

A reduced order model discretisation of the space-angle phase-space dimensions of the Boltzmann transport equation with application to nuclear reactor problems

Andrew G. Buchan^{a,*}, Ionel M. Navon^b, Liang Yang^c

^a School of Engineering and Materials Science, Queen Mary University of London, EN1 4NS, UK

^b Department of Scientific Computing, Florida State University, Tallahassee, FL, USA

^c Division of Energy and Sustainability, Cranfield University, Bedford, MK43 0AL, UK

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ABSTRACT

This article presents a new reduced order model (ROM) for fast solutions to neutron transport problems. The novelty lies in the construction of optimal basis functions spanning the space-angle phase-space dimensions of the Boltzmann transport equation (BTE). It uses Proper Orthogonal Decomposition and the method of snapshots to form the reduced basis, but here a 2-stage construction is proposed that compresses the angle, then space, dimensions sequentially. The approach alleviates the potentially limiting memory burden for BTE-based ROMs by not processing the full discretised solutions of BTE during the construction stage. The model is both accurate and efficient and is demonstrated here for eigenvalue and fixed source reactor physics problems with assumed uncertainties in material cross-section data. Reductions in problem size and solving times exceeds 5 orders of magnitude in comparison to high fidelity models, and which could potentially improve further for larger scale problems.

1. Introduction

The Boltzmann transport equation (BTE) is central to many important fields of physics including reactor physics, reactor criticality, radiation shielding, and radiative heat transfer, to name but a few. The equation describes the transport of neutrons and photons that underlie these fields, but due to the complexity of the equation and the intricate domains upon which it is solved, computational models are required to approximate its solution. Discretising the BTE for its approximation is particularly complicated by its inherent high dimensional phase-space consisting of space, angle, energy and time. The solutions to the BTE for transient problems will therefore require approximations across 7-dimensions, and very easily the resulting discrete system can be costly to solve in terms of both computer memory and solver time.

There has been a huge research effort spanning several decades in the development of efficient methods for the solving BTE. Examples include solving reduced variants of the first-order equation in simpler forms, such as diffusion theory, integral form, and second order Self-Adjoint Angular Flux (SAAF) and Even-Parity, that can allow more efficient solutions when the physics of problem suits the underlying assumptions, and when it does not introduce singularities within the differential operators. When the first-order form of the BTE is necessary, however, other efficient numerical methods are used to reduce the computational costs of the model.

* Corresponding author at: School of Engineering and Materials Science, Queen Mary University of London, EN1 4NS, UK.
E-mail address: a.buchan@qmul.ac.uk (A.G. Buchan).

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Reduced order models (ROMs) are one such area that has received much attention for resolving radiation transport problems over the last decade. The method of Proper Orthogonal Decomposition (POD) is one such ROM that has proven popular in many fields, with origins dating back some way to works of Pearson [1], and later Lumley [2], from where it has received a considerable amount of attention from within the fluid dynamics community. For example, early works include Bakewell [3] and Payne [4] for turbulent pipe flows and wakes behind cylinders. For neutron transport, early works of ROMs and PODs include [5], for transient dynamics of reactor-driven systems, [6] for one dimensional transient analysis; [7] for eigenvalue problems and reactor criticality. A fair amount of effort has been devoted to developing POD models for neutron diffusion theory and adapted to specific applications. In [8] ROMs for 3D reactor assemblies were formed with a focus of resolving control rod regions and other models for eigenvalue calculations were developed in [9]. ROMs for time dependent neutron diffusion problems were developed in [10], and in [11] a comparison between a POD neutron diffusion model and a traditional nodal methods was presented. Other related works to the nuclear fields include the application of the empirical interpolation method [12] for rod movement, and the application of non-invasive POD models through neural network auto encoders [13]. ROMs have been developed in [14] for transient analysis point kinetic models, for fuel burnup calculations [15] and reactor power profiles [16]. In [17] a ROM was proposed using dynamic mode decomposition (DMD) within a multi-physics (neutron diffusion and thermal hydraulics) framework for stability analysis of molten salt cores.

A number of works have also been developed for enabling ROMs to resolve the full transport equation enabling for the more accurate description of particle transport over diffusion and simplified spherical harmonic (SP_N) approaches. In [18] a ROM was developed for neutron transport within atmospheres in cylindrical coordinates. Here separate ROMs are formed for each angular direction and used to resolve their spatial dimension. ROMs for neutron transport in shielding applications [19], extended to domain decomposition [20], and criticality problems [21,22] have been described where, again, the spatial dependence for each angular direction are resolved. In [23] and [24], a ROM was developed for improving the angular description of radiation transport for discrete ordinate methods. ROMs directly reducing the angular dimension for neutron transport have also been developed, notably from full order models using arbitrary angular discretisations including discrete ordinates (DO), alternatively known as S_N , and spherical harmonics (P_N) approaches. Initially developed in [25] for fixed source problems, and for radiative heat transfer [26], and later the method was extended to include angle [27] and space-angle [28] domain decomposition methods for improved solver convergence and solution accuracy. Other angular ROM methods have been proposed in [29,30], and non-invasive data driven methods using DMD were presented in [17], and other non-intrusive atmospheric radiation ROMs were developed in [31].

In this article a new ROM for neutron transport is presented based on POD and the method of snapshots. It extends on the works of [28] by developing a novel method that first reduces the angular dimension over partitions on the sphere to form optimised POD angular basis functions. This is then followed by second ROM that reduces the spatial dimension of coefficients for the reduced angular basis functions. In essence this forms a set of reduced space-angle POD basis functions for neutron/photon transport problems. The method therefore collapses the space-angle phase-space dimensions of the BTE which is typically responsible for the large discrete systems formed when discretised. In addition to reducing the discrete systems by many orders of magnitude, the method also alleviates the need to process the full sized snapshot data, which can easily become infeasible for large scale problems. A demonstration of the method is presented here for two reactor applications. The first is based on a quarter core eigenvalue problem using S_N and finite elements to resolve the angle-space dimensions for its full order model training. The second is based on a pin-cell problem that is well known for producing complex angular flux profiles. Reductions in the discrete sizes exceed 5 orders of magnitude and speed up in solver times are of similar scales.

The following sections present the ROM formulation, the application to resolving the reactor problems, and a conclusion of its findings.

2. The space-angle ROM for neutron transport

The eigenvalue version of the multi-group Boltzmann transport equation for calculating the neutron multiplication is given by,

$$\begin{aligned} \Omega \cdot \nabla \psi_g(\vec{r}, \Omega) + \Sigma_{t,g}(\vec{r}) \psi_g(\vec{r}, \Omega) - \sum_{g'=1}^G \int_{\Omega'} \Sigma_{s,g' \rightarrow g}(\vec{r}, \Omega' \rightarrow \Omega) \psi_{g'}(\vec{r}, \Omega') d\Omega' \\ = \frac{\chi_g}{4\pi k_{eff}} \sum_{g'=1}^G \int_{\Omega'} \nu \Sigma_{f,g'}(\vec{r}) \psi_{g'}(\vec{r}, \Omega') d\Omega', \end{aligned} \quad (1)$$

for $g \in \{1, 2, \dots, G\}$. The solution yields the angular flux for each energy group g , $\psi_g(\vec{r}, \Omega)$, in direction Ω at position $\vec{r}$ together with the multiplication factor k_{eff} . The terms $\nu \Sigma_{f,g'}$ and $\Sigma_{s,g' \rightarrow g}$ denote the production (via fission from group g') and group to group scattering material cross-sections, respectively, and χ_g denotes the fission spectrum. The equation can also be viewed in matrix form as

$$\begin{bmatrix} \mathcal{L}_{1,1} & \mathcal{L}_{1,2} & \dots & \mathcal{L}_{1,G} \\ \mathcal{L}_{2,1} & \mathcal{L}_{2,2} & \dots & \mathcal{L}_{2,G} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{L}_{G,1} & \mathcal{L}_{G,2} & \dots & \mathcal{L}_{G,G} \end{bmatrix} \begin{bmatrix} \psi_1(\vec{r}, \Omega) \\ \psi_2(\vec{r}, \Omega) \\ \vdots \\ \psi_G(\vec{r}, \Omega) \end{bmatrix} = \frac{1}{k_{eff}} \begin{bmatrix} \mathcal{P}_{1,1} & \mathcal{P}_{1,2} & \dots & \mathcal{P}_{1,G} \\ \mathcal{P}_{2,1} & \mathcal{P}_{2,2} & \dots & \mathcal{P}_{2,G} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{P}_{G,1} & \mathcal{P}_{G,2} & \dots & \mathcal{P}_{G,G} \end{bmatrix} \begin{bmatrix} \psi_1(\vec{r}, \Omega) \\ \psi_2(\vec{r}, \Omega) \\ \vdots \\ \psi_G(\vec{r}, \Omega) \end{bmatrix} \quad (2)$$

where $\mathcal{L}_{i,j}$ contains the advection, removal and scattering operators acting on the angular flux, and $\mathcal{P}_{i,j}$ contains the operators for fission. The equation is accompanied with either void or specular reflective boundary conditions,

$$\psi_g(\vec{r}, \Omega) = 0, \quad \psi_g(\vec{r}, \Omega) = \psi_g(\vec{r}, \Omega^*), \quad \Omega \cdot n < 0, \quad \vec{r} \in \Gamma, \quad (3)$$

where Γ denotes the boundary of the domain, Ω^* is the incoming reflective angle to outgoing Ω and n is the outward pointing normal to the surface.

The full order model used in this article is formed using the discrete ordinate (S_N) angular discretisation together with discontinuous finite elements for discretising the spatial dimension. The formulation however allows a general angular discretisation of equation of $\psi_g(\vec{r}, \Omega)$ to be considered through an approximation of a sum of $\mathcal{M}$ angular basis functions $\mathcal{G}_j(\Omega)$ multiplied by the coefficients $\Psi_j(\vec{r})$,

$$\psi_g(\vec{r}, \Omega) \approx \sum_{j=1}^{\mathcal{M}} \mathcal{G}_j(\Omega) \Psi_j(\vec{r}). \quad (4)$$

Therefore the functions $\mathcal{G}_j(\Omega)$ can be used to represent the directions of the discrete ordinates, or other basis functions sets such as spherical harmonics, wavelets etc.

