Discontinuous Galerkin Methods for mass transfer through semi-permeable membranes

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with

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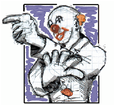

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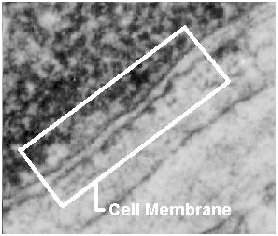
Mass transfer through semi-permeable membranes



We consider a generic problem of mass transfer of a number of solutes through a semi-permeable membrane.

Each solute is subject to:

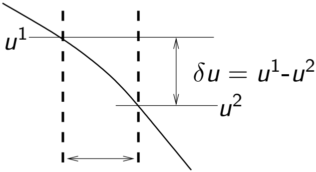
- Diffusion and/or advection on both sides of the membrane
- Reactions coupling it with the other solutes
- Mass transfer across the membrane

Membrane models

[Kedem & Katchalsky ('58), Kedem & Katchalsky ('81), Friedman ('08)]

One solute. Membrane flux J across the membrane given by:

Kedem-Katchalsky flux
$$J = P\delta u + (b - \sigma\delta u)\bar{u} = P(u)\delta u + b\bar{u},$$



$\bar{u}$ average concentration across the membrane

Thermodynamics approach: $\bar{u} = \ln(u_1/u_2)/(u_1 - u_2) \sim (u_1 + u_2)/2$

Mechanics approach: $\bar{u} = w^1 u_1 + w^2 u_2$ with $\begin{cases} w^1 + w^2 = 1 \\ w^1 \geq w^2 \quad \text{if} \quad b \geq 0 \end{cases}$.

Many solutes. $J_i = P(u_i) \sum_j \delta u_j + b\bar{u}_i$

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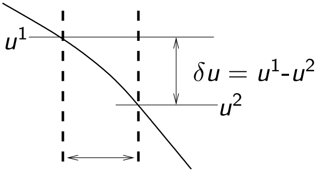

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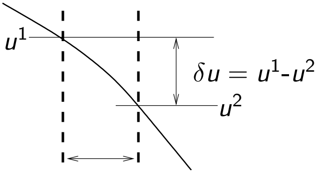

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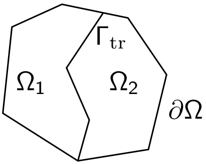
Model problem

Let $\Omega \subset \mathbb{R}^d$ be a open polygonal domain subdivided into two polygonal subdomains Ω_1 and Ω_2:

$$\Omega = \Omega_1 \cup \Omega_2 \cup \Gamma_{\mathrm{tr}}$$

$$\Gamma_{\mathrm{tr}} = \bar{\Omega}_1 \cap \bar{\Omega}_2$$



and set $\mathcal{H}^1 := [H^1(\Omega_1 \cup \Omega_2)]^n$, $n \in \mathbb{N}$.

For the time interval $[0, T]$, and for $\mathbf{u} \in L^2(0, T; \mathcal{H}^1)$, consider the system

$$\mathbf{u}_t - \nabla \cdot (A \nabla \mathbf{u} - U\mathbf{B}) + \mathbf{F}(\mathbf{u}) = \mathbf{0} \quad \text{in } (0, T] \times (\Omega_1 \cup \Omega_2),$$

with $U := \mathrm{diag}(u_1, u_2, \ldots, u_n)$, and under the assumptions

$$\mathbf{B} \in [C^1(0, T; \bar{\Omega})]^{n \times d} \qquad \text{with rows } B_i, i = 1, \ldots, n,$$

$$A := \mathrm{diag}(a_1, a_2, \ldots, a_n) \in [C(0, T; \Omega_1 \cup \Omega_2)]^{n \times n}$$

with $a_i > 0$, for all $i = 1, \ldots, n$.

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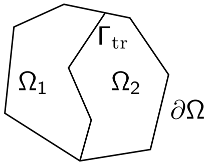

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with $a_i > 0$, for all $i = 1, \ldots, n$.

Model problem (cont.)

Initial conditions:

$$\mathbf{u}(0,x) = \mathbf{u}_0(x) \quad \text{on } \{0\} \times \Omega,$$

Boundary conditions:

$$\begin{cases} \mathbf{u} = \mathbf{g}_{\mathrm{D}} & \text{on } (0,T] \times \Gamma_{\mathrm{D}}; \\ \big(A\nabla\mathbf{u} - \chi^{-} U\mathbf{B}\big)\mathbf{n} = \mathbf{g}_{\mathrm{N}} & \text{on } (0,T] \times \Gamma_{\mathrm{N}}, \end{cases}$$

where χ^{-} is the characteristic function of the inflow part of $\partial\Omega$.

