Differential Equations and Scientific Computing, part A

# 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,

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

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:

| | | |
|---|---|---|
| $a(x_1,x_2):\Omega\to\mathbb{R}$ | *diffusion coefficient* | $(a(x_1,x_2)>0)$ |
| $c(x_1,x_2):\Omega\to\mathbb{R}$ | *rate coefficient* | $(c(x_1,x_2)\geq 0)$ |
| $f(x_1,x_2):\Omega\to\mathbb{R}$ | *source* | |
| $\gamma(x_1,x_2):\partial\Omega\to\mathbb{R}$ | *permeability* of the boundary | $(\gamma(x_1,x_2)\geq 0)$ |
| $g_D(x_1,x_2):\partial\Omega\to\mathbb{R}$ | *ambient* concentration | |
| $g_N(x_1,x_2):\partial\Omega\to\mathbb{R}$ | externally induced flux through the boundary | |

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., $\gamma\to+\infty$, 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.)

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## 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 $\Omega$,

$$-\iint_\Omega \nabla \cdot (a\nabla u) v \, dx_1 dx_2 \; + \; \iint_\Omega cuv \, dx_1 dx_2 \; = \; \iint_\Omega fv \, dx_1 dx_2,$$

i.e.,

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

We now integrate by parts,

$$-\int_{\partial\Omega} (a \frac{\partial u}{\partial x_1} n_1 + a \frac{\partial u}{\partial x_2} n_2) v \, ds \; + \; \iint_\Omega (a \frac{\partial u}{\partial x_1} \frac{\partial v}{\partial x_1} + a \frac{\partial u}{\partial x_2} \frac{\partial v}{\partial x_2}) \, dx_1 dx_2 \; +$$
$$\iint_\Omega cuv \, dx_1 dx_2 \; = \; \iint_\Omega fv \, dx_1 dx_2,$$

i.e.,

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

Use the boundary condition in (1),

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

to obtain,

$$\int_{\partial\Omega} \gamma uv \, ds \; + \; \iint_\Omega a \nabla u \cdot \nabla v \, dx_1 dx_2 \; + \; \iint_\Omega cuv \, dx_1 dx_2 \; =$$
$$\int_{\partial\Omega} (\gamma g_D - g_N) v \, ds \; + \; \iint_\Omega fv \, dx_1 dx_2.$$

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

Find $u \in V$, such that

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

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 $\Omega$ (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

$$\int_{\partial\Omega} \gamma U v\, ds \;+\; \iint_{\Omega} a\,\nabla U \cdot \nabla v\, dx_1 dx_2 \;+\; \iint_{\Omega} cUv\, dx_1 dx_2 \;= \tag{3}$$
$$\int_{\partial\Omega} (\gamma g_D - g_N) v\, ds \;+\; \iint_{\Omega} fv\, dx_1 dx_2, \quad \text{for all } v \in V_h.$$

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 $\varphi_i \in V_h,\ \varphi_i(N_j) = \delta_{ij},\ i, j = 1, \ldots, nnodes$. (Here, $\delta_{ij}$ 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*

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

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),

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

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

[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.

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

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*):

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

In *matrix form*, this reads,

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

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

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

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

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

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