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The Laputa code for lattice physics analyses

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ABSTRACT

A new lattice physics code called Laputa is currently under development at Tsinghua University. Aiming at the neutronics design of typical LWRs and advanced reactors, both the recent and traditional methodologies are integrated in the code. Laputa is able to model 2D arbitrary geometries by means of the combinational-geometry approach that has been commonly used in Monte Carlo codes. The method of characteristics (MOC), with the CMFD acceleration and OpenMP parallelism technologies, is implemented as the transport solver. The newly-proposed embedded self-shielding method (ESSM) is realized in Laputa for resonance treatment. Besides, an advanced matrix exponential method is implemented for solving the Bateman equations in the depletion module. Numerical validations against Monte Carlo solutions demonstrate that Laputa is very promising for lattice physics analyses.

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1. Introduction

The current LWR neutronics analysis generally adopts the two-step procedure consisting of the lattice physics analyses and the core calculations. The lattice physics analyses are performed on the pin/assembly level, in order to process tabulated cross-sections for the subsequent core calculations. The Laputa code is a lattice physics code developed by Institute of Nuclear and New Energy Technology (INET), Tsinghua University. The motivation of developing Laputa is to link it with an in-house core analysis code CPACT (Hu et al., 2010), and finally to provide neutronics analysis capabilities for future reactor design.

During the Laputa development, we have been trying to extend its application to not only the typical LWRs but also advanced reactors. This may be realized by incorporating the most recent methodologies and rigorous models, and trying to eliminate the unnecessary assumptions existing in the conventional lattice physics codes. Currently, the Laputa code has implemented the capabilities as follows:

- The geometry is represented by the combinational-geometry approach, which has been commonly used in many Monte Carlo codes such as MCNP (X-5 Monte Carlo Team, 2003). It enables Laputa to treat the complicated 2D geometries with general quadratic surfaces and multi-level nested lattices.
- The Laputa transport solver uses the method of characteristics (MOC) (Askew, 1972) with the acceleration technologies including the exponential function table, the CMFD acceleration and the OpenMP parallelism.
- At the current stage, Laputa uses the cross-section and depletion libraries that are converted from the Dragon-format open-source libraries (Hébert, 2014). These libraries have detailed data for resonance treatment and burnup calculation.
- A so-called embedded self-shielding method (ESSM) (Hong and Kim, 2011; Williams and Kim, 2012) is implemented for resonance treatment. The ESSM gives satisfactory accuracy without restrictions in geometry.
- By incorporating the recent progress on depletion algorithms, an efficient matrix exponential method based on the quadrature rational approximation (Pusa, 2011) is implemented for solving the burnup equations.

Laputa is written in the modern C++ programming language. Standard template libraries are generally used to improve the code's efficiency and maintainability. Besides, an open-source cross-platform graphics library called CImg (Tschumperlé, 2014) is utilized for visualization.

The methodologies and code capabilities are introduced in details in Section 2. Section 3 presents the code-to-code validations. Numerical results of various examples calculated by Laputa are compared with the Monte Carlo solutions. Finally, concluding remarks are presented in Section 4.

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2. Methodologies and code capabilities

2.1. Geometrical modeling

In order to flexibly describe the complicated reactor geometries, Laputa adopts the combinational-geometry model (X-5 Monte Carlo Team, 2003) that has been commonly existing in Monte Carlo codes. The geometry is modeled by surfaces, cells, universes and lattices, as illustrated below.

- A surface is defined by an analytic equation. Laputa supports the general quadratic surfaces such as the planes, cylinders, parabolas, hyperbolas and etc.
- A cell is defined by the intersections, unions, and complements of the areas bounded by predefined surfaces. The cell usually has a homogeneous material, or is filled with a universe that is described below.
- A universe consists of a set of non-overlapping cells which cover a complete space. One universe can be filled into a cell in another high-level universe, and coordinate transformation is allowed if needed. This feature makes it convenient to model complicated structures by using multi-level universes.
- One special kind of universe is referred as lattice, which is usually used to describe the repeated/nested geometries. Laputa currently supports the rectangle lattice and the hexagonal lattice.

With the combinational-geometry model, Laputa is able to treat a wide range of complicated reactor geometries. Besides, a geometry-plotting capability is developed to help users check geometry input. The geometry-plotting interface gives an interactive view of the system at different scales and coordinate origins.

