OTTO VON GUERICKE UNIVERSITÄT MAGDEBURG

Optimized Representative Volume Elements

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Introduction. The Representative Volume Element (RVE) method is a pragmatic approach to estimate effective properties. One imposes effective independent variables on a RVE that contains the microstructure, solves the boundary value problem numerically, and extracts average quantities.

Problem Definition

Presuming non-periodic microstructures, **good estimates** require large RVE that recover all statistical properties of the microstructure. They **are** therefore **numerically expensive**.

Objectives

Maximize the **quality** of the estimate from an RVE **over** the **numerical expense** for non-periodic microstructures.

Cooperation

Prof. Dr.-Ing. Thomas Böhlke, Karlsruhe Institut für Technologie (KIT)

Optimitze RVE Shape

There are three classical RVE boundary conditions (BC):

Isostrain BC: $\boldsymbol{u} = \overline{\boldsymbol{H}} \cdot \boldsymbol{x}_0$

Isostress / kinematic minimal BC: $\boldsymbol{t} = \overline{\boldsymbol{T}}_{1pk} \cdot \boldsymbol{n}_0 \quad \leftrightarrow \quad \overline{\boldsymbol{H}} = \int \boldsymbol{u} \otimes dA$

Pairwise periodic / antipodic coupling: $\boldsymbol{u}_+ - \boldsymbol{u}_- = \overline{\boldsymbol{H}} \cdot [\boldsymbol{x}_{0+} - \boldsymbol{x}_{0-}],\ \boldsymbol{n}_{0+} \cdot \boldsymbol{n}_{0-} = -1$

The BC are necessarily artificial. Convergence to the effective properties is obtained for RVE of increasing size due to $A_{RVE}/V_{RVE} \to 0$, i.e., the boundary influence vanishes in the absence of localization. The ratio A_{RVE}/V_{RVE} can be reduced by **using spherical RVE rather than cubical RVE**.

