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A nonlinear reduced order modelling approach to solid mechanics with application to representative volume elements

Abstract: why nonlinear MOR for FE² RVE computations?

Nonlinear model order reduction (MOR) methods like Laplacian Eigenmaps (LEM) [1] and Locally Linear Embedding (LLE) [8] are often used to extract nonlinear trends in image and speech processing [3]. There has also been successful application in fluid mechanics [7] and elastodynamics [5]. Here, we investigate the application of nonlinear MOR methods to representative volume element (RVE) computations in the context of the FE^2 method for solid mechanics.

- **Idea:** Use LEM and LLE to capture nonlinearities in solution manifolds of mechanical systems, to obtain more accurate results with fewer parameters and lower computational effort [3].
- **Application:** Representative volume element (RVE) computations for the FE^2 method [10, 4, 9].
- **Challenges:**
  - Mapping between solution space and reduced space not defined a priori [7],
  - Linearisation nontrivial [7].
- **Opportunities:**
  - Lots of data,
  - Well-defined parameter space,
  - Nonlinear, low-dimensional solution manifold.

Goal: accelerate FE² RVE computations

Instead of querying a material law, the FE^2 method performs an RVE computation at each Gauss point, in each iteration [10, 4, 9].

1. Pass macroscopic deformation gradient $\bar{\mathbf{F}}$ to RVE.
2. Impose e.g. periodic boundary conditions and compute displacements $\mathbf{u} \in \mathbb{R}^D$ in RVE; compute stress $\mathbf{P}$ and stiffness $\mathbf{A}$ fields.
3. Return average stresses $\bar{\mathbf{P}}$ and stiffnesses $\bar{\mathbf{A}}$ to macroscopic simulation.

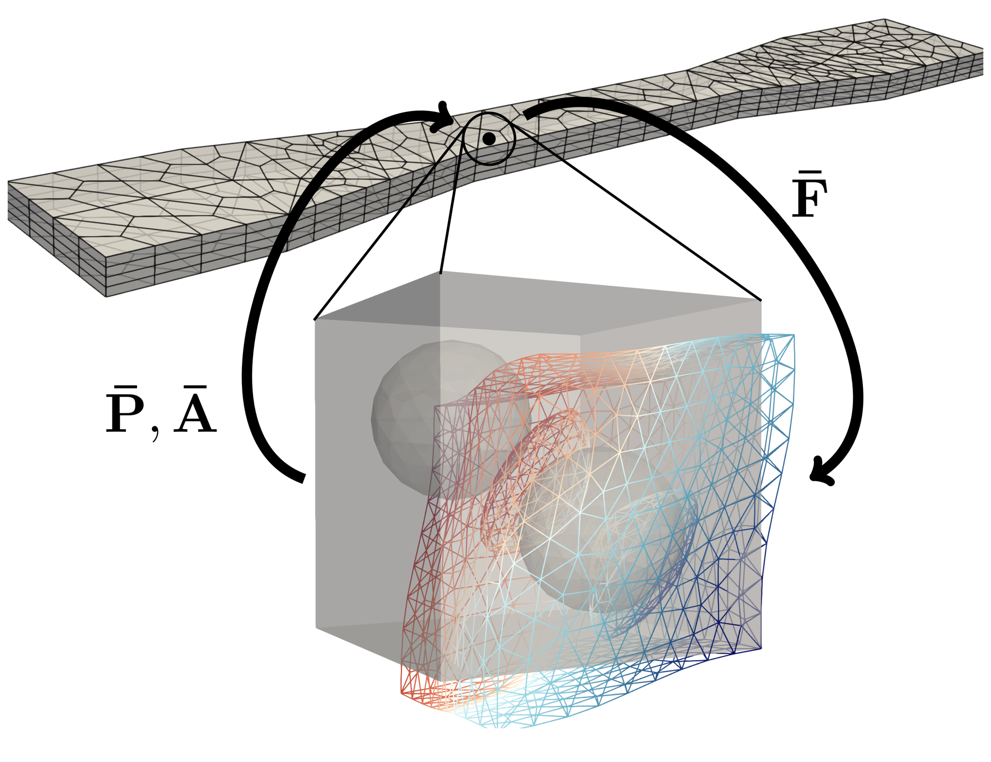


Figure 1. Schematic of the FE^2 method

Approach: Use (nonlinear) MOR to accelerate RVE computations. Do this by reducing the RVE displacement field $\mathbf{u} \in \mathbb{R}^D$ using LEM or LLE. The MOR scheme could be divided as follows:

1. **Offline phase:** Gather snapshots (full-FEM solutions) $\mathbf{U} \in \mathbb{R}^{D \times s}$ to the RVE problem to use as training data, and use LEM or LLE to obtain an embedding $\mathbf{Y} \in \mathbb{R}^{d \times s}$.
2. **Online phase:** Use the reduced model and local linearisation for projection-based MOR.

Proof of concept: numerical experiments on an RVE

In a proof-of-concept investigation, the LEM and the LLE are used to obtain reduced models for an artificial RVE. The RVE is subjected to periodic boundary conditions with load paths specified via the macroscopic displacement gradient $\bar{\mathbf{H}} = \bar{\mathbf{F}} - \mathbf{I}$ to emulate the use case in the FE^2 method.

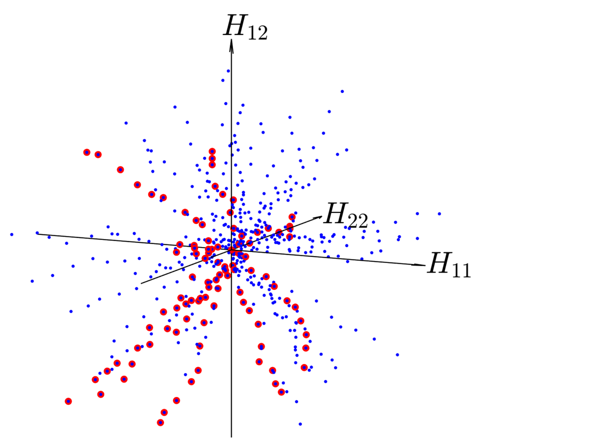


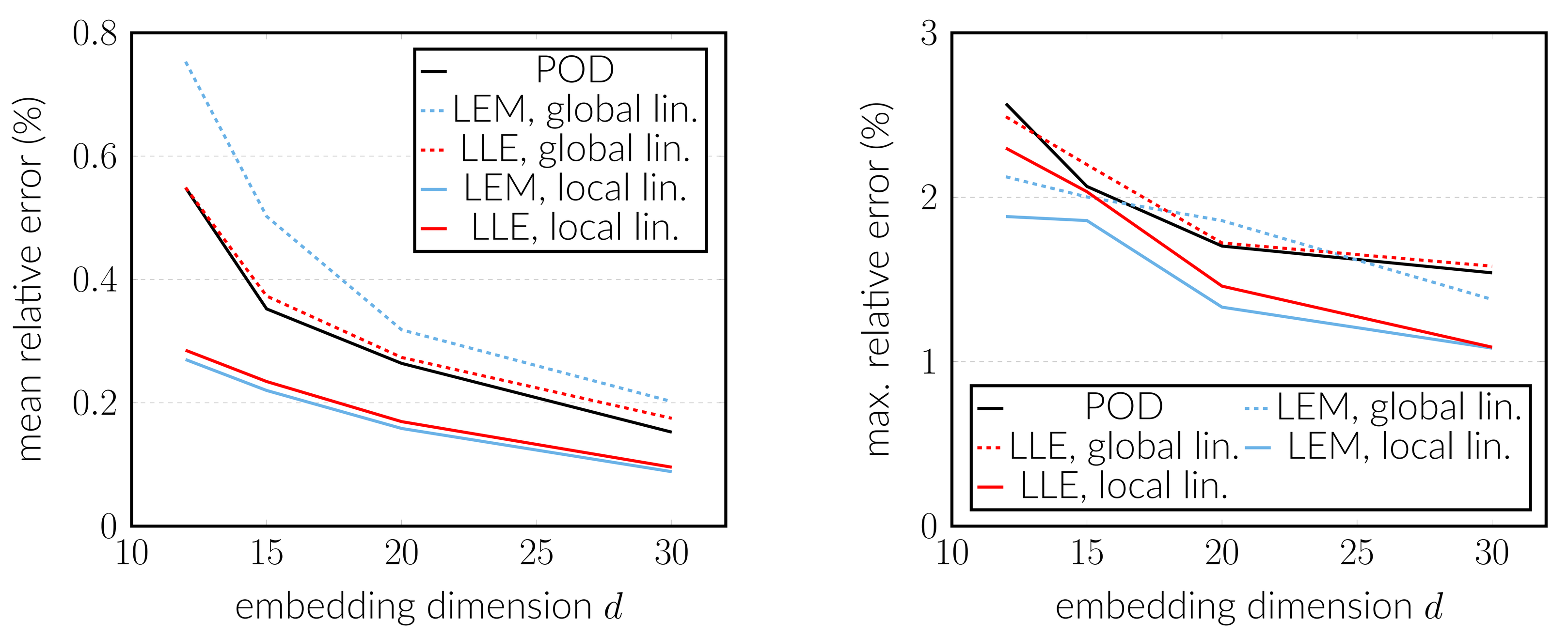
Figure 2. Three macroscopic displacement gradient components for training (red) and validation (blue) load paths