Non-linear reaction: vector field $\mathbf{F} : \mathbb{R}^n \to \mathbb{R}^n$ with

$$|\mathbf{F}(\mathbf{u}) - \mathbf{F}(\mathbf{v})| \leq C(1 + |\mathbf{u}| + |\mathbf{v}|)^{\gamma} |\mathbf{u} - \mathbf{v}|, \quad \exists \gamma \in [0,1]$$

Transmission conditions at Γ_{tr}

Transmission condition. On Γ_{tr} we impose:

$$(A\nabla\mathbf{u} - U\mathbf{B})\mathbf{n}|_{\Omega_1} = \mathbf{P}(\mathbf{u})(\mathbf{u}^2 - \mathbf{u}^1) - \{U\}_w\mathbf{B}\mathbf{n}^1$$
$$(A\nabla\mathbf{u} - U\mathbf{B})\mathbf{n}|_{\Omega_2} = \mathbf{P}(\mathbf{u})(\mathbf{u}^1 - \mathbf{u}^2) - \{U\}_w\mathbf{B}\mathbf{n}^2$$

assuming strict monotonicity and Lipschitz continuity: for some $r \geq 2$

$$\big(\mathrm{P}(\mathbf{w})[\![\mathbf{w}]\!] - \mathrm{P}(\mathbf{v})[\![\mathbf{v}]\!]\big) : [\![\mathbf{w} - \mathbf{v}]\!] \geq C_1|[\![\mathbf{w} - \mathbf{v}]\!]|^r,$$
$$\big|\mathrm{P}(\mathbf{w})[\![\mathbf{w}]\!] - \mathrm{P}(\mathbf{v})[\![\mathbf{v}]\!]\big| \leq C_2|[\![\mathbf{w} - \mathbf{v}]\!]|^{r-1}$$

Here,

$$\{U\}_w := W^1U^1 + W^2U^2, \quad \text{with } W^j = \mathrm{diag}(W_i^j),\ j = 1, 2,$$

and

$$[\![\mathbf{v}]\!] := \mathbf{v}^1 \otimes \mathbf{n}^1 + \mathbf{v}^2 \otimes \mathbf{n}^2 \qquad (\mathbf{v} \otimes \mathbf{n} = \mathbf{v}\mathbf{n}^T),$$
$$\{\mathbf{v}\} := \tfrac{1}{2}(\mathbf{v}^+ + \mathbf{v}^-).$$

Literature review

- Mass transfer transmission problems

  Calabrò & Zunino ('06), Quarteroni, Veneziani & Zunino ('01)...

- DG for parabolic problems

  Arnold ('82), Cockburn & Shu ('98), Rivière & Wheeler ('00,'02), Houston, Schwab & Süli ('02), Sun & Wheeler ('05, '06), Rivière & Girault ('06), Lasis & Süli ('07), Epshteyn & Riviére ('07), Bartels, Jensen & Müller ('09)...

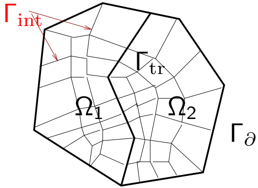
- DG reaction-diffusion(-advection) systems

  Epshteyn & Kurganov ('08), Zhu, Zhang, Newmann & Alber ('09)...

Discontinuous finite element spaces

Decomposition of Ω

- $\mathcal{T}_h$ shape-regular partition of Ω
- Each element $\kappa \in \mathcal{T}$ belongs to Ω_1 or Ω_2
- The skeleton $\Gamma = \Gamma_\partial \cup \Gamma_{\mathrm{int}} \cup \Gamma_{\mathrm{tr}}$
- $\Gamma_\partial = \Gamma_D \cup \Gamma_N$



Discontinuous finite element space:

$$S := \{v \in L^2(\Omega) : v|_\kappa \circ F_\kappa \in \mathcal{P}_{m_\kappa}(\hat{\kappa}),\ \kappa \in \mathcal{T}\}, \quad S^n := [S]^n,$$

where $\mathcal{P}_{m_\kappa}$ a space of polynomials of maximum degree m_κ.

