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Analytical and Numerical Treatment of Singularities in PDE

Edge-Corner interaction inside polyhedral singularities

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Domains and Equations

Domain Ω : **3D polyhedral** (*or with curved faces, conical points, in higher dimensions*)

Inner Operator L : **2nd order strongly elliptic, scalar or matrix-valued** (*or ord. $2m$*),
defined via a 1st order form a (usual ingredients: grad, div, curl, strain e).

Coefficients of a : **constant, or piecewise-constant in a polyhedral domain decomposition Ω_j of Ω** (*or piecewise-smooth*).

Boundary conditions B : **Dirichlet or Neumann on each face** (of Ω or of Ω_j ^a)
defining a subspace V of H^1 (**except for Maxwell**)

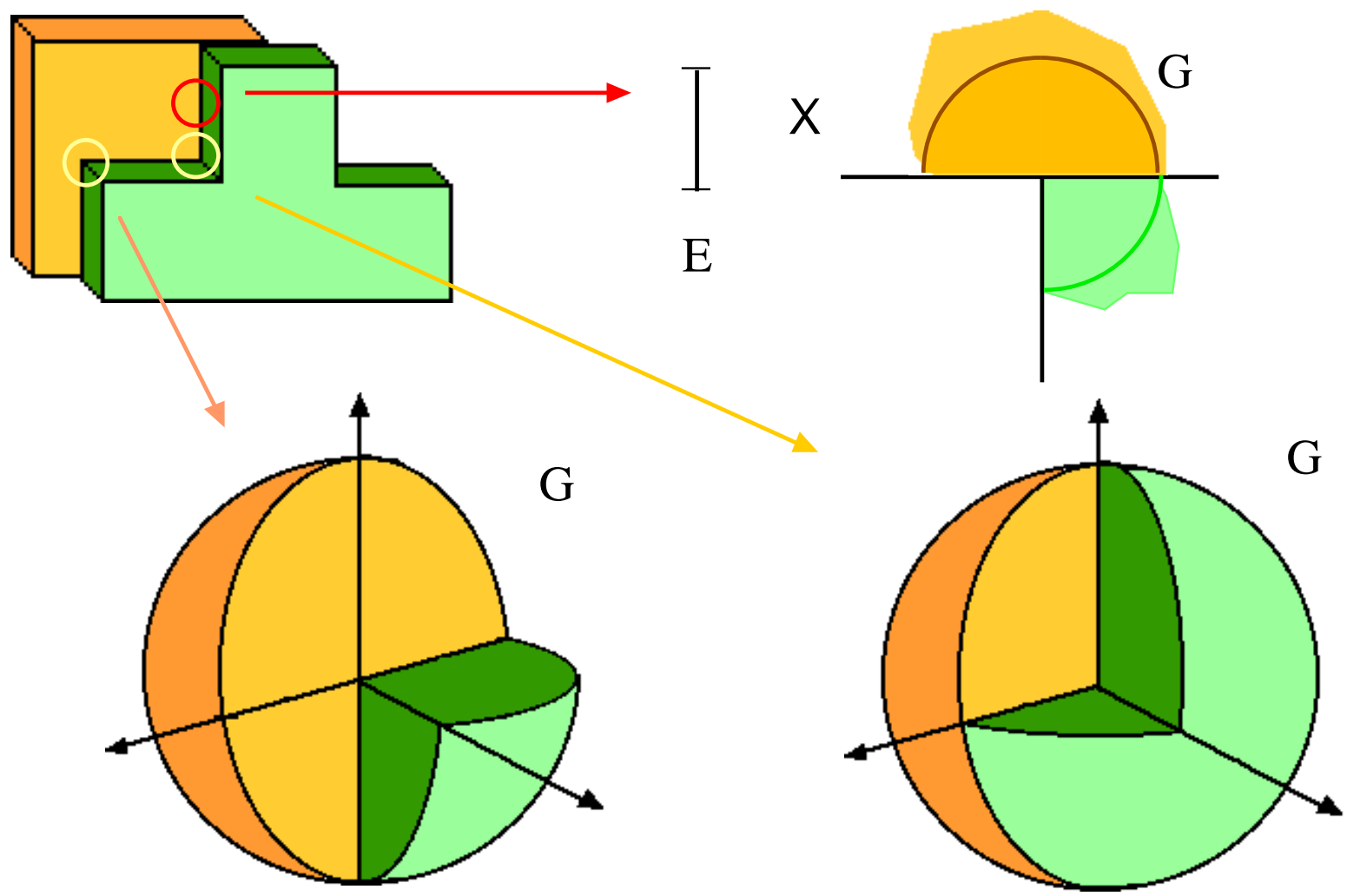
$$(\mathcal{P}) \quad u \in V, \quad \forall v \in V, \quad a(u, v) = \int_{\Omega} f v \, dx$$

i.e.

