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► To cite this version:

Felix Fritzen, Matthias Leuschner, Max Hodapp. Nonlinear homogenization using model order reduction: two-scale simulations and novel developments using the pRBMOR on GPUs. 12e Colloque national en calcul des structures, CSMA, May 2015, Giens, France. hal-01516447

HAL Id: hal-01516447

<https://hal.science/hal-01516447>

Submitted on 1 May 2017

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Nonlinear homogenization using model order reduction: two-scale simulations and novel developments using the pRBMOR on GPUs

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Résumé — Modern composite materials often consist of multiple phases arranged in a complex three-dimensional microstructure. The individual constituents are often nonlinear and path-dependent, thereby inducing many computational challenges. The recent pRBMOR [2, 3] provides a reduced order model for the rapid computation of approximate solutions to the microstructural problem. Thereby, two-scale simulations on desktop computers with off-the-shelf consumer graphic cards become feasible. The FE^{2R} method [4] and extensions of the pRBMOR for the consideration of cohesive interfaces [5] are discussed. **Mots clés** — nonlinear homogenization, model reduction, GPU programming, pRBMOR, NTFA.

1 Two-scale problem

The nonlinear homogenization problem persists in finding for an arbitrary macroscopic strain loading $\bar{\varepsilon}(t)$ the corresponding macroscopic stress $\bar{\sigma}(t)$. Due to the complex microstructural geometry and the nonlinearity of the phases therein, it is merely impossible to immediately formulate a constitutive model depending only on macroscopic (or effective) quantities. More precisely it is often required to consider the nonlinearities and the evolution of the internal state variables on the microscale in order to then compute the effective stress by means of volume averaging. Therefore, the PDE

$$\operatorname{div}(\boldsymbol{\sigma}(\boldsymbol{x}, t)) = \mathbf{0} \quad \text{in } \Omega, \quad \langle \boldsymbol{\varepsilon}(\boldsymbol{x}, t) \rangle = \bar{\boldsymbol{\varepsilon}}(t) \quad (1)$$

has to be solved, where $\langle \bullet \rangle$ is the volume averaging operator. In the following we assert that the internal variables consist of the plastic strain $\boldsymbol{\varepsilon}^p$ and the hardening vector \hat{q} . In the framework of generalized standard materials (GSM), the free energy $\psi(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \hat{q})$ and the dual dissipation potential $\phi^*(\boldsymbol{\tau}, \hat{r})$ suffice to determine all elastic and dissipative processes via

$$\boldsymbol{\sigma} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}, \quad \boldsymbol{\tau} = -\frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^p}, \quad \hat{r} = -\frac{\partial \psi}{\partial \hat{q}}, \quad \boldsymbol{\varepsilon}^p = \frac{\partial \phi^*}{\partial \boldsymbol{\tau}}, \quad \hat{q} = \frac{\partial \phi^*}{\partial \hat{r}}. \quad (2)$$

The macroscopic stress can then be computed via

$$\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle. \quad (3)$$

2 Reduced order model

Due to the often highly nonlinear and path-dependent constitutive models, the PDE (1) has to be solved using sophisticated numerical methods that produce a substantial computational cost in the sense of cpu time and memory. In order to perform actual two-scale simulations in which the macroscopic stress needs to be evaluated by recourse to RVE simulations, the computational efficiency of the latter needs to be improved by factors of 10^4 and higher. In order to achieve this ambitious goal, the authors have built a reduced order model based on the NTFA [1] : the pRBMOR [2, 3, 4]. The key ingredient of the pRBMOR is the use of global ansatz functions for the internal variables $\boldsymbol{\varepsilon}^p$, \hat{q} . Then these fields are approximated by the reduced coefficient vectors $\hat{\xi}(t)$, $\hat{\lambda}(t)$ via the operators $\hat{P}(\boldsymbol{x})$, $\hat{Q}(\boldsymbol{x})$

$$\hat{\boldsymbol{\varepsilon}}^p(\boldsymbol{x}, t) = \hat{P}(\boldsymbol{x})\hat{\xi}(t), \quad \hat{q}(\boldsymbol{x}, t) = \hat{Q}(\boldsymbol{x})\hat{\lambda}(t). \quad (4)$$

