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DAMASK: the Düsseldorf Advanced MAterial Simulation Kit for studying crystal plasticity using an FE based or a spectral numerical solver

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Abstract

The solution of a continuum mechanical boundary value problem requires a constitutive response that connects deformation and stress at each material point. Such connection can be regarded as three separate hierarchical problems. At the top-most level, partitioning of the (mean) boundary values of the material point among its microstructural constituents and the associated homogenization of their response is required, provided there is more than one constituent present. Second, based on an elastoplastic decomposition of (finite strain) deformation, these responses follow from explicit or implicit time integration of the plastic deformation rate per constituent. Third, to establish the latter, a state variable-based constitutive law needs to be interrogated and its state updated.

The Düsseldorf Advanced MAterial Simulation Kit (DAMASK) reflects this hierarchy as it is built in a strictly modular way. This modular structure makes it easy to add additional constitutive models as well as homogenization schemes. Moreover it interfaces with a number of FE solvers as well as a spectral solver using an FFT.

We demonstrate the versatility of such a modular framework by considering three scenarios: Selective refinement of the constitutive material description within a single geometry, component-scale forming simulations comparing different homogenization schemes, and comparison of representative volume element simulations based on the FEM and the spectral solver.

Keywords: CPFEM, spectral method, FFT, constitutive model

1. Introduction

The Crystal Plasticity Finite Element Method (CP-FEM [1, 2]) has gained a lot of interest in the last decade. This has led to a situation where a number of implementations of CP-FEM exist in a number of groups around the world. Most of these implementations are special purpose and not easy to use. With the Düsseldorf Advanced MAterial Simulation Kit (DAMASK) we, therefore, undertake the effort to provide a flexible and easy to use CP implementation to the scientific community to further prosper the use of this highly potent simulation method.

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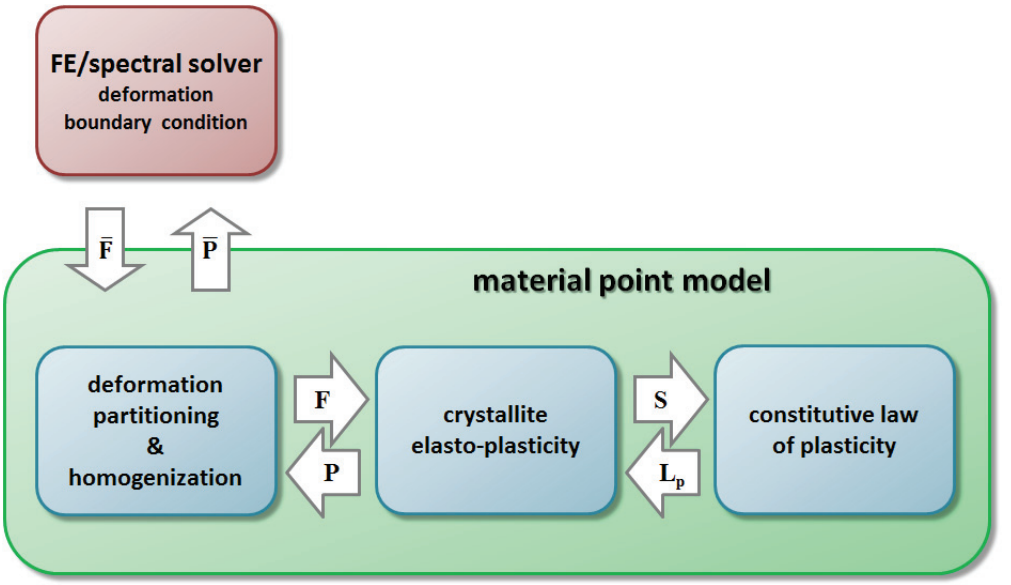

Fig. 1. Structure of the material point model.

2. Structure of the material point model

The structure of the material point model reflects the multiscale character of continuum mechanical boundary value problems and is shown in figure 1. The boundary value problem solver either FEM or spectral solver using a fast Fourier transform (FFT) determines the boundary condition in the form of an average deformation gradient $\bar{\mathbf{F}}$. The material point model needs to provide the corresponding average first Piola-Kirchhoff stress $\bar{\mathbf{P}}$.

