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Homogenization of 3D concrete microstructures based on CT image reconstruction

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OUTLINE

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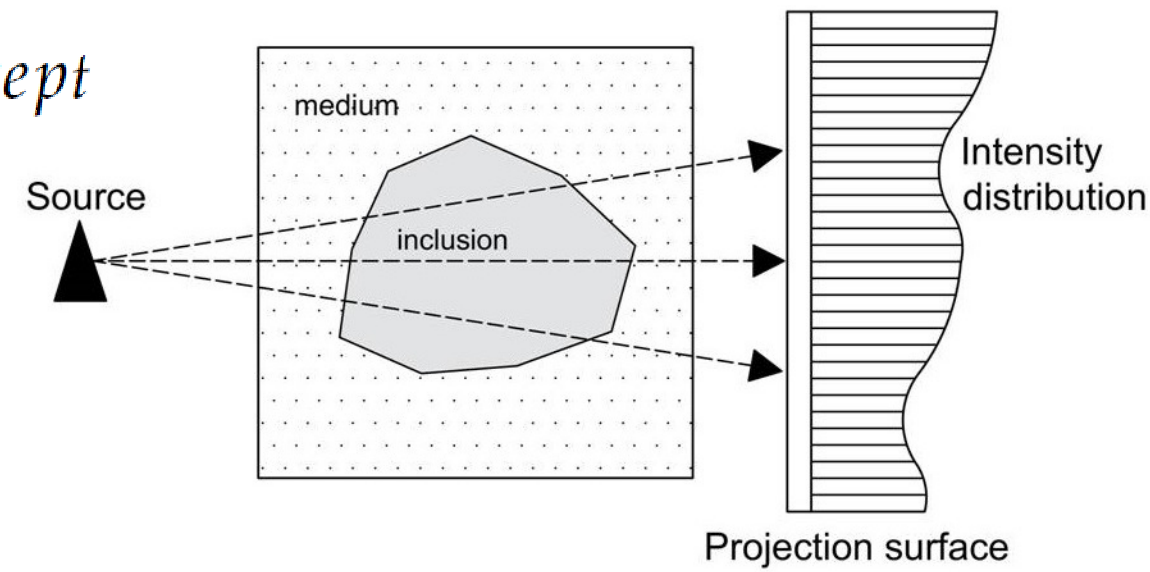
■ Reconstruction of Concrete Microstructure Based on CT Images

- Methodology

When the X-ray beam passes through a sample, some of the X-ray radiation is absorbed and scattered, while the rest penetrates through the sample. Hounsfield units (HU) is a measure of the absorbed or scattered radiation of a material and is related to the original linear attenuation coefficient measurement (μ) so as the radiodensity of distilled water at standard pressure and temperature is defined as zero HU, while the radiodensity of air, at the same conditions, is defined as -1000 HU.

$$HU = \mu \times slope + intercept$$

*The values of the rescale slope and intercept parameter are specific to the CT scanner system used.



Intensity Distribution of an X-ray array

Reconstruction of Concrete Microstructure Based on CT Images

- CT Equipment

Labarotory: Magnitiki Patron S.A.

Equipment: LightSpeed VCT of GE Medical Systems Hellas

Technical specifications for the X-ray tube:

Peak potential: 140 kV

Applied current: 180 mA

Scanner axial resolution: 0.625 mm

Output: DICOM image data

- Specifications of concrete specimen

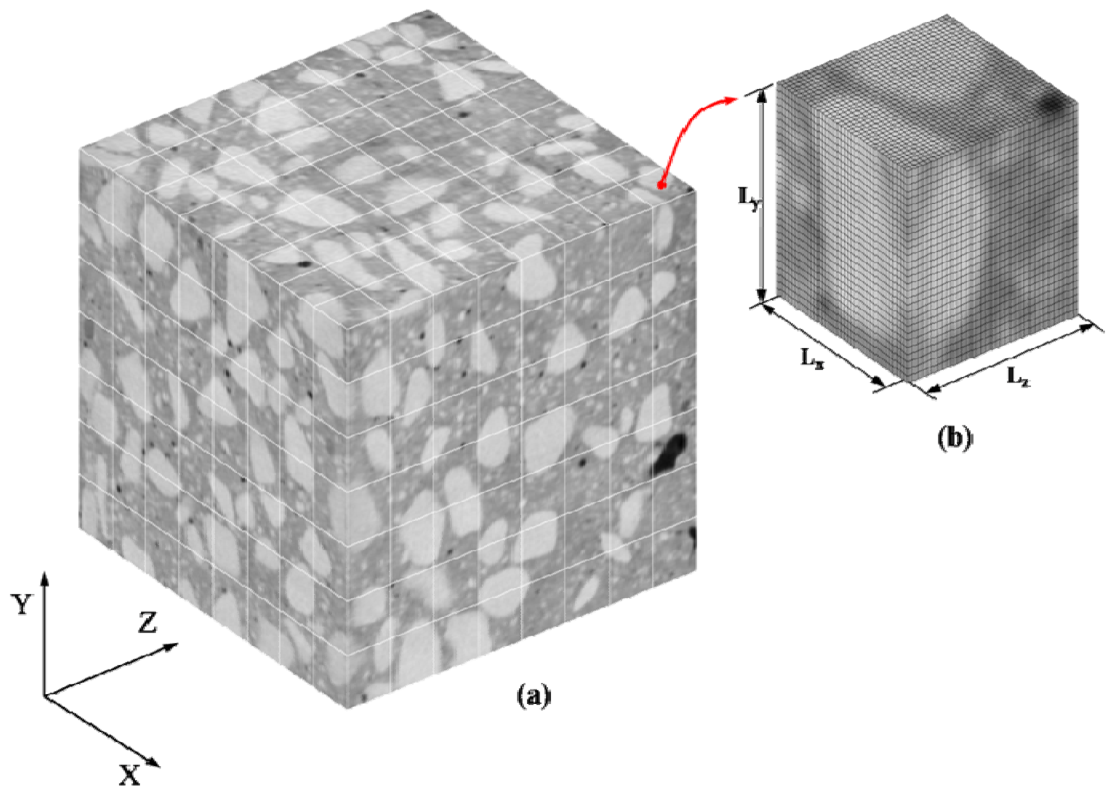
Dimensions: 136.724×136.724×131.25 mm^3

Percentage of constituent materials:

approx. 27.2% aggregates (gravels) – 30% sand – 22% cement – 20% water – 0.3% additives – 0.5 % air

Computational Homogenization

- Moving window technique



- Statistical homogeneity of the heterogeneous medium
- Separation of scales:

$$d \ll L \ll L_{macro}$$

- Extraction of Stochastic Volume Elements (SVEs) with scale factor δ:

$$\delta = L/d$$

- Voxel based finite element discretization
- Material properties assigned to finite elements based on HU

Computational Homogenization

- Computation of the random apparent elasticity tensor of 3D concrete microstructures

The stress and strain fields on a mesoscale realization of concrete $B_\delta(\omega)$ are given by:

$$\sigma(\omega,x) = \bar{\sigma} + \sigma'(\omega,x) \ , \ \ \varepsilon(\omega,x) = \bar{\varepsilon} + \varepsilon'(\omega,x)$$

where σ', ε' are the zero mean fluctuations and $\bar{\sigma}$, $\bar{\varepsilon}$ are the means of the stress and strain tensors.

At some point **X** of the macro-continuum, the above means can be computed as volume averages over $B_\delta(\omega)$:

$$\bar{\sigma}(\omega,X) = \frac{1}{V_\delta} \int_{B_\delta(\omega)} \sigma(\omega,x)\,\mathrm{d}V_\delta, \ \ \bar{\varepsilon}(\omega,X) = \frac{1}{V_\delta} \int_{B_\delta(\omega)} \varepsilon(\omega,x)\,\mathrm{d}V_\delta$$

Computational Homogenization

- Computation of the random apparent elasticity tensor of 3D concrete microstructures

The strain energy of the heterogeneous medium is calculated by:

$$\bar{\mathrm{U}} = \frac{1}{2V_\delta} \int_{B_\delta(\omega)} \sigma(\omega, x) : \varepsilon(\omega, x)\, \mathrm{d}V_\delta = \frac{1}{2}\overline{\sigma : \varepsilon} = \frac{1}{2}\bar{\sigma} : \bar{\varepsilon} + \frac{1}{2}\overline{\sigma' : \varepsilon'}$$

Hill's condition for an unbounded space domain:

$$\overline{\sigma : \varepsilon} = \bar{\sigma} : \bar{\varepsilon}$$

Hill's condition is also valid for a finite size of the domain, provided that the following constraint is satisfied:

$$\int_{\partial B_\delta} (t - \bar{\sigma} \cdot n) \cdot (u - \bar{\varepsilon} \cdot x)\, \mathrm{d}S = 0$$

Appropriate boundary conditions satisfying a priori the above constraint, e.g. *uniform kinematic, uniform static, orthogonal mixed, periodic.*

Computational Homogenization

- Computation of the random apparent elasticity tensor of 3D concrete microstructures

Generalized Hooke's law (constitutive equation):

$$\bar{\sigma}_{ij} = \bar{\mathbb{C}}_{ijkl}\bar{\varepsilon}_{kl}$$

Matrix form:

$$\bar{\sigma} = \bar{\mathbb{C}}\bar{\varepsilon} \Rightarrow \begin{bmatrix} \bar{\sigma}_{11} \\ \bar{\sigma}_{22} \\ \bar{\sigma}_{33} \\ \bar{\sigma}_{12} \\ \bar{\sigma}_{23} \\ \bar{\sigma}_{31} \end{bmatrix} = \begin{bmatrix} \bar{\mathbb{C}}_{1111} & & & & & \text{sym} \\ \bar{\mathbb{C}}_{2211} & \bar{\mathbb{C}}_{2222} & & & & \\ \bar{\mathbb{C}}_{3311} & \bar{\mathbb{C}}_{3322} & \bar{\mathbb{C}}_{3333} & & & \\ \bar{\mathbb{C}}_{1211} & \bar{\mathbb{C}}_{1222} & \bar{\mathbb{C}}_{1233} & \bar{\mathbb{C}}_{1212} & & \\ \bar{\mathbb{C}}_{2311} & \bar{\mathbb{C}}_{2322} & \bar{\mathbb{C}}_{2333} & \bar{\mathbb{C}}_{2312} & \bar{\mathbb{C}}_{2323} & \\ \bar{\mathbb{C}}_{3111} & \bar{\mathbb{C}}_{3122} & \bar{\mathbb{C}}_{3133} & \bar{\mathbb{C}}_{3112} & \bar{\mathbb{C}}_{3123} & \bar{\mathbb{C}}_{3131} \end{bmatrix} \begin{bmatrix} \bar{\varepsilon}_{11} \\ \bar{\varepsilon}_{22} \\ \bar{\varepsilon}_{33} \\ \bar{\varepsilon}_{12} \\ \bar{\varepsilon}_{23} \\ \bar{\varepsilon}_{31} \end{bmatrix}$$

where $\bar{\mathbb{C}}$ is the 4^{th} order 3D homogenized elasticity tensor with 21 independent elastic components due to symmetry of stress and strain tensors.

