Géométrie différentielle indépendante de tout système des coordonnées : application à la modélisation des interfaces imparfaites dans un contexte multi-physique

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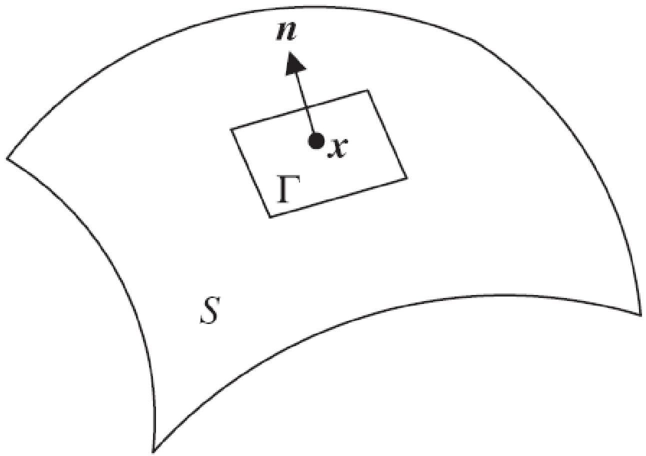
Part I

Elements of a coordinate-free differential geometry theory

• **With no loss of generality, a curved surface can be characterized as the zero level-set of a scalar-value function g:**

$$S = \{\boldsymbol{x} \in \mathbb{R}^3 \mid g(\boldsymbol{x}) = 0\}$$



• **Unit normal vector**

$$\boldsymbol{n}(\boldsymbol{x}) = \frac{\nabla g(\boldsymbol{x})}{\| \nabla g(\boldsymbol{x}) \|}$$

• **Second-order projection tensors**

$$\boldsymbol{N}(\boldsymbol{x}) = \boldsymbol{n}(\boldsymbol{x}) \otimes \boldsymbol{n}(\boldsymbol{x}),$$

$$\boldsymbol{T}(\boldsymbol{x}) = \boldsymbol{I} - \boldsymbol{N}(\boldsymbol{x}),$$

Remark: The implicit desciption of a curved surface is *strictly equivalent* to its usual parametrical description from the standpoint of differential geometry owing to the implicit function theorem.

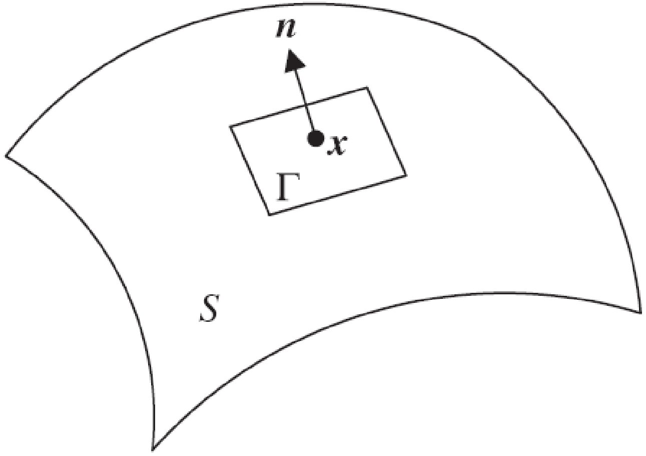
- **Weingarten's curvature tensor**

$$\boldsymbol{W} = -\nabla_s \boldsymbol{n} = -\nabla \boldsymbol{n} \cdot \boldsymbol{T} = \boldsymbol{T} \cdot \frac{(\nabla \otimes \nabla) g}{\| \nabla g \|} \cdot \boldsymbol{T}$$

- **Average and Gaussian curvatures**

$$H = tr(\mathbf{W})/2 = -(\mathrm{div}_s\, \boldsymbol{n})/2$$

$$K = \det \boldsymbol{W}$$



- Decomposition of the gradient of a scalar-valued function

$$\nabla\varphi = \nabla_N\varphi + \nabla_s\varphi, \quad \nabla_N\varphi = \boldsymbol{N}\nabla\varphi = (\nabla_n\varphi)\boldsymbol{n}, \quad \nabla_s\varphi = \boldsymbol{T}\nabla\varphi,$$

- Decomposition of the gradient of a vector-valued function

$$\nabla\mathbf{g} = \nabla_N\mathbf{g} + \nabla_s\mathbf{g}, \quad \nabla_N\mathbf{g} = (\nabla\mathbf{g})\boldsymbol{N}, \quad \nabla_s\mathbf{g} = (\nabla\mathbf{g})\boldsymbol{T}.$$

- Decomposition of the divergence of a vector-valued function

$$div\mathbf{g} = div_N\mathbf{g} + div_s\mathbf{g}, \quad div_N\mathbf{g} = \nabla\mathbf{g} : \boldsymbol{N}, \quad div_s\mathbf{g} = \nabla\mathbf{g} : \boldsymbol{T}.$$

- **Hadamard's relations** for **piecewise continuously differentiable** scalar- and vector-valued functions

$$\nabla\varphi^{(2)} - \nabla\varphi^{(1)} = \eta\boldsymbol{n} \quad \text{on } S,$$

$$\nabla\mathbf{g}^{(2)} - \nabla\mathbf{g}^{(1)} = \boldsymbol{a}\otimes\boldsymbol{n} \quad \text{on } S,$$

- **Important implications of Hadamard's relations**

$$\nabla_s\varphi^{(1)} = \nabla_s\varphi^{(2)} \quad \text{on } S$$

$$\nabla_s\mathbf{g}^{(1)} = \nabla_s\mathbf{g}^{(2)} \quad \text{on } S$$

Part II

Interfacial relations for coupled multifield phenomena

A unified formulation for coupled linear multifield phenomena

To formulate single and coupled linear phenomena in 3D media in a **unified** way, we consider r **divergence-free** vector fields and r **curl-free** vector fields:

$$div\boldsymbol{J}_{\alpha} = J_{\alpha i,i} = 0,$$

$$\boldsymbol{E}_{\alpha} = \nabla w_{\alpha} \quad \text{or} \quad E_{\alpha i} = w_{\alpha,i}$$

The constitutive law reads

$$\boldsymbol{J}_{\alpha} = \boldsymbol{L}_{\alpha\beta}\boldsymbol{E}_{\beta} \quad \text{or} \quad J_{\alpha i} = L_{\alpha i\beta j}E_{\beta j}$$

The latter can be recast in the matrix form:

A unified formulation for coupled linear multifield phenomena - II

$$\boldsymbol{J} = \mathbb{L}\boldsymbol{E}.$$

Here, $\boldsymbol{J}$ and $\boldsymbol{E}$ are two vectors of $3r$ components and $\boldsymbol{L}$ is a $3r \times 3r$ matrix. They are specified by

$$\boldsymbol{J} = \begin{bmatrix} \boldsymbol{J}_1 \\ \boldsymbol{J}_2 \\ \vdots \\ \boldsymbol{J}_r \end{bmatrix}, \quad \mathbb{L} = \begin{bmatrix} \boldsymbol{L}_{11} & \boldsymbol{L}_{12} & \cdots & \boldsymbol{L}_{1r} \\ \boldsymbol{L}_{21} & \boldsymbol{L}_{22} & \cdots & \boldsymbol{L}_{2r} \\ \vdots & \vdots & \vdots & \vdots \\ \boldsymbol{L}_{1r} & \boldsymbol{L}_{2r} & \cdots & \boldsymbol{L}_{rr} \end{bmatrix}, \quad \boldsymbol{E} = \begin{bmatrix} \boldsymbol{E}_1 \\ \boldsymbol{E}_2 \\ \vdots \\ \boldsymbol{E}_r \end{bmatrix},$$

where an element $\boldsymbol{L}_{\alpha\beta}$ of $\mathbb{L}$ is a 3×3 matrix. In what follows, the matrix $\mathbb{L}$ is assumed to invertible, so that

$$\boldsymbol{E} = \mathbb{M}\boldsymbol{J}$$

with $\mathbb{M} = \mathbb{L}^{-1}$.

