Manual to the Crystal Plasticity Finite Element Subroutine developed at the Max-Planck-Institut für Eisenforschung

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Preliminaries

1.1 Introduction

For the theory and some application examples, see Roters et al. (2010).

1.2 History of the code

?, spaghetti version,

1.3 Accessing the version controlled subroutine

Before you start: Before you are able to access the version-controlled software, you need to get a valid login to the msuhp9 server. Please ask either Berthold Beckschäfer (-922) or Achim Kuhl (-923) to set up your permissions accordingly.

1.3.1 Windows

1.3.1.1 Putty

Get yourself PuTTY and PuTTYgen from http://www.chiark.greenend.org.uk/ sgtatham/putty/-download.html Generate a RSA (SSH2) 2048 bit strong key pair with PuTTYgen. Save the private part of the key to a secure location (My Documents or such). Copy the public part from the PuTTYgen window, paste it into a text-editor and save. Append the contents of that file to `~/.ssh/authorized_keys` on any workstation you can log on to. Create a profile in PuTTY called "msuhp9" with host: msuhp9.mpie.de, your standard "MPIE
myName" username and specify the above location of your private key file as means of authentication. You should then be able to connect with this profile to msuhp9 WITHOUT password authentication!

1.3.1.2 Tortoise

Install the subversion-client Tortoise at http://tortoisesvn.net/downloads Create a directory to hold the CPFEM subroutine on your PC.

Right-Click in this folder and select "SVN checkout" from the context menu. Specify svn+ssh://msuhp9/home/svn/repos/cpfem

as the URL of the desired repository. This will use the profile named "msuhp9" from PuTTY and should hence not ask for any authentication from your end.

1.3.2 Linux workstations

1.3.2.1 Key authentication

if not already done, generate a 2048 bit RSA key pair using ssh-keygen -t rsa -b 2048 and go for the standard options offered. This will create "id_rsa" (private key) and "id_rsa.pub" (public key) within your `~/.ssh` folder.

Append `id_rsa.pub` to `~/.ssh/authorized_keys` and try logging into another workstation with ssh MPIE

myName@msuwsX (exchange X with 2...11). It should NOT require password authentication.

1.3.2.2 Checkout

create a directory to hold the subversion-controlled CPFEM routine and change into this. svn checkout svn+ssh://MPIE

myName@msuhp9.mpie.de/home/svn/repos/cpfem to copy the repository content to the current working directory – done.

familiarize yourself with svn: svn help

1.4 Style guide for programming the CPFEM subroutine

Some hints

- This manual cannot substitute proper commenting in the Fortran code. Try to include as much comments as possible directly in the code.
- When commenting, do not use cryptic comments such as *Random is random!* – an actual example from the code.

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Organization of the code

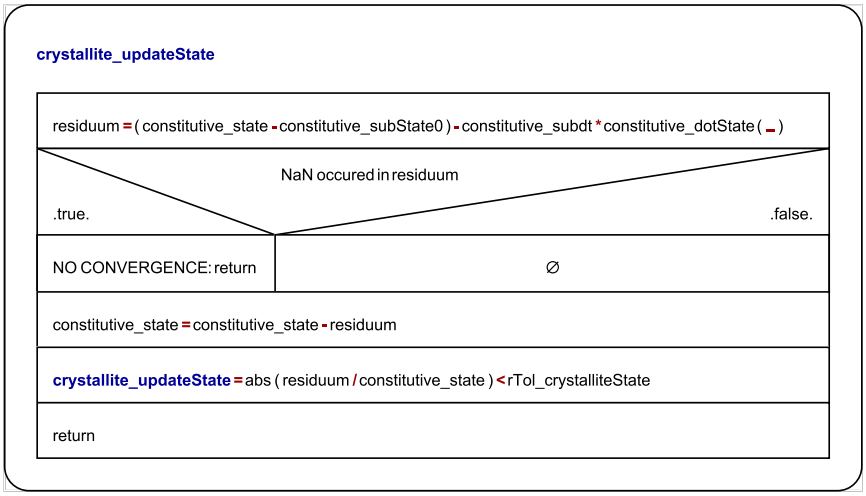

Fig. 2.1: updateState

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Homogenization schemes

If more than one grain is simulated per integration point, a homogenization scheme is required to distribute the deformation gradient of the IP to the respective grains. The simplest choice is the *isostrain approach* which simply consists in assuming the IP deformation gradient to be applicable directly to each grain.

cite RGC papers...

