Challenges in Neutron Transport Analysis for Nuclear Reactor Simulations

Anurag Gupta  
Reactor Physics Design Division

and

R.S. Modak  
Theoretical Physics Division

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Abstract

The most fundamental task in a nuclear reactor, is to follow the neutron distribution in order to maintain and control the nuclear fission chain reaction. The fundamental equation governing the average behavior of neutrons, is the linear form of Boltzmann transport equation. The core design simulations with neutron transport method are most complex and CPU-intensive jobs, in reactor design and analyses. For a designer it is imperative to perform these calculations with good accuracy and efficiency to try out various options. It is important for the code developers to use techniques involving minimum approximations and to use most recent numerical methods applied in tandem with the huge computing power available today. The present paper discusses some of these challenges.

Introduction

In nuclear reactor design, the most fundamental task is to follow the neutron distribution as a function of space, direction, energy and time, in order to maintain and control the nuclear fission chain reaction. The fundamental equation governing the average behaviour of neutrons is given by the linear form of Boltzmann transport equation, which is an integro-differential equation. The core simulations involving the solution of the neutron transport equation are very CPU-time-intensive and require the best of numerical and computational schemes. It is because of this reason, most of the preliminary core design calculations are done with diffusion theory, which is a popular approximation to the transport theory.

Because of time consuming nature of transport simulations, huge efforts have been made internationally, over many decades, to obtain a reasonable solution in acceptable CPU-times. Over the years, researchers have proposed many new discretisation schemes, numerical techniques, acceleration methods and computing styles, to reduce the computing time. These schemes are devised or modified in tandem with the availability of computing power at that moment. High performance computing tools such as sophisticated programming styles and parallel computing are regularly used, to enhance the efficiency of the computer codes.

There are several numerical schemes applied to discretise the transport equation and its variants, for a variety of
geometrical configurations. Prominent among them are finite difference, nodal, modal and finite element methods. The current international interest is to have methods that work for general geometries such as Method of Characteristics, mesh-less methods etc. Discretisation of the neutron transport equation may give rise to either a system of linear equations (source problem) or to an eigenvalue system (criticality problem). These coupled systems are huge, involving millions of unknowns and there may or may not be an explicit generation of coefficient matrices. Sophisticated numerical algorithms are available to solve these systems efficiently. One such group of methods is the Krylov subspace class of algorithms which are of current international interest. The convergence properties of the Krylov methods are usually better and they are generally suitable for parallelization.

**Challenges in Neutron Transport Simulation of a reactor core**

A nuclear reactor in practice, is a very complex device. It contains a core which may have a series of fuel rods or pins arranged in a particular fashion. There can be a moderator material to slow down the high energy neutrons, a reflector to contain the neutrons within a domain and a coolant to remove the heat. There can be several controlling devices and measurement equipment. Then there are structural and appropriate shielding materials.

The challenge is to compute the power or neutron flux in each of the fuel pellets in the fuel pins, stacked as clusters in fuel assemblies and this has to be done:

- for complicated geometries and with challenging physics,
- as a function of time over a fuel cycle,
- various core configurations, control rod situations,
- with nuclides depletion and production,
- including feedbacks from coupled heat transfer and coolant flow,
- with novel structural and support materials,
- with acceptable accuracy and efficiency.

**Complex Physics of neutron-nucleus interactions**

The physics of neutron-nucleus interaction itself is complex. The cross-sections depend on energy as shown in Fig. 1 and there are resonances which further complicate the calculations of reaction rates. Thus, the cross-sections depend very sensitively on neutron energy and material temperature. Moreover, the neutron-nucleus scattering interaction can be anisotropic in lab frame. The time-dependent calculations present further challenges: a fraction (<1%) of fission neutrons are emitted with a delay. This does not affect steady state situations, but have a huge impact on transients, in fact they dominate any time dependent behaviour of the core. Hence it is imperative to calculate precursor concentrations and decay rates along with neutron flux.

![Fig. 1: Cross section as incident neutron energy](image)

**Multi-physics Multi-scale problem**

The changes in the temperatures and densities of fuel, coolant and moderator materials, result in change in absorption and production of neutrons, leading to change in core reactivity. This leads to power gradients which further alter temperatures, densities and flows. Thus another challenge is presented in the form of a coupled multi-physics system with variable scale problems to handle (Fig. 2).
**Efforts to Solve the Problem**

Conventionally, there are two steps of numerical transport simulations: lattice and whole core. Parameters are obtained by homogenizing a lattice and fed as input to the whole core calculations (Fig. 3). This may lead to a faster solution without significant loss of accuracy but still the whole core calculations are very CPU-time-intensive.

