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MODELING OF FLUID DIFFUSION IN LAYERS WITH DOUBLE POROSITY USING HOMOGENIZATION

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Summary: The paper deals with the perfusion in hierarchically arranged double porous media constituted by transversely periodic layers. In each layer the reference periodic cell is composed of several compartments comprising the matrix, featured by permeability decreasing with the scale parameter, and several disconnected channels where the permeability is scale independent. Homogenization of the steady Darcy flow in such medium is performed by the method of periodic unfolding. The limit model involves the homogenized permeabilities associated with the channels and the transmission and drainage coefficients associated with the mass redistribution between the microstructural compartments. Due to the layered organization of the medium, the diffusion problem in 3D heterogeneous body can be replaced by a finite number of 2D problems describing the homogenized fluid redistribution in each homogenized layer. For such decomposition, coupling conditions governing the fluid exchange between the layers can be derived. This model is intended for simulations of the blood perfusion in the brain tissue.

1. Introduction

In this paper we report results on the upscaling Darcy flow in the strongly heterogeneous porous material composed of two highly permeable disconnected compartments – the *channels*, separated by the *matrix*, where in the latter one the permeability coefficients are proportional to the square of the heterogeneity scale; this is the usual ansatz of treatment the double porosity media, see (5; 1; 2; 4; 10). The model is being developed for its application in biomechanics of of the "hierarchical perfusion" in the brain tissue. We assume that the structure is formed by layers and is transversely periodic in each layer. Here we treat only the homogenization of the perfusion problem imposed in one layer. Such a homogenized model of the perfused single layer can be adapted to describe perfusion in the double porosity media consisting of several layers.

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Figure 1: The layer of the three compartment heterogeneous structure and the domain and boundary decomposition of the reference periodic cell Y.

2. Problem description

We consider diffusion problem in layer $\Omega^{\delta} \subset \mathbb{R}^3$ with small thickness $\delta \to 0$. Let $\Gamma_0 \subset \mathbb{R}^2$ be the mid-surface of Ω^{δ} spanned by coordinates $x' = (x_{\alpha}), \alpha = 1, 2$, so that

$$\Omega^{\delta} = \Gamma_0 imes] - \delta/2, + \delta/2 [$$
 .

The perfusion in the single layer is defined by solutions of the following b.v. problem:

$$\nabla \cdot (\boldsymbol{\kappa}^{\varepsilon\delta} \cdot \nabla p^{\varepsilon\delta}) = 0 \quad \text{in } \Omega^{\delta} ,$$

$$\boldsymbol{n} \cdot \boldsymbol{\kappa}^{\varepsilon\delta} \cdot \nabla p^{\varepsilon\delta} = 0 \quad \text{on } \Gamma^{\infty\delta} , \quad \boldsymbol{n} \cdot \boldsymbol{\kappa}^{\varepsilon\delta} \cdot \nabla p^{\varepsilon\delta} = g^{\varepsilon\delta\pm} \text{ on } \Gamma^{\delta+} \cup \Gamma^{\delta-} , \qquad (1)$$

where $g^{\varepsilon\pm}$ is the perfusion flux and **n** is the normal vector. The permeability $\boldsymbol{\kappa}^{\varepsilon\delta}$ is defined piecewise w.r.t. the decomposition of Ω^{δ} into three disjoint parts – two "channels" $\Omega_A^{\varepsilon\delta}$, $\Omega_B^{\varepsilon\delta}$ and the "matrix" $\Omega_M^{\varepsilon\delta}$ which separate them, $\Omega^{\delta} = interior \overline{\Omega_M^{\varepsilon\delta} \cup \Omega_A^{\varepsilon\delta} \cup \Omega_B^{\varepsilon\delta}}$, as illustrated in Fig. 1; we consider the following double porosity ansatz, cf. (5; 4; 10),

$$\boldsymbol{\kappa}^{\varepsilon\delta}(x) = \begin{cases} \boldsymbol{K}^{\varepsilon\delta}(x) & x \in \Omega_D^{\varepsilon\delta}, \quad D = A, B, \\ \varepsilon^2 \bar{\boldsymbol{\kappa}}^{\varepsilon\delta}(x) & x \in \Omega_M^{\varepsilon\delta}. \end{cases}$$
(2)

