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EFFICIENT MULTI-SCALE MODELLING OF PATH DEPENDENT PROBLEMS – COMPLAS 2017

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Abstract. With growing capabilities of computers use of multi-scale methods for detailed analysis of response with respect to material and geometric nonlinearities is becoming more relevant. In this paper focus is on MIEL (mesh-in-element) multi-scale method and its implementation with *AceGen* and *AceFEM* based on analytical sensitivity analysis. Such implementation enables efficient multi-scale modelling, consistency and quadratic convergence also for two-level path following methods for the solution of path dependent problems.

1 INTRODUCTION

Implementation of multi-scale methods is possible in various ways. Here, the numerical scheme for implementation of MIEL multi-scale method based on sensitivity analysis is presented. Implementation is done with the *Mathematica* packages *AceGen* and *AceFEM* [1]. Programs enable analytical sensitivity analysis of first and second order [2], that can be used for efficient implementation of multi-scale finite element methods, eg. FE^2 or MIEL.

2 AUTOMATIC DIFFERENTIATION BASED (ADB) NOTATION

AceGen is advanced automatic code generator, where automatic differentiation technique, automatic code optimization and generation are combined with computer algebra system *Mathematica*[3]. Size of code is reduced through control of expression swell[4]. The *AceFEM* package is a general finite element environment designed to solve multi-physics and multi-field problems.

Automation of primal and sensitivity analysis is done with *AceGen*. The automatic differentiation technique (AD) can be used for the evaluation of the exact derivatives of any arbitrary complex function via chain rule and represents an alternative solution to the numerical differentiation and symbolic differentiation. The result of AD procedure is called "computational derivative" and is written as $\frac{\hat{\delta} f(\mathbf{a})}{\hat{\delta}\mathbf{a}}$. The AD operator $\frac{\hat{\delta} f(\mathbf{a})}{\hat{\delta}\mathbf{a}}$ represents partial derivative of a function $f(\mathbf{a})$ with respect to variables $\mathbf{a}$. If, for example, alternative or additional dependencies for a set of intermediate variables $\mathbf{b}$ have to be considered for differentiation, then the AD exception is indicated by the following formalism

$$\left.\frac{\hat{\delta} f(\mathbf{a},\mathbf{b})}{\hat{\delta}\mathbf{a}}\right|_{\frac{D\mathbf{b}}{D\mathbf{a}}=\mathbf{M}}, \tag{1}$$

which indicates that during the AD procedure, the total derivatives of variables $\mathbf{b}$ with respect to variables $\mathbf{a}$ are set to be equal to matrix $\mathbf{M}$. The automatic differentiation exceptions are the basis for the ADB formulation of computational problem. The ADB notation can be directly translated to the *AceGen* input and is part of numerically efficient code automation. Details of the method and of the corresponding software *AceGen* can be found in [4], [2] and [5].

The automation of multi-scale analysis requires the automation of primal and sensitivity analysis. In primal analysis the response of the system is evaluated, whereas in sensitivity analysis the derivatives of the response, e.g. displacements, strains, stresses or work, with respect to arbitrary design parameter ϕ_i are sought. The primal problem is solved by the standard Newton-Raphson iterative procedure (see e.g. [2]). For the automation of the multi-scale methods the sensitivity analysis with respect to prescribed essential boundary conditions is needed.

3 MULTI-SCALE METHODS

Multi-scale methods are nowadays widespread in computational mechanics [6, 7, 8]. They usually originate from the demand to model heterogeneous materials, like fiber reinforced composites, particle reinforced adhesives, concrete and even metal. FE^2 is a standard two-level finite element homogenization approach [9], that is appropriate for the problems where scales are separated far enough and are only weakly coupled. FE^2 method is already implemented in *AceFEM* using sensitivity analysis, for details reader is referred to [10, 11]. In some cases for example when difference between two scales is finite, or when in the region of high gradients, the FE^2 multi-scale approach fails, thus we need to use some sort of domain decomposition method. One possibility is the mesh-in-element or MIEL scheme described e.g. by Markovič and Ibrahimbegović in [12].