A unified formulation for coupled linear multifield phenomena - III

As an example, we consider **piezomagnetoelectricity**

$$\begin{cases} \sigma_{ij} = C_{ijkl}\varepsilon_{kl} + \Pi_{kij}h_k + \Lambda_{kij}a_k, \\ d_i = \Pi_{ikl}\varepsilon_{kl} - D_{ij}h_j - K_{ij}a_j, \\ b_i = \Lambda_{ikl}\varepsilon_{kl} - K_{ij}h_j - H_{ij}a_j. \end{cases}$$

The unified formulation holds by defining

$$J_{1i} = \sigma_{1i}, \quad J_{2i} = \sigma_{2i}, \quad J_{3i} = \sigma_{3i}, \quad J_{4i} = d_i, \quad J_{5i} = b_i,$$

$$E_{\alpha i} = w_{\alpha,i}, \quad \boldsymbol{w} = (u_1, u_2, u_3, \varphi, \psi)^T,$$

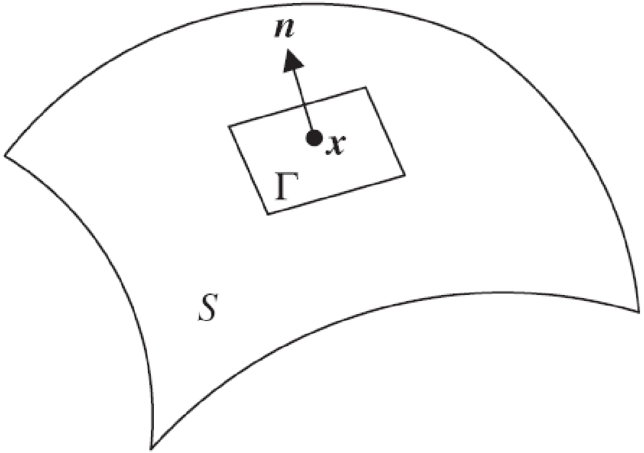
$$\mathbb{L} = [L_{\alpha i\beta j}] = \begin{bmatrix} C_{i1j1} & C_{i1j2} & C_{i1j3} & \Pi_{ji1} & \Lambda_{ji1} \\ C_{i2j1} & C_{i2j2} & C_{i2j3} & \Pi_{ji2} & \Lambda_{ji2} \\ C_{i3j1} & C_{i3j2} & C_{i3j3} & \Pi_{ji3} & \Lambda_{ji3} \\ \Pi_{i1j} & \Pi_{i2j} & \Pi_{i3j} & -D_{ij} & -K_{ij} \\ \Lambda_{i1j} & \Lambda_{i2j} & \Lambda_{i3j} & -K_{ji} & -H_{ij} \end{bmatrix}.$$

Interfacial operators - I

With respect to a curved surface, we introduce the following projection operators

$$\boldsymbol{N}(\boldsymbol{x}) = \boldsymbol{n}(\boldsymbol{x}) \otimes \boldsymbol{n}(\boldsymbol{x}), \qquad (\mathbb{P}^{\perp})_{\alpha i \beta j} = \delta_{\alpha\beta} N_{ij}, \quad (\mathbb{P}^{\parallel})_{\alpha i \beta j} = \delta_{\alpha\beta} T_{ij}$$

$$\boldsymbol{T}(\boldsymbol{x}) = \boldsymbol{I} - \boldsymbol{N}(\boldsymbol{x}), \qquad \mathbb{P}^{\perp} = \mathbf{1} \underline{\otimes} \boldsymbol{N}, \quad \mathbb{P}^{\parallel} = \mathbf{1} \underline{\otimes} \boldsymbol{T}$$



A 3D oriented smooth surface S with the unit normal vector $\boldsymbol{n}$ and tangent plane Γ at $\boldsymbol{x}$.

Remark: $\mathbb{P}^{\perp}$ and $\mathbb{P}^{\parallel}$ can be viewed as an extension of the **exterior and interior projection operators** introduced by **Hill** (1972, 1983) for the decomposition of a 3D second-rank tensor related to an interface.

Interfacial operators - II

Matrix forms and properties of the introduced projection operators:

$$(\mathbb{P}^{\perp})_{\alpha i\beta j} = \delta_{\alpha\beta} N_{ij}, \quad (\mathbb{P}^{\parallel})_{\alpha i\beta j} = \delta_{\alpha\beta} T_{ij} \quad (\mathbb{I})_{\alpha i\beta j} = \delta_{\alpha\beta}\delta_{ij}$$

$$\mathbb{P}^{\perp} = \begin{bmatrix} \boldsymbol{N} & 0 & \cdots & 0 \\ 0 & \boldsymbol{N} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \boldsymbol{N} \end{bmatrix}, \quad \mathbb{P}^{\parallel} = \begin{bmatrix} \boldsymbol{T} & 0 & \cdots & 0 \\ 0 & \boldsymbol{T} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \boldsymbol{T} \end{bmatrix} \quad \mathbb{I} = \begin{bmatrix} \delta_{ij} & 0 & \cdots & 0 \\ 0 & \delta_{ij} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \delta_{ij} \end{bmatrix}$$

$$\mathbb{P}^{\perp}\mathbb{P}^{\perp} = \mathbb{P}^{\perp}, \quad \mathbb{P}^{\parallel}\mathbb{P}^{\parallel} = \mathbb{P}^{\parallel}, \quad \mathbb{P}^{\perp}\mathbb{P}^{\parallel} = \mathbb{P}^{\parallel}\mathbb{P}^{\perp} = \mathbb{O}, \quad \mathbb{P}^{\perp} + \mathbb{P}^{\parallel} = \mathbb{I}.$$

Interfacial relations for a perfect interface - I

Assume that S is a **perfect interface** separating medium 1 and medium 2. Then,

$$\boldsymbol{w}^{(1)}|_S = \boldsymbol{w}^{(2)}|_S,$$

$$\mathbb{P}^{\perp}\boldsymbol{J}^{(1)}|_S = \mathbb{P}^{\perp}\boldsymbol{J}^{(2)}|_S$$

Applying Hadamard’s theorem to the first of the foregoing relations yields

$$\mathbb{P}^{\parallel}\boldsymbol{E}^{(1)}|_S = \mathbb{P}^{\parallel}\boldsymbol{E}^{(2)}|_S$$

Remarks:

• The last two continuity relations mean that the normal part of the flux-like vector and the tangential part of the gradient of the potentiel vector are **continuous** across a perfect interface.

• However, in general, both the tangential part of the flux-like vector and the normal part of the gradient of the potentiel vector are **discontinuous** across a perfect interface.

Interfacial relations for a perfect interface - II

One of the most important problems in mechanics of interfaces is the determination of the entire flux-like vector and potentiel gradient at one side of a perfect interface in terms of the normal part of the flux-like vector and the tangential part of the gradient of the potentiel vector. The solution to this problem is provided by

$$\boxed{\begin{aligned} \boldsymbol{E}^{(1)}|_S &= \mathbb{A}^{(1)}\boldsymbol{J}^{(2)}|_S + \mathbb{M}^{(1)}\mathbb{B}^{(1)}\boldsymbol{E}^{(2)}|_S, \\ \boldsymbol{J}^{(1)}|_S &= \mathbb{B}^{(1)}\boldsymbol{E}^{(2)}|_S + \mathbb{L}^{(1)}\mathbb{A}^{(1)}\boldsymbol{J}^{(2)}|_S, \end{aligned}}$$

with

$$\boxed{(\mathbb{A})_{\alpha i \beta j} = G_{\alpha\beta} N_{ij} \quad \text{or} \quad \mathbb{A} = \boldsymbol{G} \underline{\otimes} \boldsymbol{N}}$$

$$\boxed{Q_{\alpha\beta} = \boldsymbol{L}_{\alpha\beta}\boldsymbol{N} = L_{\alpha i \beta j} n_i n_j} \qquad \boxed{\boldsymbol{G} = \boldsymbol{Q}^{-1}}$$

$$\mathbb{A}(\mathbb{P}^{\perp}\mathbb{L}\mathbb{P}^{\perp}) = (\mathbb{P}^{\perp}\mathbb{L}\mathbb{P}^{\perp})\mathbb{A} = \mathbb{P}^{\perp}, \quad \mathbb{A}\mathbb{P}^{\perp} = \mathbb{P}^{\perp}\mathbb{A} = \mathbb{A}$$

$$\mathbb{B}(\mathbb{P}^{\parallel}\mathbb{M}\mathbb{P}^{\parallel}) = (\mathbb{P}^{\parallel}\mathbb{M}\mathbb{P}^{\parallel})\mathbb{B} = \mathbb{P}^{\parallel}, \quad \mathbb{B}\mathbb{P}^{\parallel} = \mathbb{P}^{\parallel}\mathbb{B} = \mathbb{B}$$

