<span id="page-0-0"></span>Effective Boundary Conditions for the Heat Equation with Three-dimensional Anisotropic and Optimally Aligned Coatings

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# <span id="page-1-0"></span>**[Motivations](#page-2-0)**

# **[History](#page-6-0)**

- 3 [Mathematical model](#page-7-0)
- 4 [Interior Inclusion](#page-10-0)
- 5 [Boundary Coating](#page-24-0)

# 6 [Ongoing Work](#page-29-0)

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# <span id="page-2-0"></span>Motivations : cell



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

 $\leftarrow$ 

<span id="page-3-0"></span>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 :

# <span id="page-4-0"></span>TBC

If YSZ is sprayed on by electron beam physical vapor deposition (EB-PVD) method, then parallel crystal columns that are perpendicular to the boundary form ; and between these columns a small volume fraction of elongated pores also form. (Picture taken from J.R. Nicholls K.J. Lawson, A. Johnstone, D.S. Rickerby)



<span id="page-5-0"></span>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).

- <span id="page-6-0"></span>As early as 1959, Carlaw and Jaeger, in their classic book Conduction of Heat in Solids, first derived EBCs formally ;
- Rigorous derivation was initiated by Sanchez-Palencia in 1974, to study Laplace equation and the heat equation with thin diamond-shaped inclusions ;
- In 1980, Brezis, Caffarelli and Friedman studied the case of Poisson equation ;
- In 1987, Buttazo and Kohn studied the case of thin layer of oscillating thickness ;
- Lots of follow-up work on elastic equations, electromagnetic equations, etc ;

# <span id="page-7-0"></span>Mathematical model



**Fig. 1.** The domain  $\Omega = \overline{\Omega}_1 \cup \Omega_2 \subset \mathbb{R}^N$  consists of an isotropic body  $\Omega_1$  surrounded by a layer  $\Omega_2$  of uniform thickness  $\delta$ 

4 0 3

# <span id="page-8-0"></span>Mathematical model

For any fixed  $T > 0$ ,

<span id="page-8-1"></span>
$$
\begin{cases}\nu_t - \nabla \cdot (A(x)\nabla u) = f(x,t), & (x,t) \in Q_T = \Omega \times (0,T), \\
u = 0, & (x,t) \in S_T = \partial\Omega \times (0,T), \\
u = u_0, & (x,t) \in \Omega \times \{0\}\n\end{cases}
$$
\n(1)

where  $\Omega_1$  is fixed,  $u_0 \in L^2(\Omega)$  and  $f \in L^2(Q_T)$ .  $A(x)$  is given by

$$
A(x) = \begin{cases} kI_{N \times N}, & x \in \Omega_1 \\ (a_{ij}(x))_{N \times N}, & x \in \Omega_2 \end{cases}
$$
 (2)

where k is a positive constant and  $(a_{ij})_{N\times N}$  is positive-definite. Moreover, u satisfies

$$
u_1 = u_2, \ k \frac{\partial u_1}{\partial \mathbf{n}} = A(x) \nabla u_2 \cdot \mathbf{n}
$$
 on  $\partial \Omega_1$ ,

where  $\mathbf{n} = (n_1, ..., n_N)$  is the unit outer norm [ve](#page-7-0)[cto](#page-9-0)r on  $\partial \Omega_1$ .

# <span id="page-9-0"></span>Results by Li, Rosencrans, Zhang and Wang <sup>1</sup>

- Suppose  $a_{ij}(x) = \sigma(\overline{a}_{ij}(x))$  with  $\overline{a}_{ij}(x) \in C^1(\overline{\Omega}_2)$  and  $\sigma(\delta)$  is a positive parameter.
- If  $\sigma$  is bounded and  $\lim_{\delta \to 0} \frac{\sigma}{\delta} = \alpha$ , then  $u \to v$  in  $L^2(\Omega_1 \times [0, T]),$ where  $v$  is the weak solution of

$$
\begin{cases}\nv_t - k\Delta v = f(x, t), & (x, t) \in Q_T, \\
k\frac{\partial v}{\partial \mathbf{n}} + \alpha(\sum_{i,j} \overline{a}_{ij}(x)n_i n_j)v = 0, & (x, t) \in S_T, \\
v = u_0, & x \in \Omega, t = 0\n\end{cases}
$$
\n(3)

A nature question : what is the effective boundary condition if  $\sigma \to \infty$  as  $\delta \to 0$ ?

