Manual

Material Point Model

developed at the

Max-Planck-Institut für Eisenforschung

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Contents

List of Tables

List of Figures

1 Preliminaries

1.1 Introduction

For the theory and some application examples, see **?**.

1.2 History of the code

?, spaghetti version,

1.3 Internal access to the version-controlled sources

A prerequisite for you being able to access the version-controlled software is to

1. valid login
2. membership in the `svn` group on server `musvn1`

Please ask either Berthold Beckschäfer (-922) or Achim Kuhl (-923) to set up your permissions accordingly.

1.3.1 Windows

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 "`musvn1`" with host `musvn1.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 `musvn1` WITHOUT password authentication!

Tortoise

Install the subversion-client Tortoise from http://tortoisesvn.net/downloads. Create a directory to hold the Material Point Model subroutine on your PC. Right-click in this folder and select "SVN checkout" from the context menu. Specify svn+ssh://musvn1/home/svn/repos/cpfem as the URL of the desired repository. This will use the profile named "`musvn1`" from `PuTTY` and should hence not ask for any authentication from your end.

1.3.2 Linux workstations

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 the public key to the list of known keys

```
cat ~/.ssh/id_rsa.pub >> ~/.ssh/authorized_keys
```

and try logging into another workstation with

```
ssh msuwsX
```

(exchange X with 1 . . . 13). It should *not* require password authentication.

Checkout

Create a directory to hold the subversion-controlled Material Point Model routine and change into this. Issue the command

```
svn co svn+ssh://MPIE\\yourName@musvn1/home/svn/repos/cpfem
```

to copy the repository content to the current working directory.

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.

Part I

Praxis

2

Organization of the code

Part II

Theory

3
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...

4
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

5 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 homogenization and microstructure, respectively.

Analysis options to invoke: Large Strain, Updated Lagrange. For most problems, using a constant dilatation formulation is important for robustness of the simulations.

5.1.1 Utility scripts

- marcAddUserOutput.py [¡No. of UserVars¿] marcinput — adds UserVariables to the marcinput 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.

6
Postprocessing of the results

mentat, py_post, gri, ParaView, TSL-OIM

7
Worked examples

Refer to the corresponding publications ...

A

Crystallographic orientations

A.1 Bunge Euler angles

Euler angles $(\varphi_1, \phi, \varphi_2)$—following the 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 (**?**, p. 4):

1. Rotate by φ_1 around Z, to bring X into the x_c–y_c-plane. The new intermediate axes are X', Y' and Z (unchanged).

2. Now rotate by ϕ around X', to make Z parallel with z_c. The intermediate axes are X', Y'', Z'.

3. A final rotation by φ_2 around $Z' \equiv z_\mathrm{c}$ makes the rotated axes then identical to the crystal axes.

The rotation matrix can be calculated as

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

B
Related works

B.1 Publications

B.2 PhD thesises

KuoDiss MaDiss ZaafaraniDiss

Bibliography

H.J. Bunge. *Texture Analysis in Materials Science*. Butterworths, London, 1982.

Cited on page 21.