Computational Homogenization

- Computation of the random apparent elasticity tensor of 3D concrete microstructures

Computation of the elastic components $\bar{\mathbb{C}}_{ijkl}$

Solution of 6 independent uniform kinematic boundary value problems (BVPs):

$$\boxed{\boldsymbol{u}_b = D_b^T \bar{\boldsymbol{\varepsilon}}}$$

6 independent uniform unit strain vectors are imposed

$$\bar{\varepsilon} = \left\{ \begin{bmatrix} \bar{\varepsilon}_{11} = 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ \bar{\varepsilon}_{22} = 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ \bar{\varepsilon}_{33} = 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ \bar{\varepsilon}_{12} = 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \bar{\varepsilon}_{23} = 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \bar{\varepsilon}_{31} = 1 \end{bmatrix} \right\}$$

Geometric matrix based on boundary nodes coordinates

$$D_b = \frac{1}{2} \begin{bmatrix} 2x_b & 0 & 0 \\ 0 & 2y_b & 0 \\ 0 & 0 & 2z_b \\ y_b & x_b & 0 \\ 0 & z_b & y_b \\ z_b & 0 & x_b \end{bmatrix} \quad \text{with} \quad (x_b, y_b, z_b) \in \boldsymbol{x}$$

Computational Homogenization

- Computation of the random apparent elasticity tensor of 3D concrete microstructures

Each BVP results to a system of algebraic equations:

$$\begin{bmatrix} \boldsymbol{K}_{ii} & \boldsymbol{K}_{ib} \\ \boldsymbol{K}_{bi} & \boldsymbol{K}_{bb} \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_i \\ \boldsymbol{u}_b \end{bmatrix} = \begin{bmatrix} \boldsymbol{f}_i \\ \boldsymbol{f}_b \end{bmatrix}$$

i: *interior nodes*

b: *boundary nodes*

$$\boxed{\bar{\boldsymbol{\sigma}} = \frac{1}{V}\mathbb{D}\boldsymbol{f}_b}$$

$$\boldsymbol{u}_i = \boldsymbol{K}_{ii}^{-1}\left(\boldsymbol{f}_i - \boldsymbol{K}_{ib}\boldsymbol{u}_b\right),\ \boldsymbol{f}_b = \boldsymbol{K}_{bb}\boldsymbol{u}_b + \boldsymbol{K}_{bi}\boldsymbol{u}_i$$

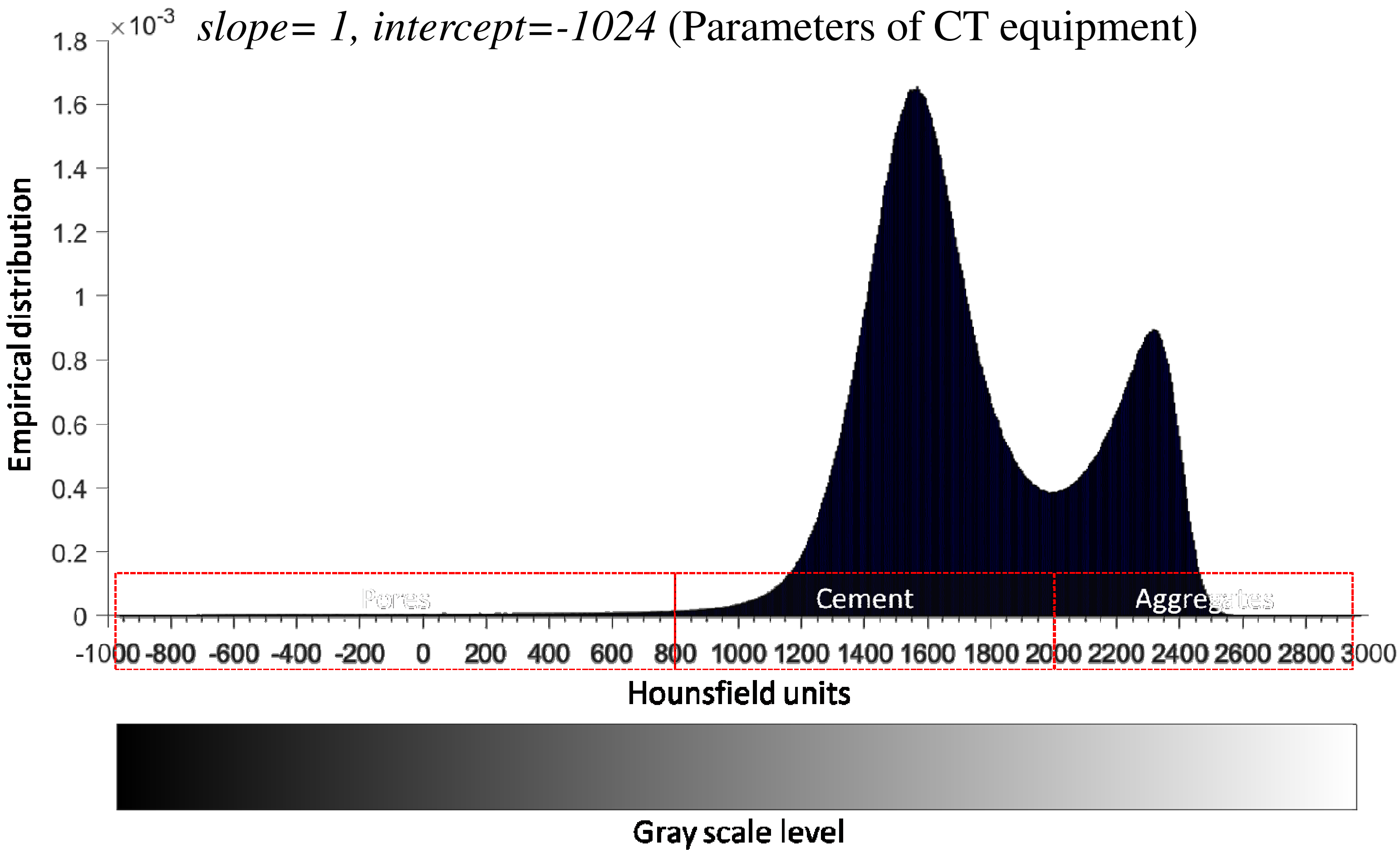
with $\mathbb{D} = \left[D_1\ D_2\ ...\ D_{n_b}\right]$

