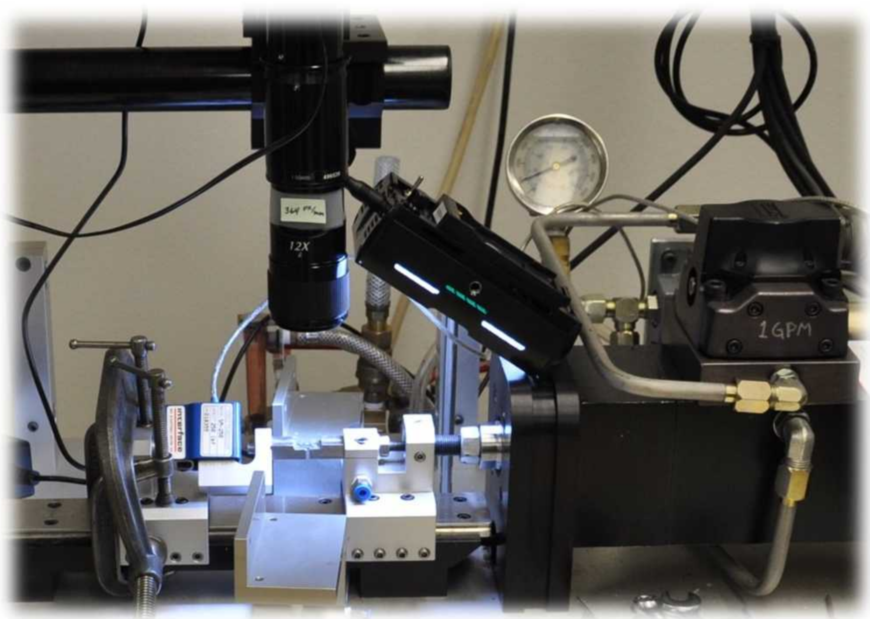
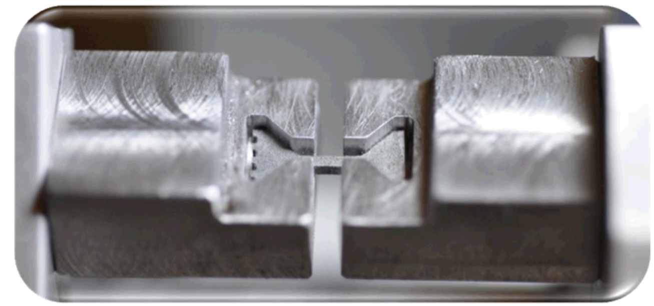
Emergent homogenization techniques and effective dynamical properties

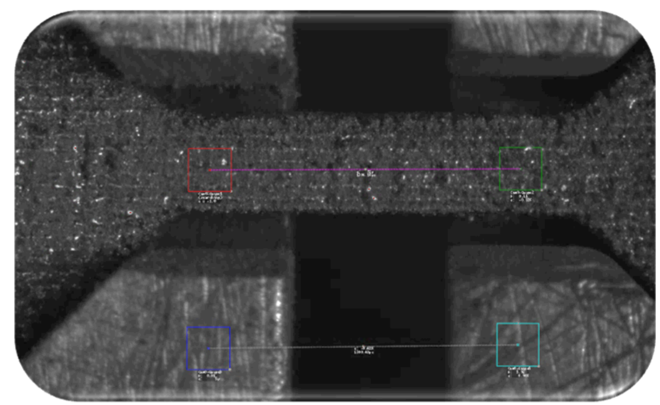
SAND2016-6973D



tensile tester [7]



grippers w/1x1 mm gage section sample for testing [7]



Sample under test [7]

Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

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Objective

Enable structure-property correlation analysis using a simplified microstructural representation:

- Generate statistically similar volume elements based on n-point correlation functions for heterogeneous material.
- Test the effect of different RVE configurations on the static and dynamic macroscale response using a quasi-explicit multiscale solver.

✧ Theory: Volume elements

- Representative volume element (RVE), is the smallest volume over which a measurement can be made that will yield a value that is representative of the whole.

