# INSTALLATION GUIDE

CalculiX Solver ccx 2.8 on Mac OS X Mavericks

### <sup>1</sup>B. Graf

*Abstract*. CalculiX comprises the solver ccx (CalculiX CrunchiX) and the graphical pre- and postprocessor cgx (CalculiX GraphiX). A step by step installation guide for ccx 2.8 on Mac OS X 10.9.5 Mavericks is provided. Installation from source is considered. The present guide is based on the general installation instructions for Unix/Linux which come with the ccx package. A basic installation of ccx is considered which is defined as follows: ccx 2.8 for multi-threading (MT), external solvers SPOOLES (serial and MT) and ARPACK (serial). The optional installation of the solvers POSIX and TAUCH, of the SGI Library as well as of a 8 byte version of ccx for large CFD problems is not subject of the present installation. Besides the aforementioned basic installation of ccx also the installation of required Mac-specific software is considered (Xcode, compilers GCC and gfortran). Except of html-help files and the installation path the installation of ccx is independent from the installation of cgx. Tests of the functionality of the installation are provided.

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<sup>1</sup>Prepared by B. Graf, based on the general installation instructions for Unix/Linux by G. Dhondt (developer of ccx, MTU Aeoro Engines, Munich, Germany).

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## **RELEASE NOTES**

Revision	Remarks
Draft, June 18, 2014	Installation of ccx 2.7 on Mac OS X 10.9.3 Mavericks.
February 10, 2015	<ul> <li>Installation of ccx 2.8 on Mac OS X 10.9.5 Mavericks. Changes:</li> <li>- GCC 4.9 (g++) used for compilation of ccx c-routines instead of previously used GCC 5.1</li> <li>- Editorial changes.</li> </ul>

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# **1. INTRODUCTION**

## 1.1 General

CalculiX comprises the solver ccx (CalculiX CrunchiX) and the graphical pre- and postprocessor cgx (CalculiX GraphiX). The present guide covers the installation of ccx on Mac OS X Mavericks (cf. [4] for the installation of cgx). Except of html-help files and the installation path the installation of ccx is independent from the installation of cgx. Accordingly, the sequence of the installation of ccx and cgx may be chosen freely.

For a brief introduction to the installation of ccx on Unix/Linux, please read the instructions by G. Dhondt [1], Section A. Based on the aforementioned reference [1] in the present document a step by step installation guide for ccx on Mac OS X is provided. Installation from source is considered. Furthermore, the installation of ccx requires the pre-installation of Mac-specific software like Xcode and compilers GCC (GNU compiler collection) and gfortran.

The present guide covers the installation of Mac-specific software as well as of the so called basic installation of ccx which according to Section 1.2 is defined as follows: installation of ccx and optional external solvers SPOOLES and ARPACK. Furthermore, in Section 1.2 also the installation of <sup>2</sup>additional (in addition to the basic installation) optional software is briefly addressed. The installation of the aforementioned additional software, however, is not subject of the present installation instructions. Accordingly, the present installation of the aforementioned Mac-specific software as well as on the afore defined basic installation of ccx.

Section 2 contains an overview of the required software and Section  $\cdot$  a summary of pre-arrangements which are required for the installation of ccx. The installation instructions are contained in Sections 4 to 7. The installation should follow the sequence as given by Sections 4 to 7. First of all, in Section 4 the installation path and the file system are explained as well as the installation of the ccx source code and html-help files. In Section 5 Mac-specific software is installed (Xcode, compilers GCC and gfortran). The external solvers SPOOLES and ARPACK are installed in the subsequent Section 6. Finally, the installation of ccx is completed in Section 7. Furthermore, Section 7 covers the following subjects: launch of ccx and test of installation, how to get started with ccx, test examples. In Section 8 the functionality of the external solvers SPOOLES and ARPACK. The final Section 9 is provided for the future documentation of hints and known Mac-specific problems. The references are provided on page 29. The release notes are provided on page i.

<sup>&</sup>lt;sup>2</sup>Installation of the additional external solvers POSIX and TAUCH, of the SGI Library as well as of a 8 byte version of ccx for large CFD problems.