Interfacial relations for a perfect interface - III

Some additional relations:

$$(\mathbb{P}^{\perp}\mathbb{L}\mathbb{P}^{\perp})_{\alpha i\beta j} = Q_{\alpha\beta}N_{ij} \quad \text{or} \quad \mathbb{P}^{\perp}\mathbb{L}\mathbb{P}^{\perp} = \boldsymbol{Q}\underline{\otimes}\boldsymbol{N}$$

$$\mathbb{L}\mathbb{A}+\mathbb{B}\mathbb{M}=\mathbb{A}\mathbb{L}+\mathbb{M}\mathbb{B}=\mathbb{I} \qquad \mathbb{B}=\mathbb{L}-\mathbb{L}\mathbb{A}\mathbb{L}$$

Remarks:

(1) The foregoing results about perfect interfaces can be viewed as extending the relevant elastic ones of Hill (1972, 1983), Laws (1977) and Walpole (1978, 1981) to the general case where a finite number of single or coupled linear phenomena are involved. For more details, please refer to

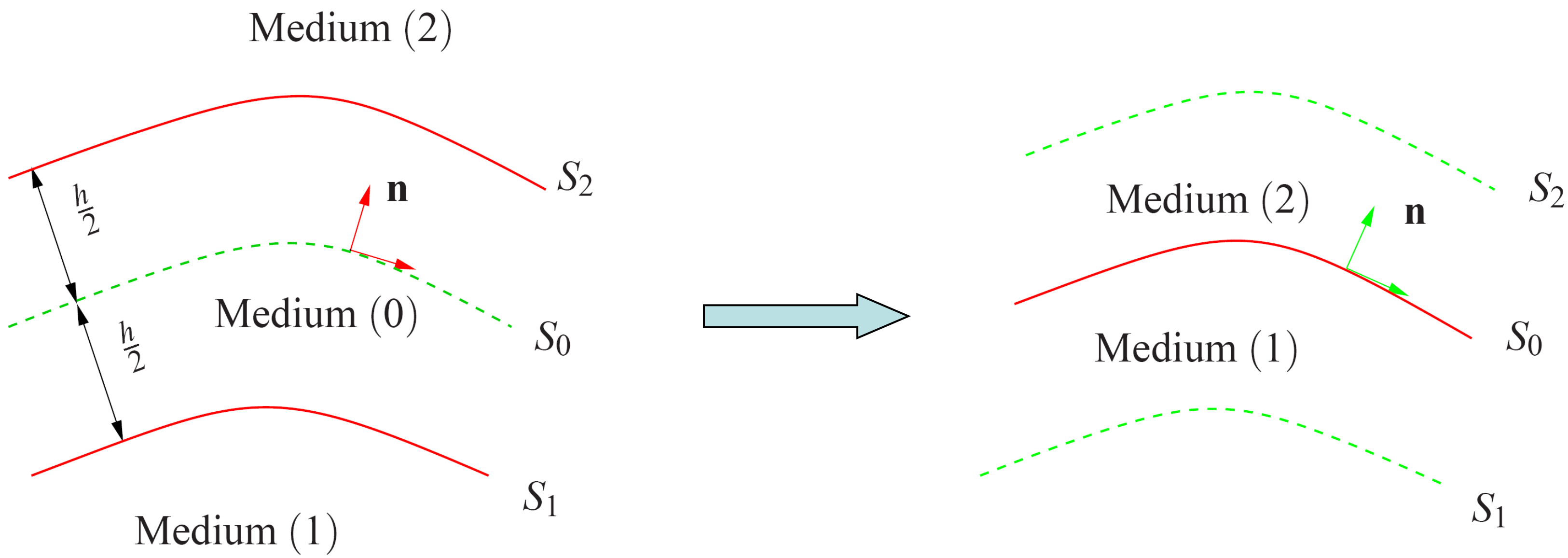
Gu S.-T., He Q.-C., Journal of the Mechanics and Physics of Solids 59, 1413-1426, 2011.

- The extended results are expected to be useful in dealing with a variety of mechanical and physical problems. In particular, we below show that they can be applied directly in deriving **imperfect interface models** and **shell models**.

Part III

Derivation of imperfect interface models for coupled multifield phenomena

Modelling of a curved thin interphase as an imperfect interface - I



(a) **Three-phase configuration**

(b) **Two-phase configuration**

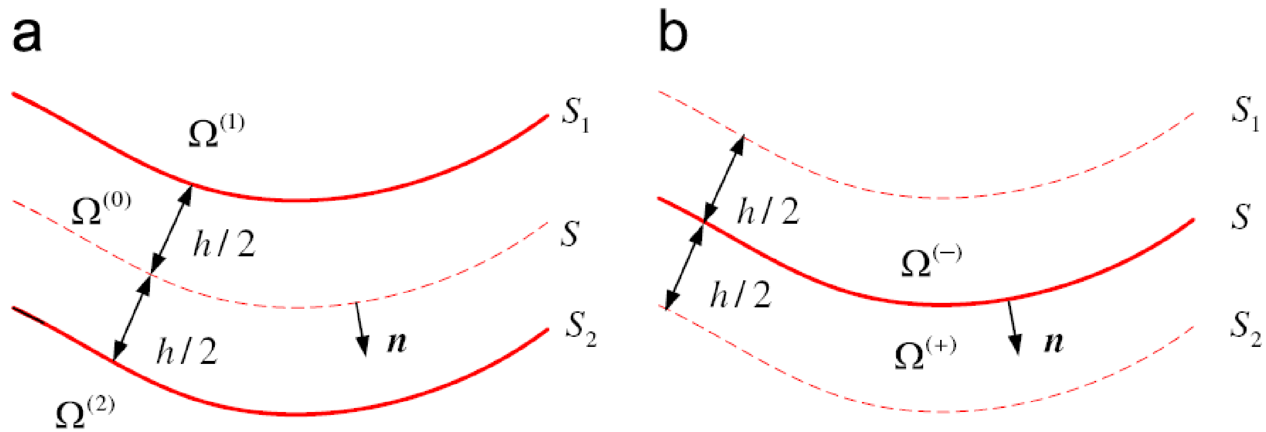
Basic idea: the interphase made of phase 0 is replaced by an imperfect interface located at S_0 whose properties are such that the relevant field jumps across the interphase bounded by surfaces S_1 and S_2 in the three-phase configuration (a) are, to within an error of order $0(h^2)$, equal to the corresponding field jumps across the zone bounded by the surfaces S_1 and S_2 in the two-phase configuration (b).