$$\bar{\boldsymbol{\sigma}} = \begin{bmatrix} \bar{\sigma}_{11} \\ \bar{\sigma}_{22} \\ \bar{\sigma}_{33} \\ \bar{\sigma}_{12} \\ \bar{\sigma}_{23} \\ \bar{\sigma}_{31} \end{bmatrix} = \begin{bmatrix} \bar{C}_{1111} & & & & & \mathrm{sym} \\ \bar{C}_{2211} & \bar{C}_{2222} & & & & \\ \bar{C}_{3311} & \bar{C}_{3322} & \bar{C}_{3333} & & & \\ \bar{C}_{1211} & \bar{C}_{1222} & \bar{C}_{1233} & \bar{C}_{1212} & & \\ \bar{C}_{2311} & \bar{C}_{2322} & \bar{C}_{2333} & \bar{C}_{2312} & \bar{C}_{2323} & \\ \bar{C}_{3111} & \bar{C}_{3122} & \bar{C}_{3133} & \bar{C}_{3112} & \bar{C}_{3123} & \bar{C}_{3131} \end{bmatrix} \begin{bmatrix} \bar{\varepsilon}_{11} = 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\mathrm{HU} = \mu \times slope + intercept$$

μ: *attenuation values obtained from CT scan*

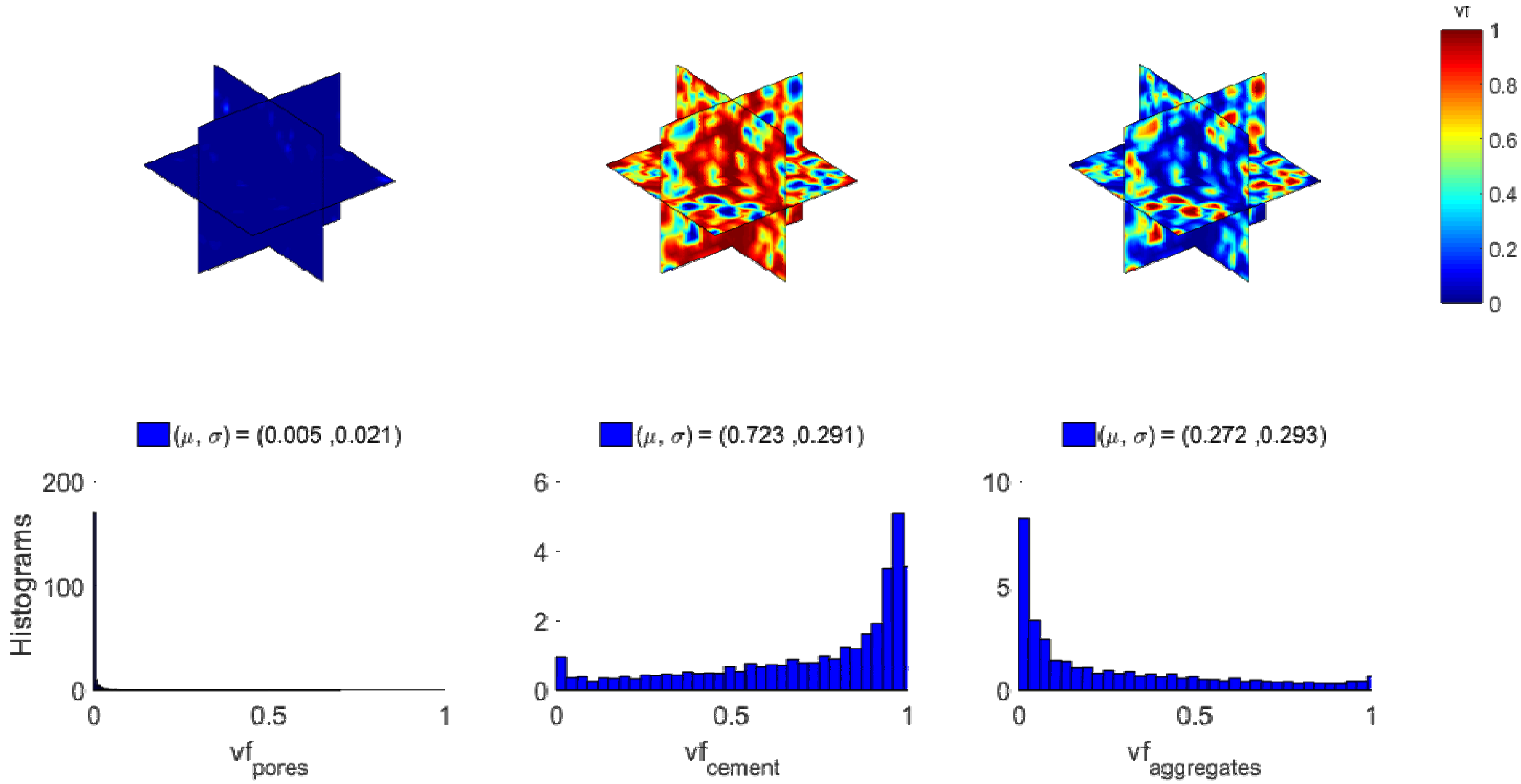
slope= 1, intercept=-1024 (Parameters of CT equipment)