## 1.2 Basic Installation of ccx and Optional Additional Software

• *Basic installation of ccx*. The so called basic installation of ccx is subject of the present instructions and comprises the following installations: ccx 2.8 for multi-threading (MT), external solvers SPOOLES (serial and MT version) and ARPACK (serial).

*Note*. As further outlined in Section 4 below, the installation of Arpack in addition requires the installation of BLAS (Basic Linear Algebra Subprograms) and LAPACK (Linear Algebra PACKage).

• *Optional additional software*. In references [1], [2] the installation as well as the capabilities of the following additional software is explained: external solvers POSIX and TAUCH, SGI Library, 8 byte version of ccx for large CFD problems. The installation of the aforementioned additional software, however, is not subject of the present installation guide.

# 2. SOFTWARE REQUIREMENTS

## 2.1 Software Releases

Unless otherwise noted, the installation has been tested for the software releases as specified below (cf. titles of subsections below for the releases).

## 2.2 Mac OS X Specific

## 2.2.1 OS X Mavericks 10.9.5

The installation was tested for version 10.9.5 of OS X Mavericks. Among others, the Unixlike Darwin OS is an inherent part of Mac OS X. The command-line interface to OS X is provided by the Terminal App (cf. Section 2.2.2 and Section 3.2 for details).

## 2.2.2 Xcode 5.1.1 – Provides Command Line Tools (Terminal) and Associated Modified GCC 5.1 (GNU Compiler Collection)

Xcode is a broad suit for software development on Mac and is provided by Apple. Several capabilities of Xcode are required for the present installation as further outlined below. However, because Xcode is not an inherent part of OS X, it needs to be installed separately from OS X (cf. Section 5.1 for the installation).

The following capabilities of Xcode are required for the present installation: (1) commandline tools (CLTs) for OS X, respectively the Terminal App, (2) modified (by Apple) version 5.1 of the GCC (GNU compiler collection). The aforementioned CLTs are provided by the Terminal App (cf. Section 3.2 for details), also denoted as Terminal or Terminal window. As will be shown below, Unix commands for software installation will be entered via Terminal. Furthermore, ccx will be launched via Terminal. Except of the c-routines of ccx, the aforementioned modified GCC 5.1 will be applied for the compilation of c-routines. For the compilation of the c-routines of ccx the unmodified GCC 4.9 is required (cf. Section 2.2.3 and Section 3.1 for details). The aforementioned CLTs and GCC 5.1 are installed together with Xcode in Section 5.1 below.

Notes. Xcode is a broad suite for software development on OS X. For the installation of cgx, however, only the so called "Command Line Tools" (CLTs) of Xcode are required (installation of Xcode requires 5 GB, whereas the installation of the CLTs requires only ca. 300 MB). Amongst others, the CLTs include the already aforementioned version 5.1 of the modified GCC. The CLTs provide commands like "make", whereas the latter is required to build executables from source.

Alternatively to Xcode, only the CLTs may be installed. The installation of the CLTs, however, is not subject of the present installation instructions. Link for download of the CLTs:

http://osxdaily.com/2014/02/12/install-command-line-tools-mac-os-x/

## 2.2.3 GCC 4.9 - Unmodified GCC (GNU Compiler Collection) for OS X Mavericks

The unmodified GCC 4.9 is required for the compilation of the c-routines of ccx and is not identical with the modified GCC 5.1 from Section 2.2.2 above (cf. also explanation of Xcode in Section 2.2.2 above and Section 3.1 below for details). GCC 4.9 will be installed in Section 5.2 below.

## 2.2.4 Fortran Compiler gfortran 4.9 for OS X Mavericks

The Fortran compiler: "gfortran" is required for the compilation of the Fortran-routines of ccx and ARPACK. For the present installation gfortran is considered as the default Fortran compiler (cf. also Section 3.1 for details). The installation of gfortran is subject of Section 5.3 below.

## 2.3 ccx 2.8 - CalculiX ChrunchiX, Version 2.8

The installation instructions for ccx are provided in Section 4 and Section 7 below. First of all, the source code of ccx is installed in Section 4. Furthermore, in Section 4 also the installation path and the file system of ccx is explained. The installation will be completed in Section 7 with the build of the binary of ccx.

