Finite Element Method Notes

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Contents

Chapter 1

Finite Element Methods

The finite element method is a method for approximating solutions to boundary value problems that has gained much popularity in the realm of numerical methods for partial differential equations. While finite element methods can be applied to a range of boundary value problems we focus our attention on Poisson's equation:

$$-\nabla \cdot (\epsilon \nabla \Phi) = f \quad \text{in} \quad \Omega \tag{1.0.1}$$

Where $\epsilon(x)$ is bounded positive-definite function. And the boundary conditions are:

$$\Phi = \Phi_D \quad \text{on} \quad \partial\Omega_D \tag{1.0.2}$$
$$-\nabla\Phi \cdot \boldsymbol{\eta} = 0 \quad \text{on} \quad \partial\Omega_N \tag{1.0.3}$$
$$\partial\Omega = \partial\Omega_D \cup \partial\Omega_N \quad \partial\Omega_D \cap \partial\Omega_N = \emptyset \tag{1.0.4}$$

Where $\partial\Omega_D$ correspond to contacts or interfaces where potentials (voltages) are applied and $\partial\Omega_N$ corresponds to oxides that act as insulators to charge flow.

Finite element methods seek weak solutions of differential equation $\Phi \in H^1(\Omega)$ by multiplying our equation by a test function $v \in H^1(\Omega)$ and integrating by parts over entire the domain

$$\int_\Omega -v \nabla \cdot (\epsilon \nabla \Phi) \, dx = \int_\Omega v \, f \, dx$$

Becomes

$$\int_\Omega \nabla v \cdot (\epsilon \nabla \Phi) \, dx - \int_{\partial\Omega_D} v \, (\epsilon \nabla \Phi \cdot \boldsymbol{\eta}) \, dx - \int_{\partial\Omega_N} v \, (\epsilon \nabla \Phi \cdot \boldsymbol{\eta}) \, dx = \int_\Omega v \, f \, dx \tag{1.0.5}$$

Using the condition of (1.0.3) we have require the Neumann boundary condition to be zero:

$$\int_\Omega \nabla v \cdot (\epsilon \nabla \Phi) \, dx - \int_{\partial\Omega_D} v \, (\epsilon \nabla \Phi \cdot \boldsymbol{\eta}) \, dx = \int_\Omega v \, f \, dx$$

In order to make our problem well-defined, we require that $v = 0$ on $\partial\Omega_D$.[1] Poisson's equation then becomes:

Find $\Phi - \Phi_D \in V = \{\phi \in H^1(\Omega) : \phi = 0 \quad \text{on} \quad \partial\Omega_D\}$. Such that for all $v \in V$ we have:

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[1] In finite element methods, Neumann (natural) boundary conditions are enforced by the formulation of problem, while Dirichlet (essential) boundary conditions are enforced by restricting our test space.

$$\int_\Omega \epsilon(x) \, (\nabla \, \Phi \cdot \nabla \, v) \, dx \; = \; \int_\Omega f \, v \, dx \tag{1.0.6}$$

In order to solve this problem we must project our infinite dimensional test space V on to a finite dimensional one $V_h = \text{span}\{\psi_1, \psi_2, \dots, \psi_N\}$, where N is the dimension of our vector space, our problem then transforms into the finite dimensional problem:

$$\text{Find } \Phi_h - \Phi_D \in V_h \text{ such that } \forall \, v_h \, \in V_h:$$

$$\int_\Omega \epsilon(x) \, (\nabla \, v_h \, \cdot \nabla \, \Phi_h \,) \, dx \; = \; \int_\Omega v_h \, f \, dx \tag{1.0.7}$$

We can rewrite this in bilinear the form of

$$\text{Find } \Phi_h - \Phi_D \in V_h \text{ such that } \forall \, v_h \, \in V_h:$$

$$a \, (v_h \, , \Phi_h \,) \; = \; F(v_h) \tag{1.0.8}$$

Where

$$a \, (\, v_h \, , \Phi_h \,) \; = \; \int_\Omega \epsilon(x) \, (\nabla \, v_h \, , \nabla \, \Phi_h \,) \, dx$$