As the material point potentially is a polycrystalline aggregate, on the homogenization level (see section 2.1) the average deformation gradient $\bar{\mathbf{F}}$ has to be partitioned into individual deformation gradients $\mathbf{F}$ for each crystal of the aggregate. As a return quantity the individual crystal stresses $\mathbf{P}$ have to be homogenized into the average stress $\bar{\mathbf{P}}$ of the material point.

Next, on the crystallite level (see section 2.2) the elasto-plasticity problem has to be solved to find the stress $\mathbf{P}$ associated with the deformation gradient $\mathbf{F}$. While this can be seen as a purely mathematical problem in its course the constitutive law of plasticity (see section 2.3) is needed to provide the plastic velocity gradient $\mathbf{L}_\mathrm{p}$ as a function of the second Piola-Kirchhoff stress $\mathbf{S}$.

2.1. Homogenization level

Figure 2 illustrates four commonly used homogenization schemes, namely the isostrain ([3] or full constraints Taylor [4]) scheme, Taylor based schemes allowing for relaxation (e.g. [5–7]), cluster models (e.g. LAMEL [8–10], GIA [11–13], or RGC [14]), and full-field homogenization by FEM [15–20] or spectral methods using an FFT [21, 22]. Out of these four classes the isostrain and the Relaxed Grain Cluster schemes are currently implemented in DAMASK.

2.2. Crystallite level

The elasto-plasticity problem is solved in a two-level integration following [23] however, with two important modifications. First, the calculation of $\mathbf{L}_\mathrm{p}$ is generalized by hiding the constitutive level (described in section 2.3). On the crystallite level, $\mathbf{L}_\mathrm{p}$ is treated as a given function of the stress $\mathbf{S}$. Second, instead of the stress, $\mathbf{S}$, $\mathbf{L}_\mathrm{p}$ is used as predictor in the Newton–Raphson scheme (figure 3) as this improves the convergence behavior, however, at the cost of a more involved 9×9 Jacobian which is lager than the 6×6 used in [23].

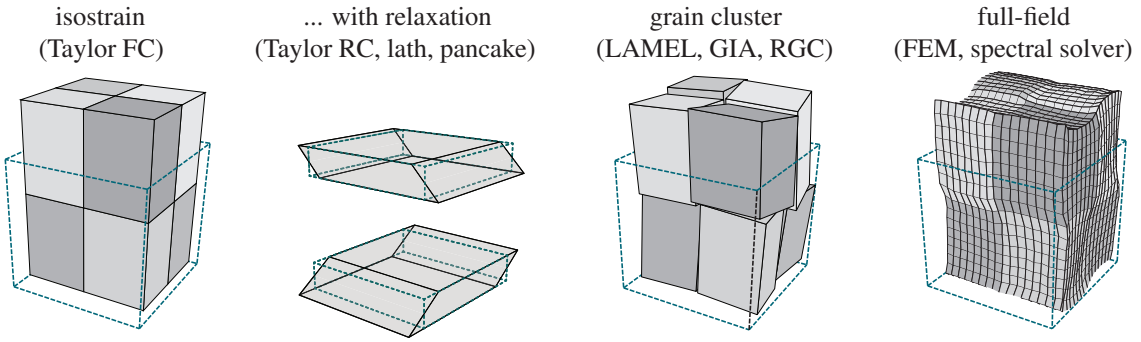

Fig. 2. Four commonly used homogenization schemes.

