

Homogenized Group Constants in the Absence of Reflective Boundary Conditions

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Outline

- Nodal calculations
- Lattice calculations
 - Homogenization
 - Discontinuity and peaking factors
 - Boundary conditions
- Multi-group diffusion equation in homogenized node
 - Numerical solution

Nodal Calculations

- System divided into nodes
- Solution based on multi-group diffusion theory

$$-D^g \Delta \phi^g(\mathbf{r}) + \bar{\Sigma}_t^g \phi^g(\mathbf{r}) = \sum_h \bar{\Sigma}_s^{h \rightarrow g} \phi^h(\mathbf{r}) + \frac{1}{k_{\text{eff}}} \bar{\chi}^g \sum_h \bar{\nu} \bar{\Sigma}_f^h \phi^h(\mathbf{r}), \quad g = 1, \dots, G$$

$$-D \Delta \phi + (\bar{\Sigma}_t - \bar{\Sigma}_s) \phi = \frac{1}{k_{\text{eff}}} \bar{F} \phi$$

- Lattice calculations \Rightarrow homogenized constants for each node
- Nodes are coupled together using *discontinuity factors* obtained from lattice calculations.

Homogenization

- Assume solution $\Phi_{\text{het}}(\mathbf{r}, E, \Omega)$ for the entire system
- Key idea in homogenization: preserve nodal reaction rates:

$$\bar{\Sigma}_{\mathbf{x},g} = \frac{\int_V d\mathbf{r} \int_{E_g}^{E_{g-1}} dE \phi_{\text{het}}(\mathbf{r}, E) \Sigma_{\mathbf{x}}(\mathbf{r}, E)}{\int_V d\mathbf{r} \int_{E_g}^{E_{g-1}} dE \phi_{\text{het}}(\mathbf{r}, E)}$$

$$\bar{\phi}_{\text{het}}^g = \int_V d\mathbf{r} \int_{E_g}^{E_{g-1}} dE \phi_{\text{het}}(\mathbf{r}, E)$$

$$\bar{\Sigma}_{\mathbf{x},g} \bar{\phi}_{\text{het}}^g = \int_V d\mathbf{r} \int_{E_g}^{E_{g-1}} dE \phi_{\text{het}}(\mathbf{r}, E) \Sigma_{\mathbf{x}}(\mathbf{r}, E)$$

- Produce homogenized constants for every node considered in the following nodal calculation

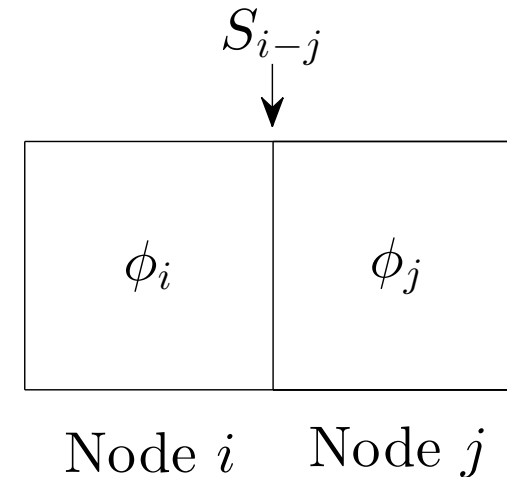
Discontinuity Factors (1)

- *Heterogeneous* flux ϕ_{het} and corresponding neutron current are known to be continuous across node boundaries
- There is no physical requirement for the *homogeneous* flux ϕ (solution of diffusion equation) to be continuous at the interfaces
- Discontinuity factors (DFs) couple the homogeneous flux ϕ to the heterogeneous flux ϕ_{het}
 \Rightarrow Continuity conditions for the nodal model

Discontinuity Factors (2)

- Definition:

$$F_{i \rightarrow j}^g = \frac{\int_{S_{i-j}} dS \int_g dE \phi_{\text{het}}(\mathbf{r}, E)}{\int_{S_{i-j}} dS \phi_i^g(\mathbf{r}, E)}$$



- *Idea:* On the boundary, ϕ_i^g multiplied by the discontinuity factor $F_{i \rightarrow j}^g$ equals ϕ_{het}^g on average.
 - Heterogeneous flux is known to be continuous across the boundaries.
 - This information is used to couple adjacent assemblies together.
- Corner DFs can be defined similarly as DFs for the sides

Pin-Power Reconstruction

- Due to homogenization, nodal solution does not provide detailed pin-by-pin flux
- It is still necessary to have an estimate for the power distribution inside the nodes
⇒ Peaking factors (PFs) couple homogeneous flux with pin-powers
- Peaking factor for pin i can be defined as:

$$p_i^g = \frac{\int_{V_i} dV \int_g dE \phi_{\text{het}}(\mathbf{r}, E) \kappa \Sigma_f(\mathbf{r}, E)}{\int_{V_i} dV \phi^g(\mathbf{r})}$$

- Power in pin i in node k can be computed as

$$P_{i,k} = \frac{\sum_g p_i^g \bar{\phi}_i^g}{P_k} P_{\text{tot}}$$

Homogenized Flux

- If boundary conditions comply with the heterogeneous calculation,

$$\overline{\phi} = \overline{\phi}_{\text{het}}$$

and DE yields the same balance equation as transport equation.

