HETEROGENEITY EFFECTS IN NEUTRON TRANSPORT COMPUTATIONS

by

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I. NATURE OF PROBLEM

One of the fundamental numerical problems involved in the design of nuclear reactors is the computation of the neutron distribution, given a distribution of neutron sources. If we postulate that all neutrons move at the same speed the neutron distribution is governed by the one-group neutron transport equation, Eq. (1):

\[ \hat{\Omega} \cdot vF(r,\hat{\Omega}) + \Sigma_t(r)F(r,\hat{\Omega}) = \int \Sigma_s(\hat{\Omega}^{-} + \hat{\Omega},r)F(r,\hat{\Omega}^{-}) \, d\hat{\Omega}^{-} + S(r,\hat{\Omega}) , \]

\[ F(r,\hat{\Omega}) = vN(r,\hat{\Omega}) . \]  

We have assumed, here, that each neutron moves in a straight line until it collides with one of the nuclei in its environment. The density of neutrons is always so small that collisions between neutrons can be ignored. As a result the neutron transport equations is linear. In Eq. (1) \( \hat{\Omega} \) is a unit vector parallel to the neutron's velocity; \( v \) is the neutron's speed, and \( N \, dr \, d\hat{\Omega} \) is the number of neutrons, in the volume element \( dr \), with velocities in the solid angle \( d\hat{\Omega} \). The function \( F \) is generally referred to as the "angular flux".

When a collision occurs many different processes can ensue. The neutron might simply be absorbed and disappear; it may be scattered, and exit from the collision with a new velocity: in some cases it will enter the nucleus and trigger a fission event in which other neutrons will be emitted. If one thinks of the neutrons as spheres, then the \( \Sigma \)'s in Eq. (1) might be regarded as the total effective cross sections subtended by all the spheres in a unit volume. Since these are only effective cross sections,
the nuclei will subtend different cross sections for different processes. Thus $\Sigma_s$ in Eq. (1), is the cross section for scattering from $\hat{\Omega}$ to $\hat{\Omega}$ at point $r$. Finally $S$ is a neutron source density, considered here as a known function of $r$ and $\hat{\Omega}$. Note that Eq. (1) is grossly oversimplified in that many processes have been neglected. In particular, fission has been neglected. If $S$ is, in fact, the rate at which fission neutrons are born, per unit volume, then $S$ will be proportional to the neutron density and the transport equation will become homogeneous. The neutron flux $F$ is, then, the solution of an eigenvalue problem.

Of course neutrons do not all have the same energy. Neutrons born in fission have a broad spectrum of energies, and lose energy in each scattering collision. Thus the transport equation, in its most general form, is an integro-differential equation in six variables. The neutron position is characterized by three variables, and the velocity by three more.

Now, it is perfectly feasible to solve the general transport equation by Monte Carlo methods, and such methods play a very important role in reactor analysis. But Monte Carlo calculations are costly, and they do not provide us with the detailed information which the reactor designer and analyst needs. Therefore, Monte Carlo is not a wholly satisfactory substitute for deterministic methods. On the other hand, to solve the multi-energy transport equation, in all its complexity, by deterministic methods alone is still prohibitively expensive. In practice, then, it is necessary to make some drastic approximations in the transport equation before it can be solved routinely by the nuclear designer. These approximations, which may all be invoked simultaneously or introduced separately, fall into three main classes. First, the cross sections, which are complicated and jagged functions of energy, are replaced by relatively smooth energy
averages of some sort. This is a very important approximation, but one which involves a great deal of reactor physics which seems inappropriate here. I will assume, therefore, that the energy-averaging process has been carried out, somehow, and say no more about it.

Secondly, the cross sections, which may be very complicated functions of position, are often replaced by cross sections which are averaged over volumes whose dimensions vary considerably from case to case. I will discuss various aspects of this averaging process in some detail later.

Finally, the transport equation may be replaced by an equation which is much easier to solve, namely the diffusion equation. To bring out the relation between the transport and diffusion equations, I will derive the diffusion equation from the transport equation in a simple one-dimensional geometry.

Suppose a reactor is composed of plates oriented perpendicular to the x-axis. Imagine that the source and the cross sections depend only on x, and not on y or z. In this case the one-group transport equation takes the form

$$\mu \frac{\partial F(x, \mu)}{\partial x} + \Sigma_t(x) F(x, \mu) = \frac{1}{2} \int_s (\hat{\Omega} + \hat{\Omega}, x) F(x, \mu^-) \, d\mu^- + \frac{1}{2} S(x) \quad (2)$$

Here $\mu$ is the cosine of the angle between $\hat{\Omega}$ and the x-axis. For simplicity I have postulated that the source is isotropic, i.e. that it is independent of $\hat{\Omega}$. Now we expand the flux, $F$, in Legendre polynomials, retaining only the first two polynomials $P_0(\mu)$ and $P_1(\mu)$, and integrate over $\mu$. After some manipulation we get Eq. (3):
\[
\frac{\partial \psi(x)}{\partial x} + \Sigma_a(x)\phi(x) = S(x) ,
\]
\[
\frac{1}{3} \frac{\partial \psi(x)}{\partial x} + \Sigma_1(x)j(x) = 0 ,
\]
where
\[
\phi(x) = \int_{-1}^{1} F(x,\mu) \, d\mu ,
\]
\[
j(x) = \int_{-1}^{1} F(x,\mu) \mu \, d\mu ,
\]
\[
\Sigma_{s0} = \frac{1}{4\pi} \int \Sigma_s(\hat{O} \to \hat{O}^- , x) \, d\hat{O}^-, 
\]
and
\[
\Sigma_{s1} = \frac{1}{4\pi} \int \Sigma_s(\hat{O} \to \hat{O}^- , x) \hat{O}^- \cdot \hat{O}^- \, d\hat{O} .
\]

