Chapter 5

Homogenization

Nuclear reactors have many levels of spatial heterogeneity. A fuel pin is comprised of cladding and many fuel pellets, an assembly is made of hundreds of fuel pins, and a reactor is made up of hundreds of assemblies. To calculate the power distribution in a reactor core is not computationally feasible when each fuel pin needs to be resolved by the spatial mesh, whether one uses finite differences or nodal calculations. This has driven the development of methods to represent the heterogeneity inside a reactor using averaged cross-sections at a scale near the assembly level. The process of determining the averaged cross-sections is known as homogenization.

The basis for most homogenization methods are assembly level calculations. In these calculations a single assembly is simulated with reflecting boundary conditions and the full heterogeneity of the assembly (this could include, for example, spatially-dependent depletion). The assembly calculation could be done with diffusion methods or transport techniques such as method-of-characteristics. An assembly calculation is required for each assembly of different composition. Once the assembly calculations are complete, homogenized parameters are then calculated, and a full-core can be simulated using a small number of nodes per assembly.

In the following sections we will develop the homogenization techniques that can be used to compute homogenized parameters that yield results for k_{eff} and assembly level power nearly equivalent to calculations the solve the full heterogeneous problem, at a much lower cost.

5.1 The Mathematical Statement of the Homogenization Problem

The starting point for homogenization is the multigroup neutron continuity equation (i.e., the zeroth angular moment of the transport equation) for the k

eigenvalue of the fully heterogeneous problem:

$$\nabla\cdot\mathbf{J}_g+\Sigma_{\mathrm{t}g}(\mathbf{r})\phi_g(\mathbf{r}) = \sum_{g'=1}^{G}\left(\Sigma_{\mathrm{s}g'\to g}(\mathbf{r}) + \frac{\chi_g\bar{\nu}\Sigma_{\mathrm{f}g'}(\mathbf{r})}{k_{\mathrm{eff}}}\right)\phi_{g'}(\mathbf{r}), \tag{5.1}$$

with appropriate boundary conditions. We would like to derive an alternative equation where the material properties (e.g., $\Sigma_{\mathrm{t}g}$) are constant over a larger regions of space than the original heterogeneous problem. Typically, the region we would like to have constant cross-sections over is a fuel assembly. The neutron continuity equation for the homogenized problem is

$$\nabla\cdot\mathbf{J}^{\mathrm{H}}_g+\Sigma^{\mathrm{H}}_{\mathrm{t}g}(\mathbf{r})\phi^{\mathrm{H}}_g(\mathbf{r}) = \sum_{g'=1}^{G}\left(\Sigma^{\mathrm{H}}_{\mathrm{s}g'\to g}(\mathbf{r}) + \frac{\chi_g\bar{\nu}\Sigma^{\mathrm{H}}_{\mathrm{f}g'}(\mathbf{r})}{k_{\mathrm{eff}}}\right)\phi^{\mathrm{H}}_{g'}(\mathbf{r}), \tag{5.2}$$

where the superscript H denotes quantities that have been averaged over a region. In common parlance, these are homogenized quantities.

We want the solution of the homogenized equation to give the same reaction rates and net leakage out of an assembly as the heterogeneous equations. If we preserve reaction rates and leakages, the overall power distribution and eigenvalue of the homogenized system will be the same as the heterogeneous system. The preservation of reaction rates in assembly i is given by the relation

$$\int_{V_i}\Sigma^{\mathrm{H}}_{\alpha g}(\mathbf{r})\phi^{\mathrm{H}}_g(\mathbf{r})\,dV = \int_{V_i}\Sigma_{\alpha g}(\mathbf{r})\phi_g(\mathbf{r})\,dV, \qquad \alpha\in\{\mathrm{t},\mathrm{s}g'\to g, f,\dots\}. \tag{5.3}$$

