# Stochastic multiscale modeling of metal foams

by Liebscher, Proppe, Redenbach and Schwarzer
(A discussion at the Soft Matter Journal Club)

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# Stochastic multiscale modeling of metal foams

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**Abstract**

A procedure for the computation of eigenfrequencies for structures made of metal foam is proposed. The heterogeneity of the foam geometry has an influence on these macroscopic properties and has to be taken into account. This is done by fitting a model of the microstructure based on Laguerre tessellations by means of

# What's a metal foam?

According to Wikipedia, a "metal foam is a cellular structure consisting of a solid metal with gas-filled pores comprising a large portion of the volume".

# Open-cell and closed-cell foams

1. The characteristic property that identifies metal foams (or foams in general) is **porosity**, i.e. the volume fraction of the 'pores' that *do not contain* the substrate against that of the metal itself.
2. The broad categorisation is based on porosity or the shape of the microstructure.
3. In open-cell foams, the cells or the pores are connected by "thin" layers of metal. Equivalently, the volume fraction of the gas to metal is *very close to one*.
4. In closed-cell foams, the cells or the pores are *disconnected* by "thick" layers of metal. Equivalently, the volume fraction of the gas to metal is *infinitesimal*.

# Representative and stochastic volume element

1. A representative volume element is a characteristic of any periodically recurring microstructure, be it foams (as is the case of interest of this paper), or for that matter, solids with periodic potential (referred to as unit cells in solid state physics or control volume element in continuum mechanics).
2. A stochastic volume element is one that fails to repeat itself for a long range of neighbourhood near itself in this space/bulk of the substrate/solid.

# What is this paper all about?

1. This paper describes a computational model that virtually performs a numerical experiment to explore the linear elastic properties of the metal foams from the images obtained from CT (computed tomography) scans.
2. In literature until then, there was a lot of interest towards microstructure models with finite element methods which included techniques such as tessellations.
3. But the issue lies in the heterogeneity of the representative volume element in the microstructures of metal foams, one eventually resorts to methodologies based on stochastic volume elements.
4. This paper introduces a simple yet unique adaptation of what one knows as the "stochastic finite element method".
5. My pivotal place of motivation in this paper lied in the integration of the geometric ramification needed in FEM along with the stochastic portrayal of the microstructure.

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# The basic strategy of the method; the algorithm

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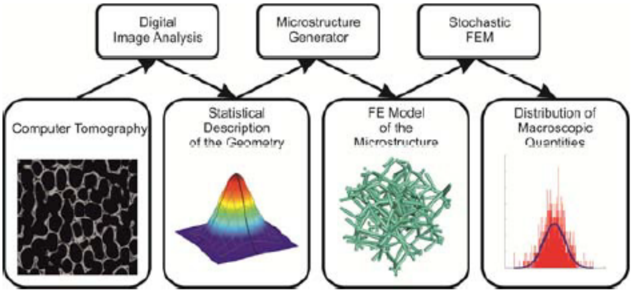



Fig. 1. Overview of the proposed computational procedure.

# Results from the CT scan

Table 1. Cell properties obtained from CT analysis

| Property | Mean | Standard deviation |
|---|---|---|
| Diameter | 5.09 mm | 0.30 mm |
| Surface Area | 80.19 $mm^2$ | 9.58 $mm^2$ |
| Volume | 49.64 $mm^3$ | 9.12 $mm^3$ |
| Facets | 13.90 | 1.48 |

# Microstructure generation and determining linear properties ....

1. As discussed before, owing to the variation in the cells, it is useful to resort to the stochastic volume element (SVE).