3.1 MIEL method

MIEL method is variant of domain decomposition methods. Here its implementation based on sensitivity analysis is presented. The finite element models at different scales communicate between each other through degrees of freedom of the finite element at

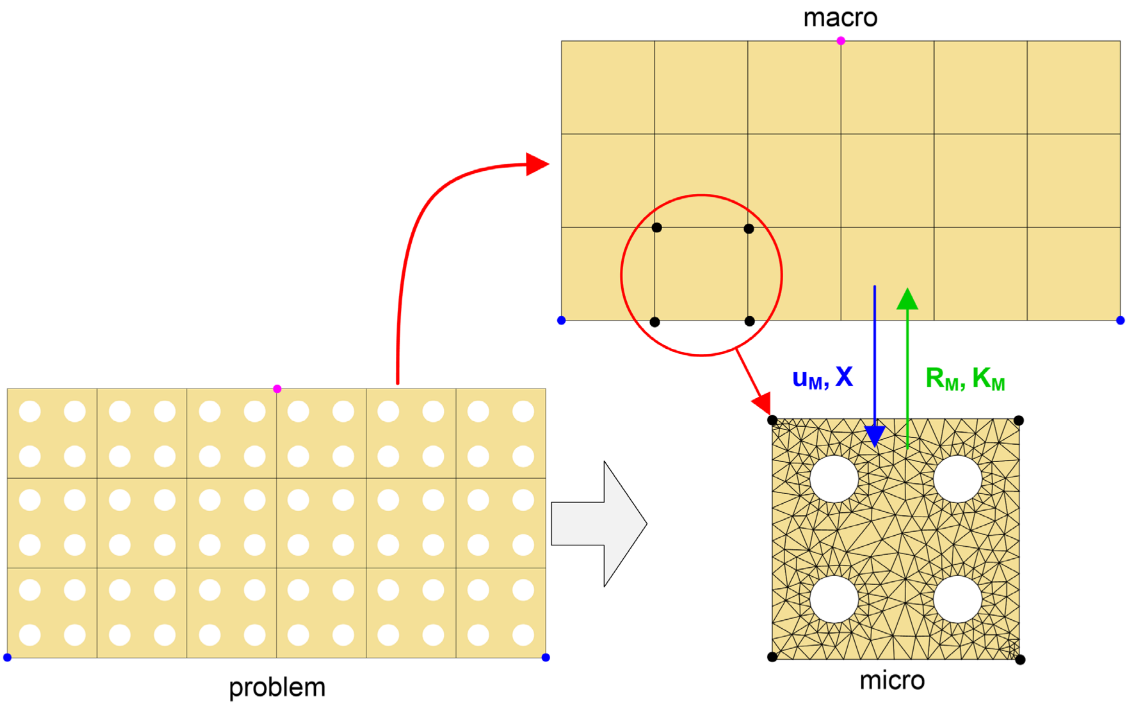


Figure 1: MIEL, problem, micro and macro level

the macro-scale. The residual and tangent matrix are for each macro element obtained directly from the micro-scale problem. Each macro element thus represents one micro problem, see Fig. 1. Macro element performs only proper transfer of components of the macro element residual vector and tangent matrix from micro scale to macro scale finite element assembly procedure. At the macro level residual and tangent are assembled from individual macro elements and macro response is calculated. Macro tangent matrix is typically evaluated using the Schur complement of the global micro matrix, which is numerical expensive operation. Here it is calculated through sensitivity analysis with respect to prescribed essential boundary conditions. Implementation in *AceFEM* enables this approach that is numerical more efficient for dense micro finite element meshes. Correctly done sensitivity analysis at micro level leads to algorithmically consistent macro tangent matrix. Quadratic convergence of problem is with that ensured also for examples, that are dependent on load-path.