The quantities \(\phi\) and \(j\) are generally referred to as the scalar flux and the current. From the definition of \(j\) it is easy to show that this quantity is, in fact, the rate at which neutrons cross a unit area whose surface is normal to the \(x\) axis. Elimination of \(j\) from Eqs. (3) leads us, finally to Eq. (4),
\[
- \frac{\partial}{\partial x} \left( \frac{\partial \phi}{\partial x} \right) + \Sigma_a \phi = S , \quad D \equiv \frac{1}{3} \Sigma_1 , \quad -D \frac{\partial \phi}{\partial x} = j ,
\]
which is the neutron diffusion equation in slab geometry.
It has been assumed, implicitly, in our derivation that the diffusion coefficient, $D$, is a differentiable function of $x$. In practice, however, this will generally not be true. At interfaces between different materials the cross sections (and, consequently, the diffusion coefficient) will generally be discontinuous. It is necessary, therefore, that Eq. (4) be supplemented by appropriate auxiliary conditions at such interfaces. The conditions normally used can be obtained by the following argument. Suppose that the cross sections are not actually discontinuous, but that they vary rapidly over a thin boundary layer. One can easily show that, as the thickness of the layer goes to zero,

$$ D^- \left. \frac{\partial \phi}{\partial x} \right|_{x_0^-} = D^+ \left. \frac{\partial \phi}{\partial x} \right|_{x_0^+}, \quad \phi \left|_{x_0^-} = \phi \left|_{x_0^+} \cdot \right. \right. $$

In Eq. (5) $D^+$ and $D^-$ are, respectively, the diffusion coefficients immediately to the left and right of the interface. Equation (5) is the interface condition normally used in neutron diffusion computations.

A straightforward generalization of the procedure just described yields the neutron diffusion equation in three dimensions, Eq. (6):

$$ -\nabla \cdot D \nabla \phi + \Sigma_a \phi = S, \quad -D \nabla \phi = J, \quad \hat{n}_0 \cdot D^- \nabla \phi \bigg|_{-} = \hat{n}_0 \cdot D^+ \nabla \phi \bigg|_{+}, \quad \phi_- = \phi_+. \quad (6) $$

In Eq. (6) $\hat{n}_0$ is a unit vector normal to the interface; $J$ is, again, the neutron current, in the sense that $J \cdot \hat{n}$ is the rate at which neutrons cross a unit area whose unit normal vector is $\hat{n}$.

Since the diffusion equation is a good deal easier to solve than the neutron transport equation it is often used in place of the transport equation in situations where the implied approximations seem to be valid.
When the diffusion equation is used, quite frequently a two-step approximation procedure is involved. In one step the transport equation is replaced by the diffusion equation: in another step (generally referred to as "homogenization") the complicated position-dependent reactor parameters are replaced by spatially smooth averages. It is important to note that these two steps do not necessarily commute: when they don't, the spatial averaging must be carried out before the diffusion approximation is introduced. Otherwise the diffusion approximation may obliterate important transport effects which are due to heterogeneities in the original problem configuration.

The heterogeneity effects I will deal with here fall into two broad classes. First, cross-section discontinuities induce singularities in the solution of the transport equation, as in the solution of the diffusion equation. Singularities in the solution of the diffusion equation have been studied intensively for some time, and a good deal is now known about them. Singularities in the solution of the transport equation are much more complicated, and not nearly as well understood. It must be expected that the presence of singularities will degrade the accuracy of numerical approximation methods and complicate the formulation of higher-order difference equations designed for use in transport computations.

Secondly, heterogeneity effects which are large enough to influence reactor analysis and design must, somehow, be taken into account when the cross sections are homogenized. Since the detailed structure of the reactor cannot be represented explicitly in most reactor computations, all significant heterogeneity effects must be incorporated into a simplified, homogenized, model reactor, a model which is computationally tractable, yet realistic enough to be useful.
II. SINGULARITIES IN THE SOLUTION OF THE TRANSPORT EQUATION

The only independent variable which appears in the diffusion equation is the scalar flux. Singularities in the solution of the diffusion equation are, by definition, singularities in the scalar flux and its derivatives. On the other hand, the character of singularities in the solution of the transport equation is often most easily understood by examining the properties of the angular flux. Consider, for example, the behavior of the angular flux in the neighborhood of a vacuum boundary. If there are no neutron sources in the vacuum, and if the boundary of the diffusing medium is convex, no neutrons will enter the medium from the vacuum. But neutrons may leak from the medium into the vacuum. It is easy to show that, if \( \hat{n} \) is normal to the surface of the diffusing medium the angular flux will generally be discontinuous, as a function of \( \hat{n} \), at \( \hat{n} \cdot \hat{n} = 0 \).