## 2.4 External Solvers SPOOLES 2.2 and ARPACK 2.1

- SPOOLES 2.2. SPOOLES is an established linear equation solver and among others, provides the following capabilities: (a) single-threading, respectively serial processing, (b) MT (multi-threading), (c) MP (multi-processing for several separate CPU's). For the present basic installation of ccx (cf. Section 1.2) the aforementioned capabilities (a) and (b) for single- and multi-threading are considered. Single- and multi-threading may be invoked with the help of user defined environment variables (cf. Section 8.2 for examples). SPOOLES will be installed for the aforementioned capabilities in Section 6.2 below.
- *ARPACK 2.1.* ARPACK (ARnoldi PACKAGE) is a collection of Fortran routines for the solution of large-scale eigenvalue problems (for details consider the link in footnote 3 below). For the considered basic installation of ccx (cf. Section 1.2) a serial version of ARPACK will be installed. The dependencies of ARPACK on BLAS and LAPACK will be further discussed in context with the installation of ARPACK in Section 6.3 below.

<sup>&</sup>lt;sup>3</sup>Link for details of ARPACK: <u>http://www.caam.rice.edu/software/ARPACK/</u>

# **3. PRE-ARRANGEMENTS FOR INSTALLATION**

# **3.1 Default Compilers GCC 5.1 and Compilers GCC 4.9 and gfortran 4.9**

- *GCC 5.1*. Except of the c-routines of ccx, the modified GCC 5.1 (GNU compiler collection) which is installed together with Xcode is considered as the default compiler for the compilation of c-routines (cf. Section 5.1 for the installation of Xcode and details concerning the version and installation path of GCC 5.1). GCC 5.1 includes versions 5.1 of the individual compilers: gcc (GNU c-compiler), g++ and clang.
- *GCC 4.9 for compilation of ccx*. GCC 4.9 from Section 2.2.3 includes versions 4.9 of the individual compilers: gcc (GNU c-compiler), g++ and clang. The aforementioned g++ will be applied in Section 7.1 for the compilation of the c-routines of ccx. GCC 4.9 will be installed in Section 5.2 below. Furthermore, details concerning the version and installation path of GCC 4.9 are given in the aforementioned Section 5.2.
- 4.9.0 for compilation of Fortran-routines. The Fortran compiler: "gfortran" will be installed in Section 5.3 and is considered as the default compiler for the compilation of the Fortran-routines of ccx and ARPACK (cf. Section 5.3 for details concerning the version and installation path of gfortran).

# 3.2 Terminal, Terminal Commands, HOME, LOGNAME, Login and Permissions

*General*. The following notes are provided for Mac users who usually don't work in Unix environments. Also search the web for more instructions concerning the below discussed subjects.

*Terminal*. First of all, as further explained below, "Terminal", respectively the Terminal App is a pre-installed application on your Mac. The notation "Terminal" or "Terminal window" here is also used for the bash (bourne-again shell) Unix-shell which is provided by the Terminal App. Terminal provides the command-line interface to OS X, respectively the interface for the input of Unix-commands which are required for the installation of cgx. Furthermore, cgx may be launched from a Terminal window (cf. Section 7.2 for details).

To open the Terminal application, double click the Terminal-App in your "/Applications/Utilities" folder. The Terminal icon then will appear in your Dock and a Terminal window will pop up on your screen. Use "Help" in the menu bar of "Terminal" to gain further instructions (how to open additional Terminal-windows, how to open further tabs in some window etc.) or visit e.g. the following site for additional instructions: http://www.maclife.com/article/feature/25\_terminal\_tips\_every\_mac\_user\_should\_know.

*Terminal Commands*. Commands, respectively Terminal commands, which are highlighted in the following with red letters, are entered after the \$-prompt in the Terminal window (cf. examples below). For execution of commands use the return key (also denoted as enter key).

*HOME*, *LOGNAME*. After a new Terminal window was opened, the shell wakes up in your home directory, denoted as HOME (shortcut ~; use keystrokes: alt + N for tilde ~). Use command env (for environment):

## \$ env <return>

to display the path to your HOME (usually: HOME=~=/Users/LOGNAME). The envcommand also displays your LOGNAME as well as the path: PWD to your current (private) working directory. The path to your current working directory, respectively current folder, also may be displayed with command: \$ pwd <return> (pwd for "print working directory").

