**A Homogenization Approach to Multi-Scale Radiative Transfer in Nano-Structures**

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**ABSTRACT**

We propose a homogenization approach for modeling thermal radiative transfer in nano-structured materials to obtain an effective radiative transport equation (RTE). The approach is based on the concept of moment-linking—the macroscopic moments of an effective RTE are matched to the moments of the underlying electrodynamic solution. Here we present the approach and discuss anticipated results and future directions.

**1. Introduction**

Radiative transfer in complex hetero-structured media has garnered much attention in the recent decade [1]. When the heterogeneous features of such media are sufficiently large, the radiative transfer equation (RTE) can be applied at discrete levels, which drastically simplifies the analysis. Recent developments provide a strong theoretical foundation for the use of the single and multiple RTE continuum approaches in macro-structured media consisting of multiple components with arbitrary-shaped discrete-level geometry and arbitrary radiative properties of the constituents [2]. Studies on predicting thermal characteristics, in particular radiative properties, of nano- and micro-structured media are nearly absent in the literature and pose serious challenges to model. Of particular interest here are the high temperature process considered in the emerging field of solar thermochemistry [3] where multiscale materials have already appeared experimentally [4].

The connection between the true electrodynamic behavior of light and the ray description that underlies the RTE in discrete and continuous random media has been explored by numerous authors and been shown to be valid in limiting cases [5,6]. In this work we propose a method for the multi-scale simulation of porous materials exhibiting wavelength-scale features where the RTE may not be strictly valid, but where the energy transfer within the media can be represented by it.

**2. Proposed methodology**

We consider the limiting case of the RTE written in terms of a phase space energy densityfor a cold scattering medium [5],



Hereis the scattering rate, is the wave-vector, is the *i*th component of the phase velocity vector, andis the scattering phase function. The permeability and permittivity of the local medium is given by and Space and time are denotedand. Note that here the phase space energy density has the units of Jm-3µm3, i.e. energy density per wave-vector, and the scattering phase function is properly normalized and should ensure that scattering only takes place within a certain wavenumber band. For the reader more comfortable with a RTE written in terms of a specific intensitywe point out that for a medium with a dilute collection of independent scatterers we havewhereis the speed of light in the background medium. We would like to connect this equation to the fields obtainable by a solution to Maxwell’s equations but we do not propose to do so by directly deriving the RTE from them. Instead, we express the coefficients defining the medium—namely  andin terms of quantities that can be readily calculated using both the RTE and Maxwell’s equations, the macroscopic moments.

The moments of the RTE are calculated by



where and are positive integers. If we assume the RTE to exist in a region of infinite extent and impose the energy density goes to zero at infinite, we can obtain a set of ordinary differential equations in time for the moments by multiplying Eq. (1) by and integrating over all wave-vectors and space:



Defining the moments for the electrodynamic problem is not as straight forward. First, we need to take a physical model that exists in configuration space only (Maxwell’s equations), and project it in a meaningful way into phase space. Ryzhik et al. [5], among others, utilizes the Wigner function for this purpose,

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The vectoris defined by and the star denotes the complex conjugate. This quantity has been shown to be analogous to the phase space density in that its zeroth and first moments in wave-vector correspond to the internal energy and the energy flux, respectively. It satisfies a RTE under limiting circumstances; see [7]. The Wigner function is not positive definite, so its interpretation as a phase space energy density is limited to the high frequency case. Regardless, the proper moments can be obtained by



**Figure 1. A concept diagram for the moment linking homogenization process in the context of a thermochemical reactor with a nano-structured active material. An effective diffusion equation was not discussed here but will be considered by an analogous approach to the RTE case considered here.**



where tr represents the trace operation.

We are now ready to state the approximation underlying the proposed homogenization process. We impose that the ODEs given by (3) fit the time dependent moments calculated by a solution to Maxwell’s equations for the geometry under study. In other words, we impose that



This imposition has been shown to give excellent agreement when approximating radiative transfer by a diffusion equation [7]. Figure 1 is a representation of the proposed scale-linking process.

**3. Future work**

With the conceptual connection between scales in place, we will set out to test it. In order to calculate the moments of the electrodynamics problem, we, in principle, need a solution to Maxwell’s equations solved on the precise geometry of infinite extent. This is, of course, impossible for most cases. To validate the theory, however, we will consider the problem of scattering from a single non-absorbing sphere whose exact solution is well known for all of space. Next we will consider the problem of an independently scattering medium as considered in the works of Mishchenko et. al [6] since it has been shown that the RTE can be rigorously derived in this limit using the Wigner function used here [5]. In order to extend the approach to cases of porous materials we propose to solve Maxwell’s equations on a large sample of the proposed geometry using computational electrodynamics. The FDTD method has been chosen because open source, scalable codes are readily available to solve this problem. The exact domain size necessary to obtain reliable moments is yet to be seen.

Some upcoming challenges will be discussed to conclude this abstract. The scattering phase function is a continuous function of the incoming and outgoing wave-vectors. It is therefore impossible to be represented exactly by a finite number of moments. An approximate expression in terms of determinable expansion coefficients will have to be decided upon. The proper way to excite a representative element of a porous system is still an outstanding problem. While an individual scatterer can be excited by a plane-wave, the analogous case for a porous element is not clear.

**References**

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