The discretisation of the angular dimension follows from inserting the approximation (4) into the BTE (1), which is then multiplied, in turn, by each angular basis function $\mathcal{G}_i(\Omega)$, for $i \in \{1, 2, \dots, \mathcal{M}\}$, and integrated over the angular dimension Ω . For each group's angular flux, $\psi_g(\vec{r}, \Omega)$, this results in the angular discretised BTE of the form,

$$(\mathbf{A} \cdot \nabla + H_g(\vec{r})) \Psi_g(\vec{r}) - S_{g,scat}(\vec{r}) = \frac{1}{k_{eff}} S_{g,fiss}(\vec{r}), \quad g \in \{1, 2, \dots, G\}. \quad (5)$$

This is a system of $\mathcal{M}$ equations involving the spatially dependent angular coefficients that have been collected into the vector $\Psi_g(\vec{r})$ of size $\mathcal{M}$. The term $\mathbf{A}$ is a vector of angular streaming matrices (A_x, A_y, A_z), each of size $\mathcal{M} \times \mathcal{M}$, that account for the angular streaming of the discretised coefficients $\Psi_g(\vec{r})$. The term $H_g(\vec{r})$ is a matrix of size $\mathcal{M} \times \mathcal{M}$ containing the discretised total cross-section and within group scattering operator for group g . The terms $S_{g,scat}(\vec{r})$ and $S_{g,fiss}(\vec{r})$ denote vectors of size $\mathcal{M}$ containing the angular discretised out of group scattering, and fission sources.

$$S_{g,scat}(\vec{r}) = \sum_{g' \neq g}^G H_{g' \rightarrow g} \Psi_{g'}(\vec{r}), \quad S_{g,fiss}(\vec{r}) = \sum_{g'=1}^G F_{g' \rightarrow g} \Psi_{g'}(\vec{r}), \quad (6)$$

where $H_{g' \rightarrow g}$ and $F_{g' \rightarrow g}$ are $\mathcal{M} \times \mathcal{M}$ scattering and fission angular discretised matrices that account for the respective scattering and fission from group g' into group g . For completeness, the angular discretised matrices in equations (5) and (6) are defined as

$$\begin{aligned} A_{x,ij} &= \int_{\Omega} \mathcal{G}_i(\Omega) \Omega_x \mathcal{G}_j(\Omega) d\Omega, \quad A_{y,ij} = \int_{\Omega} \mathcal{G}_i(\Omega) \Omega_y \mathcal{G}_j(\Omega) d\Omega, \quad A_{z,ij} = \int_{\Omega} \mathcal{G}_i(\Omega) \Omega_z \mathcal{G}_j(\Omega) d\Omega \\ H_{g,ij} &= \int_{\Omega} \mathcal{G}_i(\Omega) \Sigma_t(\vec{r}) \mathcal{G}_j(\Omega) d\Omega - \int_{\Omega} \mathcal{G}_i(\Omega) \int_{\Omega'} \Sigma_{s,g \rightarrow g'}(\vec{r}, \Omega' \rightarrow \Omega) \mathcal{G}_j(\Omega') d\Omega' d\Omega \\ (H_{g \rightarrow g'})_{i,j} &= \int_{\Omega} \mathcal{G}_i(\Omega) \int_{\Omega'} \Sigma_{s,g' \rightarrow g}(\vec{r}, \Omega' \rightarrow \Omega) \mathcal{G}_j(\Omega') d\Omega' d\Omega, \quad (F_{g \rightarrow g'})_{i,j} = \frac{\chi_g}{4\pi} \int_{\Omega} \mathcal{G}_i(\Omega) \int_{\Omega'} \Sigma_{f,g'}(\vec{r}) \mathcal{G}_j(\Omega') d\Omega' d\Omega \end{aligned}$$

where the angle is represented in the Cartesian coordinate system,

$$\Omega = (\Omega_x, \Omega_y, \Omega_z)^T = ((1 - \mu^2)^{\frac{1}{2}} \cos \omega, (1 - \mu^2)^{\frac{1}{2}} \sin \omega, \mu)^T.$$

For each group flux, $\Psi_g(\vec{r})$, in equation (5) the spatial dimension is discretised using a discontinuous finite element expansion given by,

$$\Psi_g(\vec{r}) = \sum_{j=1}^{\mathcal{N}} N_j(\vec{r}) \Psi_{g,j}, \quad (7)$$

where $N_j(\vec{r})$ is a $\mathcal{M} \times \mathcal{M}$ diagonal matrix containing the j^{th} FE basis function (linear-discontinuous in this article) defined on some finite element mesh. The vector $\Psi_{g,j}$ is of size $\mathcal{M}$ containing the angular coefficients at position j on the mesh, corresponding to energy group g . Similar to forming the angular discretised system, the spatially discretised system is formed by multiplying the system of equations (5) with each $N_i(\vec{r})$, then inserting the expansion of equation (7), and finally by integrating over the spatial element V_e associated with the discontinuous function $N_i(\vec{r})$. This results in the following space-angle discrete matrix system of size $\mathcal{N}\mathcal{M}$,

$$D_g \Psi_g - \sum_{g' \neq g} S_{g' \rightarrow g,scat} \Psi_{g'} = \frac{1}{k_{eff}} \sum_{g'} S_{g' \rightarrow g,fiss} \Psi_{g'} \quad (8)$$

where Ψ_g is the space-angle discretised vector of size $\mathcal{N}\mathcal{M}$ containing the space-angle coefficients, corresponding to energy group g . These vectors are arranged in the form,

$$\Psi_g = \begin{bmatrix} \Psi_{g,1} \\ \Psi_{g,2} \\ \vdots \\ \Psi_{g,\mathcal{N}} \end{bmatrix} \quad (9)$$

that lists the $\mathcal{M}$ angular coefficients for each spatial node in turn. The matrices D_g , $S_{g' \rightarrow g, \text{scat}}$ and $S_{g' \rightarrow g, \text{fiss}}$ are of dimension $\mathcal{N}\mathcal{M} \times \mathcal{N}\mathcal{M}$, that can be viewed as a matrices of size $\mathcal{N} \times \mathcal{N}$ containing angular discretised sub-matrices, each of size $\mathcal{M} \times \mathcal{M}$. The structure of these $\mathcal{M} \times \mathcal{M}$ sub-matrix systems are given by,

$$(D_g)_{i,j} = - \int_{V_e} \nabla N_i(\vec{r}) \cdot \mathbf{A} N_j(\vec{r}) dV + \int_{\Gamma_e, (\text{in/out})} \mathcal{N}_i(\vec{r}) (\mathbf{A} \cdot \hat{n}) N_j(\vec{r}) d\Gamma_e + \int_{V_e} N_i(\vec{r}) H(\vec{r}) N_j(\vec{r}) dV, \\ (S_{g' \rightarrow g, \text{scat}})_{i,j} = \int_{V_e} N_i(\vec{r}) H_{g' \rightarrow g} N_j(\vec{r}) dV, \quad (S_{g' \rightarrow g, \text{fiss}})_{i,j} = \int_{V_e} N_i(\vec{r}) F_{g' \rightarrow g} N_j(\vec{r}) dV, \\ \forall i, j \in \{1, \mathcal{N}\}. \quad (10)$$

Green's theorem has been applied to the advection operator resulting in a surface integral (denoted Γ_e) and volume integral over the element V_e . The term $\hat{n}$ in the surface integral denotes the outward pointing normal to the surface. This surface integral requires incoming-outgoing information of the flux to be separated in order to correctly resolve the flow of particles through the surface of adjacent elements. Here standard up-winding is applied, and thus the (in/out) subscript in the integral limits is used to denote the fact that this integral will involve the variable within element V_e or its neighbour, depending on whether it is out-flowing or in-flowing, respectively. Whilst relatively simple for the discrete ordinate method as the ray's direction naturally informs us of the direction of information flow, for other angular discretisations, a Riemann approaches can be applied [32]. Grouping the angle-spatial discretised equations from all energy groups of equation (8) results in the fully discretised system of equations,

$$L\Psi = \frac{1}{k_{eff}} P\Psi \\ \begin{bmatrix} L_{1,1} & L_{1,2} & \cdots & L_{1,G} \\ L_{2,1} & L_{2,2} & \cdots & L_{2,G} \\ \vdots & \vdots & & \vdots \\ L_{G,1} & L_{G,2} & \cdots & L_{G,G} \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_G \end{bmatrix} = \frac{1}{k_{eff}} \begin{bmatrix} P_{1,1} & P_{1,2} & \cdots & P_{1,G} \\ P_{2,1} & P_{2,2} & \cdots & P_{2,G} \\ \vdots & \vdots & & \vdots \\ P_{G,1} & P_{G,2} & \cdots & P_{G,G} \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_G \end{bmatrix} \quad (11)$$

where $L_{g,g}$ denotes the $\mathcal{M}\mathcal{N} \times \mathcal{M}\mathcal{N}$ matrix containing the discretised advection, removal, boundary and within group scattering matrices, $L_{g,g'}$, $g \neq g'$ denotes the $\mathcal{M}\mathcal{N} \times \mathcal{M}\mathcal{N}$ out of group scattering matrices, and $P_{i,j}$ is the $\mathcal{M}\mathcal{N} \times \mathcal{M}\mathcal{N}$ matrices containing the discretised fission operators. The vector Ψ is of size $\mathcal{N}\mathcal{M}G$ containing the fully discretised (space-angle-energy) BTE's coefficients. At this point, the variable denoting the discretised fluxes are becoming large and will increase further later in this article. Therefore, to help reading, Table 1 has been included that describes vector's notation, and lists their dimensions.

Whilst equation (11) details the full order model for the eigenvalue problem, the non-multiplying fixed source discretised equations are simple to form by replacing the fission term of the BTE, equation (1), with a source term $S_g(\vec{r}, \Omega)$ for each energy group g . The discretisation will follow a similar path as detailed here, but for full details the reader is referred to [27].

2.1. The space-angle ROM for the BTE

The reduced order model described in this section is based on proper orthogonal decomposition together with the method of snapshots. Snapshot data is first formed from the solutions of S realisations of some generic neutron transport problem with variations to its input parameters. In this article, the variations arise from changes in material nuclear cross-sections due to some assumed inherent uncertainties. Thus, for a given cross-section material data, obtained by probing the uncertainties, the full order model equations (11) are solved, and the resulting discrete solution vector forms a single snapshot. It is assumed that the spatial, angle and energy discretisation is kept constant throughout ensuring the each snapshot is of equal size and that each component relates to the same position in the space, angle and energy phase-space. Thus the resulting snapshot data can be viewed as the following matrix of size $\mathcal{M}\mathcal{N}G \times S$ where the full angular flux vector Ψ^s from each solution, s , forms its columns,

$$S = \begin{bmatrix} | & | & & | \\ \Psi^1 & \Psi^2 & \cdots & \Psi^S \\ | & | & & | \end{bmatrix}. \quad (12)$$

Processing the snapshot data formed from the full angle-space-energy discretised solutions in the form of (12) is not advisable since even modest sized neutron transport problems can require substantial computer memory resources. Storing and processing data of several snapshot solutions would therefore likely become infeasible using most modern computer hardware. To resolve this, the first step here is to partition the snapshot data into each energy range and to process one energy group at a time. Thus a set of G snapshot data sets are formed,

Table 1

List and description of variables. Superscripts: s relates to solution s of the snapshot data; a and r indicate variable's are arranged in vectors of angular and spatial expansion coefficients, respectively.