Similarly other variables are also discretised by appropriate schemes. The discretised transport equation is conventionally solved by the well-known inner-outer iterative procedure (Lewis and Miller, 1993). There are several computer codes developed over many decades which are based on inner-outer procedure.

**Transport Core Calculation Without Spatial Homogenization**

Traditionally, the core simulations are done in two steps: lattice and core. This procedure was followed as not enough computing power was available in the past. The accuracy of the homogenisation is a concern. With enormous computing power available today, there is a recent trend to explore the whole core simulations without any spatial homogenisation. Such simulations require the best of modelling, solution algorithms and massive parallelization techniques. Recently, an NEA benchmark (Fig. 4) was proposed to test the accuracy of modern deterministic transport methods when applied to reactor core problems without spatial homogenization (Smith et. al. 2006).

**Solution of Source Problem: the TSA and Conjugate Gradient method**

It is well-known that for optically thick and highly scattering regions, the convergence of inner iterations is very slow (Lewis and Miller, 1993) leading to large CPU times. Two major schemes have been suggested to accelerate these iterations: the Coarse Mesh Rebalancing (CMR) and the Diffusion Synthetic Acceleration (DSA). The DSA scheme was considered particularly attractive and considerable studies have been done (Adams and Larsen, 2002) on it. The Transport Synthetic Acceleration (TSA) is an improvement over the DSA, where the “corrective equation” is approximated by a transport
equation with lower quadrature order and strictly isotropic scattering rather than a diffusion equation. The TSA-CG method was applied to a variety of 2-D and 3-D cases (Gupta et al., 2008). In almost all the cases, a good speedup was obtained. Fig. 5 shows the reduction in the number of iterations with TSA-CG, for each of the 42 groups, for a representative 2-D case.

A Krylov sub-space method called Orthomin(1) was proposed by Suetomi and Sekimoto (1991) for 2-D k-eff diffusion problems. An attempt has been made to apply this method to neutron transport problems. A direct implementation of the algorithm seemed very difficult as one has to generate coefficient matrices and there will be problems such as commonly occurring negative fluxes. To overcome this, a quite different approach based on fission-sources is suggested. In this approach, the K-eigenvalue problem can be written as $P\mathbf{f} = \mathbf{Kf}$, where $P$ is a square matrix called "fission matrix" and eigenvector $\mathbf{f}$ consists of mesh-wise fission source densities. The scheme was introduced in 3-D code ATES3 (Gupta and Modak, 2005) and applied to realistic 3-D cases. It was found that the Orthomin(1) works even better when applied with TSA. Fig. 6 show the effect of Orthomin(1) and TSA schemes on the CPU-times for a run for an LWR benchmark and AHWR critical facility.

**Acceleration of K-eff Problem: Orthomin(1)**

The solution of K-eigenvalue problem is commonly required for the analysis of fission-based systems. The prime interest is to evaluate the fundamental mode eigenvalue ($K_{\text{eff}}$) and the associated shape of neutron flux. The problem is usually solved by the power iteration method, to find the fundamental mode. This involves solution of fixed source problem in each group which includes the well-known mesh-angle sweeping procedure (Lewis and Miller, 1993). Several attempts have been made (Adams and Larsen, 2002) to obtain an efficient solution of K-problem, such as shifted power iteration, coarse mesh rebalancing and Chebyshev acceleration.
General Geometry methods

One of the disadvantages that deterministic solution of neutron transport simulations have, is that they require a geometrical grid for the solution. On the other hand, stochastic Monte Carlo methods are routinely used for core calculations as they have advantage of general geometry, but their use is limited. Researchers always wished for a deterministic general geometry method and MoC is one of current international interest. In MOC, the transport equation is solved along straight lines at the discrete number of spatial angles. These lines are known as characteristics. The method has advantages in terms of parallelisation too. There exist several codes now, which use MoC to whole core calculation (Smith et al. 2006).

Conclusions

The neutron transport simulation of a reactor core is one of the most challenging jobs in reactor design and analysis. The present article offers a glimpse into how the problem is tackled. We discussed methods which are developed in-house as well as current international trends. As more and more computing power becoming available, researchers are now exploring methods without spatial homogenization, general geometry capabilities and possible use of point data libraries. Apart from stochastic Monte Carlo simulations, approaches like Method of

Characteristics and Meshless methods are now gaining momentum along with irregular grid based deterministic solutions. Advanced solution algorithms like Krylov subspace methods are becoming popular to solve coefficient matrices. Research is now more focussed on methods which use minimal approximations and provide higher accuracy.

References