And

$$F(v_h) = \int_\Omega v_h \, f \, dx$$

By writing defining $\Phi_D = \sum \Phi_j \, \psi_j$ and $v = \psi_i$ we arrive at linear system of equations:

$$A^T \mathbf{x} \; = \; \mathbf{F}$$

Where

$$A_{i,j} \; = \; \int_\Omega \epsilon(x) \, (\nabla \, \psi_i \, \cdot \nabla \, \psi_j) \, dx$$

$$\mathbf{F}_i \; = \; \int_\Omega \psi_i \, f \, dx$$

$$\mathbf{x}_i \; = \; \Phi_i$$

In order existence and uniqueness of this problem we invoke the *Lax-Milgram theorem*, and show a is bounded by Cauchy-Schwarts:

$$|a(\psi, \Phi)| = |\int_\Omega \epsilon(x) \nabla \psi \cdot \nabla \Phi \, dx|$$
$$\leq \|\epsilon\|_{L_\infty} \|\nabla \psi\|^2_{L_2(\Omega)} \|\nabla \Phi\|^2_{L_2}$$
$$\leq \|\epsilon\|_{L_\infty} \|\psi\|_{H^1(\Omega)} \|\Phi\|_{H^1(\Omega)}$$

And coercivity by Poincare's inequality:

$$|a(\Phi, \Phi)| = |\int_\Omega \epsilon(x) \, (\nabla\Phi)^2 \, , dx|$$
$$\geq \inf_\Omega |\epsilon| \, \|\nabla\Phi\|^2_{L_2(\Omega)}$$
$$\geq \inf_\Omega |\epsilon| \, \|\Phi\|^2_{H^1(\Omega)}$$

Chapter 2

Time Dependent Error Estimates

$$\partial_t u \;-\; \boldsymbol{\nabla} \cdot (D(\mathbf{x})\boldsymbol{\nabla} u) \;=\; f(\mathbf{x},t) \qquad\qquad \Omega \times (0,T] \qquad\qquad (2.0.1)$$

$$(-D\boldsymbol{\nabla} u) \cdot \boldsymbol{\eta}_N \;=\; g(u) \qquad\qquad \partial\Omega_N \times (0,T] \qquad\qquad (2.0.2)$$

$$u \;=\; u_D(\mathbf{x}) \qquad\qquad \partial\Omega_D \times (0,T] \qquad\qquad (2.0.3)$$

$$u \;=\; u_I(\mathbf{x}) \qquad\qquad \Omega \times \{t = 0\} \qquad\qquad (2.0.4)$$

Where $0 < D_* \leq D(\mathbf{x}) \leq D^*$. The boundary condition $g : H^1(\Omega) \to L^2(\partial\Omega_N)$ is Lipschitz function such that,

$$\|g(u) - g(v)\|_{L_2(\partial\Omega_N)} \;\leq\; L\|u - v\|_{H^1(\Omega)} \qquad\qquad \forall u,v \in H^1(\Omega). \qquad L > 0. \qquad (2.0.5)$$

Let $\mathcal{T}_h = \{\Omega_e\}_e$ be the triangulation of Ω. The boundary $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$ is smooth enough such that the trace identity,

$$\|v\|^2_{L^2(\partial\Omega)} \;\leq\; C_{tr}(\Omega)\|v\|^2_{H^1(\Omega)}, \qquad\qquad \forall v \in H^1(\Omega) \qquad\qquad (2.0.6)$$

holds. The semidiscrete finite element method is,

Find $u_h(t) \in H^1_D(\Omega) + u_D$ such that,

$$(v, \partial_t u_h)_\Omega \;+\; B(v, u_h) \;=\; (v, f)_\Omega \;-\; \langle v, g(u_h)\rangle_{\partial\Omega_N} \qquad \forall v \in V_h \quad a.e. \; t \in (0,T], \qquad (2.0.7)$$

$$(v, u_h(t = 0))_\Omega \;=\; (v, u_I)_\Omega \qquad\qquad \forall v \in V_h. \qquad\qquad (2.0.8)$$

Where V_h is the finite dimensional subspace of the Hilbert space $H^1_D(\Omega) \;=\; \{v \in H^1(\Omega) : v|_{\partial\Omega_D} = 0\}$. Let be V_H be the such that $v \in V_h$ then $v|_{\Omega_e} \in Q_k(\Omega_e)$ where Q_k is the tensor product of polynomials of order k. The bilinear $B : H^1 \times H^1 \to \mathbb{R}$ in (2.0.7) is coercive, meaning there exists an $\alpha \in \mathbb{R}$ such that,

$$B(v, v) \;\geq \alpha^2 \, \|v\|^2_{H^1} \qquad\qquad \forall v \in H^1(\Omega) \qquad\qquad (2.0.9)$$

Error Estimate: *If $\alpha^2 \geq 2\sqrt{L}C_{tr}$ then the finite element method defined in (2.0.7) and (2.0.8) has errors such that,*

$$\|u - u_h\|^2_{L^\infty([0,T];L^2(\Omega))} \;\leq\; Ch^k, \qquad\qquad (2.0.10)$$

for some constant $C = C(T, \alpha^2, \Omega, L) > 0$.