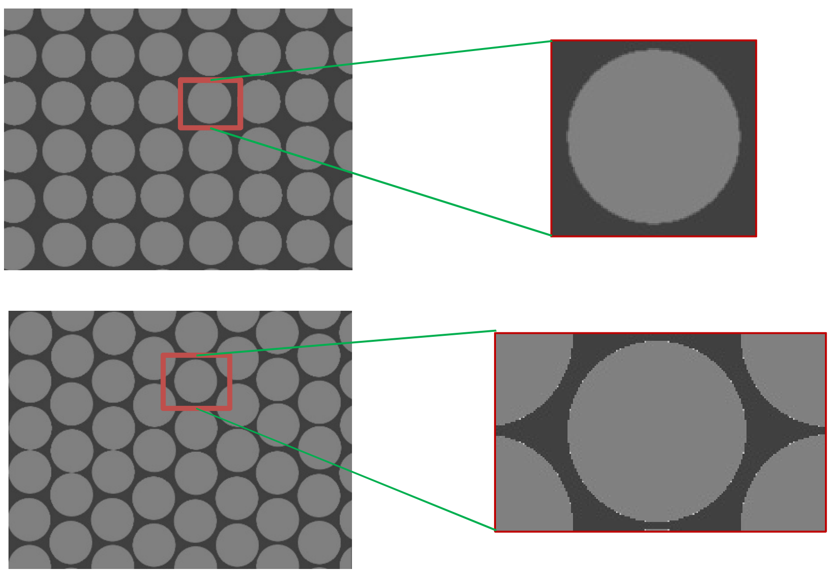


Fig. 1 Deduction of RVE for continuous fiber reinforced composite for square and hexagonal lattice

- Statistical volume element (SVE), also referred to as stochastic volume element in finite element analysis, takes into account statistics and variability in the microstructure of interest based on macroscopic property of interest.

(a) (b)

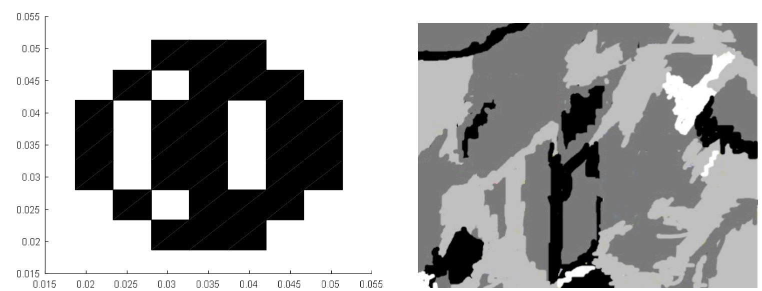


Fig. 2 Types of microstructure representation (a) Eigen microstructure – represented by discrete phases (here 0 & 1) (b) Non-eigen microstructure – represented by continuous phase

✧ Theory: Microstructural statistics

- **One-point correlation function:** probability that a randomly chosen point in the medium belongs to a phase
- **Two-point correlation function:** probability that two randomly chosen points **x**1 and **x**2 both lie in the same phase
- **Lineal-path function:** probability that the entire line segment between points **x**1 and **x**2 lies in the same phase
- **Two-point cluster function:** the probability that two randomly chosen points **x**1 and **x**2 belong to the same cluster of a phase

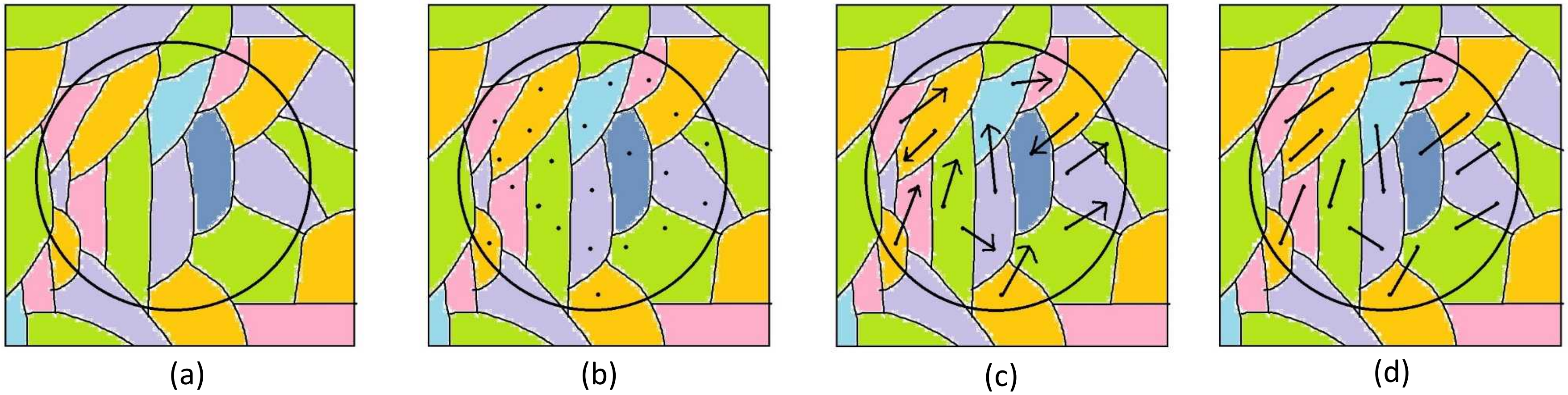
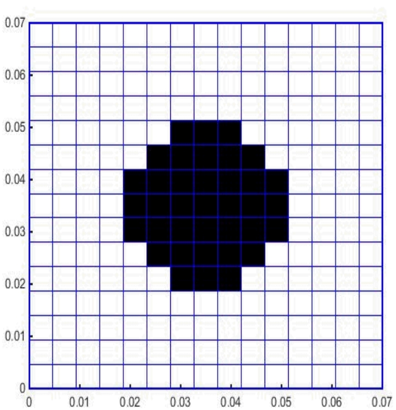