*Login*. If you are not already logged in with your LOGNAME, use command: \$ login <return> in Terminal. Afterwards, you will be asked for your LOGNAME and password to login.

*Permissions*. For several installation steps you need expanded access rights to the file system. To gain these rights, here the sudo-command will be used; syntax (examples are given below):

## \$ sudo command <return>.

Afterwards, the OS will ask you first for your password before the command is executed. If required, in the present instruction the sudo-command is set for installation commands. However, if you run into any permission-problems, first try to use sudo as specified above. If sudo doesn't work, you must login as root.

# **3.3** Editors, .bash\_profile, Editing of Hidden File .bash\_profile and Usage of .bash\_profile to Set Paths and Export Paths

*General*. The following notes are provided for Mac users who usually don't work in Unix environments. Also search the web for more instructions concerning the below discussed subjects.

*Editors*. The Finder App, respectively the "Finder" is a convenient tool for file handling on your Mac. However, many of the files on your Mac are hidden in <sup>4</sup>Finder windows, among others the file: ".bash\_profile" which is required later for the cgx installation. In the following it will be explained how hidden files may be created, opened and edited. Furthermore, the path setting in file: ".bash\_profile" is briefly explained.

*File .bash-profile*. The file .bash-profile is located in your HOME and amongst other settings contains path settings, respectively is used to <sup>5</sup>export paths. The dot in the first place

<sup>&</sup>lt;sup>4</sup>Note. Commands for displaying hidden files in Finder are available, but for several reasons will be not used here.

<sup>&</sup>lt;sup>5</sup>Note. If you open a Terminal window, the OS "exports" the path settings found in .bash\_profile and then uses these paths to search for executables. Furthermore, amongst others, the path: /usr/bin is a default path which the OS uses to search for executables.

of the file name marks file ".bash\_profile" as a hidden file which, therefore, is not displayed in the Finder window. A simple example for a .bash\_profile with path settings is given below.

*Editing of hidden files, respectively of file .bash\_profile*. The editing will be demonstrated for setting, respectively exporting paths with .bash\_profile. First, execute the following commands in Terminal (don't' type in green # comment; shortcut ~ for your HOME is used; keystrokes for typing tilde ~:  $\neg + n$ ):

\$ cd ~ <return></return>	<pre># Change directory (cd) to your home directory ~ (Home), # where your .bash_profile is located.</pre>
	<ul> <li># Long (option -l) list (command ls) displays visible files in ~.</li> <li># Note that file .bash_profile is not displayed. Command ls –l,</li> <li># therefore, displays all visible files.</li> </ul>
\$ ls -la <return></return>	# Long (option "l") list (ls) for all (option "a" for all visible and # invisible) files in ~. Now, .bash_profile is contained in the list # of files. Command ls –la, therefore, displays all visible and # invisible files.

If .bash\_profile is not listed after the execution of the last command: ls -la, then create it now with the following commands:

\$ cd ~ <return> # Change directory (cd) to your home directory HOME.

\$ touch .bash\_profile <return> # Create .bash\_profile.

**\$ ls -la <return>** *#* Verify, if .bash\_profile has been created.

Next, open .bash\_profile with editor TextEdit with commands:

\$ cd ~ <return> # Set home directory as your working directory.

**\$ open -e .bash\_profile <return>** # Opens .bash\_profile in TextEdit.

*Set paths in file .bash\_profile and export paths*. Now, we are ready for editing of the .bash\_profile, respectively to enter a new path-setting in .bash\_profile. Next an example is given, how paths may be set in .bash\_profile. For path setting you may add the following lines in your .bash\_profile:

#!/bin/bash

export PATH=\$PATH

## export PATH=\$PATH:/Users/LOGNAME/NETGEN\_INSTALL/bin

In the above lines, "export" is a Unix command, PATH an environment variable, \$PATH the value of that variable, colon ":" is used as separator between paths. The first line up-

dates the PATH variable, the second line sets the added path:

/Users/LOGNAME/NETGEN\_INSTALL/bin to some executable which is contained in directory "bin". Add as any many paths as you need. Finally, save file .bash\_profile and quit TextEdit. The required path settings for the considered software are specified in the installation instructions below.

