Effective Boundary Conditions for 3-dimensional Optimally Aligned Coatings

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Coatings may be Anisotropic : anisotropy for TBC is caused by the fashions in which the ceramic "YSZ"(yttria-stabilized zirconia) is deposited on the blade :

(Picture taken from J.R. Nicholls K.J. Lawson, A. Johnstone, D.S. Rickerby, 2002)

Distribution of phytophthora root and collar rot of alders along main rivers and streams in Bavaria. The small map above shows the location of Bavaria within Germany.

(Picture taken from M. Blaschke and T. Jung, 2004)

Motivations : cell

Figure: E. coli cell; membrane thick and diameter ratio 1:500; red-headed molecules are phospholipids

 \leftarrow

Common features :

- Domain contains a thin component;
- Diffusion tensors on different components are drastically different. Issues :
	- The multi-scale in size and different diffusion tensors lead to computational difficulty ;
	- It is hard to see the effect of the thin component;

Resolution :

Think of the thin component as widthless surface and impose "effective boundary conditions"(EBCs).

- • In 1959, Carlaw and Jaeger, in their classic book *Conduction of* Heat in Solids, first derived EBCs formally ;
- In 1974, rigorous derivation was initiated by Sanchez-Palencia to study the "interior reinforcement problem" for elliptic and parabolic equations with a thin diamond-shaped inclusion layer ;
- In 1980, Brezis, Caffarelli and Friedman studied the elliptic problem in both interior and boundary reinforcement cases ;
- In 1987, Buttazo and Kohn studied the case of thin layer of oscillating thickness ;

 \bullet \cdot \cdot ;

Lots of follow-up work on elastic equations, electromagnetic equations, etc ;

Mathematical model

Figure – $\Omega = \Omega_1 \cup \overline{\Omega}_{\delta}$. The layer Ω_{δ} is uniformly thick with thickness δ and $\Gamma(=\partial\Omega_1)\in C^2$. Ω_1 is fixed and $\partial\Omega\to\Gamma$ as $\delta\to 0$.

Mathematical model

For any fixed and finite $T > 0$, consider

$$
\begin{cases}\nu_t - \nabla \cdot (A(x)\nabla u) = f(x,t), & (x,t) \in Q_T = \Omega \times (0,T), \\
u = 0, & (x,t) \in S_T = \partial\Omega \times (0,T), \\
u = u_0, & (x,t) \in \Omega \times \{0\}\n\end{cases}
$$
\n(1)

where Ω_1 is fixed, $u_0 \in L^2(\Omega)$ and $f \in L^2(Q_T)$. $A(x)$ is given by

$$
A(x) = \begin{cases} kI_{N \times N}, & x \in \Omega_1 \\ (a_{ij}(x))_{N \times N}, & x \in \Omega_\delta \end{cases}
$$
 (2)

where $k > 0$ and $(a_{ij})_{N \times N}$ is positive-definite. Moreover, u satisfies the transmission conditions in the weak sense

$$
u_1 = u_\delta, k \frac{\partial u_1}{\partial \mathbf{n}} = A(x) \nabla u_\delta \cdot \mathbf{n}
$$
 on $\partial \Omega_1$,

where **n** is the unit outer norm vector on $\partial\Omega_1$; u_1 and u_δ are the restrictions of u on $\Omega_1 \times (0,T)$ $\Omega_1 \times (0,T)$ and $\Omega_\delta \times (0,T)$. N \rightarrow \rightarrow \rightarrow \pm \rightarrow \rightarrow \rightarrow \pm \rightarrow \rightarrow \in \sim

Optimally Aligned Coatings

Figure – $\Omega = \Omega_1 \cup \overline{\Omega}_\delta$.

- The notion of optimally aligned coatings¹ is motivated by applications in physics, ecology and cell.
- Optimally aligned coatings : for any $x \in \Omega_{\delta}$, the normal vector $\mathbf{n}(p)$ is always an eigenvector of $A(x)$.

1. S. Rosencrans and X. Wang, SIAM J. Appl. Math[, 2](#page-8-0)[006](#page-10-0) Xingri Geng (SUSTech) [Effective boundary conditions](#page-0-0) $\frac{1}{2}$ 10 / 29

Curvilinear coordinates

Figure – An illustration of the curvilinear coordinates (p, r) .

In the curvilinear coordinates (p, r) ,

$$
x = p + r \mathbf{n}(p), \quad \forall x \in \Omega_{\delta},
$$

p– projection of x onto $\partial\Omega_1$; r– distance from x to $\partial\Omega_1$.

Curvilinear coordinates Coatings in 3D

There are two assumptions of $A(x)$ in Ω_{δ} .