2. Based on the data shown in Table 1, a Laguerre tessellation was fit to the foam structure. This model is defined as follows [17]: given a set $S$ of spheres, the Laguerre cell $C(s(x,r),S)$ of a sphere $s(x,r)$ ($x$: center point, $r$: radius) belonging to this set is defined as

$$C\left(s\left(x,r\right),S\right)=\left\{y\in \mathrm{R}^3:\left\|y-x\right\|^2-r^2\le\left\|y-x'\right\|^2-r'^2,\forall s\left(x',r'\right)\in S\right\}, \quad (1)$$

where ‖ ‖ denotes the Euclidean norm. The Laguerre tessellation is the set of all non-empty Laguerre cells of spheres in $S$. It forms a space-filling system of convex polytopes. As special case the Voronoi tessellation is obtained, if all spheres have equal radii. In comparison to the Voronoi tessellation, the Laguerre tessellation allows to generate a wider range of cell patterns as cell facets are not forced to be equidistant to the cell generators.

# Microstructure generation and determining linear properties ....

1. The centres of the the Laguerre spheres are generated by the Poisson process having known the mean or average number of cells per unit volume.
2. The log-normal distribution of the radii of the cells perfectly fitted those in the image.
3. chosen for the volume distribution of the generating spheres. Its probability density function is given by

$$p(r) = \frac{\exp\left(-\frac{(\log r - m)^2}{2\sigma^2}\right)}{\sqrt{2\pi}\sigma r}, r \geq 0, \quad (2)$$

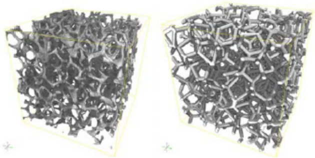
with parameters $m \in \mathbb{R}$ and $\sigma > 0$.

Estimates for the model parameters are obtained using the procedure introduced in [23]. Denote with $c_i$, $i=1,\ldots,8$, the eight quantities of Table 1 and with $\hat{c}_i(p_1, p_2)$, $i=1,\ldots,8$, estimates of these quantities obtained from Laguerre tessellations with parameters $p_1$ and $p_2$ for the sphere volume distribution. The optimal parameters are those, for which the relative distance

$$\sqrt{\sum_{i=1}^{8}\left(\frac{\hat{c}_i - c_i}{\hat{c}_i}\right)^2} \quad (3)$$

is minimized. In the application, the optimal parameters for the volume distribution were found to be $m=1.0508$ and $\sigma=0.2849$. Visualizations of one of the CT images and of the fitted model are shown in Figure 2.

# Microstructure generation and determining linear properties ....



1. Fig. 2. Visualizations of the Cu Duocel foam (left) and the model (right). Visualized are $500^3$ voxels.
2. The next step, briefly, involves the generation of the foam model using some morphological operations. (references available in the next slide ...)
3. Mesoscopic volume elements are created and loaded by boundary conditions yielding an upper (kinematic uniform boundary conditions, KUBC) and a lower bound (static uniform boundary conditions, SUBC) for the compliance tensor $S$ ($\epsilon_{ij} = S_{ijkl}\sigma_{kl}$).

# Estimating statistical averages

*4.1. Determination of the Distribution Function*

The basis for the calculation are about 100 SVEs with a side length of 25 mm. Applying KUBC and SUBC, histograms were obtained for bounds of the effective compliance tensor. For each of the SVEs, the mean value of the upper and lower bound is collected from which the empirical distribution is computed.

*4.2. Determination of the Correlation Functions*

As the linear-elastic material parameters and the mass density will serve for eigenfrequency computations of beams, they are represented by stochastic processes. The stochastic processes are assumed to be stationary due to the homogeneity of the generated microstructure geometry. In order to find the correlation functions for the linear-elastic material parameters, 15 beam structures (100 mm x 10 mm x 10 mm) made of foam are analyzed by a method of moving cubes: Cubes of the same size are cut out of each of these beams at different positions along the longitudinal axis. For each cube the material parameters are calculated so that they were determined as functions of the position x on the longitudinal axis.