Variable	Description
$\psi_g(\vec{r}, \Omega)$	Undiscretised angular flux, for energy group g .
$\Psi_g(\vec{r})$	Vector of size $\mathcal{M}$ containing angular discretised coefficients at spatial position $\vec{r}$, for energy group g .
$\Psi_{g,i}^a / \Psi_{g,i}^{a,s} / \Psi_{g,i}^{a,s}$	Vector of size $\mathcal{M}$ containing the angular coefficients at spatial node i , for energy group g .
$\Psi_{g,i}^s / \Psi_{g,i}^{s,s}$	Vector of size $\mathcal{M}\mathcal{N}$ containing space-angle discretised coefficients, for energy group g .
Ψ / Ψ^s	Vector of size $\mathcal{M}\mathcal{N}G$ containing the angle-space-energy discretised angular flux.
$\Psi_{g,q,i}^a / \Psi_{g,q,i}^{a,s}$	Vector of size $\mathcal{M}_q$ containing the subset of angle coefficients $\Psi_{g,i}^a$ restricted to partitioning O_q .
$\hat{\Psi}_{g,q,i}^a / \hat{\Psi}_{g,q,i}^{a,s}$	vector of size $\hat{\mathcal{M}}_q$ containing angular ROM coefficients for partitioning O_q .
$\hat{\Psi}_{g,q,j}^r / \hat{\Psi}_{g,q,j}^{r,s}$	Vector of size $\mathcal{N}$ containing FEM coefficients of angular ROM function j , octant q , energy group g .
$\hat{\Psi}_g$	Vector of size $\hat{\mathcal{N}}\hat{\mathcal{M}}Q$ containing the space-angle ROM coefficients for group g .
S	$\mathcal{M}\mathcal{N}G \times S$ matrix, with s^{th} column containing Ψ^s .
S_g	$\mathcal{M}\mathcal{N} \times S$ matrix, with s^{th} column containing Ψ_g^s .
S_g^a	$\mathcal{M} \times \mathcal{N}S$ matrix, with columns $\Psi_{g,i}^{a,s}$ for all nodes i and problems S .
$S_{g,q}^a$	$\mathcal{M}_q \times \mathcal{N}S$ matrix, with columns $\Psi_{g,q,i}^{a,s}$ for all nodes i and problems S .
$\hat{S}_{g,q}^a$	$\hat{\mathcal{M}}_q \times \mathcal{N}S$ matrix, with columns $\hat{\Psi}_{g,q,i}^{a,s}$ for all nodes i and problems S .
$\hat{S}_{g,q,j}^r$	$\mathcal{N} \times S$ matrix, with columns $\hat{\Psi}_{g,q,j}^{r,s}$ for all problems S .

$$S_g = \begin{bmatrix} | & | & & | \\ \Psi_g^1 & \Psi_g^2 & \dots & \Psi_g^S \\ | & | & & | \end{bmatrix} \quad \text{for } g \in \{1, 2, \dots, G\}, \quad (13)$$

where each Ψ_g^s denotes the snapshot vector of size $\mathcal{M}\mathcal{N}$, which are the space-angle coefficients of energy group g , obtained from solution s . However, even with this partitioning of the data the storage requirements are likely to exceed memory resources and so the method presented here is focused on creating a ROM using this data, but through further partitioning of it into smaller and more manageable sets by tacking the angle-space dimension sequentially.

The proposed method is to now consider the snapshot data given in equation (13) into the following re-arrange form,

$$S_g^a = \begin{bmatrix} \Psi_{g,1}^{a,1} & \Psi_{g,2}^{a,1} & \dots & \Psi_{g,\mathcal{N}}^{a,1} & \Psi_{g,1}^{a,2} & \dots & \Psi_{g,\mathcal{N}}^{a,2} & \dots & \Psi_{g,\mathcal{N}}^{a,S} \end{bmatrix}. \quad (14)$$

Here the columns of S_g^a are the vectors $\Psi_{g,j}^{a,s}$ which are the vectors of size $\mathcal{M}$ that contain the angular coefficients for energy group g , at finite element node j , for snapshot solution s - these relate directly to the coefficients in the right hand side of equation (7). In this form the data is arranged into "angular" snapshots that describe all angular distributions of the fluxes across all spatial nodes of the problems resolved. The size of the matrix S_g^a is $\mathcal{M} \times \mathcal{N}S$. To make clear the variables' meaning, superscripts a has been introduced in equation (14) to indicate the solution data is arranged in columns of angular coefficients. This notation, when used in other variables defined later in the article, implies the same meaning.

It is now possible to perform the singular value decomposition on the matrix S_g^a to form optimised POD basis functions for approximating these angular distributions. Prior to this, however, a further decomposition of this angular snapshot data is performed according to an angular partition of the surface of the unit sphere. Here the 4 or 8 octants (for 2D or 3D problems) of solid angle, denoted O_q , of the unit sphere is used,

$$\Omega = \bigcup_{q=1}^Q O_q \quad (15)$$

as shown in Fig. 1 (right). More specifically, for the S_N method, a set of vectors $\Psi_{g,q,j}^{a,s}$, for $q \in \{1, 2, \dots, Q\}$, are defined as containing those coefficients of $\Psi_{g,j}^{a,s}$ that correspond to those discrete ordinates directing into angular partition O_q , again as illustrated in Fig. 1 (left). The column size of the vectors will be denoted by $\mathcal{M}_q$, where $\sum_{q=1}^Q \mathcal{M}_q = \mathcal{M}$. Then, following the same path as that of the author's previous works [28], the angular coefficients in the matrix (14) are partitioned into the Q separate snapshot matrices according to the sphere's partitions. This set of Q snapshot matrices are defined as,

$$S_{g,q}^a = \begin{bmatrix} \Psi_{g,q,1}^{a,1} & \Psi_{g,q,2}^{a,1} & \dots & \Psi_{g,q,\mathcal{N}}^{a,1} & \Psi_{g,q,1}^{a,2} & \dots & \Psi_{g,q,\mathcal{N}}^{a,2} & \dots & \Psi_{g,q,\mathcal{N}}^{a,S} \end{bmatrix} \quad \text{for } q \in \{1, 2, \dots, Q\}, \quad (16)$$

which are of size $\mathcal{M}_q \times \mathcal{N}S$. For the flux reconstruction in a later section, we can also partition the angular basis functions $G_i(\Omega)$ according to the same partition, and so will denote the sets $\{G_{q,i}(\Omega), i \in \{1, 2, \dots, \mathcal{M}_q\}\}$ as being those related to octant q .

The partitioning defined in equation (16) serves the purpose of producing more stable angular ROM basis function sets, as detailed in [27], but also it brings the additional benefit of reducing the size of the snapshot matrix to process. At this point the snapshot data of equation (16) can still exceed computer memory resources, however it is not necessary to work with the entire data set. As the matrix provides snapshots of the angular distributions of the fluxes, at various points in space, it may be sufficient to sample this matrix and to form a reduced version of it containing a subset of its column vectors. Whilst exploring this option will be left for future works, for large scale problems (e.g. whole core analysis) this may become vital for efficient ROM construction. Having this

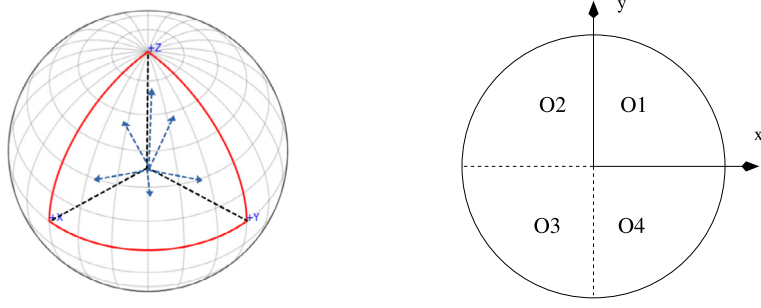


Fig. 1. Left: Surface of the unit sphere illustrating one octant of the partitioning. Discrete Ordinate rays (blue dashed arrows) pointing into the octant are grouped into the same set. Right: Sphere's surface partition numbering on the top hemisphere, octants 1-4 are listed at O1-O4. (For interpretation of the colours in the figure(s), the reader is referred to the web version of this article.)

flexibility to restrict the data matrix size allows its reduction to fit any computer resources, and provided the retained snapshots are representative of all the fluxes, the resulting ROM should still perform as expected.

One can now perform an SVD operation on the snapshot matrix $S_{g,q}^a$, or its reduced version, to form a set of optimised angular POD functions for energy group g and angular octant q ,

$$S_{g,q}^a = U_{g,q}^a \Sigma_{g,q}^a V_{g,q}^{aT}, \quad \text{for } q \in \{1, 2, \dots, Q\}. \quad (17)$$

The terms $U_{g,q}^a$ and $V_{g,q}^{aT}$ are unitary matrices of size $\mathcal{M}_q \times \mathcal{M}_q$ and $\mathcal{N}S \times \mathcal{N}S$, respectively, where the superscript T denotes the transpose. The column vectors of $U_{g,q}^a$ contain the optimised “angular” POD vectors for representing the snapshot matrix (16). The first $\hat{\mathcal{M}}_q$ column vectors of $U_{g,q}^a$ can be used as a basis set to represent the angular data, and the information content captured by the first $\hat{\mathcal{M}}$ vectors of $U_{g,q}^a$ is calculated from the metric involving the singular values of $\Sigma_{g,q}$,

$$I_{g,q} = \frac{\sum_{i=1}^{\hat{\mathcal{M}}_q} (\Sigma_{g,q}^a)_{i,i}^2}{\sum_{i=1}^{\mathcal{M}_q} (\Sigma_{g,q}^a)_{i,i}^2}. \quad (18)$$

The value of $I_{g,q}$ will tend to the value 1 as $\hat{\mathcal{M}}_q$ is increased at which point the full information content of the snapshot data has been retained. From here on, $U_{g,q}^a$ will be assumed to have been reduced to include only the first $\hat{\mathcal{M}}_q$ columns vectors, and hence is of size $\mathcal{M}_q \times \hat{\mathcal{M}}_q$, and the angular flux vector for octant q can be expressed by,

$$\Psi_{g,q}^a \approx U_{g,q}^a \hat{\Psi}_{g,q}^a, \quad \text{for } q \in \{1, 2, \dots, Q\}, \quad (19)$$

for some vector $\hat{\Psi}_{g,q}^a$ of size $\hat{\mathcal{M}}_q$. In addition, the POD angular basis functions spanning octant q are defined by the POD basis vector set, and these can be constructed by the relation,

$$\hat{\mathcal{G}}_{g,q,i}(\Omega) = \sum_{j=1}^{\mathcal{M}_q} (U_{g,q}^a)_{j,i} \mathcal{G}_{q,j}(\Omega), \quad \text{for } i \in \{1, 2, \dots, \hat{\mathcal{M}}_q\}. \quad (20)$$

One can now form a reduced form of the snapshot data (16) by its projection from the full angular space onto the reduced angular space defined equation (19). The snapshot data (16) is premultiplied by the angular POD matrix $U_{g,q}^{aT}$, to give,

$$\begin{aligned} \hat{S}_{g,q}^a &= U_{g,q}^{aT} S_{g,q}^a = U_{g,q}^{aT} \left[\Psi_{g,q,1}^{a,1} \quad \Psi_{g,q,2}^{a,1} \quad \dots \quad \Psi_{g,q,\mathcal{N}}^{a,1} \quad \Psi_{g,q,1}^{a,2} \quad \dots \quad \Psi_{g,q,\mathcal{N}}^{a,2} \quad \dots \quad \Psi_{g,q,\mathcal{N}}^{a,S} \right] \\ &= \left[\hat{\Psi}_{g,q,1}^{a,1} \quad \hat{\Psi}_{g,q,2}^{a,1} \quad \dots \quad \hat{\Psi}_{g,q,\mathcal{N}}^{a,1} \quad \hat{\Psi}_{g,q,1}^{a,2} \quad \dots \quad \hat{\Psi}_{g,q,\mathcal{N}}^{a,2} \quad \dots \quad \hat{\Psi}_{g,q,\mathcal{N}}^{a,S} \right] \end{aligned} \quad (21)$$

for $q \in \{1, 2, \dots, Q\}$. The matrix $\hat{S}_{g,q}^a$ is of dimension $\hat{\mathcal{M}}_q \times \mathcal{N}S$ - the $\hat{\cdot}$ notation has been used to denote its reduction in the angular space. The terms $\hat{\Psi}_{g,q,i}^{a,s}$ denotes the vector of size $\hat{\mathcal{M}}_q$ containing the angular projection of the angular flux vector (for group g , spatial node i , octant g and problem s) onto the reduced angular-POD space. With $\hat{\mathcal{M}}_q \ll \mathcal{M}_q \ll \mathcal{M}$, the reduced size of the snapshot matrix (21) makes it feasible to store and process. As an additional note, one may wish to construct the reduced snapshot space by evaluating $\Sigma_{g,q}^a V_{g,q}^{aT}$ in equation (17), however this would only be applicable if the entire snapshot set were used in the POD mode construction. If the aforementioned sampling approach were used, this alternative operation would only provide the reduced form of the sampled snapshot data. Hence, equation (21) is recommended as the entire data set is reduced with or without sampling of the angular snapshot data.