• Case 1. $A(x)$ has two identical eigenvalues in the tangent directions, i.e.,

$$
A(x)\mathbf{n}(p) = \sigma \mathbf{n}(p), \quad A(x)\mathbf{s}(p) = \mu \mathbf{s}(p), \tag{3}
$$

where p is the unique projection of x on $\partial\Omega_1$, and $s(p)$ is an arbitrary tangent vector at p on $\partial\Omega_1$; $(\sigma, \mu) = (\sigma(\delta), \mu(\delta))$ are two corresponding eigenvalues.

• Case 2. $A(x)$ has two different eigenvalues in the tangent directions, namely, $\partial \Omega_1 = \Gamma_1 \times \Gamma_2$, and $A(x)$ satisfies

$$
A(x)\mathbf{n}(p) = \sigma \mathbf{n}(p),
$$

\n
$$
A(x)\boldsymbol{\tau}_1(p) = \mu_1 \boldsymbol{\tau}_1(p),
$$

\n
$$
A(x)\boldsymbol{\tau}_2(p) = \mu_2 \boldsymbol{\tau}_2(p),
$$
\n(4)

 $12/29$

where τ_1, τ_2 are two orthonormal eigenvectors of $A(x)$ in the tangent plane. n[a](#page-10-0)[nka](#page-11-0)[i](#page-12-0) [Un](#page-9-0)[i](#page-10-0)[ve](#page-26-0)[rs](#page-27-0)[it](#page-9-0)[y,](#page-10-0)[Ti](#page-27-0)[anji](#page-0-0)[ng](#page-28-0) December 2, 2023

Theorem

Assume $A(x)$ is given by [\(2\)](#page-8-1) and [\(3\)](#page-11-1). Suppose

$$
\lim_{\delta \to 0} \frac{\sigma}{\delta} = \alpha \in [0, \infty] \text{ and } \lim_{\delta \to 0} \sigma \mu = \gamma \in [0, \infty].
$$

If u is the weak solution of [\(1\)](#page-8-2), then as $\delta \to 0$, $u \to v$ strongly in $C([0,T];L^2(\Omega))$, where v is the weak solution of the effective equation:

$$
\begin{cases}\nv_t - k\Delta v = f(x, t), & (x, t) \in \Omega_1 \times (0, T), \\
v(x, 0) = u_0, & x \in \partial\Omega_1,\n\end{cases}
$$
\n(5)

Case 1

Theorem

subject to the EBCs on $\partial\Omega_1 \times (0,T)$:

Remarks :

- $\triangledown_{\Gamma} v = 0$ means v is a constant in x but may depend on t;
- \mathcal{J}_D^H is the Dirichlet-to-Neumann mapping;
- \mathcal{J}_D^∞ is the fractional Laplacian.

In particular, for smooth g defined on $\partial\Omega_1$, and $H \in (0,\infty)$,

$$
\mathcal{J}_D^H[g] := \Psi_R(s,0),\tag{6}
$$

where Ψ is the solution of

$$
\begin{cases}\n\Psi_{RR} + \Delta_{\Gamma}\Psi = 0, & \partial\Omega_1 \times (0, H), \\
\Psi(s, 0) = g(s), & \Psi(s, H) = 0.\n\end{cases}
$$
\n(7)

Moreover, \mathcal{J}_D^H is linear and symmetric, and its explicit formula can be given in eigenfunctions of the Laplace-Beltrami operator $-\Delta_{\Gamma}$, from which

$$
\mathcal{J}_D^{\infty} = \lim_{H \to \infty} \mathcal{J}_D^H = -(-\Delta_{\Gamma})^{1/2}.
$$
 (8)

Definition

We say that u is a weak solution of [\(1\)](#page-8-2), if $u(x,t) \in V_{2,0}^{1,0}$ $^{71,0}_{2,0}(Q_T)$ and it holds that

$$
\mathcal{A}[u,\xi]
$$

= $-\int_{\Omega} u_0(x)\xi(x,0)dx + \int_{Q_T} (A(x)\nabla u) \cdot \nabla \xi - u\xi_t - f\xi dt dx$ (9)
=0

for any $\xi \in W^{1,1}_{2,0}$ $2.0^{1,1}_{2,0}(Q_T)$ satisfying $\xi = 0$ at $t = T$.

