Journal of Computational Physics 296 (2015) 138–157

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A POD reduced order model for resolving angular direction in neutron/photon transport problems

A.G. Buchan [a,*], A.A. Calloo [a], M.G. Goffin [a], S. Dargaville [a], F. Fang [a], C.C. Pain [a], I.M. Navon [b]

[a] Applied Modelling and Computation Group, Department of Earth Science and Engineering, Imperial College London, SW7 2AZ, UK
[b] Department of Scientific Computing, Florida State University, Tallahassee, FL 32306-4120, USA

ARTICLE INFO

Article history:
Received 20 January 2015
Received in revised form 24 April 2015
Accepted 27 April 2015
Available online 4 May 2015

Keywords:
Neutron transport
Photon transport
Boltzmann transport equation
Reduced order model
Proper orthogonal decomposition

ABSTRACT

This article presents the first Reduced Order Model (ROM) that efficiently resolves the angular dimension of the time independent, mono-energetic Boltzmann Transport Equation (BTE). It is based on Proper Orthogonal Decomposition (POD) and uses the method of snapshots to form optimal basis functions for resolving the direction of particle travel in neutron/photon transport problems. A unique element of this work is that the snapshots are formed from the vector of angular coefficients relating to a high resolution expansion of the BTE's angular dimension. In addition, the individual snapshots are not recorded through time, as in standard POD, but instead they are recorded through space. In essence this work swaps the roles of the dimensions space and time in standard POD methods, with angle and space respectively.

It is shown here how the POD model can be formed from the POD basis functions in a highly efficient manner. The model is then applied to two radiation problems; one involving the transport of radiation through a shield and the other through an infinite array of pins. Both problems are selected for their complex angular flux solutions in order to provide an appropriate demonstration of the model's capabilities. It is shown that the POD model can resolve these fluxes efficiently and accurately. In comparison to high resolution models this POD model can reduce the size of a problem by up to two orders of magnitude without compromising accuracy. Solving times are also reduced by similar factors.

1. Introduction

Computational models are important tools for our understanding of many fields of physics, they are relied upon to predict, safeguard, and optimise designs used throughout industry and academia. However despite today's large computational resources, numerical methods used to discretise the underlying equations can still require excessive computing times. Complex domains, high detail solutions or equations with high dimensionality can quickly lead to models using a large number of degrees of freedom. Solving such systems can require high computing effort, and as a direct result in reducing this burden, Reduce Order Methods (ROMs) have evolved. These are techniques that efficiently resolve problems through reduced dimensionality. One such method, which has gained much popularity in recent years, is that of Proper Orthogonal Decomposition.

* Corresponding author.
E-mail address: andrew.buchan@imperial.ac.uk (A.G. Buchan).

http://dx.doi.org/10.1016/j.jcp.2015.04.043

Proper orthogonal decomposition has evolved under a number of names from various fields. It is known as Karhunen–Loéve expansions in signal analysis and pattern recognition [1], principal component analysis in statistics [2], the method of empirical orthogonal functions in geophysical fluid dynamics [3] and meteorology [4]. All of these are model reduction techniques that offer efficient approximations of dynamical systems through using a reduced number of degrees of freedom [5–7]. The fundamental mechanics of POD are to generate optimal basis functions that represent and capture the energy, or dynamics, of a system of interest, and a way of achieving this is through the method of snapshots [8]. This involves taking snapshots of the system's state at various time instances [9], and forming optimal basis functions for their representation.

The origins of POD dates back some way to the early 1900s in the work of Pearson [10], but following the pioneering work of Lumley [11] it has received a considerable amount of attention from within the fluid dynamics community. Early applications include the work of Bakewell [12] and Payne [13] who respectively applied the techniques in turbulent pipe flow and wakes behind cylinders. Other applications include the modelling of flows around air foils [14] and through channels [15], the mixing of fluid layers [16], thermal currents [17,18] and ocean models [19]. It has been applied to the shallow water equations [20], the Euler equations [21], the full Navier–Stokes equations [22] and the various reduced versions of it including the parabolized Navier–Stokes equation [23,24]. POD has been applied to many other fields which are covered extensively in the references of the articles listed here.