Fig. 3 Depiction of microstructure statistics (a) given microstructure (b) One point correlation (c) Two point correlation (d) Lineal-path correlation

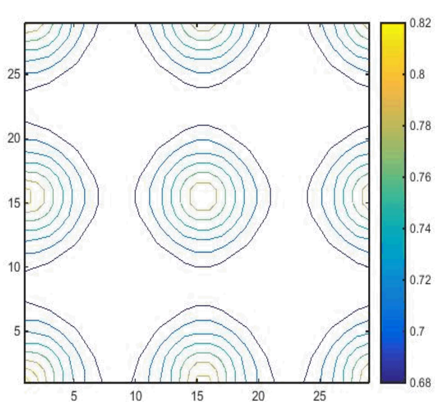
✧ Microstructure reconstruction algorithm

Phase recovery iterative algorithm

Step 1: Deduction of statistical parameter – two point correlation



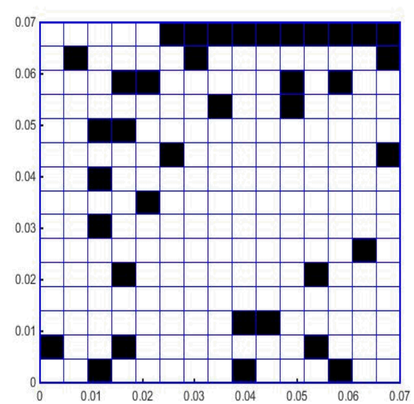
Target microstructure
- φ_1 (black phase) = 0.16
- I : target indicator function
- NxN : grid size



Target 2-point correlation

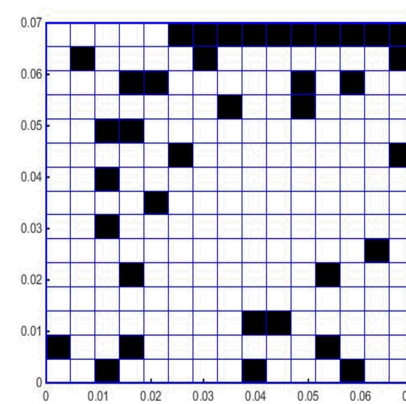
$$= \frac{1}{N^2} fft^{-1}\left[(fft(I) * fft(I)) \right]$$

Step 2: Initialize optimization



Gaussian random microstructure as initial iteration
- $\varphi_1 = 0.16$ **(constraint)**

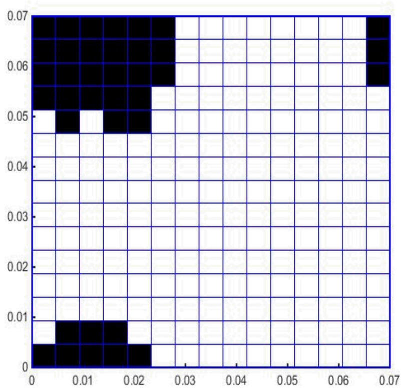
Step 3: Phase recovery iteration



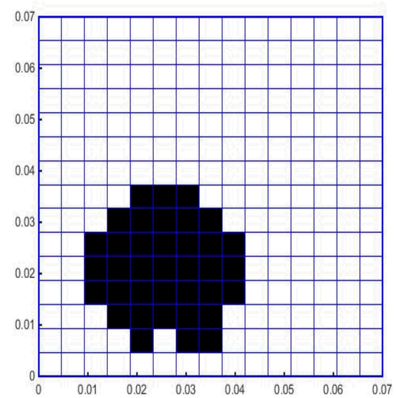
Iteration steps
- Fourier amp. & angle
- Replace amp. with target amplitude
- Assign 0's & 1's based on maximum likelihood

