Homogeneous diffusion flux solver in Serpent 2

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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

- Computationally expensive to solve transport equation in the true heterogeneous geometry of the reactor core, i.e. to compute *global heterogeneous flux*

$\Rightarrow$ Nodal calculations

  - System divided into nodes that have homogeneous properties
  - Solution based on multi-group diffusion theory

$$-D^g \triangle \phi^g(\boldsymbol{r}) + \overline{\Sigma}_{\mathrm{t}}^g \phi^g(\boldsymbol{r}) = \sum_h \overline{\Sigma}_{\mathrm{s}}^{h \to g} \phi^h(\boldsymbol{r}) + \frac{1}{k_{\mathrm{eff}}} \overline{\chi}^g \sum_h \overline{\nu\Sigma}_{\mathrm{f}}^h \phi^h(\boldsymbol{r}) \,, \quad g = 1, \ldots, G$$

$$-\boldsymbol{D} \triangle \boldsymbol{\phi} + \left(\overline{\boldsymbol{\Sigma}}_{\mathrm{t}} - \overline{\boldsymbol{\Sigma}}_{\mathrm{s}} \right) \boldsymbol{\phi} = \frac{1}{k_{\mathrm{eff}}} \overline{\boldsymbol{F}} \boldsymbol{\phi}$$

- Solution called *global homogeneous flux*
- Lattice calculations $\Rightarrow$ homogenized constants for each node

Lattice calculations

- Key idea:
  - Assume global heterogeneous $\phi_{\text{het}}^{\text{glob}}$ flux to be known
  - Preserve nodal reaction rates:

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

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

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

- **Practise**: Solve transport equation for a set of smaller sub-problems $\Rightarrow$ *local heterogeneous flux*.
- **Approximate** global heterogeneous flux $\phi_{\text{het}}^{\text{glob}}$ by local heterogeneous flux ϕ_{het}^{0} when computing the homogenized constants

Continuity conditions for nodal model

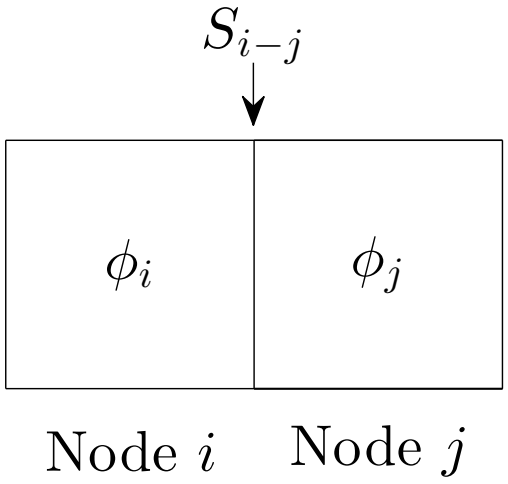
- Nodes are coupled together using *discontinuity factors* obtained from lattice calculations.
- Idea:
  - Global heterogeneous flux is known to be continuous across node boundaries
  - There is no no physical requirement for the global homogeneous flux to be continuous
  - Discontinuity factors (DFs) couple *local* homogeneous flux to *local* heterogeneous flux
- **Approximation**: DFs are used to couple *global* homogeneous flux to *global* heterogeneous flux

  $\Rightarrow$ Continuity conditions for the nodal model

Discontinuity Factors

- Definition:

$$F^g_{i\to j} = \frac{\int_{S_{i-j}} dS \phi^g_{\text{het}}(\boldsymbol{r}, E)}{\int_{S_{i-j}} dS\, \phi^g_i(\boldsymbol{r}, E)}$$



- *Idea:* On the boundary, ϕ^g_i multiplied by the discontinuity factor $F^g_{i\to j}$ equals ϕ^g_{het} on average.
- 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

  $\Rightarrow$ Peaking factors (PFs) couple local homogeneous flux with pin-powers

- Peaking factor for pin i can be defined as:

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

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

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

Data for nodal calculations

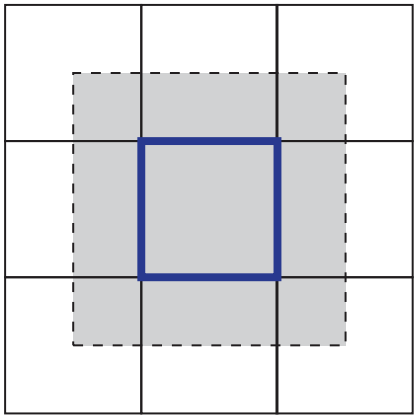
- Exact computation of homogenized constants requires global heterogeneous flux solution for the entire system.
- Exact computation of DFs and peaking factors requires global homogeneous flux in addition to the global heterogeneous flux.
- In practise, homogenized constants, DFs and peaking factors are computed based on *local* heterogeneous and *local* homogeneous fluxes (corresponding to a set of sub-problems).