Modelling of a curved thin interphase as an imperfect interface - III

Using Taylor's expansion, Hadamard's relation and the previous results obtained for a perfect interface, we can derive the following general jump relations for the imperfect interface in the two-phase configuration:

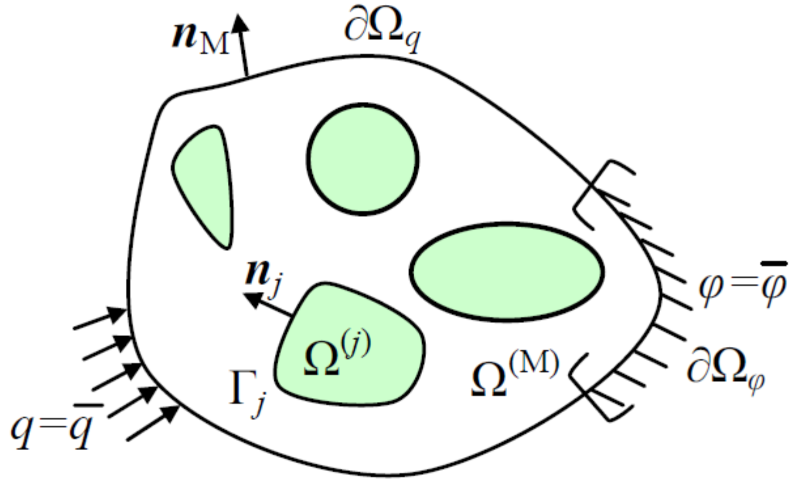
$$\boxed{[\![\boldsymbol{w}]\!] = \frac{h}{2}[(\mathbb{A}^{(0)}-\mathbb{A}^{(2)})\boldsymbol{J}^{(+)}+(\mathbb{M}^{(0)}\mathbb{B}^{(0)}-\mathbb{M}^{(2)}\mathbb{B}^{(2)})\boldsymbol{E}^{(+)}]\boldsymbol{n}+\frac{h}{2}[(\mathbb{A}^{(0)}-\mathbb{A}^{(1)})\boldsymbol{J}^{(-)}+(\mathbb{M}^{(0)}\mathbb{B}^{(0)}-\mathbb{M}^{(1)}\mathbb{B}^{(1)})\boldsymbol{E}^{(-)}]\boldsymbol{n}+\boldsymbol{0}(h^2)}$$

$$\boxed{[\![J_n]\!] = \frac{h}{2}div_s[(\mathbb{L}^{(2)}\mathbb{A}^{(2)}-\mathbb{L}^{(0)}\mathbb{A}^{(0)})\boldsymbol{J}^{(+)}+(\mathbb{L}^{(1)}\mathbb{A}^{(1)}-\mathbb{L}^{(0)}\mathbb{A}^{(0)})\boldsymbol{J}^{(-)}]+\frac{h}{2}div_s[(\mathbb{B}^{(2)}-\mathbb{B}^{(0)})\boldsymbol{E}^{(+)}+(\mathbb{B}^{(1)}-\mathbb{B}^{(0)})\boldsymbol{E}^{(-)}]+0(h^2).}$$



Remark: These two relations include as special cases the imperfect interface models derived, for example, by Sanchez-Palencia (1970), Gurtin-Murdoch (1972), Hashin (1992, 2002), Bövik (1994) and Benveniste (2006).

Particularization of the general model to transport phenomena – I



General outline of the composite material under investigation

For a transport phenomenon (thermal conduction, diffusion, …) in an isotropic multi-phase composite, the general imperfect interface model reduces to

$$[[\varphi]]_i = \frac{h}{2}\left[\left(\frac{1}{k^{(i)}} - \frac{1}{k^{(0)}}\right) q_n^{(-)} + \left(\frac{1}{k^{(M)}} - \frac{1}{k^{(0)}}\right) q_n^{(+)}\right] + 0(h^2),$$

$$[[q_n]]_i = \frac{h}{2}\left\{\left(k^{(0)} - k^{(i)}\right)\Delta_s\varphi^{(-)} + \left(k^{(0)} - k^{(M)}\right)\Delta_s\varphi^{(+)}\right\} + 0(h^2)$$

Particularization of the general model to transport phenomena - II

which can be shown to be equivalent to the simple and compact form:

$$\boxed{\begin{aligned}[[\varphi]]_i &= \frac{h}{2} a^{(i)} \langle q_n \rangle_i + 0(h^2),\\ [[q_n]]_i &= \frac{h}{2} b^{(i)} \Delta_s \langle \varphi \rangle_i + 0(h^2)\end{aligned}}$$

$$a^{(i)} = \frac{1}{k^{(M)}} + \frac{1}{k^{(i)}} - \frac{2}{k^{(0)}};$$

$$b^{(i)} = 2k^{(0)} - k^{(i)} - k^{(M)}$$

$$[[\bullet]]_i = \bullet^{(+)} - \bullet^{(-)} \qquad \langle \bullet \rangle_i = (\bullet^{(+)} + \bullet^{(-)})/2,$$

In the context of thermal conduction, this general isotropic model includes as special cases:

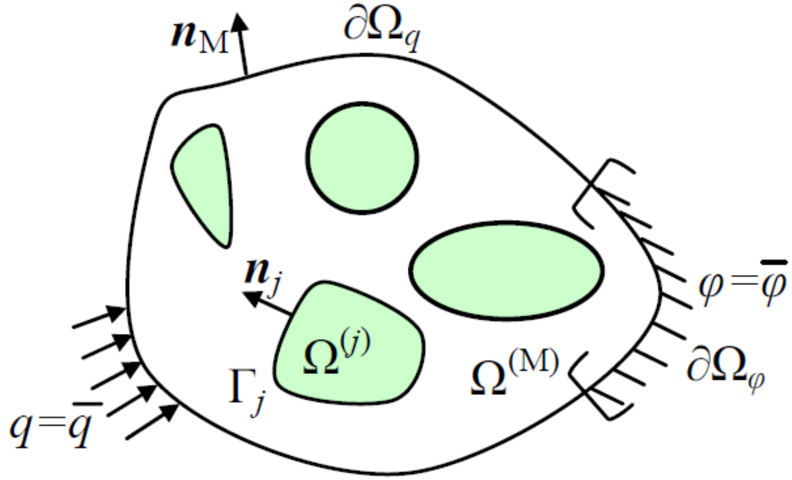
(i) Kapitza's thermal resistance model

$$\boxed{\begin{aligned}[[\varphi]]_i &= -\frac{h}{k^{(0)}} \langle q_n \rangle_i + 0(h)\\ [[q_n]]_i &= 0(h).\end{aligned}}$$

(i) Highly conducting model

$$\boxed{\begin{aligned}[[\varphi]]_i &= 0(h),\\ [[q_n]]_i &= hk^{(0)} \Delta_s \langle \varphi \rangle_i + 0(h)\end{aligned}}$$

Boundary value problem of a particulate composite : strong formulation



General outline of the composite material under investigation

Field equations:

$$div\mathbf{q}^{(l)} = 0$$

$$\mathbf{q}^{(l)} = -k^{(l)}\nabla\varphi^{(l)}$$

Interfacial relations

$$[[\varphi]]_i = \frac{h}{2}a^{(i)}\left\langle q_n\right\rangle_i + 0(h^2),$$

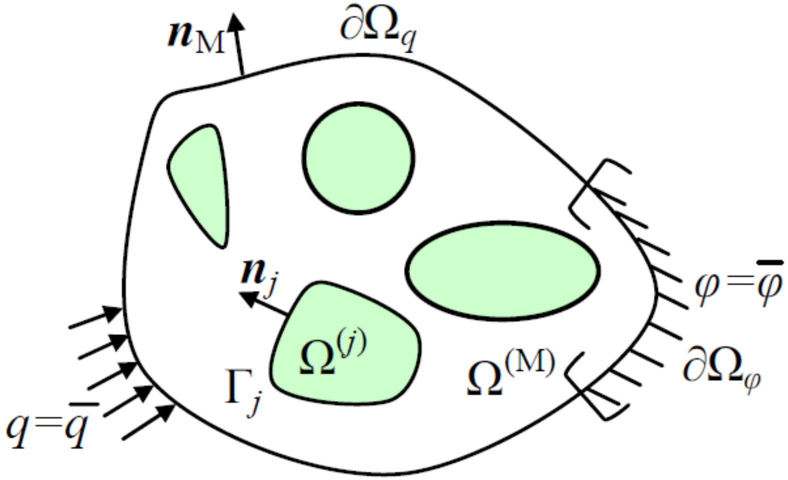
$$[[q_n]]_i = \frac{h}{2}b^{(i)}\Delta_s\left\langle \varphi\right\rangle_i + 0(h^2)$$

