Theoretical Convergence of Numerical Schemes for Coupled 3D-1D PDEs

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Abstract

Coupled 3D-1D advection-diffusion PDEs with different sets of boundary conditions are discretized. For the first set, we formulate and analyze a finite element-based scheme. For the second set, we develop and analyze a scheme that combines the finite element method for the three-dimensional equation and the interior penalty discontinuous Galerkin method for the one-dimensional equation.

Motivation

Successful liver cancer treatment depends on how drugs travel through blood vessels and spread into the surrounding tissue. Existing models often study vessel and tissue separately, missing their strong interaction. The 3D-1D coupled PDE framework is a reduced model that captures both processes together, offering deeper insights into drug distribution and guiding more effective therapies.

General Problem

Ω is the 3D domain and Λ is the 1D line embedded into Ω.

$$-\Delta u + \beta\cdot\nabla u + \kappa|\partial D|(\bar{u} - U)\delta_\Lambda = f, \qquad \text{in} \quad \Omega$$

$$-\frac{d}{ds}\left(|D|\frac{dU}{ds}\right) + \alpha|D|\frac{dU}{ds} - \kappa|\partial D|(\bar{u} - U) = g|D| \qquad \text{in} \quad \Lambda$$

- ▶ Dirac function on line Λ: δ_Λ
- ▶ Velocity fields: β and α; Source terms: $f \in L^2(\Omega)$, $g \in L^2(\Lambda)$
- ▶ Line Λ is centerline of a generalized cylinder with cross-section $D(s)$ of area $|D(s)|$ and perimeter $|\partial D(s)|$.
- ▶ Lateral average: $\bar{u}$.
- ▶ Permeability coefficient: κ: measures leakiness of blood vessels.
- ▶ Two sets of boundary conditions are considered below:

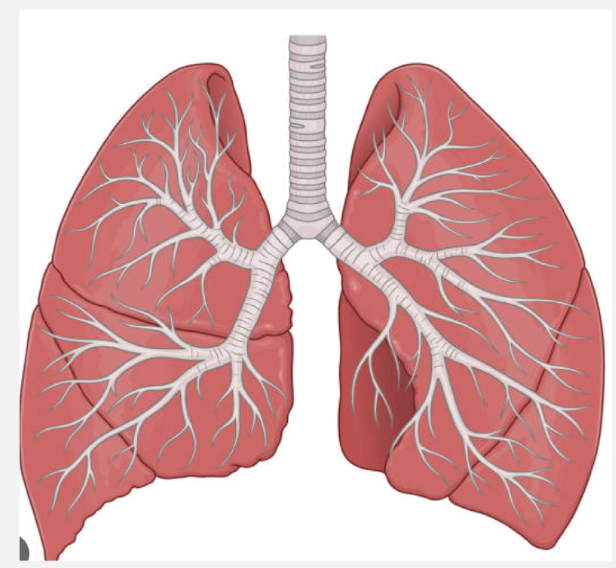
$$\mathcal{P}_I = \begin{cases} u = 0 \text{ on } \partial\Omega \\ \frac{dU}{ds} = 0 \text{ at } s = 0 \\ U = 0, \text{ at } s = L \end{cases} \qquad \mathcal{P}_{II} = \begin{cases} u = 0 \text{ on } \partial\Omega \\ \frac{dU}{ds} - \alpha U = -\alpha U_\infty \text{ at } s = 0 \\ |D(s)|\frac{dU}{ds} = 0, \text{ at } s = L \end{cases}$$

Weak Form

Let $\mathbb{V} = H_0^1(\Omega)\times H_{0,L}^1(\Lambda)$. Then, the weak form consists of finding $\mathcal{U} = (u, U) \in \mathbb{V}$ such that:

$$\int_\Omega \nabla u\cdot\nabla v + \int_\Lambda |D|\tfrac{dU}{ds}\tfrac{dV}{ds} + \int_\Omega (\beta\cdot\nabla u)v + \int_\Lambda |D|\alpha\tfrac{dU}{ds}V$$
$$+ \int_\Lambda |\partial D|\kappa(\bar{u} - U)(\bar{v} - V) = \int_\Omega fv + \int_\Lambda |D|gV, \quad \forall (v, V) \in \mathbb{V} \qquad (1)$$

Application



(a) Drug Delivery

(b) Nutrient Transport

Results for Problem $\mathcal{P}_I$

Lemma (Weighted Poincare's Inequality):

There exists a constant $\hat{C}_{P^*} > 0$ such that;

$$\forall V \in H_{0,L}^1(\Lambda); \quad \||D|^{1/2}V\|_{L^2(\Lambda)} \le \hat{C}_{P^*}\||D|^{1/2}d_sV\|_{L^2(\Lambda)}.$$

Theorem (Weak Solution):

Let $f \in L^2(\Omega)$ and $g \in L^2(\Lambda)$. Suppose that β and α satisfy the conditions:

$$\|\beta\|_{L^\infty(\Omega)} \le \frac{1}{C_P} \quad \text{and} \quad \|\alpha\|_{L^\infty(\Lambda)} \le \frac{1}{\hat{C}_{P^*}},$$

then there exists a unique solution to the weak problem (1).