The preservation of leakage is represented by a surface integral over the k^{th} face of assembly i

$$\int_{S_i^k}\hat{n}^k\cdot\mathbf{J}^{\mathrm{H}}_g\,dA = \int_{S_i^k}\hat{n}^k\cdot\mathbf{J}_g\,dA. \tag{5.4}$$

If we use Fick's law to relate $\mathbf{J}$ and ϕ in the homogeneous equation, then this

becomes

$$-\int_{S_i^k} \hat{n}^k \cdot D_g^{\mathrm{H}}(\mathbf{r}) \nabla \phi_g^{\mathrm{H}} \, dA = \int_{S_i^k} \hat{n}^k \cdot \mathbf{J}_g \, dA. \tag{5.5}$$

The relations given by Eqs. (5.3) and (5.4) are ideal. If these relations hold, then the solution to the homogeneous problem will have the same assembly powers and eigenvalue, all by solving a simpler problem. The problem is, of course, defining the homogenized parameters so that these relations hold.

5.2 Flux-Volume Weighted Homogenization

The most basic approach to homogenization is known as flux-volume weighted homogenization. What this approach does is take the reaction rate equivalence equation, Eq. (5.3), and specify that the cross-sections are constant over assembly i so that the integral of the homogenized solution simplifies. Solving the resulting equation for $\Sigma_{\alpha g}^{\mathrm{H}}$ gives the cross-section for assembly i as

$$\Sigma_{\alpha g}^{\mathrm{H}i} = \frac{\int_{V_i} \Sigma_{\alpha g}(\mathbf{r}) \phi_g(\mathbf{r}) \, dV}{\int_{V_i} \phi_g^{\mathrm{H}}(\mathbf{r}) \, dV}. \tag{5.6}$$

We still have to define the diffusion coefficient for region i, we would like to take Eq. (5.5) and solve for D_g^{H} as

$$D_g^{\mathrm{H}i} = -\frac{\int_{S_i^k} \hat{n}^k \cdot \mathbf{J}_g \, dA}{\int_{S_i^k} \hat{n}^k \cdot \nabla \phi_g^{\mathrm{H}} \, dA}. \tag{5.7}$$

There are, at least, two problems with this formulation. The first is that we need to know both the solution to the heterogeneous problem and the solution to the homogeneous problem to compute the cross-sections. Additionally, the definition of $D_g^{\mathrm{H}i}$ is somewhat incoherent because it implies that there is a different diffusion coefficient depending on which face of the assembly we consider. We could handle this by making the diffusion coefficient into a diffusion tensor or averaging the diffusion coefficient over the faces.

Flux-volume weighted homogenization technique performs an assembly-level calculation, with full heterogeneity, to get the flux $\phi_g^{\mathrm{A}i}(\mathbf{r})$ for the i^{th} assembly with reflecting boundary conditions on each side (these boundary conditions

make the problem equivalent to an infinite lattice of assemblies). In particular this solves

$$\nabla\cdot\mathbf{J}_g^{\mathrm{A}i}+\Sigma_{\mathrm{t}g}^{\mathrm{A}i}(\mathbf{r})\phi_g^{\mathrm{A}i}(\mathbf{r}) = \sum_{g'=1}^{G}\left(\Sigma_{\mathrm{s}g'\to g}^{\mathrm{A}i}(\mathbf{r}) + \frac{\chi_g\bar{\nu}\Sigma_{\mathrm{f}g'}^{\mathrm{A}i}(\mathbf{r})}{k_{\mathrm{eff}}}\right)\phi_{g'}^{\mathrm{A}i}(\mathbf{r}),\ \text{for } \mathbf{r}\in V_i, \tag{5.8}$$

$$\hat{n}\cdot\mathbf{J}_g^{\mathrm{A}i}(\mathbf{r}) = 0, \mathbf{r}\in\partial V_i.$$

We then make the approximation that the integral of the homogenized flux for the whole-core problem is equal to the integral of the assembly flux:

$$\int_{V_i}\phi_g^{\mathrm{H}i}(\mathbf{r})\,dV \approx \int_{V_i}\phi_g^{\mathrm{A}i}(\mathbf{r})\,dV. \tag{5.9}$$

An error that one occurs in this approximation is that the scalar flux for the homogenized region will have the same integral as the assembly flux. This seems reasonable except that there is no guarantee that the assembly flux (which uses a zero current boundary condition) will have the same integral as the homogenized flux in a whole-core calculation.