Discretisation in space: the transmission term

For any $\mathbf{u}, \mathbf{v} \in \mathcal{H}^1 + S^n$:

$$-\sum_{\kappa\in\mathcal{T}} \int_\kappa (\nabla\cdot(A\nabla\mathbf{u} - U\mathbf{B}))\cdot\mathbf{v} = \sum_{\kappa\in\mathcal{T}} \int_\kappa (A\nabla\mathbf{u} - U\mathbf{B}) : \nabla\mathbf{v} - \int_{\partial\kappa} (A\nabla\mathbf{u} - U\mathbf{B})\mathbf{n}\cdot\mathbf{v}.$$

yields the transmission terms:

$$-\int_{\Gamma_{\mathrm{tr}}} \left[(A\nabla\mathbf{u} - U\mathbf{B})\mathbf{n}\cdot\mathbf{v}|_{\Omega_1} + (A\nabla\mathbf{u} - U\mathbf{B})\mathbf{n}\cdot\mathbf{v}|_{\Omega_2}\right]$$

$$= \cdots = \int_{\Gamma_{\mathrm{tr}}} \left(\mathbf{P}(\mathbf{w})[\![\mathbf{u}]\!] + \{U\mathbf{B}\}_w\right) : [\![\mathbf{v}]\!].$$

In particular, in the purely diffusive case,

$$\int_{\Gamma_{\mathrm{tr}}} \mathbf{P}(\mathbf{w})[\![\mathbf{u}]\!] : [\![\mathbf{v}]\!].$$

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Reformulation of the advective transmission term

Define $\mathcal{B}^{\rm tr} := \text{diag}(b_i^{\rm tr})$ where

$$b_i^{\rm tr} = (w_i^1 - \frac{1}{2})(B_i \mathbf{n})|_{\Omega_1} \geq 0$$

we get

$$\{U\mathbf{B}\}_w \mathbf{n} = \left(\{U\mathbf{B}\} + \mathcal{B}^{\rm tr} [\![\mathbf{u}]\!]\right) \mathbf{n}$$

Thus,

$$\int_{\Gamma_{\rm tr}} (\mathbf{P}(\mathbf{w})[\![\mathbf{u}]\!] + \{U\mathbf{B}\}_w) : [\![\mathbf{v}]\!] = \int_{\Gamma_{\rm tr}} \left(\{U\mathbf{B}\} + (\mathbf{P}(\mathbf{w}) + \mathcal{B}^{\rm tr})[\![\mathbf{u}]\!]\right) : [\![\mathbf{v}]\!].$$

IPDG formulation

For $\mathbf{w} \in \mathcal{S}^n := \mathcal{H}^1 + S_h^{\mathbf{m}}$ and $\mathbf{u}_h, \mathbf{v}_h \in S_h^{\mathbf{m}}$ define

$$
\begin{aligned}
B(\mathbf{w};\mathbf{u}_h,\mathbf{v}_h) := &\sum_{\kappa\in\mathcal{T}} \int_\kappa (A\nabla\mathbf{u}_h - U_h\mathbf{B}) : \nabla\mathbf{v}_h + \int_{\Gamma_\mathrm{N}} (\chi^+ U_h\mathbf{B}) : (\mathbf{v}_h \otimes \mathbf{n}) \\
&- \int_{\Gamma_\mathrm{D}} \Big((A\nabla\mathbf{u}_h - \chi^+ U_h\mathbf{B}) : (\mathbf{v}_h\otimes\mathbf{n}) + (A\nabla\mathbf{v}_h) : (\mathbf{u}_h\otimes\mathbf{n}) - \Sigma\mathbf{u}_h\cdot\mathbf{v}_h \Big) \\
&- \int_{\Gamma_\mathrm{int}} \Big(\{A\nabla\mathbf{u}_h - U_h\mathbf{B}\} : [\![\mathbf{v}_h]\!] + \{A\nabla\mathbf{v}_h\} : [\![\mathbf{u}_h]\!] - (\Sigma + \mathcal{B})[\![\mathbf{u}_h]\!] : [\![\mathbf{v}_h]\!] \Big) \\
&+ \int_{\Gamma_\mathrm{tr}} \big(\{U\mathbf{B}\} + (\mathbf{P}(\mathbf{w}) + \mathcal{B}^\mathrm{tr})[\![\mathbf{u}]\!] \big) : [\![\mathbf{v}]\!]
\end{aligned}
$$

and

$$
l(\mathbf{v}_h) := -\int_{\Gamma_\mathrm{D}} (\mathbf{g}_\mathrm{D}\otimes\mathbf{n} : A\nabla\mathbf{v}_h + \chi^- G_\mathrm{D}\mathbf{B} : \mathbf{v}_h\otimes\mathbf{n} - \Sigma\mathbf{g}_\mathrm{D}\cdot\mathbf{v}_h) + \int_{\Gamma_\mathrm{N}} \mathbf{g}_\mathrm{N}\cdot\mathbf{v}_h,
$$

with

$\Sigma := C_\sigma A \mathtt{m}^2 \mathtt{h}^{-1}$ diagonal matrix of discontinuity-penalisation parameters,

$\mathcal{B} := 1/2\,\mathrm{diag}(|B_1\cdot\mathbf{n}|, \ldots, |B_n\cdot\mathbf{n}|)$.

