Mathematical Framework for Coupling the AMP and Denovo Codes

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INTRODUCTION

An initial validation[1] of the AMP nuclear fuel performance package previously demonstrated capabilities on par with legacy fuel performance packages. However, in order to move towards a truly predictive software package, several issues must be addressed. In this study, a strategy is proposed to use the Denovo[4] radiation transport solver to generate spatially dependent neutron flux (and thus power) distributions as a heat generation source term for AMP, providing more accuracy than current problem-independent power shapes. Because Denovo solves the transport equation on a Cartesian mesh, whereas AMP uses an unstructured hexahedral mesh, transferring solutions between codes is a problem that must be addressed. We propose a strategy using polynomial expansions of the relevant quantities as an intermediary step to facilitate transfer between meshes. This paper outlines the mathematical framework for this mapping process.

MOTIVATION

Legacy fuel performance codes (such as FRAPCON[2]) typically use a problem-independent reference shape for the spatial distribution of the heat generation rate. In particular, the radial distribution is usually assumed to be a Bessel function, the analytic solution to the neutron diffusion equation in an infinite cylinder. Although this assumption is reasonable for many problems, the inability to take into account detailed, problem-dependent power shapes is likely to be a significant limiting factor for predictive simulations.

As an example, Fig. 1 shows the thermal neutron flux computed by Denovo for a 3×3 array of PWR fuel rods where the center rod contains a strong absorber (B_4C). Although the thermal flux in the corner rods appear azimuthally symmetric, it is evident that the rods adjacent to the absorber experience a dramatic deviation from such symmetry. In addition, steep gradients near the edges of the fuel rods are unlikely to be well represented with simple functions. Using a radiation transport solver to create power generation rates for specific problems will allow investigation into assembly-level effects outside the limits of axisymmetric assumptions.

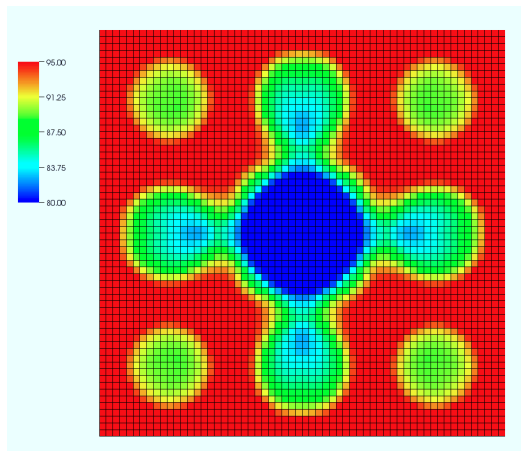

Figure 1: Thermal Neutron Flux near B_4C Rod

ZERNIKE POLYNOMIALS

The Zernike polynomials are a set of orthogonal polynomials defined on the unit disk[3]. Although they can be written purely as polynomials in x and y, the most common representation is in terms of the radial and azimuthal components, i.e.

$$Z_n^m(r,\theta) = R_n^m(r) g_m(\theta), \tag{1}$$

where Z_n^m is the Zernike polynomial of degree n and order m, R_n^m is a polynomial of degree n, and g_m is either a sine or cosine term. Although they are primarily used in the optics community, they are well suited to any application involving generally smooth quantities defined on a disk, particularly where separability of the radial and azimuthal components of the function is desirable or necessary. The Zernike polynomials form a complete set of functions on the disk so that any function f can be written as

$$f(r,\theta) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} f_n^m Z_n^m(r,\theta), \tag{2}$$

where f_n^m is the Zernike coefficient of degree n and order m for the function f. Provided that the function being represented is sufficiently smooth, the magnitude of these coefficients will decay rapidly and an accurate approximation of the function can be achieved with only a few terms in this series. Using orthogonality, the coefficients can be

computed with integrals over the disk as

$$f_n^m = \int_0^1 dr \int_0^{2\pi} d\theta Z_n^m(r,\theta) f(r,\theta). \tag{3}$$

These are the coefficients we will use to transfer solutions from a Denovo Cartesian mesh to an AMP unstructured mesh. Evaluating the integral in Eqn. 3 analytically is challenging because the intersection of Cartesian cells with the disk introduces complicated limits of integration. As an alternative, it is possible to approximate the integral using a quadrature formula on the disk. Quadrature formulas for integration on disks are readily found in the literature (e.g. 36 and 72 point formulas exactly integrating algebraic functions of degree 13 and 19, respectively[5]). It is important to note that, if a degree N expansion is desired then to maintain orthogonality it is necessary to choose a quadrature that accurately integrates functions of degree $2N$ (because the orthogonality relationship involves the product of two degree N functions). Thus, the 36 point quadrature should be sufficient for up to a degree 6 expansion and the 72 point quadrature for a degree as high as 9.

RESULTS AND FUTURE EFFORTS

In order to quantify the ability of the Zernike functions to represent neutron flux distributions, we compare specified functions to an Nth order Zernike reconstruction of those functions. The first test function is

$$F(r) = J_0\left(\frac{\nu_0 r}{R}\right), \tag{4}$$

where J_0 is the zeroth Bessel function of the first kind, ν_0 is the first root of this Bessel function, and R is the outer radius of the region. This function is the analytic solution to the diffusion equation in an infinite cylinder with radius R and also the radial flux distribution used in FRAPCON. The second test function is

$$G(x,y) = 1 + (1 + 0.4x)e^{-0.5(1-x^2-y^2)}. \tag{5}$$

This function is intended to reproduce several features likely to be present in the neutron flux distribution in a reactor lattice, such as sharp gradients near the outer boundary and significant azimuthal variation.

The reconstruction error for these functions for a range of Zernike expansion orders and for two different quadratures are shown in Fig. 2. The reconstruction error is computed using the infinity, or maximum, norm defined as

$$E = \|F - F_N\|_\infty, \tag{6}$$

where F_N is the degree N expansion of the function F. These results demonstrate that the Zernike functions are indeed a strong candidate for representing radial/azimuthal flux distributions within a fuel rod. It appears that an expansion order as low as 4–6 is sufficient to guarantee a reconstruction of the function with several digits of accuracy.

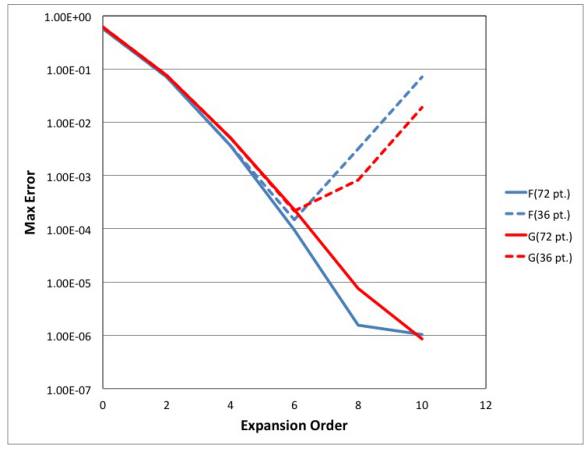

Figure 2: Convergence of Zernike Expansion

The divergence of the curves using the 36 point quadrature at $N = 6$ occurs due to a loss of orthogonality, as mentioned previously.

Preliminary functionality to compute the Zernike coefficients of a given flux distribution is now available for 2-D spatial discretizations in Denovo. Additional capability is also available in the 3-D discretizations by incorporating an axial shape function in the form of Legendre polynomial coefficients in addition to the radial/azimuthal distribution provided by the Zernike polynomials. Ongoing efforts aim to utilize these shape functions as source terms in AMP for multiphysics computations.

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