Working Notes on a 2D Thermal Model with Parallel Sensitivity Calculations

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1 Background

Mathematical models for heating/cooling of buildings typically feature large number of parameters characterizing features such as conductivity, convective coefficients, as well as geometric layout. Whereas lumped (ordinary differential equations - ODE) models are common, the treatment here will retain the distributed nature of the underlying physics (partial differential equations - PDE).

2 A Mathematical Model

We consider unsteady heat conduction in a plane. The governing partial differential equation is

$$\sigma C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right) + F(T,x,y,t),\ (x,y) \in \Omega,\ t > 0\ , \quad (1)$$

where:

- $\Omega = \{(x,y) \quad | \quad 0 \le x \le L, \quad 0 \le y \le w\} \subset \mathbb{R}^2$,
- $F(T,x,y,t)$ is a specified source term,
- σ is the areal density of the material,

- C_p is the thermal capacitance of the material, and
- $k_x > 0$ ($k_y > 0$) is the conductivity in the x direction (the y-direction).

Boundary conditions for our problem are:

$$\frac{\partial T(x,0)}{\partial y} = \frac{\partial T(x,w)}{\partial y} = 0 \ , \tag{2}$$

$$k_x \frac{\partial T(L,y)}{\partial x} = f(y) \ , \tag{3}$$

$$k_x \frac{\partial T(0,y)}{\partial x} = \alpha(y) \ \left(T(0,y) - \beta(y)\right) \ . \tag{4}$$

In the final (Robin) boundary condition we require that $\alpha(y) \geq 0$. The initial data is given by

$$T(0,x,y) = h(x,y) \ . \tag{5}$$

3 Numerical Approximation

3.1 Time discretization

Numerical solution of the problem (1 - 5) requires some type of discretization. We begin by introducing a uniform time-grid, *viz* $t_n = n\Delta t$, $n = 0, 1, ...,$ and defining $T^n(x,y) \stackrel{\triangle}{=} T(t_n, x, y)$. The time-derivative in (1) is approximated by the usual difference quotient leading to

$$(\sigma\, C_p)\, \frac{T^{n+1} - T^n}{\Delta t} = \left[\frac{\partial}{\partial x} \left(k_x \frac{\partial}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial}{\partial y} \right) \right] (\theta T^{n+1} + (1-\theta) T^n) \\ + F((\theta T^{n+1} + (1-\theta) T^n), x, y, \hat{t}) \ .$$

We have the choices:

- $\theta = 0$ - explicit Euler,
- $\theta = 1$ - implicit Euler,
- $\theta = 1/2$ - implicit mid-point rule (similar to Crank-Nicholson).

We choose the implicit Euler scheme and re-write as

$$T^{n+1} - T^n - \frac{\Delta t}{\sigma\, C_p} \left[\frac{\partial}{\partial x} \left(k_x \frac{\partial}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial}{\partial y} \right) \right] T^{n+1} \\ - \frac{\Delta t}{\sigma\, C_p} F(T^{n+1}, x, y, t_{n+1}) = 0 \ . \tag{6}$$

The (spatial) PDE (6) is to be solved at $n = 0, 1, ...$ with $T^0(x, y) = h(x, y)$, from (5).

3.2 Spatial discretization

Our numerical solution of (6) is based on a weak formulation. We multiply by a test function $\Psi(x, y)$ and integrate over the spatial domain Ω:

$$\int_\Omega \left(T^{n+1} - T^n - \frac{\Delta t}{\sigma\, C_p} F(T^{n+1}, x, y, t_{n+1}) \right) \Psi \, \mathrm{d}\omega - \frac{\Delta t}{\sigma\, C_p} \int_\Omega \left[\frac{\partial}{\partial x}\left(k_x \frac{\partial}{\partial x} \right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial}{\partial y} \right) \right] T^{n+1} \, \Psi \, \mathrm{d}\omega = 0 \; . \quad (7)$$