1. J. Li, S. Rosencrans, K. Zhang, and X. Wang, 200[9,](#page-8-0)  $\text{Proc}_{\mathcal{A}}\text{AMS} \longrightarrow \text{Rec} \longrightarrow \text{Rec}$  $\text{Proc}_{\mathcal{A}}\text{AMS} \longrightarrow \text{Rec} \longrightarrow \text{Rec}$ Xingri Geng (NUS) [Effective boundary conditions](#page-0-0) 10 / 31

# <span id="page-10-0"></span>Interior Inclusion in 3D



Figure.1:  $\Omega = \overline{\Omega}_1 \cup \overline{\Omega}_\delta \cup \Omega_2$ .

Let

$$
A(x) = \begin{cases} k_1, & x \in \Omega_1 \\ (a_{ij})_{3 \times 3}, & x \in \Omega_\delta \\ k_2, & x \in \Omega_2 \end{cases}
$$

where  $k_1$  and  $k_2$  are two positive constants independent of  $\delta > 0$ ;  $\sigma$  is a positive function of  $\delta$ ;  $\Omega$  and  $\Omega_1$  are fixed with  $\Gamma_1 \in C^2$ .

# <span id="page-11-0"></span>Optimally aligned condition



Optimally aligned coating <sup>2</sup> : for any  $x \in \Omega_{\delta}$ ,  $\mathbf{n}(p)$  is always an eigenvector. In the curvilinear coordinates  $(s, r)$ ,  $x = p + r \mathbf{n}(p) \in \Omega_{\delta}$ , suppose

<span id="page-11-1"></span>
$$
A(x)\mathbf{n}(p) = \sigma \mathbf{n}(p), \quad A(x)\mathbf{s}(p) = \mu \mathbf{s}(p), \tag{4}
$$

where **p**− the projection of x on  $\Gamma_1 = \partial \Omega_1$ ; r− distance from x to  $\Gamma_1$ ;  $s(p)$  is an arbitrary tangent vector at p on  $\partial\Omega_1$ .

2. S. Rosencrans, and X. Wang, SIAM J. Appl. Mat[h,](#page-10-0) 2[00](#page-12-0)[6](#page-10-0)  $\sigma$ Xingri Geng (NUS) [Effective boundary conditions](#page-0-0)  $SO(2)$  is  $1 \leq i \leq n$  in  $2 \leq i \leq n$ 12 / 31

<span id="page-12-0"></span>
$$
W_2^{1,0}(Q_T) = \{u \in L^2(Q_T) : \nabla u \in L^2(Q_T)\};
$$
  
\n
$$
W_{2,0}^{1,0}(Q_T) = \{u \in W_2^{1,0}(Q_T) : \text{ with trace } 0 \text{ on } S_T\};
$$
  
\n
$$
W_2^{1,1}(Q_T) = \{u \in L^2(Q_T) : u_t, \nabla u \in L^2(Q_T)\};
$$
  
\n
$$
W_{2,0}^{1,1}(Q_T) = \{u \in W_2^{1,1}(Q_T) : \text{ with trace } 0 \text{ on } S_T\};
$$
  
\n
$$
V_2^{1,0}(Q_T) = \{u \in W_2^{1,0}(Q_T) : u \in C([0,T], L^2(\Omega)\};
$$
  
\n
$$
V_{2,0}^{1,0}(Q_T) = \{u \in V_2^{1,0}(Q_T) : \text{ with trace } 0 \text{ on } S_T\};
$$

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#### <span id="page-13-0"></span>Definition

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

$$
\mathcal{A}[u,\xi]
$$
  
=  $-\int_{\Omega} u_0(x)\xi(x,0)dx + \int_{Q_T} (A(x)\nabla u) \cdot \nabla \xi - u\xi_t - f\xi dt dx$  (5)  
=0

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

#### <span id="page-14-0"></span>Lemma

$$
(i) \max_{t \in [0,T]} \int_{\Omega} u^2(x,t)dx + \int_{Q_T} \nabla u \cdot A(x) \nabla u dx dt
$$
  
\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(6)

#### <span id="page-15-0"></span>Lemma (2)

Suppose  $\Gamma_1 \in C^3$  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-8-1) satisfies the following inequalities :

$$
\int_{t_0}^{T} \int_{\Omega_{\delta}} \mu (\Delta_{\Gamma} u)^2 + \sigma (\nabla_{\Gamma} u_r)^2 \le O(1) + O(\frac{\sigma}{\mu}) + O(\frac{1}{\mu}) \tag{7}
$$

and

$$
\int_{t_0}^{T} \int_{\Omega_{\delta}} \sigma u_{rr}^2 \le O(1) + O(\frac{1}{\sigma}) + O(\frac{\mu}{\sigma})
$$
\n(8)

16 / 31

#### <span id="page-16-0"></span>Theorem (X.Chen, C.Pond and X.Wang)

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-8-1) satisfies

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

where N is a narrow neighborhood of  $\partial\Omega_1$  and  $\mathcal{N}_h = \mathcal{N} \cap \Omega_h$ .