Reflective boundary conditions

- Typical practice: consider each node separately with reflective boundary conditions ("sub-problem $=$ node")
  - $\Rightarrow$ Homogenized constants for each assembly can be computed separately.
  - $\Rightarrow$ Net currents over assembly boundaries are zero.
  - $\Rightarrow$ Diffusion equation has *constant solution* $\phi = \overline{\phi}^0_{\text{het}}$ inside the homogenized assembly.
  - $\Rightarrow$ DFs and peaking factors can be computed based on ϕ^0_{het} alone.
  - $\Rightarrow$ No need for a diffusion solver

Colorset calculations

- In some cases, reflective boundary conditions cannot be used or the approximation is poor:
  - Reflectors
  - Strong absorbers
  - Assembly positioning



$\Rightarrow$ Node must be modeled with some surroundings ("sub-problem $=$ colorset").

$\Rightarrow$ Computation of DFs and PFs requires solving the local homogeneous flux inside the node.

$\Rightarrow$ Separate deterministic calculation is required to solve the multi-group diffusion equation inside the homogenized node

  - This capability has been implemented in Serpent 2

Solutions of Homogeneous Diffusion Equation (1)

- Diffusion equation (DE) in the homogenized node

$$\begin{aligned} \boldsymbol{D}\left(\boldsymbol{\phi}_{xx}+\boldsymbol{\phi}_{yy}\right) &= \left(\overline{\boldsymbol{\Sigma}}_{\mathrm{t}}-\overline{\boldsymbol{\Sigma}}_{\mathrm{s}}-\frac{1}{k_{\mathrm{eff}}}\overline{\boldsymbol{F}}\right)\boldsymbol{\phi}=\boldsymbol{A}\boldsymbol{\phi} \\ \Leftrightarrow \quad \boldsymbol{\phi}_{xx}+\boldsymbol{\phi}_{yy} &= \boldsymbol{M}\boldsymbol{\phi}\,, \quad \boldsymbol{M}=\boldsymbol{D}^{-1}\boldsymbol{A}\,. \end{aligned}$$

- Trial function

$$\boldsymbol{\psi}(x,y)=e^{\boldsymbol{B}_1 x+\boldsymbol{B}_2 y}\boldsymbol{c}=e^{\boldsymbol{B}_1 x}e^{\boldsymbol{B}_2 y}$$

- Substitute to DE

$$\boldsymbol{\psi}_{xx}+\boldsymbol{\psi}_{yy}=\boldsymbol{B}_1^2\psi+\boldsymbol{B}_2^2\psi=\left(\boldsymbol{B}_1^2+\boldsymbol{B}_2^2\right)\psi$$

- Function ψ satisfies DE if

$$\boldsymbol{B}_1^2+\boldsymbol{B}_2^2=\boldsymbol{M}=\boldsymbol{D}^{-1}\boldsymbol{A}$$

Solutions of Homogeneous Diffusion Equation (2)

- Functions of the form

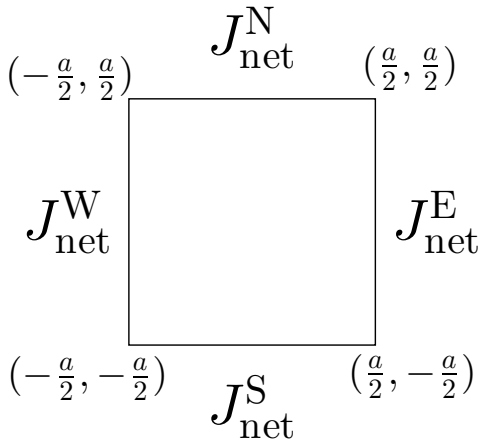
$$\psi(x,y) = e^{B_1 x + B_2 y} \ , \quad B_1^2 + B_2^2 = M \ ,$$

  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.
- Local homogeneous solution should be consistent with the nodal code.