Using this approximation, the homogenized cross-sections are computed as

$$\Sigma_{\alpha g}^{\mathrm{H}i} = \frac{\int_{V_i}\Sigma_{\alpha g}(\mathbf{r})\phi_g^{\mathrm{A}i}(\mathbf{r})\,dV}{\int_{V_i}\phi_g^{\mathrm{A}i}(\mathbf{r})\,dV}. \tag{5.10}$$

Given that we cannot satisfy the current condition are each interface of the assembly, not mention the fact that in the current on the edge of the assembly is zero in the assembly-level calculation, we need an alternate approach to define the diffusion coefficient. A common approach is to use a flux-volume weighting as we did for the cross-sections:

$$D_g^{\mathrm{H}i} = \frac{\int_{V_i}D_g(\mathbf{r})\phi_g^{\mathrm{A}i}(\mathbf{r})\,dV}{\int_{V_i}\phi_g^{\mathrm{A}i}(\mathbf{r})\,dV}. \tag{5.11}$$

The flux-volume weighted cross-sections and diffusion coefficients will only preserve the reaction rates if the reactor is an infinite lattice of the same assembly. However, if the assemblies are not part of an infinite lattice or if the

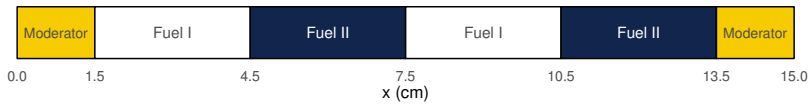

Figure 5.1: Layout for the generic assembly in the homogenization test problem.

assemblies are of different type, there is no guarantee that flux-volume weighting will give the correct solution.

We will demonstrate this using a simple, 1-D slab problem with two types of assemblies. Both assemblies are arranged with moderator regions on the outside of the slab with two types of fuel regions alternating in the middle of the slab, as shown in Figure 5.1. The difference between the two assemblies is that the "Fuel II" region in Assembly A is fuel and is a control element in Assembly B. The numerical values of the material properties for these assemblies are given in Table 5.1.

Table 5.1: Material Properties for the Homogenization Test Problem. Multi-group quantities are given in the format: (group 1, group 2). For all regions, $\chi_1 = 1$, $\chi_2 = 0$.

	Moderator	Fuel I	Fuel II (Assembly A)	Fuel II (Assembly B)
D_g (cm)	(1.530, 0.295)	(1.4, 0.375)	(1.4, 0.375)	(1.11, 0.185)
$\Sigma_{\mathrm{r}g}$ (cm^{-1})	(0.0005, 0.009)	(0.009, 0.060)	(0.009, 0.070)	(0.08375, 0.950)
$\nu\Sigma_{\mathrm{f}g}$ (cm^{-1})	(0,0)	(0.0051, 0.08)	(0.0057, 0.1)	(0,0)
$\Sigma_{\mathrm{s}1\to2}$ (cm^{-1})	0.0310	0.0180	0.0170	0.00375

The solution for a single assembly of type A with reflecting boundary conditions is shown in Figure 5.2. For this simulation we performed a critical buckling search to make k_{eff} close to unity. The homogenized cross-sections for this assembly are given in Table 5.2. We performed the same calculation for assembly B with the results shown in Figure 5.3 and the homogenized quantities for this assembly are given in Table 5.2. Note that the numerical solution to the homogenized problem and the heterogeneous problem for both assemblies gives the same value of k_{eff} and the fission reaction rate.