3. X.Chen, C.Pond and X.Wang, Arch.Ration.Mech.[An](#page-15-0)[al.\(](#page-17-0)[2](#page-15-0)[01](#page-16-0)[2\)](#page-17-0) Xingri Geng (NUS) [Effective boundary conditions](#page-0-0)  $S$   $\left(\frac{20 \text{ Hz}}{20 \text{ Hz}}\right)$   $\left(\frac{20 \text{ Hz}}{20 \text{ Hz}}\right)$   $\left(\frac{20 \text{ Hz}}{20 \text{ Hz}}\right)$ 17 / 31

# <span id="page-17-0"></span>Main results

## Theorem (Geng)

<sup>a</sup> Denote  $A_0(x) = k_1, x \in \Omega_1$  and  $A_0 = k_2, x \in \Omega \setminus \overline{\Omega}_1$ . Suppose  $\Gamma_1 \in C^3$ 

$$
\lim_{\delta \to 0} \frac{\sigma}{\delta} = b \in [0, \infty], \quad \lim_{\delta \to 0} \sigma \delta = a \in [0, \infty],
$$
  
\n
$$
\lim_{\delta \to 0} \sigma \mu = \gamma \in [0, \infty], \quad \lim_{\delta \to 0} \mu \delta = \beta \in [0, \infty].
$$
\n(9)

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

<span id="page-17-1"></span>
$$
\begin{cases}\nv_t - \nabla \cdot (A_0(x)\nabla v) = f(x,t), & (x,t) \in Q_T, \\
v = 0, & (x,t) \in S_T, \\
v = u_0, & x \in \Omega, t = 0,\n\end{cases}
$$
\n(10)

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

a. Xingri Geng, submitted

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# <span id="page-18-0"></span>Main results

## Theorem (Geng)



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# <span id="page-19-0"></span>Theorem (Geng)



#### <span id="page-20-0"></span>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;
- $\Delta_{\Gamma_1}$  is the Laplacian-Beltrami;
- $\mathcal{J}^H$  is called Dirichlet-to-Neumann map;
- Lots of new and exotic EBCs emerge, including the fractional Laplacian-Beltrami and the Dirichlet-to-Neumann mapping.

<span id="page-21-0"></span>Let  $q(s)$  be a function on  $\partial\Omega_1$  and  $\Psi$  is defined by

$$
\begin{cases}\n\Psi_{RR} + \Delta_{\Gamma}\Psi = 0, & \partial\Omega_1 \times (0, H), \\
\Psi(s, 0) = g(s), & \Psi(s, H) = g(s).\n\end{cases}
$$
\n(11)

Moreover,

$$
\mathcal{J}^H[g] := \Psi_R(s,0),\tag{12}
$$

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where  $\mathcal{J}^H$  is symmetric for  $H \in (0, \infty)$  and

$$
\mathcal{J}^{\infty} = \lim_{H \to \infty} \mathcal{J}^H = -(-\Delta_{\Gamma_1})^{1/2}.
$$
 (13)

 $\mathcal{J}^H$  can be given in eigenfunctions of the Laplace-Beltrami operator.

#### <span id="page-22-0"></span>Theorem (Isotropic case)

(i) If  $\lim_{\delta \to 0} \frac{\sigma}{\delta} = b \in [0, \infty]$  and  $\sigma \to 0$ , then

$$
k_1 \frac{\partial v_1}{\partial n} = b(v_1 - v_2), \quad k_1 \frac{\partial v_1}{\partial n} = k_2 \frac{\partial v_2}{\partial n}.
$$

(ii)If  $\lim_{\delta \to 0} \sigma \delta = a \in [0, \infty)$  and  $\sigma \ge O(1) > 0$ , then

$$
v_1 = v_2, \quad k_1 \frac{\partial v_1}{\partial n} - k_2 \frac{\partial v_2}{\partial n} = a \Delta_{\Gamma_1} v.
$$

