

ROBIN BOUNDARY CONDITIONS IN 2D

1. MODELING

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

$$(1) \quad \begin{aligned} -\nabla \cdot (a\nabla u) + cu &= f, & x = (x_1, x_2) \in \Omega \subset \mathbb{R}^2, \\ -n \cdot (a\nabla u) &= \gamma(u - g_D) + g_N, & x = (x_1, x_2) \in \Gamma = \partial\Omega, \end{aligned}$$

where $u = u(x_1, x_2)$, denoting the *concentration* of the substance, is the unknown function that we wish to compute. The following functions are *data* to the problem:

$$\begin{aligned} a(x_1, x_2) : \Omega &\rightarrow \mathbb{R} & \text{diffusion coefficient} & & (a(x_1, x_2) > 0) \\ c(x_1, x_2) : \Omega &\rightarrow \mathbb{R} & \text{rate coefficient} & & (c(x_1, x_2) \geq 0) \\ f(x_1, x_2) : \Omega &\rightarrow \mathbb{R} & \text{source} & & \\ \\ \gamma(x_1, x_2) : \partial\Omega &\rightarrow \mathbb{R} & \text{permeability of the boundary} & & (\gamma(x_1, x_2) \geq 0) \\ g_D(x_1, x_2) : \partial\Omega &\rightarrow \mathbb{R} & \text{ambient concentration} & & \\ g_N(x_1, x_2) : \partial\Omega &\rightarrow \mathbb{R} & \text{externally induced flux through the boundary} & & \end{aligned}$$

We first consider the case $g_N(x) = 0$ for all $x = (x_1, x_2) \in \partial\Omega$, for which Robin boundary conditions are a mathematical model of the physical fact that *the flux through the boundary, $-n \cdot (a\nabla u) = -a \frac{\partial u}{\partial n}$ where $n(x) = (n_1(x_1, x_2), n_2(x_1, x_2))$ denotes the outward unit normal on $\partial\Omega$, is proportional to the concentration difference between the domain boundary and its surroundings.* Note that, since n is taken to be the outward unit normal, a *positive* sign corresponds to an *outward* flux. 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 where $\gamma = 0$, implying zero flux through the boundary: $-n \cdot (a\nabla u) = 0$, or, since $a > 0$: $n \cdot \nabla u = \frac{\partial u}{\partial n} = 0$.

Dirichlet boundary condition: This boundary condition physically corresponds to the case of very *high permeability*, i.e., $\gamma \rightarrow +\infty$, implying that the concentration at the boundary adapts to the ambient concentration: $u = g_D$. (The special case $u = 0$, is referred to as a *homogeneous* Dirichlet boundary condition.)

We may also imagine a situation 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: $-n \cdot (a\nabla u) = g_N$. (Again, since n is taken to be the outward unit normal, a *positive* value of g_N corresponds to an *outward* flux.)

2. VARIATIONAL FORMULATION

To *derive* the variational formulation of (1), we multiply the differential equation by a *test function* $v = v(x_1, x_2)$ and integrate over Ω ,

$$- \iint_{\Omega} \nabla \cdot (a \nabla u) v \, dx_1 dx_2 + \iint_{\Omega} c u v \, dx_1 dx_2 = \iint_{\Omega} f v \, dx_1 dx_2,$$

i.e.,

$$- \iint_{\Omega} \left(\frac{\partial}{\partial x_1} \left(a \frac{\partial u}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left(a \frac{\partial u}{\partial x_2} \right) \right) v \, dx_1 dx_2 + \iint_{\Omega} c u v \, dx_1 dx_2 = \iint_{\Omega} f v \, dx_1 dx_2.$$