Step 4: Invoking periodic structure constraint

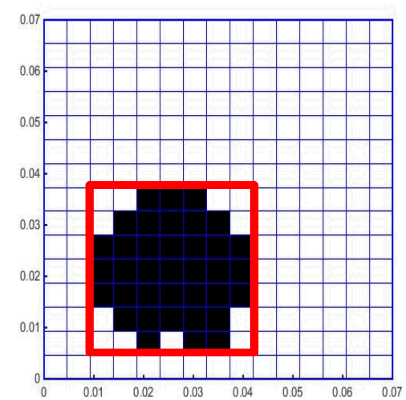
Step 5: Selection of cluster of particles



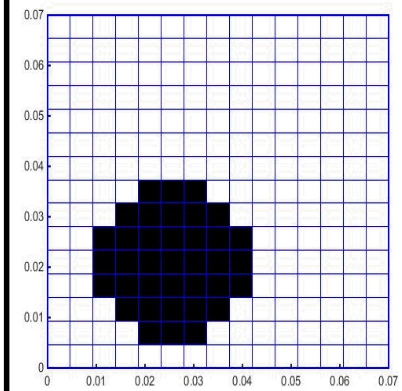
Optimized microstructure
- φ_1 = 0.16
- Error $\triangleq \left\| \text{Target-Recon} \right\|_F = 0.032$



Reconstructed with periodic boundary condition



Optimization is performed only on the selected cluster through Simulated Annealing



Final reconstructed microstructure

✧ Theory: FE^2 method

- Finite element squared (FE^2) method is a computational homogenization approach, which is based on the solution of two boundary value problems, one for the macroscopic and one for the RVE scale.

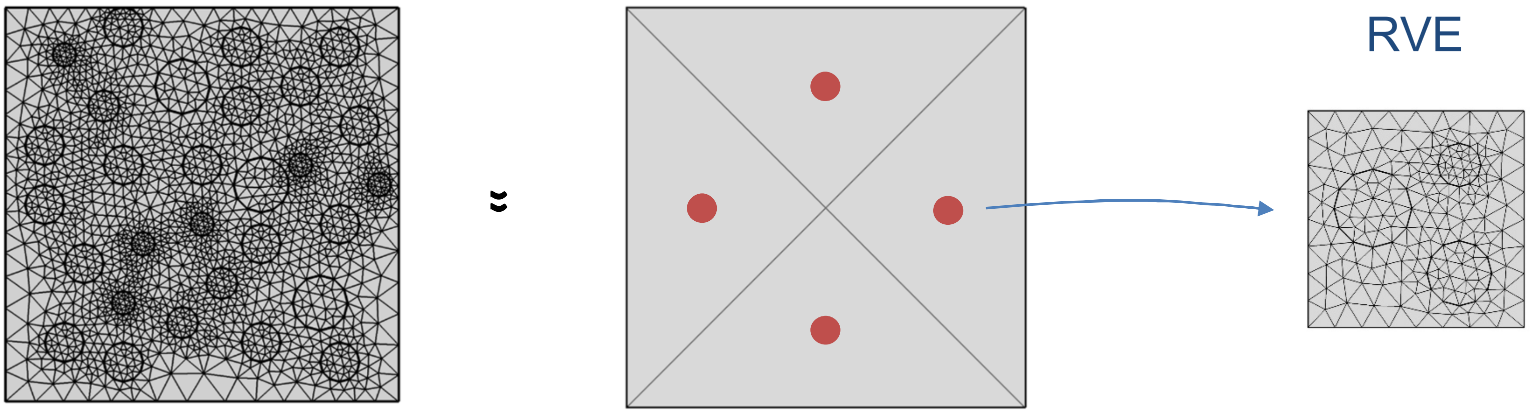
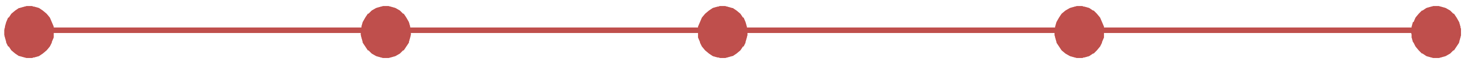


Fig. 4 Schematic figure of single scale and multiscale finite element mesh.