The effect of this discontinuity on the scalar flux can be treated analytically in a simple model problem usually called the "Milne problem". The Milne problem configuration is sketched in Fig. 1. In the simplest form of the Milne problem neutrons are assumed to be monoenergetic, and the medium in which they move is a pure scatterer. That is to say that all collisions are scattering collisions: no neutrons are absorbed. An infinite plane source of neutrons is located at an infinite distance to the left of the planar boundary. It can be shown that as one moves to the left the scalar flux becomes, asymptotically, a linear function of \( x \). Near the boundary there is, however, a small zone in which the flux is not linear. In fact the scalar flux drops rapidly near the boundary, and its derivatives at the boundary are all infinite. It is to be expected that, unless special steps are taken to deal with this singularity, its presence will slow the convergence of any finite element or difference
approximation. The nature of this singularity is discussed in a paper by Abu-Shumays and Bareiss, who have developed a finite element approximation which incorporates the singularity into one of the basic functions. Numerical experiments show that the inclusion of such a basis function improves the performance of the finite element method, in this case, quite effectively.

But it should be noted that from a practical point of view, the Milne problem is not very important, not, at least, in reactor computations. And, as one might expect, practical problems are considerably more complicated. There is, however, a problem of some practical interest which is similar to the Milne problem. Suppose an infinite absorbing slab is embedded in an infinite medium, as in Fig. 2. In the slab, \( \Sigma_s = 0 \), i.e. all neutrons which collide in the slab are absorbed. You see that there are neutron sources in Regions 1 and 2 on either side of the slab, but not in the slab itself. Now consider the fluxes, at point P, in the two indicated directions. Most of the neutrons with velocities parallel to \( \hat{\alpha}_1 \), have travelled a long distance through the absorbing slab. The angular flux \( F(\hat{\alpha}_1) \) will therefore be small. On the other hand, neutrons moving along \( \hat{\alpha}_2 \) have not passed through the slab, and therefore \( F(\hat{\alpha}_2) \) may be relatively large. As in the Milne problem the angular flux will, generally, be discontinuous at \( \hat{\alpha} \cdot \hat{n} = 0 \). Not very much is known at this time, about the corresponding singularity in the scalar flux at the surface of the slab.

As soon as we turn our attention from slab geometry to other geometries the situation becomes still more complicated. It seems pointless, here, to try to enumerate all the singularities which might be encountered in transport computations. Instead I will consider, as an illustrative
example, the singular behavior of the angular flux at a corner point. It is easy to show that, in a simple model problem, the angular flux cannot have well-defined spatial derivatives at corners.

In Fig. 3 you see an infinite, purely absorbing, medium with constant cross sections, divided into two regions. If $\Omega_x$ and $\Omega_y$ are positive the angular flux, $F(\Omega_x, y)$, is continuous across the $x$ and $y$ interfaces. It follows that $\partial F/\partial x$ is continuous across the horizontal interface while $\partial F/\partial y$ is continuous across the vertical interface. At $P_1$, the flux satisfies the transport equation

$$\frac{\Omega_x}{\partial x} \frac{\partial F}{\partial x} + \frac{\Omega_y}{\partial y} \frac{\partial F}{\partial y} + \Sigma_t F = \frac{1}{4\pi},$$

while at $P_2$

$$\frac{\Omega_x}{\partial x} \frac{\partial F}{\partial x} + \frac{\Omega_y}{\partial y} \frac{\partial F}{\partial y} + \Sigma_t F = 0.$$
Now let \( P_1 \) approach \( P_2 \). If the partial derivatives exist at the corner point then, because of their continuity properties, it must be true that

\[
\frac{\partial F}{\partial x}{|}_{p_1} \rightarrow \frac{\partial F}{\partial x}{|}_{p_2}, \quad \frac{\partial F}{\partial y}{|}_{p_1} \rightarrow \frac{\partial F}{\partial y}{|}_{p_2}. \tag{9}
\]

But it is impossible for the flux to satisfy Eqs. (7), (8), and (9) simultaneously. It is clear, then, that the spatial derivatives of the angular flux at the corner must be undefined in at least one of the regions.

Figure 4 represents a more complicated configuration, where four regions meet at a point. The dotted line in Fig. 4 is drawn from the corner point, in a direction parallel to some arbitrary unit vector, \( \hat{n} \). Here \( \hat{n} \) is another unit vector, perpendicular to \( \hat{\alpha} \). It can be shown that, generally, the directional derivative \( \hat{n} \cdot \nabla F(p, \hat{\alpha}) \) is discontinuous at all points on the dotted line. This pathological behavior of the angular flux was first noted by Aruszewski, Kulokowski and Mika,\(^3\) who refer to the dotted line as a "singular characteristic". Of course each direction, \( \hat{\alpha} \), defines its own singular characteristic, along which the normal derivative of \( F(\hat{\alpha}) \) is discontinuous. The effects of corner points on the derivatives of the angular flux are closely examined in a recent paper by Kellogg.\(^4\)

Usually, in practice, the neutron transport equation is treated by what is called the "S\(_N\) method". Aruszewski, Kulokowski and Mika have shown\(^3\) that the indicated singularities in the angular flux have a deleterious effect on the accuracy of the difference equations normally used in the S\(_N\) method. These authors have proposed an alternative differencing scheme which takes into account the presence of the singular characteristics, and their test results using this scheme are encouraging. On the
other hand their difference equations are rather complicated and have never been tested in any full-scale, production-oriented, transport code. Apparently the discontinuities along the singular characteristics also have a noticeable deleterious effect in finite element calculations. Reed, at Los Alamos Scientific Laboratory, has studied the accuracy of finite element methods as applied, in various forms, to the transport equation. He finds that in a series of simple test problems the errors in scalar fluxes seem to be $O(h)$, whatever the order of his basis polynomials. Apparently theoretical results on the accuracy of the finite element method near corners (in transport computations) are totally lacking.