Proof:
Let $P : H^1_D \to V_h$ be the projection that satisfies the elliptic projection property,

$$B(v, u - Pu) \;=\; 0 \qquad\qquad \forall v \in V_h \qquad\qquad (2.0.11)$$

And has the approximation properties,

$$\|u - Pu\|_{L^2(\Omega)} \leq Ch^{k+1} \qquad \text{and} \qquad \|u - Pu\|_{H^1(\Omega)} \leq Ch^k \tag{2.0.12}$$

The function $u(t) \in H^1 + u_D$ also satisfies the finite element method,

$$(v, \partial_t u)_\Omega + B(v, u) = (v, f)_\Omega - \langle v, g(u)\rangle_{\partial\Omega_N} \qquad \forall v \in V_h \qquad a.e.\ t\ \in (0, T] \tag{2.0.13}$$
$$(v, u(t=0))_\Omega = (v, u_I)_\Omega \qquad \forall v \in V_h \tag{2.0.14}$$

Subtracting the (2.0.7) from (2.0.13) we have,

$$(v, \partial_t(u - u_h)) + B(v, u - u_h) \leq |\langle v, g(u) - g(u_h)\rangle_{\partial\Omega_N}| \qquad a.e.\ t \tag{2.0.15}$$

Define $e_I(t) = u(t) - Pu(t)$ and $e_A(t) = Pu(t) - u_h(t)$ and using the elliptic projection property then the above becomes,

$$(v, \partial_t e_A) + B(v, e_A) \leq |(v, \partial_t e_I)| + |\langle v, g(u) - g(u_h)\rangle_{\partial\Omega_N}| \qquad a.e.\ t \tag{2.0.16}$$

Taking $v = e_A(t)$ and using the coercivity property of $B(\cdot, \cdot)$ we have,

$$\frac{d}{dt}\|e_A\|_{L^2(\Omega)}^2 + 2\alpha^2\|e_A\|_{H^1(\Omega)}^2 \leq 2\,|(e_A, \partial_t e_I)| + 2\,|\langle e_A, g(u) - g(u_h)\rangle_{\partial\Omega_N}| \qquad a.e.\ t \tag{2.0.17}$$

We now use Young's inequality to obtain,

$$\frac{d}{dt}\|e_A\|_{L^2(\Omega)}^2 + 2\alpha^2\|e_A\|_{H^1(\Omega)}^2 \leq \|e_A\|_{L^2(\Omega)}^2 + 4\|\partial_t e_I\|_{L^2(\Omega)}^2 + \frac{1}{\delta}\|e_A\|_{L^2(\partial\Omega_N)}^2 + \delta\|g(u) - g(u_h)\|_{L^2(\partial\Omega_N)}^2 \tag{2.0.18}$$

Using the Lipschitz property of $g(\cdot)$ we have,

$$\frac{d}{dt}\|e_A\|_{L^2(\Omega)}^2 + 2\alpha^2\|e_A\|_{H^1(\Omega)}^2 \leq \|e_A\|_{L^2(\Omega)}^2 + 4\|\partial_t e_I\|_{L^2(\Omega)}^2 + \frac{1}{\delta}\|e_A\|_{L^2(\partial\Omega_N)}^2 + \delta L\|u - u_h\|_{H^1(\Omega)}^2 \tag{2.0.19}$$

Using the Trace identity (2.0.6) on the second to last term and the triangle inequality on the last term,

$$\frac{d}{dt}\|e_A\|_{L^2(\Omega)}^2 + 2\alpha^2\|e_A\|_{H^1(\Omega)}^2 \leq \|e_A\|_{L^2(\Omega)}^2 + 4\|\partial_t e_I\|_{L^2(\Omega)}^2 + \left(\frac{C_{tr}^2}{\delta} + \delta L\right)\|e_A\|_{H^1(\Omega)}^2 + \delta L\|e_I\|_{H^1(\Omega)}^2 \tag{2.0.20}$$