- Balance equation:

$$-J_{\text{net}} + (\overline{\Sigma}_{\text{t}} - \overline{\Sigma}_{\text{s}}) \overline{\phi} = \frac{1}{k_{\text{eff}}} \overline{F\phi}$$

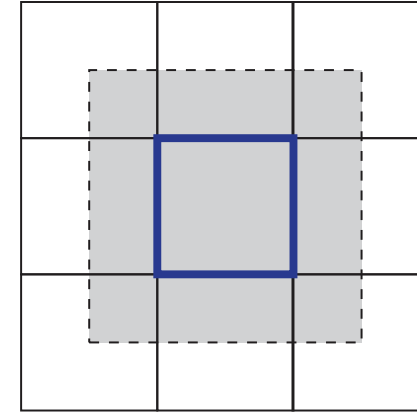
Data for nodal calculations (1)

- Exact computation of homogenized constants requires heterogeneous solution for the entire system.
- Exact computation of DFs and peaking factors requires homogeneous flux inside the node in addition to the heterogeneous solution.
- Typically it is assumed that assemblies can be modeled without their actual surroundings as a part of an *infinite lattice* using reflective boundary conditions.
 - ⇒ Homogenized constants for each assembly can be computed separately.
 - ⇒ Net currents over assembly boundaries are zero.
 - ⇒ Diffusion equation has *constant solution* $\phi = \bar{\phi}_{\text{het}}^0$ inside the assembly.
 - ⇒ DFs and peaking factors can be computed based on ϕ_{het}^0 alone.

Data for nodal calculations (2)

- In some cases, reflective boundary conditions cannot be used or the approximation is poor:

- Reflectors
- Strong absorbers
- Assembly positioning



- ⇒ Node must be modeled with some surroundings.
- ⇒ Computation of DFs and PFs requires solving the homogeneous flux inside the node.
- ⇒ Separate deterministic calculation is required to solve the multi-group diffusion equation inside the homogenized node
 - This capability will be implemented in Serpent

Solution of Homogenized Flux

- Multi-group diffusion equation in 2D

$$\begin{aligned} -D\Delta\phi + (\bar{\Sigma}_t - \bar{\Sigma}_s) \phi &= \frac{1}{k_{\text{eff}}} \bar{F} \phi \\ \Leftrightarrow D\Delta\phi &= A\phi \end{aligned}$$

- In addition to homogenized group constants, the solution depends on *boundary conditions*.
- Typically, boundary conditions are specified as *net currents* across (parts of) the boundaries:

$$-D^g \int_S \frac{\partial \phi^g}{\partial n} dS = J_{\text{net},S}^g$$

(Here n is the inward-pointing normal vector and $J_{\text{net}}^g > 0$ if the net flow of neutrons is into the node)

Solutions of Diffusion Equation (1)

- Diffusion equation (DE) in the homogenized node

$$D (\phi_{xx} + \phi_{yy}) = \left(\bar{\Sigma}_t - \bar{\Sigma}_s - \frac{1}{k_{\text{eff}}} \bar{F} \right) \phi = A \phi$$
$$\Leftrightarrow \phi_{xx} + \phi_{yy} = M \phi, \quad M = D^{-1} A .$$

- Trial function

$$\psi(x, y) = e^{B_1 x + B_2 y} c = e^{B_1 x} e^{B_2 y}$$

- Substitute to DE

$$\psi_{xx} + \psi_{yy} = B_1^2 \psi + B_2^2 \psi = (B_1^2 + B_2^2) \psi$$

- Function ψ satisfies DE if

$$B_1^2 + B_2^2 = M = D^{-1} A$$

Solutions of Diffusion Equation (1)

- Functions of the form

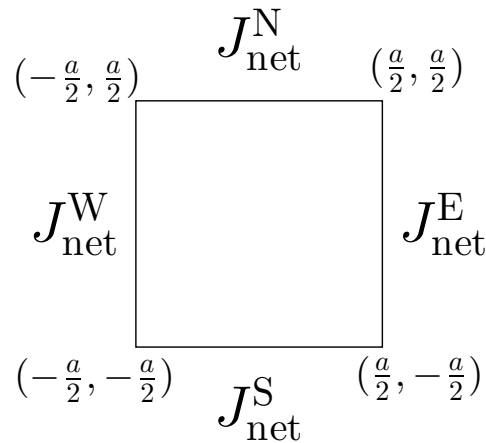
$$\psi(x, y) = e^{B_1 x + B_2 y}, \quad B_1^2 + B_2^2 = M,$$

satisfy DE. These functions are called *basis functions*.