We now integrate by parts,

$$\begin{aligned} - \int_{\partial\Omega} \left(a \frac{\partial u}{\partial x_1} n_1 + a \frac{\partial u}{\partial x_2} n_2 \right) v \, ds + \iint_{\Omega} \left(a \frac{\partial u}{\partial x_1} \frac{\partial v}{\partial x_1} + a \frac{\partial u}{\partial x_2} \frac{\partial v}{\partial x_2} \right) dx_1 dx_2 + \\ \iint_{\Omega} c u v \, dx_1 dx_2 = \iint_{\Omega} f v \, dx_1 dx_2, \end{aligned}$$

i.e.,

$$- \int_{\partial\Omega} (n \cdot (a \nabla u)) v \, ds + \iint_{\Omega} a \nabla u \cdot \nabla v \, dx_1 dx_2 + \iint_{\Omega} c u v \, dx_1 dx_2 = \iint_{\Omega} f v \, dx_1 dx_2.$$

Use the boundary condition in (1),

$$-n \cdot (a \nabla u) = \gamma(u - g_D) + g_N, \quad x = (x_1, x_2) \in \partial\Omega,$$

to obtain,

$$\begin{aligned} \int_{\partial\Omega} \gamma u v \, ds + \iint_{\Omega} a \nabla u \cdot \nabla v \, dx_1 dx_2 + \iint_{\Omega} c u v \, dx_1 dx_2 = \\ \int_{\partial\Omega} (\gamma g_D - g_N) v \, ds + \iint_{\Omega} f v \, dx_1 dx_2. \end{aligned}$$

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

Find $u \in V$, such that

$$\begin{aligned} \int_{\partial\Omega} \gamma u v \, ds + \iint_{\Omega} a \nabla u \cdot \nabla v \, dx_1 dx_2 + \iint_{\Omega} c u v \, dx_1 dx_2 = \\ (2) \quad \int_{\partial\Omega} (\gamma g_D - g_N) v \, ds + \iint_{\Omega} f v \, dx_1 dx_2, \quad \text{for all } v \in V, \end{aligned}$$

where V denotes the vector space of functions $v = v(x_1, x_2)$ that are sufficiently regular for the integrals in (2) to exist.

3. THE FINITE ELEMENT METHOD (FEM)

3.1. Discretization. Introducing the vector space, V_h , of *continuous, piecewise linear* functions on a *triangulation*, $\mathcal{T}_h = \{K_i\}_{i=1}^{ntri}$, of Ω (which is assumed to have a polygonal boundary), with the corresponding set of nodes, $\mathcal{N}_h = \{N_i\}_{i=1}^{nnodes}$, we now state the *cG(1) method*¹ as the following *discrete* counterpart of (2):

Find $U \in V_h$, such that

$$(3) \quad \begin{aligned} & \int_{\partial\Omega} \gamma U v \, ds + \iint_{\Omega} a \nabla U \cdot \nabla v \, dx_1 dx_2 + \iint_{\Omega} c U v \, dx_1 dx_2 = \\ & \int_{\partial\Omega} (\gamma g_D - g_N) v \, ds + \iint_{\Omega} f v \, dx_1 dx_2, \quad \text{for all } v \in V_h. \end{aligned}$$

3.2. Ansatz. We now seek a solution, $U(x_1, x_2)$, to (3), expressed in the basis of *tent functions* $\{\varphi_i\}_{i=1}^{nnodes} \subset V_h$, defined by $\varphi_i \in V_h$, $\varphi_i(N_j) = \delta_{ij}$, $i, j = 1, \dots, nnodes$. (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*

$$(4) \quad U(x_1, x_2) = \sum_{j=1}^{nnodes} \xi_j \varphi_j(x_1, x_2),$$

and seek to determine the coefficient vector,

$$\xi = \begin{bmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_{nnodes} \end{bmatrix} = \begin{bmatrix} U(N_1) \\ U(N_2) \\ \vdots \\ U(N_{nnodes}) \end{bmatrix},$$

of nodal values of $U(x_1, x_2)$, in such a way that (3) is satisfied.