2.2. MOC implementation

Due to its advantage in handling complicated geometry, the method of characteristics (MOC) is widely used for neutron transport calculations. General introductions on the MOC can be found in many existing references. In this section, we focus on the implementation of MOC in the Laputa code.

2.2.1. Cyclic tracking

Laputa uses the cyclic tracking approach, which is also known as the long characteristic method. Azimuthal angles are specifically disposed in order that the tracking paths at symmetrical azimuthal angles are linked to be closed cycles. The cyclic tracking approach gives convenience to the boundary condition treatment. As for the reflective boundary, one track's incoming flux at the boundary surface is equal to the outgoing flux of the symmetrical track in the cycle, and therefore no interpolation need be done. For simplicity, it is currently required that the reflective boundaries are rectangular surfaces. The design of cyclic tracking becomes somewhat complicated in case of hexagonal or other types of boundary surfaces, which is still under development in Laputa.

Similar to the geometry-plotting function mentioned in, a track-plotting function is provided by Laputa to dynamically look at the tracks. For example, Fig. 1 gives the geometry plotting and track plotting of a super-cell structure.

2.2.2. Exponential function table

During the MOC transport sweeps, a very time-consuming part is calculating the exponential function $e^{-\Sigma_t s}$, where Σ_t is the total cross-section at the current energy group and material, and s is the segment length. Laputa replaces the native std::exp() function with an exponential table as follows.

At the initial stage, a list of e^{-y} is pre-calculated at an increment of $\Delta y = 0.001$ in the range of [0.001, 20]. That is, the exponential table is indexed as

$$\begin{aligned} &T[i] = e^{-y} \\ &i = 1000y, \quad 0.001 \leqslant y \leqslant 20 \end{aligned} \tag{1}$$

At the stage of calling exponential function e^{-x}, the exponent is divided into two parts:

$$\begin{aligned} &y = \mathrm{int}(1000x) \\ &\varepsilon = x - 0.001y < 0.001 \end{aligned} \tag{2}$$

If $y > 20$, simply let $e^{-x} = 0$. Otherwise, the following expression is used to calculate the exponential function:

$$e^{-x} = e^{-(y+\varepsilon)} = e^{-y}e^{-\varepsilon} \approx e^{-y}(1-\varepsilon) = (1-\varepsilon)T[1000y] \tag{3}$$

Numerical tests suggest that the exponential function table can save about 30% computational time without visible accuracy reduction.

2.2.3. Acceleration technologies

The Coarse Mesh Finite Difference (CMFD) acceleration has been applied very successfully to nodal methods (Smith, 1983). CMFD is also very useful for MOC criticality calculations in the large system with a high dominance ratio. The basic idea of CMFD is solving the diffusion equation using diffusion coefficients that preserve the neutron currents from the MOC solution. In the code implementation, however, we found that numerical instability may arise if the diffusion coefficients are evaluated from a far-from-converged MOC solution. Under such case, Laputa temporarily switches off the CMFD acceleration and restarts it at the next cycle.

Another acceleration technology is the parallel MOC computation. At the current stage, Laputa adopts a shared-memory parallelism with the OpenMP framework. The OpenMP implementation requires small modifications to the MOC subroutines and therefore is easy to maintain. However, the speedup gained by a pure OpenMP parallelism is limited, because the number of cores in a single node is not so many. In this regard, the MPI + OpenMP parallelism would be favorable for large-scale calculations.

2.3. Data library

At the previous stage, Laputa used the WIMS-format open-source library (IAEA/NDS, 2014) for self-shielding, transport and burnup calculations. The WIMS format has a simple structure and small capacity, and is relatively easy to implement. However, the WIMS-format library has been found to have restrictions in resonance treatment, depletion chains and some other physical models. Consequently, we turn to the open-source Dragon-format library, which essentially eliminates those mentioned restrictions. Table 1 gives comparisons between the WIMS-format and Dragon-format libraries.

The Dragon-format SHEM 361-group library is processed into sequenced isotope-dependent data blocks. Besides, an index file is produced for a quick access to data blocks. It is quite similar to the xdir file which used by MCNP to access the ACE libraries. The benefit of using an index-type library is that the code can load the minimal data as required, instead of loading the whole data.

2.4. Resonance treatment

Resonance treatment, i.e. the self-shielding calculation, might be one the most challenging tasks in deterministic transport calculations. The accuracy of the effective cross-section is crucial to the validity of lattice physics analyses. The various approaches to resonance calculations are generally classified into three categories:

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