

# On the usage of HDF5 in the DAMASK crystal plasticity toolkit

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## ABSTRACT

Crystal plasticity is a multi-scale problem. Most engineering simulations live on the component scale, i.e. usually in the meter range. The mechanical properties of crystalline materials are, however, determined on the scale of single grains, i.e. usually in the micrometer range. Therefore, some form of homogenization is usually applied to bridge the gap from the crystal to the component level.

The Düsseldorf Advanced MATERIAL Simulation Kit (DAMASK, [1, 2]) reflects this multi-scale nature of crystal plasticity by its hierarchical structure. Each material point (integration point in case of FEM or Fourier point in case of spectral solvers) is potentially considered to be a polycrystal. This means that its constitutive response, i.e. stress due to a given deformation, needs to be determined by applying a homogenization treatment to the constitutive responses of the individual crystals forming that polycrystal. The response of the single crystals is determined by their state defined by a set of state variables depending on the constitutive model used for their description.

The simulation output needs to store both the geometry information as well as material point data as selected by the user. The output frequency can also be freely chosen by the user. A HDF5 data structure is adapted to store output data in a manner that reflects DAMASK's hierarchical concept. The structure is flexible so that for every material point, potentially different data on the homogenization level (macro scale) as well as data of individual grains (micro scale) can be stored, interpreted and visualized. Besides the structure of the stored data we also discuss more general aspects of data storage, like lean data vs. fat data.

## REFERENCES

- [1] F. Roters, P. Eisenlohr, C. Kords, D.D. Tjahjanto, M. Diehl, D. Raabe: "DAMASK: the Düsseldorf Advanced MATERIAL Simulation Kit for studying crystal plasticity using an FE based or a spectral numerical solver", *Procedia IUTAM* **3** (2012) 3-10.
- [2] <http://damask.mpie.de>