MA50177: Scientific Computing
Case Study

Nonlinear Thermal Conduction – Inexact Newton Methods

This assignment is about practical aspects of solving sparse systems of nonlinear equations

$$\mathbf{F}(U) \;=\; \mathbf{0} \tag{1}$$

using the inexact Newton's method. In particular we will use parallel Newton–CG and look at a case study on nonlinear thermal combustion in a self–heating medium in a partially insulated square domain. This problem arises when investigating critical parameter values for underground repositories of self–heating waste which are partially covered by buildings. Beyond certain critical parameter values the steady state solutions may become very large or even unbounded leading to an explosion in the medium. For more information see Greenway & Spence [2] and Adler [1]. (See also the first two pages of [2] which are attached.)

The Problem – Nonlinear Thermal Conduction

We are concerned with finding solutions of the (dimensionless) nonlinear thermal conduction equation

$$F(u, \lambda, \beta) \;:=\; -\frac{\partial^2 u}{\partial x_1^2} \;-\; \frac{\partial^2 u}{\partial x_2^2} \;-\; f(u, \lambda, \beta) \;=\; 0 \qquad \text{in } \Omega := [0, 1]^2, \tag{2}$$

subject to the following mixed boundary conditions on $\partial\Omega$:

$$
\begin{aligned}
u &= 0 & \text{if } x_1 > \delta \ \text{and} \ x_2 = 1 \\
\frac{\partial u}{\partial x_1} &= 0 & \text{if } x_1 = 0 \ \text{or} \ x_1 = 1 \\
\frac{\partial u}{\partial x_2} &= 0 & \text{otherwise}
\end{aligned}
\tag{3}
$$

PSfrag replacements
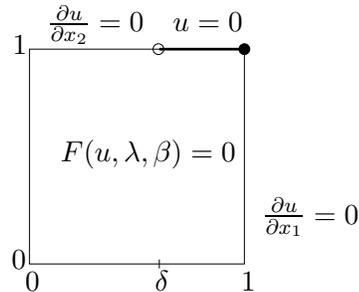
for $0 \le \delta < 1$. The nonlinear function

$$f(u, \lambda, \beta) \;:=\; \lambda \, \exp\left(\frac{u}{1 + \beta u}\right) \tag{4}$$

is the Arrhenius reaction rate which depends on the two parameters λ and β.

The relationship between the dimensionless variables in (2–4) and the physical quantities are given by Adler [1]. We note that u is a dimensionless temperature excess and λ the Frank–Kamenetskii parameter; β is the dimensionless activation energy and δ the dimensionless half–width of an insulating strip.

Finite Difference Discretisation

As for the linear reaction–diffusion equation on Problem Sheet 7, suppose that Ω is subdivided into small equal squares of size $h \times h$ with $h := 1/m$. The interior and boundary nodes of the mesh are given by $\boldsymbol{p}_{i,j} := (ih, jh)$, with $i, j = 0, \ldots, m$. Let $m_\delta := [\delta m] \in \mathbb{N}$ be the integer part of δm (i.e. largest integer $\leq \delta m$). Then $m_\delta h \leq \delta$ and $(m_\delta + 1)h > \delta$, and so all the points $\boldsymbol{p}_{i,m}$ with $i > m_\delta$ lie on the Dirichlet boundary.

The finite difference approximation to the above problem is now to seek approximations $U_{i,j}$ to $u(\boldsymbol{p}_{i,j})$ such that

$$-\frac{(U_{i-1,j} - 2U_{i,j} + U_{i+1,j})}{h^2} \;-\; \frac{(U_{i,j-1} - 2U_{i,j} + U_{i,j+1})}{h^2} \;-\; f(U_{i,j}, \lambda, \beta) \;=\; 0.$$

As on Sheet 7, we can discretise the Neumann boundary condition $\frac{\partial u}{\partial x_2} = 0$ at the nodes
$\boldsymbol{p}_{i,0}$, $i = 0, \ldots, m$, by using the finite difference approximation

$$\frac{U_{i,0} - U_{i,-1}}{h} \;=\; 0 \;.$$

Therefore the second derivative at $\boldsymbol{p}_{i,0}$ becomes

$$-\frac{(-U_{i,0} + U_{i,1})}{h^2} \qquad \text{instead of} \qquad -\frac{(U_{i,-1} - 2U_{i,0} + U_{i,1})}{h^2}.$$

We can proceed in a similar way at the other Neumann boundary nodes $\{\boldsymbol{p}_{i,m} : i = 0, \ldots, m_\delta\}$, $\{\boldsymbol{p}_{0,j} : j = 0, \ldots, m\}$ and $\{\boldsymbol{p}_{m,j} : j = 0, \ldots, m-1\}$, e.g.

$$-\frac{(U_{m-1,j} - 2U_{m,j} + U_{m+1,j})}{h^2} \qquad \text{is replaced by} \qquad -\frac{(U_{m-1,j} - U_{m,j})}{h^2} \;.$$

The Dirichlet boundary nodes $\boldsymbol{p}_{i,m}$, $i = m_\delta + 1, \ldots, m$, on the other hand, are discarded as on Problem Sheet 7, since $U_{i,m} = 0$ at those points.