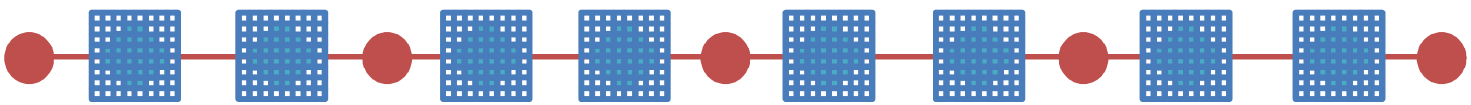
- A multiscale solver is recently formulated in the spirit of FE^2 and is capable to deal with general loading conditions, including inertia effects. Each time incremental problem can be solved exactly with a single Newton-Raphson iteration with a constant Hessian, representing a quasi-explicit multiscale solver (QEMS).

✧ Quasi-explicit multiscale solver

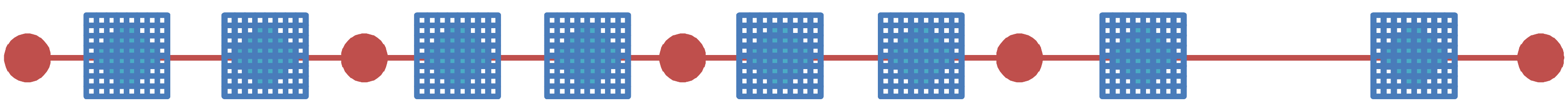
Step-0 Consider a 1-D macroscopic mesh with n elements and n+1 nodes.



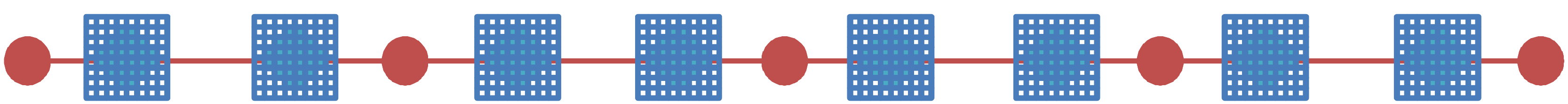
Step-1 Setup initial configuration (two RVEs per 1-D element).



Step-2 Apply increment to the macroscopic boundary conditions.
Get boundary condition for all RVEs and solve RVE as BVP.



Step-3 Compute macroscopic force and update macroscopic nodes.



Step-4 Solve all RVE problems in the current macroscopic configuration.
Update information for the next time step.

✧ Improvement of QEMS

- The original multiscale solver uses explicit Newmark method, which is conditionally stable. Instead of using same time step, different time steps could be used in the multiscale solver. In the step 4 of the flow chart, the boundary condition for all the RVE could be applied adaptively.