Rearranging terms we have,

$$\frac{d}{dt}\|e_A\|_{L^2(\Omega)}^2 + \left(2\alpha^2 - \frac{C_{tr}^2}{\delta} - \delta L\right)\|e_A\|_{H^1(\Omega)}^2 \leq \|e_A\|_{L^2(\Omega)}^2 + 4\|\partial_t e_I\|_{L^2(\Omega)}^2 + \delta L\|e_I\|_{H^1(\Omega)}^2 \tag{2.0.21}$$

Taking $2\alpha^2 - \frac{C_{tr}^2}{\delta} - \delta = \alpha^2$ we obtain the quadratic form,

$$L\delta^2 - \alpha^2\delta + C_{tr}^2 = 0, \tag{2.0.22}$$

which has a real positive solution if $\alpha^2 \geq 2\sqrt{L}C_{tr}$. With these choices then (2.0.21) becomes

$$\frac{d}{dt}\|e_A\|_{L^2(\Omega)}^2 + \alpha^2\|e_A\|_{H^1(\Omega)}^2 \leq \|e_A\|_{L^2(\Omega)}^2 + 4\|\partial_t e_I\|_{L^2(\Omega)}^2 + \delta\left(\alpha^2, C_{tr}\right)L\|e_I\|_{H^1(\Omega)}^2 \tag{2.0.23}$$

Integrating over $(0, t)$ with $t \leq T$ yields,

$$\|e_A(t)\|_{L^2(\Omega)}^2 + \alpha^2 \int_0^t \|e_A\|_{H^1(\Omega)}^2 ds \leq \int_0^t \|e_A\|_{L^2(\Omega)}^2 ds \qquad (2.0.24)$$

$$+ \int_0^t \left(\|e_A(0)\|_{L^2(\Omega)}^2 + 4\|\partial_t e_I\|_{L^2(\Omega)}^2 + \delta \left(\alpha^2, C_{tr} \right) L \|e_I\|_{H^1(\Omega)}^2 \right) ds \qquad (2.0.25)$$

Using a Gromwall's inequality, the approximation properties (2.0.12) and the fact the $\|e_A(0)\|_{L^2(\Omega)}^2 = 0$ we have,

$$\|e_A(t)\|_{L^2(\Omega)}^2 + \alpha^2 \int_0^t \|e_A\|_{H^1(\Omega)}^2 ds \leq C(t, \alpha^2, \Omega, L) h^{2k} \qquad (2.0.26)$$

where the dependency on constants dependency on Ω comes from the Trace theorem constant $C_{tr}(\Omega)$. Then taking the maximum over all $t \in (0, T)$ we have,

$$\|e_A\|_{L^\infty([0,T];L^2(\Omega))} \leq C(T, \alpha^2, \Omega, L) h^k \qquad (2.0.27)$$

Using the triangle inequality $\|u - u_h\|_{L^\infty([0,T];L^2(\Omega))} \leq \|e_A\|_{L^\infty([0,T];L^2(\Omega))} + \|e_I\|_{L^\infty([0,T];L^2(\Omega))}$ gives the desired results.

Chapter 3

Mixed Finite Element Methods

The problem with the general finite element approximation of Φ is that $\nabla\Phi$ must come from post processing and we cannot control the accuracy or continuity of $\nabla\Phi$. This is necessary not only for use in solving the drift diffusion equation, but also when we are working with a semiconductor-electrolyte system as will be explained in the next section.

One way to overcome these limitations is to use a mixed finite element approach to solve Poisson's equation. In the mixed formulation we are solving the problem as in (1.0.1), but we define define the a new variable related to the electric field as:

$$\mathbf{E} = -\epsilon\,\nabla\,\Phi$$

Then (1.0.1) becomes the system:

$$\nabla\,\cdot\,\mathbf{E}\,=\,f \tag{3.0.1}$$

$$\epsilon^{-1}\,\mathbf{E} + \nabla\,\Phi = 0 \tag{3.0.2}$$

With the boundary conditions:

$$\Phi\,=\,\Phi_D \qquad \text{on} \quad \partial\Omega_D \tag{3.0.3}$$

$$\mathbf{E}\cdot\boldsymbol{\eta} = 0 \qquad \text{on} \quad \partial\Omega_N \tag{3.0.4}$$

$$\partial\Omega = \partial\Omega_D \cup \partial\Omega_N \qquad \partial\Omega_D \cap \partial\Omega_N = \emptyset \tag{3.0.5}$$