Constant Current on Every Boundary

- Boundary condition: $-\boldsymbol{D}\frac{\partial}{\partial n}\boldsymbol{\Phi}(x,y) = \boldsymbol{J}^{S}_{\mathrm{net}}/S = \mathrm{const.}$, when $(x,y) \in S$.
  - For example, $\boldsymbol{\phi}_x(x,y) = -\boldsymbol{D}^{-1}\boldsymbol{J}^{\mathrm{W}}_{\mathrm{net}}/a$ when $x = -a/2$



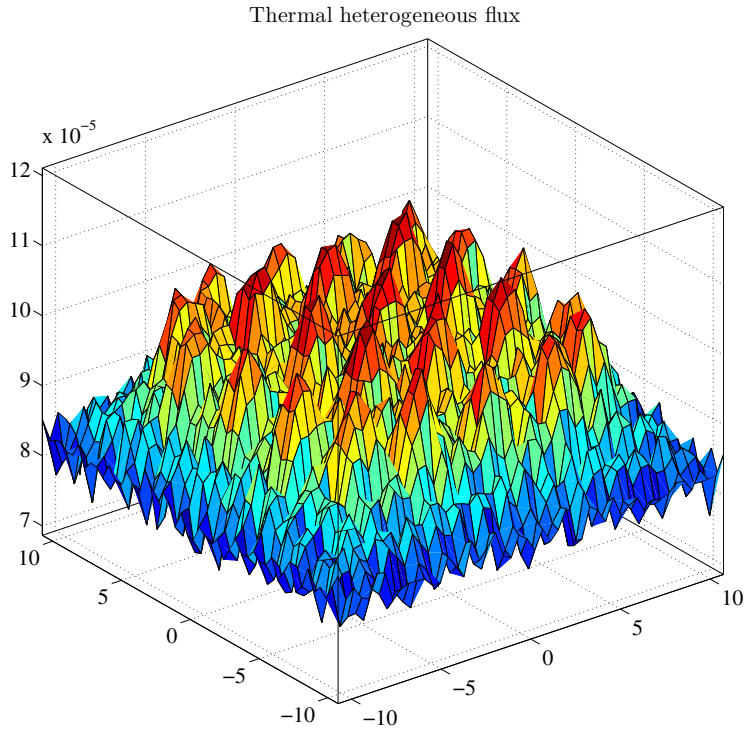
- Solution must be of the form:

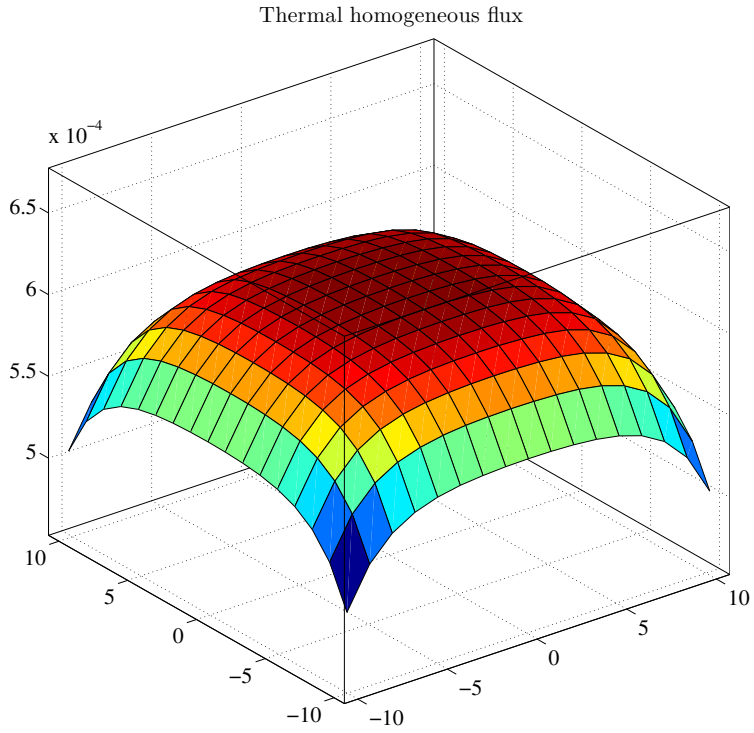
$$\phi(x,y) = e^{\sqrt{\boldsymbol{A}}x}\boldsymbol{c}_1 + e^{-\sqrt{\boldsymbol{A}}x}\boldsymbol{c}_2 + e^{\sqrt{\boldsymbol{A}}y}\boldsymbol{c}_3 + e^{-\sqrt{\boldsymbol{A}}y}\boldsymbol{c}_4$$

- Unknown coefficient vectors $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_4$ are solved from 4 boundary conditions
- In this case, the solution is unique.