In this article the method of POD is applied in a very unique way to solve radiation transport problems. It is applied to the Boltzmann Transport Equation (BTE), which describes the transport of radiation, in order to reduce the problem of high dimensionality (which plagues many radiation transport (RT) models). The problem of high dimensionality arises from several factors, one of the main being the equation having a 7 dimensional phase-space (their discretisation lead to high numbers of unknowns). Radiation problems are also made difficult by their geometries being complex (e.g. reactors are formed of thousands of pins and shields have complex duct systems) and solutions requiring high resolution. POD can therefore be of benefit to these radiation problems as it possesses the appropriate properties to efficiently resolve them. In addition, the BTE is a linear equation which side-steps completely the issue of non-efficient operations caused by non-linear operators. This means that additional treatment of the non-linear terms, recent examples including those of quadratic expansion [25], DEIM [26] and Residual-DEIM [27], are not necessary here.

The novelty in the method presented here is in the use of POD to resolve the direction of particle travel. The two angular dimensions of the BTE are resolved using POD basis functions formed from the method of snapshots. Unusually the snapshots are taken through space, rather than the traditional time, and this in turn allows for time-independent problems to be solved (although it should be mentioned that time dependent problems can still be solved). This has similarities with that of [23,24], which solves the two dimensional time independent parabolized Navier–Stokes equation using a spatial dimension as though it were time. The work here shows how the POD model can be constructed efficiently. It is also shown how the same full model methods can be used to resolve the remaining dimensions of the BTE. This is particularly important as it makes the implementation of the POD model simple as it is almost non-intrusive.

The application of ROMs to radiation problems is still quite rare, although there has been some development in recent years. In [28] POD models have been applied to simulate the dynamics of an accelerator driven system (ADS), and in [29] a useful comparison of POD and modal methods were made. In the work of [30] POD was applied to solving eigenvalue problems for reactor physics applications. The work of [31] applied a Karhunen–Loéve approach to form basis functions that efficiently resolve the energy dependence in reactor physics problems.

The sections of this article are set out as follows. In Section 2 the Boltzmann transport equation is introduced and a description of the high resolution discretisation of the space and angle dimensions is given. This section then describes the process of recording the snapshot data and forming the new reduced order model. In Section 3 two numerical examples are presented. These are specifically chosen to pose complex problems for the POD model to resolve, they also form realistic radiation transport problems. Section 4 completes this article with a conclusion of its findings.

2. The POD formulation for angular discretisation

The following sections describe transport equation together with a review of the full model's discretisation methods. Following this the formulation of the POD model is presented.

2.1. The Boltzmann transport equation

In this article the steady-state, mono-energetic Boltzmann transport equation is considered,

$$\hat{\mathbf{\Omega}} \cdot \nabla\psi(\boldsymbol{r}, \hat{\mathbf{\Omega}}) + \Sigma_t(\boldsymbol{r})\psi(\boldsymbol{r}, \hat{\mathbf{\Omega}}) = \int\limits_{\hat{\mathbf{\Omega}}'} \mathrm{d}\mathbf{\Omega}' \Sigma_s(\boldsymbol{r}, \hat{\mathbf{\Omega}}' \to \hat{\mathbf{\Omega}})\psi(\boldsymbol{r}, \hat{\mathbf{\Omega}}') + S(\boldsymbol{r}, \hat{\mathbf{\Omega}}). \tag{1}$$

This is a linear equation but with five-dimensions (as energy and time are omitted) that describes the state of the angular flux ψ in term of the spatial position, $\boldsymbol{r}$, and the angular direction, $\hat{\mathbf{\Omega}}$. The angular flux defines the number of neutral particles at position $\boldsymbol{r}$ travelling in direction $\hat{\mathbf{\Omega}}$ multiplied by their velocity. The terms in the equation define the change in flux due to particle streaming, absorption, scattering and external sources, respectively. The focus of this article is on the discretisation of the angular dimension of this equation. This is formed of a polar angle, θ (which is also expressed in the