2.1. Dilated weak formulation

The weak formulation of (1) is introduced by the following identity: given $g^{\varepsilon\delta\pm} \in L^2(\Gamma^{\pm\delta})$, find $p^{\varepsilon\delta} \in H^1(\Omega^{\delta})/\mathbb{R}$ such that

$$\sum_{D=A,B} \int_{\Omega_D^{\varepsilon\delta}} \nabla q \cdot \boldsymbol{K}^{\varepsilon\delta} \cdot \nabla p^{\varepsilon\delta} + \int_{\Omega_M^{\varepsilon\delta}} \nabla q \cdot \varepsilon^2 \bar{\boldsymbol{\kappa}}^{\varepsilon\delta} \cdot \nabla p^{\varepsilon\delta} = \int_{\Gamma^{+\delta} \cup \Gamma^{-\delta}} g^{\pm\varepsilon\delta} q \, \mathrm{dS}_x \quad \forall q \in H^1(\Omega^{\delta}) .$$
(3)

Since (1) is the Neumann type problem, its solution exists provided the boundary fluxes are equilibrated:

$$\int_{\Gamma^{\pm\varepsilon\delta}} g^{\varepsilon\delta\pm} \,\mathrm{dS}_x = 0 \;. \tag{4}$$

If this *solvability condition* is satisfied, due to (2), for $\varepsilon > 0$ the existence of solutions results from the Lax–Milgram theorem. Since $p^{\varepsilon\delta}$ is defined up to a constant, to obtain a unique solution, we may impose the following condition,

$$\int_{\Omega_A^{\varepsilon\delta}} p^{\varepsilon\delta} = 0 , \qquad (5)$$

which will also be used to obtain a priori estimates of the solution. Obviously, in the above condition we could replace A by B.

Dilated formulation Variational equality (3) can be written equivalently in the dilated configuration where instead of Ω^{δ} the layer is represented by domain $\Omega = \Gamma_0 \times] - 1/2, +1/2[$ having unit thickness. For given $g^{\varepsilon \pm} \in L^2(\Gamma^{\pm})$, find $p^{\varepsilon} \in H^1(\Omega)/\mathbb{R}$ such that

$$\sum_{D=A,B} \int_{\Omega_D^{\varepsilon}} \nabla q \cdot \mathbf{K}^{\varepsilon} \cdot \nabla p^{\varepsilon} + \int_{\Omega_M^{\varepsilon}} \nabla q \cdot \varepsilon^2 \bar{\mathbf{\kappa}}^{\varepsilon} \cdot \nabla p^{\varepsilon} = \frac{1}{\delta} \int_{\Gamma^+ \cup \Gamma^-} g^{\pm \varepsilon} q \, \mathrm{dS}_x \quad \forall q \in H^1(\Omega) \,. \tag{6}$$

2.2. Periodic microstructure — representative cell

We set $\Xi =]0, 1[^2, I_z =] - 1/2, 1/2[$ and introduce the reference periodic cell, $Y = \Xi \times I_z$. The periodic *dilated* structure of layer Ω is generated by cells $Y^{\varepsilon} = \varepsilon \Xi \times I_z = \{(\varepsilon y', z) \in \mathbb{R}^2 \times \mathbb{R}, (y', z) \in Y\}$. The periodic structure decomposing Ω is generated by the following decomposed structure of Y: let $Y_A, Y_B, Y_M \subset Y$ be mutually disjoint open bounded such that

$$Y = Y_M \cup \left(\sum_{D=A,B} Y_D\right) \cup \left(\sum_{D=A,B} \partial_M Y_D\right) \ , \partial_M Y_D = \partial_D Y_M = \overline{Y_D} \cap \overline{Y_M}, \quad D = A, B \ . \ (7)$$

Any of the (dilated) subdomains Ω_D^{ε} , D = A, B, M is generated as the lattice:

$$\Omega_D^{\varepsilon} = \bigcup_{k \in \mathbb{K}^{\varepsilon}} \left(Y_D^{\varepsilon} + \varepsilon \sum_{\alpha = 1, 2} k_{\alpha} \vec{e}_{\alpha} \right) , \quad Y_D^{\varepsilon} = \{ (\varepsilon y', z) \in Y^{\varepsilon}, \ (y', z) \in Y_D \} , \tag{8}$$

where $\vec{e}_{\alpha} = (\delta_{\alpha 1}, \delta_{\alpha 2}, 0)$ and $\mathbb{K}^{\varepsilon} = \{(k_{\alpha}), \alpha = 1, 2, k_{\alpha} \in \mathbb{Z} : (Y^{\varepsilon} + \sum_{\alpha = 1, 2} k_{\alpha} \vec{e}_{\alpha}) \subset \Omega\}$, where $\delta_{\alpha\beta}$ is the Kronecker symbol.

