



“Virtual density” and traditional boundary perturbation theories: Analytic equivalence and numeric comparison



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ABSTRACT

We compare and contrast “virtual density” perturbation theory with the traditional boundary perturbation theory developed by Pomraning, Larsen, and Rahnama in the context of diffusion theory. First, after reviewing that literature, we mathematically prove that virtual density perturbations and traditional boundary perturbations are precisely equivalent for arbitrary 1-D problems, which constitute non-uniform isotropic expansions. We also mathematically prove that these two perturbation theories are equivalent for 2-D boundary shift problems, which constitute non-uniform anisotropic expansions. Extension of this proof to swellings or 3-D problems is straightforward. We compare the two theories numerically for a series of alternating uranium and sodium 1-D slabs in finite difference diffusion, and we show that virtual density theory predicts reactivities much more accurately and efficiently than traditional boundary perturbation theory. Boundary perturbation theory is often very inaccurate on a coarse mesh but converges to the virtual density solution as the mesh becomes finer. We also compare the two theories for axial assembly swelling in an abbreviated FFTF benchmark with a coarse mesh. Here we find that reactivity coefficients obtained via virtual density perturbation theory agree with reference solutions to within 0.1%, while those obtained via boundary perturbation theory exhibit sporadic accuracy – sometimes in the range of 1–5% error, more frequently in the range 5–20% error, and occasionally well over 100% error in control rod assemblies. We conclude that although virtual density perturbation theory and boundary perturbation theory are analytically equivalent, boundary perturbations in diffusion theory are often thwarted in coarse mesh finite difference solutions due to inaccurate flux gradients along mesh cell surfaces in heterogeneous cores.

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1. Introduction

Our original “virtual density” paper numerically validated non-uniform anisotropic virtual density theory against “virtual mesh” diffusion reference cases (Reed et al., 2018). Now we seek to ascertain how well virtual density theory performs relative to traditional boundary perturbation theory. Showing that our new theory works is nice, but showing how it compares to previous methods could “seal the deal”. This paper assumes that the reader is familiar with the original virtual density paper and refers back to that paper multiple times (Reed et al., 2018).

First, however, we demonstrate the analytic equivalence of virtual density perturbation theory and traditional boundary perturbation theory. This is important, because it represents an

analytic “proof” that “virtual density” theory is valid – if theory A has already been proven, and we subsequently prove that theory B is equivalent to theory A, we have therefore also proven that theory B is valid. Our original virtual density paper presented the theory based on physical and mathematical reasoning but provided no formal derivation (Reed et al., 2018). We now present that here.

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

2. A review of traditional boundary perturbation theory

Most classical perturbation theory literature is centered around one class of perturbations: material density changes. However, there is a second major class of perturbations: geometry changes. Pomraning aptly characterized the fundamental distinction

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between these two perturbation classes (Pomraning, 1983). Let $\epsilon \ll 1$ be a small perturbation parameter. Then material density perturbations are $O(\epsilon)$ cross-section changes over $O(1)$ volumes. In contrast, geometry perturbations are $O(1)$ cross-section changes over $O(\epsilon)$ volumes. Thus, geometry perturbations are inherently more difficult, because they require relatively large changes in cross-sections.

Komata published the first major paper on geometric perturbation theory in 1977 (Komata, 1977). He showed that one can convert a boundary perturbation into a boundary condition perturbation (Rahnema and Ravetto, 1998). This obviates part of the problem, but, of course, it only applies to external boundaries (where boundary conditions exist).

2.1. First order transport and diffusion (1980s)

Pomraning, Larsen, and Rahnema carried out most of the seminal work on boundary perturbation theory in both diffusion and transport simultaneously. Their first paper “Boundary Perturbation Theory” succeeded in becoming the revered authority (Larsen and Pomraning, 1981). Larsen and Pomraning derived explicit first order perturbation expressions (in both diffusion and transport) to evaluate reactivities due to small perturbations in the external boundary of a reactor. Their result for one-group diffusion is

$$\Delta\rho = \frac{\int dS |\vec{r}' - \vec{r}| D (\hat{n} \cdot \nabla \phi^\dagger) (\hat{n} \cdot \nabla \phi)}{\int dV \phi^\dagger \nu \Sigma_f \phi} \quad (1)$$

Here we have negated the vacuum boundary extrapolation condition. The denominator contains the usual core-wide fission source integration, identical to that in classic perturbation theory. The numerator contains a surface integral over the unperturbed surface S . The quantity $|\vec{r}' - \vec{r}|$ is the magnitude of the distance between the unperturbed surface \vec{r} and the perturbed surface \vec{r}' . The unit vector \hat{n} is perpendicular to the unperturbed surface. Although we have only written this for one energy group, the extension to multigroup is simple – simply sum up the numerator and denominator over all energy groups.