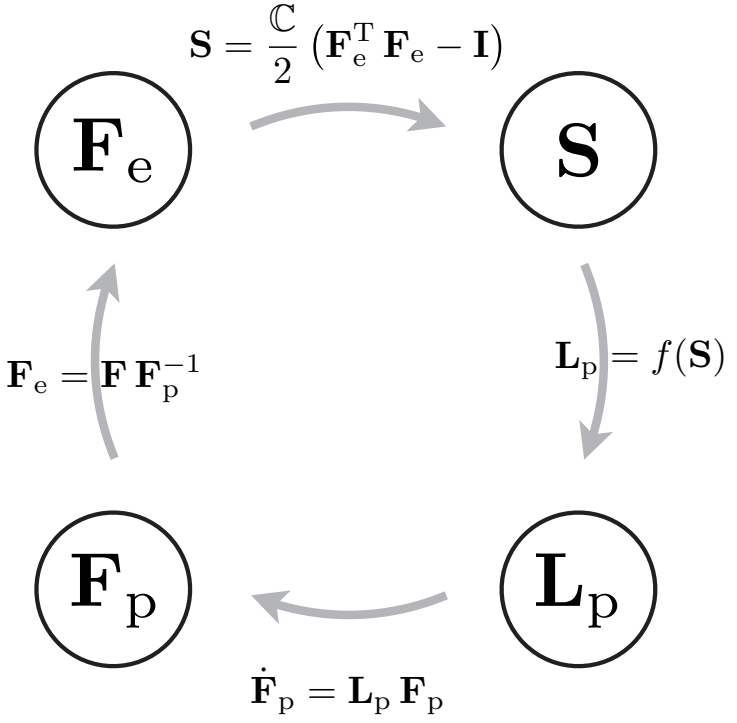

Fig. 3. Calculation scheme to determine $\mathbf{S}$ as a function of $\mathbf{F}$.

2.3. Constitutive level

The constitutive law is the core of any crystal plasticity implementation. It determines the material behavior and whether the model is empiric, phenomenological, or physics based. The main tasks of any constitutive model are to define the state variables and calculate $\mathbf{L}_\mathrm{p}$ as a function of $\mathbf{S}$ as well as its tangent $\partial\mathbf{L}_\mathrm{p}/\partial\mathbf{S}$. Usually, there is only one kind of constitutive law used in a crystal plasticity implementation. In DAMASK, however, due to its modular nature and the generalization of $\mathbf{L}_\mathrm{p}$ described in the previous section, a number of different constitutive laws can be included concurrently. At the time being, a simple J_2 based isotropic model, a phenomenological power law formulation [23], a dislocation density based formulation (the latter two include twinning), and a non-local model including dislocation fluxes are already implemented within DAMASK.

2.4. Material configuration

Two parameters have to be specified at each material point to define its constitutive behavior. The first parameter specifies the homogenization scheme (see section 2.1) to be used for this material point, the second specifies the microstructure to be used. A microstructure can consist of one or several constituents, where each constituent is defined by a pair of phase and texture. The phase determines which constitutive law to use (see section 2.3) and the texture specifies the orientation information. A texture can be either specified by texture components [24] or by providing a discrete representation of the orientation distribution function (ODF) which can be used to sample the required number of orientations using the hybridIA scheme introduced in [25].

3. Application examples

In this section we show three application examples. The first two use the FEM as solver while the third one is a comparison of representative volume element (RVE) simulations based on the FEM and the spectral solver.

3.1. Selective refinement of the constitutive material description within a single geometry

A unique feature of DAMASK is the ability to combine several constitutive laws within one geometry. Figure 4 shows the results of such a simulation. An aluminium oligo-crystal was deformed under plane strain compression [26]. The figure shows the dislocation density and the compressive strain where for the upper row the whole geometry was modeled using the dislocation density based constitutive law, while for the lower row a modular assignment of constitutive laws was used as illustrated in figure 5. The assignment of constitutive laws in this example is based on the assumption, that the region around the triple point as indicated in figure 4 is of special interest. The modular simulation saves about 30% computation time while maintaining the quality of the results in the chosen region of interest. This kind of simulation, frequently called direct CPFEM simulation, does not involve any homogenization. Within DAMASK this is formally treated as using the isostrain homogenization, however, with a single grain.