- Matrix square root: If $C^2 = A$, C is a matrix square root of A
- Examples of basis functions: $e^{\sqrt{M}x}$, $e^{-\sqrt{M}y}$ and $e^{\sqrt{\frac{M}{2}}(x+y)}$
- General solution of DE is a linear combination of all basis functions. Boundary conditions determine the coefficients of the basis functions.
- When constructing a solution to DE, the number of boundary conditions must equal the number of basis functions.

Case 1: Constant Current on Every Boundary

- Boundary condition: $-D \frac{\partial}{\partial n} \Phi(x, y) = J_{\text{net}}^S / S = \text{const.}$, when $(x, y) \in S$.
 - For example, $\phi_x(x, y) = -D^{-1} J_{\text{net}}^W / a$ when $x = -a/2$



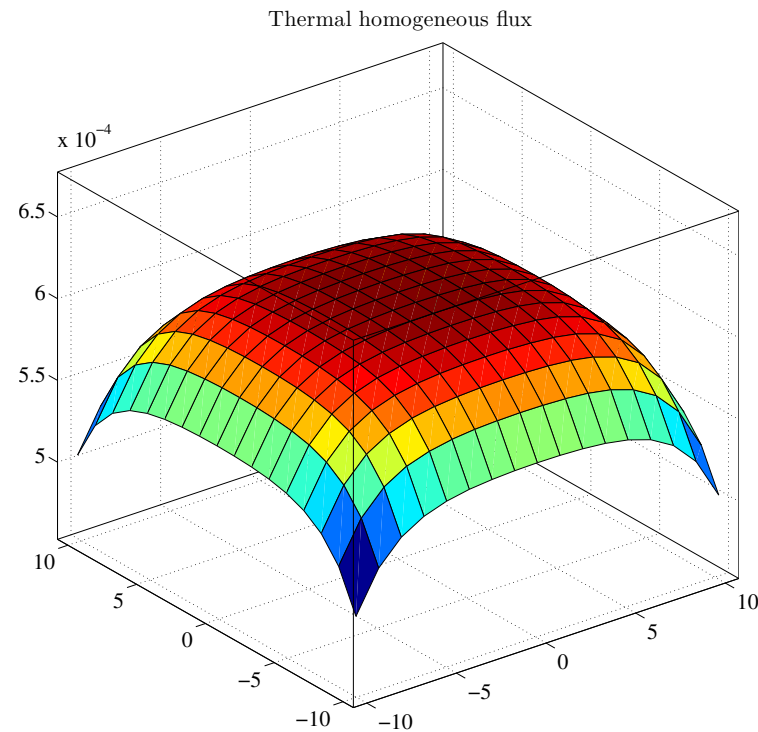
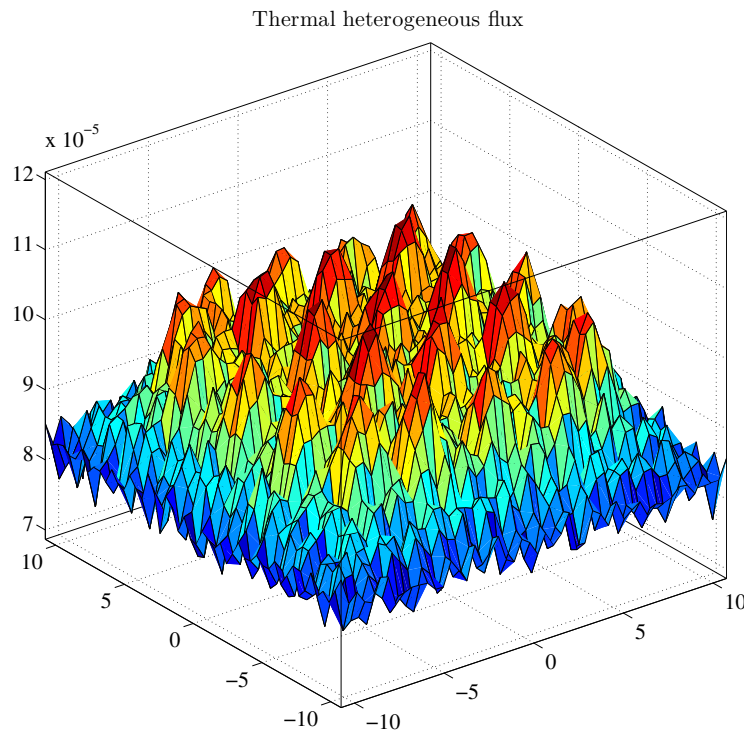
- Solution must be of the form:

$$\phi(x, y) = e^{\sqrt{A}x} c_1 + e^{-\sqrt{A}x} c_2 + e^{\sqrt{A}y} c_3 + e^{-\sqrt{A}y} c_4$$

- Unknown coefficient vectors c_1, \dots, c_4 are solved from 4 boundary conditions
- In this case, the solution is unique.