1. Compute RVE snapshots (full-FEM solutions) $\mathbf{U} \in \mathbb{R}^{D \times s}$ for 10 training load paths (red dots).
2. Obtain embedding $\mathbf{Y} \in \mathbb{R}^{d \times s}$ via LEM or LLE.
3. Compute RVE solutions for 50 validation load paths (blue dots), using the reduced model.
4. Compare to results obtained via full-FEM computations. Evaluate the relative error between reduced and full-FEM solutions.
5. Compare relative errors obtained via the LEM and LLE to those obtained via the Proper Orthogonal Decomposition (POD), see e.g. [6, 11].

Experiments are conducted on the simple artificial RVE with two pores in Figure 1, with:

- $D \approx 6000$ as well as $D \approx 20000$ DOFs,
- Quadratic tetrahedral elements,
- Compressible neo-Hooke material model [2],
- $E = 1000$, $\nu = 0.25$.

Results: relative error for RVE experiments



Tools, Data, and Acknowledgements

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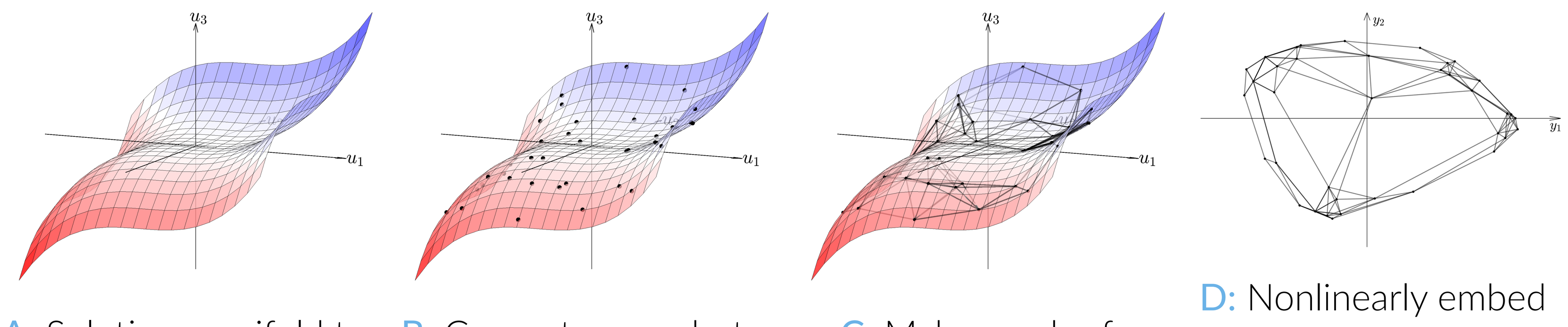
All FE and MOR scripts were run with our in-house FElix toolbox. Python routines, results data, and visualisations are archived on GitHub.