The final stage of the space-angle ROM construction is to form a reduced basis of the snapshot data that captures the spatial variation of each angular POD basis function. The snapshot data in equation (21) is, in effect, the original snapshot data projected onto the angular ROM space. By its construction, the j^{th} row of $\hat{S}_{g,q}^a$ will contain the spatial information of the j^{th} angular POD function (relating to octant q) for each of the S problems forming the snapshot data. More specifically, the j^{th} row would be a vector of size $1 \times \mathcal{N}S$ that can also be viewed as being partitioned into set of S consecutive vectors of size $\mathcal{N}$. The s^{th} vector of this partitioning relates to the s^{th} snapshot solution. The $\mathcal{N}$ values of the s^{th} vector would be the values of the j^{th} angular POD function that forms the s^{th} snapshot solution over the $\mathcal{N}$ nodes of FEM mesh. Thus, for each angular POD function in turn, the spatial information can be extracted and formed into its own snapshot matrix. That is, for angular ROM function j , of group g and octant q , the corresponding j^{th} row of $\hat{S}_{g,q}^a$ can be recast into the following matrices of dimension $\mathcal{N} \times S$,

$$\hat{S}_{g,q,j}^r = \begin{bmatrix} \hat{\Psi}_{g,q,j}^{r,1} & \hat{\Psi}_{g,q,j}^{r,2} & \dots & \hat{\Psi}_{g,q,j}^{r,S} \end{bmatrix} \quad \text{for } j \in \{1, 2, \dots, \hat{\mathcal{M}}_q\}, \quad q \in \{1, 2, \dots, Q\}, \quad (22)$$

where $\hat{\Psi}_{g,q,j}^{r,s}$ is a vector of size $\mathcal{N}$ containing the spatial coefficients (on the FEM mesh) of the angular POD function j on octant q for energy group g , obtained from the full model solution s . The superscript r notation is now used to indicate that the matrix column vectors correspond to coefficients on the nodes of the FEM mesh - i.e. they are describing the spatial variation of a ROM angular coefficient. It is now feasible to store this information in computer memory as the size of each snapshot matrix (22) is of the same order as any other POD method, applied to some scalar variable, using a full order FEM model. An SVD of the snapshot matrix (22) can now be performed to extract the POD modes representing the spatial variation in each angular POD modes,

$$\hat{S}_{g,q,j}^r = U_{g,q,j}^r \Sigma_{g,q,j}^r V_{g,q,j}^{rT} \quad \text{for } j \in \{1, 2, \dots, \hat{\mathcal{M}}_q\}, \quad q \in \{1, 2, \dots, Q\}. \quad (23)$$

The matrix $U_{g,q,j}^r$ is of dimension $\mathcal{N} \times \mathcal{N}$ where again, in a similar fashion to the angular reduction, the first $\hat{\mathcal{N}}_{g,q,j}$ columns of $U_{g,q,j}^r$ are used to form the spatial POD basis vectors. The matrix $U_{g,q,j}^r$ will be assumed to be restricted to contain the first $\hat{\mathcal{N}}_{g,q,j}$ column vectors. Thus the spatial variation of the j^{th} angular POD coefficient of octant q , energy group g can be expressed as,

$$\hat{\Psi}_{g,q,j}^r \approx U_{g,q,j}^r \hat{\hat{\Psi}}_{g,q,j}^r, \quad \forall j \in \{1, 2, \dots, \hat{\mathcal{M}}_q\}, \quad q \in \{1, 2, \dots, Q\}, \quad (24)$$

where $\hat{\hat{\Psi}}_{g,q,j}^r$ is a vector of size $\hat{\mathcal{N}}_{g,q,j}$ containing the spatial POD coefficients that expands the angular POD function. The double hat $\hat{\hat{\cdot}}$ notation is used to denote the fact that the vector relates to two reduction projections, i.e. in both angle and space. The ROM spatial basis functions can also be reconstructed through the relations,

$$\hat{N}_{g,q,j,i}(\vec{r}) = \sum_{k=1}^{\mathcal{N}} (U_{g,q,j}^r)_{k,i} N_k(\vec{r}) \quad i \in \{1, 2, \dots, \hat{\mathcal{N}}_{g,q,j}\} \quad (25)$$

which form the i^{th} spatial basis function for expanding the j^{th} angular POD function for angular octant q for energy group g . Importantly, this approach has now constructed a distinct set of spatial POD modes that are optimised to resolve the spatial dependence of their respective angular POD basis functions. Thus, in summary, the space-angle dimensions of the angular flux can now be expanded fully using optimised POD basis functions where equations (20) form the set of optimised angular basis functions, and equations (25) form the corresponding set of optimised spatial functions for each angular POD function. The angular flux can now be approximated through the expansion,

$$\psi_g(\vec{r}, \Omega) = \sum_{q=1}^Q \sum_{j=1}^{\hat{\mathcal{M}}_{g,q}} \hat{G}_{g,q,j}(\Omega) \sum_{i=1}^{\hat{\mathcal{N}}_{g,q,j}} \hat{N}_{g,q,j,i}(\vec{r}) \hat{\hat{\Psi}}_{g,q,j,i} \quad (26)$$

where $\hat{\hat{\Psi}}_{g,q,j,i}$ denotes the coefficients of the ROM model. Alternatively this may also be expressed as a matrix vector mapping between the full order model discretised coefficients and the coefficients of the ROM. This will be denoted here as:

$$\Psi_g = U_g \hat{\hat{\Psi}}_g, \quad (27)$$

where U_g is the matrix that maps the vector of space-angle ROM coefficients $\hat{\hat{\Psi}}_g$ to the full model's space-angle coefficients Ψ_g , for each energy group g . Whilst the theory presented here allows for arbitrary and varying ROM angular and spatial sizes, i.e. arbitrary values for $\hat{\mathcal{M}}_q$ and $\hat{\mathcal{N}}_{g,q,j}$, respectively, for simplicity fixed sizes will be used from here on. The angular and spatial ROM sizes will be denoted by $\hat{\mathcal{M}}$ and $\hat{\mathcal{N}}$, respectively, and so the matrix U_g will be of size $\mathcal{M}\mathcal{N} \times \hat{\mathcal{N}}\hat{\mathcal{M}}Q$.

2.2. Off-line ROM construction and on-line solver

The ROM model for the BTE can now be formulated using the space-angle POD basis functions defined in the previous section. This is achieved through a method that generates pre-computed POD matrices for resolving the operators of the BTE, which themselves can then be combined to form the ROM's discrete equations during the online solving stage. Whilst this approach of exploiting the linear nature of the BTE has been used by a number of works mentioned in this article, it is the use of these new space-angle basis

functions that make this formulation unique. Construction begins by considering the fully discretised equations (11), and separating out the operators. The operators of equation (11) can be considered as,

$$L_{g,g} = L_{g,g}^{adv} + L_{g,g}^{bc} + \sum_m \Sigma_{t,g,m} L_{g,g,m}^{rem} + \sum_m \Sigma_{s,g \rightarrow g,m} L_{g,g,m}^{scat} \quad (28)$$

$$L_{g,g'} = \sum_m \Sigma_{s,g' \rightarrow g,m} L_{g,g',m}^{scat}, \quad \text{for } g \neq g' \quad (29)$$

$$P_{g,g'} = \sum_m \frac{\chi_g}{4\pi} \nu \Sigma_{f,g',m} P_{g,g',m}^{fiss} \quad (30)$$

where the RHS terms of equation (28) denote the discretised matrices (of size $\mathcal{M}\mathcal{N}$) for advection, boundary conditions, removal and scattering, respectively, relating to each energy group g . Note the superscript notation (*adv*, *bcm*, *rem*, *scat*, *fiss*) has been used to clearly indicate what part of the transport processes the operators relate to. The summation over m within the removal and scattering operators arises from these terms being further decomposed to represent the discretised matrices from each material region of a given problem. Furthermore, since they are decomposed for each material, the cross-sections for each material m , denoted as $\Sigma_{t,g,m}$ and $\Sigma_{s,g \rightarrow g,m}$, can be pulled out of the matrices since they will be constants within their respective integrals of equations (10). For example, the removal component of the scatter removal term in equation (11), related to material m , can be recast as,

$$\Sigma_{t,g,m} (L_{g,g,m}^{rem})_{i,j} = \Sigma_{t,g,m} \int_{V_e} N_i(\vec{r}) H N_j(\vec{r}) \delta(\vec{r}, \vec{r}_m) dV \quad \forall i, j \in \{1, \mathcal{N}\},$$

where the function $\delta(\vec{r}, \vec{r}_m)$ has the value 1 if position $\vec{r}$ contains material m , and 0 otherwise, and where H is the angular mass matrix of size $\mathcal{M} \times \mathcal{M}$,

$$H_{ij} = \int_{\Omega} \mathcal{G}_i(\Omega) \mathcal{G}_j(\Omega) d\Omega \quad \forall i, j \in \{1, \mathcal{M}\}.$$

Similarly, in equations (30), the group to group scattering and fission matrix for material m are expressed as,

$$\Sigma_{s,g' \rightarrow g,m} (L_{g,g',m}^{scat})_{i,j} = \Sigma_{s,g' \rightarrow g,m} \int_{V_e} N_i(\vec{r}) H_{g' \rightarrow g,m}^{scat} N_j(\vec{r}) \delta(\vec{r}, \vec{r}_m) dV, \quad \forall i, j \in \{1, \mathcal{N}\},$$

and

$$\frac{\chi_g}{4\pi} \nu \Sigma_{f,g',m} (P_{g,g',m}^{fiss})_{i,j} = \frac{\chi_g}{4\pi} \nu \Sigma_{f,g',m} \int_{V_e} N_i(\vec{r}) H N_j(\vec{r}) \delta(\vec{r}, \vec{r}_m) dV, \quad \forall i, j \in \{1, \mathcal{N}\},$$

where

$$(H_{g' \rightarrow g,m}^{scat})_{i,j} = \int_{\Omega} \mathcal{G}_i(\Omega) \int_{\Omega'} S_{g' \rightarrow g,m}^{scat}(\vec{r}, \Omega' \rightarrow \Omega) \mathcal{G}_j(\Omega') d\Omega' d\Omega \quad \forall i, j \in \{1, \mathcal{M}\},$$

and $S_{g' \rightarrow g,m}^{scat}(\vec{r}, \Omega' \rightarrow \Omega)$ denotes the scattering angle probability distribution for material m and for energy group g' into g .