Case 1: Constant Current on Every Boundary

- Forcing the homogeneous current to a constant value on each boundary can lead to overestimation or underestimation of homogeneous flux near the corners
- Some nodal codes use corner ADFs in addition to surface ADFs



Case 2: N Boundary Conditions

- General idea: Choose N boundary conditions and N basis functions and solve the coefficients of the basis functions
 - Boundary conditions can be formed by dividing the boundary into N parts:

$$-D \int_{S_i} \frac{\partial}{\partial n} \phi(x, y) dS = J_{\text{net}}^{S_i} ,$$

where $S_i \subset \partial V$ is some part of the boundary.

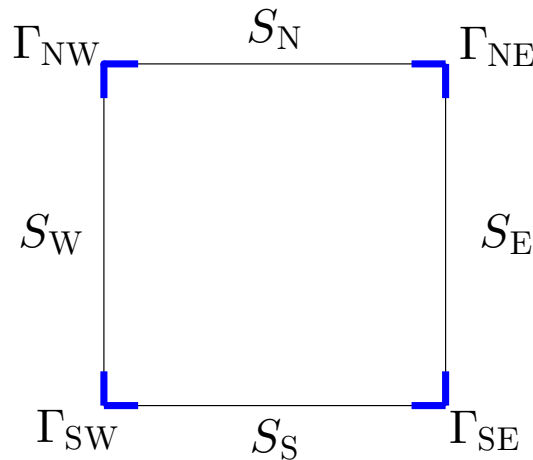
- Normal derivative of the homogeneous flux doesn't need to be forced to a *constant* value on any part of the boundary

Method to be implemented in Serpent

- 8 boundary conditions and 8 basis functions
- Basis functions:

$$f_x^\pm = e^{\pm\sqrt{A}x}, f_y^\pm = e^{\pm\sqrt{A}y}, f_{x+y}^\pm = e^{\pm\sqrt{\frac{A}{2}}(x+y)}, f_{x-y}^\pm = e^{\pm\sqrt{\frac{A}{2}}(x-y)}$$

- Boundary conditions:
 - $\int_S \mathbf{J}_{\text{hom}}(\mathbf{r}) dS = \mathbf{J}_{\text{net},S}$ for each boundary surface
 - $\int_\Gamma \mathbf{J}_{\text{hom}}(\mathbf{r}) dS = \mathbf{J}_{\text{net},\Gamma}$ for each corner



