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Large-scale Monte Carlo neutron transport calculations with thermal hydraulic feedback

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ABSTRACT

The Monte Carlo method provides the most accurate description of the particle transport problem. The criticality problem is simulated by following the histories of individual particles without approximating the energy, angle or the coordinate dependence. These calculations are usually done using homogeneous thermal hydraulic conditions. This is a very crude approximation in the general case. In this paper, the method of internal coupling between neutron transport and thermal hydraulics is presented. The method is based on dynamic material distribution, where coordinate dependent temperature and density information is supplied on the fly during the transport calculation. This method does not suffer from the deficiencies characteristic of the external coupling via the input files. In latter case, the geometry is split into multiple cells having distinct temperatures and densities to supply the feedback. The possibility to efficiently simulate large scale geometries at pin-by-pin and subchannel level resolution was investigated. The Wielandt shift method for reducing the dominance ratio of the system and accelerating the fission source convergence was implemented. During the coupled iteration a detailed distribution of the fission heat deposition is required by the thermal hydraulics calculation. Providing reasonable statistical uncertainties for tallies having large numbers of bins, is a complicated task. This problem was resolved by applying the Uniform Fission Site method. Previous investigations showed that the convergence of the coupled neutron transport/thermal hydraulics calculation is limited by the statistical uncertainty and exhibits strong nonuniform behavior. The stochastic approximation scheme was used to stabilize the convergence. In combination with the Uniform Fission Site method, uniform convergence was achieved.

1. Introduction

The increase of computer power enabled detailed nuclear reactor core simulations Smith and Forget (2013). High fidelity tools capable of simulating the processes occurring in nuclear cores have been developed worldwide Ivanov et al. (2014), Kotlyar et al. (2009), Weber et al. (2007) and Bernnat (2012). Since Monte Carlo transport provides the most accurate solution using only minimum approximations, it is the most natural candidate for estimating the fission heat distribution. Varying temperature fields require temperature correction of both the single and the double differential nuclear data. The main obstacles that have prohibited the high resolution simulation of large scale geometries have been the complications related to the introduction of the thermal hydraulic feedback. The code coupling has been done by the input files. In the case of **MCNP**, this requires splitting the geometry into artificial subvolumes. This is necessary, because to change the temperature in **MCNP** one provides distinct materials having nuclear cross sections prepared in advance at the temperatures of interest. This is a rather cumbersome procedure that requires the definition of a large number of cells. In the case of a single fuel pin, if axially 20 axial nodes are to be simulated, the coolant and the fuel cells have to be split in 20 subvolumes, where 40 different materials having the proper temperatures should be supplied. It is clear that this strategy is highly inefficient for a full core geometry. The large inputs created by the external coupling methodologies take hours for **MCNP** to process.

The varying moderator temperatures should be taken into account by providing the proper temperature dependent thermal scattering data. In contrast to the single differential data, double differential data can not be processed at arbitrary temperatures, because one has to provide the corresponding oscillation spectrum for the bound hydrogen nucleus. Therefore, a consistent methodology for correcting the temperature dependence of the thermal scattering data is needed.

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Simulating large scale geometries requires the introduction of effective variance reduction techniques and proper assessment of the fission source convergence. Since the fission heat deposition is tallied on a mesh having pin-by-pin resolution, obtaining reasonable variance for all tally bins requires simulating massive number of neutron histories if analog transport is run. Due to the nonuniform distribution of the relative error, simple increase of the number of histories is a very inefficient strategy. In this, case the variance is improved in the central part of the core and the improvement becomes insignificant moving towards the core periphery. To overcome this deficiency an effective variance reduction scheme is needed.

Monte Carlo criticality calculations use power iteration for estimating the dominant eigenvalue. The convergence of the power iterations is determined by the dominance ratio of the system. Large loosely coupled geometries have dominance ratio close to unity. In this case converging the fission source distribution is problematic. If the convergence is not achieved before tallying, the estimated scores are biased.

Coupled Monte Carlo calculations show nonuniform convergence behavior. To accelerate the convergence various relaxation schemes have been applied. By using under relaxation of the thermal hydraulics parameters it is possible to significantly accelerate the convergence of the coupled calculation. In all the cases, however, the convergence is directly correlated to the variance of the fission heat distribution. The variance causes osculations between the coupled iterations. Therefore, to improve the convergence behavior the variance of all tally bins needs to be improved. Due to the correlation between tally variance and convergence, ensuring uniform convergence of the coupled scheme is difficult. To ensure convergence the maximum variance of all fission heat bins should be less than the targeted convergence. These difficulties show that a relaxation scheme capable of lifting the correlation between statistical uncertainty and convergence is needed.

Temperature dependence of the nuclear cross sections.

2. Temperature dependence of the single differential nuclear data

One of the most powerful features of the Monte Carlo codes is the use of continuous energy nuclear data. Cross sections are reconstructed from resonance parameters and are stored on an energy grid with many thousands of energy points. This is a major difference in comparison with deterministic codes, where the energy dependence is usually averaged over an energy interval.