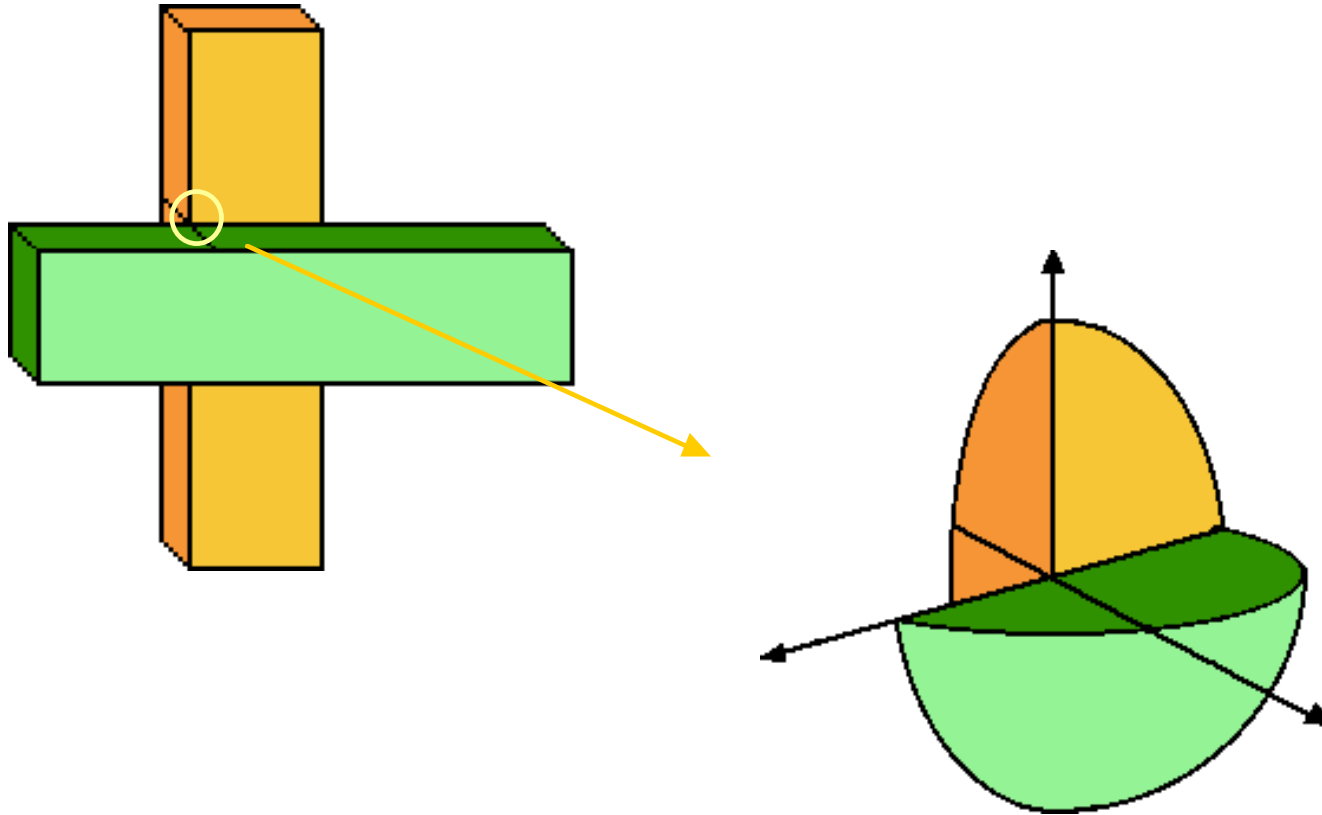
$$(\mathcal{P}) \quad \begin{cases} Lu = f & \text{in } \Omega_j, \\ Bu = 0 & \text{on } \partial\Omega \cap \partial\Omega_j, \quad [u] = [Nu] = 0 & \text{on } \partial\Omega_j \setminus \partial\Omega \end{cases}$$

^a*Careful! Mixed boundary conditions on a smooth domain are a trap!*

Vertices and Edges



A non-Lipschitz polyhedron



Example: Electrostatic Potential in (Heterogeneous) Media

Domain Ω , 3D-polyhedron. $\Omega = \cup_j \Omega_j$, Ω_j 3D-polyhedron.

