On the usage of HDF5 in the DAMASK crystal plasticity toolkit

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Outline

• Structure of DAMASK Material Point Model
• Simulation Configuration + Output
• Visualization Workflow
  – Current Implementation
  – Implementation Using HDF5
• Example Using Current Status of HDF5 Implementation
• Summary and Outlook
Crystal Plasticity is a multi-scale problem!
Material Point Model

solver for
• equilibrium
• compatibility

material point model

deformation partitioning & homogenization

F P

F P

F P

F e

S Lp

crystallite elasto-plasticity

constitutive law
• elasticity
• plasticity

Usage of HDF5 in DAMASK
Configuration of a Simulation

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Usage of HDF5 in DAMASK

homogenization

microstructure

constituation
  • lattice type
  • elasticity
  • parameter
  • output
  ...

phase + texture

phase + texture

<crystallite >

[all]
(output) phase
(output) texture
(output) volume
(output) eulerangles # orientation as Bunge triple in degree
(output) grainrotation # deviation from initial orientation as axis
(output) f # deformation gradient tensor; synonyms
(output) fe # elastic deformation gradient tensor
(output) fp # plastic deformation gradient tensor
...

[none]
Material Point output array

- can be different for every element (integration point)
- memory is allocated according to the largest array

<table>
<thead>
<tr>
<th>part</th>
<th>variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>homogenization</td>
<td>( N )</td>
</tr>
<tr>
<td>grain</td>
<td>( M )</td>
</tr>
</tbody>
</table>

HomogenizationCount: 22  
GrainCount: 9  
CrystalliteCount: 30  
Texture: 31  
ConstitutiveCount: 32  
Orientation: 33  
Grainrotation: 43  
Ph: 44  

...
Usage of HDF5 in DAMASK

Visualization Workflow (old)

1. Use FEM post processing software
   - MSC: Mentat
   - ABQ: Abaqus CAE
   - Spectral: none

2. Write Material Point array to binary file
   - Marc: *.t16
   - ABQ: *.odb
   - Spectral: *.spectralOut

3. Extract data of interest into ASCII file
   - Marc & Spectral: postResults.py
   - ABQ: none

4. Post process data
   - Collection of python scripts, e.g. addMises.py

5. Visualize data
   - Your favorite software, e.g. Origin, MatLab, Excel
   - 3Dvisualize.py => *.vtk
   - ParaView

Excessive data copying
Slow data access due to simple ascii file format
Excessive data copying

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Visualization Workflow (new)

write Material Point array + geometry information + etc. to HDF5 file

post process data

generate XDMF file for data of interest

visualize data

Benefits:

✓ no excessive data copying
✓ faster data access
✓ common workflow for all solvers
Material Configuration File

2 homogenizations
1 with output, 1 without

3 sets of output
1 empty, 2 with different sizes

3 phases
each with different outputs

combinations of phases and textures

orientation information
Structure of HDF5 File

Currently everything is stored as scalar values. Vectors and tensors are possible in HDF5. Issues with visualization.

Thanks to Gerd Heber, member of the HDF5 Group.
Visualization Example

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Usage of HDF5 in DAMASK
Some Points of Importance

- Keep original data
- Only add data during post processing
- Store history
- Store data at nodes and/or IPs
- Geometry: which information to store?
  - Initial positions + displacements vs. current positions
  - Connectivity
- Minimize data conversion/ transformation
What do we have:

✓ Working scheme for DAMASK
  ➢ HDF5
  ➢ xdmf
  ➢ ParaView

What do we want:

✓ “general” and “self explanatory” file format
  ➢ HDF5 or something else?
    – if HDF5 ...
      ... someone needs to take care of xdmf
      ... or alternative tool

✓ multi-physics capability
  ➢ HDF5 can do it
Düsseldorfer Advanced MAterial Simulation Kit, DAMASK

- Available as freeware according to GPL 3
- Integrates into MSC.Marc and Abaqus (std. and expl.)
- Standalone spectral solver
- Web: https://DAMASK.mpie.de
- Email: DAMASK@mpie.de