III. HOMOGENIZATION

So far I have simply assumed that the cross sections used in the flux computation are given functions of position, and have said nothing about their physical significance. In fact, these cross sections may be local cross sections in individual fuel pins, plates, or other reactor constituents, or they may be cross sections which have been averaged, somehow, over many different constituents. Individual reactor components are often represented explicitly in computations covering small subregions of a reactor, but it is generally impossible to incorporate fine details of the reactor's structure in computations which treat the reactor as a whole. In computations involving the whole reactor the cross sections and diffusion coefficients are usually average parameters which, in some sense, embody properties of all the materials in a fairly large, heterogeneous, subregion of the reactor. Many different processes have been used to obtain such homogenized parameters, and none are rigorously justifiable. All rely, to some extent, on engineering judgment. For the sake
of simplicity I will not attempt to describe any homogenization procedure
in full detail. I will, however, describe those features of a typical
homogenization process which seem to me to be most interesting and impor-
tant. Figure 5 represents schematically the core of a hypothetical reac-
tor, viewed from above. Each small square in the core is a subassembly
which might contain a fuel pin, as in A, or fuel plates as in B. The core
is, of course, finite in height, and surrounded by a blanket or reflector
region which is not shown. In this grossly oversimplified reactor each
subassembly would probably be homogenized, so that the core would be repre-
sented as a uniform, homogeneous medium, surrounded by a homogeneous
reflector or blanket.

The homogenization procedure would take a particularly simple form if
the core were infinite in all directions so that the homogenized reactor
would consist, simply, of an infinite homogeneous medium. I think it is
instructive to examine a homogenization procedure which might be used in
such a case.

Suppose, for example, that the subassembly is made up of plates, as
in Fig. 5B. Suppose, further, that the whole reactor is critical, i.e.
that the number of neutrons produced, per second, by fission is exactly
equal to the number captured. For simplicity we again assume that all
neutrons have the same energy. In this case the neutron transport
equation takes the form

$$
\hat{\Omega} \cdot \nabla F + \Sigma_t F = \frac{1}{4\pi} \Sigma_s \phi + \frac{1}{4\pi} \nu \Sigma_f \phi, \quad \phi = \int F \, d\hat{\Omega}. \quad (10)
$$

In Eq. (10) I have taken the scattering to be isotropic, i.e. I have
assumed that the probability that a neutron will be scattered into the
solid angle $d\hat{\Omega}$ is equal to $\frac{1}{4\pi} \, d\hat{\Omega}$: $\Sigma_s$ is the scattering cross section,
$\kappa_f$ is the fission cross section and $v$ is the average number of neutrons produced in a single fission event.

An operating reactor is held critical through the action of control rods and other control mechanisms. On the other hand we cannot expect that the model reactor represented in our computations will also be critical. Therefore, it is necessary to introduce into our computations a parameter which artificially maintains criticality, and appears in the transport equation as an eigenvalue. For computational purposes, then, we modify the transport equation as in Eq. (11):

$$\hat{\Omega} \cdot \nabla F + \Sigma_{f} F = \frac{1}{4\pi} \Sigma_s \phi + \frac{1}{4\pi\lambda} \gamma \Sigma_f \phi . \quad (11)$$

Equation (11), with its boundary conditions, determines a set of permissible values for $\lambda$. If our model is reasonably realistic, the maximum $\lambda$ will be close to one (perhaps within one or two percent of one) and the corresponding flux, $F$, will be reasonably close to the true flux in the reactor.

Suppose that at some point on a subassembly boundary, $\hat{n}$ is a unit vector normal to the boundary. For every vector, $\hat{\Omega}$, at the subassembly boundary one can define a mirror image vector, $\hat{\Omega}^-$, as in Eq. (12):

$$\hat{\Omega}^- = \hat{\Omega} - 2\hat{n}(\hat{\Omega} \cdot \hat{n}) . \quad (12)$$

Because of the symmetry properties of our hypothetical subassembly (properties often found in real subassemblies), one can show that, at each boundary point, $r_B$, the angular flux must satisfy Eq. (13):

$$F(\hat{\Omega}, r_B) = F(\hat{\Omega}^-, r_B) . \quad (13)$$
Given this condition it is not necessary to solve the transport equation over the whole reactor configuration. Equation (13) can be regarded as a boundary condition imposed on the flux in a single subassembly (or "cell"), and Eq. (11) can be solved in a single cell with this boundary condition.