Shortly after deriving this formula for external surfaces, the trio began to study internal interface perturbations – slightly moving an internal boundary between two materials so that one material “substitutes” the other. However, Rahnema and Pomraning discovered an “anomaly” in the application of boundary perturbation theory to these internal interface shifts. Specifically, classic first order perturbation theory does not correctly predict the first derivative of reactivity as it does for material density changes. This “anomaly” does not appear in transport theory – it is an artifact of the diffusion approximation that appears at internal material interfaces (Rahnema and Pomraning, 1981). They corrected the “anomaly” and proposed a general expression for an internal interface perturbation in one-group diffusion:

$$\Delta\rho = \frac{\int dS |\vec{r}' - \vec{r}| Q}{\int dV \phi^\dagger \nu \Sigma_f \phi}$$

where

$$Q = (D_R - D_L) \nabla \phi_R^\dagger \cdot \nabla \phi_L + \phi^\dagger \left[\left(\frac{1}{k} \nu \Sigma_f - \Sigma_a \right)_L - \left(\frac{1}{k} \nu \Sigma_f - \Sigma_a \right)_R \right] \phi. \quad (2)$$

This applies to an internal interface shift to the right. The subscripts R and L denote quantities evaluated immediately to the right and left of the boundary. Note that although the flux gradient is discontinuous across the interface, the flux itself is always continuous. In terms of a material density perturbation, one could consider the R quantities to be the unperturbed case while the L quantities are the perturbed case. When a surface moves to the

right, the L quantities replace the R quantities. Also note that Eqs. (1) and (2) have an additional minus sign that does not appear in the literature, but this is only because $\Delta(1/k) = -\Delta\rho$.

Later on, Pomraning revisited this “anomaly” and derived another corrected first order perturbation formula for an internal interface shift in one-group diffusion theory (Pomraning, 1983):

$$\Delta\rho = \frac{\int dS |\vec{r}' - \vec{r}| Q}{\int dV \phi^\dagger \nu \Sigma_f \phi} \quad (3)$$

where

$$Q = -\frac{D}{D'} dD \nabla \phi^\dagger \cdot \nabla \phi + \phi^\dagger \left[\frac{1}{k} d(\nu \Sigma_f) - d\Sigma_a \right] \phi.$$

Here $d\Sigma_a = \Sigma_{a,L} - \Sigma_{a,R}$ and $d(\nu \Sigma_f) = \nu \Sigma_{f,L} - \nu \Sigma_{f,R}$. Similarly, $dD = D_L - D_R$, $D = D_R$, and $D' = D_L$. The two unperturbed flux gradients are evaluated to the right of the perturbation, because the rightward region is the unperturbed region. Conservation of (real and adjoint) current across the interface can allow one to convert the leakage term in Eq. (3) to that in Eq. (2). Note that Eq. (3) is precisely equivalent to Eq. (2). Pomraning simply re-formulates the perturbation in terms of a material density change.

Pomraning notes that Eq. (3) is fully general to both material density and boundary perturbations. In the case of a small material density perturbation, one can estimate $D/D' \approx 1$. Then the numerator in Eq. (3) is identical to a classic first order perturbation formula (for material densities).

These expressions in Eqs. (1)–(3) correctly predict the first order (one-group diffusion) reactivity due to small perturbations in external and internal boundaries. However, the predictions will only be correct if one has obtained very accurate (real and adjoint) flux gradients on the unperturbed boundary.

Rahnema and Pomraning derived one-group first order perturbation formulas for changes in various quantities (anything that is a linear functional of the flux – not just eigenvalue) due to changes in external boundaries in fixed-source problems (Rahnema and Pomraning, 1983). Rahnema and Pomraning later wrote a paper generalizing these methods to full multigroup transport and diffusion (Rahnema and Pomraning, 1983). This leap was crucial, as previous papers had demonstrated the methods only for simple one-group examples.

Pomraning showed that one can obtain first order estimates for reactivities due to non-analytic perturbations in the external boundaries of a reactor (Pomraning, 1983). The previous methods allowed for only an analytic continuous extension of the material adjacent to the external boundary, but Pomraning’s work here allows for adding arbitrary material compositions to the external boundary such that the boundary perturbation is “non-analytic”.

At last, Rahnema and Pomraning presented multigroup transport and diffusion perturbation formulas for internal interface perturbations coupled with material density perturbations (Rahnema, 1984). This was the final step in demonstrating that first order boundary perturbation theory was possible for both internal and external boundaries in both transport and diffusion.

2.2. Higher order transport and diffusion (1990s–2000s)

After the initial flurry of work by Pomraning, Larsen, and Rahnema, the literature is mostly silent on the topic for about a dozen years. Rahnema revisited the internal interface problem in the mid-1990s, and he re-derived the first order expressions via the “crossmultiplication” method (Rahnema, 1996).

Then, Gheorghiu and Rahnema developed the first higher order (variational) estimates of reactivity due to boundary perturbations (Gheorghiu and Rahnema, 1997; Gheorghiu and Rahnema, 1998). This work covers both transport and diffusion, but it is only valid

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