The 2$^{\text{nd}}$ term in (7) is integrated by parts

$$\int_\Omega \left[\frac{\partial}{\partial x}\left(k_x \frac{\partial}{\partial x} \right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial}{\partial y} \right) \right] T^{n+1} \, \Psi \, \mathrm{d}\omega = - \int_\Omega \left(k \nabla T^{n+1} \cdot \nabla \Psi \right) \mathrm{d}\omega + \int_{\partial\Omega} \left(k \nabla T^{n+1} \cdot \hat{n} \right) \Psi \, \mathrm{d}\sigma \; , \quad (8)$$

where in the boundary integral, $\hat{n}$ is an outward normal to the surface, and the integration is in an anti-clockwise sense around the region Ω. Imposing the specified boundary conditions (2 - 4), the boundary term in (8) evaluates to

$$\int_{\partial\Omega} \left(k \nabla T^{n+1} \cdot \hat{n} \right) \Psi \, \mathrm{d}\sigma = \int_0^w f(y) \Psi(L, y) \, \mathrm{d}y - \int_w^0 \alpha(y) \left[T^{n+1}(0, y) - \beta(y) \right] \Psi(0, y) \, \mathrm{d}y \; . \quad (9)$$

In the following we restrict attention to the case wherein the source term F does not depend on T.

3.3 Galerkin Finite Element

We seek an approximate solution of the form

$$T_N^n(x, y) = \sum_{\jmath=1}^{N} z_\jmath^n \, \Phi_\jmath(x, y) \; . \quad (10)$$

Substitute the approximation (10) into the weak-form and use for test functions $\Psi = \Phi_\imath$ leads to:

$$\sum_\jmath z^{n+1} \int_\Omega \Phi_\jmath(x,y)\ \Phi_\imath(x,y)\ \mathrm{d}\omega - \sum_\jmath z^n \int_\Omega \Phi_\jmath(x,y)\ \Phi_\imath(x,y)\ \mathrm{d}\omega$$
$$- \frac{\Delta t}{\sigma\, C_p} \int_\Omega F(x,y,t_{n+1})\Phi_\imath\ \mathrm{d}\omega + \frac{\Delta t}{\sigma\, C_p} \sum_\jmath z^{n+1} \int_\Omega (k\nabla\Phi_\jmath \cdot \nabla\Phi_\imath)\ \mathrm{d}\omega$$
$$-\frac{\Delta t}{\sigma\, C_p}\left[\int_0^w f(y)\Phi_\imath(L,y)\ \mathrm{d}y - \int_w^0 \alpha(y)\left(\sum_\jmath z_\jmath^{n+1}\Phi_\jmath(0,y) - \beta(y)\right)\Phi_\imath(0,y)\ \mathrm{d}y\right] \ = \ 0$$
$$\text{for } \imath = 1, 2, ..., N\ . \quad (11)$$

Gathering terms leads to

$$\sum_\jmath \Bigg[\int_\Omega \Phi_\jmath(x,y)\ \Phi_\imath(x,y)\ \mathrm{d}\omega$$
$$+\frac{\Delta t}{\sigma\, C_p}\left(\int_\Omega (k\nabla\Phi_\jmath \cdot \nabla\Phi_\imath)\ \mathrm{d}\omega + \int_w^0 \alpha(y)\,\Phi_\jmath(0,y)\,\Phi_\imath(0,y)\ \mathrm{d}y\right)\Bigg]\, z_\jmath^{n+1}$$
$$-\sum_\jmath \left[\int_\Omega \Phi_\jmath(x,y)\ \Phi_\imath(x,y)\ \mathrm{d}\omega\right] z_\jmath^n - \left[\frac{\Delta t}{\sigma\, C_p}\int_\Omega F(x,y,t_{n+1})\Phi_\imath\ \mathrm{d}\omega\right]$$
$$-\frac{\Delta t}{\sigma\, C_p}\left[\int_0^w f(y)\Phi_\imath(L,y)\ \mathrm{d}y + \int_w^0 \alpha(y)\beta(y)\Phi_\imath(0,y)\ \mathrm{d}y\right] = 0$$
$$\text{for } \imath = 1, 2, ..., N\ . \quad (12)$$

In matrix terminology

$$(\mathbf{M}_1 + \mathbf{M}_2)\ z^{n+1}\ -\ \mathbf{M}_1\, z^n\ +\ \mathbf{F}(t_{n+1})\ +\ \mathbf{b} = 0\ . \quad (13)$$