Boundary conditions

$$\varphi = \overline{\varphi} \text{ on } \partial\Omega_\varphi,$$
$$q_n = \overline{q}_n \text{ on } \partial\Omega_q$$

Boundary value problem of a particulate composite : weak formulation

$$\int_{\Omega} k\nabla\varphi \cdot \nabla\left(\delta\varphi\right) dv + \frac{h}{2}\sum_{j=1}^{m}\int_{\Gamma_j} b^{(j)}\nabla_s \left\langle\varphi\right\rangle_j \cdot \nabla_s \left\langle\delta\varphi\right\rangle_j ds - \frac{2}{h}\sum_{j=1}^{m}\int_{\Gamma_j} \frac{1}{a^{(j)}}[[\varphi]]_j[[\delta\varphi]]_j ds$$
$$= \; -\int_{\partial\Omega_q} q_n \delta\varphi ds. \tag{29}$$



General outline of the composite material under investigation

Remark: the weak form contains one term relatated to the interfacial jump of the prime variable and another term relative to the interfacial average of the dual variable.

Boundary value problem of a particulate composite : discretization

Level-set description of an interface and its discretization:

$$\Gamma = \{\mathbf{x} \in \mathbb{R}^3 | \phi(\mathbf{x}) = 0\} \qquad \phi^h(\mathbf{x}) = \sum_{s=1}^{n_e} N_s(\mathbf{x})\phi_s$$

$$\mathbf{n}^h(\mathbf{x}) = \frac{\nabla\phi^h(\mathbf{x})}{||\nabla\phi^h(\mathbf{x})||} \quad \text{with} \quad \nabla\phi^h(\mathbf{x}) = \sum_{s=1}^{n_e} \frac{\partial N_s(\mathbf{x})}{\partial \mathbf{x}}\phi_r$$

Extended finite element method (XFEM) approximation of the prime variable:

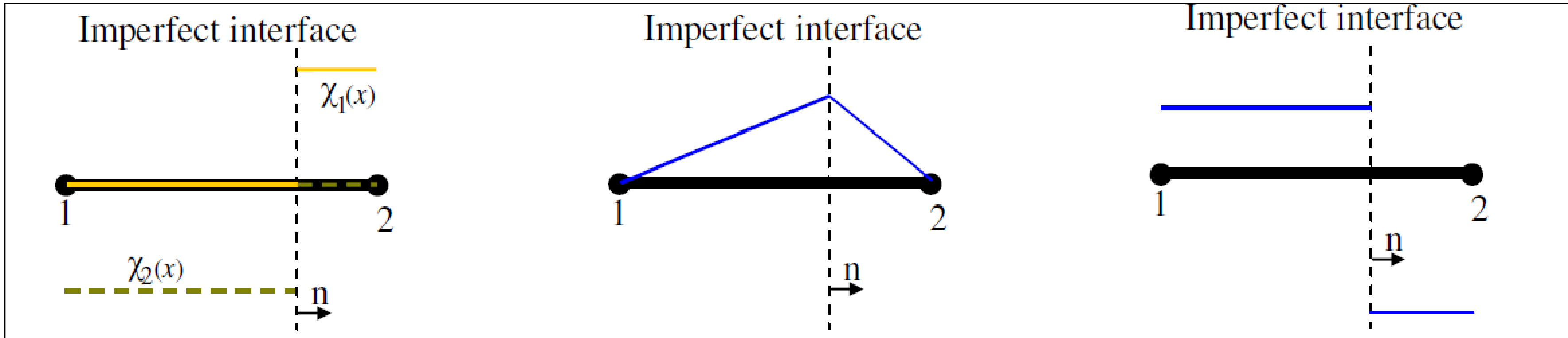
$$\boxed{\varphi^h(\mathbf{x}) = \sum_{s=1}^{n_{nd}} N_s(\mathbf{x})\varphi_s + \sum_{p=1}^{m_{nd}} N_p(\mathbf{x})\chi_p(\mathbf{x})\overline{\varphi}_p + \sum_{p=1}^{m_{nd}} N_p(\mathbf{x})\psi_p(\mathbf{x})\overline{\overline{\varphi}}_p}$$

$$\boxed{\chi_p(\mathbf{x}) = sign(\phi(\mathbf{x})) - sign(\phi_p)}$$

$$\boxed{\psi_p(\mathbf{x}) = \sum_{s=1}^{n_e} N_s(\mathbf{x})|\phi_s| - |\sum_{s=1}^{n_e} N_s(\mathbf{x})\phi_s|}$$

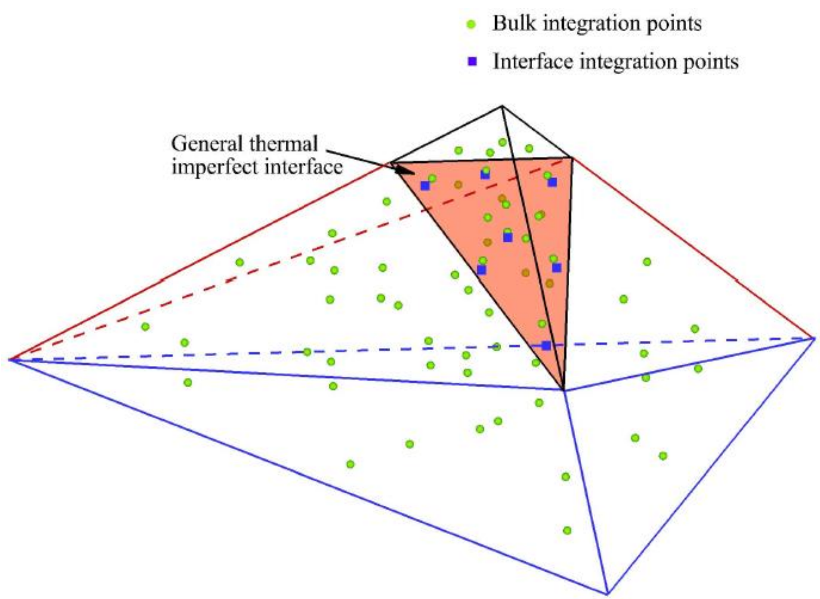
Geometrical interpretation of the enrichment functions and integration procedure for an element intercepted by an interface

1D interpretation of the enrichement functions



(a) Enrichment function $\chi_p(x)$ (b) Enrichment function $\psi_p(x)$ (c) Enriched shape function $\frac{\partial \psi_p(x)}{\partial x}$

Sudivision of an intercepted element, bulk and interfacial integrations



Boundary value problem of a particulate composite : discrete equations

Final system of linear equations:

$$\boxed{(\mathbf{K} + \mathbf{K}_s)\,\mathbf{\Phi} = \mathbf{F}}$$

$$\boxed{\mathbf{K} = \sum_{s=1}^{n_{em}} \int_{\Omega_s^e} \mathbf{B}^T \mathbf{K}_s^{(l)} \mathbf{B}\, d\Omega_s^e}$$

$$\boxed{\mathbf{K}_s = \sum_{j=1}^{m} \sum_{j'=1}^{n_s} \int_{\Gamma^e_{j\text{-}j'}} [\frac{h}{2} b^{(j)} \widetilde{\mathbf{B}}_{j'}^T \mathbf{T}^{(j')} \widetilde{\mathbf{B}}_{j'} - \frac{2}{h} a^{(j)} \widetilde{\mathbf{N}}_{j'}^T \widetilde{\mathbf{N}}_{j'}] dS^e}$$

$$\boxed{\mathbf{F} = -\int_{\partial\Omega_q} \mathbf{N}^T \bar{q}_n \, dS}$$

Remark: we retrieve as special cases the relsults for the Kapitza and HC models by taking appropriate values for a(j) and b(j).

