Stochastic multiscale modeling of metal foams

by Liebscher, Proppe, Redenbach and Schwarzer
(A short review on the method of computation)

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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. The authors primarily aim to compute the eigenfrequency of the structures from metal foams, and the generic elastic properties such as shear modulus, bulk modulus etc.
2. But intuitionally too, I asked myself: "How are the eigenfrequencies and elastic properties of a material related?" For example, the relationship between the Young's modulus from flexural vibration for circular section

$$E = 1.6067 \frac{D^3}{L^4} m f^2 T_1 \tag{1}$$

where E is the Young's modulus, L and D being the length and the diameter of the rod respectively, m being the mass, f being the resonance frequency for flexion and T_1 being a correction factor for the fundamental flexural mode related to D, L and μ, the Poisson's ratio. (References available in the next slide ....)

Some references

1. ASTM (American Society for Testing and Materials) E1876-15, "Standard Test Method for Dynamic Young's Modulus, Shear Modulus, and Poisson's Ratio by Impulse Excitation of Vibration", ASTM International, West Conshohocken, PA, USA 2015
2. ASTM E1875, "Standard Test Method for Dynamic Youngs Modulus, Shear Modulus, and Poissons Ratio by Sonic Resonance", ASTM International, West Conshohocken, PA, USA, 2013
3. ASTM C215-19, "Standard Test Method for Fundamental Transverse, Longitudinal, and Torsional Resonant Frequencies of Concrete Specimens", ASTM International, West Conshohocken, PA, USA, 2019
4. O. A. Quaglio, J. M. da Silva, E. da Cunha Rodovalho, L. de Vilhena Costa, "Determination of Young's Modulus by Specific Vibration of Basalt and Diabase", Advances in Materials Science and Engineering, vol. 2020, Article ID 4706384, 8 pages, 2020

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.

What is this paper all about?

1. This paper introduces a simple yet unique adaptation of what one knows as the "stochastic finite element method".
2. 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.

The basic strategy of the method; the algorithm

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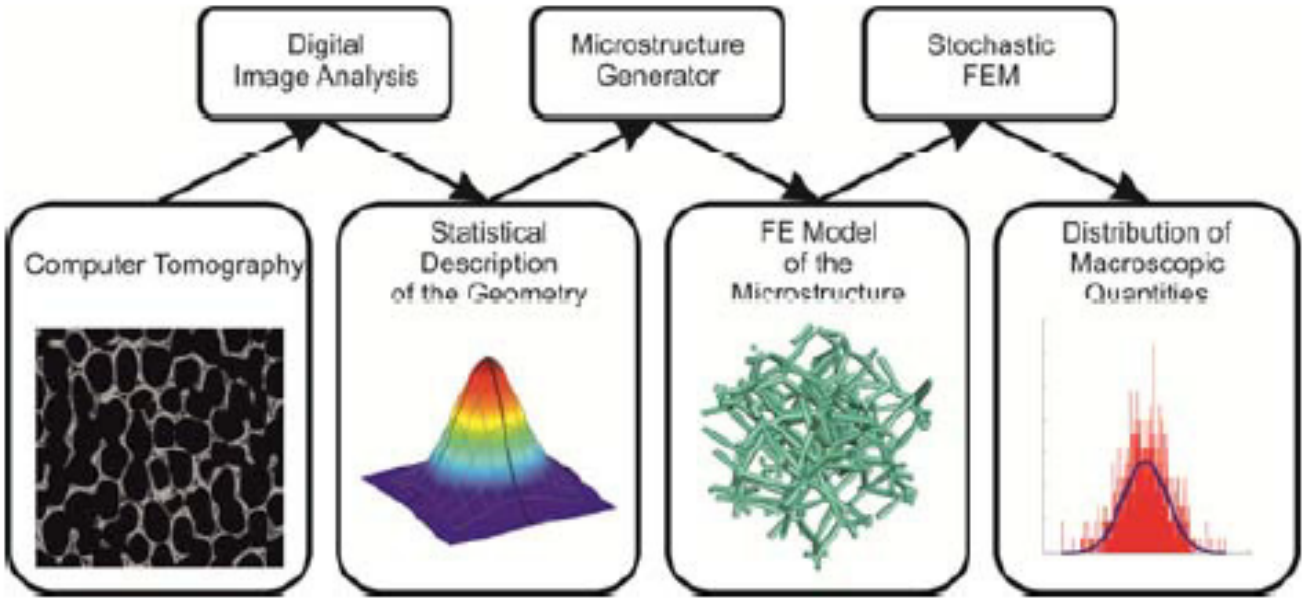


Fig. 1. Overview of the proposed computational procedure.

