TMA225 Differential Equations and Scientific Computing for Kb2, part A

ROBIN BOUNDARY CONDITIONS

1. Modeling

As an example, we consider the following mathematical model of a stationary *reaction-diffusion process* involving a single substance,

$$
\begin{aligned}
-(au')' + cu &= f, \qquad\qquad x_{\min} < x < x_{\max}, \\
a(x_{\min})u'(x_{\min}) &= \gamma(x_{\min})(u(x_{\min}) - g_D(x_{\min})) + g_N(x_{\min}), \\
-a(x_{\max})u'(x_{\max}) &= \gamma(x_{\max})(u(x_{\max}) - g_D(x_{\max})) + g_N(x_{\max}),
\end{aligned} \tag{1}
$$

where $u(x)$, denoting the *concentration* of the substance, is the unknown function that we wish to compute. The following functions are *data* to the problem:

$a(x)$:	*diffusion coefficient*	$(a(x) > 0)$
$c(x)$:	*rate coefficient*	$(c(x) \geq 0)$
$f(x)$:	*source*	
$\gamma(x_{\min}),\ \gamma(x_{\max})$:	*permeability* at the end-points	$(\gamma \geq 0)$
$g_D(x_{\min}),\ g_D(x_{\max})$:	*ambient* concentration	
$g_N(x_{\min}),\ g_N(x_{\max})$:	externally induced flux through the boundary	

First, we consider the case $g_N(x_{\min}) = g_N(x_{\max}) = 0$, for which Robin boundary conditions are a mathematical model of the physical fact that *the outward flux is proportional to the concentration difference between the domain boundary and its surroundings*. We have the following *special cases*:

Homogeneous Neumann boundary condition: This boundary condition physically corresponds to the case of an *impermeable* boundary, i.e., one for which $\gamma = 0$, implying zero flux through the boundary: $u' = 0$.

Dirichlet boundary condition: This boundary condition physically corresponds to the case of a very *high permeability*, i.e., $\gamma \to +\infty$, implying that the concentration at the boundary adapts to the ambient concentration: $u = g_D$.

We can also imagine a case where we externally control the flux through the boundary. This case can be modelled by choosing $\gamma = 0$ and $g_N \neq 0$:

Inhomogeneous Neumann boundary condition: This boundary condition prescribes the flux through the boundary:
$a(x_{\min})u'(x_{\min}) = g_N(x_{\min})$, $-a(x_{\max})u'(x_{\max}) = g_N(x_{\max})$.

2. Variational Formulation

To *derive* the variational formulation of (1), we multiply the differential equation by $v(x)$ and integrate over $[x_{\min},\ x_{\max}]$,

$$
-\int_{x_{\min}}^{x_{\max}} (au')'v\,dx + \int_{x_{\min}}^{x_{\max}} cuv\,dx = \int_{x_{\min}}^{x_{\max}} fv\,dx.
$$

Date: September 11, 2002.

We now integrate by parts,

$$[-(au')v]_{x=x_{\min}}^{x=x_{\max}} \; + \; \int_{x_{\min}}^{x_{\max}} au'v'\,dx \; + \; \int_{x_{\min}}^{x_{\max}} cuv\,dx \; = \; \int_{x_{\min}}^{x_{\max}} fv\,dx.$$

Use the boundary conditions in (1),

$$\begin{aligned} a(x_{\min})u'(x_{\min}) \quad &= \quad \gamma(x_{\min})(u(x_{\min}) - g_D(x_{\min})) + g_N(x_{\min}), \\ -a(x_{\max})u'(x_{\max}) \quad &= \quad \gamma(x_{\max})(u(x_{\max}) - g_D(x_{\max})) + g_N(x_{\max}), \end{aligned}$$

to obtain,

$$\gamma(x_{\max})u(x_{\max})v(x_{\max}) \; + \; \gamma(x_{\min})u(x_{\min})v(x_{\min}) \; + \; \int_{x_{\min}}^{x_{\max}} au'v'\,dx \; + \; \int_{x_{\min}}^{x_{\max}} cuv\,dx \; =$$

$$(\gamma(x_{\max})g_D(x_{\max}) - g_N(x_{\max}))v(x_{\max}) \; + \; (\gamma(x_{\min})g_D(x_{\min}) - g_N(x_{\min}))v(x_{\min}) \; + \; \int_{x_{\min}}^{x_{\max}} fv\,dx.$$

We now state the following *variational formulation* of (1):