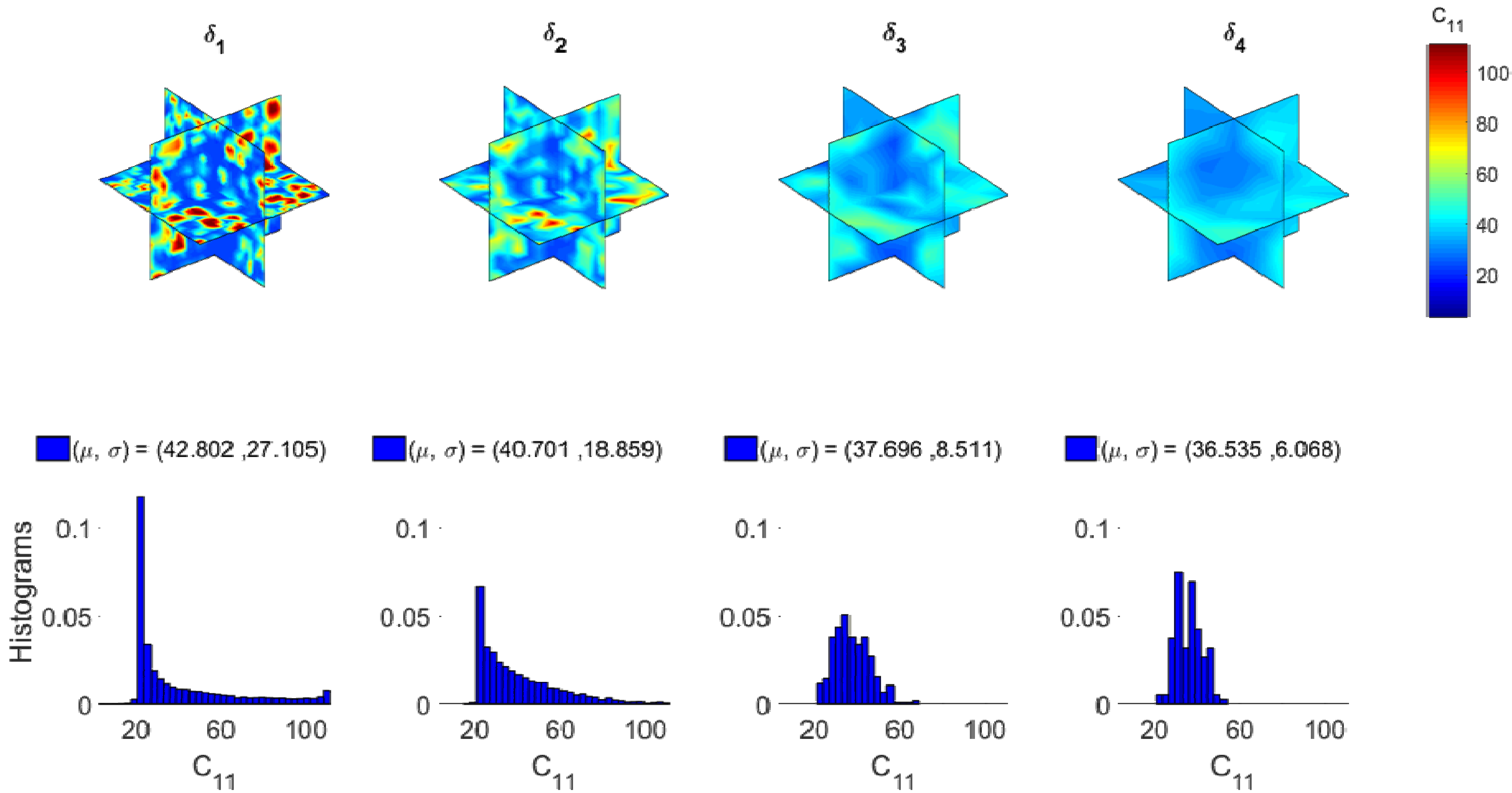
Empirical distribution of Hounsfield unit (HU) values derived from all CT images

Table 1. Size of window and total number of SVEs corresponding to each δ_i examined.