Each Ω_j is formed by an homogeneous medium: Constant electric permittivity ε_j .

Electrostatic potential u solution of the variational problem:

$$(\mathcal{P}) \quad u \in H_0^1(\Omega), \quad \forall v \in H_0^1(\Omega), \quad a(u, v) = \int_{\Omega} f v \, dx$$

with the bilinear form a

$$a(u, v) = \sum_j \int_{\Omega_j} \varepsilon_j \operatorname{grad} u \cdot \operatorname{grad} v \, dx.$$

Corresponding electrostatic field (solution of Maxwell equations at zero frequency)

$$E = \operatorname{grad} u$$

Vertex and edge singularities

For a polyhedron Ω and an operator L with constant coefficients.

With curved faces or variable coefficients, the edge singularities vary along their edge.

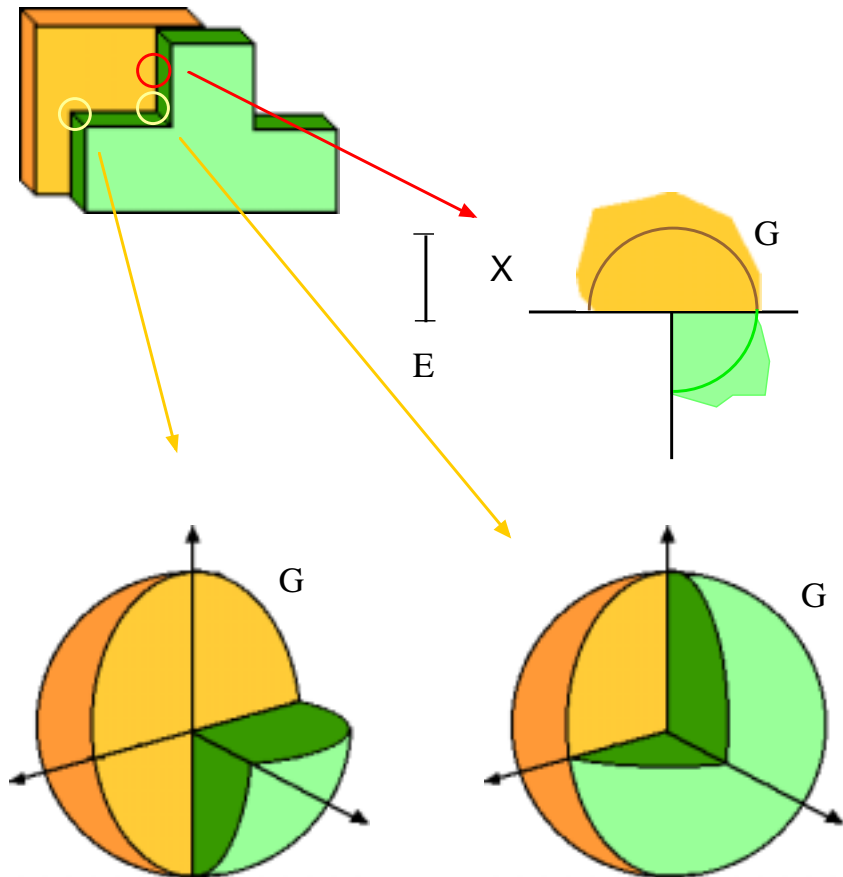
Corner c \longleftrightarrow **Polar coord.** $(\rho, \vartheta) \in \mathbb{R}_+ \times G_c$
centered in c .

$$\left\{ \begin{array}{ll} \text{Singularity Exponents} & \lambda \in \Lambda[c] \\ \text{Singular Functions} & U_{c,\lambda} = \rho^\lambda U_{c,\lambda}(\vartheta) \end{array} \right.$$

Edge e \longleftrightarrow **Cylindrical coord.**

$(r, \theta, z) \in \mathbb{R}_+ \times (0, \omega_e) \times e$.

$$\left\{ \begin{array}{ll} \text{Singularity Exponents} & \lambda \in \Lambda[e] \\ \text{Singular Functions} & U_{e,\lambda} = r^\lambda U_{e,\lambda}(\theta) \end{array} \right.$$



How to find Singular Functions

Corner c : Singular Function $U_{c,\lambda} = \rho^\lambda U_{c,\lambda}(\vartheta)$ in the cone

$$\Gamma_c = \{\mathbb{R}^3 \ni x \simeq (\rho, \vartheta) \in \mathbb{R}_+ \times G_c\}$$

Edge e : Singular Function $U_{e,\lambda} = r^\lambda U_{e,\lambda}(\theta)$ in the sector

$$\Gamma_e = \{\mathbb{R}^2 \ni y \simeq (r, \theta) \in \mathbb{R}_+ \times (0, \omega_e)\}$$

Singularities are special solutions of problem (\mathcal{P}) :

- With zero right hand sides,
- In infinite **cones Γ_c (for the corner c) or sectors Γ_e (for the edge e)**,
- Homogeneous in **ρ (for corners) or in r (for edges)**.