The upper and lower boundaries of Y are denoted by $\partial Y^{\pm} = \Xi \times z^{\pm}$ where $z^{\pm} = \pm 1/2$. Further, we introduce the boundary segments $\partial^{\pm}Y = \overline{\Xi \times z^{\pm}}$ and define

$$\partial_{\pm}Y_D = \partial^{\pm}Y \cap \partial Y_D , \quad D = A, B, M .$$
 (9)

Channels represented by Y_D , D = A, B have branches intersecting $\partial_{\pm} Y$ at surfaces \mathcal{A}_D^k (channel inlets, outlets), $k \in J_D$, where J_D is the index set, so that

$$\partial_{\pm} Y_D = \bigcup_{k \in J_D} \mathcal{A}_D^k . \tag{10}$$

3. Homogenization result

The homogenized layer is described by macroscopic model involving homogenized coefficients which characterize permeability of the layer and fluid redistribution between different compartments. The homogenized coefficients are determined by the microstructure of the layer and by solutions of the microscopic problems.

3.1. Microscopic problems – corrector basis functions

In this section we introduce the so-called corrector basis functions as the solutions of a local microscopic problems which are imposed in channels Y_D , D = A, B, and in the matrix Y_M . Below we use these functions to define the homogenized coefficients involved in the homogenized macroscopic problem.

Microscopic problem in Y_D . For corrector functions associated with the channel inlet, outlet surfaces \mathcal{A}_D^k , $k \in J_D$, we need the following space decomposition employed below in (13). Any $q \in H^1(\mathcal{Y}) \cap H^1(Y_D)$ can be written as

$$q = \sum_{k \in J_D} q^k \quad \text{where } q^k \in \mathcal{V}^k \equiv \{ \psi \in H^1(\mathcal{Y}) \cap H^1(Y_D) \mid \psi = 0 \text{ on } \partial Y \setminus \mathcal{A}^k \} .$$
(11)

Note that $\bigcup_{i \in J_D} \mathcal{V}^i = H^1(\mathcal{Y}) \cap H^1(Y_D)$.

1. Find $\pi_D^\beta \in H^1(\mathcal{Y})/\mathbb{R}$ for $\beta = 1, 2$ such that

$$\int_{Y_D} \left(\mathbf{K} \cdot \nabla_y^h \pi_D^\beta \right) \cdot \nabla_y^h \phi = - \int_{Y_D} \left(\mathbf{K} \cdot \nabla_y^h \phi \right)_\beta \quad \forall \phi \in H^1(\mathcal{Y}),$$
(12)

2. We define function $\gamma_D^k \in H^1(\mathcal{Y}) \cap H^1(Y_D)$ using the split

$$\gamma_D^k = \hat{\gamma}_D^k + \tilde{\gamma}_D^k , \quad \hat{\gamma}_D^k \in \mathcal{V}^k , \tag{13}$$

where for any $k \in J_D$ functions $\hat{\gamma}_D^k$, $\tilde{\gamma}_D^k$ are solutions of the following problems:

(a) Find $\hat{\gamma}_D^k$ such that

$$\int_{Y_D} \left(\mathbf{K} \cdot \nabla_y^h \hat{\gamma}_D^k \right) \cdot \nabla_y^h q = \frac{1}{h} \int_{\mathcal{A}^k} \tilde{\chi}_D^k q \, \mathrm{dS}_y \qquad \forall q \in \mathcal{V}^k \;, \tag{14}$$