Examples

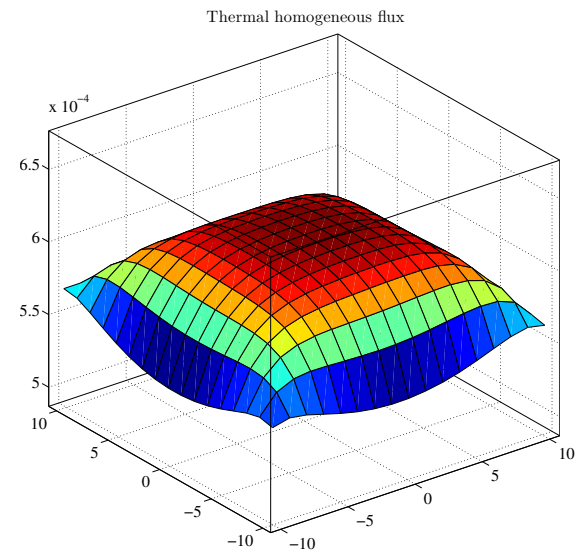
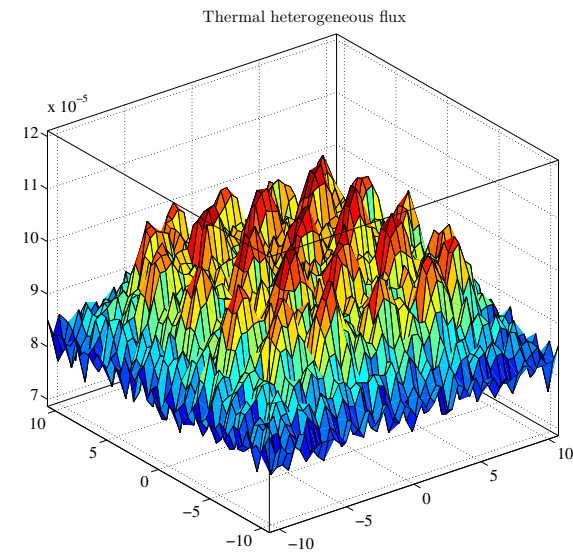
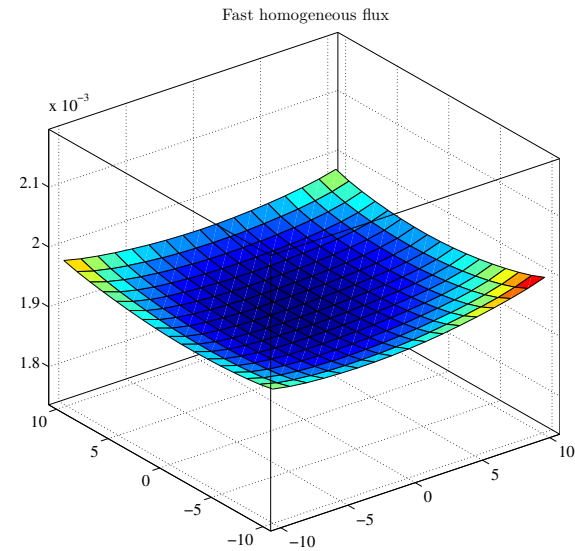
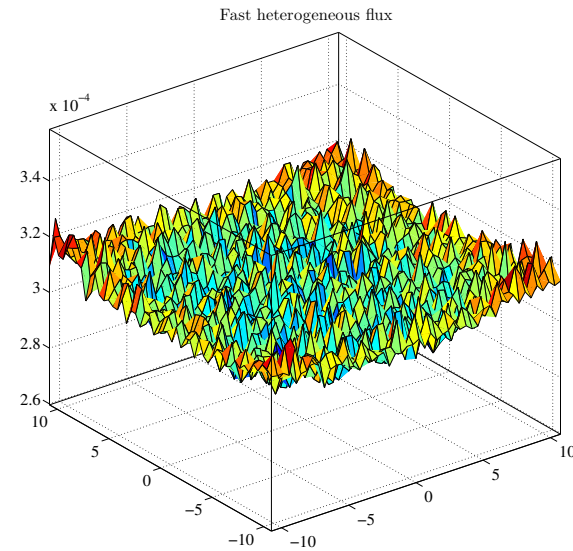
- The Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS)

- Example 1: Red (in the middle)
- Example 2: Blue w. 6 absorber pins
- Example 3: Reflector I