Note that if the source term in (1) has a finite limit ($\lim_{t\to\infty} F(t,x,y) = F^\infty(x,y)$) and $\lim_{t\to\infty} \mathbf{F}(t) = \mathbf{F}^\infty$ then (13) has a steady-state solution that satisifies

$$\mathbf{M}_2 z^{\mathrm{ss}} + \mathbf{F}^\infty + \mathbf{b} = 0\ . \quad (14)$$

3.3.1 Quadratic Functions on Triangular Elements

We impose a regular $n_x \times n_y = ((2\ell+1)\times(2m+1))$ grid on Ω ($\ell, m \geq 1$). Using the odd-labeled points we generate $\ell\ m$ rectangles; diagonals divide these into $2\ \ell\ m$ triangles. Figure 1 shows the case $n_x = 21, n_y = 13$

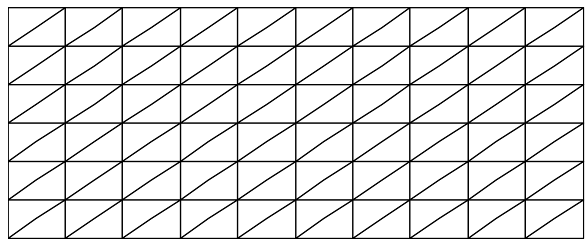


Figure 1: 21×13 Grid

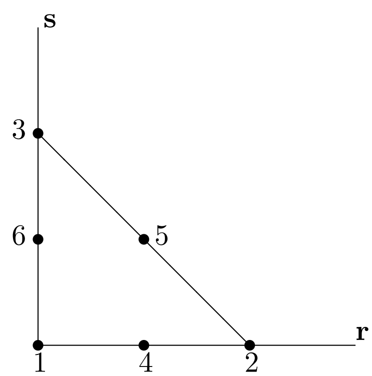


Figure 2: Computational Triangle

($\ell = 10, m = 6$). Grid points at the center of each line segment are not shown.

A typical computational triangle is shown in Figure 2. Note that the vertex points are numbered 1 - 3 in order as one traverses the edges of the triangle in counter-clockwise fashion. The center points are similarly numbered 4 - 6.

We construct six quadratic functions: three of these interpolate values at vertex points (H_1, H_2, H_3), and three interpolate values at the segment

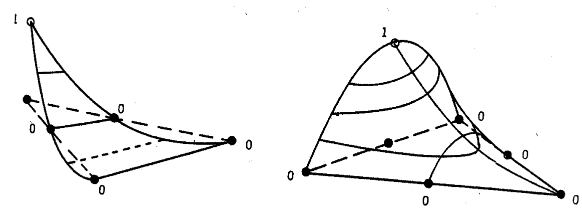


Figure 3: Basic Quadratic Functions

center points (H_4, H_5, H_6).

$$
\begin{aligned}
H_1(r,s) &= 1 - 3r + 2r^2 - 3s + 4rs + 2s^2 \\
H_2(r,s) &= -r + 2r^2 \\
H_3(r,s) &= -s + 2s^2 \\
H_4(r,s) &= 4r - 4r^2 - 4rs \\
H_5(r,s) &= 4rs \\
H_6(r,s) &= 4s - 4rs - 4s^2
\end{aligned}
$$

Figure 3 displays the shape of these local interpolating functions for the vertex points (left) and the segment center points (right) [1, from p 139].

3.4 Example Results

Example 1

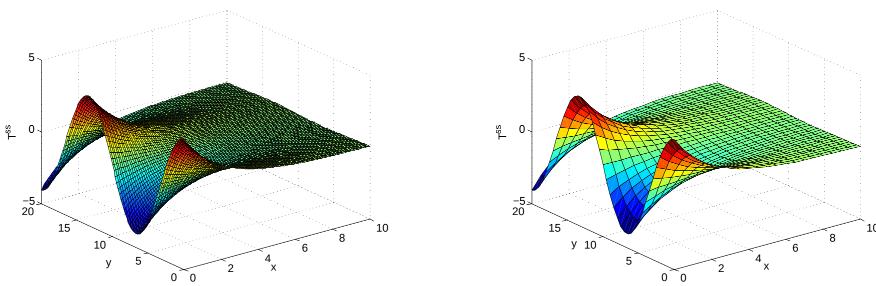
We first consider a case with $\Omega = [0,\ 10] \times [0,\ 20]$ with $\sigma = C_p = k_x = k_y = 1$, and $F \equiv 0$.. On the right boundary we take $f = 0$, while on the left boundary we take $\alpha = \hat{\alpha}$ (a constant), $\beta(y) = \hat{\beta} \cos \frac{p\pi y}{w}$. In this case a standard separation of variables analysis leads to a steady-state solution:

$$
T^{\text{ss}}(x,y) = \frac{\hat{\alpha}\hat{\beta}\ \cos\frac{p\pi y}{w}\ \cosh\frac{p\pi(L-x)}{w}}{\hat{\alpha}\cosh\frac{p\pi L}{w} + \frac{p\pi}{w}\sinh\frac{p\pi L}{w}}\ . \tag{15}
$$

Figure 4 compares surface plots of the analytic solution (4a) and the numerical approximation at $t = 400$ on a 21×41 grid (4b). Figure 5 compares line plots of the analytic solution and the same numerical approximation along lines at $x = 0$ (5a) at $x = 2$ (5b). It appears that the approximation for the steady-state solution (at least) is quite good.

Example 2

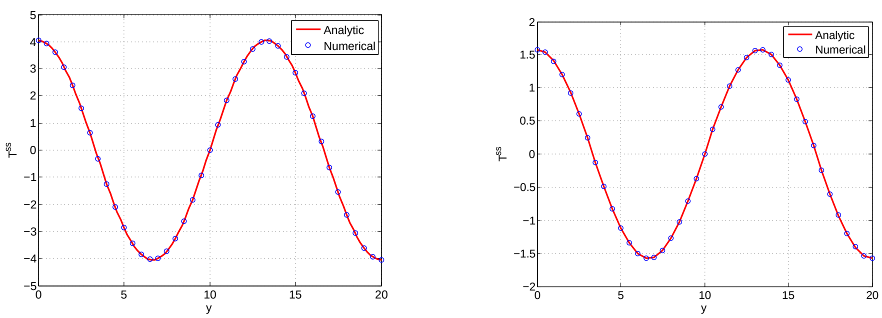
For our second example we change $\Omega = [0,\ 10] \times [0,\ 4]$ and introduce several



(a) Analytic Solution

(b) 21×41 grid

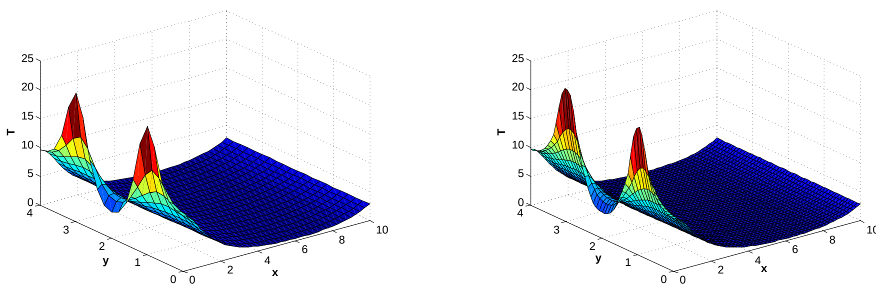
Figure 4: Surface Plot of Steady State Solutions



(a) $x = 0$

(b) $x = 2$

Figure 5: Steady State Solutions at Two Values of x



(a) 41×21 (b) 51×51

Figure 6: Example 2 - Solution at $t = 2$

'zones' along the $x = 0$ boundary with the parameters α and β varying in step fashion (see 4). Specifically, we have:

$$\alpha(y) = \begin{cases} 4 & \text{if } 0.8 \leq y \leq 1.2 \\ 2 & \text{if } 1.6 \leq y \leq 2.4 \\ 4 & \text{if } 2.8 \leq y \leq 3.2 \\ 0 & \text{otherwise, and} \end{cases}$$

$$\beta(y) = \begin{cases} 35 & \text{if } 0.8 \leq y \leq 1.2 \\ 35 & \text{if } 2.8 \leq y \leq 3.2 \\ 0 & \text{otherwise.} \end{cases}$$

On the right boundary we have:

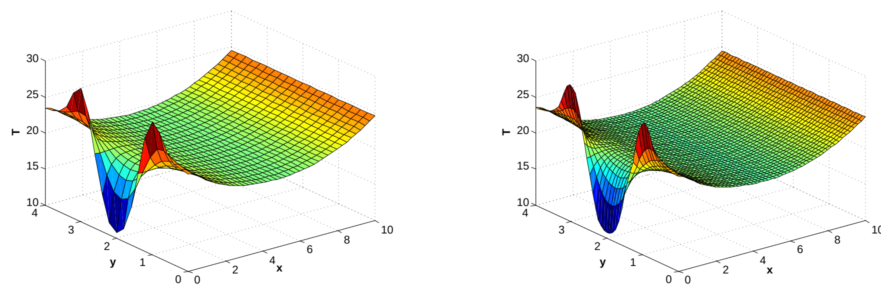
$$k \frac{\partial T}{\partial x}|_{x=10} = 2 \ ,$$

whereas along the upper and lower boundaries we use (2). The initial condition is $T(x, y, 0) = 0$.

Figure 6 compares the numerical results at $t = 2$ for a 41×21 grid (6a) and a 51×51 grid (6b). Figure 7 compares the numerical results on the same grids at $t = 42$.

4 Sensitivity

Here we focus on sensitivity of the solution to parameters in the boundary conditions (2 - 4). More specifically, we suppose that the functions α, β, f depend smoothly on parameters $q \in \mathbf{Q} \subset \mathbb{R}^p$. Since the solution depends



(a) 41×21 (b) 51×51

Figure 7: Example 2 - Solution at $t = 42$

on the parameter q we have $T : \mathbb{R}^+ \times \Omega \times \mathbf{Q} \mapsto \mathbb{R}$. We assume that T depends smoothly on q and write:

$$S_k(t, x, y; q) \stackrel{\triangle}{=} \frac{\partial T}{\partial q_k}|_{(t,x,y;q)} \ . \tag{16}$$

Assuming sufficient smoothness, we can obtain a model for S_k by differentiating a model for T. We choose to apply this procedure to the weak-form (7 - 9):

$$\begin{aligned} &\frac{\sigma\, C_p}{\Delta t} \int_\Omega \left(S_k^{n+1} - S_k^n\right)\ \Psi\ \mathrm{d}\omega - \int_\Omega \left(k \nabla S_k^{n+1} \cdot \nabla \Psi\right)\ \mathrm{d}\omega \\ &+ \int_0^w \frac{\partial f(y;q)}{\partial q_k} \Psi(L, y)\ \mathrm{d}y + \int_0^w \frac{\partial \alpha(y;q)}{\partial q_k} \left[T^{n+1}(0, y) - \beta(y)\right] \Psi(0, y)\ \mathrm{d}y \\ &\qquad + \int_0^w \alpha(y) \left[S_k^{n+1}(0, y) - \frac{\partial \beta(y;q)}{\partial q_k}\right] \Psi(0, y)\ \mathrm{d}y \ , \end{aligned} \tag{17}$$

where $S_k^n(x, y; q) = S_k(t_n, x, y; q)$. Here, as above, we have assumed that the source term F, does not depend on T (nor on q).

We use the Galerkin finite element scheme from § 3.3 and approximate $S_k^n(x, y; q)$ by the finite sum

$$S^n(x, y) \approx \sum_{\jmath=1}^{N} u_\jmath^n\, \Phi_\jmath(x, y) \ .$$

Note that we have suppressed both the k index (which labels the components of the parameter vector q) and the explicit dependence on the parameter q.

The weak-form (17) leads to:

$$\frac{\sigma\,C_p}{\Delta t}\sum_{\jmath} u_{\jmath}^{n+1}\int_{\Omega}\Phi_{\jmath}(x,y)\Phi_{\imath}(x,y)\,\mathrm{d}\omega - \frac{\sigma\,C_p}{\Delta t}\sum_{\jmath} u_{\jmath}^{n}\int_{\Omega}\Phi_{\jmath}(x,y)\Phi_{\imath}(x,y)\,\mathrm{d}\omega$$
$$+\sum_{\jmath} u_{\jmath}^{n+1}\int_{\Omega} k\nabla\Phi_{\jmath}(x,y)\cdot\nabla\Phi_{\imath}(x,y)\,\mathrm{d}\omega + \int_0^w \frac{\partial f}{\partial q}\,\Phi_{\imath}(L,y)\,\mathrm{d}y$$
$$+\sum_{\jmath} z_{\jmath}^{n+1}\int_0^w \frac{\partial\alpha}{\partial q}\Phi_{\jmath}(0,y)\Phi_{\imath}(0,y)\,\mathrm{d}y + \int_w^0 \frac{\partial\alpha}{\partial q}\beta(y)\Phi_{\imath}(0,y)\,\mathrm{d}y$$
$$+\sum_{\jmath} u_{\jmath}^{n+1}\int_0^w \alpha(y)\Phi_{\jmath}(0,y)\Phi_{\imath}(0,y)\,\mathrm{d}y\int_w^0 \alpha(y)\frac{\partial\beta}{\partial q}\Phi_{\imath}(0,y)\,\mathrm{d}y = 0\;. \quad (18)$$

