§2.1 PDEs and Their Equivalent Formulations

§2.1.1 Diffusion and Reaction Equation

$$\begin{cases} \mathcal{L}u \equiv -\nabla\cdot(A\nabla u) + au = f & \text{in } \Omega \subset \mathbb{R}^d \\ u|_{\Gamma_D} = g_D \text{ and } \vec{n}\cdot(A\nabla u)|_{\Gamma_N} = g_N \end{cases}$$

where (1) Ω is a connected, bounded domain with Lipschitz boundary

$$\partial\Omega = \Gamma_D \cup \Gamma_N \quad \text{s.t. } \Gamma_D \cap \Gamma_N = \phi$$

(2) $A = (a_{ij})_{d\times d}$ - sym is diffusion coefficient, a is reaction coefficient.

(3) f, g_D, and g_N are given scalar-valued functions defined on Ω, Dirichlet boundary Γ_D, and Neumann boundary Γ_N, respectively.

(4) $\vec{n}$ is the unit outward vector normal to $\partial\Omega$.

(5) ∇ is the gradient operator defined by $\nabla u = \left(\frac{\partial u}{\partial x_1}, \cdots, \frac{\partial u}{\partial x_d}\right)^T$

(6) $\nabla\cdot$ is the divergence operator defined ~~by~~ for a vector field $\vec{v} = (v_1, \cdots, v_d)^T$ by

$$\nabla\cdot\vec{v} = \frac{\partial v_1}{\partial x_1} + \cdots + \frac{\partial v_d}{\partial x_d}.$$

<u>Lemma (formula of integration by part)</u>

$$\int_\Omega (\nabla\cdot\vec{v})\, u\, dx = -\int_\Omega \vec{v}\cdot\nabla u\, dx + \int_{\partial\Omega} (\vec{v}\cdot\vec{n})\, u\, ds$$

§2.1.1.1 Variational (Weak) Formulation

$$\int_\Omega f v\, dx = \int_\Omega \left[-\nabla\cdot(A u) + a u \right] v\, dx$$
$$= \int_\Omega \left[A\nabla u\cdot\nabla v + a u v \right] dx - \int_{\Gamma_N} g_N v\, ds - \int_{\Gamma_D} (\vec{n}\cdot A\nabla u) v\, ds$$

For any v satisfying $v|_{\Gamma_D} = 0$

$$\int_\Omega \left(A\nabla u\cdot\nabla v + a u v \right) dx = \int_\Omega f v\, dx + \int_{\Gamma_N} g_N v\, ds$$

(1) Solution spaces

Sobolev space $H^1(\Omega) = \left\{ v \in L^2(\Omega) \,\middle|\, \int_\Omega v^2 + |\nabla v|^2 < +\infty \right\}$

$$u \in H^1_g(\Omega) = \left\{ v \in H^1(\Omega) \,\middle|\, v|_{\Gamma_D} = g \right\}$$
$$v \in H^1_0(\Omega) = \left\{ v \in H^1(\Omega) \,\middle|\, v|_{\Gamma_D} = 0 \right\}$$

(2) Bilinear and linear forms

$$a(u,v) \equiv \int_\Omega \left(A\nabla u\cdot\nabla v + a u v \right) dx \quad \text{and} \quad f(v) = \int_\Omega f v\, dx + \int_{\Gamma_N} g_N v\, ds$$

bilinear $\quad a(\alpha_1 u_1 + \alpha_2 u_2, v) = \alpha_1 a(u_1, v) + \alpha_2 a(u_2, v), \quad \alpha_i \in R$

$\qquad a(u, \beta_1 v_1 + \beta_2 v_2) = \beta_1 a(u, v_1) + \beta_2 a(u, v_2), \quad \beta_i \in R$

linear $\quad f(\alpha_1 v_1 + \alpha_2 v_2) = \alpha_1 f(v_1) + \alpha_2 f(v_2), \quad \alpha_i \in R.$

(3) Boundary conditions

Dirichlet B.C. $\quad u|_{\Gamma_D} = g_D \quad$ essential

Neumann B.C. $\quad (A\nabla u)\cdot\vec{n}|_{\Gamma_N} = g_N \quad$ natural

- Variational Formulation (VF)

Find $u \in H^1_g(\Omega)$ s.t. $a(u,v) = f(v) \quad \forall v \in H^1_0(\Omega)$.