The nuclear cross sections depend on the relative velocity in the center of mass frame. Temperature motion of the target nuclei results in Doppler effect, one of the most important phenomena in reactor physics. The temperature dependence of the nuclear data is determined by the following convolution with the Maxwell–Boltzmann distribution $P(\mathbf{v},T)d\mathbf{v}$ McFarlane and Muir (1993), McFarlane and Kahler (2010)

$$\begin{aligned}\rho v\sigma(v,T) &= \int d\mathbf{v}'\rho|\mathbf{v}-\mathbf{v}'|\sigma(|\mathbf{v}-\mathbf{v}'|)P(\mathbf{v}',T)\\ P(\mathbf{v},T)d\mathbf{v} &= \left(\frac{M}{2kT\pi}\right)^{\frac{3}{2}}\exp\left(-\frac{M}{2kT}v^2\right)d\mathbf{v}.\end{aligned} \tag{1}$$

Here $\mathbf{v}$ is the neutron velocity, $\mathbf{v}'$ denotes the velocity of the target nucleus and $\mathbf{v}-\mathbf{v}'$ is the relative velocity. Clearly the cross-section depends of the relative velocity between the neutrons and the target nuclei. As the nuclei are in thermal motion, the relative velocity can change. This difference between the relative velocities rises to the Doppler deviation effect. The effect of Doppler broadening is shown in Fig. 1 for the 6.675 eV resonance of U_{92}^{238}. The resonances tend to become wider and reduce their amplitude. Exception are the v^{-1} cross section that remain unchanged. In general the area under a resonance does changes unless $E \gg \frac{kT}{A}$, where A is the mass number. In fact, each resonance develops v^{-1} tail. Constant cross section (for example, elastic scattering) develops a v^{-1} tail at low energies after Doppler-broadening McFarlane and Kahler (2010).

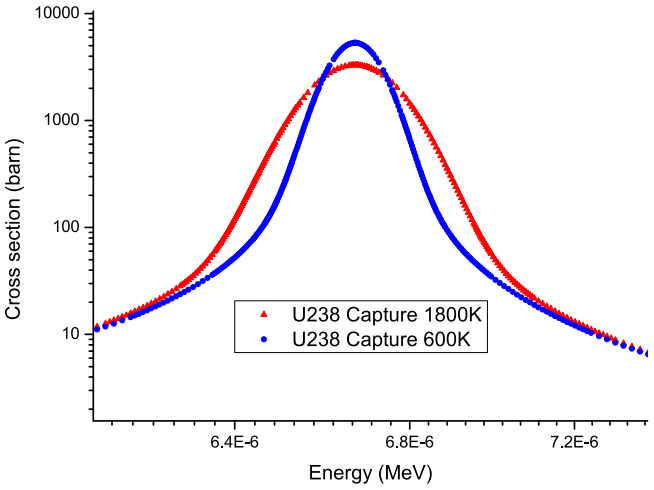

Fig. 1. Capture cross section for U_{92}^{238} evaluated at 600 K and 1800 K.

In principle, nuclear data processing codes like NJOY McFarlane and Kahler (2010) can process the single differential data at all desired temperatures. However, in some cases this might be an impossible task. In the case of a coupled calculation, where the thermal hydraulic calculation supplies fuel temperatures in the range 570–1200 K. Evaluating the data at 1 K increments for he entire range would pose serious memory storage challenges. The main problem being the presence of large amount of double precision data allocated on the heap. This will slow down the computation significantly, therefore, another method for correcting the temperature dependence is needed.

The temperature dependence of the nuclear data can be taken into account using pseudo material mixing Donnely (2011a). This method consists in mixing nuclear data evaluated at different temperatures, bracketing the temperature of interest. Doing so, the number of materials is doubled. This method relies on the stochastic nature of the computation. The probability for interaction with a particular type of nuclide is given by the weight of that nuclide. Modifying the weights of the different temperature evaluations changes the interaction probability. In practical terms this yields an effective cross section (2)

$$\Sigma_{\text{pseudo}}(T_{\text{actual}}) = f_{\text{low}}\Sigma_{\text{low}}(T_{\text{low}}) + f_{\text{high}}\Sigma_{\text{high}}(T_{\text{high}}). \tag{2}$$

The weights determining the concentrations of the 'low' and 'high' temperature evaluations are given by (3)

$$\begin{aligned}f_{\text{high}} &= 1 - f_{\text{low}}\\ f_{\text{low}} &= \frac{\sqrt{T_{\text{high}}} - \sqrt{T_{\text{actual}}}}{\sqrt{T_{\text{high}}} - \sqrt{T_{\text{low}}}}.\end{aligned} \tag{3}$$

The consistency of this methodology was verified Ivanov et al. (2013a, 2012) by comparing calculations performed with NJOY-BROADR processed data at specific temperature, and calculations performed with interpolated cross-sections at the same temperature by using pseudo materials. For the actual tests a 17×17 PWR fuel assembly with 24 guide tubes was used. Two cases were studied with UOX and MOX fuel. MOX fuel was chosen because the mixture of uranium and plutonium isotopes is expected to give higher sensitivity to thermal spectrum shifts than the UOX fuel. The MOX fuel contained 14 wt% plutonium, and the UOX was

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