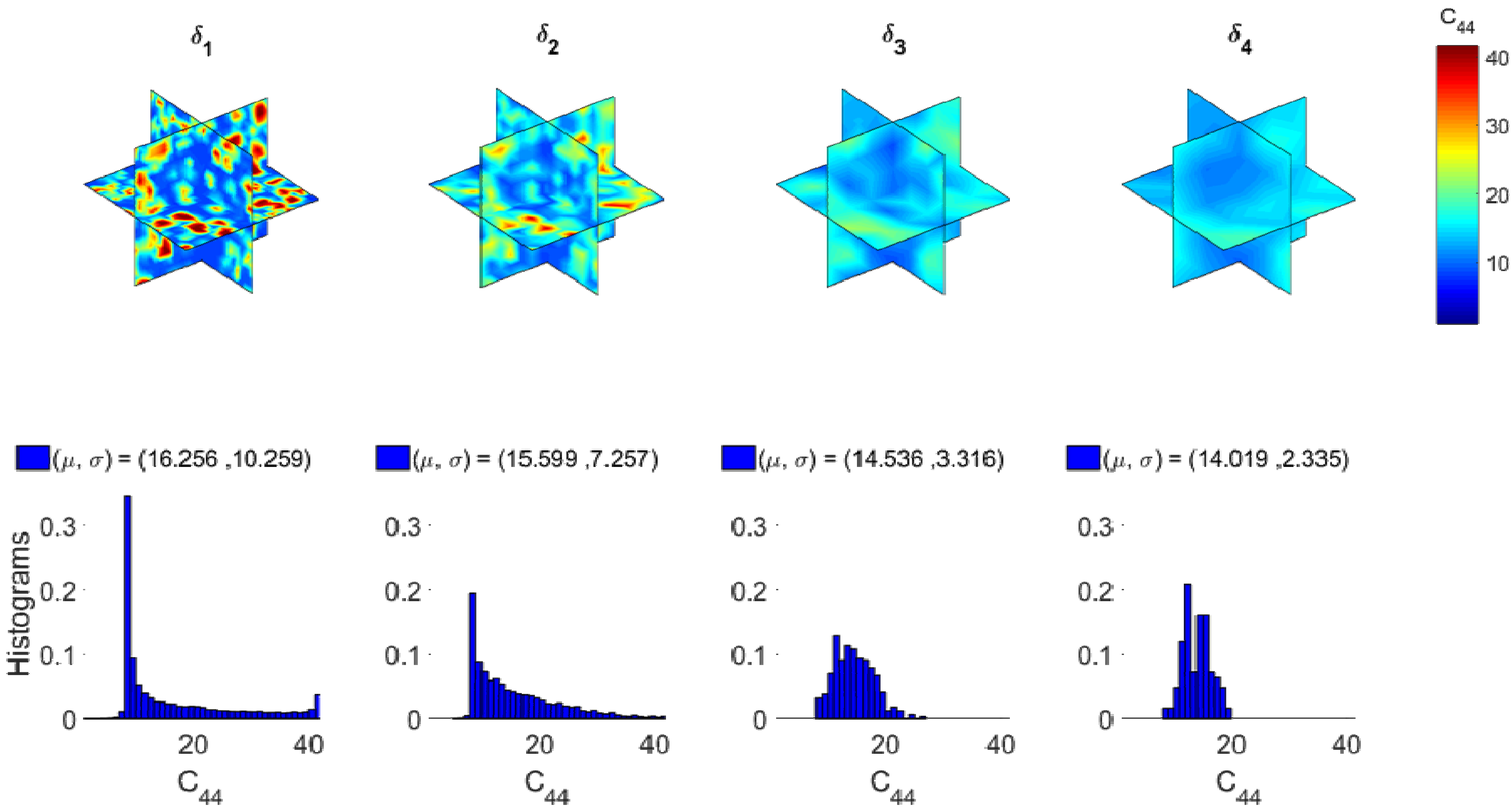
δ_i	$L_x \times L_y \times L_z$ (mm^3)	No. SVEs
δ_1	$4.88 \times 4.88 \times 6.25$	16,464
δ_2	$9.77 \times 9.77 \times 8.75$	2940
δ_3	$19.53 \times 19.53 \times 18.75$	343
δ_4	$27.34 \times 27.34 \times 26.25$	125



Random fields and histograms of volume fraction (vf) of concrete constituents for δ_1