(b) Find $\tilde{\gamma}_D^k = \sum_{j \in J_D} \tilde{\gamma}_D^{kj}$, where $\tilde{\gamma}_D^{kj} \in \mathcal{V}^j$, such that $\{\gamma_D^{kj}\}_j, j \in J_D$ solves

$$\sum_{j\in J_D} \int_{Y_D} \left(\mathbf{K} \cdot \nabla_y^h \tilde{\gamma}_D^{kj} \right) \cdot \nabla_y^h q^i = (\delta_{ki} - 1) \int_{Y_D} \left(\mathbf{K} \cdot \nabla_y^h \hat{\gamma}_D^k \right) \cdot \nabla_y^h q^i \qquad \forall q^i \in \mathcal{V}^i \ , \forall i \in J_D$$
(15)

Microscopic problem in Y_M . We introduce corrector basis functions $\eta_A, \eta_B \in H^1(\mathcal{Y}) \cap H^1(Y_M)$ and $\gamma^{+/-} \in H^1_{\#0}(\mathcal{Y}, Y_M)$ which satisfy the following Dirichlet conditions:

for
$$D = A, B$$
, $\eta_D = \delta_{DR}$ on $\partial_M Y_R$, $R = A, B$,
 $\gamma^{+/-} = 0$ on $\partial_M Y_A \cup \partial_M Y_B$. (16)

The following two subproblems are verified by $\gamma^{+/-}$ and η_D :

1. Find $\eta_D \in H^1(\mathcal{Y}) \cap H^1(Y_M)$, D = A, B with condition (16)₁ satisfied, such that

$$\int_{Y_M} \left(\bar{\boldsymbol{\kappa}} \cdot \nabla^h_y \eta_D \right) \cdot \nabla^h_y \phi = 0 \quad \forall \phi \in H^1_{\#0}(\mathcal{Y}, Y_M)$$
(17)

Due to conditions $(16)_1$,

$$\eta_B = 1 - \eta_A , \qquad (18)$$

so that η_B can be obtained easily once η_A is resolved, thus, only one problem (17) needs to be solved for either D = A, or D = B. On integrating by parts in (17), assuming enough regularity, the following boundary conditions hold for η_D , D = A, B:

$$\boldsymbol{n} \cdot \bar{\boldsymbol{\kappa}} \cdot \nabla_{\boldsymbol{y}}^{h} \eta_{D} = 0 \quad \text{on } \partial_{\pm} Y_{M} .$$
⁽¹⁹⁾

On $\partial_D Y_M$ the Dirichlet conditions are given by (16)₁.

2. Find $\gamma^+ \in H^1_{\#0}(\mathcal{Y}, Y_M)$ such that

$$\int_{Y_M} \left(\bar{\kappa} \cdot \nabla_y^h \gamma^+ \right) \cdot \nabla_y^h \phi = \frac{1}{h} \int_{\partial_+ Y_M} \phi \mathrm{dS}_y \quad \forall \phi \in H^1_{\#0}(\mathcal{Y}, Y_M).$$
(20)

Analogous problem can be defined to compute γ^- ; for this the r.h.s. integral is evaluated over ∂Y_M^- . Let us summarize that problem (20) is featured by the following boundary conditions:

$$\gamma^{+} = \gamma^{-} = 0 \quad \text{on } \partial_{A}Y_{M} \cup \partial_{B}Y_{M},$$

$$\boldsymbol{n}^{+/-} \cdot \bar{\boldsymbol{\kappa}} \cdot \nabla_{y}^{h} \gamma^{+/-} = 1 \quad \text{on } \partial_{+/-}Y_{M},$$

$$\boldsymbol{n}^{-/+} \cdot \bar{\boldsymbol{\kappa}} \cdot \nabla_{y}^{h} \gamma^{+/-} = 0 \quad \text{on } \partial_{-/+}Y_{M},$$

(21)

where \mathbf{n}^{\pm} is the unit normal vector on $\partial_{\pm}Y$ outward to Y_M and notation +/-, or -/+ means the respective alternatives.

3.2. Homogenized coefficients

Using the corrector basis functions the following homogenized coefficients are introduced which describe permeability properties of the layer (for detailed derivation see (7)).

• The *in-plane permeability* of channel D = A, B:

$$\mathcal{K}^{D}_{\alpha\beta} = \int_{Y_{D}} \left(\mathbf{K} \cdot \nabla^{h}_{y} (\pi^{\alpha}_{D} + y_{\alpha}) \right) \cdot \nabla^{h}_{y} (\pi^{\beta}_{D} + y_{\beta}) , \qquad \alpha, \beta = 1, 2 , \qquad (22)$$

where the symmetric form follows from (12) on substituting there $\phi = \pi_D^{\beta}$.