					R	P	N	M	L	K	J	H	G	F	E	D	C	B	A					
								III	III	III	III	III	III	III	III	III								
							III	III	III	I	I	I	I	I	II	III	III	III						
1				III	III	II	II			6		6		6		II	II	III	III					
2		III	III	II				16		20		20		16			II	III	III					
3		III	II		15	16		16		16		16		16		15		II	III					
4	III	III	II		16			16		12		12		16		16		II	III	III				
5	III	II		16		16		12		12		12		12		16		16		I	III			
6	III	I	6		16		12		12		12		12		12		16		6	I	III			
7	III	I		20		12		12		16		12		12		12		20		I	III			
8	III	I	6		16		12		16		16		16		12		16		6	I	III			
9	III	I		20		12		12		16		12		12		12		20		I	III			
10	III	I	6		16		12		12		12		12		12		16		6	I	III			
11	III	I		16		16		12		12		12		12		16		16		II	III			
12	III	III	II		16		16		12		12		12		16		16		II	III	III			
13		III	II		15	16		16		16		16		16		15		II	III					
14		III	III	II			16		20		20		16				II	III	III					
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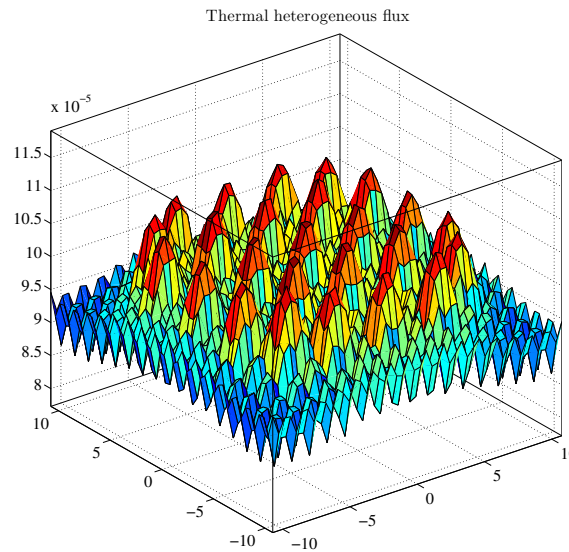
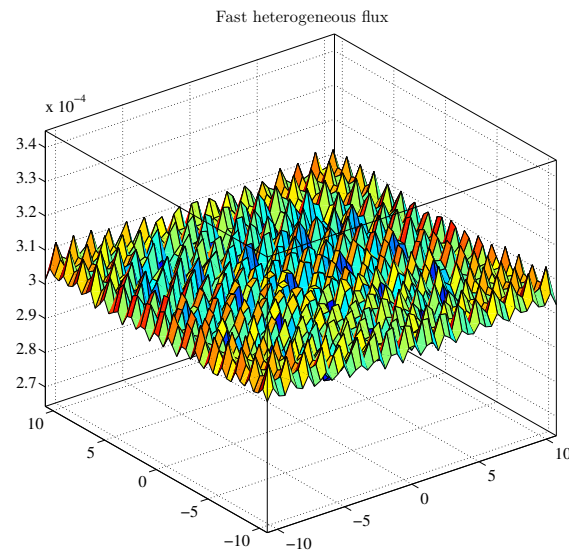
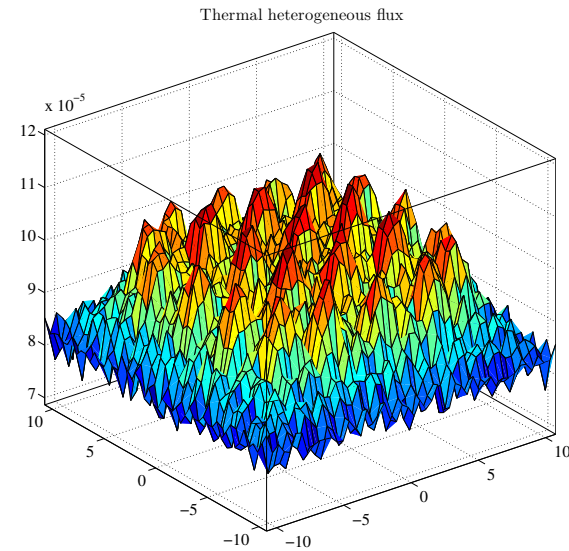
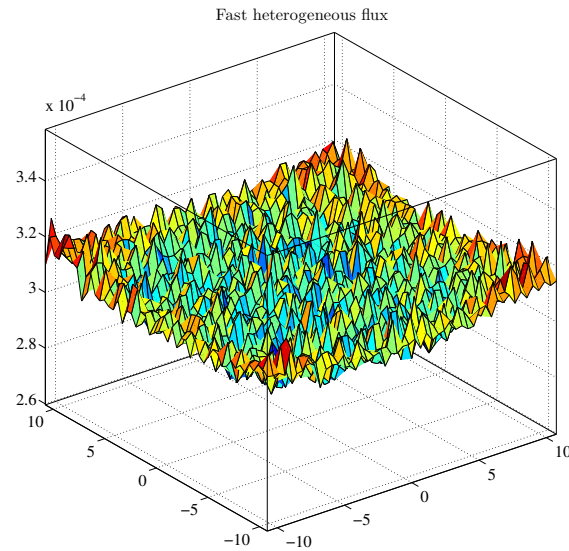
Example 1

2.5 assembly widths of surroundings.



Example 1

Top: surroundings included. Bottom: reflective boundary.