The POD model is now constructed by the projection of the full model in equations (11) using the space-angle ROM matrices in equations (27). That is, the reduced systems of equations of (11) are formed by inserting the ROM projection of equation (27), and pre-multiplying by U_g^T ,

$$\begin{aligned} \hat{L}\hat{\Psi} &= \frac{1}{k_{eff}} \hat{P}\hat{\Psi} \\ \begin{bmatrix} \hat{L}_{1,1} & \hat{L}_{1,2} & \dots & \hat{L}_{1,G} \\ \hat{L}_{2,1} & \hat{L}_{2,2} & \dots & \hat{L}_{2,G} \\ \vdots & \vdots & & \vdots \\ \hat{L}_{G,1} & \hat{L}_{G,2} & \dots & \hat{L}_{G,G} \end{bmatrix} \begin{bmatrix} \hat{\Psi}_1 \\ \hat{\Psi}_2 \\ \vdots \\ \hat{\Psi}_G \end{bmatrix} &= \frac{1}{k_{eff}} \begin{bmatrix} \hat{P}_{1,1} & \hat{P}_{1,2} & \dots & \hat{P}_{1,G} \\ \hat{P}_{2,1} & \hat{P}_{2,2} & \dots & \hat{P}_{2,G} \\ \vdots & \vdots & & \vdots \\ \hat{P}_{G,1} & \hat{P}_{G,2} & \dots & \hat{P}_{G,G} \end{bmatrix} \begin{bmatrix} \hat{\Psi}_1 \\ \hat{\Psi}_2 \\ \vdots \\ \hat{\Psi}_G \end{bmatrix} \end{aligned} \quad (31)$$

where each sub-matrix is constructed by,

$$\hat{L}_{g,g'} = U_g^T L_{g,g'} U_{g'} \quad \text{and} \quad \hat{P}_{g,g'} = U_g^T P_{g,g'} U_{g'} \quad (32)$$

Next the decomposition relations in equations (28) and (30) are substituted into equations (32) to form:

$$U_g^T L_{g,g} U_g = U_g^T L_{g,g}^{adv} U_g + U_g^T L_{g,g}^{bc} U_g + \sum_m \Sigma_{t,g,m} U_g^T L_{g,g}^{rem} U_g + \sum_m \Sigma_{s,g \rightarrow g,m} U_g^T L_{g,g}^{scat} U_g, \quad (33)$$

$$U_g^T L_{g,g'} U_{g'} = \sum_m \Sigma_{s,g' \rightarrow g,m} U_g^T L_{g,g'}^{scat} U_{g'} \quad U_g^T P_{g,g'} U_{g'} = \sum_m \frac{\chi_g}{4\pi} \nu \Sigma_{f,g',m} U_g^T P_{g,g'}^{fiss} U_{g'}, \quad (34)$$

Table 2
Nuclear material cross-section data for the BWR core.

Material	Group	Σ_t	$\nu\Sigma_f$	$\Sigma_{s,g \rightarrow 1}$	$\Sigma_{s,g \rightarrow 2}$	χ
I	Group 1	0.26260	0.00460	0.23190	0.02533	1.0
	Group 2	1.57978	0.10910	0.00000	1.47946	0.0
II	Group 1	0.26288	0.00461	0.22790	0.02767	1.0
	Group 2	1.75254	0.08675	0.00000	1.68205	0.0
III	Group 1	0.26476	0.00466	0.23046	0.02617	1.0
	Group 2	1.59413	0.10210	0.00000	1.51067	0.0
IV	Group 1	0.26476	0.00466	0.23046	0.02617	1.0
	Group 2	1.59413	0.10210	0.00000	1.52078	0.0
V	Group 1	0.26518	0.00000	0.21691	0.04754	-
	Group 2	2.09380	0.00000	0.00000	2.07468	-

which can be re-cast as,

$$\hat{L}_{g,g} = \hat{L}_{g,g}^{adv} + \hat{L}_{g,g}^{bc} + \sum_m \Sigma_{t,g,m} \hat{L}_{g,g}^{rem} + \sum_m \Sigma_{s,g \rightarrow g,m} \hat{L}_{g,g}^{scat} \quad (35)$$

$$\hat{L}_{g,g'} = \sum_m \Sigma_{s,g' \rightarrow g,m} \hat{L}_{g,g'}^{scat} \quad \hat{P}_{g,g'} = \sum_m \frac{\chi_g}{4\pi} \nu \Sigma_{f,g',m} \hat{P}_{g,g'}^{fiss}. \quad (36)$$

The sub-matrices listed in equation (35) and (36) are of dimension $\hat{M}Q\hat{N} \times \hat{M}Q\hat{N}$, which can be computed and stored during the off-line stage construction of the ROM. Note that the nuclear cross-section data for each material have been extracted from the matrices and so are not included within the their construction. This make constructing a ROM for a new problem, with an arbitrary set of material data, simple and efficient. One can now form, during the online-stage of the ROM model, the sub-matrices $\hat{L}_{g,g'}$ and $\hat{P}_{g,g'}$, in equations (35) and (36), by simply multiplying the sub-matrices for scattering, removal and fission by their respective material cross-sections, and performing the summations. When combined into the whole system of equations (31), the resulting eigenvalue problem is projected into the ROM space and can be solved using any eigenvalue algorithm of choice to obtain the solution.

The formulation presented here has developed the ROM for solving the eigenvalue version of the BTE. Extending the method to resolving fixed source problems is straightforward as one can simply replace the RHS fission terms of equations (1) with a fixed source $s_g(\vec{r}, \Omega)$ which, when discretised in angle and space, results in replacing the RHS of equations (11) with the discretised vector of size $\mathcal{N}\mathcal{M}$ for each group flux. This can be split into components representing different sources that can each be projected onto the ROM space, for each group g , by its pre-multiplication with the mapping operator U_g^T .

3. Numerical examples

In this section two numerical examples are presented to demonstrate the capabilities of the ROM at resolving neutron transport problems for reactor physics applications. The first involves solving an eigenvalue problem for a 2 dimensional quarter reactor core, the second a fixed source problem resembling an array of fuel pins. These examples were chosen to showcase the ROM's capability to resolve complex solutions that can form in both the space-angle dimensions. In the following analysis a ROM with $\hat{M}$ angular basis functions per octant and $\hat{N}$ spatial basis functions per angle function will be denoted as ROM $_{\hat{M},\hat{N}}$.

3.1. BWR quarter reactor core

This example aims to demonstrate the ROM's ability at simulating reactor cores by resolving the quarter core BWR eigenvalue problem presented in Fig. 2. The core is composed of 4 regions of varying fuel compositions that are surrounded by a reflector shield. The material cross-sections comprise of 2-energy group data which is listed in Table 2. These will be considered as their nominal (or expected) values when, later, there are assumed uncertainties within them. To construct the snapshot data, a full-order model was employed, utilizing an S_{32} discrete ordinate angular discretisation alongside a discontinuous finite element spatial discretisation over a uniform mesh of 66×66 quadrilateral elements. This discretisation has 544 angular directions and approximately 17k spatial nodes, totalling around 18.9m degrees of freedom (DoF) for the 2 energy group problem.

The snapshot data used to construct the ROM was obtained by probing uncertainties in the cross-section data and resolving the perturbed problem using the full order model. Two cross-sections were randomised within the main fuel region (material 1: $\Sigma_{t,1}$ and $\nu\Sigma_{f,2}$) and outer shield (material 5: $\Sigma_{s,1 \rightarrow 2}$ and $\Sigma_{t,2}$), using a $\pm 2.5\%$ variation, with uniform probability, centred over their nominal values. Provided this didn't result in non-physical cross-section values, the solutions were stored for the snapshot matrix, two of which were build using 20 and 40 realisations of the problem. For testing purposes, the solutions to a further 50 unseen problems (to those used in the POD construction) were resolved using the same randomisation in the material data. Fig. 3 (left) presents the 2 group scalar flux solution to one of the unseen problem using the full order model.

Fig. 4 presents the singular values from the angular and spatial POD compression for each of the 4 octant regions. Interestingly, in the angular POD compression, the singular values for each octant decay at a very similar rate, and their magnitude has dropped by over three orders of magnitude using only 7 basis functions for energy group 1, and 4 for group 2. The singular values from the

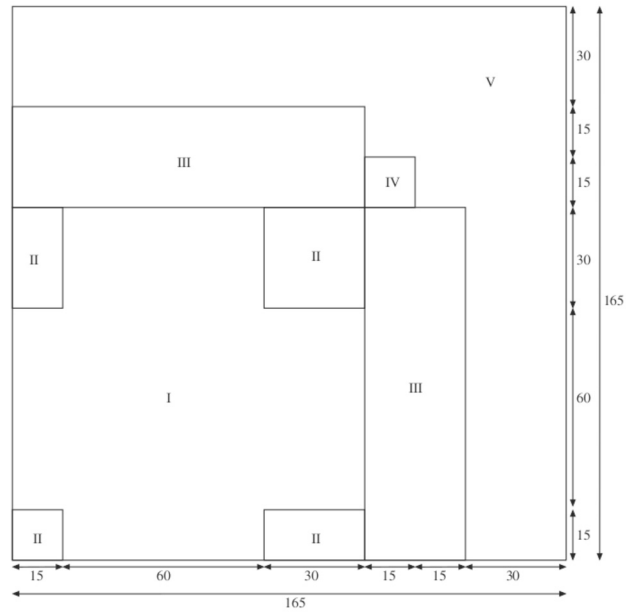


Fig. 2. Quarter core geometry with dimensions listed in centimetres. The domain composed of 5 regions of varying fuels (regions I-IV) and a shield (region V). Vacuum boundary conditions are applied to top and right sides, reflective conditions applied to left and bottom.

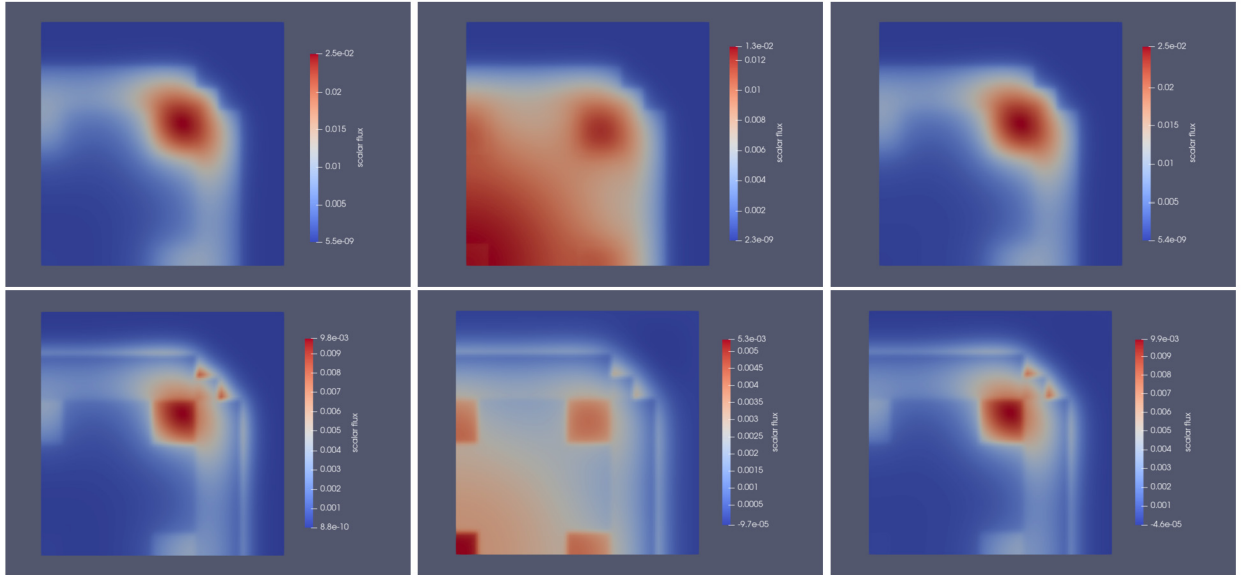


Fig. 3. Scalar flux profiles of the group 1 (top) and group 2 (bottom) solutions from the full order model (left), $ROM_{5,2}$ (middle) and $ROM_{5,7}$ (right) for an unseen problem.

spatial compression are shown for angular basis functions 1, energy group 1, and angular basis functions 4 of energy group 2. It is shown that these values also decay at the same rate for both energy group fluxes, and that their values have reduced by 4 orders of magnitude by the 8th singular value. These sharp decays in the singular values for both the angle and space domains suggest the ROM is capable of capturing the detail of the problem using a relatively small basis function set.