• The Barenblatt transmission coefficient:

$$\mathcal{G} := \mathcal{G}^{A} = \int_{\partial_{A}Y_{M}} \boldsymbol{n}^{[M]} \cdot \bar{\boldsymbol{\kappa}} \cdot \nabla_{y}^{h} \eta_{A} \, dS_{y} = -\int_{\partial_{A}Y_{M}} \boldsymbol{n}^{[M]} \cdot \bar{\boldsymbol{\kappa}} \cdot \nabla_{y}^{h} \eta_{B} \, dS_{y} = -\mathcal{G}^{AB} \, . \tag{23}$$

Moreover, it holds that $\mathcal{G}^A = \mathcal{G}^B = \mathcal{G}$, thereby also $\mathcal{G}^{AB} = \mathcal{G}^{BA} = -\mathcal{G}$; this result is a simple consequence of $\eta_B = 1 - \eta_A$.

• The *Matrix drainage* coefficient ($\mathcal{F}^{B+/-}$ defined in analogy):

$$\mathcal{F}^{A+/-} = \int_{\partial_A Y_M} \boldsymbol{n}^{[M]} \cdot \bar{\boldsymbol{\kappa}} \cdot \nabla_y^h \gamma^{+/-} \, \mathrm{dS}_y \tag{24}$$

• The *Branch saturation* coefficient ($S^{B,k}_{\alpha}$ defined in analogy for $k \in J_B$):

$$\mathcal{S}_{\alpha}^{A,k} = \int_{Y_A} (\mathbf{K} \cdot \nabla_y^h \gamma_A^k)_{\alpha} = \int_{Y_A} (\mathbf{K} \cdot \nabla_y^h \gamma_A^k) \cdot \nabla_y^h y_{\alpha} , \quad k \in J_A .$$
(25)

It is worth noting that $\mathcal{G}^D, \mathcal{F}^{D+/-}$ vanish, when $\mathbf{n}^{[M]} \cdot \bar{\mathbf{\kappa}}(y) \to 0$ for $y \in \partial_D Y_M$. In such a case channel Y_D has impermeable boundary $\partial_M Y_D$, so that neither drainage through $\partial_{\pm} Y_M$, nor via the other channel is possible.

3.3. Macroscopic problem on layer Γ_0

The macroscopic problem describes in terms of the channel pressures $p^{0,A}$ and $p^{0,B}$ the fluid redistribution in the homogenized layer represented by the midsurface Γ_0 . The data of the problem are the fluid fluxes prescribed on the "upper" and "lower" boundaries of the layer; in the limit model these fluxes are represented by the *channel branch fluxes* $g_D^k \in L^2(\Gamma_0)$ for $k \in J_k$, D = A, B describing fluxes through surfaces \mathcal{A}_D^k , and by the *matrix* fluxes $g^+, g^- \in L^2(\Gamma_0)$ which describe the fluid exchange through $\partial_{\pm}Y_M$, i.e. the dual porosity and the exterior.

The limit equations involve fluxes \tilde{g}_D^k which are introduced using $g_D^k \in L^2(\Gamma_0)$ (defined independently each of the others) as follows

$$\bar{g}_D = \frac{\sum_{k \in J_D} g_D^k |\mathcal{A}^k|}{\sum_{l \in J_D} |\mathcal{A}^l|} , \quad \tilde{g}_D^k = g_D^k - \bar{g}_D , \qquad (26)$$

a.e. on Γ_0 .