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

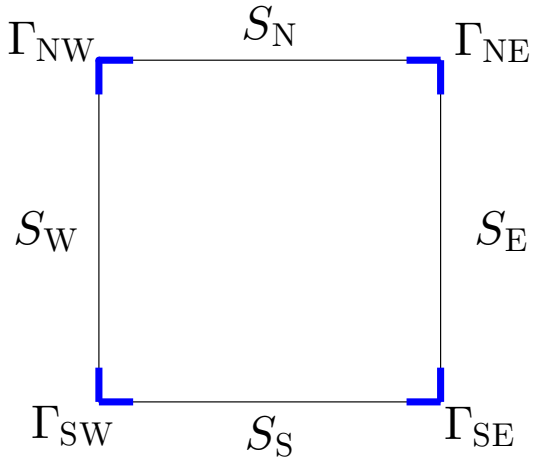




Method implemented in Serpent

- Boundary conditions:
  - $\int_S \boldsymbol{J}_{\mathrm{hom}}(\boldsymbol{r})\, dS = \boldsymbol{J}_{\mathrm{net},S}$ for each boundary surface
  - $\int_\Gamma \boldsymbol{J}_{\mathrm{hom}}(\boldsymbol{r})\, dS = \boldsymbol{J}_{\mathrm{net},\Gamma}$ for each corner
- Rectangular geometry:
  - 8 boundary conditions and 8 basis functions
  - Basis functions:

$$\boldsymbol{f}^{\pm}_{\mathrm{x}} = e^{\pm\sqrt{\boldsymbol{A}}x}\,, \boldsymbol{f}^{\pm}_{\mathrm{y}} = e^{\pm\sqrt{\boldsymbol{A}}y}\,, \boldsymbol{f}^{\pm}_{\mathrm{x+y}} = e^{\pm\sqrt{\frac{\boldsymbol{A}}{2}}(x+y)}\,, \boldsymbol{f}^{\pm}_{\mathrm{x-y}} = e^{\pm\sqrt{\frac{\boldsymbol{A}}{2}}(x-y)}$$