Lemma (First order estimates)

$$
(i) \max_{t \in [0,T]} \int_{\Omega} u^2(x,t)dx + \int_{Q_T} \nabla u \cdot A(x) \nabla u dx dt
$$

\n
$$
\leq C(T) \left(\int_{\Omega} u_0^2 dx + \int_{Q_T} f^2 dx dt \right);
$$

\n
$$
(ii) \max_{t \in [0,T]} t \int_{\Omega} \nabla u \cdot A(x) \nabla u(x,t) dx + \int_{Q_T} tu_t^2 dx dt
$$

\n
$$
\leq C(T) \left(\int_{\Omega} u_0^2 dx + \int_{Q_T} f^2 dx dt \right).
$$
\n(10)

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Lemma (Second order estimates)

Suppose $\Gamma \in C^3$ and $f \in L^2(Q_T)$ with $u_0 \in L^2(\Omega)$. Then, for any fixed $t_0 > 0$, the weak solution u of [\(1\)](#page-8-2) satisfies the following inequalities :

$$
\int_{t_0}^{T} \int_{\Omega_\delta} \mu (\Delta_{\Gamma} u)^2 + \sigma (\nabla_{\Gamma} u_r)^2 \le O(1) + O(\frac{\sigma}{\mu}) + O(\frac{1}{\mu}).\tag{11}
$$

Lemma (Higher order estimates)

Let $m \geq 2$ be an integer and $\alpha \in (0,1)$. Suppose that $\partial \Omega_1 \in C^{m+\alpha}$ and $f \in C^{m-2+\alpha,(m-2+\alpha)/2}(\overline{\Omega}_h \times [0,T])$ $(h = 1, \delta, 2)$, and $a_{ij} \in C^{m-1+\alpha,(m-1+\alpha)/2}(\overline{\Omega}_h\times [0,T]), \text{ then for any }t_0>0, \text{ the weak}$ solution u of [\(1\)](#page-8-2) satisfies

$$
u \in C^{m+\alpha, (m+\alpha)/2)}(\overline{\mathcal{N}}_h \times [t_0, T])
$$

where [N](#page-18-0) is a narrow neig[h](#page-18-0)borhood of $\partial\Omega_1$ and $\mathcal{N}_h = \mathcal{N} \cap \Omega_h$ $\mathcal{N}_h = \mathcal{N} \cap \Omega_h$ $\mathcal{N}_h = \mathcal{N} \cap \Omega_h$. Na[nkai](#page-17-0) U[ni](#page-10-0)[ve](#page-26-0)[rs](#page-27-0)[it](#page-9-0)[y,](#page-10-0)[Ti](#page-27-0)[anji](#page-0-0)[ng](#page-28-0) Decem Main Steps :

- \bullet Step 1. Existence and uniqueness of weak solution of (1) ;
- Step 2. Energy estimates of the weak solution of [\(1\)](#page-8-2) and prove $u \to v$ strongly in $C([0,T]; L^2(\Omega))$ as $\delta \to 0$;
- Step 3. Show that v is the weak solution of [\(5\)](#page-12-1) with related EBCs;
	- Harmonic extension²: construct a test function such that $\overline{\xi}(s, r, t) = \psi(s, r, t)$ in $\overline{\Omega}_{\delta}$,

$$
\begin{cases}\n\sigma\psi_{rr} + \mu\Delta_{\Gamma}\psi = 0, & \Gamma \times (0,\delta), \\
\psi(s,0,t) = \xi(s,0,t) & \psi(s,\delta,t) = 0\n\end{cases}
$$
\n(12)

- By rescaling, $\Psi(s, R) = \psi(s, \sqrt{\mu/\sigma}r, t)$
- Step 4. Existence and uniqueness of the weak solution of the effective equation [\(5\)](#page-12-1) with related EBCs ;

EBCs in 3D

Similarly, if the layer is of interior inclusion, denote

$$
A(x) = \begin{cases} k_1, & x \in \Omega_1 \\ (a_{ij})_{N \times N}, & x \in \Omega_\delta \\ k_2, & x \in \Omega_2 \end{cases}
$$

where k_1 and k_2 are two positive constants independent of $\delta > 0$.

Figure – $\Omega = \Omega_1 \cup \overline{\Omega}_\delta \cup \Omega_2$. Ω and Ω_1 are fixed with $\Gamma_1 \in C^2$.

EBCs in 3D

Denote

$$
A_0(x) = \begin{cases} k_1, & x \in \Omega_1, \\ k_2, & x \in \Omega \backslash \overline{\Omega}_1. \end{cases}
$$

Suppose $\Gamma_1 \in C^2$, and

$$
\lim_{\delta \to 0} \frac{\sigma}{\delta} = b \in [0, \infty], \lim_{\delta \to 0} \sigma\mu = \gamma \in [0, \infty], \lim_{\delta \to 0} \mu\delta = \beta \in [0, \infty].
$$

As $\delta \to 0$, $u \to v$ strongly in $C([0,T]; L^2(\Omega))$, where v is the weak solution of

$$
\begin{cases}\nv_t - \nabla \cdot (A_0(x)\nabla v) = f(x,t), & (x,t) \in Q_T, \\
v = 0, & (x,t) \in S_T, \\
v = u_0, & x \in \Omega, t = 0,\n\end{cases}
$$

subject to the effective boundary conditions on $\Gamma_1 \times (0,T)$:

EBCs for interior inclusion in 3D

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EBCs for interior inclusion in 3D

Remarks :

- $\sigma \delta^3 \to 0$ can be removed if $\frac{\mu}{\sigma}$ does not vanish as $\delta \to 0$;
- $\nabla_{\Gamma_1} v = 0$ means v is a constant in x but may depend on t;
- Δ_{Γ_1} is the Laplacian-Beltrami operator;
- \mathcal{J}_1^H , \mathcal{J}_2^H and \mathcal{J}^H are Dirichlet-to-Neumann mappings that can be defined as \mathcal{J}_D^H ;

•
$$
\mathcal{J}_1^{\infty} = \mathcal{J}^{\infty} = -(-\Delta_{\Gamma_1})^{1/2}
$$
 and $\mathcal{J}_2^{\infty} = 0$.

EBCs for 3-dimensional optimally aligned coatings Case 2

Theorem

Suppose that Γ is a topological torus and $A(x)$ is given in [\(2\)](#page-8-1) and satisfies [\(4\)](#page-11-2). Let $u_0 \in L^2(\Omega)$ and $f \in L^2(Q_T)$ with functions being independent of δ . Assume further that without loss of generality, $\mu_1 > \mu_2$. Moreover, σ, μ_1 , and μ_2 satisfy

$$
\lim_{\delta \to 0} \frac{\mu_2}{\mu_1} = c \in [0, 1], \quad \lim_{\delta \to 0} \frac{\sigma}{\delta} = \alpha \in [0, 1],
$$

$$
\lim_{\delta \to 0} \sigma \mu_i = \gamma_i \in [0, \infty], \quad \lim_{\delta \to 0} \mu_i \delta = \beta_i \in [0, \infty], \quad i = 1, 2.
$$

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Case 2

Theorem

(i) If $c \in (0,1]$, then as $\delta \to 0$, $u \to v$ weakly in $W_2^{1,0}$ $i_{2}^{1,0}(\Omega_{1}\times(0,T)),$ strongly in $C([0,T];L^2(\Omega_1))$, where v is the weak solution of [\(5\)](#page-12-1) subject to the effective boundary conditions :

Figure – $EBCs$ on $\partial\Omega_1$ for $c=0$

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EBCs in 3D

Case 2

Theorem

(*ii*) If $c = 0$ and $\lim_{\delta \to 0} \delta^2 \mu_1/\mu_2 = 0$, then $u \to v$ weakly in

 $W^{1,0}_2$ $2^{(1,0)}(\Omega_1\times(0,T))$, strongly in $C([0,T];L^2(\Omega_1))$, where v is the weak solution of [\(5\)](#page-12-1) subject to the effective boundary conditions :

Figure – EBCs on $\partial\Omega_1 \times (0,T)$ for $c=0$

Exotic EBCs

 $\mathcal{K}_D^H[g](s) := \Phi_R(s,0)$, where Φ is the unique bounded solution of

$$
\begin{cases} \Phi_{RR} + \Phi_{s_1s_1} + c\Phi_{s_2s_2} = 0, & \Gamma \times (0, H), \\ \Phi(s, 0) = g(s), & \Phi(s, H) = 0. \end{cases}
$$

 $\Lambda_D^H[g](s) := \Phi_R^0(s,0)$, where Φ^0 is the unique bounded solution of

$$
\begin{cases} \Phi_{RR}^0 + \Phi_{s_1s_1}^0 = 0, & \Gamma \times (0, H), \\ \Phi^0(s, 0) = g(s), & \Phi^0(s, H) = 0. \end{cases}
$$

 $\mathcal{D}_{D}^{H}[g](s_2) := \Phi_R(s_2, 0)$, where $\Phi(s_2, R)$ is the bounded solution of

$$
\begin{cases} \Phi_{RR} + \Phi_{s_2 s_2} = 0, & \Gamma_2 \times (0, H), \\ \Phi(s_2, 0) = g(s_2), & \Phi(s_2, H) = 0. \end{cases}
$$

Ongoing Work

It is natural to find the EBC involving the fractional Laplacian of any order.

• Suppose

$$
A(x)\mathbf{n}(p) = \sigma d(x)^a \mathbf{n}(p),
$$

$$
A(x)\mathbf{s}(p) = \mu d(x)^a \mathbf{s}(p),
$$

where a is a constant; $d(x)$ is the distance of x onto $\partial\Omega$; p is the unique projection of x on $\partial\Omega$, and $s(p)$ is an arbitrary tangent vector at p on $\partial\Omega$.

Figure – $\Omega = \Omega_1 \cup \overline{\Omega}_{\delta}$. Ω and Ω are fixed.

THANK YOU !