Benchmark problem: comparison between the numerical and analytical results

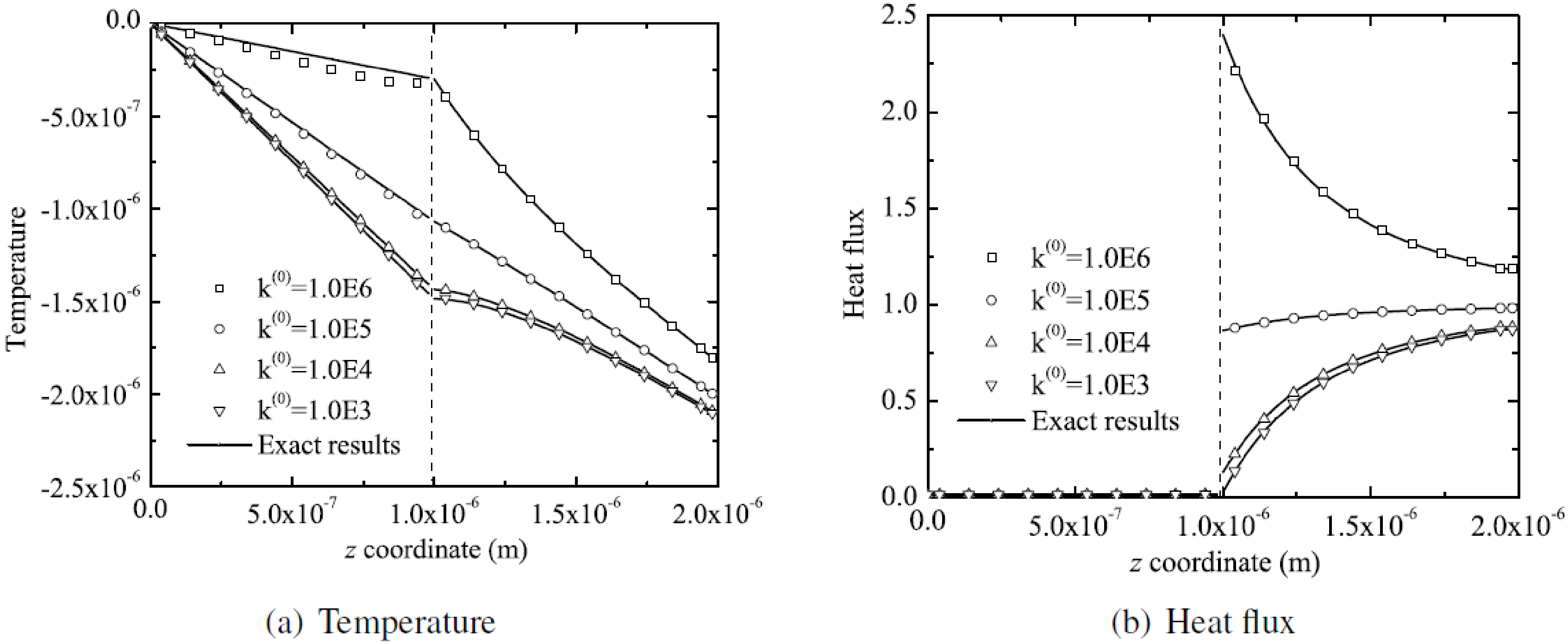
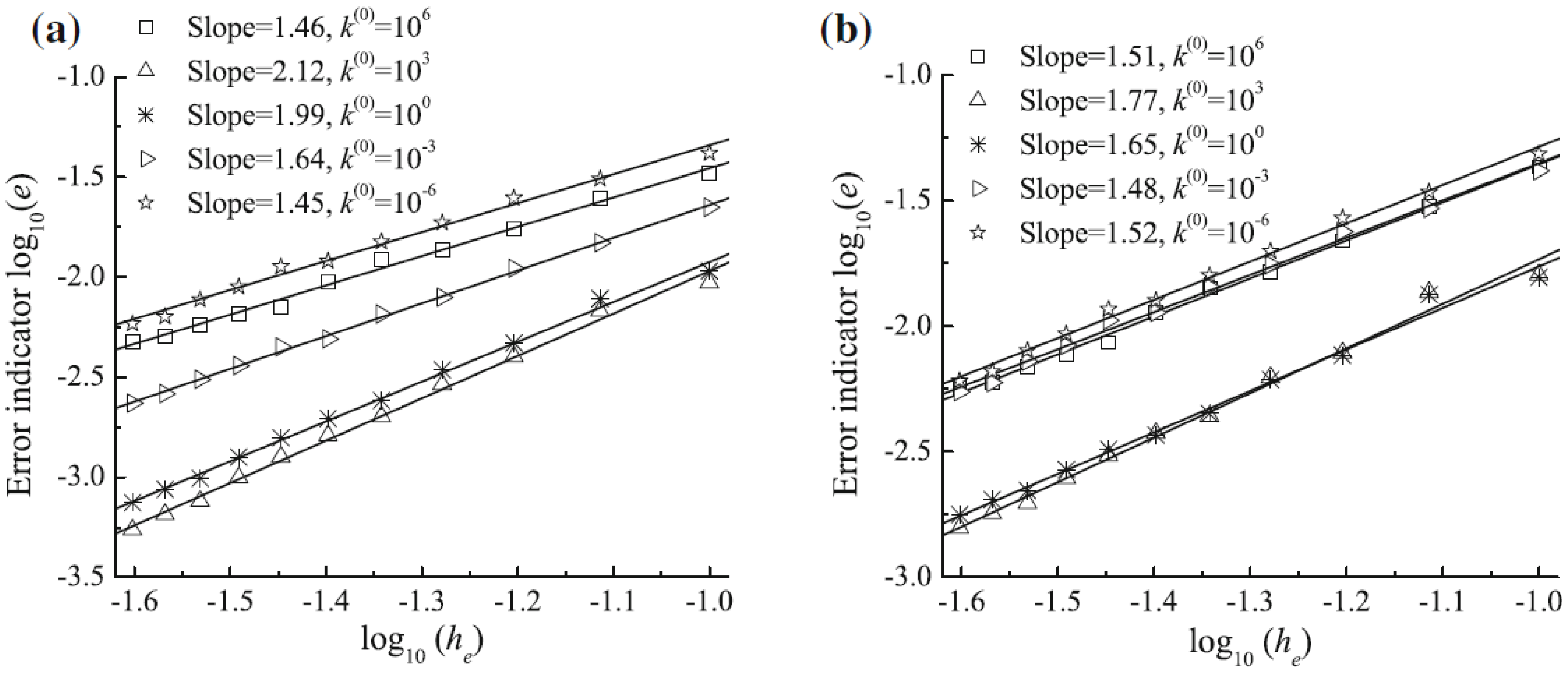


Figure 9. Comparison of the theoretical and predicted results along z axis with x=0, y=0 of the spherical benchmark for different surface conductivities.