Figs. 5 and 6 present a sample of the angular and spatial ROM basis functions. To avoid an excessive number of plots, just the upper right octant angular basis functions are presented for both energy groups.¹ They show both groups angular basis functions to have similar profiles, and that they are very smooth initially and increase in complexity and detail further into the expansion set. Similar patterns are observed in the spatial ROM functions which, again to avoid excessive plots, are presented only for the 1st angular

¹ These and all subsequent angular flux profiles are viewed looking down on the north hemisphere with orientation as that shown in Fig. 1.

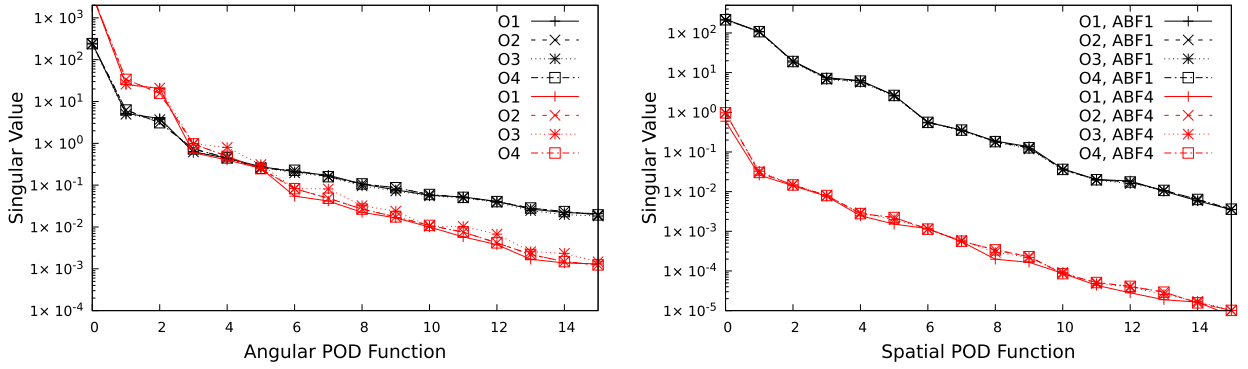


Fig. 4. Left: Singular Values from the POD Angular Compression for group 1 (black) and group 2 (red) snapshot data. Right: Singular values from the spatial compression for group 1 angular basis function (ABF) 1 (black) and group 2 ABF 4 (red). Ox in the legend denotes Octant x.

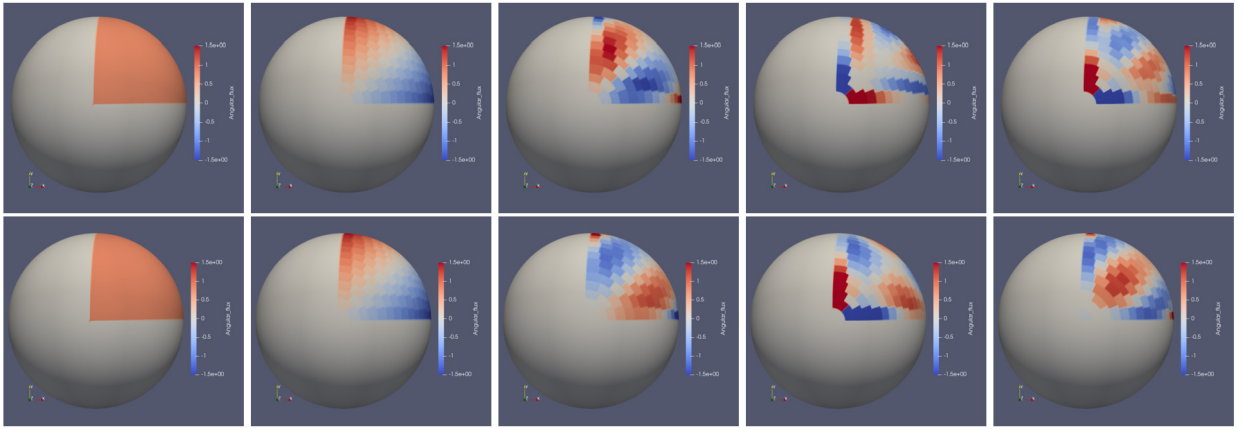


Fig. 5. Angular flux POD basis functions for energy group 1 (top) and 2 (bottom) for angular octant 1. Left-to-right are basis functions 1, 2, 7, 9 and 11.

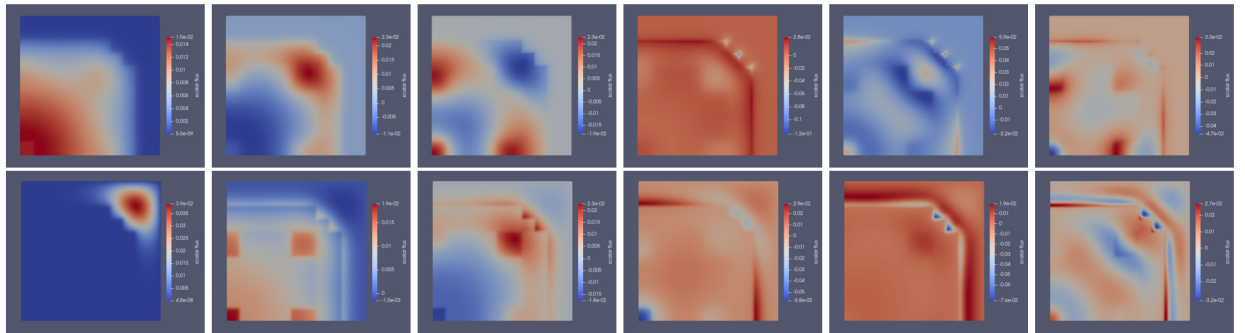


Fig. 6. Spatial POD basis functions for energy group 1 (top) and 2 (bottom) for angular POD function 1 of angular octant 1. Left-to-right are basis functions 1, 2, 3, 6, 8 and 10.

ROM function corresponding to Fig. 5. Here there are clear differences in the group 1 and group 2 spatial ROM basis functions. The initial basis functions encapsulate the overall features, whereas the subsequent ones concentrate on finer details, particularly around the core-shield interface. The scalar flux solutions obtained from the ROM are presented in Fig. 3 for comparison with the full order model solution to the unseen problem. The ROM_{5,2} (80 DoF) shows that using a very low number of spatial ROM basis functions can still provide a reasonable approximation, but there are clear visible difference in the scalar flux in comparison to the full-order model solution. However, the solutions obtained using ROM_{5,7} (280 degrees of freedom) have significantly mitigated these errors, demonstrating a close comparison with the full-order model. Fig. 7 presents and compares the angular flux profiles from the full-order and ROM models at some selected point within the domain. The full-order model's angular flux exhibits a smoothly varying profile across the sphere and the ROM_{5,2} has captured these general features, with some visible differences. Once again the ROM_{5,7} compares very closely to the full-order model whilst increasing the resolution to ROM_{11,9} (792 DoF) all but eliminates any visible difference.

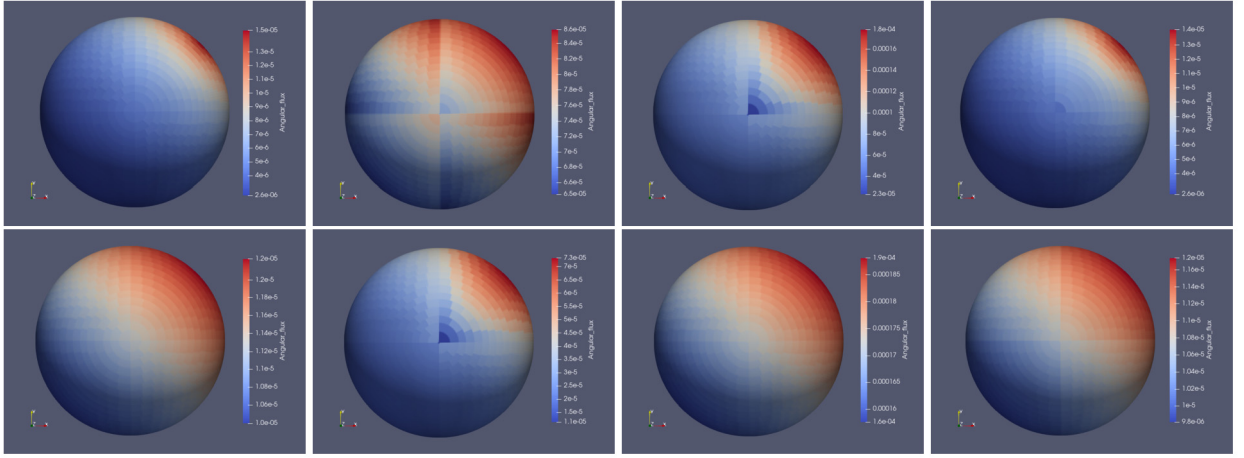


Fig. 7. Group 1 (top) and 2 (bottom) angular flux profiles at position $(x,y)=(1.4,1.4)$ m. Left to right: Comparison between S_{32} , $ROM_{5,2}$, $ROM_{5,7}$, $ROM_{11,9}$.

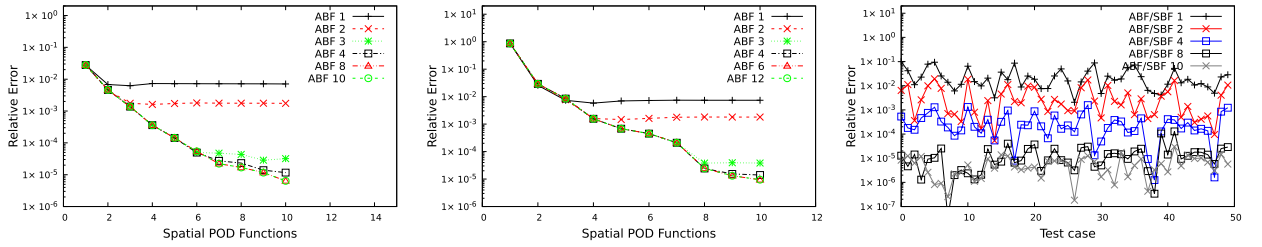


Fig. 8. Left and Middle: The ROM's average relative error in predicted k_{eff} for varying spatial resolution where the angular basis functions (ABF) per octant are held fixed - results were obtained using the snapshot data of size 20 and 40 respectively. Right: ROM relative error in predicted k_{eff} for all 50 unseen test cases using varying ABF and spatial basis function (SBF) expansions using snapshot size 20.