How to unwind a solution manifold with nonlinear MOR methods

For a set of full-FEM snapshot solutions $\mathbf{U} \in \mathbb{R}^{D \times s}$ to an RVE problem, the LEM and LLE can find a low-dimensional embedding $\mathbf{Y} \in \mathbb{R}^{d \times s}$. The goal is the data-based identification of a reduced space $\mathbf{y} \in \mathbb{R}^d$ to parametrise the solution manifold while respecting its nonlinearity. For example, an LEM workflow might look as follows [1]:

1. Compute s full-FEM snapshots solutions $\mathbf{U} \in \mathbb{R}^{D \times s}$ for the RVE problem.
2. Make a graph $\mathbf{G}$ with Gaussian weights $\mathbf{W} \in \mathbb{R}^{s \times s}$ for $\mathbf{U}$ using a k-nearest neigbours algorithm.
3. Compute the graph Laplacian $\mathbf{L} = \mathbf{D} - \mathbf{W}$, were $\mathbf{D}$ is a diagonal matrix with $D_{ii} = \sum_j W_{ij}$.
4. Compute the eigenvalues λ_i and eigenvectors $\mathbf{v}_i$ of the scaled graph Laplacian $\tilde{\mathbf{L}} = \mathbf{D}^{-1}\mathbf{L}$.
5. The eigenvectors for the 2$^{\text{nd}}$ to $s+1^{\text{th}}$ lowest eigenvalues yield the embedding: $\mathbf{Y} = [\mathbf{v}_2, \dots, \mathbf{v}_{s+1}]^T \in \mathbb{R}^{d \times s}$.



A: Solution manifold to be approximated (in solution space $\mathbf{u} \in \mathbb{R}^D$)

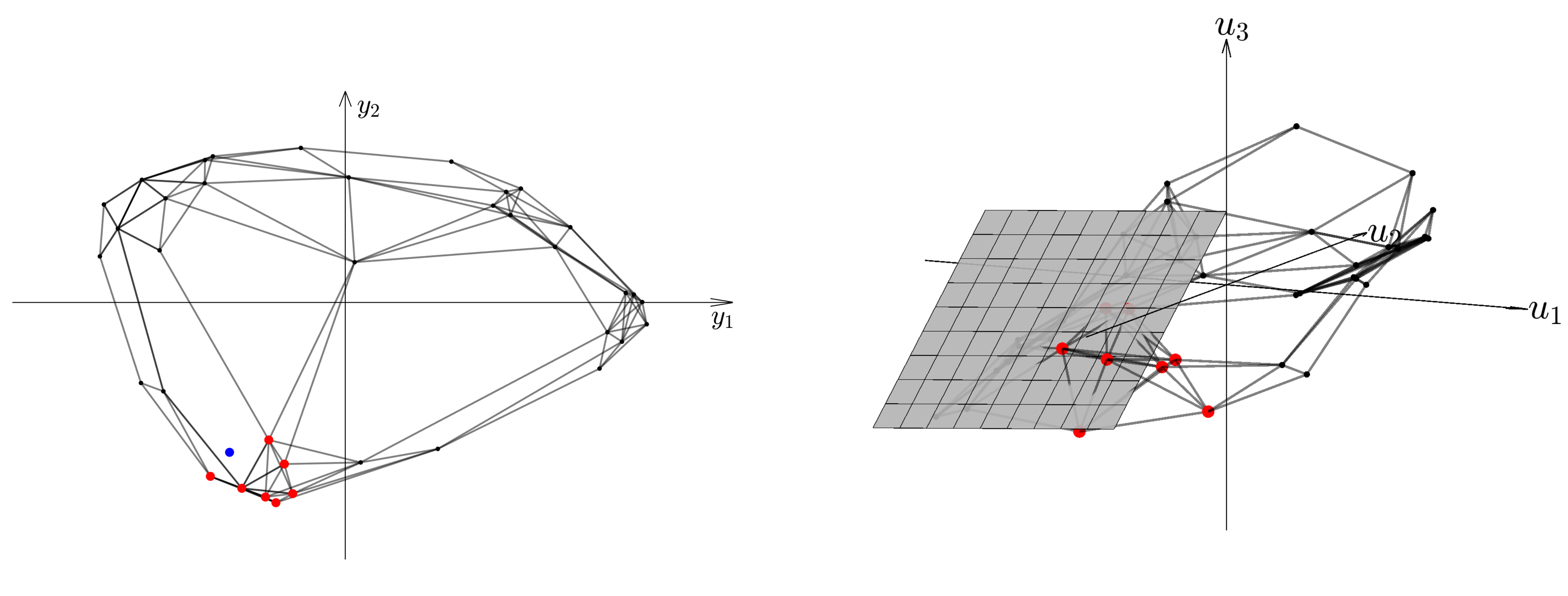
B: Compute snapshots (full FE solutions to RVE problem)