We use these two types of assemblies to form a slab reactor comprised of two B assemblies surrounded by an assembly of type A and a reflector, as shown in Figure 5.4. The reflector is modeled using an albedo boundary with $\alpha = 0.156627$. When solving this problem with fully heterogeneity we get $k_{\mathrm{eff}} = 1.0001548$ and a fission power ratio (fission power in assembly A divided by fission power in assembly B) of 4.93115. The solution, using a reflecting

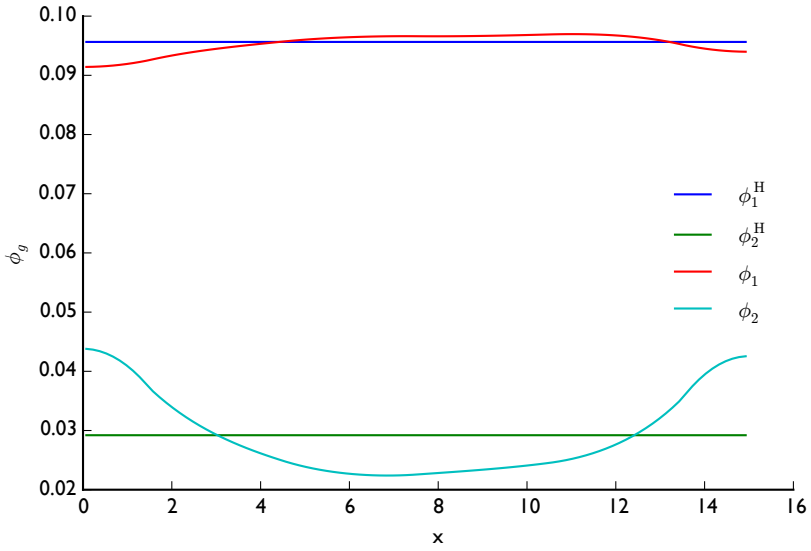

Figure 5.2: Scalar flux solution for an infinite lattice comprised of assemblies of type A. The solution for the homogenized assembly is also shown.

Table 5.2: The assembly homogenized quantities for Assembly A and B based on infinite lattice calculations.

	Assembly A	Assembly B
D_g (cm)	(1.42536998,0.35252385)	(1.33417596, 0.32942652)
Σ_{rg} (cm^{-1})	(0.00734119, 0.04920257)	(0.03149932, 0.07895485)
$\nu\Sigma_{fg}$ (cm^{-1})	(0.0043473, 0.06458608)	(0.00230837,0.03964929)
$\Sigma_{s1\to2}$ (cm^{-1})	0.02013269	0.01647865

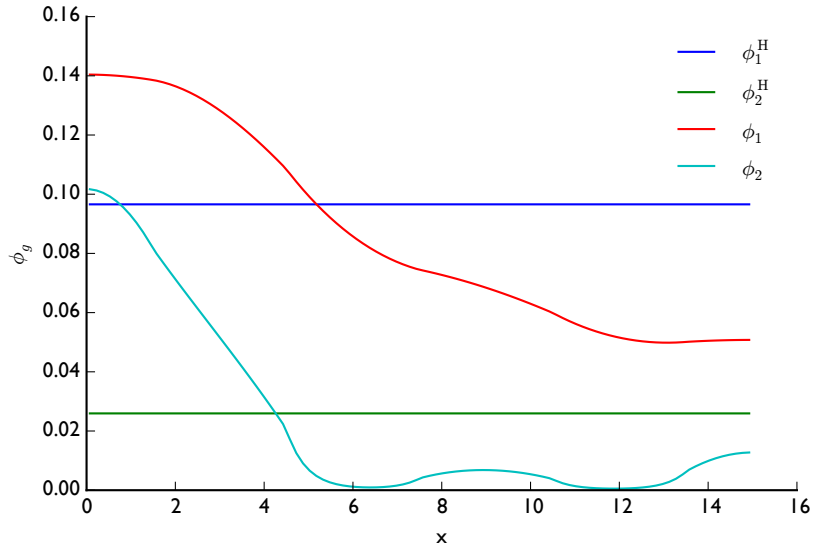

Figure 5.3: Scalar flux solution for an infinite lattice comprised of assemblies of type B. The solution for the homogenized assembly is also shown.