Table 3
ROM solver times for the BWR problem (seconds).

angle\space	2	4	6	8	10
2	1.89×10^{-3}	4.36×10^{-3}	1.24×10^{-2}	1.01×10^{-2}	2.19×10^{-2}
5	4.73×10^{-3}	1.71×10^{-2}	5.26×10^{-2}	7.40×10^{-2}	1.16×10^{-1}
8	1.35×10^{-2}	4.89×10^{-2}	9.97×10^{-2}	2.32×10^{-1}	3.63×10^{-1}

The left and middle graphs of Fig. 8 present the relative errors in the eigenvalue when the ROM's angular resolution is held constant and the spatial resolution is increased. Here the error was calculated to be the average relative error in K_{eff} in the 50 unseen test cases, and the two graphs present the results using snapshot data of size 20 and 40. The results show that 5 or more angular ROM basis functions per octant is sufficient to obtain angular convergence in the eigenvalue error, and that in combination with 8 spatial basis functions, the relative errors are reduce to 10^{-5} . The ROM's performance using the two snapshots data sets are quite similar and result in similar accuracy, although the larger snapshot set created a ROM that was a little slower to converge. But this indicates that the ROM for this type of reactor problem can be trained using a relatively modest number of snapshot data. The right graph of Fig. 8 presents the eigenvalue errors for each of the 50 unseen problems for varying ROM space-angle resolution. These show that for a fixed space-angle size, the errors are largely the same for all test cases. This is important because there were no spurious cases for which the ROM was unable to resolve as accurately as the others. This provides confidence that the model can effectively resolve this reactor-type problem within the specified bounds of uncertainty used in its training.

Table 3 lists the computational times for solving the ROM with varying space and angle resolution. These include the time to construct the ROM matrices, from the pre-computed matrices, and execute the eigenvalue solver for which the numpy linear algebra package was used [33]. The typical full order model solver times were in the order of 10^4 seconds to solve a single problem. However it is stressed that this might not be representative of an optimal solver time since only sweep-based solvers were used with no acceleration techniques, in addition to high solver tolerances to ensure sufficient solution convergence. Thus these solver times should be considered as an indicator. However, even so, the results demonstrate considerable efficiency gains using the ROM. For example, the $ROM_{5,8}$, accurate to within 10^{-5} error, is of 5 orders of magnitude faster to solve compared to the full order model. Furthermore, it should also be mentioned that the numpy-based solver resolved all eigenvalues and eigenvectors, and so the ROM's efficiency potentially be improved if only the single dominant eigenvalue was computed.

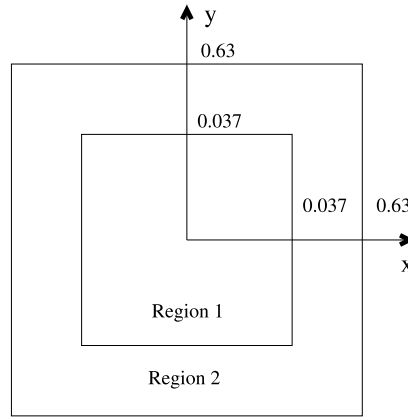


Fig. 9. Problem geometry of pin cell problem with dimensions in centimetres. Reflective boundary conditions are applied to all sides.

Table 4
Nuclear material cross-section data.

Material	Group	Σ_t	Σ_s	source
I	Group 1	0.064132	0.008642	1.0
II	Group 1	0.083524	0.057843	0.0

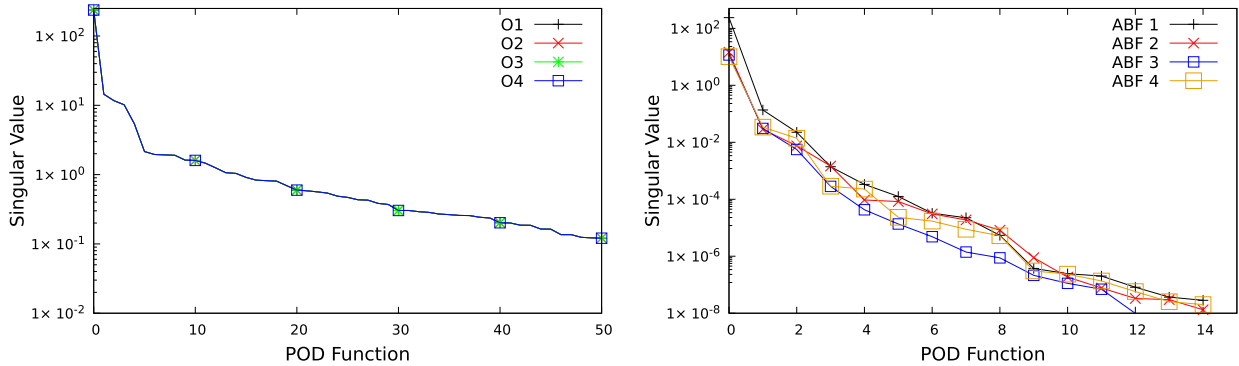


Fig. 10. Singular Values of the angular POD compression (left), and spatial POD compression (right) for the first 4 angular ROM basis functions for octant 1.

3.2. Fixed source pin cell problem

In this example a simple fixed source problem representing a fuel pin cell is resolved. The problem domain is presented in Fig. 9 showing a fuel cell surrounded by a moderator region, with reflective boundary conditions applied to all sides. The single energy group material cross-section data for each regions are listed in Table 4, these will be considered the material's nominal values when uncertainties are applied. The problem has been selected as it is very similar to the Adam's pin-cell problem [34] that is well known for producing complex angular flux distributions. Thus it will provide a good examination of the ROM's ability to resolve these different types of fluxes that did not form in the previous example. The full model used to construct the snapshot data employed an S_{32} discrete ordinate discretisation together with a 63×63 quadrilateral FEM mesh. This equates to approximately 8.6m DoF. In total, 15 solutions were computed to form the snapshot data. Each problem varied by introducing uncertainty within all 4 material cross-sections of Table 4, applying a $\pm 2.5\%$ with uniform distribution. The singular values for the angle and spatial POD compression are presented in Fig. 10. The angular POD singular values follow the same profiles for each octant which is expected due to the problem's symmetry. They show a sharp reduction over the first 5 values, but the decay slows to a lower rate soon after. The spatial compression, however, shows extremely rapid reduction in singular values, reducing by 6 orders of magnitude by the 6th value. These singular value profiles are to be expected and actually provide indicator to where the complexity in the problem lies. That is, the angular dimension is more complex to resolve than the spatial dimension, hence the slower rate of reduction in the angular singular values.

An unseen problem was analysed using the nominal value material cross-section of Table 4. A comparison of the scalar flux solutions from the full order model and ROM_{5,5} and ROM_{10,5} are presented in Fig. 11. Visually all three solutions appear very similar, with the higher order angular ROM being almost identical to the full-order model. Fig. 12 presents the angular flux solutions at 4 different locations within the domain, and provide comparisons between the full order model, S_6 , ROM_{6,4} and ROM_{10,4}. These

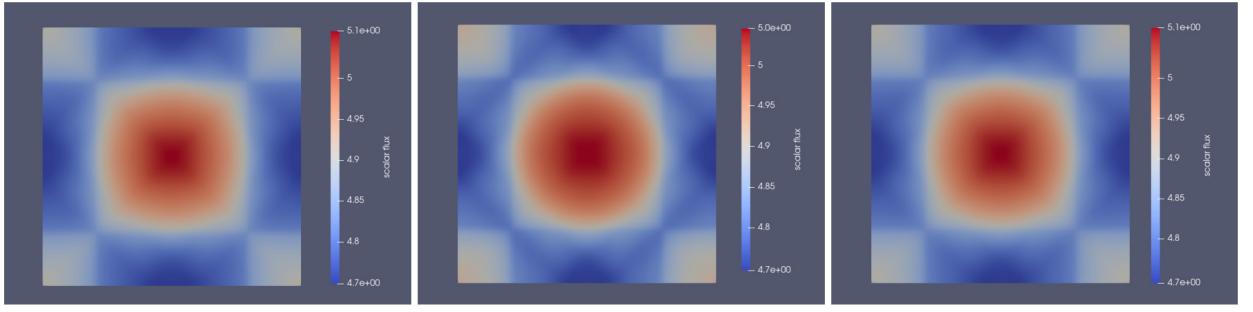


Fig. 11. Scalar flux solutions of the pin cell problem. Left to right: S_{32} , $ROM_{5,5}$, and $ROM_{10,5}$.

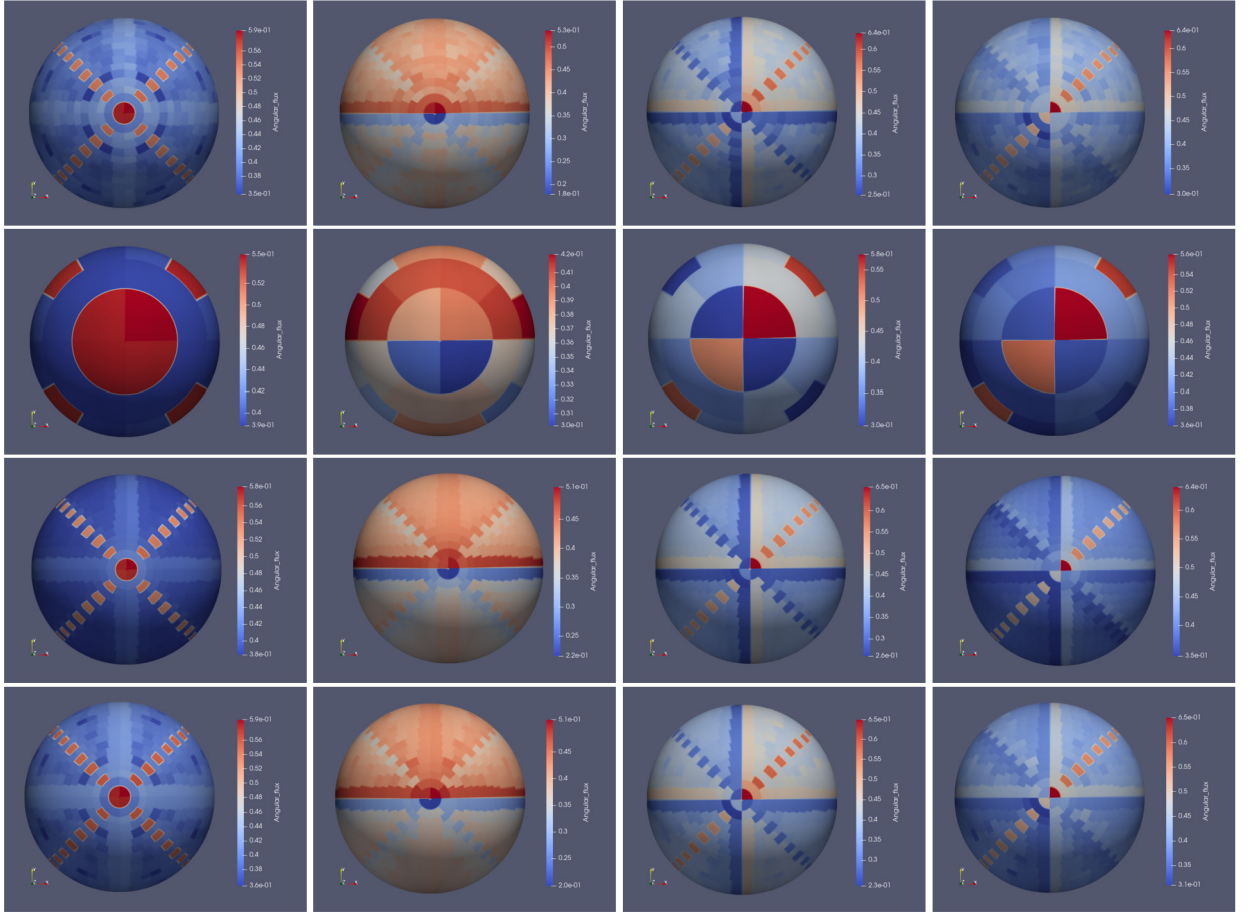


Fig. 12. Left to right: Angular flux solutions of the pin cell problem at positions (0.64,0.64), (0.64,1.0), (1.04,1.04) and (0.8,0.8) cm. Top to bottom: solutions from S_{32} , S_6 , $ROM_{6,5}$, $ROM_{10,5}$.

profiles demonstrate the complexity within the angular flux solutions. The $ROM_{6,4}$ and S_6 are included as both have the same DoF in the angular domain, but it is clearly shown how the ROM is superior in capturing the complex detail. The higher resolution ROM is in close agreement with the full-order solution, demonstrating that for complex angular flux profiles, the ROM can perform well using a modest number of basis functions.