ADFs for Example 1

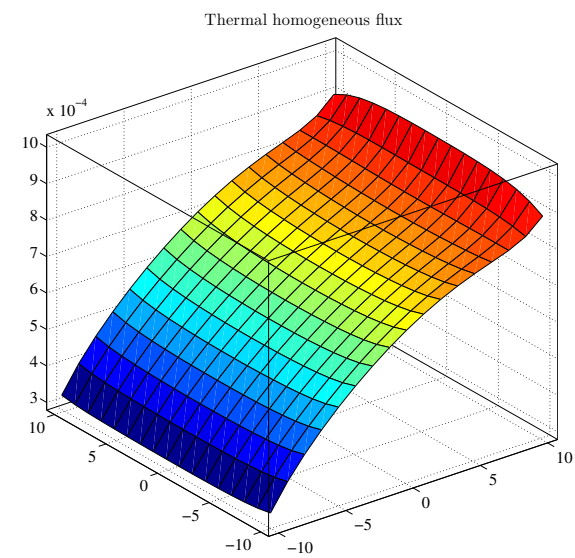
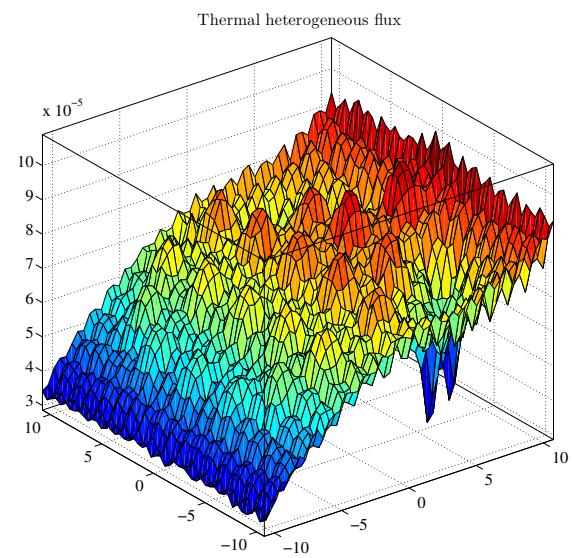
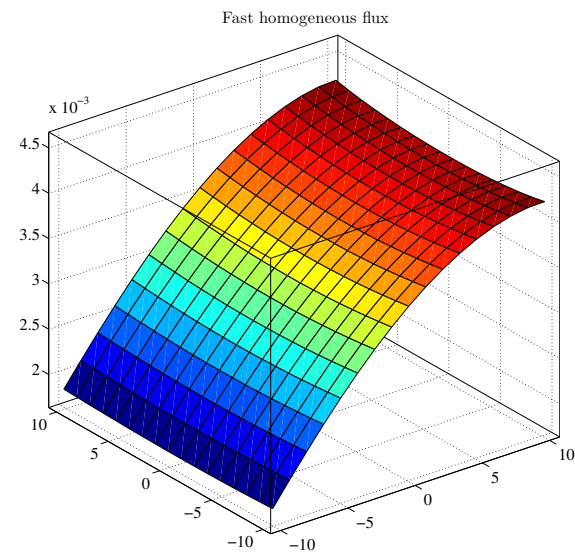
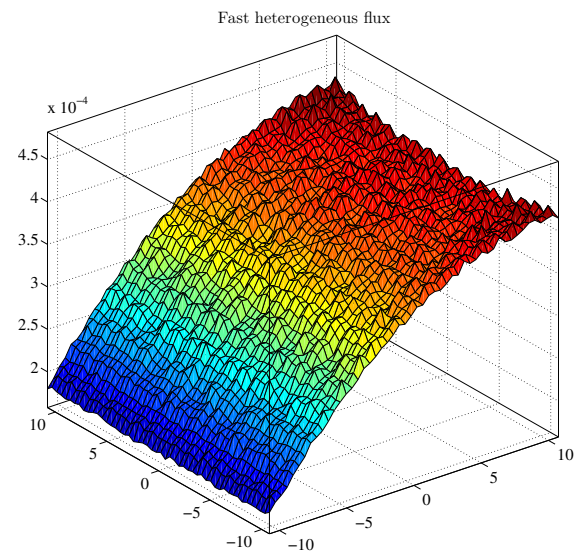
- 2.5 assembly widths of surroundings

Fast	1.0017	1.0030	1.0030	1.0007
Thermal	0.9916	0.9869	0.9936	0.9949

- Reflective boundary conditions

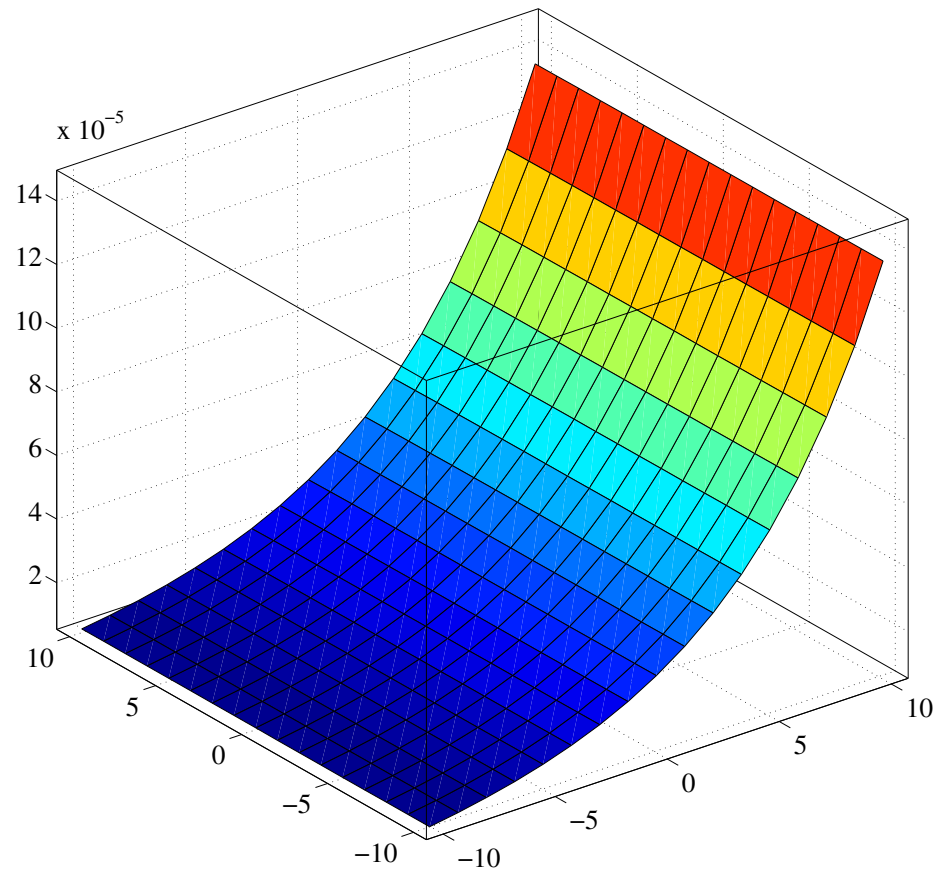
Fast	0.9973	0.9970	0.9971	0.9977
Thermal	0.9968	0.9980	0.9970	0.9970