The problem of finding the singularities is a spectral problem

- ★ in the spherical polygon G_c for the corner c ,
- ★ in the intervals $(0, \omega_e)$ for the edge e .

.../...

Vertex Mellin Symbols

Vertex c (of Ω or Ω_j). In polar coordinates $(\rho, \vartheta) \in \mathbb{R}_+ \times G_c$

$$L = \rho^{-2} \mathcal{L}_c(\vartheta; \rho \partial_\rho, \partial_\vartheta), \quad \text{and} \quad B = \rho^{-\deg B} \mathcal{B}_c(\vartheta; \rho \partial_\rho, \partial_\vartheta).$$

Mellin Symbol and associated problem:

$$\mathbb{C} \ni \lambda \longmapsto \mathcal{L}_c(\vartheta; \lambda, \partial_\vartheta) =: \mathcal{L}_c(\lambda) \quad \text{and} \quad \mathbb{C} \ni \lambda \longmapsto \mathcal{B}_c(\vartheta; \lambda, \partial_\vartheta) =: \mathcal{B}_c(\lambda).$$

$$\mathcal{P}[c, \lambda] \begin{cases} \mathcal{L}_c(\lambda) U = F & \text{in } G_c, \\ \mathcal{B}_c(\lambda) U = 0 & \text{on } \partial G_c, \quad [U] = [\mathcal{N}_c U] = 0 & \text{on } \partial G_{c,j} \setminus \partial G_c \end{cases}$$

The ellipticity of problem (\mathcal{P}) implies the solvability of $\mathcal{P}[c, \lambda]$ in $H^1(G_c)$ **except for λ in a discrete set $\Lambda[c]$** . We repeat each $\lambda \in \Lambda[c]$ according to $\dim \ker \mathcal{P}[c, \lambda]$ and denote by $U_{c,\lambda}$ a basis of $\ker \mathcal{P}[c, \lambda]$.

The *singularity exponents* λ and the associated base *singular functions* at c are

$$\lambda \in \Lambda[c] \quad \text{with} \quad \operatorname{Re} \lambda > -\frac{1}{2} \quad \text{and} \quad U_{c,\lambda} = \rho^\lambda u_{c,\lambda}(\vartheta).$$

Edge Mellin Symbols

Edge e (of Ω or of Ω_j). In cylindrical coordinates $(r, \theta, z) \in \mathbb{R}_+ \times (0, \omega) \times e$,

$$L = r^{-2} \mathcal{L}_e(\theta; r\partial_r, \partial_\theta) + r^{-1} \mathcal{L}_1(\theta; r\partial_r, \partial_\theta, \partial_z) + \mathcal{L}_2(\theta; r\partial_r, \partial_\theta, \partial_z).$$

Mellin Symbol and associated problem:

$$\mathbb{C} \ni \lambda \longmapsto \mathcal{L}_e(\theta; \lambda, \partial_\theta) =: \mathcal{L}_e(\lambda) \quad \text{and} \quad \mathbb{C} \ni \lambda \longmapsto \mathcal{B}_e(\theta; \lambda, \partial_\theta) =: \mathcal{B}_e(\lambda).$$

$$\mathcal{P}[e, \lambda] \begin{cases} \mathcal{L}_e(\lambda) U = F & \text{in } G_e, \\ \mathcal{B}_e(\lambda) U = 0 & \text{on } \partial G_e, \quad [U] = [\mathcal{N}_e U] = 0 & \text{on } \partial G_{e,j} \setminus \partial G_e \end{cases}$$

The ellipticity of problem (\mathcal{P}) implies the solvability of $\mathcal{P}[e, \lambda]$ in $H^1(G_e)$ **except for λ in a discrete set $\Lambda[e]$** . **We repeat each $\lambda \in \Lambda[c]$ according to $\dim \ker \mathcal{P}[e, \lambda]$ and denote by $U_{e,\lambda}$ a basis of $\ker \mathcal{P}[e, \lambda]$.**

The *singularity exponents* λ and the associated base *singular functions* along e are

$$\lambda \in \Lambda[e] \quad \text{with} \quad \operatorname{Re} \lambda > 0 \quad \text{and} \quad U_{e,\lambda} = r^\lambda U_{e,\lambda}(\theta).$$

Singular Functions of the Laplace operator

When Ω has a constant coefficient ε .