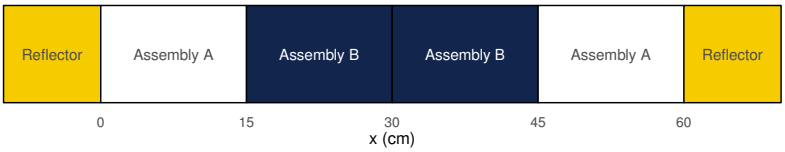

Figure 5.4: Layout for the slab reactor problem. The reflector is modeled with an albedo boundary condition using $\alpha = 0.156627$.

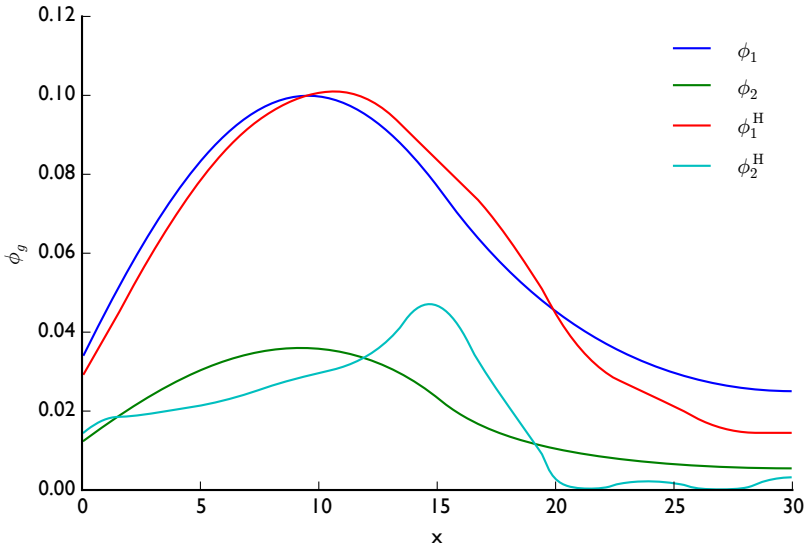

Figure 5.5: Solution to the slab reactor problem from both a heterogeneous and homogenized calculation. For the heterogeneous problem $k_{\text{eff}} = 1.0001548$, and for the homogenized solution $k_{\text{eff}} = 0.896229$.

boundary at $x = 30$ cm, is shown in Figure 5.5 We also can solve the same problem using the homogenized cross-sections we computed using the assembly calculations. This solution is also shown in Figure 5.5. The overall shape of the solution in the homogenized calculation is fundamentally different than that in the heterogeneous calculation. For example, the peak in the thermal flux in assembly A, is in the middle of the assembly in the homogeneous case and near the assembly interface in the heterogeneous case. For the homogenized calculation we get $k_{\text{eff}} = 0.896229$, an error of 10393 pcm, not to mention that the homogenized reactor is subcritical whereas the heterogeneous reactor is supercritical. The power ratio for the homogenized reactor is 4.64775, a 6% difference.

Clearly, there is room for improvement in the homogenized calculation. We will next detail a means to improve the homogenization by adding an extra degree of freedom in the solution process.

5.3 Discontinuity Factors

As the results above showed, quantities homogenized by scalar fluxes computed in assembly calculations cannot capture the solution to heterogeneous reactor

problems. As one can see in Figure 5.5, the value of the heterogeneous scalar flux in the thermal group at the assembly interface is above the average value in Assembly A, and above the average value in Assembly B. Furthermore, at $x = 30$ the value of the heterogeneous, thermal scalar flux is below the average value in that assembly. If one looks back at the assembly calculations used in the homogenization, the solutions have the same properties, but we lost this information in the homogenization process.