3.2. Deep drawing of dual phase steel

Deep drawing of a dual phase steel has been simulated using the isostrain and RGC homogenization schemes (see section 2.1). In both cases 25% of the total number of grains where treated as Martensite while the rest was assigned the properties of Ferrite. The RGC simulations used $2 \times 2 \times 2$ grain clusters with abitraty orientation. Three different parameter sets have been used: 1) penalty free, i.e. no penalty for incompatible $\mathbf{F}$ within the cluster; 2) compatible, i.e. very high penalty to assure compatibility; 3) best fit, i.e. best fit to the experimental uniaxial stress–strain curve. The results are shown in figure 6. As the material is rather isotropic there is not much difference in the predicted cup profiles and all simulations are close to the experiment. However, for the punch force the situation is different[1]. As could be expected

[1]The absolut value of the punch force also depends on the friction model used. As in the experiment Teflon sheets were used for lubrication, Coulomb friction with a low friction coefficient of $\mu = 0.04$ was used in the simulation.

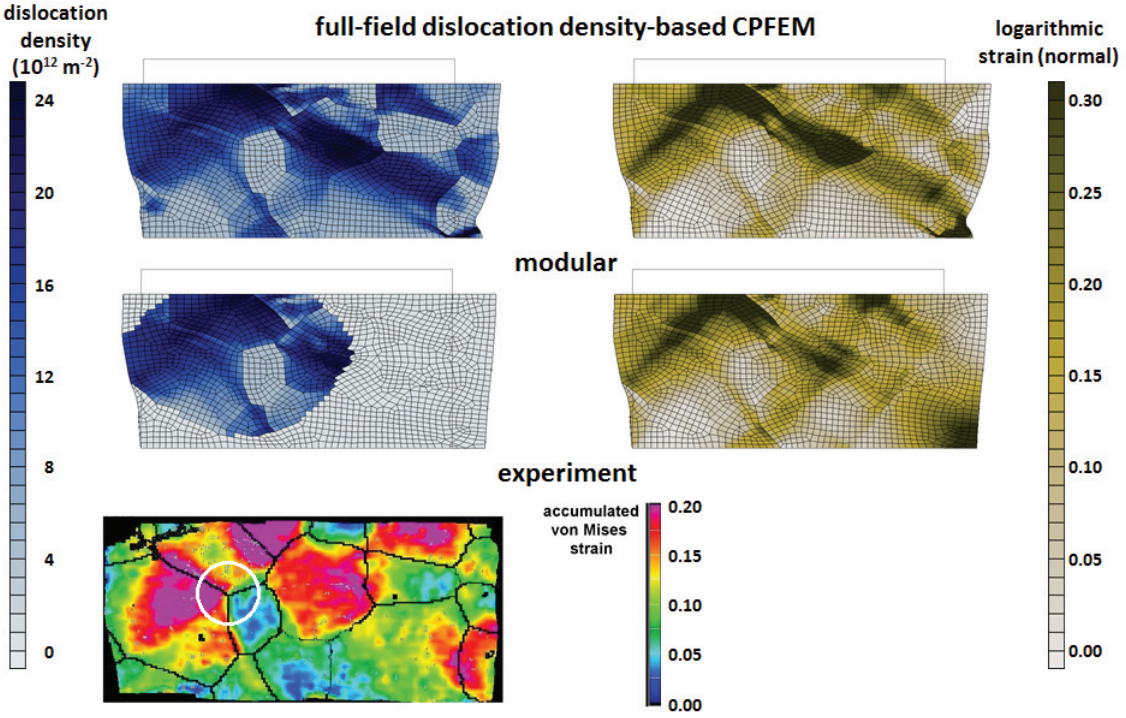

Fig. 4. Comparison of full-field and modular simulation results.