If we integrate Eq. (11) over a single cell we get Eq. (14):

\[
\tilde{\phi} = \left(\frac{1}{V_{\text{cell}}} \right) \int_{\text{cell}} \phi \, dV ,
\]

\[
\tilde{\phi} = \left(\frac{1}{\phi V_{\text{cell}}} \right) \int_{\text{cell}} \Sigma_t \phi \, dV ,
\]

\[
\tilde{\phi} = \left(\frac{1}{\phi V_{\text{cell}}} \right) \int_{\text{cell}} \Sigma_s \phi \, dV ,
\]

\[
\nu_{\Sigma_f} = \left(\frac{1}{\phi V_{\text{cell}}} \right) \int \nu_{\Sigma_f} \phi \, dV .
\]  \hspace{1cm} (14)

It will be seen that Eq. (14) is simply the neutron transport equation for an infinite homogeneous medium with absorption cross section \( \tilde{\Sigma}_a \), and fission production cross section \( \nu_{\Sigma_f} \). Thus \( \tilde{\Sigma}_a \) and \( \nu_{\Sigma_f} \) are uniform cross sections for an infinite homogeneous medium which has the same eigenvalue as the original infinite lattice. If the core is very large (though not infinite) one might expect that the same \( \tilde{\Sigma}_a \) and \( \nu_{\Sigma_f} \) could still be used as homogenized core cross sections. But the homogenization prescription
defined by Eqs. (14) has a serious, and perhaps obvious, defect. In a real reactor, neutrons will leak from the core into the adjoining reflector or blanket. You will note, first, that we have not taken this leakage into account in any way in our very primitive homogenization procedure. Secondly, in any diffusion computation of the reactor eigenvalue, and of flux shapes in the reactor, we will need diffusion coefficients for the core, blanket, and reflector. I have, so far, suggested no procedure for the computation of such diffusion coefficients. In fact, the problems involved in computing homogenized diffusion coefficients are among the most difficult problems of reactor physics.

When one examines the prescriptions which I suggested earlier for the homogenization of absorption and fission cross sections, two ad hoc prescriptions for the computation of homogenized diffusion coefficients come to mind, both equally plausible. Recall that in a homogeneous medium, the diffusion coefficient is given by Eq. (15):

\[
D \equiv 1/3 \, \Sigma_1 \, , \quad \Sigma_1 \equiv \Sigma_t - \Sigma_{s1} \, ,
\]

\[
\Sigma_{s1} \equiv \frac{1}{4\pi} \int \Sigma_{s}(\Omega \rightarrow \Omega') \hat{\Omega} \cdot \hat{\Omega}' \, d\Omega' \, . \tag{15}
\]

One might think it reasonable to define the homogenized diffusion coefficient as a flux-weighted average of the local diffusion coefficients as in Eq. (16):

\[
\tilde{D} = \left( \frac{1}{\bar{\phi}_{cell}} \right) \int_{cell} D\phi \, dV \, . \tag{16}
\]
On the other hand it may seem just as reasonable to compute a homogenized diffusion coefficient from flux-weighted average cross sections, as in Eq. (17):

\[
\bar{D} = \left( \frac{1}{3} \bar{\Sigma}_1 \right), \quad \bar{\Sigma}_1 = \left( \frac{1}{\bar{\phi}_{cell}} \right) \int_{cell} \Sigma_1 \phi.
\]

As a matter of fact both definitions have been used in practice, as well as other more complicated ad hoc prescriptions. If \( \Sigma_1 \) does not change radically from region to region all the various ad hoc prescriptions tend to give much the same homogenized diffusion coefficients. Further, if the leakage rate from the core is small (as it is in most large power reactors) small differences in \( \bar{D} \) have little effect on computed eigenvalues or flux shapes. Unfortunately there are situations in which \( \Sigma_1 \) varies sharply as a function of position, and in which leakage from the core is quite important. This is true, for example, in a gas-cooled fast reactor. In such a reactor the coolant, which is generally helium, flows through many channels which are otherwise empty, and are interspersed throughout the system. These channels constitute excellent escape routes through which neutrons stream out of the core. Heterogeneities are not normally so important in the LMFBR, the liquid metal fast breeder reactor, which is cooled by liquid sodium. However, in the analysis of hypothetical accidents it is necessary to deal with situations in which some or all of the sodium has actually boiled out of the core. If this were to occur we would again be left with nearly empty coolant channels, severe heterogeneities, and important leakage effects. In such situations ad hoc prescriptions for homogenized diffusion coefficients are not always adequate, and
more sophisticated homogenization techniques may be required. Before we can discuss such techniques it will be necessary to introduce the "buckling" concept, a fundamental concept of reactor physics. For the sake of simplicity, I will continue to confine my attention, here, to a one-group model reactor, though everything I have to say applies, as well, to a multi-energy reactor.

It is generally true that, near the center of a large homogeneous reactor core, the scalar flux (approximately) satisfies the Helmholtz equation, \( \nabla^2 \phi = -B^2 \phi \), for a value of \( B \) determined only by the core cross sections. The constant \( B^2 \) is usually referred to as the "buckling". Any real solution of the Helmholtz equation may be written in the form of an integral over the unit sphere, as in Eq. (18):

\[
\phi(r) = \int d\hat{b} \ g(\hat{b}) \ e^{iB\hat{b} \cdot r} . \tag{18}
\]

Correspondingly one can Fourier analyze the angular fluxes as in Eq. (19):

\[
F(r,\hat{\omega}) = \int d\hat{b} \ f(\hat{\omega},\hat{b}) \ e^{iB\hat{b} \cdot r} , \tag{19}
\]

Here \( \hat{b} \) is a unit vector, while \( f \) and \( g \) are arbitrary functions subject only to the constraints \( g(-\hat{b}) = g^*(\hat{b}) \), \( f(\hat{\omega},-\hat{b}) = f^*(\hat{\omega},\hat{b}) \). If the reactor core is roughly rectangular the fluxes may be expected to take on the

\[ \text{This "folk theorem" plays a peculiar role in reactor physics. It is assumed to be true, is often observed to be true in reactor experiments, and has been verified in innumerable transport and diffusion computations. Yet this "fundamental theorem of reactor physics" is discussed very little in the reactor physics literature. For more insight into the physics underlying the buckling concept see, for example, Ref. 6.} \]
particularly simple form

\[ \phi(r) = c_1 \cos(B \cdot r + c_2) = R\{g e^{iB \cdot r}\}, \]  

(20)

\[ F(r,\hat{n}) = R\{f(\hat{n}) e^{iB \cdot r}\}, \]  

(21)

where \(f\) and \(g\) are generally complex.