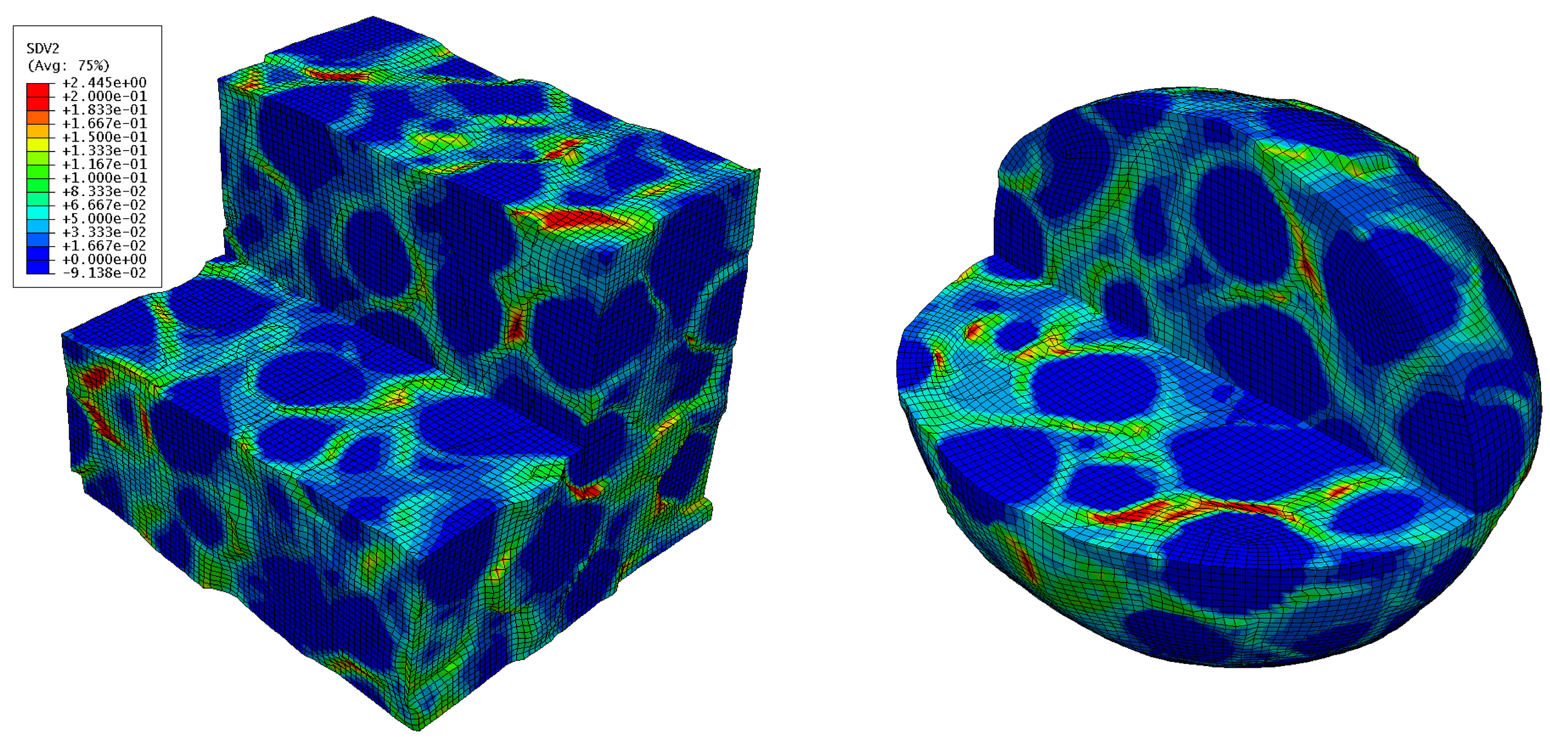


Figure 1. Cubical and spherical RVE of an isotropic, elastoplastic matrix material without hardening, with stiffer, isotropic, elastic, spherical inclusions of equal diameter, dispersed homogeneously, after 10% of effective strain in a uniaxial tension test (color indicates eq. plastic strain).

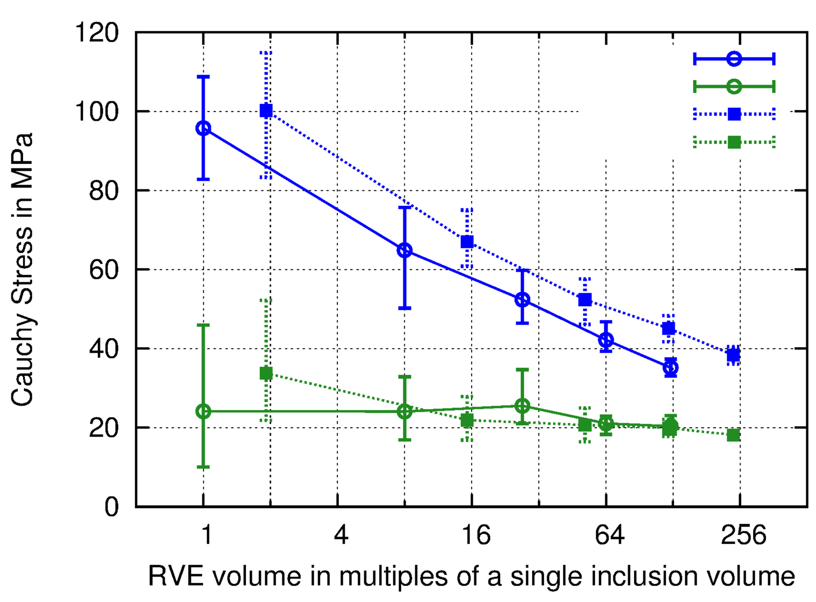


Figure 2. Effective tension stress at 10% of strain for periodic BC (green) and isostrain BC (blue). Convergence is better for spherical RVE (see legend).