To activate the changes, respectively to export the new paths in .bash\_profile use commands:

\$ cd ~ <return> # Set home directory.

\$ source .bash\_profile <return>

in current Terminal window. Alternatively, you may open a new Terminal window, because as soon as a new Terminal window is opened the OS will automatically execute the commands in .bash\_profile, i.e. export path settings etc.).

Control the path settings with the following command:

\$ echo \$PATH <return>.

Notes. The OS also automatically searches the default paths: /usr/bin as well as /usr/local/bin for executables. Instead of TextEdit, also one of the command line editors may be used (vim-editor etc.).

# 4. INSTALLATION PATH AND INSTALLATION OF CCX FILES

## 4.1 General

In the present section the ccx source code and html-help files will be downloaded. The installation path may be chosen according to Section 4.2. Furthermore, the file system for the installation of cgx and ccx as well of the external solvers is explained in Section 4.2.

## After the installation of ccx files continue installation in the sequence of Section 5 to Section 7.

## 4.2 Installation Path "calculix\_inst\_path" and File System

## Installation Path

Both ccx and cgx as well as the external solvers are installed for the same installation path. Choose option A or option B for the installation <sup>6</sup>path "calculix\_inst\_path":

- Option A (default installation path):

"calculix\_inst\_path" =/usr/local

- Option B (example for user defined path):

"calculix\_inst\_path"=~/Applications=/Users/LOGNAME/Applications

Option A is in compliance with the Unix file system hierarchy standard and also is the default path for the installation of ccx. For option B the path may be chosen freely. For option B an example is given above, for which ccx will be installed in directory "Applications" under your home directory "~" (cf. Section 3.2 for the home directory).

Because in ccx the paths are set relative to directory "src" of ccx\_2.8 (cf. file system in Fig. 1), neither for option A nor for option B paths must be set for the installation of ccx in Section 7.1.

Prior to the installation the directories of the path "calculix\_inst\_path" must exist. Create them now, if necessary. Use the Finder to create directories or the sequence of Unix commands: \$ cd "path\_to\_Directory" <return> (change to directory: "path\_to\_Directory" under which a subdirectory has to be created), then type: \$ mkdir "dir\_name" <return> to create the subdirectory "dir\_name". Furthermore, use: \$ ls –l <return> to list contents of some directory, use sudo before commands (e.g. sudo mkdir) if the permission for making of directories is denied.

<sup>&</sup>lt;sup>6</sup>Note. The notation "calculix\_inst\_path" here is used for documentation reasons only and, therefore, is not an environment variable for the installation of cgx. Otherwise stated, replace "calculix\_inst\_path" in commands with full path specification according to options A, B.

cgx 2.8

doc examples netgen src

CalculiX

(downloaded source code and html-help

files stored in directories "CalculiX")

cgx file system

glut-3.5

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libSNL

**"calculix\_inst\_path"** (chosen installation path according to Section 4.2 for installation of directory "CalculiX" with source code and help files of cgx and ccx)

external solvers

ccx file system

ccx\_2.8

doc src test

ссх

(html-help files)

**SPOOLES.2.2** 

spooles.a

(library spooles.a)

**ARPACK** 

Libarpack Mac.a

(library libarpack\_Mac.a)

### File System

cgx

(html- help files)

After the installation of the ccx source code and the external solvers the file system for the present ccx installation looks as depicted in Fig. 1. Calculix (ccx and cgx) and the external solvers, therefore, must be installed for the installation path "calculix\_inst\_path" from Section 4.2. The ccx source code is contained in directory "src", the html-help files in directory "ccx" and the test examples in directory "test". Furthermore, the libraries of the external solvers are build in directories "SPOOLES.2.2" and "ARPACK" as depicted in Fig. 1.

## 4.3 Install ccx Files

Steps a, b:

- (a) Download the following packages from Calculix site <u>http://www.dhondt.de/</u>:
  - "the source code" ccx\_2.8.src.tar.bz2,
  - "the documentation html" ccx\_2.8.htm.tar.bz2,
  - "test examples" ccx\_2.8.test.tar.bz2.

The files will be downloaded on your Desktop.