Edge e with opening $\omega_e = \{G_e = (0, \omega_e)\}$

$$\left\{ \begin{array}{l} \text{Singularity Exponents} \quad \lambda \in \Lambda[e] = \left\{ \frac{\ell\pi}{\omega_e} \mid \ell \in \mathbb{N} \right\} \\ \text{Singular Functions} \quad U_{e,\lambda} = r^\lambda \sin(\lambda\theta). \end{array} \right.$$

Corner c with solid angle G_c .

Eigenpairs of the Laplace-Beltrami Dirichlet problem on G_c : $\{\mu_\ell, U_\ell(\vartheta)\}$

$$\left\{ \begin{array}{l} \text{Singularity Exponents} \quad \lambda \in \Lambda[c] = \left\{ -\frac{1}{2} + \sqrt{\mu_\ell + \frac{1}{4}} \mid \ell \in \mathbb{N} \right\} \\ \text{Singular Functions} \quad U_{c,\lambda} = \rho^{\lambda_\ell} U_\ell(\vartheta). \end{array} \right.$$

Shift Theorem

For smooth domains, there holds

$$f \in H^{\sigma-1}(\Omega) \implies u \in H^{\sigma+1}(\Omega).$$

Let $H_{\star}^s(\Omega)$ be the closure in $H^s(\Omega)$ of the smooth functions with their support outside the union of edges $\bigcup \bar{e}$. There holds

$$f \in H_{\star}^{\sigma-1}(\Omega) \implies u \in H_{\star}^{\sigma+1}(\Omega)$$

if and only if $\sigma < \sigma[\Omega, a]$

$$\sigma[\Omega, a] = \min \left\{ \min_{c \text{ corner}} \xi_c + \frac{1}{2}, \min_{e \text{ edge}} \xi_e \right\}$$

with

ξ_c the least (real part) $> -\frac{1}{2}$ of the exponents $\lambda \in \Lambda[c]$ and

ξ_e the least (real part) > 0 of the exponents $\lambda \in \Lambda[e]$.

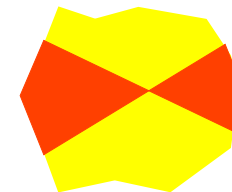
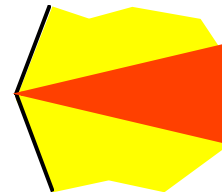
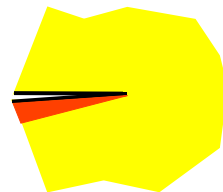
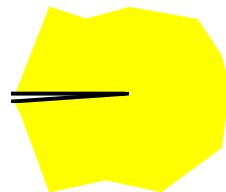
The shift Theo. in standard Sobolev spaces has to take polynomial RHS into account.

Edge regularity of electrostatic potential in heterogeneous media

Optimal Minima for ξ_e

(Regularity $H^{1+\xi_e}$ for potential and H^{ξ_e} for electric field) :

Exterior Angle	1 material	2 materials	3 materials	4 materials
$\leq \frac{\pi}{2}$	2	1	0	0
Convex	1	$\frac{1}{2}$	0	0
Any	$\frac{1}{2}$	$\frac{1}{4}$	0	0
None	∞	$\frac{1}{2}$	$\frac{1}{4}$	0



Expansion Theorem: first layer of singularities

For $\sigma > \sigma[\Omega, a]$ with $\sigma < \boxed{1 + \sigma[\Omega, a]}$ and a smooth RHS $f \in H_\star^\infty(\Omega)$

$$u - \left(\sum_{\text{c corner}} \chi_c u_c + \sum_{\text{e edge}} \chi_e u_e \right) \in H_\star^{\sigma+1}(\Omega),$$

with the cut-off $\chi_c = \chi_c(\rho)$ and $\chi_e = \chi_e(r/\rho)$. The corner and edge contributions are:

$$u_c = \sum_{\substack{\lambda \in \Lambda[c] \\ -1/2 < \lambda < \sigma - 1/2}} \gamma_{c,\lambda} U_{c,\lambda} \quad \text{and} \quad u_e = \sum_{\substack{\lambda \in \Lambda[e] \\ 0 < \lambda < \sigma}} \gamma_{e,\lambda}(z) U_{e,\lambda}$$

where

- $\gamma_{c,\lambda} \in \mathbb{R}$ are the vertex coefficients
- $e \ni z \mapsto \gamma_{e,\lambda}$ are the edge coefficients along e . They are $C^\infty(e)$ (inside e).