Find $u(x) \in H^1([x_{\min},\, x_{\max}]) := \left\{ v(x) : \int_{x_{\min}}^{x_{\max}} v(x)^2\,dx < \infty,\; \int_{x_{\min}}^{x_{\max}} v'(x)^2\,dx < \infty \right\}$, such that

$$\gamma(x_{\max})u(x_{\max})v(x_{\max}) \; + \; \gamma(x_{\min})u(x_{\min})v(x_{\min}) \; + \; \int_{x_{\min}}^{x_{\max}} au'v'\,dx \; + \; \int_{x_{\min}}^{x_{\max}} cuv\,dx \; =$$

(2) $$(\gamma(x_{\max})g_D(x_{\max}) - g_N(x_{\max}))v(x_{\max}) \; + \; (\gamma(x_{\min})g_D(x_{\min}) - g_N(x_{\min}))v(x_{\min}) \; +$$

$$\int_{x_{\min}}^{x_{\max}} fv\,dx, \quad \forall v \in H^1([x_{\min},\, x_{\max}]).$$

3. The Finite Element Method (FEM)

3.1. **Discretization.** Introducing the vector space, V_h, of *continuous*, *piecewise linear* functions on a partition, $x_{\min} = x_1 < x_2 < \ldots < x_{N-1} < x_N = x_{\max}$, of $[x_{\min},\, x_{\max}]$, we now state the *cG(1) method*[1] as the following *discrete* counterpart of (2):

Find $U(x) \in V_h$, such that

$$\gamma(x_N)U(x_N)v(x_N) \; + \; \gamma(x_1)U(x_1)v(x_1) \; + \; \int_{x_1}^{x_N} aU'v'\,dx \; + \; \int_{x_1}^{x_N} cUv\,dx \; =$$

(3) $$(\gamma(x_N)g_D(x_N) - g_N(x_N))v(x_N) \; + \; (\gamma(x_1)g_D(x_1) - g_N(x_1))v(x_1) \; +$$

$$\int_{x_1}^{x_N} fv\,dx, \quad \forall v \in V_h.$$

[1]In *cG(1)*, the letter *c* stands for *continuous* and the number *1* stands for *linear*, expressing the fact that this finite element method is based on continuous, piecewise linear approximation. The letter *G* stands for *Galerkin*. Boris Grigorievich Galerkin (1871 - 1945) was a Russian mathematician who made pioneering contributions to the field of numerical solution of differential equations. The *Galerkin method* is the method of rewriting the differential equation in variational form, and discretize this. A Finite Element Method (FEM), is a Galerkin method that utilises piecewise polynomials as approximating functions.

3.2. **Ansatz.** We now seek a solution, $U(x)$, to (3), expressed in the basis of *hat functions* $\{\varphi_i\}_{i=1}^N \subset V_h$, defined by $\varphi_i \in V_h,\ \varphi_i(x_j) = \delta_{ij},\ i,j = 1,\ldots,N$. (Here, δ_{ij} denotes the *Kronecker delta function*, which is defined by the property $\delta_{ij} = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{if } i \neq j. \end{cases}$) In other words, we make the *Ansatz*

$$U(x) = \sum_{j=1}^{N} \xi_j \varphi_j(x), \tag{4}$$

and seek to determine the coefficient vector,

$$\xi = \begin{bmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_N \end{bmatrix} = \begin{bmatrix} U(x_1) \\ U(x_2) \\ \vdots \\ U(x_N) \end{bmatrix},$$

of nodal values of $U(x)$, in such a way that (3) is satisfied.

3.3. **Construction of discrete system of linear equations.** We substitute (4) into (3),

$$\begin{aligned}
&\gamma(x_N)\xi_N v(x_N) \ + \ \gamma(x_1)\xi_1 v(x_1) \ + \ \sum_{j=1}^{N} \xi_j \left\{ \int_{x_1}^{x_N} a\,\varphi_j' v'\,dx \ + \ \int_{x_1}^{x_N} c\,\varphi_j v\,dx \right\} \ = \\
&(\gamma(x_N)g_D(x_N) - g_N(x_N))v(x_N) \ + \ (\gamma(x_1)g_D(x_1) - g_N(x_1))v(x_1) + \\
&\int_{x_1}^{x_N} f v\,dx, \quad \forall v \in V_h.
\end{aligned} \tag{5}$$