We can introduce this information back in to the homogenized calculation by modifying the homogenized calculation at the assembly interface. What we would like to do is modify the problem so that the reaction rates in an infinite lattice would not be modified and so that we can make the net current between assemblies in the homogeneous solution is the same as that in the heterogeneous problem. We might be tempted to try to modify the definition of the diffusion coefficient so that the current in the heterogeneous problem is preserved, but there are several interfaces for a given assembly (up to 6 in 3-D) so that we would need to have several different coefficients for a given assembly.

Rather than introduce different diffusion coefficients, we can define an extra degree of freedom at each interface that will work with the flux-volume weighted diffusion coefficients we defined above. At the interface between two assemblies the heterogeneous scalar flux will have a value that is different that the interfacial scalar flux computed by a homogenized calculation. Therefore we define a *discontinuity factor* f for each side of that interface. In the x direction, the values of f at interface $i + 1/2$ would be

$$f^-_{gi+1/2} = \frac{\phi_g(x^-_{i+1/2})}{\phi^{\mathrm{H}}_g(x^-_{i+1/2})}, \qquad f^+_{gi+1/2} = \frac{\phi_g(x^+_{i+1/2})}{\phi^{\mathrm{H}}_g(x^+_{i+1/2})}, \tag{5.12}$$

where the superscript $\pm$ denotes if we are on the left or right of the interface. The discontinuity factors are defined so that the product of a discontinuity factor and the homogenized scalar flux at the interface will be equal to the heterogeneous scalar flux there.

The discontinuity factors can be implemented in nodal diffusion solvers. In nodal diffusion, one simply changes the continuity of scalar flux condition to be the continuity of the scalar flux times a discontinuity factor. That is, at the nodal interface we enforce the condition $f^-_{gi+1/2}\phi^{\mathrm{H}}_g(x^-_{i+1/2}) = f^+_{gi+1/2}\phi^{\mathrm{H}}_g(x^+_{i+1/2})$ in a homogenized node.

We can also use discontinuity factors in the CMFD acceleration technique.

To do this we re-write the CMFD current to be

$$J_{xg}(x_{i+1/2})^{\mathrm{H}} = -D_{gi}^{\mathrm{H}} \frac{f_{gi+1/2}^{-}\phi_{gi+1/2}^{\mathrm{H}} - \phi_{gi}^{\mathrm{H}}}{h_x/2} = -D_{gi+1}^{\mathrm{H}} \frac{\phi_{gi}^{\mathrm{H}} - f_{gi+1/2}^{+}\phi_{gi+1/2}^{\mathrm{H}}}{h_x/2}. \tag{5.13}$$

Solving for $\phi_{gi+1/2}$ and substituting this back in we get

$$J_{xg}(x_{i+1/2})^{\mathrm{H}} = -\frac{2D_{gi}^{\mathrm{H}} D_{gi+1}^{\mathrm{H}}}{h_x} \frac{f_{gi+1/2}^{-}\phi_{gi+1}^{\mathrm{H}} - f_{gi+1/2}^{+}\phi_{gi}^{\mathrm{H}}}{f_{gi+1/2}^{+}D_{gi+1}^{\mathrm{H}} + f_{gi+1/2}^{-}D_{gi}^{\mathrm{H}}}. \tag{5.14}$$

Notice that if the discontinuity factors are equal, then the current reduces to the expression we previously derived that uses the harmonic mean of the diffusion coefficients.

$$J_{xg}(x_{i+1/2}) = -\frac{2D_{gi}^{\mathrm{H}} D_{gi+1}^{\mathrm{H}}}{h_x} \frac{f_{gi+1/2}^{-}\phi_{gi+1}^{\mathrm{H}} - f_{gi+1/2}^{+}\phi_{gi}^{\mathrm{H}}}{f_{gi+1/2}^{+}D_{gi+1}^{\mathrm{H}} + f_{gi+1/2}^{-}D_{gi}^{\mathrm{H}}} - \tilde{D}_{i+1/2} \frac{f_{gi+1/2}^{+}\phi_{i}^{\mathrm{H}} + f_{gi+1/2}^{-}\phi_{i+1}^{\mathrm{H}}}{h_x}. \tag{5.15}$$