Example 2

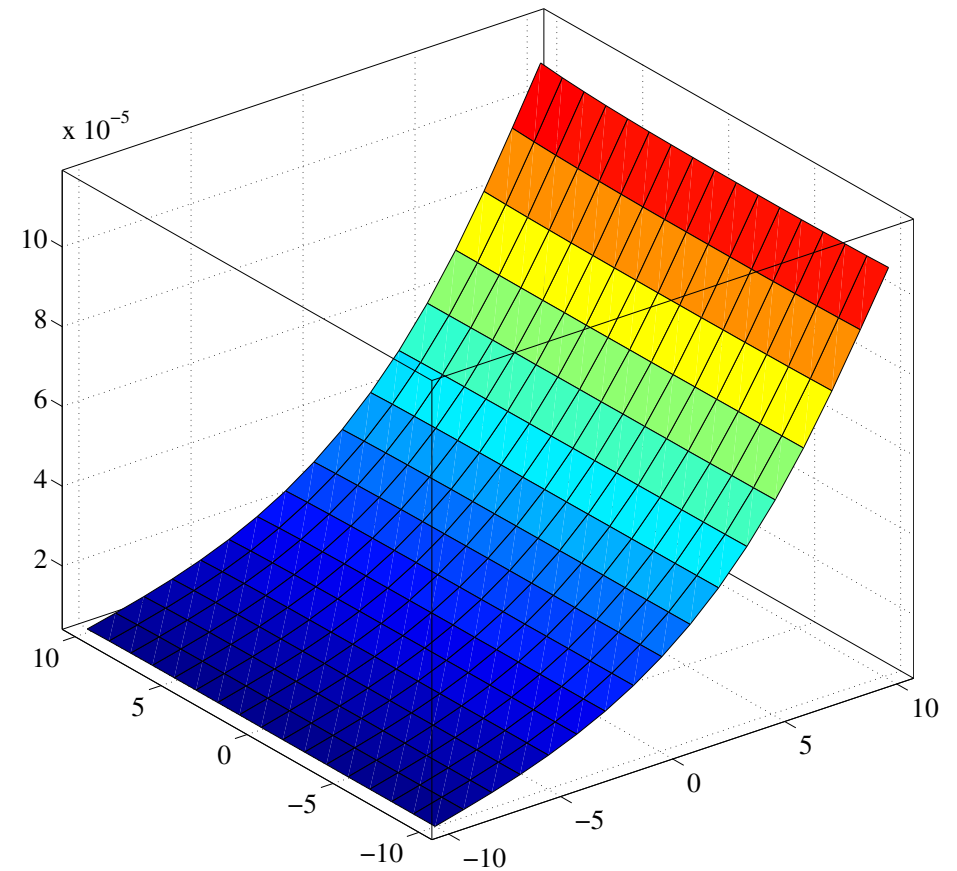


Example 3

Fast homogeneous flux



Thermal homogeneous flux



Numerical solution of homogeneous flux (1)

- Starting point: Homogenized constants and boundary conditions
- Form matrix M :

$$M = D^{-1} \left(\bar{\Sigma}_t - \bar{\Sigma}_s - \frac{1}{k_{\text{eff}}} \bar{F} \right)$$

- Compute square root of M
 - Explicit formulas for small matrices
 - Iterative methods for larger matrices
- Compute basis functions
 - Matrix exponential
 - Matrices are small and well-behaved
- Form equations corresponding to boundary conditions
 - Requires numerical integration

Numerical solution of homogeneous flux (2)

- Solve coefficients of the basis functions
 - Requires a linear solver
- Numerical building blocks:
 - Matrix square root algorithm
 - Matrix exponential algorithm
 - Numerical integration method
 - Linear solver
- After implementing these numerical methods, it is easy to refine the method by changing the boundary conditions and/or basis functions. Also, solution method can be extended to more complex geometries and 3D.