The links for the download of the Installation Guide [1] and User's Guide [2] are provided together with the list of references on page 29.

(b) Next, install downloaded packages. First drag packages: "ccx\_2.8.src.tar.bz2", "ccx\_2.8.htm.tar.bz2" and "ccx\_2.8.test.tar.bz2" from Desktop to the installation directory: "calculix\_inst\_path" from Section 4.2 (cf. also the file system in Fig. 1). Then use Terminal commands (without comments) to extract the files from the packages one by <sup>7</sup>one as follows:

**\$** cd "calculix\_inst\_path" <return> # Set directory for installation of ccx.

\$ bunzip2 ccx\_2.8.src.tar.bz2 <return> # Unzip package with source code.

**\$ bunzip2 ccx\_2.8.test.tar.bz2 <return>** # Unzip package with test examples.

\$ bunzip2 ccx\_2.8.htm.tar.bz2 <return> # Unzip package with html-help files.

The directories: "src" with the source code, "doc" with the html-documentation and "test" with the test examples now are installed under the path (cf. also Fig. 1 for the file system): "calculix\_install\_path"/CalculiX/ccx\_2.8.

<sup>&</sup>lt;sup>7</sup>Note. Wildcards don't work for tar-command.

# **5. INSTALL MAC-SPECIFIC SOFTWARE**

# 5.1 Xcode 5.1.1 and Associated Modified GCC 5.1

Xcode may be downloaded for free from "Categories" in the App Store. Follow installer instructions. The Xcode App will be installed in your "Applications" folder.

As already mentioned before in Section 2.2.2, the modified GCC 5.1 (GNU compiler collection) comes together with Xcode and is installed under the default path: /usr/bin. The modified GCC 5.1 includes the individual compilers: gcc (GNU c-compiler), g++, Clang. GCC 5.1 will be applied according to Section 3.1.

The installation of GCC 5.1 now will be tested exemplarily for g++. If the installation was successful, after the execution of the Terminal command: which g++ -return the path to the default g++ compiler is displayed as follows:

/usr/bin/g++

After execution of Terminal command:  $g_{++} - v < return > (option - v for version)$  the screen output for the version of  $g_{++}$  should look as follows:

Configured with: --prefix=/Applications/Xcode.app/Contents/Developer/usr --with-gxx-include-dir=/usr /include/c++/4.2.1 Apple LLVM version 5.1 (clang-503.0.40) (based on LLVM 3.4svn) Target: x86\_64-apple-darwin13.2.0 Thread model: posix

# 5.2 Unmodified GCC 4.9

The unmodified GCC 4.9 (GNU compiler collection) will be applied according to Section 3.1. GCC 4.9 for OS X will be installed according to point 2 of the instructions: https://wiki.helsinki.fi/display/HUGG/Installing+the+GNU+compilers+on+Mac+OS+X

Installation steps 1 - 4:

- (1) Download pre-build GCC 4.9, respectively gunzipped file gcc-4.9-bin.tar.gz from site: http://sourceforge.net/projects/hpc/files/hpc/gcc/gcc-4.9-bin.tar.gz/download?use\_mirror=cznic&download=
- (2) Open Terminal window and change to download directory (usually directory "Downloads" or directory "Desktop") of gcc-4.9-bin.tar.gz. If for example gcc was downloaded on your Desktop use terminal command:

\$ cd ~/Desktop <return>.

(3) If gcc-4.9-bin.tar.gz was not automatically unzipped, then unzip file with Terminal command:

\$ gunzip gcc-4.9-bin.tar.gz <return>

(4) For installation of GCC 4.9 use terminal command (without comment):

\$ sudo tar xvf gcc-4.9-bin.tar -C / <return> # Installs GCC 4.9 under default directory: # /usr/local/bin.

After step 4, among others the compilers gcc and g++ are installed in /usr/local/bin.