Almost invariably derivations of homogenized diffusion coefficients start from a generalization of Eqs. (20) and (21). Most methods for computing homogenized diffusion coefficients can be regarded as variants of the Benoist method, so I will discuss this method first.

Suppose that an infinite lattice of some sort contains a distributed neutron source whose density has the following separable form,

\[ S(r,\hat{n}) = s(r) \cos(B \cdot r) = R\{s(r) e^{iB \cdot r}\}, \]  

(22)

where the (real) function, \(s(r)\) has the periodicity of the lattice. The flux in this lattice is governed by the transport equation, Eq. (23):

\[ \hat{\omega} \cdot \nabla F + \Sigma_t F = \frac{1}{4\pi} \Sigma_s \phi + \frac{1}{4\pi} S, \quad \phi = \int F \, d\hat{n}. \]  

(23)

To solve Eq. (23) we make the substitution shown in Eq. (24):

\[ F = R\{f(r,\hat{n}) e^{iB \cdot r}\}, \quad f = R + iI. \]  

(24)

Here \(R\) and \(I\) are the real and imaginary parts of the complex function, \(f\). It is easy to show that \(R\) and \(I\) satisfy Eqs. (25) and (26):
\[ \Omega \cdot \nabla R + \Sigma R = \frac{1}{4\pi} \Sigma_s \psi + i\hat{\Omega} \cdot B I + \frac{1}{4\pi} s, \quad \psi = \int R \, d\Omega, \quad (25) \]

\[ \Omega \cdot \nabla I + \Sigma I = \frac{1}{4\pi} \Sigma_s x - i\hat{\Omega} \cdot B R, \quad \chi = \int I \, d\Omega. \quad (26) \]

Now we will assume that \( R \) and \( I \) can be expanded in Taylor series in the components of the vector \( B \). It should be noted that this is by no means an innocuous assumption. There are very important situations in which such an expansion is not possible,\(^7,8\) so that alternative methods of attack are required.\(^8,9\) But if a series expansion is possible, then, to leading order in \( B \), Eqs. (25) and (26) are equivalent to Eqs. (27) and (28):

\[ \hat{\Omega} \cdot \nabla R + \Sigma R = \frac{1}{4\pi} \Sigma_s \psi + \frac{1}{4\pi} s, \quad (27) \]

\[ \hat{\Omega} \cdot \nabla I + \Sigma I = \frac{1}{4\pi} \Sigma_s x - \hat{\Omega} \cdot B R, \quad I = B \, \hat{I}, \quad x = B \, \hat{x}. \quad (28) \]

It will be seen that Eqs. (27) and (28) are formally identical with the conventional transport equation. Further \( R \) and \( I \) have the periodicity of the lattice, so that they satisfy simple boundary conditions on each cell boundary. Therefore it is possible to solve these equations via transport computations which are confined to a single cell, and need not extend over the entire lattice.

Now suppose, for simplicity, that the lattice cells are rectangular, and that their bounding surfaces are parallel to the coordinate planes. Let \( L_x \) be the total number of neutrons leaking out of a cell, per second, across the two boundaries normal to the \( x \) axis. It can be shown that, to leading order in \( B \), \( L_x \) is given by Eq. (29):
L_x = \cos(B \cdot r_0) B_x^2 \left[ \int j_{xx} \, dV + \int_{\text{cell}} (x - x_0) \frac{\partial}{\partial x} j_{xx} \, dV \right],

\begin{equation}
    j_{xx} = -\int \hat{a}_x \hat{r} \, d\hat{a},
\end{equation}

where \( r_0 \) lies at the center of the cell.

Now suppose we were to replace the lattice by a homogeneous medium. Suppose that, in this medium, the scalar flux has the simple form

\( \phi(r) = c \cos B \cdot r. \)

Imagine a rectangular region in this infinite medium which is coextensive with one of the cells of the lattice. Suppose we want the average flux in this region to be equal to the average flux in the cell, and the leakage, \( L_x \), from the region to be equal to the leakage, \( L_x \), from the cell. Further, the leakage rates in the homogeneous medium are to be computed in a diffusion approximation. Now, in diffusion theory, the leakage rate in the \( x \) direction, in a homogeneous medium, is given by Eq. (31)

\begin{equation}
    \frac{\partial j_x}{\partial x} = -\frac{\partial}{\partial x} D \frac{\partial \phi}{\partial x} = -D \frac{\partial^2 \phi}{\partial x^2},
\end{equation}

and the leakage out of the rectangular region is given by Eq. (32):

\begin{equation}
    L_{x(\text{HOM})} = -\int_R D \frac{\partial^2 \phi(\text{HOM})}{\partial x^2} \, dV.
\end{equation}

