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Title: Resolving Rapid Variation in Energy for Particle Transport

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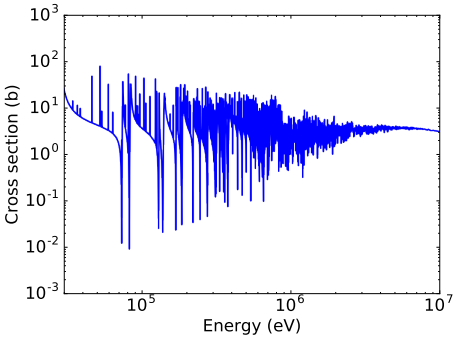
Resolving the rapid variation in energy in neutron and thermal radiation transport is needed for the predictive simulation capability in high-energy density physics applications. Energy variation is difficult to resolve due to rapid variations in cross sections and opacities caused by quantized energy levels in the nuclei and electron clouds. In recent work [2], we have developed a new technique to simultaneously capture slow and rapid variations in the opacities and the solution using homogenization theory, which is similar to multiband (MB) [1, 3] and to the finite-element with discontiguous support (FEDS) method [4], but does not require closure information. We demonstrated the accuracy and efficiency of the method for a variety of problems. We are researching how to extend the method to problems with multiple materials and the same material but with different temperatures and densities. In this highlight, we briefly describe homogenization theory and some results.

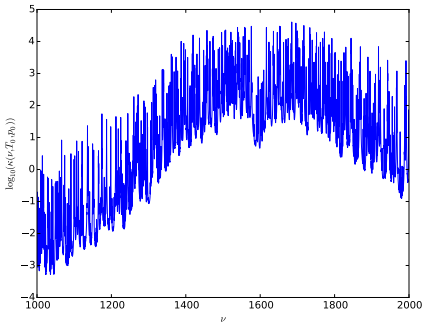
Background and Motivation

Neutron transport (NT) and thermal radiative transfer (TRT) play key roles in various scientific and engineering problems. For example, NT is important in nuclear reactors, fusion applications, and shielding. TRT is important in many astrophysical systems, in planetary atmospheres, and in fusion applications. The Boltzmann transport equation encompasses both sets of physics, with appropriate speeds and source terms for NT or TRT, and tracks particles in a six-dimensional phase space that includes particle position, direction, and energy. NT and TRT solutions are rarely analytic, requiring the use of computers to solve approximations to the Boltzmann transport equation, which involves discretization in all of the variables.

The discretization in energy is difficult due to resonances (lines) in the cross sections (opacities) arising from quantized energy levels in the nucleus (atom). These are shown in the cross section and opacity plots below.



Total cross section (barns) for iron-56



Total opacity (cm^2/g) for water vapor

Anticipated Impact

Using a homogenization framework, we have derived a homogenized continuous-in-energy equation, which we then discretized using a multiband-like approach that first divides energy into coarse groups. We choose groups to be

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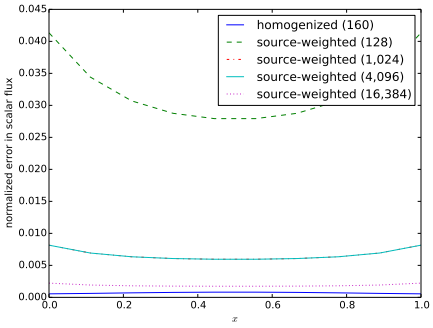
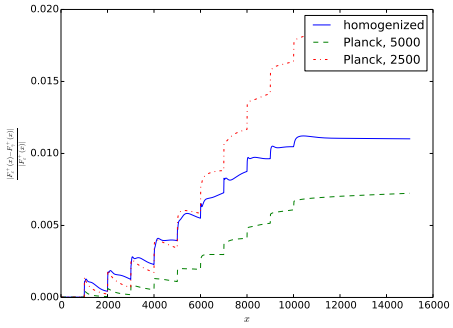
large compared to the characteristic cross section spacing but small compared to the macroscopic energy scale of interest. A key tool is the Young's measure, which within a group describes the probability that the cross section assumes a particular value. Our framework yields a multiband-like transport equation and cross sections without the need for a closure. Errors for a NT shielding problem in iron and an atmospheric TRT problem show homogenization theory to be accurate and efficient.



Solution error for a NT shielding calculation as a function of position for 4 energy groups and 40 bands per group



Relative solution error for an atmospheric TRT calculation as a function of position using 10 energy groups and 5 bands per group compared to a standard multigroup method with 2,500 and 5,000 energy groups

Path Forward

Future work will generalize the process to include problems with resonant scattering cross sections. We are currently extending the method to incorporate correlations of cross sections for the same material but with different temperatures and densities.

Acknowledgements

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References

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[2] TS Haut, C Ahrens, A Jonko, R Lowrie, and A Till. A new multigroup method for cross-sections that vary rapidly in energy. *arXiv preprint arXiv:1604.01451*, 2016.

[3] S. E. Strom and R. L. Kurucz. A Statistical Procedure for Computing Line-Blanketed Model Stellar Atmospheres with Applications to the F5 IV Star Procyon. *J. Quant. Spectrosc. Radiat. Transfer*, 6:591–607, 1966.

[4] A. T. Till, M. Hanuš, J. E. Morel, and M. L. Adams. Comparisons of the Finite-Element-with-Discontiguous-Support Method to Continuous-Energy Monte Carlo for Pin-Cell Problems. In *International Conference on the Physics of Reactors (PHYSOR) - Unifying Theory and Experiments in the 21st Century*, Sun Valley, Idaho, USA, May 2016. American Nuclear Society.