Note: This expansion is valid if the inverses of Mellin symbols have poles of degree 1 in the exponents of singularities. If there exist poles with degree ≥ 2 , other singular functions with logarithmic terms $\rho^\lambda \log^k \rho$ or $r^\lambda \log^k r$ appear.

Expansion Theorem: more layers of singularities

For $\sigma \geq 1 + \sigma[\Omega, a]$ and a smooth RHS $f \in H_\star^\infty(\Omega)$

$$u - \left(\sum_{c \text{ corner}} \chi_c u_c + \sum_{e \text{ edge}} \chi_e u_e \right) \in H_\star^{\sigma+1}(\Omega),$$

with the corner and edge contributions:

$$u_c = \sum_{\substack{\lambda \in \Lambda[c] \\ -1/2 < \lambda < \sigma - 1/2}} \gamma_{c,\lambda} U_{c,\lambda} \quad \text{and} \quad u_e = \sum_{\substack{\lambda \in \Lambda[e] \\ 0 < \lambda + p < \sigma}} \sum_{p \in \mathbb{N}_0} d_z^p \gamma_{e,\lambda}(z) U_{e,\lambda}^p$$

where

- $\gamma_{c,\lambda} \in \mathbb{C}$ are the vertex coefficients (with more terms)
- $e \ni z \mapsto \gamma_{e,\lambda}$ are the edge coefficients along e (with more terms)
- For $p = 0$, $U_{e,\lambda}^0 = U_{e,\lambda}$.
For $p \geq 1$, the new singularities $U_{e,\lambda}^p$ have the form $U_{e,\lambda}^p = r^{\lambda+p} U_{e,\lambda}^p(\theta)$.

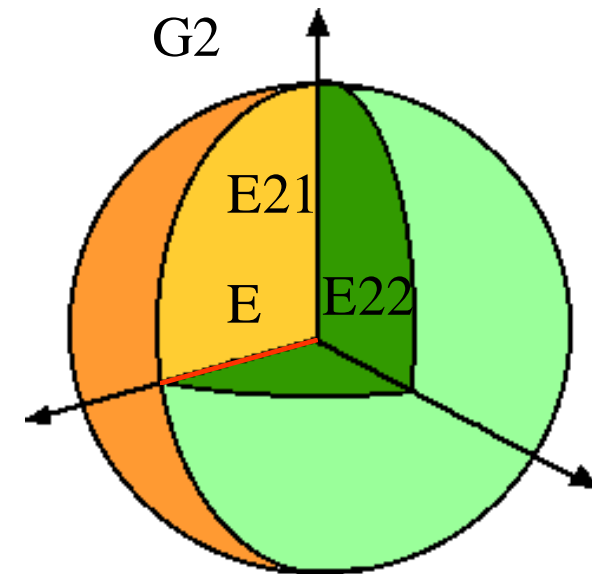
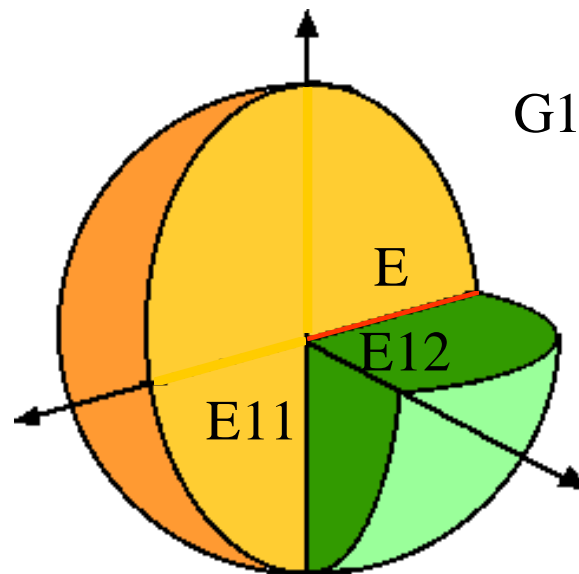
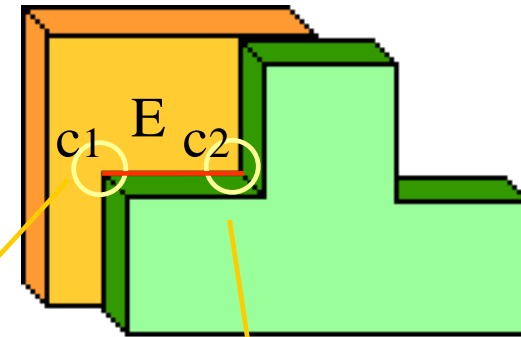
Vertex – Edge interaction: the geometry

The edge E has the vertices $c1$ and $c2$ as end points.