Here \( R \) is the volume of the rectangular region coextensive with the given cell. Note that the flux and leakage rates, here, are fluxes and leakage rates in the \textit{homogeneous} medium. Since we have assumed that the flux is separable we may write
\[ L_{x,\text{(HOM)}} = D B^2 V_{\text{cell}} \bar{\phi}_{\text{(HOM)}} = D B^2 V_{\text{cell}} \bar{\phi}, \quad (33) \]

where \( \bar{\phi} \), on the extreme right-hand side of Eq. (33) is now the average flux in the lattice cell. Equating the leakage rates in the lattice and in the homogeneous medium we are led to define the homogenized diffusion coefficient, to leading order in \( B \), as in Eq. (34):

\[
D_x = \left[ \int_{\text{cell}} j_{xx} \, dV + \int_{\text{cell}} (x - x_0) \frac{\partial}{\partial x} j_{xx} \, dV \right] \left/ \int_{\text{cell}} \psi \, dV \right.,
\]

\[ \psi = \int d\Omega \, \bar{R}. \quad (34) \]

Thus the \( x \) diffusion coefficient is now determined entirely by the two coupled transport equations for \( R \) and \( I \).

It should be noted, however, that the Benoist method gives us different diffusion coefficients in different directions. These diffusion coefficients embody the various properties of the lattice as seen by neutrons streaming in different directions. If, for example, a reactor contains empty channels parallel to the \( z \)-axis we must expect that neutrons will stream preferentially in the \( z \)-direction, so that \( D_z \) will be greater than \( D_x \) or \( D_y \). When the diffusion coefficients are direction-dependent (or "anisotropic") the diffusion equation takes the form shown in Eq. (35):

\[
- \frac{\partial}{\partial x} D_x \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial y} D_y \frac{\partial \phi}{\partial y} - \frac{\partial}{\partial z} D_z \frac{\partial \phi}{\partial z} + k \phi = S. \quad (35)
\]
Average absorption cross sections and fission production rates may still be defined as flux-weighted averages, just as in an infinite lattice with $\beta = 0$, although slightly more refined procedures are often used.

As you may recall, I have already pointed out the homogenization process and the introduction of the diffusion approximation are operations which do not necessarily commute. You will note that the Benoist method involves the solution of the transport equation in the heterogeneous lattice cell. The homogenized diffusion coefficients, which are designed for use in the diffusion equation, are derived from solutions of the transport equation. It is easy to think of situations where the diffusion approximation must not be introduced until the homogenization process has been completed. Suppose, again, that empty channels run through the core in the z-direction. In these channels the cross sections vanish, so that the local diffusion coefficient is infinite. Now, in a diffusion approximation, the z-leakage rate at each point would be given by the expression $L_z(r) = DB^2 \phi(r)$, so that the total z-leakage rate from the cell would be infinite. On the other hand, the Benoist method, based on a transport computation in the lattice, will give a finite leakage rate except in those pathological cases where the Benoist Taylor series expansion is invalid. Many other peculiar anomalies occur when the diffusion approximation is applied directly to heterogeneous lattice cells. On the other hand, the homogenized lattice can often be treated by diffusion theory, even when the heterogeneous lattice cannot.

So far I have discussed homogenization only in an infinite homogeneous medium. In a multiregion reactor homogenized diffusion coefficients and cross sections would be computed separately over several large subregions in which the lattice structure is fairly uniform. The resulting average parameters would then be used in a multiregion diffusion calculation in
which the reactor would be represented as a collection of large homogeneous regions. Such a computational procedure is certainly not beyond reproach. After all, if a well-defined buckling exists anywhere in a reactor it exists only near the center of a large core. Yet the homogenized diffusion coefficient must be used everywhere in the reactor, even near the boundary of the core where, strictly speaking, there is no buckling. Even if one assumes that a well-defined buckling exists some interesting objections to the Benoist method remain. In discussing the Benoist method I referred repeatedly to a unit cell. But in an infinite lattice there is no uniquely defined unit cell. The same lattice can generally be constructed from many different unit cells. Unfortunately different definitions of the unit cell imply different values of the Benoist diffusion coefficients. Given the usual prescriptions for homogenizing absorption and fission cross sections, it turns out that the different diffusion coefficients lead to slightly different lattice eigenvalues for any specified buckling. Under such circumstances it seems most important that the Benoist method (as well as other similar homogenization prescriptions) be checked extensively against experiment, and against Monte Carlo computations. There is some experimental evidence that the Benoist method is adequate for use in nuclear design and analysis, but in my opinion, the range of validity of the method has still not been thoroughly investigated.

Now, before closing, I want to turn briefly to a method which is related to Benoist's, but looks totally different. In earlier sections of this paper I have written the transport equation for a reactor in differential form, as in Eq. (36):
The same equation can also be written in integral form as in Eq. (37):

\[ \lambda S_f(r) = \int K(r' - r) S_f(r') \, dr'. \quad (37) \]

In Eq. (37) \( S_f(r) \) is the fission source density at \( r \), i.e. \( S_f(r) \) is equal to \( \nu E_f(r) \phi(r) \). Further, the kernel \( K(r' - r) \) is a Green's function which has the following significance. Suppose there is an isotropic \( \delta \) function source of fission neutrons at \( r' \). Each of the fission neutrons born at \( r' \) will diffuse through the reactor until it is absorbed. At the point where it is absorbed it may trigger a fission, producing offspring which I will call "second-generation neutrons": \( K(r' - r) \) is the birth rate of second-generation neutrons produced at \( r \) by the \( \delta \)-function source at \( r' \). Of course second-generation neutrons will produce third-generation neutrons, and so on, but only the production rate of second-generation neutrons is to be included in the kernel, \( K \).