Now, mixed finite element methods seek weak solutions of both Φ and $\mathbf{E}$ by multiplying our (3.0.1) by a test function $v \in L_2(\Omega)$ (3.0.2) by a test function $\mathbf{p} \in H(\text{div}, \Omega)$ then integrating by parts over entire the domain for just (3.0.2):

$$\int_\Omega v\,(\nabla\,\cdot\,\mathbf{E})\,dx \,=\, \int_\Omega v\,f\,dx \tag{3.0.6}$$

$$\int_\Omega \mathbf{p}\,\cdot\,\epsilon^{-1}\,\mathbf{E}\,dx + \int_{\partial\Omega_N}(\mathbf{p}\,\cdot\,\boldsymbol{\eta})\,\Phi\,dx + \int_{\partial\Omega_D}(\mathbf{p}\,\cdot\,\boldsymbol{\eta})\,\Phi\,dx - \int_\Omega(\nabla\,\cdot\,\mathbf{p})\,\Phi\,dx = 0 \tag{3.0.7}$$

If we enforce the boundary conditions and the restrict $\mathbf{p}\cdot\boldsymbol{\eta} = 0$, on $\partial\Omega_N$, so that $\mathbf{p}$ and $\mathbf{E}$ are in the space function space, then we have the weak formulation:

Find $(\Phi\,,\mathbf{E}\,) \in L_2(\Omega)\,\times\,V$ such that for all $(v,\mathbf{p}) \in L_2(\Omega)\,\times\,V$:

$$\int_\Omega v \, (\nabla \cdot \mathbf{E}) \, dx \; = \; \int_\Omega v \, f \, dx \tag{3.0.8}$$

$$\int_\Omega \mathbf{p} \cdot \epsilon^{-1} \, \mathbf{E} \, dx \; + \; \int_\Omega (\nabla \cdot \mathbf{p}) \, \Phi \, dx \; = \; \int_{\partial \Omega_N} (\mathbf{p} \cdot \boldsymbol{\eta}) \, \Phi_D \; dx \tag{3.0.9}$$

Where $V \; = \; \{\, \boldsymbol{\phi} \in H(\mathrm{div}\,;\, \Omega) : \boldsymbol{\phi} \cdot \boldsymbol{\eta} = 0 \quad \text{on} \quad \partial \Omega_N \}$

Now we wish to project our functions onto a finite dimensional vector space. However, we allow Φ and $\mathbf{E}$ to be in different vector spaces. Therefore we write:

$$\Phi = \sum_J \Phi_J \, \psi_J, \qquad \mathbf{E} = \sum_J E_J \boldsymbol{\Upsilon}_J$$

Where $\psi \in L_2(\Omega)$ and we enforce that $\boldsymbol{\Upsilon} \in V$ be continuous across element nodes. We also take $\mathbf{p} = \boldsymbol{\Upsilon}_I$ and $v = \psi_I$ this changes the weak formulation into:

$$\sum_I E_I \underbrace{\left(\int_\Omega (\nabla \cdot \boldsymbol{\Upsilon}_I) \, \psi_J \, dx \right)}_{A_{10}} = \underbrace{\int_\Omega f \, \psi_J \, dx}_{F}$$

And

$$\epsilon^{-1} \sum_I E_i \underbrace{\int_\Omega \boldsymbol{\Upsilon}_I \cdot \boldsymbol{\Upsilon}_J \, dx}_{A_{00}} + \sum_I \Phi_I \underbrace{\int_\Omega \psi_I \, (\nabla \cdot \boldsymbol{\Upsilon}_J)}_{A_{01}} = \underbrace{\int_{\partial \Omega} \Phi_D \, \boldsymbol{\Upsilon}_I \cdot \, \boldsymbol{\eta} \, ds}_{V} = 0$$

Then we write the two linear systems as one larger linear system:

$$\begin{bmatrix} A_{10} & 0 \\ \epsilon^{-1} A_{00} & -A_{01} \end{bmatrix} \begin{bmatrix} \Phi_{DOF} \\ E_{DOF} \end{bmatrix} = \begin{bmatrix} 0 \\ F \end{bmatrix} + \begin{bmatrix} V \\ 0 \end{bmatrix} \tag{3.0.10}$$

However, this time we cannot use the *Lax-Milgram theorem* to prove existence and uniqueness of the solutions.