The test of the installation will be explained exemplarily for g++. If the installation was successful the Terminal command: \$ which /usr/local/bin/g++ <return> will display the path to the unmodified GNU g++ compiler as follows (screen output):

/usr/local/bin/g++

Using built-in specs. COLLECT\_GCC=/usr/local/bin/g++ COLLECT\_LTO\_WRAPPER=/usr/local/libexec/gcc/x86\_64-apple-darwin14.0.0/4.9.2/lto-wrapper Target: x86\_64-apple-darwin14.0.0 Configured with: ./gcc-4.9-20141029/configure --enable-languages=c++,fortran Thread model: posix gcc version 4.9.2 20141029 (prerelease) (GCC)

As already explained in Section 3.1 above, the unmodified g++4.9 will be applied only for the compilation of the c-routines of ccx in Section 7.1 below. The path for g++: /usr/local/ bin/g++ will be set in the Makefile of ccx (cf. Section 7.1 for details).

# **5.3** Fortran Compiler gfortran 4.9

The Fortran compiler gfortran 4.9 will be applied according to Section 3.1. Download the pre-built binary of gfortran 4.9 for OS X Mavericks from site: <u>http://hpc.sourceforge.net/</u>.

The zipped tar-file gfortran-4.9-bin.tar.gz will be downloaded on your Desktop. Install compiler with the following Terminal commands (without comments):

\$ cd ~/Desktop <return> # Change to directory Desktop.

## \$ gunzip gfortran-4.9-bin.tar.gz <return> # Unzip gfortran-4.9-bin.tar.gz to # gfortran-4.9-bin.tar.

\$ sudo tar -xvf gfortran-4.9-bin.tar -C / <return> # Installs gfortran for default path:

# /usr/local. Binary "gfortran", therefore,

# located under directory:

# /usr/local/bin/gfortran.

After the execution of the last command the binary "gfortran" will be installed under the default path: /usr/local/bin/gfortran. No additional path settings required.

Next, test the installation of binary "gfortran" and the installed version. Change to some working directory and use Terminal commands (without comments):

**\$ which gfortran <return> #** Displays path to binary "gfortran".

**\$** gfortran -v <return> # Display version (option "-v") of gfortran.

The installation of gfortran was successful if the path is displayed as follows:

/usr/local/bin/gfortran

### and the version of gfortran as follows:

Using built-in specs. COLLECT\_GCC=gfortran COLLECT\_LTO\_WRAPPER=/usr/local/libexec/gcc/x86\_64-apple-darwin14.0.0/4.9.2/lto-wrapper Target: x86\_64-apple-darwin14.0.0 Configured with: ../gcc-4.9-20141029/configure --enable-languages=c++,fortran Thread model: posix

# 6. INSTALL EXTERNAL SOLVERS

## 6.1 General

According to the definition of the basic installation of ccx from Section 1.2, the external solvers SPOOLES and ARPACK will be installed.

## 6.2 **SPOOLES 2.2**

• *General*. SPOOLES is an linear equation solver (cf. Section 2.4 for details). For the basic installation of ccx the library spooles.a with the single- and multi-threading (MT) routines of SPOOLES is required. SPOOLES will be installed for the chosen installation path from Section 4.2 and the library spooles.a will be build in directory "spooles.2.2" (cf. Fig. 1 for the file system): "calculix\_inst\_path"/spooles.2.2/spooles.a.

The present installation instruction of SPOOLES is based on the instruction: "Install" which may be downloaded from site: <u>http://netlib.sandia.gov/linalg/spooles/spooles.2.2.html</u>

- *Installation*. Steps a to f:
  - (a) Download SPOOLES package "spooles.2.2.tgz" from site:

http://netlib.sandia.gov/linalg/spooles/spooles.2.2.html

The package: "spools.2.2.tgz" will be downloaded on your Desktop.

- (b) Install source files. Double click icon: "spooles.2.2.tgz" to unzip package, then drag unzipped directory: "spooles.2.2" from Desktop to the installation directory according to your installation path: "calculix\_inst\_path". The file system for the installation of SPOOLES now should look as depicted in Fig. 1.
- (c) Modify files Lock.h, drawTree.c, Make.inc:
  - Backup files prior to modifications.
  - File "Lock.h" set thread type to POSIX. Location of file: "calculix\_inst\_path"/ spooles.2.2/Lock/Lock.h. Open file with an editor of your choice and then check, if after line (without quotes): "#define TT\_POSIX 2" the line: "#define THREAD\_TYPE TT\_POSIX" is already set for the required thread type POSIX. If not, insert line (without quotes): "#define THREAD\_TYPE TT\_POSIX" after existing line "#define TT\_POSIX 2". Save file and quit editor.
  - File "makeGlobalLib" replace file name "drawtree.c" in considered file with "drawtree.c" (cf. [1]). Location of file: "calculix\_inst\_path"/spooles.2.2/Tree/src /makeGlobalLib. Open file "makeGlobalLib" with an editor of your choice. Then find "drawtree.c" and replace it with "tree.c" (without quotes). Save file.