Now suppose that

\[ S_f(r') = s(r) e^{iB \cdot r} , \quad (38) \]

and that \( s(r) \) has the periodicity of the lattice. Substituting from Eqs. (38) into Eq. (37), we get Eq. (39):

\[ \lambda s(r) = \int K(r' - r) e^{iB \cdot (r' - r)} s(r') \, dr'. \quad (39) \]

If, in Eq. (39), we set \( B = 0 \) we get Eq. (40):
\[ \lambda_0 s_0(r) = \int K(r' \rightarrow r) s_0(r') \, dr'. \]

Now Eqs. (39) and (40) are integral equations with slightly different kernels and, as \( B \rightarrow 0 \), we ought to be able to estimate the eigenvalue, \( \lambda \), by perturbation theory. Perturbation theory leads us, in fact, to Eq. (41):

\[
\lambda - \lambda_0 \equiv \Delta = -\left(1/S_T\right) \int dr \, s_0^*(r) \int K(r' \rightarrow r) \left[ 1 - e^{iB \cdot (r' - r)} \right] s_0(r') \, dr',
\]

\[ S_T = \int dr \, s_0^*(r) s_0(r). \quad (41) \]

Here \( s_0^*(r) \) is the adjoint fission source which is the solution of the adjoint integral equation, Eq. (42):

\[ \lambda_0 s_0^*(r) = \int K(r' \rightarrow r) s_0^*(r') \, dr'. \]

It is now easy to show that the fractional change in \( \lambda \) is given by Eq. (43):

\[
\frac{\Delta}{\lambda_0} = -\frac{\int dr \, s_0^*(r) \int K(r' \rightarrow r) \left[ 1 - e^{iB \cdot (r' - r)} \right] s_0(r') \, dr'}{\int dr \, s_0^*(r) \int K(r' \rightarrow r) s_0(r') \, dr'}. \quad (43)
\]

At this point I am going to assume that the lattice cell has three planes of symmetry, each symmetry plane being normal to the \( x \), \( y \), or \( z \) axis. I will assume, further, that the numerator on the rhs of Eq. (43) can be expanded in a Taylor series in \( B \). It turns out, then, that the perturbed eigenvalue is given, to leading order in \( B \), by Eq. (44):
\[
\frac{\Delta}{\lambda_0} = -\frac{1}{2} \left( B_x^2 \bar{z}^2 + B_y^2 \bar{y}^2 + B_z^2 \bar{z}^2 \right),
\]

\[
\bar{\bar{\ell}}^2_{x,y,z} = \frac{\int dr \ s_0^*(r) \int K(r^- + r)(r^-_{x,y,z} - r_{x,y,z})^2 s_0(r^-) \ dr^-}{\int dr \ s_0^*(r) \int K(r^- + r) s_0(r) \ dr}.
\]

The quantities \(\bar{\bar{\ell}}^2_x, \bar{\bar{\ell}}^2_y,\) and \(\bar{\bar{\ell}}^2_z\) are mean-square distances from birth to fission, weighted by the value of the adjoint source at the point where fission occurs.

Equation (44) is interesting for three reasons. First, it establishes a conceptually simple relation between the leakage rate, for a given \(B^0\), and the geometry of the lattice. Secondly, it is convenient for Monte Carlo computations since estimates of the mean-square distances in Eq. (44) yield a direct estimate of the leakage rate as a function buckling. I know of no other simple way to impose a specified buckling in a Monte Carlo eigenvalue calculation. Finally, Eq. (44) clarifies the relation between leakage rates and mean-square path lengths. Some such relation seems to have been assumed in important early work by Behrens, but never stated precisely. Theoretical clarification of Behrens' work still seems to be of interest, since his method is still useful. It should be noted that Eq. (44) generalizes to lattices a relation long known to be valid for infinite homogeneous media.

I think it is natural to ask what can be deduced via perturbation theory if the cell does not have the symmetry properties I have postulated. You see that the right-hand side of Eq. (41) will generally be complex and, if the cell is not symmetric, one cannot show that \(\Delta\) will be real. Moreover, one can construct an asymmetric cell such that if a core
no matter how large is composed of such cells, a well-defined buckling will not exist anywhere in the core. Now all homogenization methods, so far as I know, rely on the existence of a buckling. Thus it is not at all certain, in principle, that any method available today can be applied to lattices of nonsymmetric cells.

It seems very clear that the homogenization problems of reactor physics still urgently need a good deal of attention. Perhaps there are, in the interdisciplinary group attending this conference, specialists from other disciplines who can bring, to these reactor physics problems, a fresh point of view and a new approach.
REFERENCES

Diffusing medium ($\Sigma_a = 0$)
Plane source at $x = -\infty$

Fig. 1. Simple Milne problem configuration.
Fig. 2. Source-free absorbing slab imbedded in a scattering medium.
Fig. 3. Infinite absorbing medium with a source in Region 1 and no source in Region 2.
Fig. 4. Singular characteristic extending from a corner point:  
\( \hat{n} \cdot \nabla F \) is discontinuous along dotted line.
FIG. 5. Core Lattice Structure Viewed From Above

a. Schematic of Pin Subassembly

b. Schematic of Plate Subassembly