Micromechanical properties of the problem then show that the stress and strain on the microscale are linear functions of the applied macroscopic strain $\bar{\varepsilon}(t)$ and the mode activity vector $\hat{\xi}(t)$. Hence, all microscopic fields can be computed as linear functions of the macroscopic state $\bar{S} = \{\bar{\varepsilon}, \hat{\xi}, \hat{\lambda}\}$. Following the procedure first derived in [2] and extended towards nonuniform hardening modes in [3], a mixed incremental pseudo potential

$$\bar{\Pi}^* = \langle \psi(t) - \psi(t_n) \rangle + \left(\hat{\xi}(t) - \hat{\xi}(t_n) \right) \cdot \hat{\tau} + \left(\hat{\lambda}(t) - \hat{\lambda}(t_n) \right) \cdot \hat{R} - \Delta t \langle \phi^*(\tau, \hat{r}) \rangle \quad (5)$$

is defined. The saddle point of $\bar{\Pi}^*$ defines the new values of the reduced coefficient vectors $\hat{\xi}$, $\hat{\lambda}$ and, simultaneously, the corresponding effective driving forces $\hat{\tau}$, \hat{R} . Similar to the NTFA, the effective stress $\hat{\sigma}$ can be written as a linear function of the effective strain and of the vector $\hat{\xi}$

$$\hat{\sigma} = \hat{C}\hat{\varepsilon} - \hat{A}^T\hat{\xi}. \quad (6)$$

The number of plastic modes N and hardening modes M was shown to be both fairly small, i.e. on the order of 10-100 for three-dimensional problem settings. Thereby, a massive reduction of the memory requirements is attained. However, the computation of the reduced degrees of freedom $\hat{\xi}$, $\hat{\lambda}$ requires millions of algebraic operations. Still the computational savings are on the order of 100 and higher.

3 GPU acceleration

- A detailed analysis of the algebraic operations involved in the homogenization procedure reveals that
- the algebraic operations are small and have the same dimension at all evaluation points,
 - the operations are very simple, i.e. single precision floating point arithmetics are sufficient and the operations are mostly linear,
 - there is no execution path branching,
 - the operations are mostly *memory bound*, i.e. a high memory bandwidth is required.

These properties qualify the algorithm for parallelization on modern many core systems. The authors decided to use modern graphic cards since they provide a superior memory bandwidth at a fairly reasonable price. For the implementation we decided on the Nvidia CUDA framework. The library that we developed in [3] contains batched linear algebraic operations and functions for the batched evaluation of the thermodynamic potentials and of their first and second gradients. Overall, the use of the GPU allowed for another acceleration on the order of 100 over a single core CPU version. In total, the computational time is reduced by factors on the order of 10^4 with respect to a highly tuned finite element implementation.

4 FE^{2R} method

The aforementioned gains are sufficient to put realistic two-scale simulations into service. However, the algorithmic tangent operator is required in order to use the pRB MOR in the context of two-scale finite element simulations.

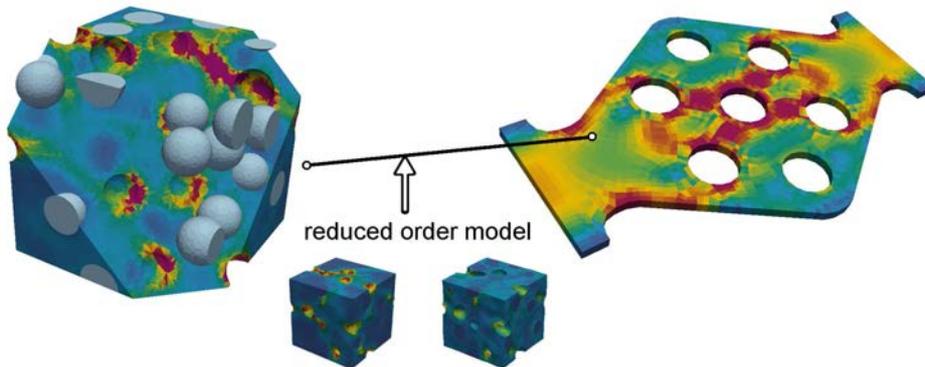


FIGURE 1 – FE^{2R} method for viscoplastic materials with pores and elastic inclusions

Only recently the algorithmic tangent operator for the pRBMOR was proposed in [4]. It can be computed at basically no additional computational expense. In combination with a robust time integration scheme, the pRBMOR was used to form the FE Square Reduced method (FE^{2R}). Further details can be found in [4]. An example of an FE^{2R} simulation is shown in Figure 1.

5 Future fields of application

While the pRBMOR can make accurate predictions of viscoplastic composites and porous materials, practical applications often involve additional physical phenomena. A possible extension of the pRBMOR is envisaged in terms of cohesive interfaces. The authors have proposed a potential based framework for cohesive zones [5], the Standard Dissipative Cohesive Zone framework (SD-CZ). Basically, the GSM framework is adopted for the interface. Thereby, novel aspects such as unilateral interface opening, elastic degradation of the bonding layer etc. can be considered. We discuss the incorporation of SD-CZ type models into the pRBMOR and present preliminary results for materials with tension-compression-asymmetry.

Acknowledgement

The authors highly acknowledge the funding of this work in the context of the Excellence Initiative for the KIT Young Investigator Group Computer Aided Material Modeling. Further, the work is generously supported by the German Research Foundation (DFG) under grant DFG-FR2702/3-1, within the context of the Emmy Noether Junior Research Group EMMA (DFG-FR2702/6-1) and the scientific network CoSiMOR (www.cosimor.de ; grants DFG FR2702/4-1, FR2702/7-1).

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