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).

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.

2.

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.

chosen for the volume distribution of the generating spheres. Its probability density function is given by

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

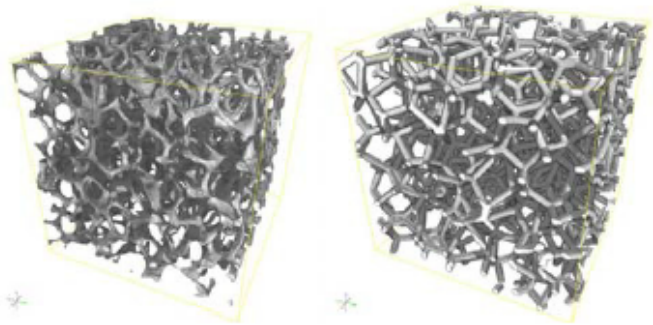
with parameters $m \in \mathbb{R}$ and $\sigma > 0$.

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

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

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 ($\epsilon_{ij} = S_{ijkl}\sigma_{kl}$).

Some references on the morphological operations

1. Kanaun S, Tkachenko O., "Effective conductive properties of open-cell foams", International Journal of Engineering Science, 2008;46:551571
2. Soille P., "Morphological image analysis", Springer Verlag, 1999
3. Liebscher A, Redenbach C., "Statistical analysis of the local strut thickness of open cell foams", Image Analysis & Stereology, 2013
4. Jang WY, Kraynik A, Kyriakides S., "On the microstructure of open-cell foams and its effect on elastic properties", International Journal of Solids and Structures, 2008;45:18451875
5. Kanaun S, Tkachenko O., "Mechanical properties of open cell foams: simulations by Laguerre tessellation procedure", International Journal of Fracture, 2006;140:305312.