Let $\mathbf{p}_{Me}$ be a vector of unknowns in the nodes of the macro element, $\mathbf{p}_{me}$ a vector of unknowns in the nodes of the characteristic micro problem element and W strain energy function. The outer shape of the micro problem is the same as the shape of the corresponding macro element. The prescribed essential boundary conditions (displacements) are identical to the displacements at the boundary of the corresponding macro element. The integration point contribution (g-th integration point in the e-th element of the micro

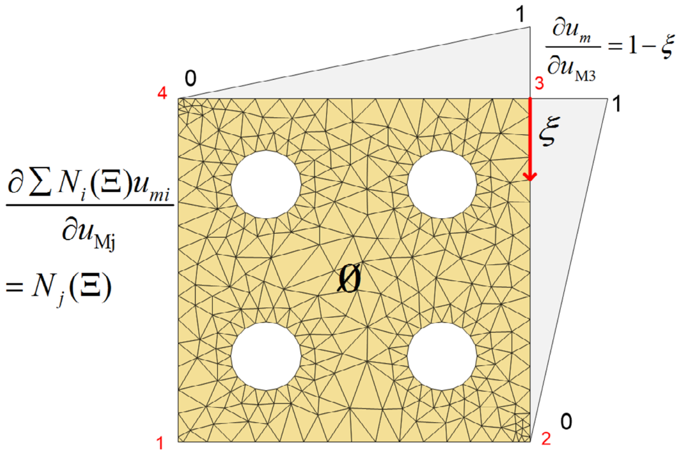


Figure 2: Characteristic velocity field for MIEL

mesh) to the macro residual and macro tangent matrix is then

$$\mathbf{R}_{Mg} = \frac{\partial W(\mathbf{p}_{me}(\mathbf{p}_{Me}))}{\partial \mathbf{p}_{Me}} = \frac{\partial W}{\partial \mathbf{p}_{me}} \frac{D\mathbf{p}_{me}}{D\mathbf{p}_{Me}} \tag{2}$$

$$\mathbf{K}_{Mg} = \frac{\partial \mathbf{R}_{Mg}}{\partial \mathbf{p}_{Me}} = \frac{\partial^2 W}{\partial \mathbf{p}_{me}{}^2} \frac{D\mathbf{p}_{me}}{D\mathbf{p}_{Me}} + \frac{\partial W}{\partial \mathbf{p}_{me}} \frac{D^2\mathbf{p}_{me}}{D\mathbf{p}^2_{Me}}. \tag{3}$$

The implicit dependencies $\frac{D\mathbf{p}_{me}}{D\mathbf{p}_{Me}}$ and $\frac{D^2\mathbf{p}_{me}}{D\mathbf{p}^2_{Me}}$ are obtained by the first and second order sensitivity analysis. Thus, the sensitivity analysis based automation of the MIEL scheme requires the second order sensitivity analysis for a set of sensitivity parameters $\mathbf{p}_{Me}$. The ADB form of (2) and (3) then leads to

$$\mathbf{R}_{Mg} = \left.\frac{\hat{\delta}\mathbf{W}}{\hat{\delta}\mathbf{p}_{Me}}\right|_{\frac{D\mathbf{p}_{me}}{D\mathbf{p}_{Me}} = D_{\mathbf{p}_{Me}}\mathbf{p}_{me}} \tag{4}$$

$$\mathbf{K}_{Mg} = \left.\frac{\hat{\delta}\mathbf{R}_{Mg}}{\hat{\delta}\mathbf{p}_{Me}}\right|_{\frac{D\mathbf{p}_{me}}{D\mathbf{p}_{Me}} = D_{\mathbf{p}_{Me}}\mathbf{p}_{me},\ \frac{D(D_{\mathbf{p}_{Me}}\mathbf{p}_{m})}{D\mathbf{p}_{Me}} = D_{\mathbf{p}_{Me}\mathbf{p}_{Me}}\mathbf{p}_{me}} \tag{5}$$

where data structures $D_{\mathbf{p}_{Me}}\mathbf{p}_{me} = \frac{D\mathbf{p}_{me}}{D\mathbf{p}_{Me}}$ and $D_{\mathbf{p}_{Me}\mathbf{p}_{Me}}\mathbf{p}_{me} = \frac{D^2\mathbf{p}_{me}}{D\mathbf{p}^2_{Me}}$ are the results of the first and second order sensitivity analysis.

