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# PARTICLE METHODS FOR THE DYNAMICS OF POROUS BIOFILMS WITH HETEROGENEOUS RHEOLOGY AND ITS INTERACTION WITH LUNG EPITHELIUM

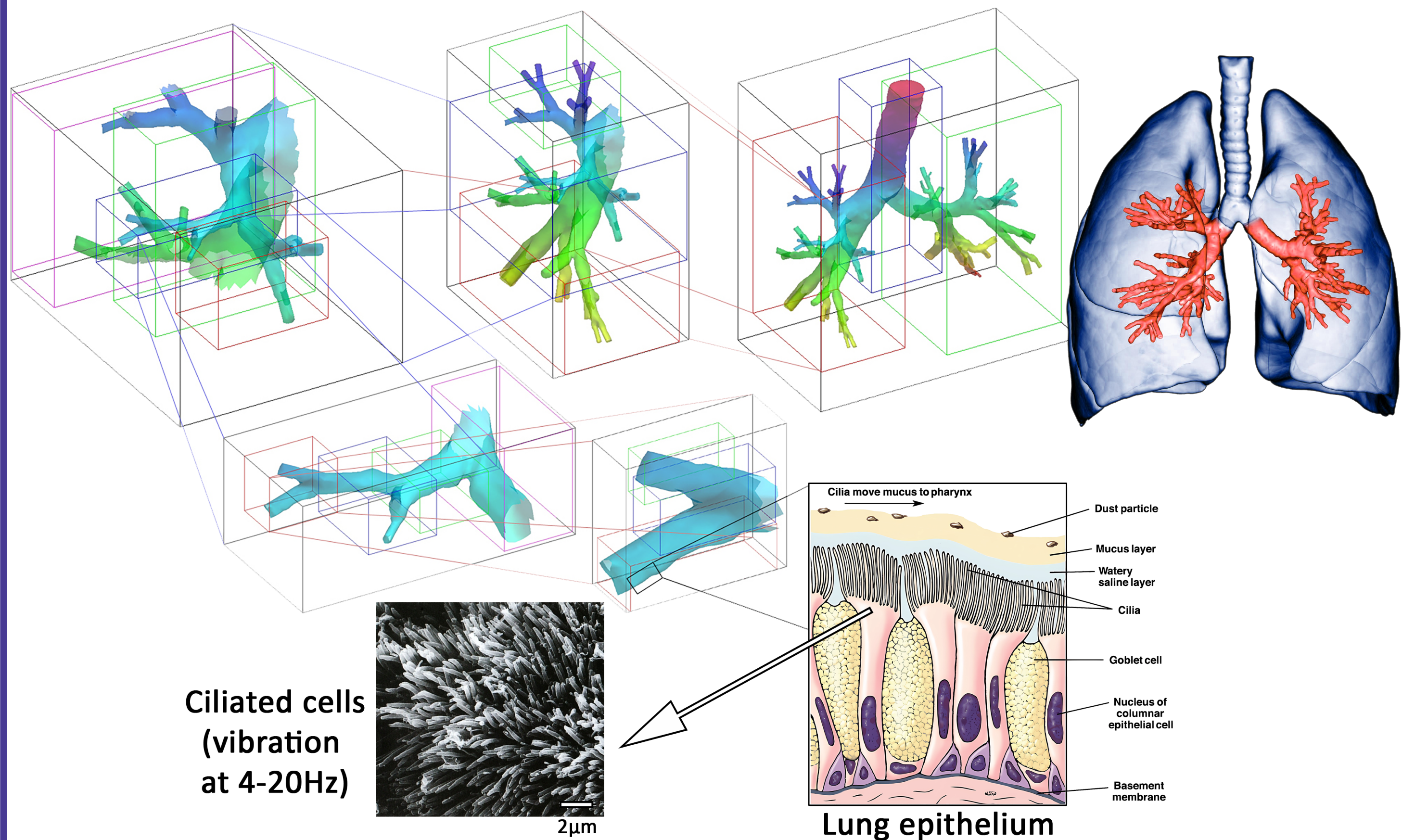
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## CONTEXT: UPSCALING FLOW AROUND LUNG CELLS



Multiscale description of human lung from trachea ( $\sim 2\text{cm}$ ) to its epithelium at the 6-7th generations ( $\sim 10\mu\text{m}$  high), one cilia being  $100\text{nm}$  wide (sketch inspired from [8]).