Benchmark problem: convergence analysis

Error funnction:

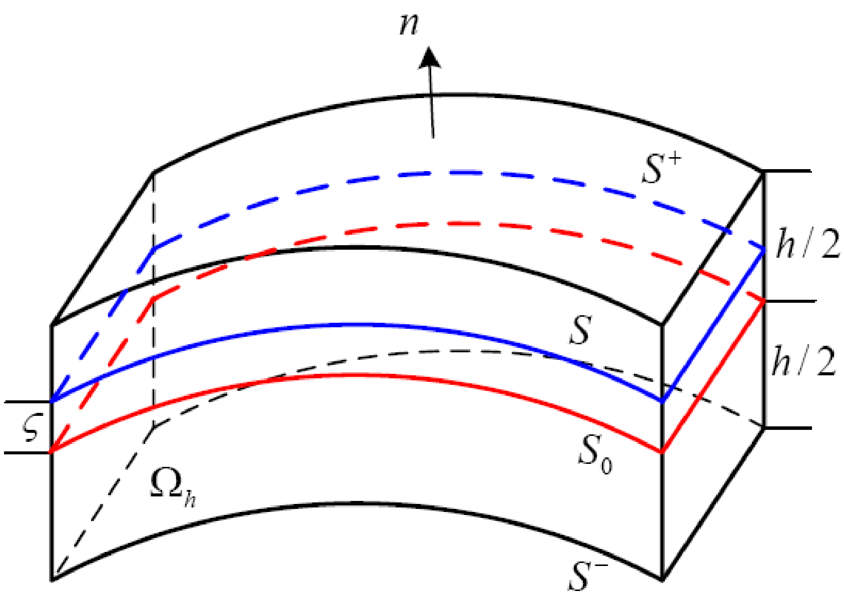
$$e = \frac{\sqrt{\frac{1}{V}\int_{\Omega} |\varphi^{h_e} - \varphi|^2 dV + \frac{1}{S}\int_{\Gamma} |[[\varphi]]^{h_e} - [[\varphi]]|^2 dS}}{\sqrt{\frac{1}{V}\int_{\Omega} \varphi^2 dV + \frac{1}{S}\int_{\Gamma} [[\varphi]]^2 dS}}$$



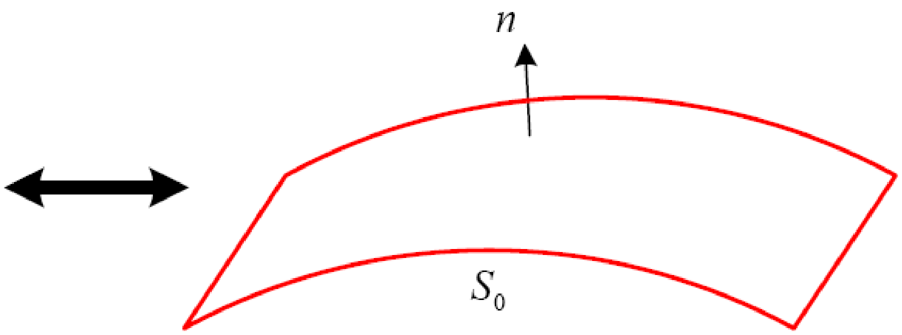
Part IV

Derivation of plate and shell models for coupled multifield phenomena

Derivation of shell models from a 3D thin solid



(a) 3D curved thin solid



(b) Curved median surface

Basic idea: A 3D thin solid of uniform thickness h in the configuration (a) is replaced by its median surface S_0 in the configuration (b), endowed with the properties such that **the energy stored in the former is, to within an error of order 0(h^4), equal to the one stored in the latter**.

Key to establishing a shell model: express every quantity defined in the 3D thin solid in terms of appropriate quantities defined on S_0.

Elements of a coordinate-free differential geometry theory - III

- **Upper and lower surfaces**

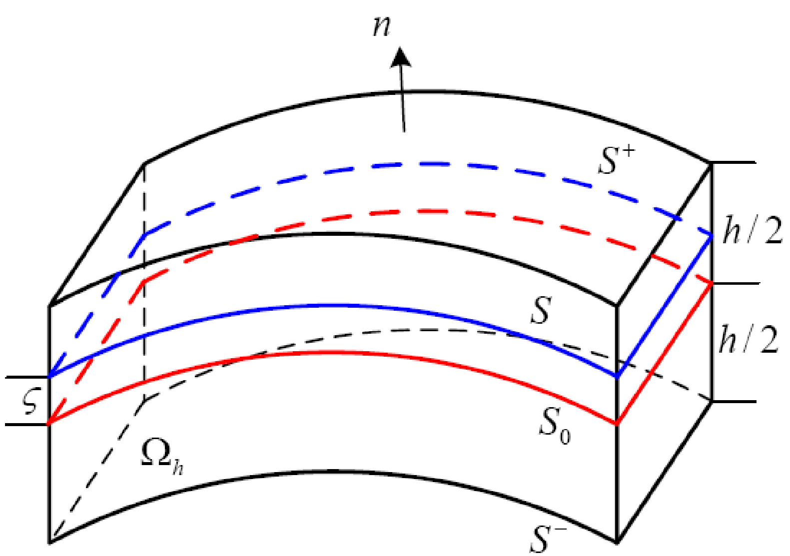
$$S^+ = \{\boldsymbol{x} \in \mathbb{R}^3 \mid \boldsymbol{x} = \boldsymbol{x}_0 + \frac{h}{2}\boldsymbol{n}(\boldsymbol{x}_0), \quad \boldsymbol{x}_0 \in S_0\}$$

$$S^- = \{\boldsymbol{x} \in \mathbb{R}^3 \mid \boldsymbol{x} = \boldsymbol{x}_0 - \frac{h}{2}\boldsymbol{n}(\boldsymbol{x}_0), \quad \boldsymbol{x}_0 \in S_0\}$$

- **A generic surface**

$$S = \{\boldsymbol{y} \in \mathbb{R}^3 \mid \boldsymbol{y} = \boldsymbol{x}_0 + \varsigma\boldsymbol{n}(\boldsymbol{x}_0), \quad \boldsymbol{x}_0 \in S_0, \quad -\frac{h}{2} < \varsigma < \frac{h}{2}\}$$

- **Normal gradient of the unit normal vector**



$$\nabla_n \boldsymbol{n} = \nabla \boldsymbol{n} \cdot \boldsymbol{n} = 0$$

Taylor's expansions - I

- **Taylor's expansion of the generalized displacement vector**

$$\boldsymbol{w}\left(\boldsymbol{x}\right) = \boldsymbol{w}|_{\boldsymbol{x}_0} + \varsigma \nabla_n \boldsymbol{w}|_{\boldsymbol{x}_0} + \frac{\varsigma^2}{2!}\nabla_n^2 \boldsymbol{w}|_{\boldsymbol{x}_0} + \frac{\varsigma^3}{3!}\nabla_n^3 \boldsymbol{w}|_{\boldsymbol{x}_0} + \cdots$$

with

$$\varsigma = (\boldsymbol{x} - \boldsymbol{x}_0)\cdot \boldsymbol{n} \qquad \nabla\varsigma = \boldsymbol{n}$$

$$\nabla_n^r \boldsymbol{w} = \nabla\left(\nabla_n^{r-1}\boldsymbol{w}\right)\cdot \boldsymbol{n}$$

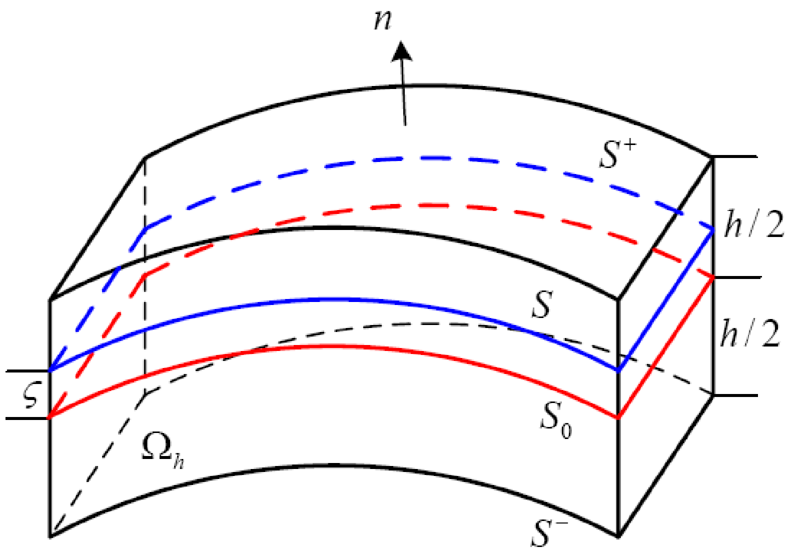
- **Taylor's expansion of the derivative of the generalized strain vector**

$$\begin{aligned} \boldsymbol{E} \quad &= \quad \nabla_s \boldsymbol{w}|_{\boldsymbol{x}_0} + \nabla_n \boldsymbol{w}|_{\boldsymbol{x}_0} \otimes \boldsymbol{n} + \varsigma\left[\nabla_s\left(\nabla_n \boldsymbol{w}|_{\boldsymbol{x}_0}\right) + \nabla_n^2 \boldsymbol{w}|_{\boldsymbol{x}_0} \otimes \boldsymbol{n}\right] \\ &\quad + \frac{\varsigma^2}{2!}\left[\nabla_s\left(\nabla_n^2 \boldsymbol{w}|_{\boldsymbol{x}_0}\right) + \nabla_n^3 \boldsymbol{w}|_{\boldsymbol{x}_0} \otimes \boldsymbol{n}\right] + 0(\varsigma^3). \end{aligned}$$