Solving for $\tilde{D}_{i+1/2}$ gives

$$\tilde{D}_{i+1/2} = -\frac{D_{gi}^{\mathrm{H}}(-2D_{gi+1}^{\mathrm{H}} f_{gi+1/2}^{-}\phi_{gi+1}^{\mathrm{H}} + 2D_{gi+1}^{\mathrm{H}} f_{gi+1/2}^{+}\phi_{gi}^{\mathrm{H}} + f_{gi+1/2}^{-} h_x J_{xg}^{\mathrm{node}}(x_{i+1/2})) + D_{gi+1}^{\mathrm{H}} f_{gi+1/2}^{+} h_x J_{xg}^{\mathrm{node}}(x_{i+1/2})}{(D_{gi}^{\mathrm{H}} f_{gi+1/2}^{-} + D_{gi+1}^{\mathrm{H}} f_{gi+1/2}^{+})(f_{gi+1/2}^{-}\phi_{gi+1}^{\mathrm{H}} + f_{gi+1/2}^{+}\phi_{gi}^{\mathrm{H}})} \tag{5.16}$$

5.3.1 Calculating the discontinuity factors

The discontinuity factors are defined in terms of the homogenized and heterogeneous solution for the full core problem. Of course we will not typically have the whole core heterogeneous solution to define the discontinuity factors. Therefore, we would like to use a single assembly calculation to define the discontinuity factors. As we can see in Figures 5.2 and 5.3, the solution to the homogenized, single assembly problem is completely flat, making the solution equal to the average. Therefore, we can define a discontinuity factor as the ratio between the assembly scalar flux averaged along the edge and the average scalar flux from the homogenized calculation.

This definition of the discontinuity factor is an approximation, though in practice it is an effective strategy. Where this definition is deficient can be at

Table 5.3: Discontinuity Factors calculated different ways: row 1 is the discontinuity factor from the full heterogeneous reactor, row 2 uses an infinite lattice calculation for each assembly type, row 3 uses the actual reactor boundary conditions on one side of assembly A, and row 4 is the discontinuity factor from the flux-volume weighted homogenized solution without prescribed discontinuity factors.

	Assembly A ($x = 30^-$ cm)	Assembly B ($x = 30^+$ cm)
Exact	(1.03999816659, 1.71921099472)	(2.21717457747, 4.8714351949)
Infinite Lattice of Assemblies	(0.982684871456, 1.45667328119)	(1.45393848272 3.91874887014)
Assembly A with albedo BC	(0.996683026551, 1.49138771059)	“”
Homogenized Calculation	(0.943989455075, 0.812236497011)	(1.8701676062, 2.34579514378)

assemblies that are on the edge of the reactor. For these assemblies, one can improve the discontinuity factor by doing an assembly calculation using the reactor boundary condition at one face and reflecting conditions on the other faces.

For the test problem we solved in the previous section, we can look at what the discontinuity factors are under different circumstances. We can compute the “exact” discontinuity factors by looking at the assembly interface value divided the average homogenized solution over the assembly, or we can use assembly calculations to estimate the discontinuity factors either in an infinite lattice or by imposing the actual albedo BC's on the left side of assembly A. We can compare these discontinuity factors to the ratios of the interface value divided by the average in the homogenized result without discontinuity factors. These numbers for the interface at $x = 30cm$ are given in Table 5.3. In this table we can see that the assembly-level calculations give discontinuity factors that are much closer to the exact values than effective discontinuity factors that we see in the homogenized calculation without discontinuity factors.

Exercises for the student will demonstrate how discontinuity factors impact that solution to this problem.