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COMPUTATIONAL HOMOGENIZATION USING HIGH-PERFORMANCE, REDUCED-ORDER MODELING

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One of the major challenges in the macro-scale continuum description of heterogeneous materials, such as composites and polycrystalline metals, lies in the determination of macroscopic constitutive relations that accurately reflects the properties and geometrical arrangement of the distinct phases at the finer scale. It is well-known that, under certain hypotheses (namely, scale separation and periodicity or statistical homogeneity), this constitutive link can be systematically established by solving, for *each* point at the coarse scale, a Boundary Value Problem (BVP) on a certain Representative Volume Element (RVE) of the material. In a strain-driven formulation of this BVP, the macro-strain at a given point acts as "loading parameter", in the form of appropriate essential boundary conditions, whereas the associated macro-stress is obtained through volume averaging —i.e., *homogenization*— of the corresponding micro-stress field.

In the present work, we propose to solve this RVE equilibrium problem using the so-called *Reduced-Basis* (RB) *approximation*. Generally speaking, the reduced-basis approximation is a class of *Galerkin* approximation procedure that employs *globally supported basis functions*. These basis functions *or modes* are not constructed from either polynomials or transcendental functions, as in classical Rayleigh-Ritz methods, but rather are determined from a larger set of *previously* computed —using *the finite element* (FE) method, for instance— solutions of the BVP at appropriately selected values of the input of interest (in this case, the macroscopic strains).

The main original elements of the proposed Reduced-Order Model (ROM) are fundamentally three. Firstly, the reduced set of empirical, globally-supported shape functions are constructed from pre-computed Finite Element (FE) snapshots by applying, rather than the standard Proper Orthogonal Decomposition (POD), a partitioned version of the

POD that accounts for the elastic/inelastic character of the solution. Secondly, we show that, for purposes of fast evaluation of the nonaffine term (in this case, the stresses), the widely adopted (in other model reduction contexts) approach of replacing such a term by a low-dimensional interpolant constructed from POD modes, obtained, in turn, from FE snapshots, leads invariably to ill-posed formulations. We demonstrate that, to avoid this ill-posedness, one has to enrich the approximation space for the interpolant with the span of the gradient of the displacement shape functions. Likewise, we show that spectral properties of the Jacobian matrix of the governing equation are influenced by the number and particular placement of sampling points used in the interpolation. The third innovative ingredient of the present paper is a points selection algorithm that does acknowledge this peculiarity and chooses the sampling points guided, not only by accuracy requirements, but also by stability considerations.

The implementation of the proposed methodology is quite straightforward. Taking as departure point an existing FE code, one has only to replace the typical loop over elements in the FE code by a loop over the pre-selected sampling points $\{\mathbf{x}_{\mathcal{I}_1}, \mathbf{x}_{\mathcal{I}_2}, \dots \mathbf{x}_{\mathcal{I}_p}\}$. The stress vectors and corresponding constitutive tangent matrices obtained at each stage of the loop are stored in global arrays $\hat{\boldsymbol{\Sigma}}$ and $\hat{\mathbb{C}}$, respectively; then, the residual vector and the Jacobian matrix are computed as $\hat{\mathbb{B}}^{**^T}\hat{\boldsymbol{\Sigma}}$ and $\hat{\mathbb{B}}^{**^T}\hat{\mathbb{C}}\hat{\mathbb{B}}^{*}$, respectively, $\hat{\mathbb{B}}^{**^T}$ and $\hat{\mathbb{B}}^{*}$ being operators calculated in the offline stage, prior to the overall multiscale analysis. These operators encode the *essential* information regarding the geometrical arrangement and interaction of the distinct phases and/or pores at the fine scale. Once convergence is achieved, the macroscopic stress value is simply calculated as $\boldsymbol{\sigma_M} = \mathbb{T}\hat{\boldsymbol{\Sigma}}$ ($\mathbb{T}$ is another pre-computed operator). The *operation count in both solving this reduced-order cell equation and updating the macroscopic stress vector depends exclusively on the number of basis functions* n_u and the *number of sampling points* p—it is independent of the underlying finite element mesh. Likewise, *storage of history data (internal variables) is only required at the pre-selected sampling points*. Computational savings accrue, thus, not only in terms of number of operations, but also in terms of memory requirements.

The efficiency of the proposed approach is assessed in the solution of a cell problem corresponding to a highly complex porous metal material under plane strain conditions. Results obtained convincingly show that the computational complexity of the proposed ROM is independent of the size and geometrical complexity of the considered representative volume, with gains in performance with respect to finite element analyses of above three orders of magnitude, and approximation errors below 10% —hence the appellation *High-Performance* ROM.