- Similar approach for hexagonal geometry

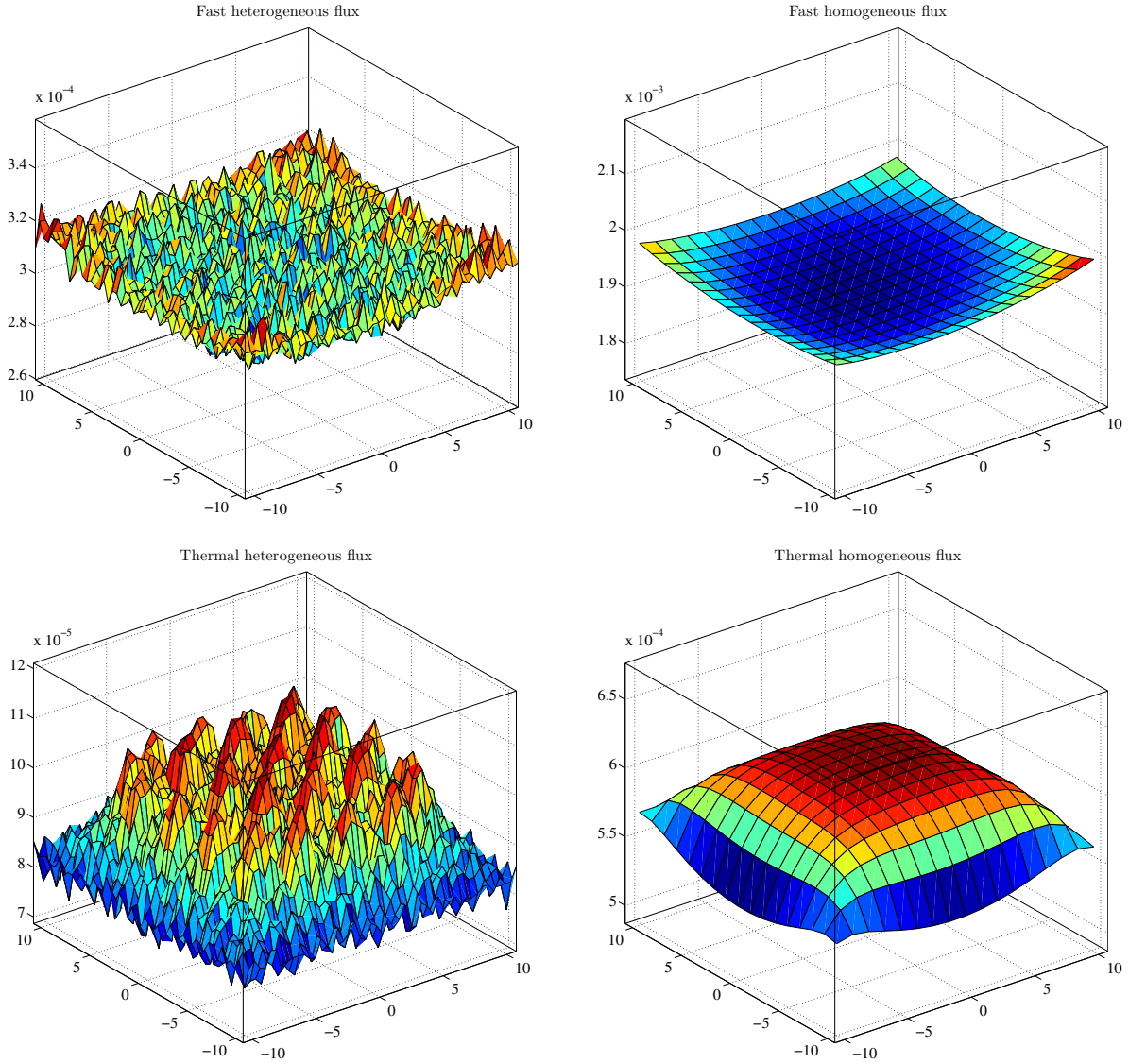
Example 1

- The Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS), red assembly (in the middle)

	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	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		16		16		I	III
6	III	I	6		16		12		12		12		12		16		6	I	III
7	III	I		20		12		12		16		12		12		20		I	III
8	III	I	6		16		12		16		16		12		16		6	I	III
9	III	I		20		12		12		16		12		12		20		I	III
10	III	I	6		16		12		12		12		12		16		6	I	III
11	III	I		16		16		12		12		12		16		16		II	III
12	III	III	II		16		16		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	
15			III	III	II	II		6		6		6		II	II	III	III		
				III	III	III	II	I	I	I	I	I	I	III	III	III			
						III	III	III	III	III	III	III	III	III					

