards answering the third and fourth questions.
  - We investigate the use of the Analytical Discrete Ordinates (ADO) spectral nodal method for solving the spectral approximation of the nonclassical transport equation in slab geometry.

The CAPES Print Team Contributions

- **An improved spectral approach for solving the nonclassical neutral particle transport equation.** Leonardo R.C. Moraes, Japan K. Patel, Ricardo C. Barros and Richard Vasques. Journal of Quantitative Spectroscopy and Radiative Transfer, vol. 490(-), 2022, p. 108282.
  - Our contribution in this work is an improved modification of the SA. The main focus of the modified SA lies in a slight modification of the nonclassical angular flux representation as a truncated Laguerre series. This leads, in some cases, to a considerable decrease in the Laguerre truncation order required to generate accurate solutions, thus improving efficiency.

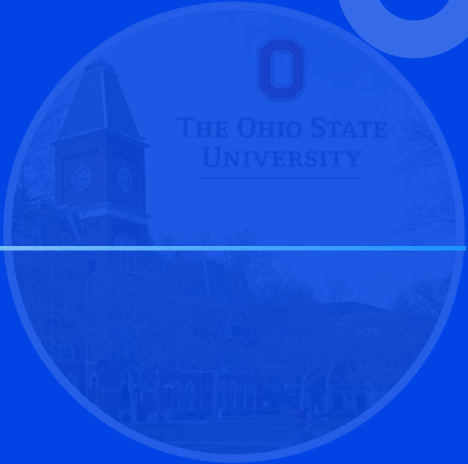
- **On the occurrence of linearly dependent eigenvectors in nonclassical transport calculations.** Leonardo R.C. Moraes, Richard Vasques and Ricardo C. Barros. Journal of Quantitative Spectroscopy and Radiative Transfer, vol. 295(-), 2023, p. 108407.
  - Described here is the occurrence of linearly dependent eigenvectors in the analytical solution of the spectral approximation of the nonclassical transport equation in the S_N formulation. To the best of our knowledge, this characteristic does not arise in the analytical solution of the classical S_N transport equations. This was a warning that classical analytical numerical methods, such as the spectral nodal methods, need to be modified for application to nonclassical transport calculations in order to address this issue.

The CAPES Print Team Contributions

- **On the use of spherical harmonic approximations in nonclassical particle transport problems**. Sunday A. Agbo, Leonardo R.C. Moraes and Richard Vasques. Journal of Quantitative Spectroscopy and Radiative Transfer, vol. 324, 2024, p. 109048.
  - In this work, they describe the application of the spherical harmonic expansion to the nonclassical transport equation to derive a system of equations for the nonclassical flux angular moments, namely nonclassical spherical harmonic approximations (NSHA). This yields a system of equations for the nonclassical flux angular moments structured similarly to the classical P_N equations.

- **A nonclassical model to eigenvalue neutron transport calculations**. Leonardo R.C. Moraes, Ricardo C. Barros and Richard Vasques. **Preprint**.
  - Aiming at contributing to the PBNR global calculations, in this work we present an extension of the nonclassical transport model to eigenvalue criticality calculations.

Future Work



Future Work

- Capes Print project ends next month. This has been our research team's contribution over the past six years (2018-2024). I think this is a significant contribution, considering the long pandemic period the world went through.

- Recently we have submitted to CNPq the two-year project entitled *Development of numerical methods for neutral particle transport calculations based on the generalized linear Boltzmann model using innovative computational techniques.*

- The Brazilian Council for Scientific and Technological Development (CNPq) is a Brazilian governmental agency that sponsors research work.

Future Work

Instituto Politécnico · The Ohio State University

- The result shall come out by the end of this year. Should the project succeed to be approved, we shall have the financial support to continue working together on neutral particle transport with a focus on:
  - Working on techniques to define the path-length distribution function $p(\mathbf{\Omega}, s)$ for PBNR global calculations.
  - Using machine learning to optimize the efficiency of the non-classical transport calculations; e.g., optimizing the choice of N in the S_N models and the order M of the expansion of the nonclassical angular flux in Laguerre polynomials.
  - Study of different spectral basis functions for the Spectral Approach method (robustness).
  - Deal with statistically heterogeneous media.

Acknowledgments

This is the wrap-up report I would like to share with you.
Thank you all very much.