The left graph of Fig. 13 presents the 2-norm error in the scalar flux solution vector as a function of angular resolution. It compares the ROM with S_N for varying angular resolution when the spatial resolution was kept constant. The S_N model used the same FEM mesh as the full-order model whilst 3 ROM spatial resolutions were studied using 1, 3 and 5 spatial basis functions. The ROM provides about 1 to 1.5 order of magnitude reduction in the solution error in comparison to S_N for the same angular size. Furthermore only small gains in error reduction are found by increasing the ROM's spatial resolution. These results again supports the idea that this is an angular complex problem to resolve. The right graph of Fig. 13 presents the scalar flux errors as a function of CPU solver time.

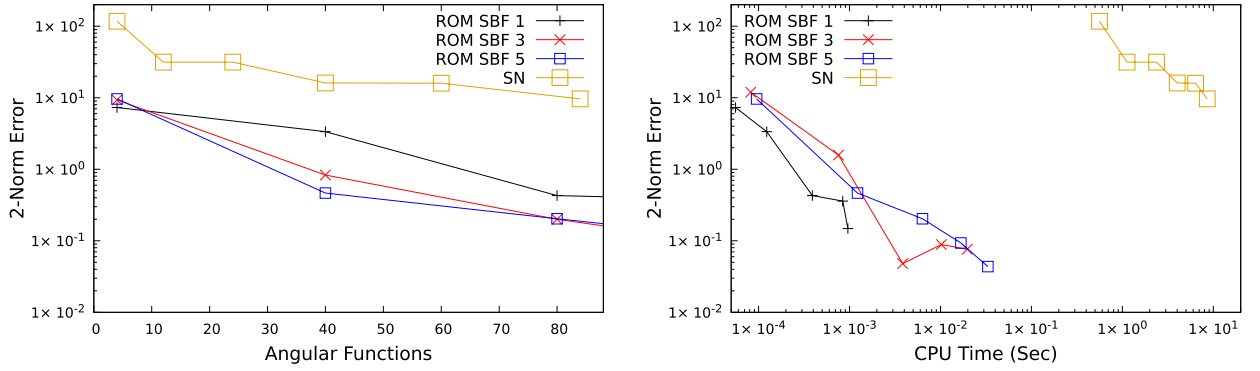


Fig. 13. Scalar flux solutions errors as a function of angle resolution (left) and time (right). Comparisons made with S_N and ROM using 1, 3 and 5 spatial POD basis functions (SBF) per angular basis functions.

Table 5

Comparison of model and projection error measures in the angular flux solution. ABF denotes angular basis functions per octant, SBF denoted the spatial basis functions per angular function.

	Projection Error			Model Error		
	SBF 1	SBF 3	SBF 5	SBF 1	SBF 3	SBF 5
ROM resolution						
ABF 1	11.6	11.6	11.6	11.7	12.6	12.7
ABF 10	2.0	2.0	2.0	3.8	3.0	2.6
ABF 20	1.0	1.0	1.0	1.5	1.7	1.8

Again the same ROM and S_N models are compared and the graph shows a huge reductions in solver times using the ROMs, for the same solution errors, that have exceeded 5 orders of magnitude.

Table 5 provides a comparison between the ROM's modelling errors and its projection errors for varying angular and spatial resolution. The errors are defined as,

$$e^m = \|\Psi - U\hat{\Psi}\|_2 \quad \text{and} \quad e^p = \|\Psi - UU^T\Psi\|_2, \quad (37)$$

where the vectors Ψ , $\hat{\Psi}$ and operators U relate to the full angular flux vectors of equation (27), where the subscript g has been omitted for simplicity. The model error e^m measures (in the 2-norm sense) the difference in the angular flux vectors of the exact (full model) solution and the ROM solution when projected onto the full model space. The projection error e^p measures the difference between the full model's angular flux solution and its projected form - i.e. when first mapped onto the ROM space, and then back to the full space, by pre-multiplying the exact solution by UU^T . As previously shown, the reductions in errors are largely affected from increasing the angular resolution. For low angular resolution, the model and projection errors are of very similar size which indicates the model introduces negligible errors in comparison to what the ROM can realistically achieve. However, as the angular resolution is increased, the ROM model does introduce additional errors but these are not excessive as they are all within a factor of 2 in comparison to the projection error. This provides assurances that the model described in equation (32) can form accurate solutions for a given ROM resolution, but also that there is room for future developments for improving accuracy further.

A final analysis compares the accuracy of the ROM model against the ROM when the solution coefficients are computed via interpolation of the projected snapshots, with respect to the material cross-sections. Similarly it also compares the ROM accuracy against a full order model that is generated via interpolation of the snapshot data, again with respect to the material cross-sections. To conduct this analysis, a new snapshot data set was formed from 16 full model solutions where the four nominal cross-sections of Table 4 were varied, one at a time, by $\pm 2.5\%$. The unseen problem was then defined to be that using the nominal material cross-section values which, since being at the mid-points of the snapshot data, meant the interpolated solutions of the full model, Ψ^{int} , and ROM, $\hat{\Psi}^{int}$, could be constructed via a simple average,

$$\Psi^{int} = \frac{1}{16} \sum_{s=1}^{16} \Psi^s \quad \text{and} \quad \hat{\Psi}^{int} = \frac{1}{16} \sum_{s=1}^{16} U\Psi^s. \quad (38)$$

The ROM errors are presented in Table 6 for varying model sizes. As previously seen for this problem, the angle resolution is the dominant factor in reducing model errors. Furthermore the ROM solution generated via interpolation shows modest reductions in error in comparison to the ROM. Here the difference is just under a factor 2 for the lower ROM expansion sizes, but this reduces to a factor of just 1.2 as the resolution is increased. Compared against the interpolated full order model, the errors of the highest resolution ROMs, and interpolated ROMs, are within a factor of 3 to 4 greater, respectively.

Table 6

Comparison of angular flux error in the interpolated (Int.) full order model, interpolated ROM solution and ROM model.

	ROM Int. Error		ROM Model Error		FOM Int. Error
ROM resolution	SBF 1	SBF 3	SBF 1	SBF 3	
ABF 1	11.7	11.7	11.7	12.6	–
ABF 10	2.0	2.0	3.8	3.0	–
ABF 20	1.0	1.0	1.4	1.7	–
ABF 40	0.34	0.34	0.41	0.46	–
ABF 60	0.13	0.13	0.16	0.17	0.04

4. Conclusion

This article has presented a new reduced order model for resolving the space-angle dimensions of the Boltzmann transport equation. The novelty lies in the construction of optimised basis functions that first resolve the angular distributions of the angular flux, followed by a second set of optimised spatial basis functions that resolve the spatial variation of the optimised angular functions. The ROM was based on the use of proper orthogonal decomposition, together with the method of snapshots, which used the solutions of a full-order model using finite elements and discrete ordinates. The model has been applied to two reactor physics type applications, the first an eigenvalue problem of quarter core resembling a BWR, and the second a fixed source neutronics problem of a fuel pin surrounded by a moderator. The two problems were selected as they exhibit different types of complexities in their flux solution profiles, thus they examine a range of problems that may occur in general reactor applications.

It has been demonstrated here that the ROM is capable of resolving the two problems studied both efficiently and accurately. Here the reductions in model size exceeded 5 orders of magnitude which led to similar sized reductions in computer solver times in comparison to a full-order model. A powerful aspect of this ROM is that the separation of the space-angle functions allows flexibility in choosing the resolution applied to each dimension. The fuel pin example showed the angular dimension required higher resolution than the spatial dimension, whilst for the reactor core the resolution was about the same. This flexibility allows appropriate resolution to be applied which, in turn, helps to keep the size of the ROM to a minimum.

Interestingly it was shown for the two problems studied the number of snapshots required to build the ROM was modest in size. Only a few tens of full-order solutions were required to construct a ROM that could then accurately predict other problems with variations in their material cross-sections. The numerical examples presented here were centred on probing assumed uncertainties in the material data and the analysis has shown the approach to be effective for the uncertain ranges considered. This demonstration also provides weight that the approach would likely be effective in other analysis involving moderately varying nuclear materials, such as including feedback effects due to temperature changes, or small changes to fuel compositions. However, further testing, and possibly additional model developments, would be needed for other applications for larger variations in material data, for example in fuel burnup calculations, moving control rods and core-level calculations with varying positions of burnable poisons within assemblies. Further analysis showed interpolation of the ROM basis functions, with respect to the material cross-section used in generating the snapshot data, yielded modest improvements in accuracy in comparison to the ROM model based on Galerkin projection. Furthermore, for the pin-cell problem, the higher resolution ROM errors were within a factor of 4 greater than those when using interpolation of the snapshot data. This result, and that of the projection error analysis, first suggests that there is room for further improvements, perhaps by alternative ROM formulations, e.g. Petrov-Galerkin approaches, or by just using interpolation for problems when appropriate. Secondly it provides the user with a choice in whether the small errors incurred by the ROM is out weighed by the computational efficiencies it provides as an alternative of working directly with the full model space. Such model developments for improvements, together with the extension to larger whole core problems, will be the study of future works. At such a stage of development, it would be appropriate to compare the method against other ROMs for core analysis mentioned in this article, as well as other rapid modelling approaches such as [35].

CRediT authorship contribution statement

Andrew G. Buchan: Writing – review & editing, Writing – original draft, Software, Methodology, Investigation, Funding acquisition, Formal analysis. **Ionel M. Navon:** Writing – review & editing, Methodology. **Liang Yang:** Writing – review & editing, Visualization, Software.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Andrew Buchan reports financial support was provided by Engineering and Physical Sciences Research Council. Andrew Buchan reports a relationship with Engineering and Physical Sciences Research Council that includes: funding grants. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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A reduced order model discretisation of the space-angle phase-space dimensions of the Boltzmann transport equation with application to nuclear reactor problems

Buchan, Andrew G.; Navon, Ionel M.; Yang, Liang

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