Vertices $c1 - c2 \longleftrightarrow$ spherical polygons $G1 - G2$.

Corners of $G1 \longleftrightarrow$ edges E , $E11$ and $E12$.

Corners of $G2 \longleftrightarrow$ edges E , $E21$ and $E22$.



Vertex – Edge interaction: edge coefficients

We have

$$u = \left(\sum_{c \text{ corner}} \chi_c u_c + \sum_{e \text{ edge}} \chi_e u_e \right) \in H_{\star}^{\sigma+1}(\Omega),$$

with the corner and edge contributions:

$$u_c = \sum_{\substack{\lambda \in \Lambda[c] \\ -1/2 < \lambda < \sigma - 1/2}} \gamma_{c,\lambda} U_{c,\lambda} \quad \text{and} \quad u_e = \sum_{\substack{\nu \in \Lambda[e] \\ 0 < \nu + p < \sigma}} \sum_{p \in \mathbb{N}_0} d_z^p \gamma_{e,\nu}(z) U_{e,\nu}^p$$

For the edge $e = \{z \in (z_1, z_2)\}$, the edge coefficients satisfy

$$\delta^{\alpha-\sigma}(z) d_z^{\alpha} \gamma_{e,\nu} \in L^2(e), \quad \forall \alpha \in \mathbb{N}_0$$

where $\delta = (z - z_1)(z_2 - z)$ is \simeq the distance to the endpoints of e .

When σ increases, the corner coefficients are only more numerous.

When σ increases, the edge coefficients depend on σ .

Should write instead:

Vertex – Edge interaction: edge coefficients

We have

$$u = \left(\sum_{c \text{ corner}} \chi_c u_c + \sum_{e \text{ edge}} \chi_e u_e \right) \in H_{\star}^{\sigma+1}(\Omega),$$

with the corner and edge contributions:

$$u_c = \sum_{\substack{\lambda \in \Lambda[c] \\ -1/2 < \lambda < \sigma - 1/2}} \gamma_{c,\lambda} U_{c,\lambda} \quad \text{and} \quad u_e = \sum_{\substack{\nu \in \Lambda[e] \\ 0 < \nu + p < \sigma}} \sum_{p \in \mathbb{N}_0} d_z^p \gamma_{e,\nu}^{(\sigma)}(z) U_{e,\nu}^p$$

For the edge $e = \{z \in (z_1, z_2)\}$, the edge coefficients satisfy

$$\delta^{\alpha-\sigma}(z) d_z^{\alpha} \gamma_{e,\nu}^{(\sigma)} \in L^2(e), \quad \forall \alpha \in \mathbb{N}_0$$

where $\delta = (z - z_1)(z_2 - z)$ is \simeq the distance to the endpoints of e .

When σ increases, the corner coefficients are only more numerous.

When σ increases, the edge coefficients $\gamma_{e,\nu}^{(\sigma)}$ are more and more flat.

Vertex – Edge interaction: stress intensity functions

We have

$$u = \left(\sum_{c \text{ corner}} \chi_c \tilde{u}_c + \sum_{e \text{ edge}} \chi_e \tilde{u}_e \right) \in H_{\star}^{\sigma+1}(\Omega),$$

with the corner and edge contributions:

$$\tilde{u}_c = \sum_{\substack{\lambda \in \Lambda[c] \\ -1/2 < \lambda < \sigma - 1/2}} \gamma_{c,\lambda} \tilde{U}_{c,\lambda}^{(\sigma)} \quad \text{and} \quad \tilde{u}_e = \sum_{\substack{\nu \in \Lambda[e] \\ 0 < \nu + p < \sigma}} \sum_{p \in \mathbb{N}_0} d_z^p \tilde{\gamma}_{e,\nu}(z) U_{e,\nu}^p$$

For the edge $e = \{z \in (z_1, z_2)\}$, the edge coefficients satisfy

$$\delta^\alpha(z) d_z^\alpha \tilde{\gamma}_{e,\nu} \in L^2(e), \quad \forall \alpha \in \mathbb{N}_0$$

where $\delta = (z - z_1)(z_2 - z)$ is \simeq the distance to the endpoints of e .

When σ increases, the corner functions are more and more flat.

The edge coefficients (stress intensity functions) $\tilde{\gamma}_{e,\nu}$ are more numerous.