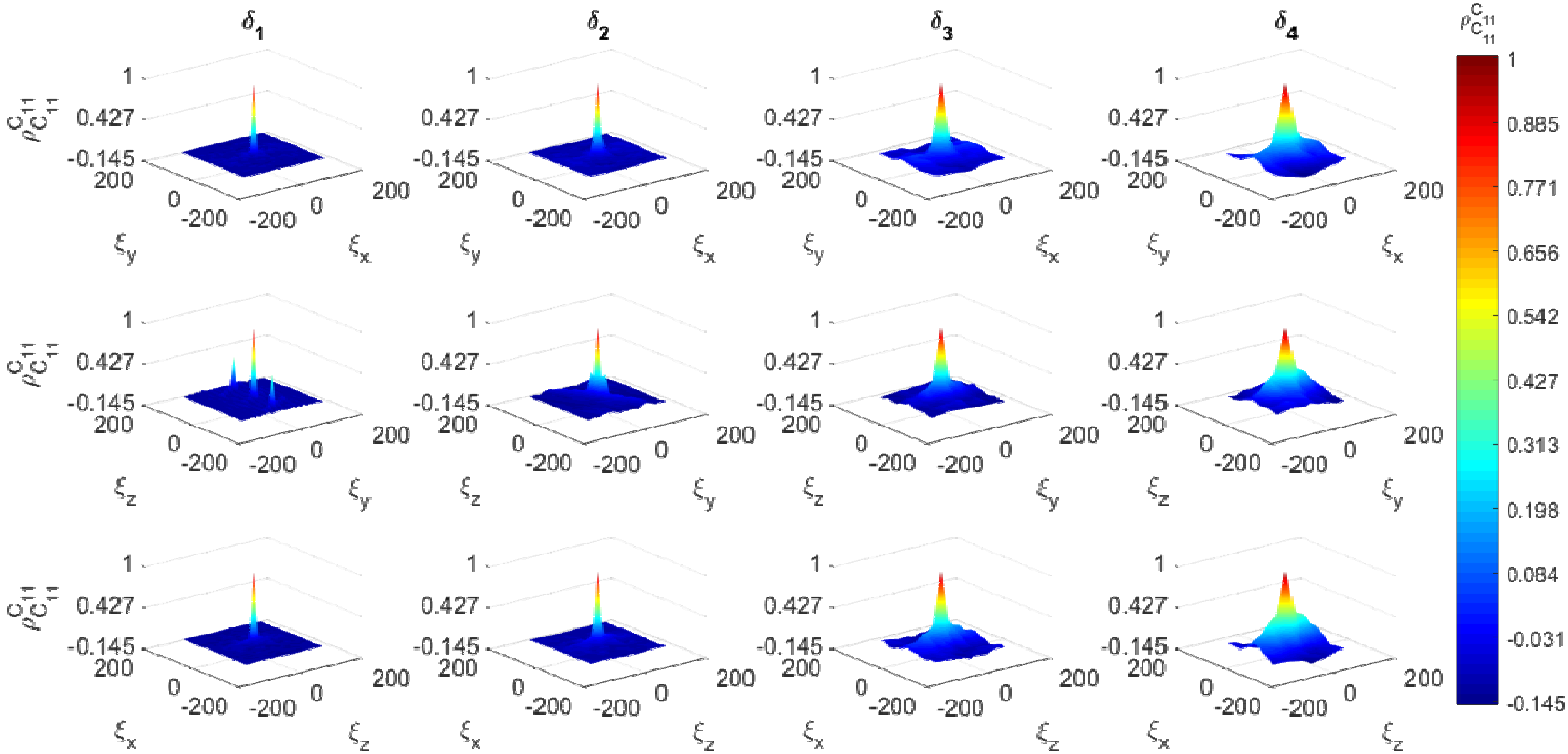
Random fields and histograms of C_{11}



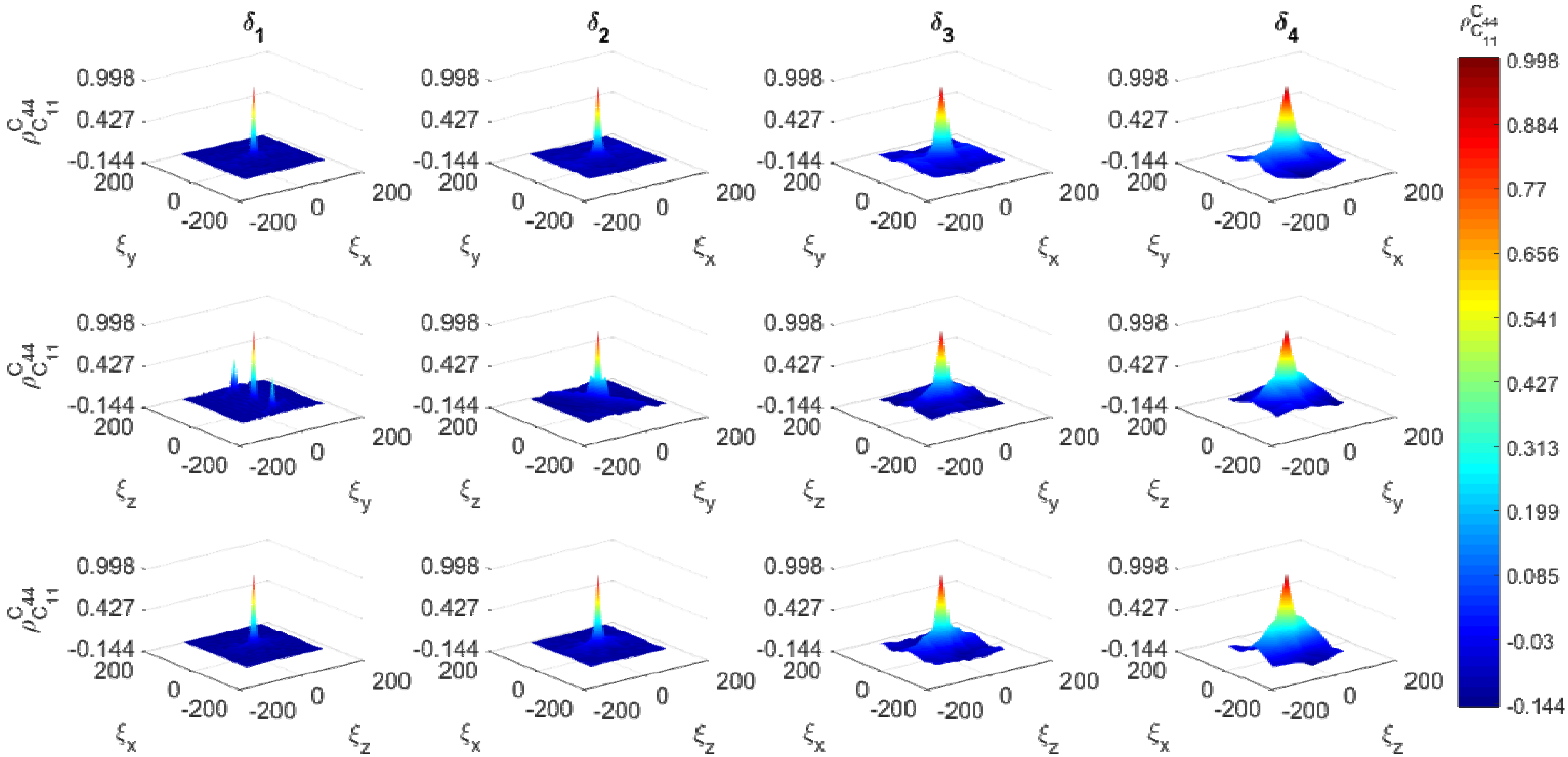
Random fields and histograms of C_{44}

$$\hat{\rho}_A^B(\xi_x, \xi_y, \xi_z) = \frac{1}{n-1}\sum_{i=0}^{n_{wx}}\sum_{j=0}^{n_{wy}}\sum_{k=0}^{n_{wz}}\left(\frac{A\left(x^i, y^j, z^k\right) - \hat{\mu}_A}{\hat{\sigma}_A}\right)\left(\frac{B\left(x^i+\xi_x, y^j+\xi_y, z^k+\xi_z\right) - \hat{\mu}_B}{\hat{\sigma}_B}\right)$$