9

Chapter 4

Local Discontinuous Galerking Methods

We discuss the local discontinuous Galerkin (LDG) method to approximate solutions of the Poisson equation:

$$
\begin{aligned}
-\nabla \cdot (\,\nabla u\,) &= f(\mathbf{x}) && \text{in } \Omega, \\
-\nabla u \cdot \mathbf{n} &= g_N(\mathbf{x}) && \text{on } \partial\Omega_N \\
u &= g_D(\mathbf{x}) && \text{on } \partial\Omega_D.
\end{aligned}
\tag{4.0.1}
$$

We first introduce some notation. Let $\mathcal{T}_h = \mathcal{T}_h(\Omega) = \{\,\Omega_e\,\}_{e=1}^{N}$ be the general triangulation of a domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$, into N non-overlapping elements Ω_e of diameter h_e. The maximum size of the diameters of all the elements is $h = \max(\,h_e\,)$. We define $\mathcal{E}_h$ to be the set of all element faces and $\mathcal{E}_h^i$ to be the set of all interior faces of elements which do not intersect the total boundary $(\partial\Omega)$. We define $\mathcal{E}_D$ and $\mathcal{E}_N$ to be the sets of all element faces and on the Dirichlet and Neumann boundaries respectively. Let $\partial\Omega_e \in \mathcal{E}_h^i$ be a interior boundary face element, we define the unit normal vector to be,

$$
\mathbf{n} \;=\; \text{unit normal vector to } \partial\Omega_e \text{ pointing from } \Omega_e^- \to \Omega_e^+.
\tag{4.0.2}
$$

We take the following definition on limits of functions on element faces,

$$
w^-(\mathbf{x})\,|_{\partial\Omega_e} \;=\; \lim_{s\to 0^-} w(\mathbf{x}+s\mathbf{n}), \qquad\qquad
w^+(\mathbf{x})\,|_{\partial\Omega_e} \;=\; \lim_{s\to 0^+} w(\mathbf{x}+s\mathbf{n}).
\tag{4.0.3}
$$

We define the average and jump of a function across an element face as,

$$
\{f\} \;=\; \frac{1}{2}(f^- + f^+), \qquad \text{and} \qquad [\![f]\!] \;=\; f^+\mathbf{n}^+ + f^-\mathbf{n}^-,
\tag{4.0.4}
$$

and,

$$
\{\mathbf{f}\} \;=\; \frac{1}{2}(\mathbf{f}^- + \mathbf{f}^+), \qquad \text{and} \qquad [\![\mathbf{f}]\!] \;=\; \mathbf{f}^+ \cdot \mathbf{n}^+ + \mathbf{f}^- \cdot \mathbf{n}^-,
\tag{4.0.5}
$$

where f is a scalar function and $\mathbf{f}$ is vector-valued function. We note that for a faces that are on the boundary of the domain we have,

$$
[\![f]\!] \;=\; f\,\mathbf{n} \qquad \text{and} \qquad [\![\mathbf{f}]\!] \;=\; \mathbf{f}\cdot\mathbf{n}.
\tag{4.0.6}
$$

We denote the volume integrals and surface integrals using the $L^2(\Omega)$ inner products by $(\,\cdot\,,\,\cdot\,)_\Omega$ and $\langle\,\cdot\,,\,\cdot\,\rangle_{\partial\Omega}$ respectively.

As with the mixed finite element method, the LDG discretization requires the Poisson equations be written as a first-order system. We do this by introducing an auxiliary variable which we call the current

flux variable $\mathbf{q}$:

$$\nabla \cdot \mathbf{q}_n \;=\; f(\mathbf{x}) \qquad\qquad \text{in } \Omega, \tag{4.0.7}$$

$$\mathbf{q}_n \;=\; -\nabla u \qquad\qquad \text{in } \Omega, \tag{4.0.8}$$

$$\mathbf{q}_n \cdot \mathbf{n} \;=\; g_N(\mathbf{x}) \qquad\qquad \text{on } \partial\Omega_N, \tag{4.0.9}$$

$$u = g_D(\mathbf{x}) \qquad\qquad \text{on } \partial\Omega_D. \tag{4.0.10}$$

In our numerical methods we will use approximations to scalar valued functions that reside in the finite-dimensional broken Sobolev spaces,

