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The "virtual density" theory of neutronics

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ABSTRACT

Sustainable nuclear energy will likely require fast reactors to complement the current light water reactor paradigm. In particular, breed-and-burn sodium fast reactors (SFRs) offer a unique combination of fuel cycle and power density features. Unfortunately, large breed-and-burn SFRs are plagued by positive sodium void worth. In order to mitigate this drawback, one must quantify various sources of negative reactivity feedback, among which geometry distortions (bowing and flowering of fuel assemblies) are often dominant. These distortions arise mainly from three distinct physical phenomena: irradiation swelling, thermal swelling, and seismic events.

Distortions are notoriously difficult to model, because they break symmetry and repeating patterns. Currently, no efficient and fully general method exists for computing neutronic effects of distortions. Computing them directly via diffusion would require construction of exotic meshes that seldom exist within the neutronics community. Many deterministic transport methods are geometrically flexible but tightly constrained by assumptions of symmetry and repeating patterns. Monte Carlo offers the only high-fidelity approach to arbitrary geometry, but resolving minute reactivities and flux shift tallies within large heterogeneous cores requires CPU years per case and is thus prohibitively expensive. Currently, the most widely-used methods consist of various approximations involving weighting the uniform radial swelling reactivity coefficient by the power distribution. These approximations agree fairly well with experimental data for flowering in some cores, but they are not fully general and cannot be trusted to work for arbitrary distortions in generic cores. Boundary perturbation theory, developed in the 1980s, is fully general and mathematically rigorous, but it is inaccurate for coarse mesh diffusion and has never been applied in industry.

Our solution is the "virtual density" theory of neutronics, which alters material density (isotropically or anisotropically) instead of explicitly changing geometry. While geometry is discretized, material densities occupy a continuous domain; this allows density changes to obviate the greatest computational challenges of geometry changes. Although primitive forms of this theory exist in Soviet literature, they are only applicable to cases in which entire cores swell uniformly. Thus, we conceive a much more general and pragmatic form of virtual density theory to model non-uniform and localized geometry distortions via perturbation theory. In this work, we develop and implement virtual density theory entirely in the context of diffusion.

In order to efficiently validate virtual density perturbation theory, we conceive the "virtual mesh" method for diffusion theory. This new method involves constructing a slightly perturbed "fake" mesh that produces correct first-order reactivity and flux shifts due to anisotropic swelling or expansion of individual mesh cells. First order reactivities computed on a virtual mesh agree with continuous energy Monte Carlo to within 1σ uncertainty.

We validate virtual density theory via the virtual mesh method in 3-D coarse mesh models of the Fast Flux Test Facility (FFTF) and Jōyō benchmarks using the MATLAB-PETSc-SLEPc (MaPS) multigroup finite difference diffusion code, which we developed for this purpose. We model a panoply of non-uniform anisotropic swelling scenarios, including axial swelling of individual assemblies, axial swelling of each mesh cell in proportion to its fission power, and radial core flowering with arbitrary axial dependence. In 3-D coarse mesh Cartesian cores with explicit coolant gaps, we model individual assembly motion, assembly

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row motion with arbitrary axial dependence, and assembly row "s-shape" bowing. In all cases, we find that virtual density perturbation theory predicts reactivity coefficients that agree with virtual mesh reference cases to within 0.01%. These reactivity coefficients are two to four orders of magnitude more accurate than those computed via boundary perturbation theory. In general, this virtual density perturbation method can precisely predict reactivity coefficients due to anisotropic swelling or expansion of any core region in any direction.

1. A review of uniform isotropic virtual density theory

1.1. Introduction

Core reactivities are sensitive to geometry distortions arising from three distinct phenomena: (1) irradiation swelling of fuel throughout core lifetime, (2) thermal swelling of fuel during transients, and (3) mechanical oscillations during seismic events. Performing comprehensive reactivity analysis of these distortions requires methods for rapidly computing a multitude of small shifts. Traditionally, these reactivity effects have been studied via boundary perturbation theory developed by Pomraning, Larsen, Rahnema, and Favorite (Larsen and Pomraning, 1981; Rahnema and Pomraning, 1983; Rahnema and Pomraning, 1983; Rahnema, 1984; Favorite and Bledsoe, 2010). However, those methods were never applied to full-core 3-D reactor models, and there is evidence to suggest that multiple boundary perturbations interfere with one another (Favorite, 2010).