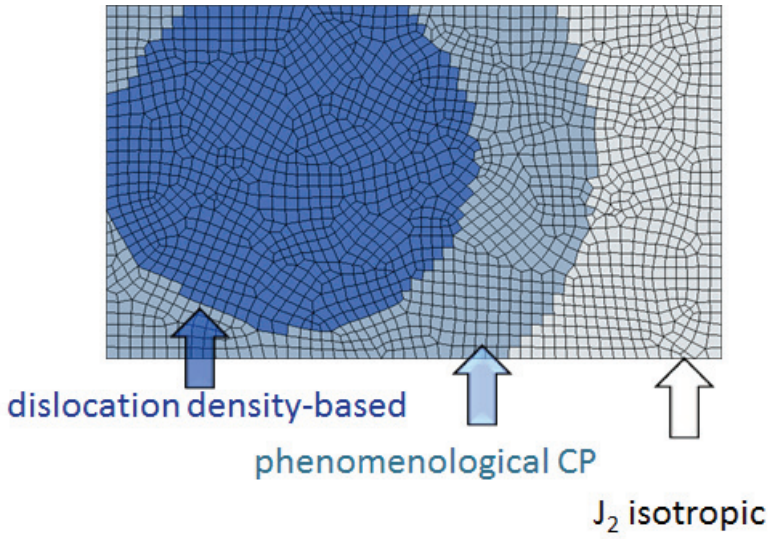

Fig. 5. Assignment of constitutive laws used for the modular simulation.

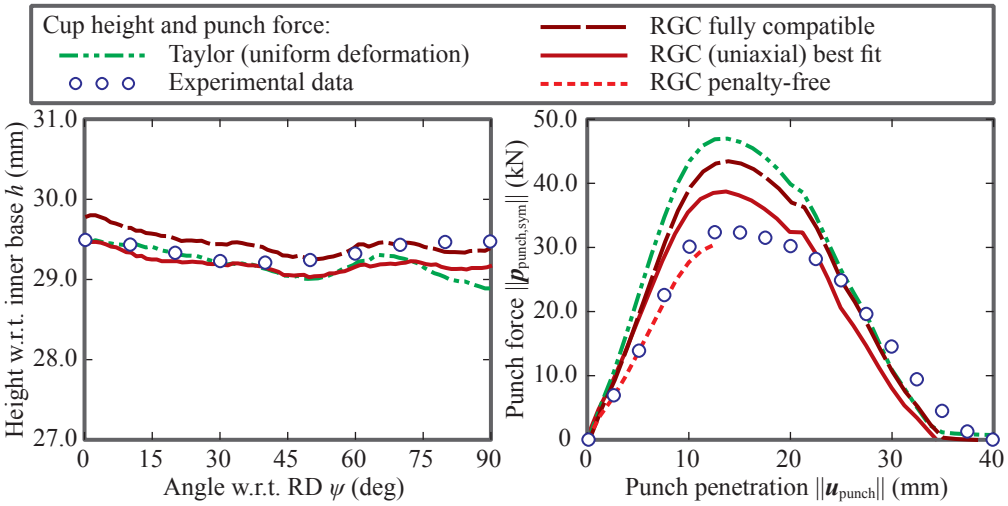

Fig. 6. Results of a simulation of the deep drawing of a dual phase steel comparing different homogenization schemes. Left: cup profile Right: punch force

the isostrain scheme highly overpredicts the punch force. In contrast the experimental result lies within the region covered by the RGC scheme. The fact the "best fit" parameter set still overpredicts the experimentally found values is probably due to the fact that the bending stiffness of the sheet is overpredicted as there were only five linear elements used over the sheet thickness.

3.3. Comparing RVE calculations using the FEM and the spectral solver

Representative volume element simulations are of high interest for application in the so called "virtual laboratory" [27], where they are used to replace extensive experimental testing for calibrating continuum-scale yield surface models. DAMASK provides interfaces to two commercial FE solvers (MSC.Marc and Abaqus Std./Expl.) as well as to a spectral solver using an FFT. It, therefore, for the first time allows a direct comparison of both solvers, where exactly the same code is used for the material point response. The comparison is done based on a RVE with 100 randomly oriented grains (figure 7). Simple shear to about 20% shear deformation is performed. Figure 7 shows the distribution of shear stress (in terms of the first Piola–Kirchhoff stress) for a typical RVE with a resolution of $10 \times 10 \times 10$ elements. While both solvers show very similar results, at this low resolution the underlying grain structure is hardly visible. However, the spectral solver is not only faster than the FE solver (about two orders of magnitude) but it is also substantially less memory intensive. Therefore, the maximum RVE dimension that can be handled is much larger for the spectral solver. The figure, therefore, also shows the distribution of the shear stress for the two maximum dimensions that could be achieved on similar hardware with each method, that is $32 \times 32 \times 32$ for the FE solver and $192 \times 192 \times 192$ for the spectral solver. While the grain structure can just be recognized from the FE simulation, it is clearly visible for the spectral method, where even in-grain gradients are resolved in great detail.