Semidiscrete IPDG method

The symmetric IPDG in space method reads: find $\mathbf{u}_h \in L^2(0, T; S_h^{\mathbf{m}})$ such that

$$\langle (\mathbf{u}_h)_t, \mathbf{v}_h \rangle + B(\mathbf{u}_h; \mathbf{u}_h, \mathbf{v}_h) + \langle \mathbf{F}(\mathbf{u}_h), \mathbf{v}_h \rangle = l(\mathbf{v}_h), \quad \text{for all} \quad \mathbf{v}_h \in L^2(0, T; S_h^{\mathbf{m}}).$$

The method is analysed in the standard norms

$$L^\infty(0, T; L^2(\Omega)), \quad L^2(0, T; \mathcal{S}).$$

where on $\mathcal{S}$ the DG-norm

$$|||\mathbf{w}||| := \Big(\sum_{\kappa \in \mathcal{T}} \big(\|\sqrt{A}\nabla \mathbf{w}\|_\kappa^2 + \|\sqrt{D}\mathbf{w}\|_\kappa^2 \big) + \|\sqrt{\Sigma}[\![\mathbf{w}]\!]\|_{\Gamma_{\rm D}\cup\Gamma_{\rm int}}^2 + \|\sqrt{\mathcal{B}}[\![\mathbf{w}]\!]\|_{\Gamma\backslash\Gamma_{\rm tr}}^2 + \|\sqrt{\mathcal{B}^{\rm tr}}[\![\mathbf{w}]\!]\|_{\Gamma_{\rm tr}}^2 + \|[\![\mathbf{w}]\!]\|_{L^r(\Gamma_{\rm tr})}^r \Big)^{1/2}$$

is defined.

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$$+ \|\sqrt{\mathcal{B}}[\![\mathbf{w}]\!]\|_{\Gamma \setminus \Gamma_{\mathrm{tr}}}^2 + \|\sqrt{\mathcal{B}^{\mathrm{tr}}}[\![\mathbf{w}]\!]\|_{\Gamma_{\mathrm{tr}}}^2 + \|[\![\mathbf{w}]\!]\|_{L^r(\Gamma_{\mathrm{tr}})}^r \Big)^{1/2}$$

is defined.

A-priori error bounds

Theorem

Assume that A *is positive definite and that* $\gamma \in [0,1]$ *if* $d = 3$, $\mathbf{u} \in \mathcal{H}^1$ *and* $u|_\kappa \in H^1(0,T;[H^{k_\kappa+1}(\kappa)]^n)$, *and that the mesh* $\mathcal{T}_h$ *is fine enough. Then, we have*

$$\|\mathbf{e}\|^2_{L^\infty(0,T;L^2(\Omega))} + C\|\mathbf{e}\|^2_{L^2(0,T;\mathcal{S})} \leq \delta^2 \mathrm{e}^{\tilde{C}T},$$

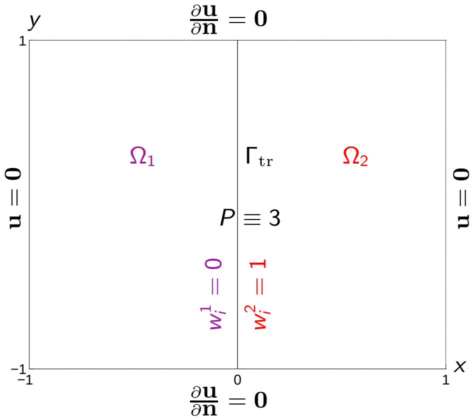
where

$$\delta^2 \leq C(\mathbf{u},A,\mathbf{B},\mathbf{F}) \int_0^T \sum_{\kappa\in\mathcal{T}} h_\kappa^{s_\kappa} \left(|\mathbf{u}|^2_{[H^{k_\kappa+1}(\kappa)]^n} + |\mathbf{u}|^2_{[H^{k_\kappa+1/2}(\Gamma_{\mathrm{tr}}\cap\bar{\kappa})]^n} + |\mathbf{u}_t|^2_{[H^{k_\kappa+1}(\kappa)]^n} \right),$$

for $1 \leq s_\kappa \leq \min\{m_\kappa, k_\kappa\}$.