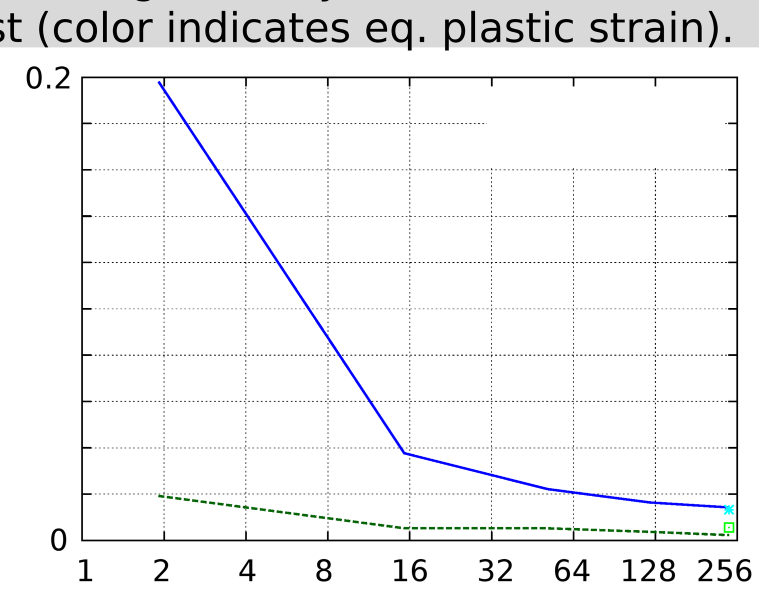


Figure 3. Ratio of the norms of anisotropic and isotropic part of eff. stiffness tetrad over RVE vol. in singel inclusion vol., cubical and spherical RVE with periodic and antipodal BC (blue and green).

Optimize Boundary Conditions

The generalized BC:

Partition the RVE surface into *n* parts. The independent variable is $\overline{\boldsymbol{H}}$. Impose kinematic minimal BC on each part individually.

By using simply non-connected **stochastic partitionings**, one obtains the stochastic BC. The stiffness can be adjusted by the size of the partitions.

Depending on the partitioning, one can **scale between** the **stiff isostrain BC** (infinite fine partitioning) and the **soft isostress BC** (no partitioning). The periodic/antipodal BC are obtained by contracting a partition of two not simply connected sections to opposing points.

The **Hill-Mandel-condition is satisfied** for any partitioning.

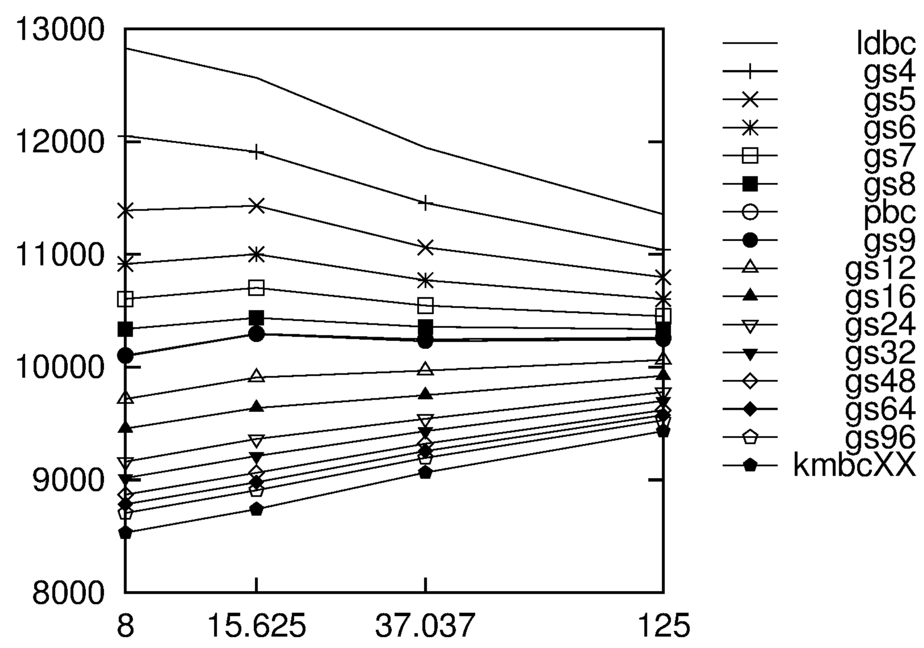


Figure 4. Effective Young's modulus in MPa converges as the RVE size is increased. gs*n* corresponds to generalized stochastic BC with a **coupling of *n* surface points**. *n*=3 gives isostrain BC (ldbc), $n \to \infty$ gives isostress BC (kmbcXX). ***n*=9 gives a stiffness virtually identical to the periodic/antipodal BC**.