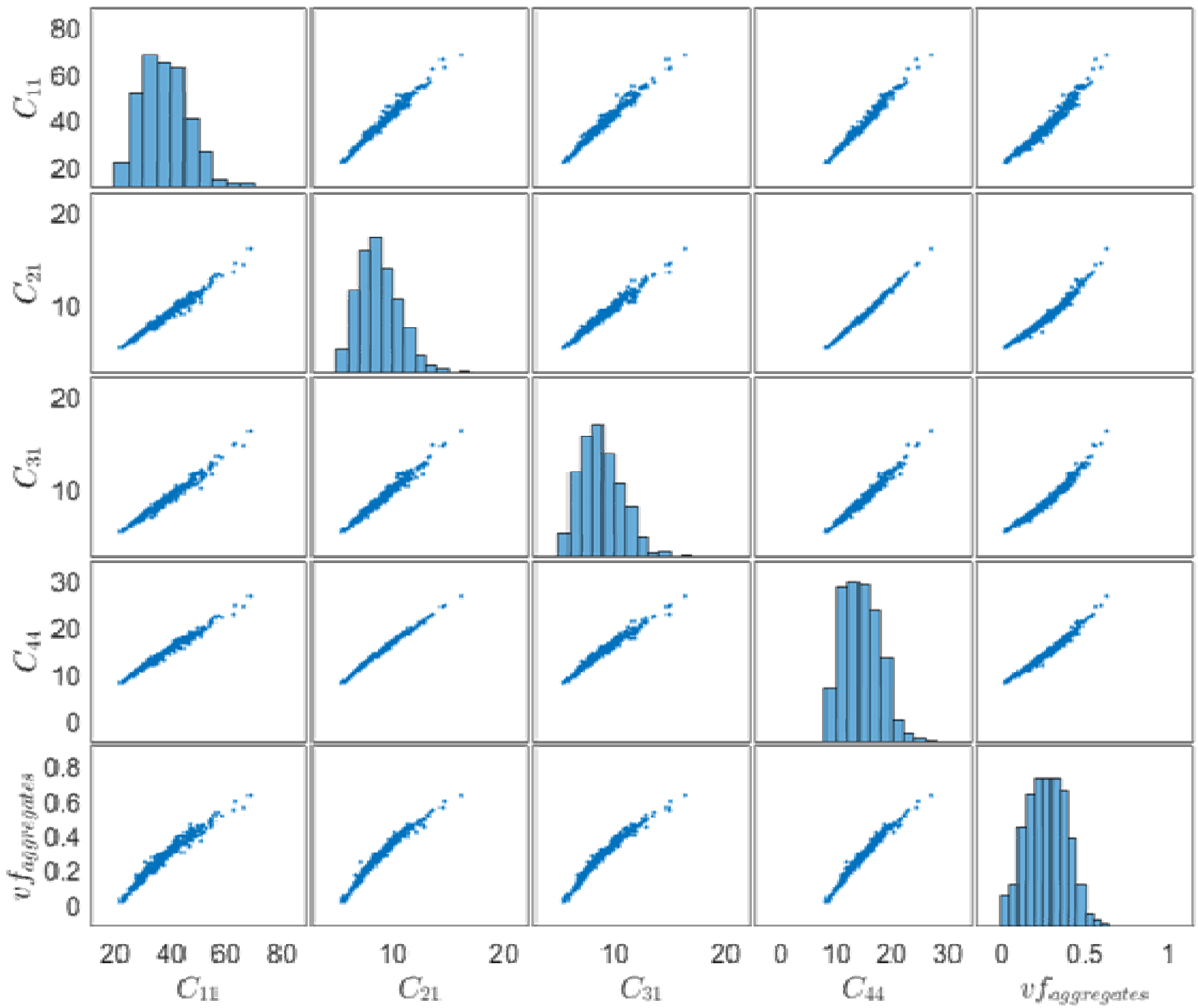
$$-n_{wx}\Delta\xi_x \le \xi_x \le n_{wx}\Delta\xi_x\ ,\ -n_{wy}\Delta\xi_y \le \xi_y \le n_{wy}\Delta\xi_y\ ,\ -n_{wz}\Delta\xi_z \le \xi_z \le n_{wz}\Delta\xi_z$$



Auto-correlation function of C_{11}



Cross-correlation function between C_{11} and C_{44}



Scatter plots of elasticity components and volume fraction of aggregates for δ_3

Conclusions

✓ The random spatially varying apparent elasticity tensor of 3D concrete microstructures has been computed using CT images of a cubic specimen for the reconstruction of concrete microstructure and computational homogenization.

✓ A complete probabilistic description of the spatial variation of the elastic properties of concrete has been achieved through computation of the respective mesoscale random fields.

✓ A moderate to large variability of the local volume fraction of the constituents (pores, cement paste and aggregates) has been observed depending on the scale factor δ considered.

✓ This was reflected on the moderate to high COV of the apparent axial and shear stiffness, meaning that microstructural uncertainty can lead to substantial random spatial variation of the mechanical properties of concrete.

✓ The computed random material property fields can be used for the stochastic FE analysis of concrete structures.

➢ Stefanou, G., Savvas, D., & Metsis, P. (2021). Random Material Property Fields of 3D Concrete Microstructures Based on CT Image Reconstruction. Materials, 14(6), 1423

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