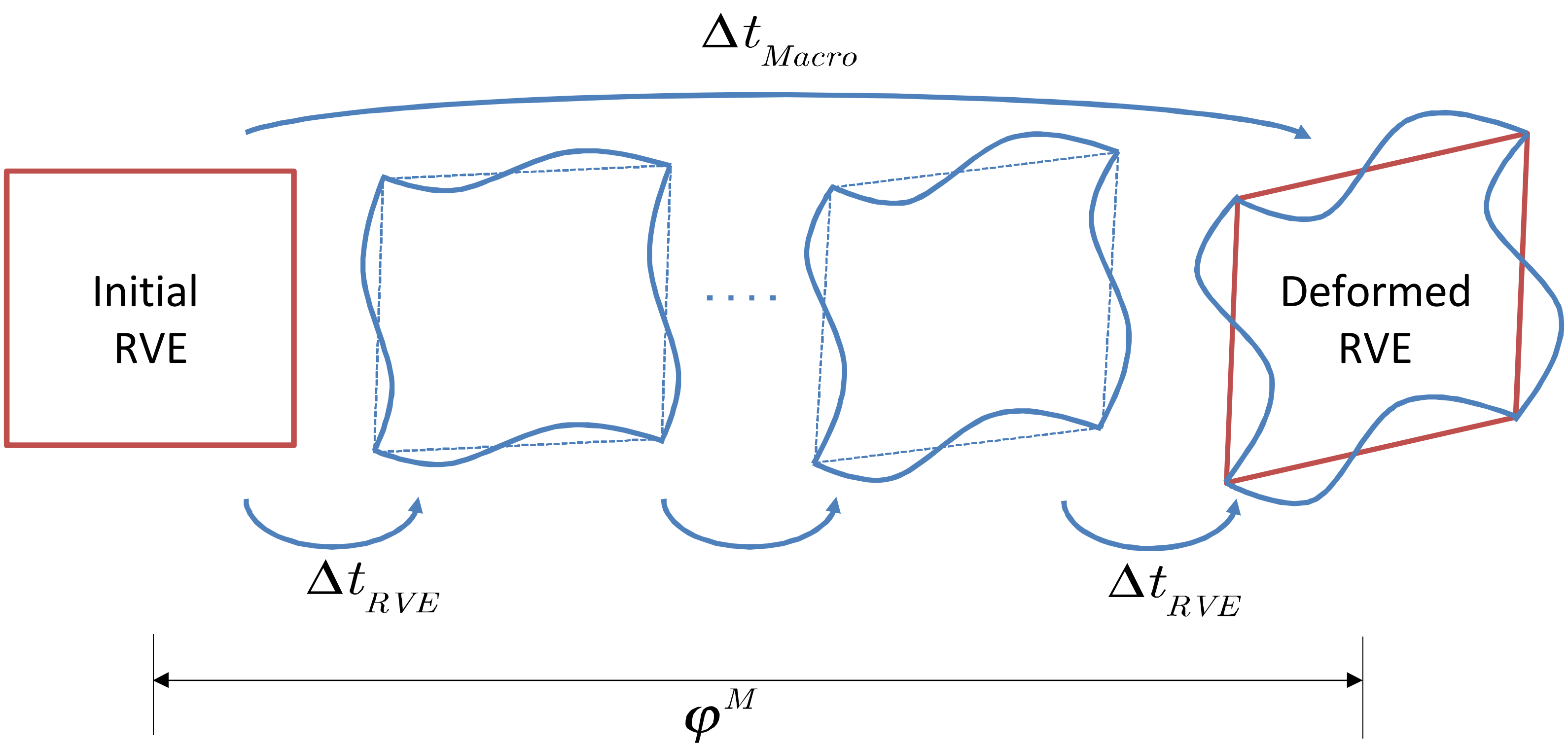
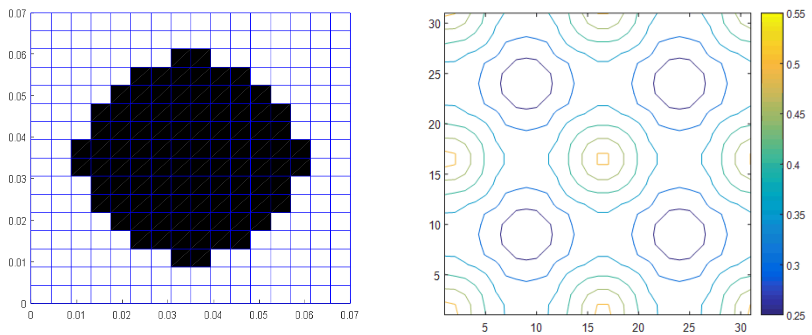


Fig. 5 Schematic figure of sub-cycling in multiscale solver.

✧ Case Study

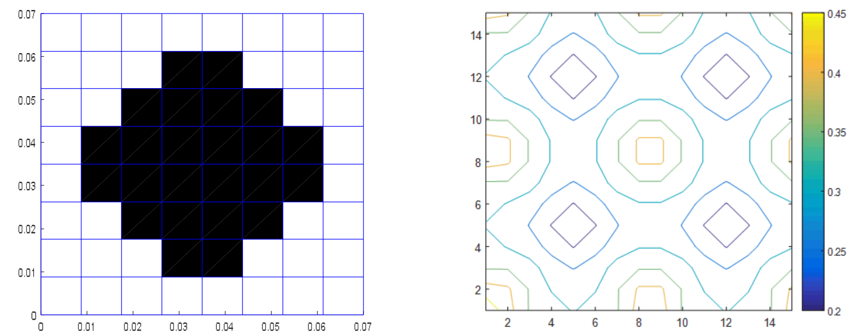
- Problem Description

A microstructure with a circular inclusion is studied with both a 16X16 and a 8X8 pixel grid. These microstructures represent actual and pixelated volume element image. The coarser mesh microstructure is generated iteratively by minimizing difference in two point correlation with the volume fraction constraint. QEMS is used to test the macroscopic response of the two sets of RVEs.



(a) (b)

Fig. 6 (a) Microstructure with circular inclusion on 16X16 pixel grid.
(b) Two point correlation of microstructure.



(a) (b)

Fig. 7 (a) Microstructure with circular inclusion on 8X8 pixel grid.
(b) Two point correlation of microstructure.