4. Summary

The Düsseldorf Advanced MAterial Simulation Kit (DAMASK) is a highly modular crystal plasticity implementation. Due to this modular character it is very flexible and can be easily extended, e.g. by adding additional constitutive laws, homogenization schemes, or solver interfaces.

DAMASK can be applied from the single grain to the component scale as shown by two application examples. The incorporation of several constitutive laws offers the unique possibility to create models using selective refinement or coarsening of the constitutive description. Moreover, the combination with a spectral

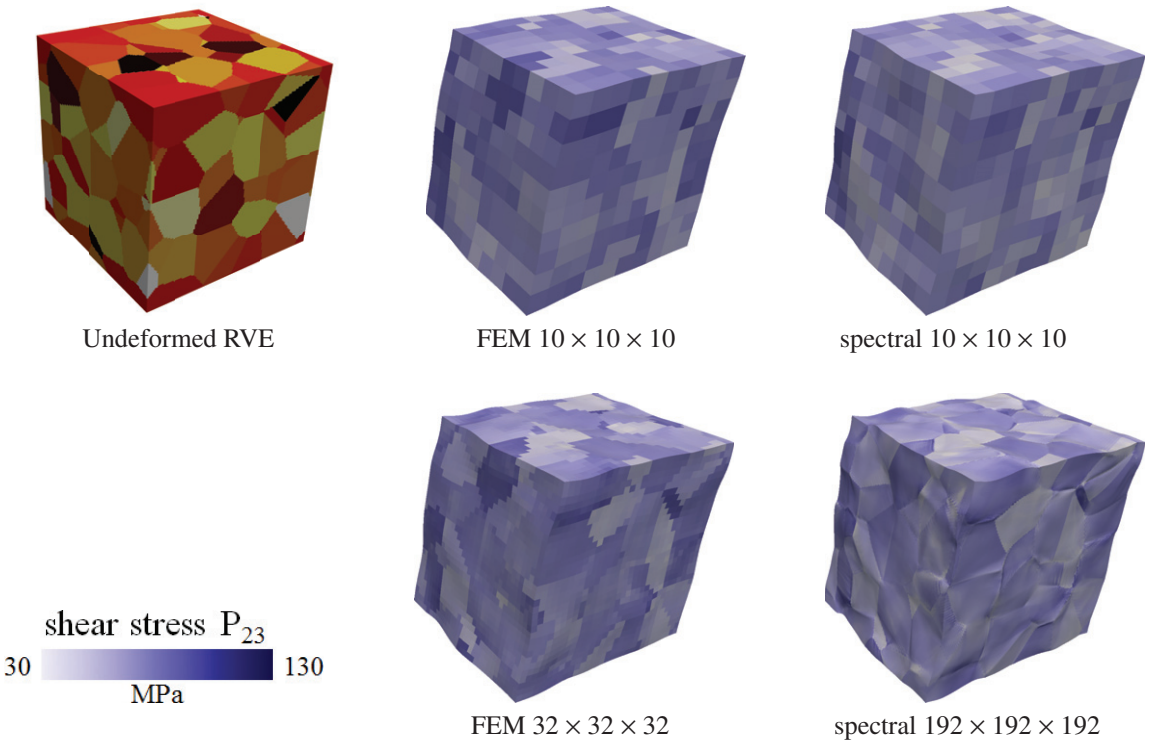

Fig. 7. Comparison of shear stress distribution after approximately 20% shear.

solver using an FFT offers high potential in the application for RVE simulations, which are of great interest for the so called ”virtual laboratory.”

Appendix A. How to obtain DAMASK

DAMASK is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

DAMASK is distributed in the hope that it will be useful, but without any warranty; without even the implied warranty of merchantability or fitness for a particular purpose. See the GNU General Public License for more details (`http://www.gnu.org/licenses/`).

If you are interested in obtaining a copy of DAMASK you can download it from `damask.mpie.de`, where you also find additional information.

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