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

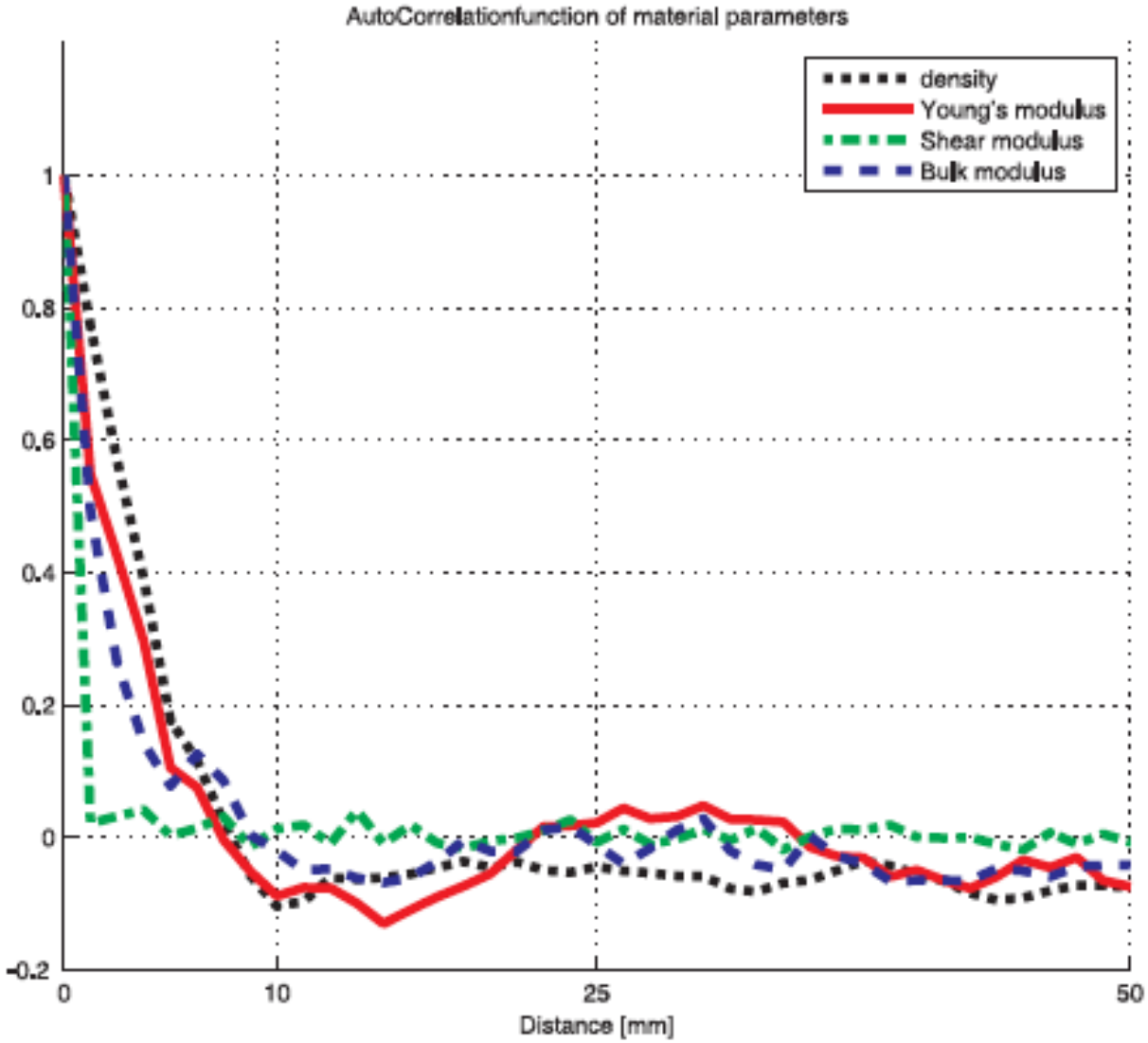
$$E_0(x) = \frac{E(x) - \mu_E}{\sigma_E}, \tag{5}$$

where μ_E and σ_E are the mean value and the standard deviation of the Young's modulus, respectively. Then, for each field the autocorrelation data

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

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 Δ. The results for the material parameters are shown in Figure 3.

Estimating statistical averages



Kahrunen-Loeve transform

According to Wikipedia, "in case of a centered stochastic process $X_{t, t\in[a,b]}, (E[X_t] = 0 \forall t \in [a, b])$ satisfying a technical continuity condition, X_t admits a decomposition",

$$X_t = \sum_{k=1}^{\infty} Z_k e_k(t) \tag{2}$$

where Z_k are pairwise uncorrelated random variables and the functions $e_k(t)$ are continuous real-valued functions on $[a, b]$ that are pairwise orthogonal in $L^2[a, b]$"

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)

Some concluding remarks and advertisements

1. So is the method 'good' or 'bad': Rather subjective.
2. It's good because the treatment of the inherent randomness of the system in question has been captured well.
3. It's not clear whether they have repeated the 'numerical experiment' several times before being assured of the correctness of the verification.
4. Also, personal questions whether it is better than using the same scheme with the randomness along with the finite difference grid; comparing the time and space complexity of the FDA and FEA??

Some concluding remarks and advertisements

1. Survey paper on stochastic FEA: "Practical Application of the Stochastic Finite Element Method" by Jose D. A. Mena (Oak Ridge National Lab), L. Margetts (University of Manchester), P. Mummery (University of Manchester)
2. I am developing a repository *ShrohanMohapatra/softMatterAlgos* with all of my attempts to code all the schemes discussed in the class such as Monte Carlo, molecular dynamics, Brownian dynamics, SCFT (for a dilute homopolymer solution) etc.

Thank you!!!