C: Make graph of snapshot data

D: Nonlinearly embed graph using LEM or LLE (in reduced space $\mathbf{y} \in \mathbb{R}^d$)

Challenge: Mapping $\mathbf{u} = M(\mathbf{y})$ from reduced space $\mathbf{y} \in \mathbb{R}^d$ to solution space $\mathbf{u} \in \mathbb{R}^D$ not known!

How to (locally) linearise nonlinear MOR methods



1: Find neighbours (red) to current point (blue) in reduced space

2: Linearise mapping of neighbouring points from reduced to solution space

Solution: Local linearisation of mapping from reduced space $\mathbf{y} \in \mathbb{R}^d$ to solution space $\mathbf{u} \in \mathbb{R}^D$ via coordinates of N neighbouring solutions in reduced space $\mathbf{Y}_N \in \mathbb{R}^{d \times N}$ and solution space $\mathbf{U}_N \in \mathbb{R}^{D \times N}$

$$\psi = \mathbf{U}_N \mathbf{W}_N \mathbf{Y}_N^T (\mathbf{Y}_N \mathbf{W}_N \mathbf{Y}_N^T)^{-1}, \quad \mathbf{W}_N = \mathbf{I}_N - \frac{1}{N}\mathbf{1}_N,$$

such that the increment in solution space can be computed as

$$\Delta \mathbf{u} = \psi \Delta \mathbf{y}.$$

An alternative is the global linearisation scheme proposed in [7], with $\psi = \mathbf{U}\mathbf{Y}^T(\mathbf{Y}\mathbf{Y}^T)^{-1}$.

How to use LEM and LLE for nonlinear projection-based MOR

When Newton's method is used to solve an RVE problem, in each iteration, the stiffness matrix $\mathbf{K} \in \mathbb{R}^{D \times D}$ and residuum $\mathbf{g} \in \mathbb{R}^D$ must be assembled and the linear equation system

$$\mathbf{K}\Delta\mathbf{u} = -\mathbf{g},$$

solved for the unknown displacement increment $\Delta\mathbf{u} \in \mathbb{R}^D$ [10, 4, 9].

With LEM or LLE and local linearisation, the search for solutions can instead be projected onto the approximated tangent to the solution manifold via

$$\underbrace{\psi^T \mathbf{K} \psi}_{\mathbf{K}_r} \Delta\mathbf{y} = -\underbrace{\psi^T \mathbf{g}}_{\mathbf{g}_r}.$$

Here, $\Delta\mathbf{y} \in \mathbb{R}^d$ is the increment in the reduced variables which aim to parametrise the solution manifold, and $\mathbf{K}_r \in \mathbb{R}^{d \times d}$ and $\mathbf{g}_r \in \mathbb{R}^d$ are the reduced stiffness matrix and residuum.

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