Since $\{\varphi_i\}_{i=1}^N \subset V_h$ is a *basis* of V_h, (5) is equivalent to,

$$\begin{aligned}
&\gamma(x_N)\xi_N \varphi_i(x_N) \ + \ \gamma(x_1)\xi_1 \varphi_i(x_1) \ + \ \sum_{j=1}^{N} \xi_j \left\{ \int_{x_1}^{x_N} a\,\varphi_j' \varphi_i'\,dx \ + \ \int_{x_1}^{x_N} c\,\varphi_j \varphi_i\,dx \right\} \ = \\
&(\gamma(x_N)g_D(x_N) - g_N(x_N))\varphi_i(x_N) \ + \ (\gamma(x_1)g_D(x_1) - g_N(x_1))\varphi_i(x_1) + \\
&\int_{x_1}^{x_N} f \varphi_i\,dx, \quad i = 1,\ldots,N,
\end{aligned} \tag{6}$$

which is a quadratic system of N linear equations and N unknowns. Introducing the notation

$$a_{ij} = \int_{x_1}^{x_N} a\,\varphi_j' \varphi_i'\,dx,$$

$$m_{c\,ij} = \int_{x_1}^{x_N} c\,\varphi_j \varphi_i\,dx,$$

$$b_i = \int_{x_1}^{x_N} f \varphi_i\,dx,$$

and taking into account that $\varphi_i(x_1) = \begin{cases} 1, & \text{if } i = 1, \\ 0, & \text{if } i \neq 1, \end{cases}$ and $\varphi_i(x_N) = \begin{cases} 1, & \text{if } i = N, \\ 0, & \text{if } i \neq N, \end{cases}$ we can write the system of equations (6), as:

$$\left\{ \begin{array}{rcccrcl} (\gamma(x_1) + a_{11} + m_{c\,11})\xi_1 & + & \dots & + & (a_{1\mathrm{N}} + m_{c\,1\mathrm{N}})\xi_\mathrm{N} & = & b_1 + \gamma(x_1)g_D(x_1) - g_N(x_1) \\ (a_{21} + m_{c\,21})\xi_1 & + & \dots & + & (a_{2\mathrm{N}} + m_{c\,2\mathrm{N}})\xi_\mathrm{N} & = & b_2 \\ \vdots & \vdots & & & \vdots & \vdots & \\ (a_{\mathrm{N\text{-}1}\,1} + m_{c\,\mathrm{N\text{-}1}\,1})\xi_1 & + & \dots & + & (a_{\mathrm{N\text{-}1}\,\mathrm{N}} + m_{c\,\mathrm{N\text{-}1}\,\mathrm{N}})\xi_\mathrm{N} & = & b_{\mathrm{N\text{-}1}} \\ (a_{\mathrm{N}1} + m_{c\,\mathrm{N}1})\xi_1 & + & \dots & + & (a_{\mathrm{NN}} + m_{c\,\mathrm{NN}} + \gamma(x_\mathrm{N}))\xi_\mathrm{N} & = & b_\mathrm{N} + \gamma(x_\mathrm{N})g_D(x_\mathrm{N}) - g_\mathrm{N}(x_\mathrm{N}) \end{array} \right.$$

In *matrix form*, this reads,

$$(A + M_c + R)\,\xi = b + rv,$$

where $A = \begin{bmatrix} a_{11} & \dots & a_{1\mathrm{N}} \\ \vdots & \ddots & \vdots \\ a_{\mathrm{N}1} & \dots & a_{\mathrm{NN}} \end{bmatrix}$ is the *stiffness matrix*,

$M_c = \begin{bmatrix} m_{c\,11} & \dots & m_{c\,1\mathrm{N}} \\ \vdots & \ddots & \vdots \\ m_{c\,\mathrm{N}1} & \dots & m_{c\,\mathrm{NN}} \end{bmatrix}$ is the *mass matrix*,

$R = \begin{bmatrix} \gamma(x_1) & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & \gamma(x_\mathrm{N}) \end{bmatrix}$ contains the *boundary contributions* to the system matrix,

$b = \begin{bmatrix} b_1 \\ \vdots \\ b_{\mathrm{N}} \end{bmatrix}$ is the *load vector*, and

$rv = \begin{bmatrix} \gamma(x_1)g_D(x_1) - g_N(x_1) \\ 0 \\ \vdots \\ 0 \\ \gamma(x_{\mathrm{N}})g_D(x_{\mathrm{N}}) - g_N(x_{\mathrm{N}}) \end{bmatrix}$ contains the *boundary contributions* to the right hand side.