## FROM DNS OF THE PORE SCALE REACTIVE FLOWS

The superficial velocity  $u$  follows the Darcy-Brinkman-Stokes equation in a porosity field  $\varepsilon$ , which defines a pure liquid phase where  $\varepsilon = 1$  and a solid matrix where  $\varepsilon$  is small :

$$\varepsilon^{-1} \frac{\partial(\rho u)}{\partial t} + \varepsilon^{-1} \text{div}(\varepsilon^{-1} \rho u \otimes u) - \varepsilon^{-1} \text{div}(2\mu D(u)) + \mu^* K^{-1} u = f - \nabla p \quad (1)$$

along with  $\text{div} u = 0$ , using the usual notations. The permeability  $K$  of the lower scale is driven by the Kozeny-Carman relation  $K(\varepsilon) = K_0 \varepsilon^3 (1 - \varepsilon)^{-2}$ . Given the scales, it reduces to

$$-\text{div}(2\mu D(u)) + \mu^* K_0^{-1} \frac{(1 - \varepsilon)^2}{\varepsilon^2} u = \varepsilon(f - \nabla p) \quad (2)$$

An acid of concentration  $C$  dissolves a solid of molar volume  $m$  at rate  $r$  following

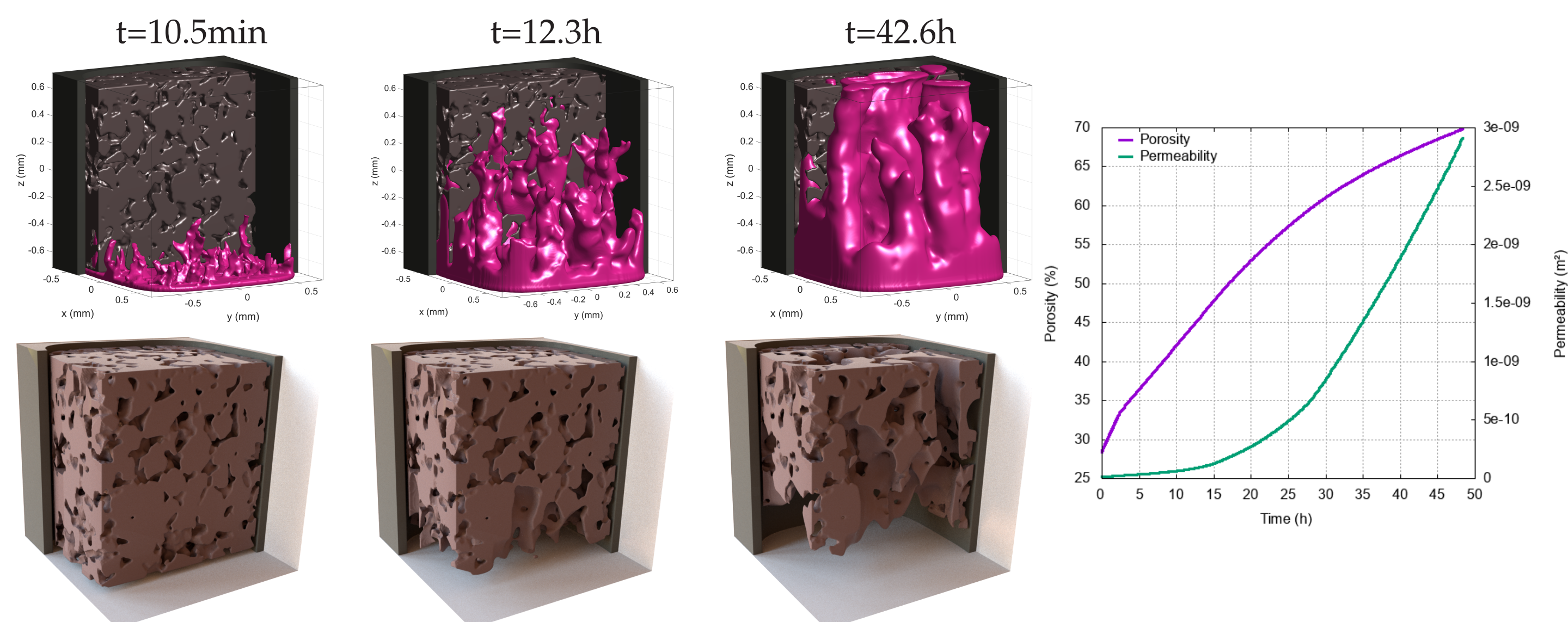
$$\frac{\partial C}{\partial t} + \text{div}(\varepsilon^{-1} u C) - \text{div}(d_m \varepsilon^{1+\beta} \nabla \varepsilon^{-1} C) = -r(C, \varepsilon) \quad \text{and} \quad \frac{\partial \varepsilon}{\partial t} = -m r(C, \varepsilon) \quad (3)$$