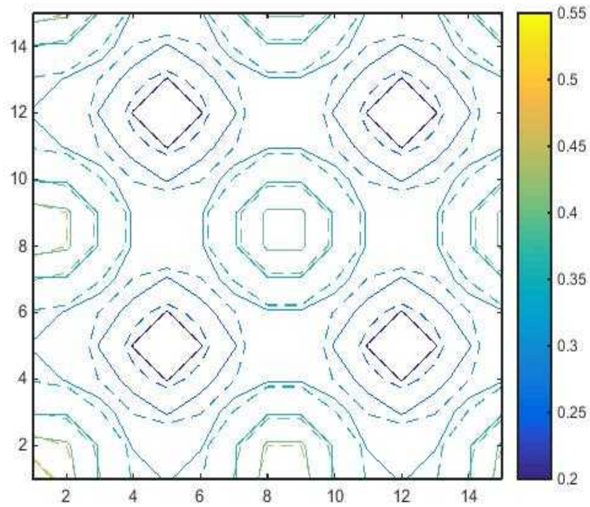


Fig. 8 Comparison of two point correlation deduced from original 8X8 pixel grid (-) and interpolated from 16X16 (--) pixel grid.

- Comparison of original and interpolated correlation shows the approximation during the mesh coarsening
- Interpolated values are higher than original data in general
- Two point correlation for r=0 (or 1 point correlation) are close for both cases
- Direct interpolation can cause distortion in complex asymmetric volume element

- Computational results

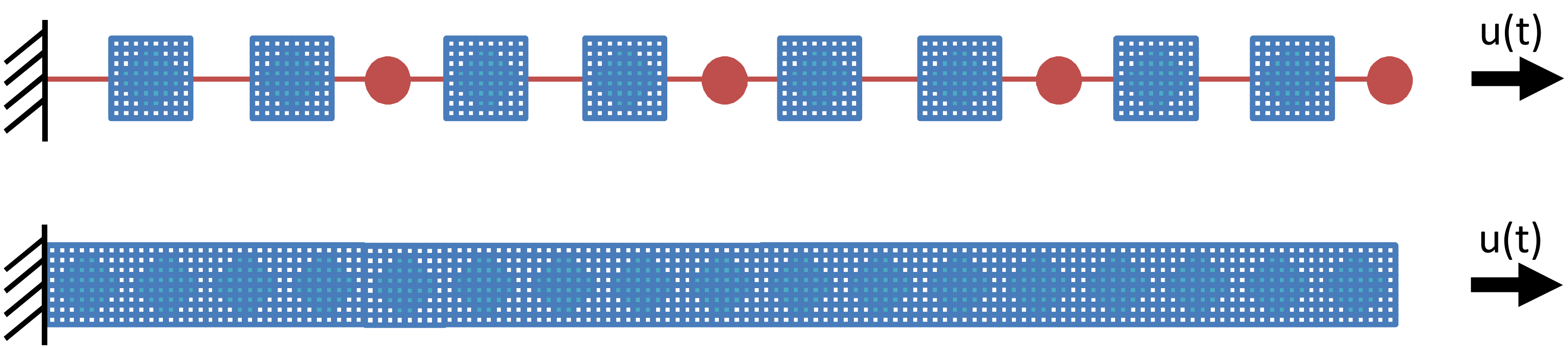


Fig. 9 Multiscale and single scale finite element model.

Quasi-static response by multiscale solver (MS)