Vertex – Edge interaction: expansion of corner singularities

Case $\sigma < \sigma[\Omega, a] + 1$. In the corner contribution

$$u_c = \sum_{\substack{\lambda \in \Lambda[c] \\ -1/2 < \lambda < \sigma - 1/2}} \gamma_{c,\lambda} U_{c,\lambda}(x) = \sum_{\substack{\lambda \in \Lambda[c] \\ -1/2 < \lambda < \sigma - 1/2}} \boxed{\gamma_{c,\lambda} \rho^\lambda} U_{c,\lambda}\left(\frac{x}{\rho}\right)$$

the angular function $U_{c,\lambda}$ has singularities at the corners of G_c (\leftrightarrow edges $\bar{e} \ni c$):

$$U_{c,\lambda}\left(\frac{x}{\rho}\right) = \sum_{\bar{e} \ni c} \sum_{\substack{\nu \in \Lambda[e] \\ 0 < \nu < \sigma}} \boxed{a_{e,\nu}^{c,\lambda}} U_{e,\nu}\left(\frac{r}{\rho}, \theta\right) = \tilde{u}_{c,\lambda}^{(\sigma)} \in H_\star^{\sigma+1}(G_c).$$

Note that $U_{e,\nu}\left(\frac{r}{\rho}, \theta\right) = \boxed{\rho^{-\nu}} U_{e,\nu}(r, \theta)$. Expansion of the corner singularities

$$u_c = \sum_{\substack{\lambda \in \Lambda[c] \\ -1/2 < \lambda < \sigma - 1/2}} \sum_{\bar{e} \ni c} \sum_{\substack{\nu \in \Lambda[e] \\ 0 < \nu < \sigma}} \boxed{\gamma_{c,\lambda} \rho^\lambda} \boxed{a_{e,\nu}^{c,\lambda}} \boxed{\rho^{-\nu}} U_{e,\nu}(r, \theta) = \tilde{u}_c.$$

Vertex – Edge interaction: expansion of Stress Intensity Functions

The expansion of the corner singularities

$$u_c = \sum_{\substack{\lambda \in \Lambda[c] \\ -1/2 < \lambda < \sigma - 1/2}} \sum_{\bar{e} \ni c} \sum_{\substack{\nu \in \Lambda[e] \\ 0 < \nu < \sigma}} \boxed{\gamma_{c,\lambda} \rho^\lambda} \boxed{a_{e,\nu}^{c,\lambda}} \boxed{\rho^{-\nu}} U_{e,\nu}(r, \theta) = \tilde{u}_c$$

gives the stress intensity functions of u_c along the edges e such that $\bar{e} \ni c$:

They are

$$\boxed{a_{e,\mu}^{c,\lambda}} \boxed{\gamma_{c,\lambda} \rho^\lambda} \boxed{\rho^{-\nu}}$$

Note that $\rho = z - z_1$ is a suitable coordinate along the edge(s) e .

Therefore, we find the expansion at the corner c of the stress intensity functions:

$$\tilde{\gamma}_{e,\nu}(\rho) = \sum_{\substack{\lambda \in \Lambda[c] \\ -1/2 < \lambda < \sigma - 1/2}} \boxed{a_{e,\mu}^{c,\lambda} \gamma_{c,\lambda} \rho^\lambda \rho^{-\nu}} = \gamma_{e,\nu}^{(\sigma)}(\rho)$$

Are Stress Intensity Functions bounded ?

The interesting SIF are those associated with the first edge exponent ν_1 .

The SIF $\tilde{\gamma}_{e,\nu}$ is bounded iff $\lambda_1 \geq \nu_1$ with λ_1 the first corner exponent.

- Example of Laplace Dirichlet.

Fichera corner: $\lambda_1 \simeq 0.45418$ and $\nu_1 = \pi/(3\pi/2) = 2/3$.

Screen problem: $\Gamma_c = \mathbb{R}^3 \setminus S_\omega$ (S_ω plane sector of opening ω).

$\nu_1 = 1/2$ and $\lambda_1 = \lambda_1(\omega)$ where λ_1 is increasing

$$\lambda_1(0) = 0 \quad \text{and} \quad \lambda_1(2\pi) = 1 \quad (\text{and also } \lambda_1(\pi) = 1/2).$$

- Maxwell (electric).

Same difference $\lambda_1 - \nu_1$ than for Laplace-Dirichlet, since the first electric singularities are the gradients of the Laplace-Dirichlet singularities:

$$E_{c,\lambda} = \nabla_{x,y,z} U_{c,\lambda+1}^{\Delta,\text{Dir}} \quad \text{and} \quad E_{e,\lambda} = \nabla_{x,y} U_{e,\lambda+1}^{\Delta,\text{Dir}}.$$