where  $d_m$  is molecular diffusion of the acid and  $\beta$  is the index of tortuosity within the solid.

Using a particle method for (3) means that we describe the fluid by a set of volumes  $v_p$ , concentrations  $c_p$ , and locations  $\xi_p$ . Then, one gets the *particle formulation* of (3) :

$$\frac{dC_p}{dt} = [\text{div}(d_m \varepsilon^{1+\beta} \nabla \varepsilon^{-1} C) - C u \cdot \nabla \varepsilon^{-1}]_{\xi_p}, \quad \frac{d\xi_p}{dt} = \varepsilon^{-1} u(\xi_p), \quad \frac{dv_p}{dt} = [\text{div}(\varepsilon^{-1} u)]_{\xi_p} v_p \quad (4)$$

with back and forth high order interpolations from the grid used to solve (2).



Dissolution of a 5% porous calcite body ( $1.43\text{mm}$  wide) at  $\text{pH}=2$ , following model (2, 3). See [2] for more details and the validation of the numerical method (4) in [3]. The resulting porosity/permeability is displayed to the right.

## TO THE DNS OF LUNG CELLS WITH PCL/MUCUS BIOFILM

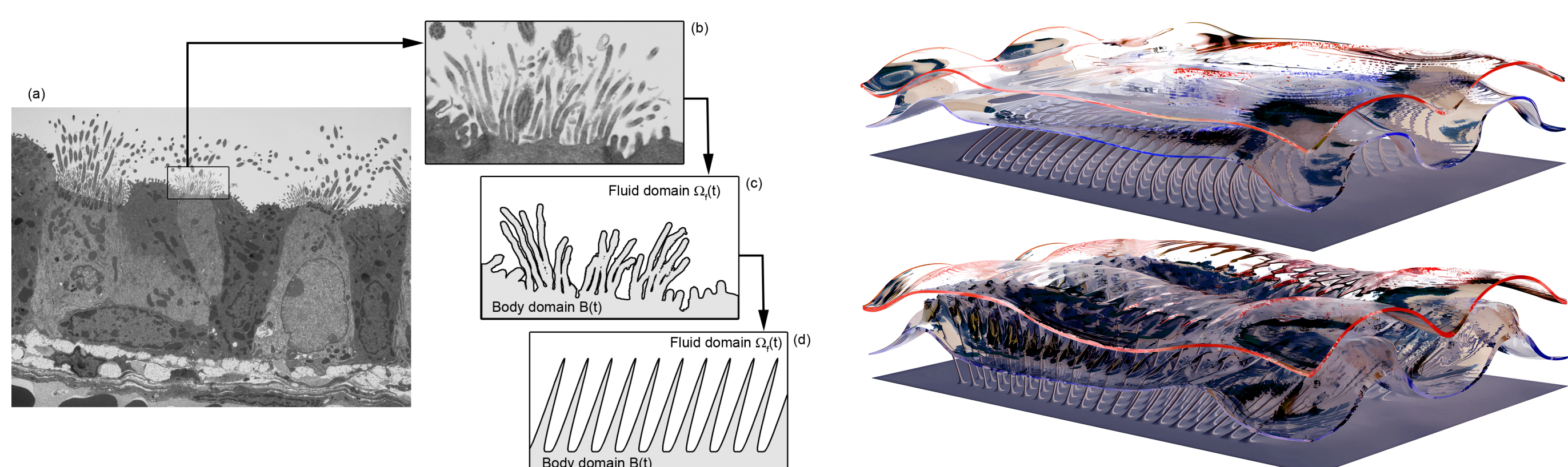
The lung epithelium (the ciliated cells  $B(t)$ ) is surrounded by a Newtonian periciliary liquid (PCL) of viscosity  $\mu_\infty$  and a miscible shear-thinning mucus composed of mucin proteins at concentration  $C$ .