The limit problem involving the homogenized coefficients (22)-(25) is described by two equations describing the in-plane redistribution in channels A and B (the Einstein summation convention is applied for repeated indices $\alpha, \beta = 1, 2$). Given fluxes \bar{g}_D and \tilde{g}_D^k , $k \in J_k$, D = A, B and g^+, g^- , compute $p^{0,A}, p^{0,B} \in H^1(\Gamma_0)$ such that

$$\int_{\Gamma_0} \mathcal{K}^A_{\alpha\beta} \partial^x_{\alpha} p^{0,A} \partial^x_{\beta} q + \int_{\Gamma_0} \mathcal{G}^A \left(p^{0,A} - p^{0,B} \right) q$$

$$= \frac{1}{h} \int_{\Gamma_0} q \, \bar{G}_A - \sum_{k \in J_A} \int_{\Gamma_0} \mathcal{S}^{A,k}_{\alpha} \tilde{g}^k_A \partial^x_{\alpha} q - \int_{\Gamma_0} \left(\mathcal{F}^{A+} g^+ + \mathcal{F}^{A-} g^- \right) q \quad \forall q \in H^1(\Gamma_0)$$
(27)

$$\int_{\Gamma_0} \mathcal{K}^B_{\alpha\beta} \partial^x_{\alpha} p^{0,B} \partial^x_{\beta} q + \int_{\Gamma_0} \mathcal{G}^B \left(p^{0,B} - p^{0,A} \right) q$$

= $\frac{1}{h} \int_{\Gamma_0} q \, \bar{G}_B - \sum_{k \in J_B} \int_{\Gamma_0} \mathcal{S}^{B,k}_{\alpha} \tilde{g}^k_B \partial^x_{\alpha} q - \int_{\Gamma_0} \left(\mathcal{F}^{B+} g^+ + \mathcal{F}^{B-} g^- \right) q \quad \forall q \in H^1(\Gamma_0) .$

In-plane permeability	$\mathcal{K}^A = \begin{bmatrix} 4.115 & 0.0\\ 0.0 & 4.250 \end{bmatrix} \times 10^{-3}$
	$\mathcal{K}^B = \begin{bmatrix} 4.382 & 0.0\\ 0.0 & 5.699 \end{bmatrix} \times 10^{-3}$
Barenblatt transmission	$\mathcal{G} = 4.144$
Matrix drainage	$\mathcal{F}^A = \begin{bmatrix} -0.199 & -0.317 \end{bmatrix}$
	$\mathcal{F}^B = \begin{bmatrix} -0.368 & -0.265 \end{bmatrix}$
Branch saturation	$\mathcal{S}^{A,1} = [0.090 \ -1.469] \times 10^{-3}$
	$\mathcal{S}^{B,1} = \begin{bmatrix} 0.026 & 2.581 \end{bmatrix} \times 10^{-3}$
	$\mathcal{S}^{A,2} = \begin{bmatrix} 0.043 & -1.709 \end{bmatrix} \times 10^{-3}$
	$\mathcal{S}^{B,2} = \begin{bmatrix} 0.008 & 0.682 \end{bmatrix} \times 10^{-3}$
	$\mathcal{S}^{A,3} = \begin{bmatrix} 0.0217 & 3.829 \end{bmatrix} \times 10^{-3}$
	$\mathcal{S}^{B,3} = \begin{bmatrix} 0.024 & -4.115 \end{bmatrix} \times 10^{-3}$

Table 1: Homogenized coefficients of the 3D microstructure.

For detailed development of the model we refer to (7). The model is implemented numerically in our in-house developed software SfePy which is based on the finite element method, see http://sfepy.kme.zcu.cz, http://sfepy.org

4. Numerical illustrations

In this section we give an illustrative example of a specific double porosity microstructure and the associated homogenized coefficients introduced above. The geometry of the representative volume element (periodic cell) Y at the microscopic scale is depicted in Fig. 2. The RVE consists of matrix represented by Y_M and two embedded channels A (red), B (blue). In Figs. 3 and 4 we show computed corrector functions $\pi_A^{1,2}$ (see (12)) in channel A and $\gamma^{+,-}$ (see (20)) in matrix Y_M . The homogenized coefficients (22)-(25) of the 3D microstructure are in Table 1.

The homogenization procedure leading to model (27) is described in (7). In a forthcoming publication we shall explain in detail numerical aspects of the multiscale modeling for the case of multiple layers.

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Figure 2: Geometry of the reference periodic cell Y: two channels A, B embedded in matrix Y_M .



Figure 3: Corrector functions $\pi_A^{1,2}$ in channel A (left: π_A^1 , right: π_A^2).



Figure 4: Corrector functions $\gamma^{+,-}$ in matrix Y_M (left: γ^+ , right: γ^-).

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