Taylor's expansions - II

- **Generalized strain energy**

$$\Xi_h = \frac{1}{2}\int_{\Omega_h} \boldsymbol{E} : \mathbb{L} : \boldsymbol{E}\, dv$$



- **Taylor's expansion of the generalized strain energy**

$$\begin{aligned}\Xi_h \quad = \quad & \frac{h}{2}\int_{S_0} \left[\nabla_s \boldsymbol{w} + \nabla_n \boldsymbol{w} \otimes \boldsymbol{n}\right] : \mathbb{L} : \left[\nabla_s \boldsymbol{w} + \nabla_n \boldsymbol{w} \otimes \boldsymbol{n}\right] ds \\ & + \frac{h^3}{24}\left\{\int_{S_0} \left[\nabla_s \boldsymbol{w} + \nabla_n \boldsymbol{w} \otimes \boldsymbol{n}\right] : \mathbb{L} : \left[\nabla_s \left(\nabla_n^2 \boldsymbol{w}\right) + \nabla_n^3 \boldsymbol{w} \otimes \boldsymbol{n}\right] ds\right. \\ & \left. + \int_{S_0} \left[\nabla_s \left(\nabla_n \boldsymbol{w}\right) + \nabla_n^2 \boldsymbol{w} \otimes \boldsymbol{n}\right] : \mathbb{L} : \left[\nabla_s \left(\nabla_n \boldsymbol{w}\right) + \nabla_n^2 \boldsymbol{w} \otimes \boldsymbol{n}\right] ds\right\} + 0\left(h^3\right)\end{aligned}$$

Plate and shell models - I

- **Key to deriving plate and shell models**

  To obtain plate and shell models, all the quantities must be defined on the median surface. Since normal gradients defined on the median surface do not make sense when the 3D thin solid has been replaced by its median surface, they have to be expressed in terms of some appropriate surface gradients. This can be accomplished in a general way by using the interfacial relations obtained in the first part.

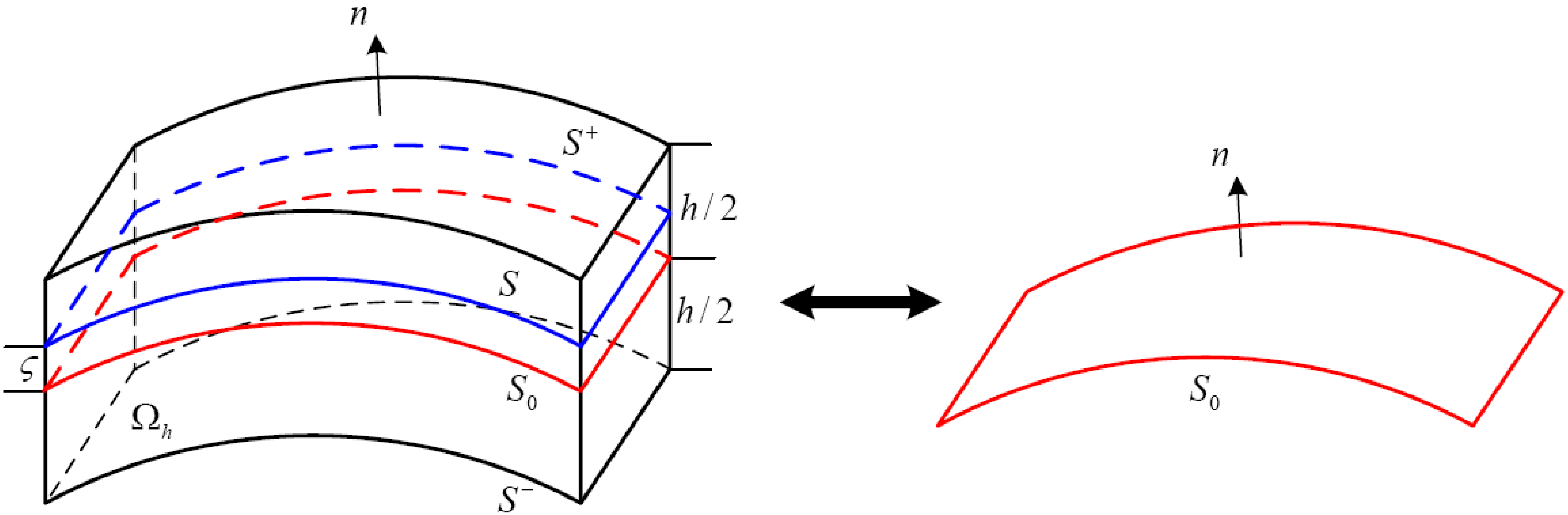


Plate and shell models - II

- **A general shell model is given by**

$$\Xi_h = \Xi_{mem} + \Xi_{bending} + \Xi_{couple}$$

$$\Xi_{membrane} = \frac{h}{2}\int_{S_0} (\nabla_s \boldsymbol{w} : \mathbb{B} : \nabla_s \boldsymbol{w})\, ds.$$

$$\Xi_{bending} = \frac{h^3}{24}\int_{S_0} [\nabla_s (\boldsymbol{n} \cdot \mathbb{M} : \mathbb{B} : \boldsymbol{E}) : \mathbb{B} : \nabla_s (\boldsymbol{n} \cdot \mathbb{M} : \mathbb{B} : \boldsymbol{E}) + (\nabla_s \boldsymbol{w}.\boldsymbol{W}) : \mathbb{L} : \mathbb{A} : \mathbb{L} : (\nabla_s \boldsymbol{w}.\boldsymbol{W})]\, ds$$

$$\Xi_{couple} = \frac{h^3}{24}\int_{S_0} \{\nabla_s \boldsymbol{w} : \mathbb{B} : \nabla_s [\boldsymbol{n} \cdot \mathbb{M} : \mathbb{B} : \nabla_s (\boldsymbol{n} \cdot \mathbb{M} : \mathbb{B} : \boldsymbol{E})] + \nabla_s \boldsymbol{w} : \mathbb{B} : \nabla_s [\boldsymbol{n} \cdot \mathbb{M} : \mathbb{B} : (\nabla_s \boldsymbol{w}.\boldsymbol{W})]\}\, ds$$

Remarks:

- **The derived shell model is coordinate-free. No curvilinear coordinates are used.**
- **The material forming the shell is linear but can be multi-physical while being generally anisotropic.**

Concluding remarks

- **In contrast with most of the works about the derivation of interfacial relations and shell models, our approach is coordinate-free. Consequently, a system of Cartesian coordinates or any other system of coordinates can be used to carry out computations.**

- **The interfacial relations established for perfect interfaces turn out to be the key to modelling of an interphase as an imperfect interface and to deriving plate and shell models. This last point was unexpected.**

- **The numerical approach based on XFEM and LST is proved to be powerful for the treatment of imperfect interfaces.**

- **In deriving imperfect interface models or plate and shell models, elasticity and multifield phenomena such piezoelectricity have been treated in a unified and compact way.**

- **The general shell model established in this work can be viewed as an generalization of the well-known Koiter's shell model.**

Some references

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- **Liu, J.T., He, B., Gu, S.T., He, Q.-C., 2018. Implementation of a physics-based general elastic imperfect interface model in the XFEM and LSM context. International Journal for Numerical Methods in Engineering 115, 1499-1525.**