Model (2, 3) is still valid but in this case, the fluid is not reacting ( $r = 0$ ) and  $K(\varepsilon) = \mathbf{1}_{B(t)}/\varepsilon$ . Here (2) and (3) are coupled by means of the Carreau relationship defining the viscosity of the heterogeneous non-Newtonian fluid (see [5] for instance) :

$$\mu(\alpha, D) = \mu_\infty + \mu_\infty \left[ \left( \frac{B}{\mu_\infty} \right)^\alpha d_0^{1-N} - 1 \right] \left[ 1 + 2 \frac{D : D}{d_0^2} \right]^{\alpha(N-1)/2} \quad (5)$$

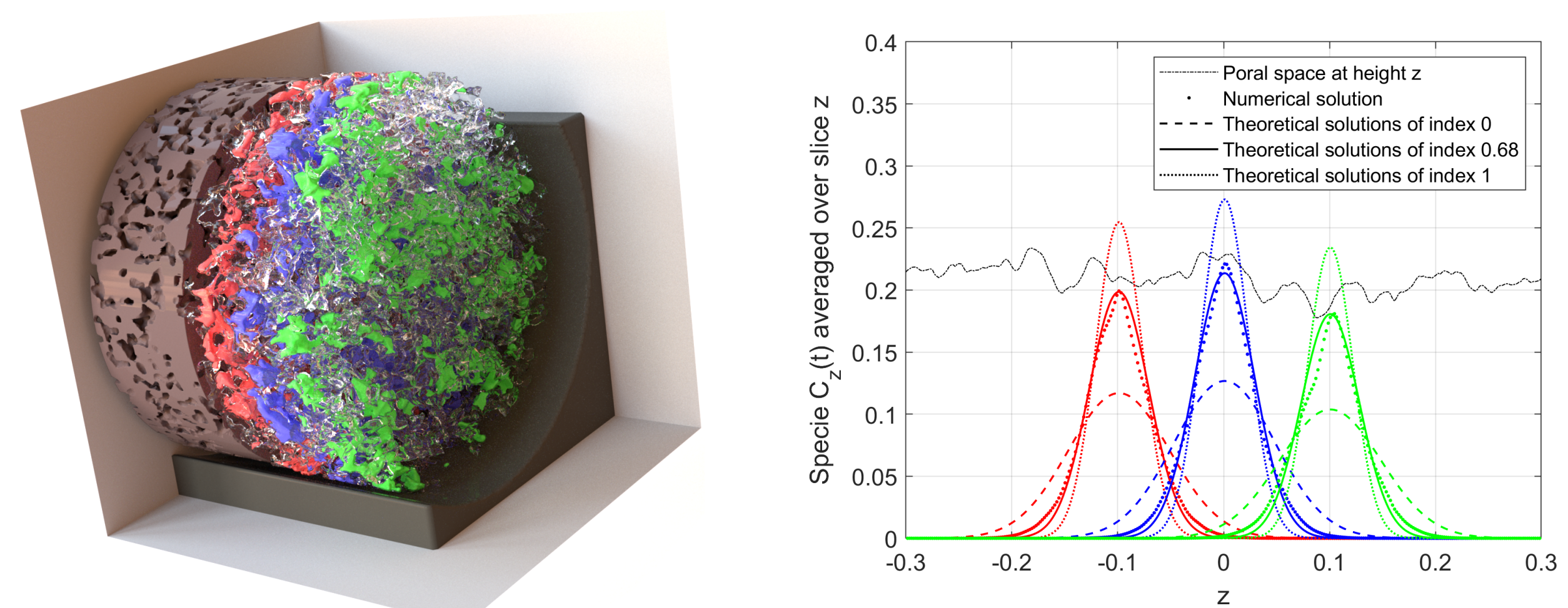
where  $D$  is the shear-rate and  $\alpha = C/C_0$  the renormalized concentration of mucin ( $d_0$  is the cut-off frequency and  $C_0$  the maximum admissible concentration of mucins).