- **Finite Element Scheme:** Let $\mathbb{V}_h = V_h^\Omega \times V_h^\Lambda$ be the discrete space. Then the finite element solution to (1) involves finding:

$$\mathcal{U}_h \in \mathbb{V}_h, \quad \mathcal{A}(\mathcal{U}_h, \mathcal{V}_h) = \mathcal{F}(\mathcal{V}_h) \quad \forall \mathcal{V}_h \in \mathbb{V}_h. \qquad (2)$$

Lemma (Existence and Uniqueness of FEM solution):

Let $f \in L^2(\Omega)$ and $g \in L^2(\Lambda)$. Suppose that β and α satisfy the conditions:

$$\|\beta\|_{L^\infty(\Omega)} \le \frac{1}{2C_P} \quad \text{and} \quad \|\alpha\|_{L^\infty(\Lambda)} \le \frac{1}{2\hat{C}_{P^*}}. \qquad (*)$$

Then, there exists a unique solution to (2).

Theorem (Error Estimate):

Suppose $u \in H^{\frac{3}{2}-\varepsilon}(\Omega), U \in H^2(\Lambda)$. Under the assumptions below:

$$\|\beta\|_{L^\infty(\Omega)} \le \frac{9}{10(1+2C_P)} \quad \text{and} \quad \|\alpha\|_{L^\infty(\Lambda)} \le \frac{9}{10(1+2\hat{C}_{P^*})},$$

there exists a constant C independent of u, U and h such that

$$\|\nabla(u-u_h)\|_{L^2(\Omega)}^2 + \||D|^{\frac{1}{2}}d_s(U-U_h)\|_{L^2(\Lambda)}^2$$
$$+ \||\partial D|^{\frac{1}{2}}\kappa^{\frac{1}{2}}(\bar{u} - \bar{u}_h - (U-U_h))\|_{L^2(\Lambda)}^2$$
$$\le C(h^{1-2\varepsilon}|u|_{H^{\frac{3}{2}-\varepsilon}(\Omega)}^2 + h^2|U|_{H^2(\Lambda)}^2).$$

Results for Problem $\mathcal{P}_{II}$

- **FEM-DG Scheme:** Let $\tilde{\mathbb{V}}_h = \mathbf{V}_h^\Omega \times \mathcal{D}_k(\mathcal{T}_\Lambda^h)$. $\mathcal{D}_k(\mathcal{T}_\Lambda^h)$ is the space of discontinuous piecewise polynomial. Our numerical scheme consists of finding $\mathcal{U}_h \in \tilde{\mathbb{V}}_h$ such that:

$$a_\Omega(u_h, v_h) + c_\Omega(u_h, v_h) + a_{DG}(U_h, V_h) + b_\Lambda(\bar{u}_h - U_h, \bar{v}_h - V_h)$$
$$= (f, v_h)_\Omega + \int_0^L |D(s)|g(s)V(s) + \alpha|D(0)|U_\infty V(0)$$
$$\forall \mathcal{V}_h \in \tilde{\mathbb{V}}_h \qquad (3)$$

▶ $a_{DG}(U_h, V_h)$ is the DG bilinear form of the diffusion and the advection terms in 1D with some boundary terms.

Lemma (Coercivity):

Suppose $\varepsilon = 1$ and $\sigma \ge 0$. Then

$$\forall V_h \in \mathcal{D}_k(\mathcal{T}_\Lambda^h) : a_{DG}(V_h, V_h) \ge |V_h|_{DG}^2, \qquad (4)$$

where

$$|V_h|_{DG} = \left(\sum_{i=0}^{N-1}\int_{s_i}^{s_{i+1}} |D(s)|(V_h'(s))^2 ds + \sum_{i=1}^{N-1}\frac{\sigma}{h}[V_h(s_i)]^2\right)^{\frac{1}{2}}.$$

Lemma (Existence and Uniqueness):

Let $f \in L^2(\Omega)$ and $g \in L^2(\Lambda)$. Suppose that β satisfies $(*)$ and $\varepsilon = 1$. Then, there exists a unique solution to the problem (3).

- **The FDG Norm:** Assume the exact solution $\mathcal{U} = (u, U) \in H_0^1(\Omega)\times H^2(\Lambda)$. We define the $\|\cdot\|_{FDG}$

$$\|\mathcal{V}\|_{FDG}^2 = \|v\|_{H^1(\Omega)}^2 + |V|_{DG}^2 + \||\partial D|^{\frac{1}{2}}\kappa^{\frac{1}{2}}(\bar{v} - V)\|_{L^2(\Lambda)}^2.$$

Theorem (Error Estimate)

Suppose $\mathcal{U} \in H^{\frac{3}{2}-\varepsilon}(\Omega)\times H^2(\Lambda)$. Let $\mathcal{U}_h$ be our discrete solution. Assume β satisfies $(*)$. Then, there exists constants K_1 and K_2, independent of h, such that the following error estimate holds:

$$\|\mathcal{U} - \mathcal{U}_h\|_{FDG}^2 \le K_1 h^{1-2\varepsilon}|u|_{H^{\frac{3}{2}-\varepsilon}(\Omega)}^2 + K_2 h^2|U|_{H^2(\Lambda)}^2.$$

Future Work and Acknowledgment

- Implementation of the numerical schemes.
- Developing a more robust scheme using the DG-DG methods.
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