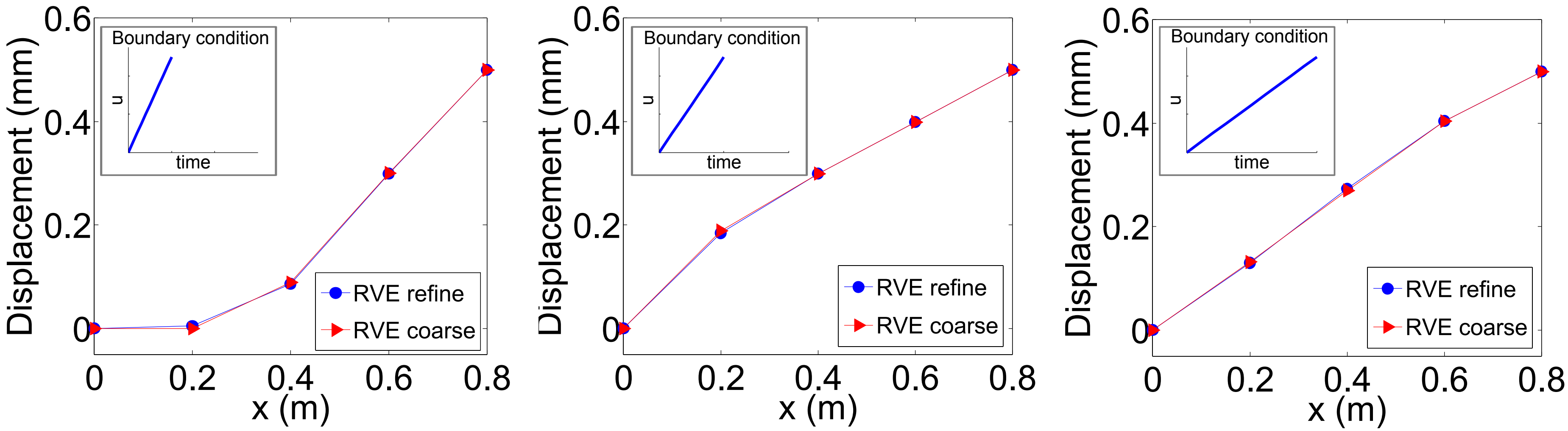


Fig. 10 Displacement distribution along macroscopic domain at final time with different loading rate.

Dynamic response and effective Young's modulus

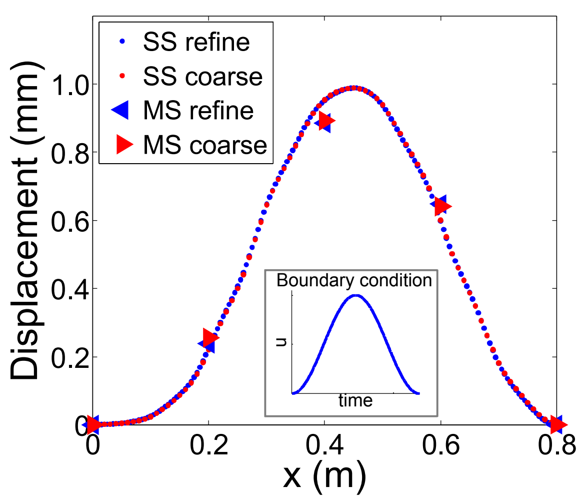


Fig. 11 Displacement distribution along the macroscopic domain at final time.

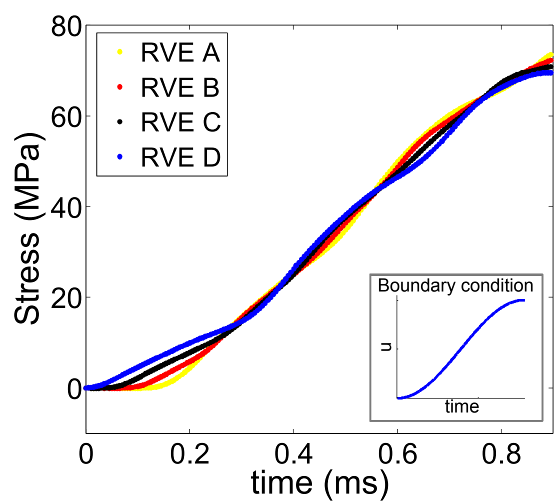


Fig. 12 Time evolution of the volume average of stress along the macro domain.

Materials	E (GPa)	density (kg/m³)
Inclusion	20	1000
Matrix (steel)	200	7000
Effective $\rho(\lambda / T)^2$	114.9	4750
Effective σ / ε	116.8	4750

Table. 1 Material properties of the composite and the calculated Young's modulus.

Conclusions

- Using the 2-point correlation function via fft, along with simulated annealing, a microstructure can be recreated with various grid sizes.
- With the coarsening procedure, while keeping the similar statistic property of RVEs, the presented macroscopic displacement distribution is similar.
- Effective Young's modulus computed by the wavelength and evolution of static stress are shown to be in good agreement.

References

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4. Liu, C. and Reina C., Discrete averaging relations for micro to macro transition, Journal of Applied Mechanics, 2016, 83(8), 081006.
5. Liu, C. and Reina C., Computational homogenization of heterogeneous media under dynamic loading, arXiv preprint arXiv: 1510.02310.
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7. The credit of the photo of experimental instruments belongs to Brad Boyce and Brad Salzbrenner of Sandia National Labs.

Suggested Layout of slides:

Title (slide 1) Authors (slide 2)

Objective (slide 3)

- Theory: volume… (slide 4)
- Theory: Micro… (slide 5)
- Microstructure… (slide 6-7)

- Theory: : FE^2… (slide 8)
- QEMS (slide 9)
- Improvement… (slide 10)

- Case study

slide 11 slide 12 slide 13

Conclusion (slide 14) References (slide 15)

Another Suggested Layout of slides:

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slide 11   slide 12   slide 13

Conclusion (slide 14)   References (slide 15)