For the complete formulation of the prescribed boundary condition sensitivity problem, we need the first and second order prescribed boundary condition velocity fields $D_{\phi_i}\bar{\mathbf{p}}_e$ and $D_{\phi_i\phi_j}\bar{\mathbf{p}}_e$ for details see e.g.[2]. Let $\bar{\mathbf{p}}_m$ be a vector of unknowns at the boundary of micro problems with prescribed essential boundary conditions, thus $\bar{\mathbf{p}}_m = \bar{\mathbf{p}}_m(\mathbf{p}_{Me})$. The set of sensitivity parameters of the MIEL problem is $\boldsymbol{\phi} = \mathbf{p}_{Me}$. The components of $D_{\phi_i}\bar{\mathbf{p}}_e$ are obtained by the differentiation of $\bar{\mathbf{p}}_m(\mathbf{p}_{Me})$ with respect to $\mathbf{p}_{Me}$. Let us assume the standard interpolation of the unknown field u on the boundary of the macro element

$$u = \sum N_i(\Xi)\, u_i, \tag{6}$$

where $N_i(\Xi)$ are the shape functions and u_i the nodal unknowns and $\frac{\partial u}{\partial u_i} = N_i(\Xi)$. Thus, the components of the first order boundary condition velocity field $D_{\phi_i}\bar{\mathbf{p}}_e$ are the values of the macro element shape functions at the position of the boundary nodes of the micro mesh, see Fig. 2. For boundary condition in form of linear combination (6), the second order velocity field is zero $D_{\phi_i\phi_j}\bar{\mathbf{p}}_e = \mathbf{0}$.

4 EFFICIENCY IMPROVEMENT

Numerical efficiency of multi-scale methods can be improved in different ways. First improvement was done at individual macro problem, with replacing calculation of Schur complement with sensitivity analysis based calculation of macro tangent matrix. For densely meshed micro-structure calculation of the Schur complement inflicts high memory allocation and is time consuming, which is not the case for the sensitivity analysis based implementation. In case of MIEL method this is due to the fact that the number of sensitivity parameters remains the same, regardless of the density of the micro mesh, whereas the size of the Schur complement grows with the number of the nodes on the boundary of the micro problem.

Further optimisation can be done with use of unified sensitivity based approach to multi-scale modelling, that is enabled by automatic-differentiation-based (ADB) formulation for an arbitrary nonlinear, time dependent coupled problem (e.g. general finite strain plasticity). Different multi-scale methods FE^2, MIEL and also single scale schemes can be used together in one model. With that optimal domain discretization is possible. For example, MIEL that is numerically most demanding can be used only where it is needed, other ways FE^2 or single-scale method can be used.

In *AceFEM* solving of nonlinear problems is done implicitly with a Newton-Raphson type iterative solution procedure. Since we have two scales, we have in general a path following procedure at both scales, resulting in two-level path following procedure. Traditionally, each step at macro level is followed by only one step at micro level. Sensitivity analysis based multi-scale analysis allows extension to more general case, where each macro step can be followed by an arbitrary number of micro substeps.

Implementation of the presented multi-scale computational approach in *AceFEM* is fully parallelized for multi-core processors. Micro problems are distributed on kernels by evaluating each individual micro problem always at the same kernel. With parallelized computation, computational time for complex problems can be significantly reduced. The setup is also appropriate for the implementation on clusters.

