ROBIN BOUNDARY CONDITIONS

1. MODELING

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

$$-(au')' + cu = f, \qquad x_{\min} < x < x_{\max},$$

$$(1) \quad \begin{aligned} a(x_{\min})u'(x_{\min}) &= \gamma(x_{\min})(u(x_{\min}) - g_D(x_{\min})) + g_N(x_{\min}), \\ -a(x_{\max})u'(x_{\max}) &= \gamma(x_{\max})(u(x_{\max}) - g_D(x_{\max})) + g_N(x_{\max}), \end{aligned}$$

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 $[x_{\min}, x_{\max}]$,

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

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),

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

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

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

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

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

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

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

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

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

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[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 $\delta_{ij} = \left\{ \begin{array}{ll} 1, & \text{if } i = j, \\ 0, & \text{if } i \neq j. \end{array} \right.$) In other words, we make the *Ansatz*

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

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),

$$\gamma(x_N)\xi_N v(x_N) \; + \; \gamma(x_1)\xi_1 v(x_1) \; + \; \sum_{j=1}^N \xi_j \left\{ \int_{x_1}^{x_N} a\, \varphi_j' v'\, dx \; + \; \int_{x_1}^{x_N} c\, \varphi_j v\, dx \right\} =$$

$$(5) \qquad (\gamma(x_N)g_D(x_N) - g_N(x_N))v(x_N) \; + \; (\gamma(x_1)g_D(x_1) - g_N(x_1))v(x_1) +$$

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

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

$$\gamma(x_N)\xi_N \varphi_i(x_N) \; + \; \gamma(x_1)\xi_1 \varphi_i(x_1) \; + \; \sum_{j=1}^N \xi_j \left\{ \int_{x_1}^{x_N} a\, \varphi_j' \varphi_i'\, dx \; + \; \int_{x_1}^{x_N} c\, \varphi_j \varphi_i\, dx \right\} =$$

$$(6) \qquad (\gamma(x_N)g_D(x_N) - g_N(x_N))\varphi_i(x_N) \; + \; (\gamma(x_1)g_D(x_1) - g_N(x_1))\varphi_i(x_1) +$$

$$\int_{x_1}^{x_N} f\varphi_i\, dx, \quad i = 1, \ldots, N,$$

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:

$$\begin{cases} (\gamma(x_1) + a_{11} + m_{c\,11})\xi_1 & + & \ldots & + & (a_{1N} + m_{c\,1N})\xi_N & = & b_1 + \gamma(x_1)g_D(x_1) - g_N(x_1) \\[2mm] (a_{21} + m_{c\,21})\xi_1 & + & \ldots & + & (a_{2N} + m_{c\,2N})\xi_N & = & b_2 \\[2mm] & \vdots & \vdots & & \vdots & & \vdots \\[2mm] (a_{N\text{-}1\,1} + m_{c\,N\text{-}1\,1})\xi_1 & + & \ldots & + & (a_{N\text{-}1\,N} + m_{c\,N\text{-}1\,N})\xi_N & = & b_{N\text{-}1} \\[2mm] (a_{N1} + m_{c\,N1})\xi_1 & + & \ldots & + & (a_{NN} + m_{c\,NN} + \gamma(x_N))\xi_N & = & b_N + \gamma(x_N)g_D(x_N) - g_N(x_N) \end{cases}$$

In *matrix form*, this reads,

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

where $A = \begin{bmatrix} a_{11} & \ldots & a_{1N} \\ \vdots & \ddots & \vdots \\ a_{N1} & \ldots & a_{NN} \end{bmatrix}$ is the *stiffness matrix*,

$M_c = \begin{bmatrix} m_{c\,11} & \ldots & m_{c\,1N} \\ \vdots & \ddots & \vdots \\ m_{c\,N1} & \ldots & m_{c\,NN} \end{bmatrix}$ is the *mass matrix*,

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

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b = \begin{bmatrix} b_1 \\ \vdots \\ b_N \end{bmatrix} \text{ is the } \textit{load vector}, \text{ and}
$$

$$
rv = \begin{bmatrix} \gamma(x_1)g_D(x_1) - g_N(x_1) \\ 0 \\ \vdots \\ 0 \\ \gamma(x_N)g_D(x_N) - g_N(x_N) \end{bmatrix} \text{ contains the } \textit{boundary contributions} \text{ to the right hand side.}
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