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Constitutive Laws

4.1 phenoPowerlaw

4.1.1 The material file for phenoPowerlaw

4.2 dislotwin

4.3 The non-local model

4.4 The material file: material.config

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Application notes for different finite elements systems

5.1 MSC.MARC/Mentat

In MARC the CPFEM routine is interfaced through the `hypela2` subroutine. The routine `makeMe.py` produces the interface files such as `mpie_cpfem_marc2008r1.f90` that will can be called by the different MARC releases.

Necessary changes in the submit scripts

Model definition for using the subroutine: In MARC, state variable 1 defines the temperature in Kelvin. State variables 2 and 3 define the microstructure and texture, respectively.

Analysis options to invoke: Large Strain, Updated Lagrange.

5.1.1 Utility scripts

- marcAddUserOutput.py [<No. of UserVars>] <model>_<job>.dat— adds UserVariables to the <model>_<job>.dat file under the "post" section

5.1.2 Practical hints

A copy of the subroutine on the home directory on the SAN makes the routine accessible from all workstations under /san/arbitraryfoldername/code/*.f90 . Under windows it is beneficial to keep an additional local copy of the routine to work with TortoiseSVN, since the change of folder icons seems to not work on the SAN.

5.2 Troubleshooting

5.2.1 Inside out element error

An inside out element error can occur if the number of increment is chosen too small. This was observed for revision 539 using the pheno-powerlaw constitutive formulation on a particle in mesh problem.

5.3 Abaqus

Differences to Marc.

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Postprocessing of the results

mentat, py_post, gri, ParaView, TSL-OIM

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Worked examples

Refer to the corresponding publications ...

Appendix A

Crystallographic orientations

A.1 Bunge Euler angles

Euler angles (φ_1, Φ, φ_2) – in Bunge convention – rotate the sample coordinate system (X, Y, Z or RD, TD, ND) into the crystal coordinate system (x_c, y_c, z_c). Three successive rotations are carried out in the following way (Bunge, 1982, pg. 4):

1. Rotate by angle φ_1 around Z, to bring X into the x_c–y_c-plane. The new intermediate axes are X', Y' and Z (Z is unchanged).
2. Now rotate Φ degrees around X', to make Z parallel with z_c. The intermediate axes are X', Y'', Z'.
3. A rotation by angle φ_2 around Z' makes the rotated axes then identical to the crystal axes.

The rotation matrix can be calculated as

$$\boldsymbol{g} = \begin{pmatrix} \cos\varphi_1 \cos\varphi_2 - \sin\varphi_1 \sin\varphi_2 \cos\Phi & \sin\varphi_1 \cos\varphi_2 + \cos\varphi_1 \sin\varphi_2 \cos\Phi & \sin\varphi_2 \sin\Phi \\ -\cos\varphi_1 \sin\varphi_2 - \sin\varphi_1 \cos\varphi_2 \cos\Phi & -\sin\varphi_1 \cos\varphi_2 + \cos\varphi_1 \cos\varphi_2 \cos\Phi & \cos\varphi_2 \sin\Phi \\ \sin\varphi_1 \sin\Phi & -\cos\varphi_1 \sin\Phi & \cos\Phi \end{pmatrix}$$

Appendix B

Related works

B.1 Publications

B.2 PhD thesises

KuoDiss MaDiss ZaafaraniDiss

Bibliography

Bunge, H. *Texture Analysis in Materials Science*. Butterworths Publishers, London (1982). 19

Roters, F., Eisenlohr, P., Hantcherli, L., Tjahjanto, D.D., Bieler, T.R., and Raabe, D. Overview of constitutive laws, kinematics, homogenization, and multiscale methods in crystal plasticity finite element modeling: theory, experiments, applications. *Acta Materialia*, 58(4), 1152–1211 (2010). doi-link. 5