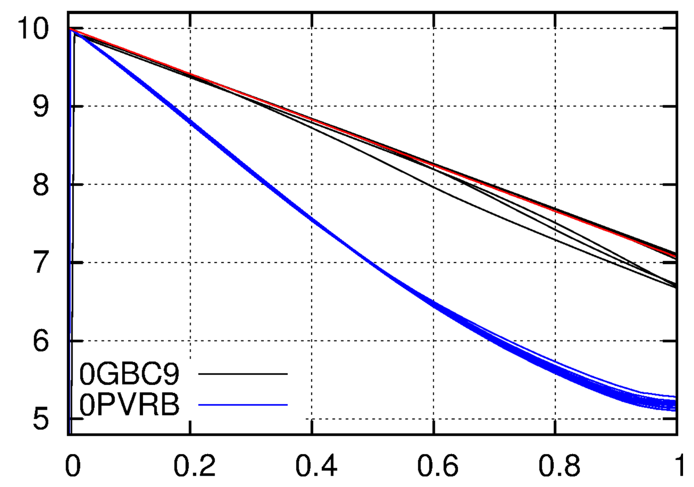
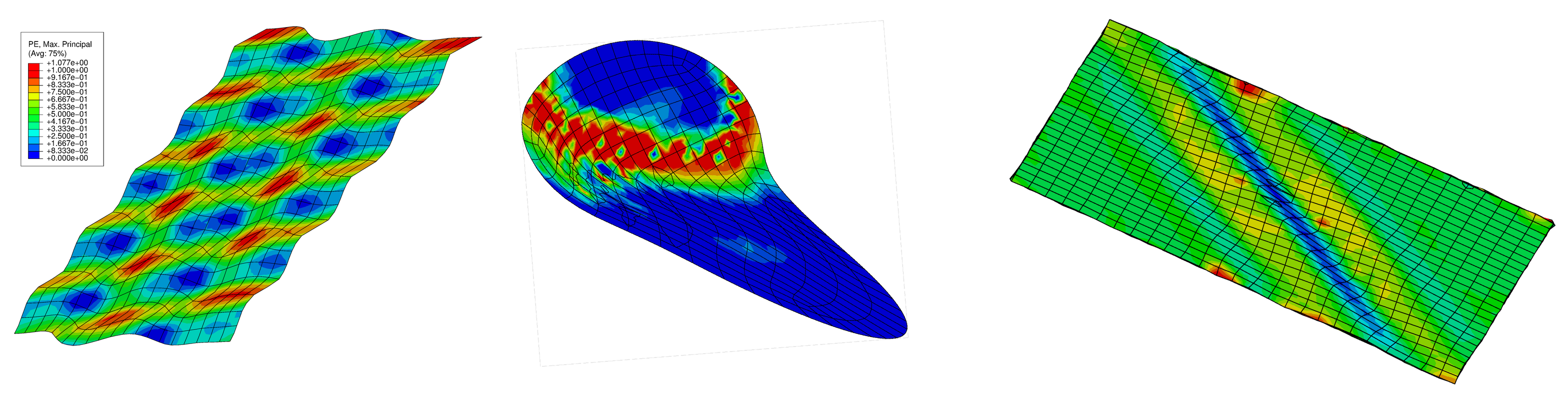


Figure 5. v. Mises stress in MPa over effective shear strain for a hom. RVE with softening elastoplastic material with periodic/antipodal BC (blue) and stochastic BC with *n*=9 (black). Both BC are equally stiff for the elastic properties (see Fig. 4), but localization prevents the periodic BC from being close to the true effective material law (red).

The stochastic BC allow to adjust the resistence against non-localized deformations and against localization to some extend independently. The stochastic node coupling diffuses shear bands that reach the boundary, preventing a loss of representativity, as can be seen in the lower right figure:



Summary

Shape optimization:
- spherical RVE give better convergence by reducing the boundary effect
- spherical RVE allow for BC of moderate stiffness without introducing an artificial anisotropy

Generalized BC:
- allow for stochastic BC of moderate stiffness with high resistance against localization at the same time
- combine the best properties of periodic BC and isostrain BC

Publications

R. Glüge, M. Weber, A. Bertram: Comparison of spherical and cubical statistical volume elements with respect to convergence, anisotropy and localization behavior, Computational Materials Science, (2012), 63, 91-104

R. Glüge, M. Weber: Numerical Properties of Spherical and Cubical Representative Volume Elements with Different Boundary Conditions, Technische Mechanik 33, 97-103 (2013)

R. Glüge: Generalized boundary conditions on representative volume elements and their use in determining the effective material properties, Computational Materials Science, (2013), 79, 408-416

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