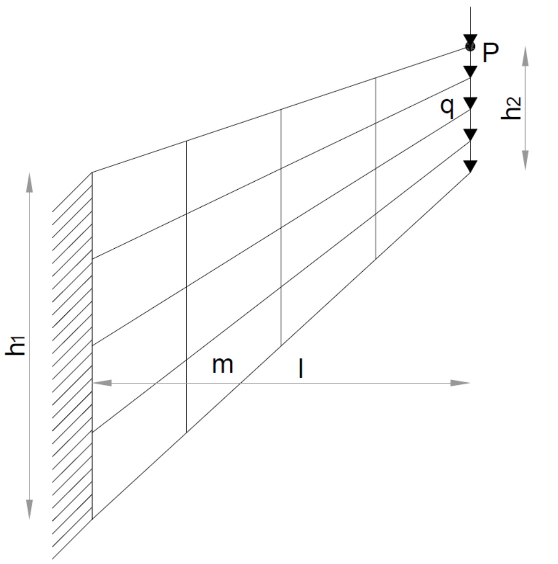
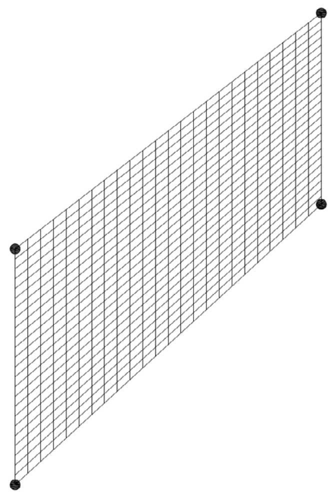
5 NUMERICAL EXAMPLE

Multi-scale MIEL method was tested on Cook membrane benchmark problem, to verify consistency and efficiency of micro-macro coupling. The homogeneous micro structure is chosen intentionally for the benchmark purposes. Effect of macro mesh density and use of different finite elements were investigated. With *AceGen*, the codes of analytical first and second order sensitivity analysis are generated automatically. Examples were calculated with *AceFEM*, where whole MIEL scheme is implemented including communication between macro and micro scale. Essential boundary condition of macro mesh are sent to micro problem and interpolated over the edge. Important is that essential boundary condition velocity fields are set correctly.

5.1 Description of example

In Tab. 1 characteristics of problem on macro and micro level are described. Geometry, constraints and load are defined at macro level, whereas material properties are defined at micro level. Displacements are fixed on one side and on the other distributed load in vertical direction is added. Division of macro mesh had been variated, while division on micro level was the same in all computations. For mesh at macro and micro level two-dimensional quadrilateral elements with 4 nodes Q1 and with 8 nodes Q2S were used. Converged mesh density on micro level was used, so that results for different macro mesh densities can be compared.

Table 1: Macro and micro problem for MIEL

macro problem	micro problem
Geometry $h_1 = 44$ mm; $h_2 = 16$ mm; $l = 48$ mm; $t = 1$ mm Constraints: $X = 0$: $u = v = 0$ Load: $q = 0.1$ N/mm^2 	Material $E = 1$ N/mm^2 $\nu = 0$ *micro mesh of macro element marked with m 

5.2 Consistency of micro-macro coupling

Consistent coupling between micro and macro scale was verified with comparison of upper right point P displacement on the Cook membrane test. Vertical displacement was compared for different macro mesh densities. For single scale analysis results for linear and quadratic elements are shown. For MIEL three combinations were investigated. MIEL Q1-Q1: Q1 element at macro and Q1 element at micro level, MIEL Q2S-Q1: Q2S element at macro and Q1 element at micro level and MIEL Q2S-Q2S: Q2S element at macro and Q2S element at micro level. Convergence of result is faster for MIEL, than for single-scale analysis, comparison is shown in Fig. 3. Overall convergence of Q2S elements with quadratic interpolation is faster than with Q1. Results show that for meshing at micro level use of Q2S elements is not preferable, because small improvement of convergence does not compensate for increased computational time. In Fig. 4 results for strain Exx of example MIEL Q2S-Q1 are shown.