In this model, only two "patient specific" parameters remain: the bulk viscosity  $B$  and the shear-thinning index  $N$  (see the clinical context thereafter).



Cilia  $B(t)$  and fluid domain  $\Omega(t)$  in motion (picture to the left, from [6]), driving the mucus (isosurfaces of mucin concentration on the picture to the right, see [4] for more details).

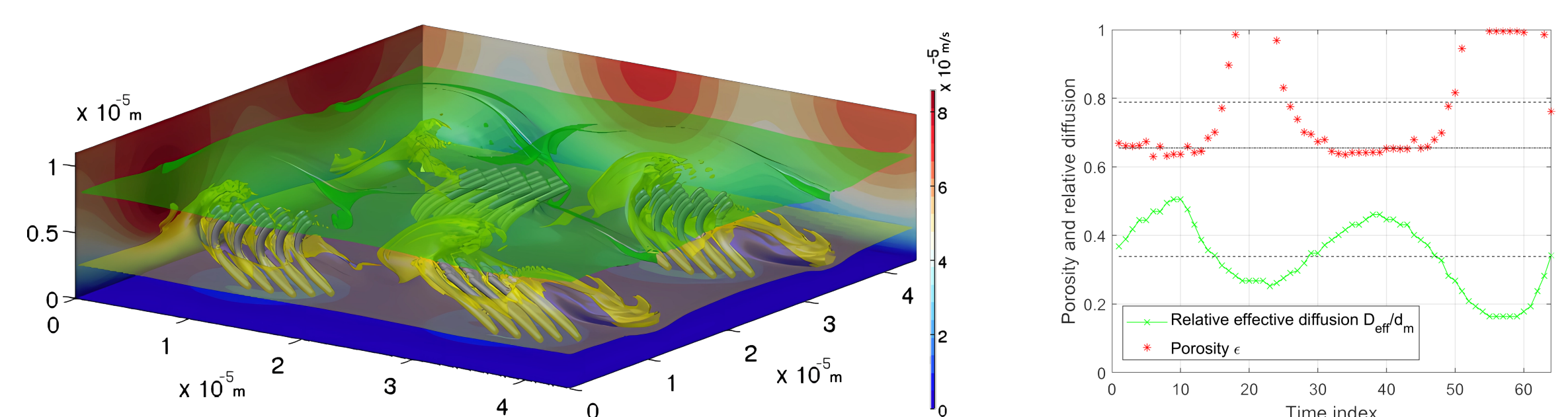
## FROM THE UPSCALING OF THE PORE SCALE DIFFUSION



Diffusion in this sandstone, which is 21% porous, leads to a *tortuosity index* of  $\beta = 0.68$ . This means that the upscaled diffusion coefficient in an homogeneous medium is  $\varepsilon^\beta$  times the molecular diffusion (taken from [1]).

## TO THE UPSCALING OF THE DIFFUSION WITHIN LUNG CELL

Diffusion within ciliated cell with time-dependent geometry is upscaled and computed using the same technique as above. It is required in order to estimate the mucin slip-through dynamics. The resulting tortuosity index  $\beta(t)$  is shown to be relatively time independent.