Assumptions (1) $a(\cdot,\cdot)$ is elliptic (coercive) in V

$\iff \exists\, \alpha > 0$ s.t. $\alpha \|v\|_V^2 \leq a(v,v) \quad \forall v \in V$.

(2) $a(\cdot,\cdot)$ is symmetric $\iff a(u,v) = a(v,u) \quad \forall u, v \in V$

(3) $a(\cdot,\cdot)$ is bounded $\iff \exists\, M > 0$ s.t. $|a(u,v)| \leq M \|u\|_V \|v\|_V, \ \forall u,v \in V$

(4) $f(\cdot)$ is bounded $\iff \exists\, C > 0$ s.t. $|f(v)| \leq C \|v\|_V, \ \forall v \in V$

Theorem Under the assumptions (1)–(4), (VF) has a unique solution.

- Minimization Formulation (MF)

Find $u \in H^1_g(\Omega)$ s.t. $J(u) = \min\limits_{v \in H^1_g(\Omega)} J(v)$

where $J(v) = \frac{1}{2} a(v,v) - f(v)$ is the energy functional.

Theorem Assume that $a(\cdot,\cdot)$ is sym. and semi-positive definite.

$\implies$ (VF) $\iff$ (MF)

Proof "$\Leftarrow$" Assume that $u = \operatorname{argmin}\limits_{v \in H^1_g(\Omega)} J(v)$.

For any $v \in V$, define $g(t) = J(u + tv) = J(u) + t\,[a(u,v) - f(v)] + \frac{1}{2} t^2 a(v,v)$

$\Rightarrow 0 = g'(0) = a(u,v) - f(v)$ (VF)

"$\Rightarrow$" $\forall v \in H^1_g(\Omega)$, $J(v) = J(u + (v-u)) = J(u) + [a(u, v-u) - f(v-u)] + \frac{1}{2} a(v-u, v-u)$

$= J(u) + \frac{1}{2} a(v-u, v-u) \geq J(u)$

$\Rightarrow J(u) = \min\limits_{v} J(v)$.

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- Least-squares Formulations

(1) Bramble-Schatz LS (1970)

BS functional $\mathcal{L}(v;\vec{f}) = \| f + \nabla\cdot(A\nabla v) - av \|^2_{0,\Omega} + \| v - g_D \|^2_{\frac{3}{2},\Gamma_D} + \| \vec{n}\cdot(A\nabla v) - g_N \|^2_{\frac{1}{2},\Gamma_N}$

solution space $\quad V = H^2(\Omega)$

BSLS Formulation $\quad$ Find $u \in H^2(\Omega)$ s.t. $\mathcal{L}(u;\vec{f}) = \min\limits_{v\in H^2(\Omega)} \mathcal{L}(v;\vec{f})$

Theorem $\exists\, \alpha>0, M>0$ s.t. $\alpha \|v\|^2_{2,\Omega} \le \mathcal{L}(v;\vec{0}) \le M\|v\|^2_{2,\Omega} \quad \forall\, v\in H^2(\Omega)$

~~limitations In general, the solution u is not in $H^2(\Omega)$ whose functions have twice 2nd-order weak derivative.~~

solution properties of elliptic PDEs $\quad -\nabla\cdot(A\nabla u) + au = f$ in $\Omega \subset \mathbb{R}^d$ $(d=2,3)$

(1) $u \in H^{1+\alpha}(\Omega)$ with $\alpha > \frac{1}{2} - \varepsilon$ for all ε.

(2) often $u \notin H^2(\Omega)$

(3) $f \in L^2(\Omega) \Longrightarrow A\nabla u \in H(\mathrm{div};\Omega) = \left\{ \vec{v} \in L^2(\Omega)^d \;\middle|\; \nabla\cdot\vec{v} \in L^2(\Omega) \right\}$

$\Longrightarrow$ the interface condition $0 = [\![\vec{n}_\Gamma \cdot (A\nabla u)]\!]_\Gamma$

e.g. elliptic interface problem $\quad = \vec{n}^+_\Gamma \cdot (A\nabla u^+)_\Gamma + \vec{n}^-_\Gamma \cdot (A\nabla u^-)_\Gamma$

(4) the interface Γ is in general unknown,

its location is known for some linear problems.

challenge $\quad$ when Γ is unknown, how to enforce the interface condition?

