1 Prototype equation

1.1 Geometry

Let Ω be a bounded 2-dimensional region. Let Γ be a 1-dimensional curve that devides Ω into two subregions, denoted as Ω_1 and Ω_2. Let $\partial\Omega_D$ and $\partial\Omega_N$ denote its Dirichlet and Neumann boundaries, respectively.

1.2 Diffusion-reaction equation for excitons

Consider the following equation defined on Ω:

$$-\nabla\left(a(x)\nabla u\right) + c(x)u = f(x) \tag{1}$$

and boundary conditions are:

$$u = u_D \qquad \forall x \in \Omega_D \tag{2}$$

$$\frac{\partial u}{\partial n} = g_N \qquad \forall x \in \Omega_N \tag{3}$$

In particular, u is not assumed to have continuous "flux" across $\Gamma = \overline{\Omega}_1 \cap \overline{\Omega}_2$, i.e.

$$u_1 = u_2 = u_\Gamma \qquad \forall x \in \Gamma \tag{4}$$

$$\frac{\partial u_1}{\partial n_{12}} - \frac{\partial u_2}{\partial n_{12}} = -ku_\Gamma \qquad \forall x \in \Gamma \tag{5}$$

The physical meaning here is that, if u is the density of excitons, then near the interface Γ, u has a drainage rate of "ku".

To use Finite Element Method, one needs to write down the weak form. Let v be a test function on Ω, then

$$\int_\Omega a(x)\nabla u \cdot \nabla v\, dx + \int_\Omega c(x)uv\, dx + \int_\Gamma kuv\, ds = \int_\Omega fv dx \tag{6}$$

In FEM, the region Ω is decomposed into the union of disjoint triangles. Both u and v are approximated by piecewise linear polynomials.

2 Linear system assembly

In this section, we write down the detailed formula of assembling coefficient matrix. In particular, the 3 integrals above are replaced by the matrices A, C, and D.

2.1 Quadrature rule: 1D and 2D

Consider an integral over a triangular region with vertices $\{v_0,v_1,v_2\}$

$$I = \int_T f \, dx \tag{7}$$

Then first-order quadrature rule is

$$I \approx |T| * (f_0 + f_1 + f_2)/3 \tag{8}$$

where f_i denotes the function value $f(x_i, y_i)$.

We then consider an integral over a segment, for example an edge e of a triangle with end nodes being $\{ v_0, v_1\}$. And we have 1st-order quadrature rule

$$I = \int_e f \, ds \tag{9}$$

$$\approx |e| \frac{f_0 + f_1}{2} \tag{10}$$

These quadrature rules are exact for linear polynomials and are used for assembling all the matrices below.

2.2 Matrices and vectors

2.2.1 Matrix A

Let ϕ_i be the linear basis Lagrange polynomial with 1 on the i-th node and 0 on all other nodes. Then

$$A_{ij} = \int_\Omega a(x) \nabla \phi_i \nabla \phi_j \, dx \tag{11}$$

In practice, this is done by looping through all triangular elements T's. For each T, one identify its vertices i, j, k, and calculate the contribution of T to all 9 entries in A: $A_{\alpha\beta}$ where α and β can be either i, j, or k.

For example, assume triangle T has vertices 0,1,and 2. We denote the coordinates of these vertices by $\overrightarrow{r}_0$, $\overrightarrow{r}_1$ and $\overrightarrow{r}_2$. We compute 2 quantities: $A_{00}(T)$ and $A_{01}(T)$. Other cases can be obtained by switching subscripts between 0, 1, and 2.

1. $A_{00}(T)$
   First, note by a linear transformation, one can transform v_0, v_1 and v_2 easily to a reference triangle with vertices (0,0), (1,0), and (0,1). In this way, we compute

$$\nabla \phi_0 \cdot \nabla \phi_0 = \frac{|\overrightarrow{r}_2 - \overrightarrow{r}_1|^2}{4\,|T|^2} \tag{12}$$

And hence,

$$\int_T a(x)\nabla\phi_0 \cdot \nabla\phi_1 \, dx = |T| \cdot \frac{(a_0 + a_1 + a_2)}{3} \cdot \frac{\left|\overrightarrow{r}_2 - \overrightarrow{r}_1\right|^2}{4\,|T|^2} \tag{13}$$

$$= \frac{a_0 + a_1 + a_2}{12\,|T|} \left|\overrightarrow{r}_2 - \overrightarrow{r}_1\right|^2 \tag{14}$$

2. $A_{01}(T)$
   Similar to $A_{01}(T)$, we again make use of the reference triangle and obtained

$$\nabla\phi_0 \cdot \nabla\phi_1 = -\frac{(\overrightarrow{r}_2 - \overrightarrow{r}_0) \cdot (\overrightarrow{r}_2 - \overrightarrow{r}_1)}{4\,|T|^2} \tag{15}$$

   and thus

$$\int_T a(x)\nabla\phi_0 \cdot \nabla\phi_1 \, dx = -\frac{a_0 + a_1 + a_2}{12\,|T|} \, (\overrightarrow{r}_2 - \overrightarrow{r}_0) \cdot (\overrightarrow{r}_2 - \overrightarrow{r}_1) \tag{16}$$

   Note the "-" sign on the right-hand side and symmetry in the formulation.

2.2.2 Matrix C

Applying the simple quadrature rule, we conclude the matrix C is diagonal, i.e. $A_{ij} = 0$ if $i \neq j$. We then compute the contribution to A_{ii} from element T if v_i is a vertex belonging to T.

$$A_{ii}(T) = \int_T c(x)\phi_i\phi_i \, dx \tag{17}$$

$$= |T| \, \frac{c_i}{3} \tag{18}$$

2.2.3 Matrix D

Similar structure takes place in D. In fact D is sparser than C, for it's only non-zero entries corresponds to the nodes on the interface Γ defined above. Furthermore, applying a 1st-order quadrature rule for line integral, we have

$$\int_e k\phi_i\phi_j \, ds = \delta_{ij} \, |e| \frac{k_i}{2} \tag{19}$$

where $|e|$ is the length of edge e.

2.2.4 Right-hand side vector

$$\int_T f(x)\phi_i \, dx = |T| \frac{f_i}{3} \tag{20}$$

2.3 Dirichlet boundary conditions

Finally, we identify the nodes on Dirichlet boundaries. We modify the linear system defined above on both sides (assuming v_i is a node on Dirichlet boundaries):

- Left side:
  We re-write the i-th row as a unit vector with i-th entry being 1 and 0's elsewhere.

- Right side:
  Corresponding to the modification to the coefficient matrix on the left side, we change the i-th entry of right-hand side vector to be the Dirichlet boundary value $u_D(v_i)$