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

$$(5) \quad \begin{aligned} & \sum_{j=1}^{nnodes} \xi_j \left\{ \int_{\partial\Omega} \gamma \varphi_j v \, ds + \iint_{\Omega} a \nabla \varphi_j \cdot \nabla v \, dx_1 dx_2 + \iint_{\Omega} c \varphi_j v \, dx_1 dx_2 \right\} = \\ & \int_{\partial\Omega} (\gamma g_D - g_N) v \, ds + \iint_{\Omega} f v \, dx_1 dx_2, \quad \text{for all } v \in V_h. \end{aligned}$$

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

¹In *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.

$$(6) \quad \sum_{j=1}^{nnodes} \xi_j \left\{ \int_{\partial\Omega} \gamma \varphi_j \varphi_i ds + \iint_{\Omega} a \nabla \varphi_j \cdot \nabla \varphi_i dx_1 dx_2 + \iint_{\Omega} c \varphi_j \varphi_i dx_1 dx_2 \right\} = \\ \int_{\partial\Omega} (\gamma g_D - g_N) \varphi_i ds + \iint_{\Omega} f \varphi_i dx_1 dx_2, \quad i = 1, \dots, nnodes,$$

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

$$r_{i,j} = \int_{\partial\Omega} \gamma \varphi_j \varphi_i ds,$$

$$a_{i,j} = \iint_{\Omega} a \nabla \varphi_j \cdot \nabla \varphi_i dx_1 dx_2,$$

$$m_{c\ i,j} = \iint_{\Omega} c \varphi_j \varphi_i dx_1 dx_2,$$

$$rv_i = \int_{\partial\Omega} (\gamma g_D - g_N) \varphi_i ds,$$

$$b_i = \iint_{\Omega} f \varphi_i dx_1 dx_2,$$

we can write the system of equations (6), as (we denote $nnodes$ by nn):

$$\left\{ \begin{array}{l} (r_{1,1} + a_{1,1} + m_{c\ 1,1})\xi_1 + \dots + (r_{1,nn} + a_{1,nn} + m_{c\ 1,nn})\xi_{nn} = rv_1 + b_1 \\ (r_{2,1} + a_{2,1} + m_{c\ 2,1})\xi_1 + \dots + (r_{2,nn} + a_{2,nn} + m_{c\ 2,nn})\xi_{nn} = rv_2 + b_2 \\ \vdots \\ (r_{nn,1} + a_{nn,1} + m_{c\ nn,1})\xi_1 + \dots + (r_{nn,nn} + a_{nn,nn} + m_{c\ nn,nn})\xi_{nn} = rv_{nn} + b_{nn} \end{array} \right.$$

In *matrix form*, this reads,

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

where $R = \begin{bmatrix} r_{1,1} & \dots & r_{1,nn} \\ \vdots & \ddots & \vdots \\ r_{nn,1} & \dots & r_{nn,nn} \end{bmatrix}$ contains the *boundary contributions* to the system matrix,

$$A = \begin{bmatrix} a_{1,1} & \cdots & a_{1,nn} \\ \vdots & \ddots & \vdots \\ a_{nn,1} & \cdots & a_{nn,nn} \end{bmatrix} \text{ is the } \textit{stiffness matrix},$$

$$M_c = \begin{bmatrix} m_{c\,1,1} & \cdots & m_{c\,1,nn} \\ \vdots & \ddots & \vdots \\ m_{c\,nn,1} & \cdots & m_{c\,nn,nn} \end{bmatrix} \text{ is the } \textit{mass matrix},$$

$$rv = \begin{bmatrix} rv_1 \\ \vdots \\ rv_{nn} \end{bmatrix} \text{ contains the } \textit{boundary contributions} \text{ to the right-hand side, and}$$

$$b = \begin{bmatrix} b_1 \\ \vdots \\ b_{nn} \end{bmatrix} \text{ is the } \textit{load vector}.$$