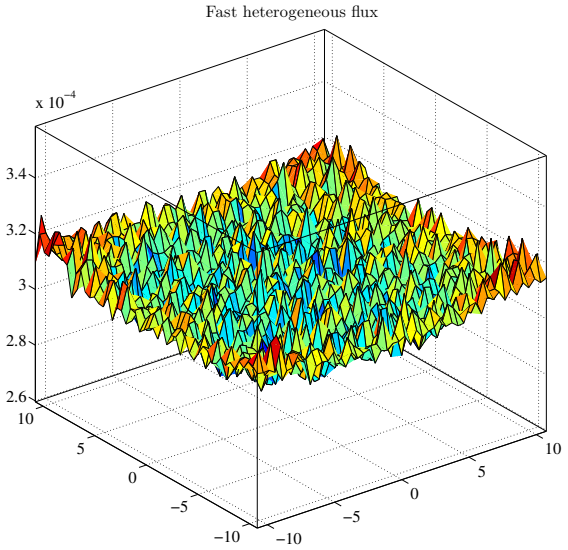
Example 1

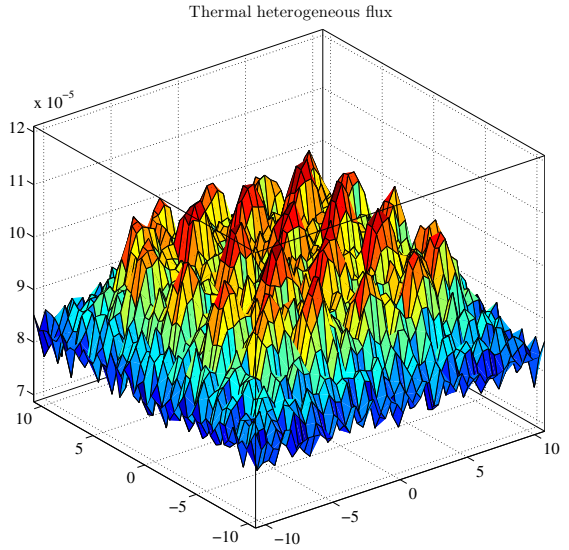
2.5 assembly widths of surroundings.

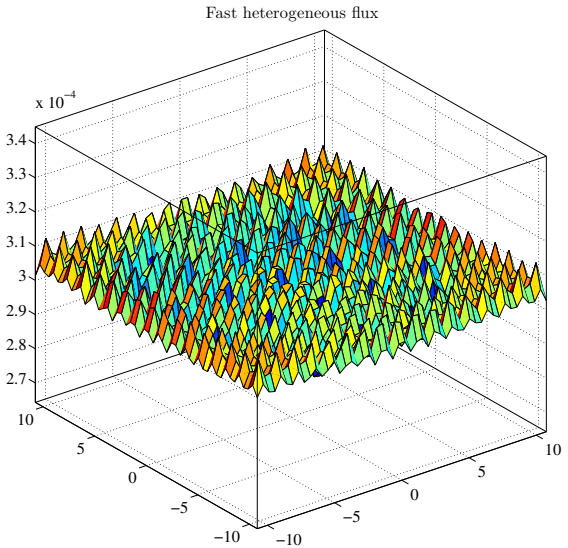


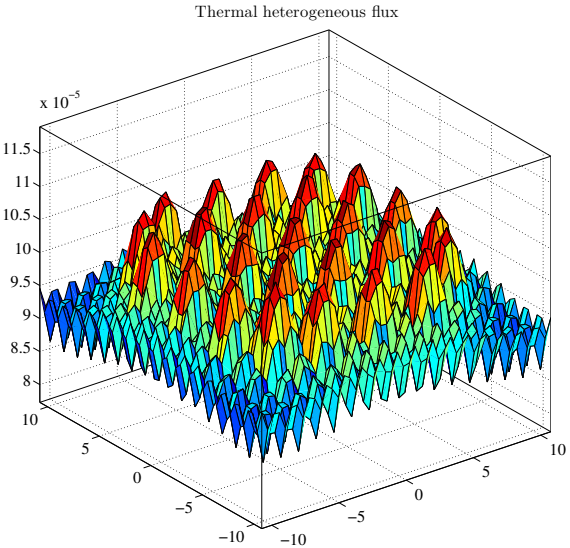
Example 1

Top: surroundings included. Bottom: reflective boundary.