Define the $N \times N$ matrix $\mathbf{M}_3$ by

$$\mathbf{M}_3 = \frac{\Delta t}{\sigma\,C_p}\int_0^w \frac{\partial\alpha}{\partial q}(y)\,\Phi_{\jmath}(0,y)\,\Phi_{\imath}(0,y)\,\mathrm{d}y\;,$$

and, the vectors $\mathbf{b}^0,\ \mathbf{b}^L \in \mathrm{I\!R}^N$ by

$$\mathbf{b}_{\imath}^0 = \frac{\Delta t}{\sigma\,C_p}\int_w^0 \frac{\partial(\alpha\,\beta)}{\partial q}(y)\,\Phi_{\imath}(0,y)\,\mathrm{d}y$$
$$\mathbf{b}_{\imath}^L = \frac{\Delta t}{\sigma\,C_p}\int_w^0 \frac{\partial f}{\partial q}(y)\,\Phi_{\imath}(L,y)\,\mathrm{d}y\;.$$

Equation (18) can be written in matrix form as

$$(\mathbf{M}_1+\mathbf{M}_2)u^{n+1} - \mathbf{M}_1 u^n + \mathbf{M}_3 z^{n+1} + \mathbf{b}^0 + \mathbf{b}^L = 0\;. \quad (19)$$

Since our initial condition for the temperature field does not depend on the parameter (q), we have $S^0(x,y) = 0$, hence $u^0 = 0 \in \mathrm{I\!R}^N$. Note that Equation (19) includes terms from the temperature distribution (z^{n+1}). One strategy is to solve the pair (13, 19) as a coupled system.

4.1 Numerical Example

Here we consider the sensitivity of the steady-state solution of Example 2 to the value of the α parameter on the central interval $(1.6 \le y \le 2.4)$. The steady-state solution for the temperature distribution is found from (13) as

$$\mathbf{M}_2\, z^{\mathrm{ss}} = -(\mathbf{F}+\mathbf{b})\;,$$

and the steady-state solution for the sensitivity is found from (19) as

$$\mathbf{M}_2\, u^{\mathrm{ss}} = -(\mathbf{M}_3 z^{\mathrm{ss}} + \mathbf{b}^0 + \mathbf{b}^L)\;.$$

The resulting sensitivity (distribution) is shown in Figure 8.

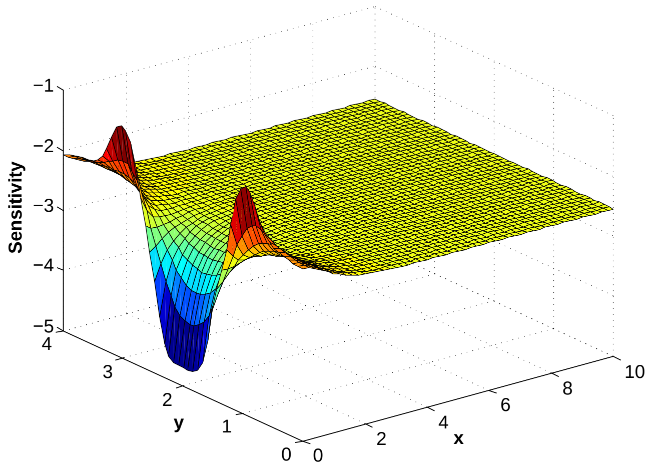


Figure 8: Steady sensitivity on a 51 × 51 grid

References

[1] J.E. Akin, *Finite Elements for Analysis and Design*, Academic Press, 1994