For the computation of autocorrelation data, the 15 received fields for example for the Young's modulus $E(x)$ are normalized by

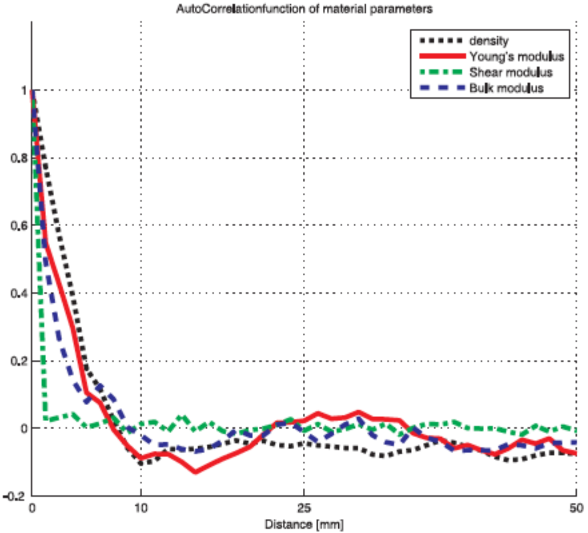
$$E_0(x) = \frac{E(x) - \mu_E}{\sigma_E}, \quad (5)$$

where $\mu_E$ and $\sigma_E$ are the mean value and the standard deviation of the Young's modulus, respectively. Then, for each field the autocorrelation data

$$\tilde{C}_E(\Delta) = \int_0^\ell \mathrm{E}_0(x)\, \mathrm{E}_0(x+\Delta)\, \mathrm{d}x \quad (6)$$

is calculated as a function of the distance $\Delta = x_2 - x_1$ and the mean value over all 15 fields is taken at each distance $\Delta$. The results for the material parameters are shown in Figure 3.

# Estimating statistical averages



# Random field representation

## 5. Random field representation

The non-Gaussian random field is represented by a truncated KLE:

$$\alpha(x,\theta) = \sum_{i=1}^{M} \sqrt{\lambda_i}\, \xi_i(\theta) f_i(x), \tag{13}$$

where $f_i(x)$ are deterministic eigenfunctions that are obtained by solving a homogeneous Fredholm integral equation of the 2nd kind:

$$\int_D C(x_2 - x_1) f_i(x_1)\, \mathrm{d}x_1 = \lambda_i f_i(x_2) \tag{14}$$

for the previously determined covariance function $C(x)$. For the representation of the covariance function adopted here, an analytical solution of equation (14) is still possible, cf. [33]. $\xi_i(\theta)$ are uncorrelated random variables with zero mean and unit variance that are obtained iteratively by adapting the empirical marginal distribution to the previously determined one. The truncated KLE has the advantage that the random variables enter linearly in the expression for the random fields. Samples of $\xi_i(\theta)$ are generated by a procedure described in [34]. It consists of the following steps:

- Given samples $\xi_i^k(\theta_m)$, $m = 1, 2, ..., n$, for $\xi_i(\theta)$, generate samples of the non-Gaussian random field (13).
- Estimate the empirical marginal distribution function $\hat{F}^k(y;x)$ of the random field.
- Transform each sample of the random field by $\eta^k(x,\theta_m) = F^{-1}\left(\hat{F}^k(\alpha(x,\theta_m);x)\right)$. $\eta^k(x,\theta_m)$ matches the target marginal distribution $F$.
- Generate new samples $\tilde{\xi}_i^{k+1}$ for $\xi_i(\theta)$ from

$$\tilde{\xi}_i^{k+1}(\theta_m) = \frac{1}{\sqrt{\lambda_i}} \int_D \left( \eta^k(x,\theta_m) - \frac{1}{n}\sum_{l=1}^{n} \eta^k(x,\theta_l) \right) f_i(x)\, \mathrm{d}x \tag{15}$$

- Standardize $\tilde{\xi}_i^{k+1}$ to unit variance and reorthogonalize the samples by product-moment based shuffling of the sampling.

# Simulation v/s experiment

Table 3. Comparison of bending eigenfrequencies for beams (250 mm x25 mm x 25 mm) made of Cu Duocel®

| Bending mode | Simulation | Experiments |
|---|---|---|
| First | 333 Hz (2.6% COV) | 322 Hz (1.5% COV) |
| Second | 864 Hz (3.7% COV) | 839 Hz (6.2% COV) |

Thank you!!