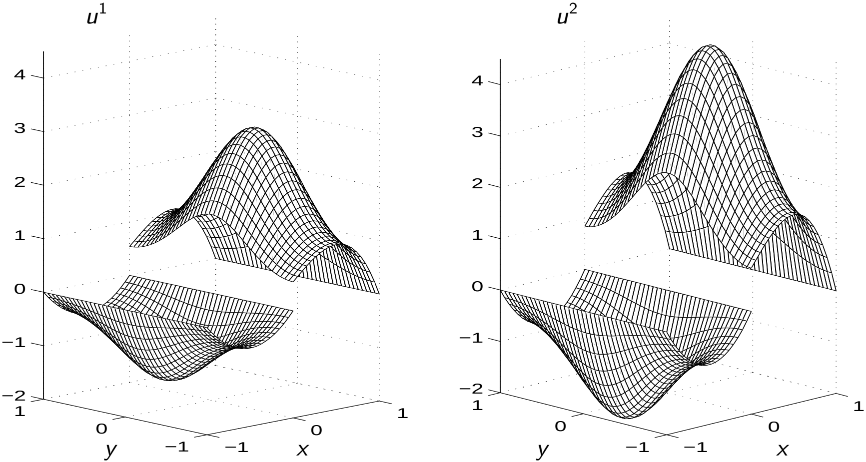
Remark. We do not require any mesh quasi-uniformity assumptions.

Numerical example ($d = 2$ $n = 2$)



$$\mathbf{u}_t - \Delta \mathbf{u} - \mathbf{u}_x = \mathbf{F}(x, y, t) + \begin{pmatrix} \overset{\Omega_1}{(u^1)^2 - u^2(1 - u^2)} & \Big| & \overset{\Omega_2}{-u^2} \\ u^1 & \Big| & u^1 \end{pmatrix}$$

Exact solution $(t = 1)$



$$\mathbf{u} = \begin{pmatrix} \cos t \\ \sin t \end{pmatrix} e^{(y^2-1)^2} \begin{cases} 4x(1+x) & \text{in } \Omega_1, \\ (-4x^3+3x+1) & \text{in } \Omega_2. \end{cases}$$

Convergence tables

# elements	# dofs	$L^2(0,T;\mathcal{S})$		$L^\infty(0,T;L^2(\Omega))$	
$m \equiv 1$					
16	128	7.620e+00	1.05	8.293e-01	-
64	512	3.617e+00	1.08	2.400e-01	1.79
256	2048	1.737e+00	1.06	6.497e-02	1.89
1024	8192	8.477e-01	1.03	1.693e-02	1.94
4096	32768	4.183e-01	1.02	4.323e-03	1.97
$m \equiv 2$					
16	288	1.014e+00	2.24	5.422e-02	-
64	1152	2.289e-01	2.15	8.367e-03	2.70
256	4608	5.529e-02	2.05	1.312e-03	2.67
1024	18432	1.389e-02	1.99	1.775e-04	2.89
4096	73728	3.792e-03	1.87	2.270e-05	2.97

Convection dominated scalar problem ($p = 1/2$, $w_1 = .9$, $w_2 = .1$)

$\varepsilon = 0.1$

$\varepsilon = 0.01$

$$\begin{cases} u_t - \varepsilon \Delta u + u_x = 0 \\ (\epsilon \nabla u - \chi^- u(1,0)) \cdot \mathbf{n}|_{\partial\Omega} = 0 \end{cases}$$

Coupling of parabolic and hyperbolic equations

C. & Natalini, J. of Theoretical Biology (to appear)

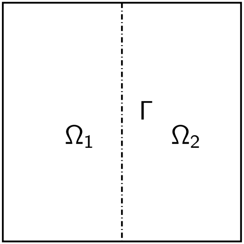
Lotka-Volterra System

We consider the system of two-equations

$$\begin{cases} (u_1)_t = 0.1\Delta u_1 + u_1(1 - 1.5u_2) \\ (u_2)_t = 0.1\Delta u_2 - u_2(1 - 1.5u_1) \end{cases}$$

in $\Omega_1 \cup \Omega_2$ with permeabilities

$$p_1 = 0.25$$
$$p_2 = 0.5$$



Lotka-Volterra reaction-diffusion system

Lotka-Volterra with $p_1 = .2, \quad p_2 = 20$

Numerical simulations - credits

- FEM code based on deal.II [Bangerth, Hartmann & Kanschat ('07)].
- Meshing Cubit (Sandia National Laboratories)
- Visualisation VisIt (Lawrence Livermore National Laboratory)

Special thanks to L. Heltai (the deal.II wizard) for his advice and to T. Leicht for granting us permission to use his hybrid deal.II.