(2) First-Order System Least-Squares (FOSLS)

FOS
$$\begin{cases} \vec{\sigma} + A\nabla u = \vec{0} & \text{in } \Omega \\ \nabla\cdot\vec{\sigma} + a u = f & \text{in } \Omega \end{cases} \qquad \begin{cases} u|_{\Gamma_D} = g_D \\ \vec{n}\cdot\vec{\sigma}|_{\Gamma_N} = -g_N \end{cases}$$

FOSLS-functional

$$G(\vec{\tau}, v; \vec{f}) = \|A^{-\frac{1}{2}}\vec{\tau} + A^{\frac{1}{2}}\nabla v\|^2_{0,\Omega} + \|a^{-\frac{1}{2}}(\nabla\cdot\vec{\tau} + av - f)\|^2_{0,\Omega} + \|v - g_D\|^2_{\frac{1}{2},\Gamma_D} + \|\vec{n}\cdot\vec{\tau} + g_N\|^2_{-\frac{1}{2},\Gamma_N}$$

solution spaces

$u \in H^1(\Omega)$ and $\vec{\sigma} \in H(\mathrm{div};\Omega)$

FOSLS Find $(\vec{\sigma}, u) \in H(\mathrm{div};\Omega) \times H^1(\Omega)$ s.t.

$$G(\vec{\sigma}, u; \vec{f}) = \min_{(\vec{\tau}, v)\in H(\mathrm{div})\times H^1} G(\vec{\tau}, v; \vec{f}).$$

Theorem $\exists\ \alpha > 0,\ M > 0$ such that $\forall\ (\vec{\tau}, v) \in H(\mathrm{div};\Omega)\times H^1(\Omega)$

$$\alpha |||(\vec{\tau}, v)|||^2 \equiv \alpha\left(\|\vec{\tau}\|^2_{H(\mathrm{div})} + \|v\|^2_{H^1(\Omega)}\right) \le G(\vec{\tau}, v; \vec{0}) \le M\, |||(\vec{\tau}, v)|||^2.$$

Proof
$$G(\vec{\tau}, v; \vec{0}) = \|A^{-\frac{1}{2}}\vec{\tau} + A^{\frac{1}{2}}\nabla v\|^2 + \|a^{-\frac{1}{2}}\nabla\cdot\vec{\tau} + a^{\frac{1}{2}}v\|^2 + \|v\|^2_{\frac{1}{2},\Gamma_D} + \|\vec{\tau}\cdot\vec{n}\|^2_{-\frac{1}{2},\Gamma_N}$$

$$= \|A^{-\frac{1}{2}}\vec{\tau}\|^2 + \|A^{\frac{1}{2}}\nabla v\|^2 + \|a^{-\frac{1}{2}}\nabla\cdot\vec{\tau}\|^2 + \|a^{\frac{1}{2}}v\|^2 + \|v\|^2_{\frac{1}{2},\Gamma_D} + \|\vec{\tau}\cdot\vec{n}\|^2_{-\frac{1}{2},\Gamma_N}$$

$$+ 2\left[(\vec{\tau}, \nabla v) + (\nabla\cdot\vec{\tau}, v)\right] \longrightarrow 2\left[\int_{\Gamma_D}(\vec{n}\cdot\vec{\tau})v\,ds + \int_{\Gamma_N}(\vec{n}\cdot\vec{\tau})v\,ds\right]$$

$$\ge \|A^{-\frac{1}{2}}\vec{\tau}\|^2 + \|a^{-\frac{1}{2}}\nabla\cdot\vec{\tau}\|^2 - 2C\|\vec{\tau}\|_{H(\mathrm{div})}\|v\|_{\frac{1}{2},\Gamma_D} + \|v\|^2_{\frac{1}{2},\Gamma_D} \qquad \le 2C\|\vec{\tau}\|_{H(\mathrm{div})}\|v\|_{\frac{1}{2},\Gamma_D} + 2C\|v\|_{H^1}\|\vec{\tau}\cdot\vec{n}\|_{-\frac{1}{2},\Gamma_N}$$

$$+ \|A^{\frac{1}{2}}\nabla v\|^2 + \|av\|^2 - 2C\|v\|_{H^1}\|\vec{\tau}\cdot\vec{n}\|_{-\frac{1}{2},\Gamma_N} + \|\vec{\tau}\cdot\vec{n}\|^2_{-\frac{1}{2},\Gamma_N}$$

$$\begin{cases} \|\vec{n}\cdot\vec{\tau}\|_{-\frac{1}{2},\Gamma_D} \le C\|\vec{\tau}\|_{H(\mathrm{div})} \\ \|v\|_{\frac{1}{2},\Gamma_N} \le C\|v\|_{H^1} \end{cases}$$