$$W_{h,k} \;=\; \left\{ w \in L^2(\Omega) \,:\, w|_{\Omega_e} \in \mathcal{Q}_{k,k}(\Omega_e), \quad \forall \Omega_e \in \mathcal{T}_h \right\}, \tag{4.0.11}$$

where $\mathcal{Q}_{k,k}(\Omega_e)$ denotes the tensor product of discontinuous polynomials of order k on the element Ω_e. We use approximations of vector valued functions that are as,

$$\mathbf{W}_{h,k} \;=\; \left\{ \mathbf{w} \in \left(L^2(\Omega)\right)^d \,:\, \mathbf{w}|_{\Omega_e} \in \left(\mathcal{Q}_{k,k}(\Omega_e)\right)^d, \quad \forall \Omega_e \in \mathcal{T}_h \right\} \tag{4.0.12}$$

We seek approximations for densities $u_h \in W_{h,k}$ and gradients $\mathbf{q}_h \in \mathbf{W}_{h,k}$. Multiplying (??) by $w \in W_{h,k}$ and (??) by $\mathbf{w} \in \mathbf{W}_{h,k}$ and integrating the divergence terms by parts over an element $\Omega_e \in \mathcal{T}_h$ we obtain,

$$-(\nabla w \,,\, \mathbf{q}_h)_{\Omega_e} + \langle w \,,\, \mathbf{q}_h \rangle_{\partial\Omega_e} \;=\; (w \,,\, f)_{\Omega_e} \,,$$

$$(\mathbf{w} \,,\, \mathbf{q}_h)_{\Omega_e} - (\nabla \cdot \mathbf{w} \,,\, u_h)_{\Omega_e} + \langle \mathbf{w} \,,\, u_h \rangle_{\partial\Omega_e} \;=\; 0,$$

Summing over all the elements leads to the **weak formulation**:

Find $u_h \in W_{h,k}$ and $\mathbf{q}_h \in \mathbf{W}_{h,k}$ such that,

$$-\sum_e (\nabla w,\, \mathbf{q}_h)_{\Omega_e} + \langle [\![w]\!] \,,\, \widehat{\mathbf{q}_h} \rangle_{\mathcal{E}_h^i} + \langle [\![w]\!] \,,\, \widehat{\mathbf{q}_h} \rangle_{\mathcal{E}_D \cup \mathcal{E}_N} \;=\; (w,\, f)_\Omega \tag{4.0.13}$$

$$\sum_e (\mathbf{w} \,,\, \mathbf{q}_h)_{\Omega_e} - \sum_e (\nabla \cdot \mathbf{w},\, u_h)_{\Omega_e} + \langle [\![\mathbf{w}]\!] \,,\, \widehat{u_h} \rangle_{\mathcal{E}_h^i} + \langle [\![\mathbf{w}]\!] \,,\, \widehat{u_h} \rangle_{\mathcal{E}_D \cup \mathcal{E}_N} \;=\; 0 \tag{4.0.14}$$

for all $(w, \mathbf{w}) \in W_{h,k} \times \mathbf{W}_{h,k}$.

The terms $\widehat{\mathbf{q}_h}$ and $\widehat{u_h}$ are the numerical fluxes. The numerical fluxes are introduced to ensure consistency, stability, and enforce the boundary conditions weakly. The flux $\widehat{u_h}$ is,

$$\widehat{u_h} \;=\; \begin{cases} \{u_h\} \;+\; \boldsymbol{\beta} \cdot [\![u_h]\!] & \text{in } \mathcal{E}_h^i \\ u_h & \text{in } \mathcal{E}_N \\ g_D(\mathbf{x}) & \text{in } \mathcal{E}_D \end{cases} \tag{4.0.15}$$

The flux $\widehat{\mathbf{q}_h}$ is,

$$\widehat{\mathbf{q}_h} \;=\; \begin{cases} \{\mathbf{q}_h\} \;-\; [\![\mathbf{q}_h]\!] \boldsymbol{\beta} \;+\; \sigma \, [\![u_h]\!] & \text{in } \mathcal{E}_h^i \\ g_N(\mathbf{x})\,\mathbf{n} & \text{in } \mathcal{E}_N \\ \mathbf{q}_h \;+\; \sigma\,(u_h - g_D(\mathbf{x}))\,\mathbf{n} & \text{in } \mathcal{E}_D \end{cases} \tag{4.0.16}$$