Let us order the indices (i,j) lexicographically again, i.e $(0,0), (1,0), \ldots, (m,0), (0,1), \ldots,$ $(m,1), \ldots, (0,m), \ldots, (m_\delta, m)$. Then the above equations form a system of

$$N \;:=\; m*(m+1) \;+\; m_\delta \;+\; 1$$

nonlinear linear equations in N unknowns:

$$\mathbf{F}(\boldsymbol{U}) \;:=\; A_\delta\,\boldsymbol{U} \;-\; f(\boldsymbol{U}, \lambda, \beta) \;=\; 0 \tag{5}$$

where $\boldsymbol{U} := (U_{0,0}, U_{1,0}, \ldots, U_{m_\delta,m})^T \in \mathbb{R}^N$ and A_δ is the $N \times N$ matrix

$$A_\delta \;:=\; \frac{1}{h^2}\begin{pmatrix} B & -I & & & & \\ -I & C & -I & & & \\ & -I & C & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & C & -I_\delta^T \\ & & & & -I_\delta & B_\delta \end{pmatrix}$$

with

$$
B := \begin{pmatrix} 2 & -1 & & & & \\ -1 & 3 & -1 & & & \\ & -1 & 3 & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & 3 & -1 \\ & & & & -1 & 2 \end{pmatrix}, \quad C := \begin{pmatrix} 3 & -1 & & & & \\ -1 & 4 & -1 & & & \\ & -1 & 4 & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & 4 & -1 \\ & & & & -1 & 3 \end{pmatrix}.
$$

The $(m_\delta + 1) \times m$ matrix I_δ is given by $[I\ 0]$, and the $(m_\delta + 1) \times (m_\delta + 1)$ matrix B_δ consists of the first $m_\delta + 1$ rows and columns of B.

> **Note that a routine which assembles the matrix $A(\delta)$ for $\delta = 0.5$ (as on Problem Sheet 7) will be provided. Values of $\delta \neq 0.5$ are only needed in the last part of the assignment.**

Inexact Newton Method

To solve the system of nonlinear equations (5) we will use the *Inexact Newton Method* (as discussed in the lecture in Week 10).

Algorithm Newton: Choose an *initial guess* $\boldsymbol{U}_0 \in \mathbb{R}^n$ and a *tolerance* $\tau > 0$.

Set $\boldsymbol{r}_0 = \mathbf{F}(\boldsymbol{U}_0)$ and $k = 0$.
do
     if $(\|\boldsymbol{r}_k\| \leq \tau)$ exit   *(stopping criterion)*   (N0)
     Solve $\mathbf{F}'(\boldsymbol{U}_k)\boldsymbol{s}_k = -\boldsymbol{r}_k$.   *(calculation of Newton step)*   (N1)
     $\boldsymbol{U}_{k+1} = \boldsymbol{U}_k + \boldsymbol{s}_k$ *(solution update)*   (N2)
     $\boldsymbol{r}_{k+1} = \mathbf{F}(\boldsymbol{U}_{k+1})$ *(residual update)*   (N3)
     $k = k + 1$
end do

To solve the linear systems in Step (N1) for each k, we will use the Conjugate Gradient (CG) method with initial guess $\mathbf{0}$ and stopping criterion

$$
\|\boldsymbol{r}_j^{lin}\| \leq \varepsilon_k \|\boldsymbol{r}_0^{lin}\| \tag{6}
$$

where $\boldsymbol{r}_j^{lin}$ denotes the <u>linear</u> residual after j inner iterations. Two reasonable choices for the tolerance ε_k in the stopping criterion (6) for CG above are:

1. fixed tolerance: $\varepsilon_k = 10^{-5}$

2. variable tolerance:

$$\varepsilon_k = \min(\bar{\varepsilon}, \gamma * \|\mathbf{F}(\boldsymbol{x}_k)\|^2 / \|\mathbf{F}(\boldsymbol{x}_{k-1})\|^2)$$

with $\varepsilon_0 = \bar{\varepsilon} = 0.1$ and $\gamma = 0.9$ (as defined in the lecture in Week 10).

For more details on the inexact Newton method and on the iterative solution of systems of nonlinear equations in general see Kelley [3].

References

[1] Adler J., Thermal–explosion theory for a slab with partial insulation, *Combustion and Flame* **50**, 1983, pp. 1–7. (Library: `PER66`)

[2] Greenway P. and Spence A., Numerical calculation of critical points for a slab with partial insulation, *Combustion and Flame* **62**, 1985, pp. 141–156. (Library: `PER66`)

[3] Kelley CT., *Iterative Methods for Linear and Nonlinear Equations*, SIAM, Philadelphia, 1995. (Library: `512.978KEL`)