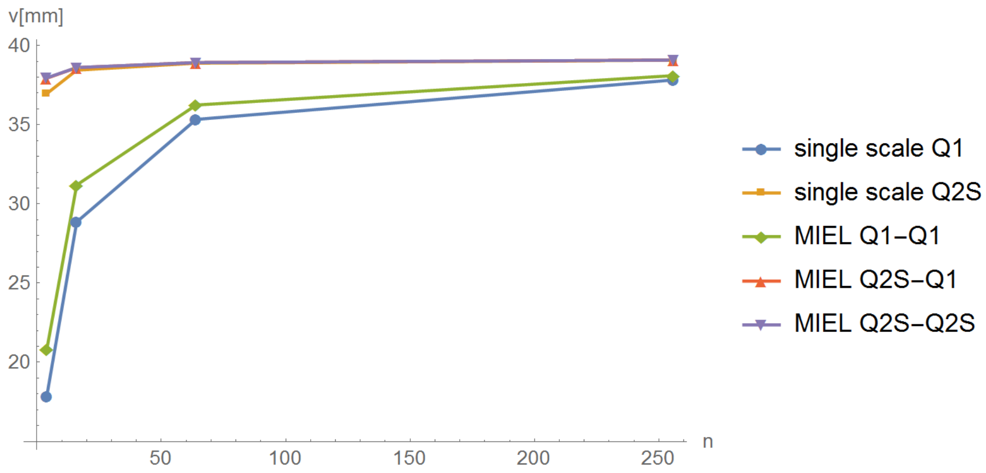


Figure 3: Convergence of result for vertical displacement

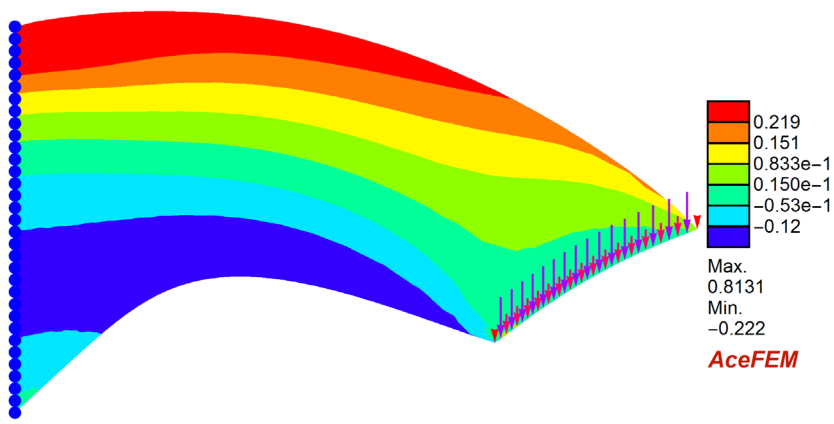


Figure 4: Results for strains Exx

6 CONCLUSIONS

In this work, basic principles of multi-scale MIEL method and possibilities for numerical improvement were described. In a conventional way of computing macroscopic tangent matrix a Schur complement is needed. As an alternative, the boundary condition sensitivity analysis was used to obtain macroscopic tangent matrix, for which second order sensitivity is needed. Numerical examples were calculated with *AceFEM*. Consistency of micro-macro coupling was shown on a Cook membrane example. Use of finite elements with quadratic interpolation is recommended for macro elements, whereas for micro mesh, elements with linear interpolation are preferred. Codes of the finite element for analytical first and second order sensitivity analysis are generated automatically with *AceGen*. For densely meshed micro-structures, the sensitivity analysis based calculation is numerically more efficient than Schur complement. This is due to the fact that the size of the Schur complement grows with the number of the nodes on the boundary of the micro problem, whereas the number of sensitivity parameters remains the same regardless of the density of the micro mesh. Traditionally, in multi-scale methods solved with two-level path-following procedure one macro time step is followed by one micro time step. Sensitivity analysis based multi-scale analysis allows that each macro step can be followed by an arbitrary number of micro substeps.

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