See Chapter 2 of Mark Reed's doctoral thesis (Reed, 2014), upon which this paper is based, for a thorough literature review of pre-existing geometric distortion modeling methods, especially boundary perturbation theory.

Thus, we introduce the "virtual density" theory of neutronics as a new perturbation method based on fundamentally different principles. Essentially, this virtual density theory converts geometric perturbations into equivalent material density perturbations, which are more accurate and much simpler to evaluate. In this section, we introduce and validate this technique for uniform isotropic cases, which include (1) swellings and expansions of simple analytic problems and (2) swellings of 2-D heterogeneous full-core models (isotropic swelling of 3-D core models is unrealistic).

In this work, we use the term "boundary" to include both "internal interfaces" and "external boundaries" as defined by Pomraning, Larsen, Rahnema, and Favorite. This is because, as we shall see, virtual density theory makes no distinction between these two types of perturbations.

1.2. The virtual density concept

For now, let us consider an idealized uniform core swelling in which every material in the entire reactor swells by the same factor. Of course, in real scenarios the liquid coolant would not swell at the same rate as other materials, but we will neglect that effect for now. Let the reactor volume be V, and let any given material atom density be N. If mass is conserved, then N will vary inversely proportional to V.

$$N \propto \frac{1}{V} \tag{1}$$

If we let λ be any given neutron mean free path in the core, then λ will vary proportional to V. Let Σ_t and σ_t be the macroscopic and microscopic total cross-sections, respectively.

$$\lambda \propto \frac{1}{\Sigma_t} = \frac{1}{N\sigma_t} \propto V \tag{2}$$

During this core swelling, the neutron mean free path increases at a rate greater than the rate at which all linear core dimensions increase. Thus, the net reactivity will be negative – the negative reactivity effect due to reduced material densities overcomes the positive reactivity effect due to increased core size, and so the net effect is increased leakage. This is true for any arbitrary reactor (homogenous or heterogeneous) except an array of infinite 1-D slabs, for which the net reactivity is precisely zero.

If we wished to keep reactivity constant during a uniform swelling of an arbitrary reactor, we would need to scale up the neutron mean free path proportional to the core linear dimensions ($V^{1/3}$).

$$\lambda \propto V^{1/3} \rightarrow N \propto V^{-1/3} \tag{3}$$

Thus, if we uniformly swell the core volume V and simultaneously reduce all core material densities proportional to $V^{1/3}$, the neutron leakage rate does not change. Of course, it follows that the relative magnitudes of neutron fluxes between internal core regions do not change such that the spatial neutron distribution does not change. Furthermore, because the relative proportions of all materials in the core are fixed, the neutron energy spectrum is also fixed. Thus, the reactor is essentially "scaled up" with no change to reactivity, spatial flux distributions, or local flux spectra.

1.2.1. Three axioms

Intuitively, we can summarize this generic principle with three closely-related axioms:

Axiom 1: Swelling all linear dimensions of any reactor by a certain factor while simultaneously reducing all material densities by that same factor will result in exactly zero change to reactivity and relative flux distributions.

Axiom 2: The reactivity and flux distribution effects of a uniform core swelling (or contraction) can be exactly replicated by manipulating material densities with no change to core geometry.

Axiom 2 is a direct logical consequence of Axiom 1. While Axiom 1 states that we can *counteract* a dimension change with a density change, Axiom 2 states that we can *replicate* a dimension change with a density change. Naturally, this begs for a third axiom:

Axiom 3: If any arbitrary dimensional change can be *counteracted* by a material change, then that same dimension change can be *replicated* by a different material density change.

These three axioms encapsulate the basic virtual density theory for isotropic expansions and swellings.

1.2.2. Definitions: "swelling", "expansion", "isotropic", "anisotropic", "uniform", "non-uniform"

Throughout this paper, we define a *swelling* as a dimension change with a corresponding density change that conserves mass. Thermal enlargement of a solid is one example of a swelling. In contrast, we define an *expansion* as a dimension change without