The term $\boldsymbol{\beta}$ is a constant vector which does not lie parallel to any element face in $\mathcal{E}_h^i$. For $\boldsymbol{\beta} = 0$, $\widehat{\mathbf{q}_h}$ and $\widehat{u_h}$ are called the central or Brezzi et. al. fluxes. For $\boldsymbol{\beta} \neq 0$, $\widehat{\mathbf{q}_h}$ and $\widehat{u_h}$ are called the LDG/alternating fluxes. The term σ is the penalty parameter that is defined as,

$$\sigma \;=\; \begin{cases} \tilde{\sigma}\,\min\left(h_{e_1}^{-1}, h_{e_2}^{-1}\right) & \mathbf{x} \in \langle \Omega_{e_1}, \Omega_{e_2} \rangle \\ \tilde{\sigma}\,h_e^{-1} & \mathbf{x} \in \partial\Omega_e \cap \in \mathcal{E}_D \end{cases} \tag{4.0.17}$$

with $\tilde{\sigma}$ being a positive constant.

We can now substitute (**??**) and (**??**) into (**??**) and (**??**) to obtain the solution pair $(u_h, \mathbf{q}_h)$ to the semi-discrete LDG approximation to the drift-diffusion equation given by:

Find $u_h \in W_{h,k}$ and $\mathbf{q}_h \in \mathbf{W}_{h,k}$ such that,

$$
\begin{aligned}
a(\mathbf{w}, \mathbf{q}_h) \;+\; b^T(\mathbf{w}, u_h) \;&=\; G(\mathbf{w}) \\
b(w, \mathbf{q}_h) \;+\; c(w, u_h) \;&=\; F(w)
\end{aligned}
\tag{4.0.18}
$$

for all $(w, \mathbf{w}) \in W_{h,k} \times \mathbf{W}_{h,k}$. This leads to the linear system,

$$
\begin{bmatrix} A & -B^T \\ B & C \end{bmatrix} \begin{bmatrix} \mathbf{U} \\ \mathbf{Q} \end{bmatrix} = \begin{bmatrix} \mathbf{G} \\ \mathbf{F} \end{bmatrix}
\tag{4.0.19}
$$

Where $\mathbf{U}$ and $\mathbf{Q}$ are the degrees of freedom vectors for u_h and $\mathbf{q}_h$ respectively. The terms $\mathbf{G}$ and $\mathbf{F}$ are the corresponding vectors to $G(\mathbf{w})$ and $F(w)$ respectively. The matrix in for the LDG system is non-singular for any $\sigma > 0$.

The bilinear forms in (**??**) and right hand functions are defined as,

$$
b(w, \mathbf{q}_h) \;=\; -\sum_e (\nabla w, \mathbf{q}_h)_{\Omega_e} + \langle \llbracket w \rrbracket, \{\mathbf{q}_h\} - \llbracket \mathbf{q}_h \rrbracket \boldsymbol{\beta} \rangle_{\mathcal{E}_h^i} + \langle w, \mathbf{n} \cdot \mathbf{q}_h \rangle_{\mathcal{E}_D}
\tag{4.0.20}
$$

$$
a(\mathbf{w}, \mathbf{q}_h) \;=\; \sum_e (\mathbf{w}, \mathbf{q}_h)_{\Omega_e}
\tag{4.0.21}
$$

$$
-b^T(w, \mathbf{q}_h) \;=\; -\sum_e (\nabla \cdot \mathbf{w}, u_h)_{\Omega_e} + \langle \llbracket \mathbf{w} \rrbracket, \{u_h\} + \boldsymbol{\beta} \cdot \llbracket u_h \rrbracket \rangle_{\mathcal{E}_h^i} + \langle w, u_h \rangle_{\mathcal{E}_N}
\tag{4.0.22}
$$

$$
c(w, u_h) \;=\; \langle \llbracket w \rrbracket, \sigma \llbracket u_h \rrbracket \rangle_{\mathcal{E}_h^i} + \langle w, \sigma u_h \rangle_{\mathcal{E}_D}
\tag{4.0.23}
$$

$$
G(\mathbf{w}) \;=\; -\langle \mathbf{w}, g_D \rangle_{\mathcal{E}_D}
\tag{4.0.24}
$$

$$
F(w) \;=\; (w, f) - \langle w, g_N \rangle_{\mathcal{E}_N} + \langle w, \sigma g_D \rangle_{\mathcal{E}_D}
\tag{4.0.25}
$$