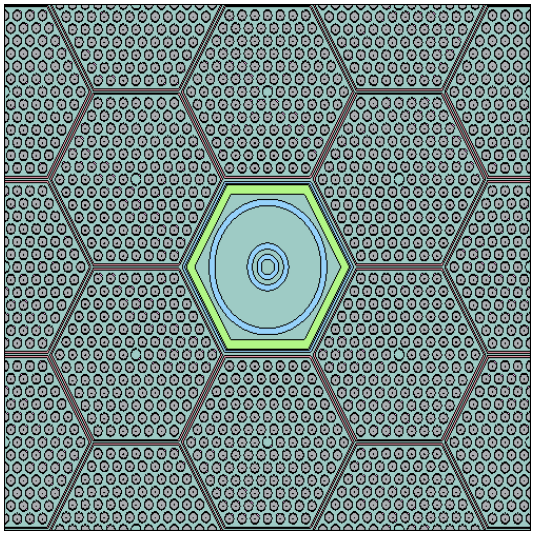


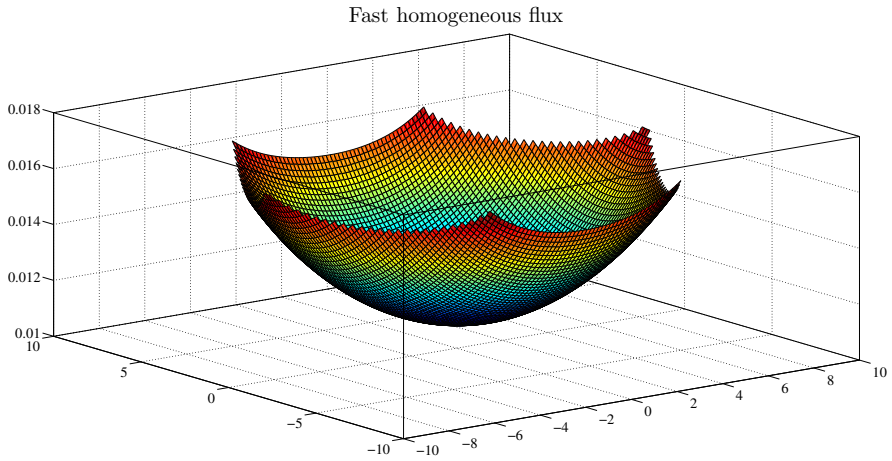


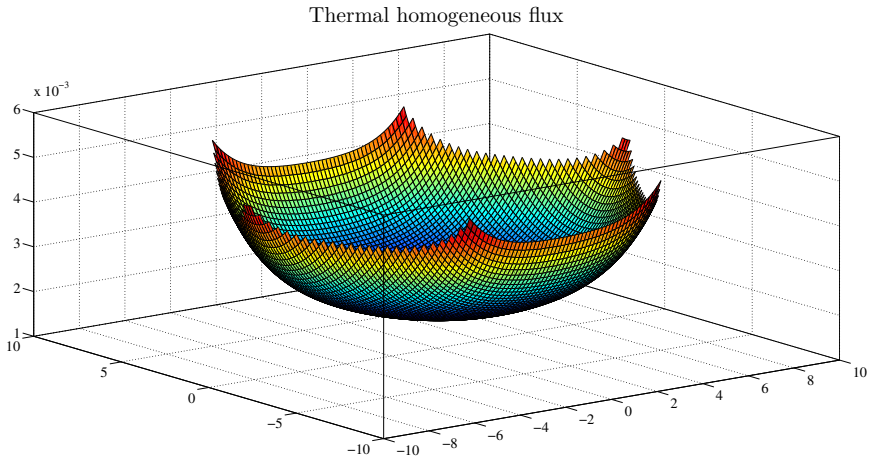




Example 2




Fast homogeneous flux
0.018
0.016
0.014
0.012
0.01
10
5
0
−5
−10
−10
−8
−6
−4
−2
0
2
4
6
8
10


Thermal homogeneous flux
x 10^−3
6
5
4
3
2
1
10
5
0
−5
−10
−10
−8
−6
−4
−2
0
2
4
6
8
10

Numerical solution of homogeneous flux in Serpent

- Starting point: Homogenized constants and boundary conditions
- Form matrix $\boldsymbol{M}$:

$$\boldsymbol{M} = \boldsymbol{D}^{-1}\left(\overline{\boldsymbol{\Sigma}}_{\mathrm{t}} - \overline{\boldsymbol{\Sigma}}_{\mathrm{s}} - \frac{1}{k_{\mathrm{eff}}}\overline{\boldsymbol{F}}\right)$$

- Compute *complex* Schur form $\boldsymbol{M} = \boldsymbol{U}\boldsymbol{T}\boldsymbol{U}^{*}$
  - Hessenberg reduction and QR decomposition based on Householder transformations
  - QR updates with Wilkinson shift

$\Rightarrow$ Matrix functions (matrix square root, matrix exponential) can be computed efficiently with Parlett method

- Form boundary conditions
- Solve coefficients (Gaussian elimination with partial pivoting)
- Compute DFs and PFs based on local homogeneous solution

Summary

- In the absence of reflective boundary conditions, the computation of discontinuity and peaking factors requires solving diffusion equation for the homogenized node.
  - General solution is a linear combination of matrix functions (called basis functions)
  - Coefficients of basis functions computed based on boundary conditions
  - Boundary conditions should be consistent with nodal code
- Method implemented in Serpent 2:
  - 2D
  - Rectangular and hexagonal geometry
  - Boundary and corner net currents as boundary condition
- Future work:
  - Need for other types of boundary conditions?
  - Extend methodology to 3D.