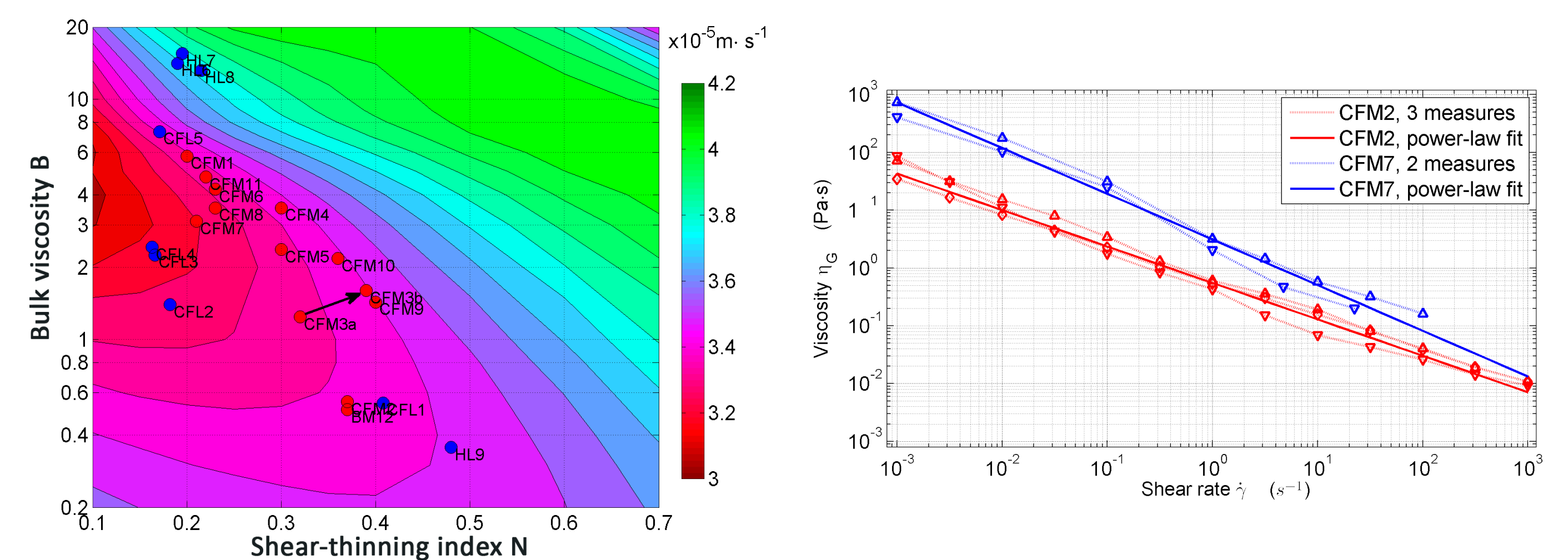


Cilia carpet with time-dependent geometry (left picture, from [7]) and resulting time-dependant effective diffusion and porosity (right picture). This leads to a *tortuosity index* at  $\beta \simeq 0.4$  when not in flat shape configuration.

## CLINICAL CONTEXT: MONITORING OF THERAPIES FOR CYSTIC-FIBROSIS

Rheology coefficients  $B$  and  $N$  have been measured from expectoration samples of cystic fibrosis patients. Experiments were carried out on a Mars III rheometer equipped with a cone and plate geometry (angle  $1^\circ$ , diameter  $35\text{mm}$ ) which required a small volume of fluid ( $0.2\text{ml}$ ).

It has been shown in [5] that numerical simulation of mucus dynamics are coherent with clinical data: slow mucus motion coincides with CF patients, while the highest mucus motions correspond to healthy people.



$(B, N)$  phase diagram with clinical data from [5] (figure to the left). Examples of robust estimation of coefficients  $B$  and  $N$  by rheometry, using aliquoting of mucus samples (figure to the right).

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