(iii) If  $\lim_{\delta \to 0} \sigma \delta = \infty$ , then

$$
v_1 = v_2, \quad \nabla_{\Gamma_1} v = 0, \quad \int_{\Gamma_1} (k_1 \frac{\partial v_1}{\partial n} - k_2 \frac{\partial v_2}{\partial n}) ds = 0,
$$

where  $v_1$  and  $v_2$  are the restrictions of v on  $\Omega_1 \times (0,T)$  and  $(\Omega \backslash \Omega_1) \times (0,T)$ , respectively. [S](#page-23-0)[ci](#page-21-0)[CA](#page-22-0)[D](#page-23-0)[E](#page-9-0)[,](#page-10-0) [U](#page-23-0)[ni](#page-24-0)[v](#page-9-0)[er](#page-10-0)[si](#page-23-0)[ty](#page-24-0) [of](#page-0-0) [Icel](#page-30-0)and, R

<span id="page-23-0"></span>Main Steps :

- Step 1 : existence and uniqueness of weak solution of  $(1)$ ;
- Step 2 : energy estimates of the weak solution of [\(1\)](#page-8-1) and prove  $u \to v$  strongly in  $C([0,T]; L^2(\Omega))$  as  $\delta \to 0$ ;
- Step 3 : show that  $v$  is the exact weak solution of [\(10\)](#page-17-1) with related EBCs ;
	- Construct a test function such that  $\overline{\xi}(s, r, t) = \psi(s, r, t)$  in  $\Omega_{\delta}$ ,

$$
\begin{cases}\n\sigma\psi_{rr} + \mu\Delta_{\Gamma}\psi = 0, & \Gamma_1 \times (0,\delta), \\
\psi(s,0,t) = g_1(s) & \psi(s,\delta,t) = g_2(s)\n\end{cases}
$$
\n(14)

- 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 [\(10\)](#page-17-1) with related EBCs ;

## <span id="page-24-0"></span>Boundary layers Two identical tangent thermal conductivity



Fig. 1. The domain  $\Omega = \overline{\Omega}_1 \cup \Omega_2 \subset \mathbb{R}^N$  consists of an isotropic body  $\Omega_1$  surrounded by a layer  $\Omega_2$  of uniform thickness  $\delta$ 

#### Theorem (Boundary case)

<sup>a</sup> Suppose  $A(x)$  is given by [\(4\)](#page-11-1). If u is the weak solution of [\(1\)](#page-8-1), 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(15)

a. Xingri Geng, Submitted

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#### <span id="page-25-0"></span>Theorem (Boundary case)

subject to the following effective boundary conditions :



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<span id="page-26-0"></span>Assume  $\partial\Omega_1$  is a topological torus, namely,  $\partial\Omega_1 = \Gamma_1 \times \Gamma_2$ , and  $A(x)$ satisfies

$$
A(x)\mathbf{n}(p) = \sigma \mathbf{n}(p),
$$
  
\n
$$
A(x)\mathbf{t}_1(p) = \mu_1 \mathbf{t}_1(p),
$$
  
\n
$$
A(x)\mathbf{t}_2(p) = \mu_2 \mathbf{t}_2(p),
$$
\n(16)

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where  $t_1, t_2$  are two orthonormal eigenvectors of  $A(x)$  in the tangent plane. WOLG, suppose  $\mu_1 > \mu_2$  and  $\frac{\mu_2}{\mu_1} \to c \in [0, 1]$ .

- If  $c \in (0, 1]$ , EBCs are similar as above;
- If  $c = 0$  with  $\frac{\mu_2/\mu_1}{\delta^2} \to 0$ , new results arise.

<span id="page-27-0"></span>

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



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

<span id="page-28-0"></span>For  $H \in (0, \infty)$ ,  $\Lambda_D^H[g] := \Phi_R(s, 0)$  and  $\Lambda_D^{\infty} := \lim_{H \to \infty} \Lambda_D^H$ , where  $\Phi(s, R)$ is the bounded solution of

$$
\begin{cases}\n\Phi_{RR} + \Phi_{s_1s_1} = 0, & \partial\Omega_1 \times (0, H), \\
\Phi(s, 0) = g(s), & \Phi(s, H) = 0.\n\end{cases}
$$
\n(17)

Moreover,  $\mathcal{D}_D^H[g] := \Psi_R(s_2, 0)$  and  $\mathcal{D}_D^{\infty} := \lim_{H \to \infty} \mathcal{D}_D^H$ , where  $\Psi(s_2, R)$  is the bounded solution of

$$
\begin{cases} \Psi_{RR} + \Psi_{s_2 s_2} = 0, & \Gamma_2 \times (0, H), \\ \Psi(s_2, 0) = g(s_2), & \Psi(s_2, H) = 0. \end{cases}
$$
\n(18)

<span id="page-29-0"></span>

Use the idea of EBCs to derive new model for other nonlinear equations such as the Fisher-KPP equation and reaction diffusion systems.

# <span id="page-30-0"></span>THANK YOU !