Note. File "drawTree.c" does not exist under path: "calculix\_inst\_path"/spooles.2.2/Tree/src.

- File "Make.inc" – modify code. Location of file: "calculix\_inst\_path"/spooles.2.2/Make.inc. Open file with an editor of your choice, then activate green lines (remove "#" at first place) and deactivate red lines (add "#" at first place) as depicted below:

```
# place your favorite compiler here
# for solaris
#
CC = gcc
# CC = /usr/lang-4.0/bin/cc
# for sgi
#
\# CC = cc
# for hp
# CC = /opt/mpi/bin/mpicc
#_
         _____
#
# set the compiler flags
#
# OPTLEVEL =
# OPTLEVEL = -g -v
# OPTLEVEL = -O
# OPTLEVEL = -xO5 - v
OPTLEVEL = -O3
\# OPTLEVEL = -O4
# CFLAGS = -Wall -g
# CFLAGS = -Wall -pg
# CFLAGS = $(OPTLEVEL) -D POSIX C SOURCE=199506L
# CFLAGS = $(OPTLEVEL)
CFLAGS = -Wall $(OPTLEVEL)
#
#.
```

Save file and quit editor.

(d) Build serial library spools.a. Use Terminal commands (without comments):

\$ cd "calculix\_inst\_path"/spooles.2.2 <return> # Set directory.

Note. The last command generates several warnings which may be ignored.

(e) Build multi-threading (MT) library and merge library in spools.a. Use Terminal commands (without comments):

\$ cd calculix\_inst\_path/spooles.2.2/MT/src <return> # Set directory.

# Consider that the next command "makeLib" is case sensitive:

\$ make makeLib <return> # Creates library and merges MT library in library # spooles.a from previous step (d).

Note. The last command automatically removes all object files. Warnings may be ignored.

(f) Repeat installation of libraries. If you want to repeat the installation for some reason, first make the installation clean. Use Terminal commands (without comments):

\$ cd "calculix\_inst\_path"/spooles.2.2 <return> # Set directory.

**\$ make clean <return>** # Removes object files and file "library.a"

• Test installation. The installation of SPOOLES will be tested in Section 8.2 below.

# 6.3 ARPACK 2.1

• *General*. ARPACK (ARnoldi PACKAGE) is a collection of Fortran routines for the solution of large-scale eigenvalue problems (cf. Section 2.4 for details). For the considered basic installation of ccx (cf. Section 1.2) a serial version of ARPACK will be installed. ARPACK will be installed for the chosen installation path from Section 4.2 and the library Libarpack\_Mac.a will be build in directory "ARPACK" (cf. Fig. 1 for the file system): "calculix\_inst\_path"/ARPACK/libarpack\_Mac.a.

According to Section 1.2 above, libraries for BLAS (Basic Linear Algebra Subprograms) and LAPACK (Linear Algebra PACKage) are required for the installation of ARPACK. Basically, the following two options a, b exist to provide the aforementioned libraries: (a) compile ARPACK with the routines for BLAS and LAPACK which come with the ARPACK-package, (b) link ARPACK to libraries for BLAS and LAPACK. For the reasons outlined in the note below, option (a) has been chosen, i.e. build of a selfcontained library for ARPACK which includes the required routines for BLAS and LAPAC.

The present installation instruction of ARPACK is based on the "README" which is downloaded with the ARPACK-package.

Note. As already outlined above, alternatively to option (a) ARPACK may be installed according to option (b) with links to libraries of BLAS and LAPACK. Options for links: (1) link against libraries which come with OS X, (2) Install source for BLAS and LAPACK separately, build libraries, then link against these libraries, (3) build libraries with the routines of BLAS and LAPACK which come with ARPACK, then link against these libraries. The aforementioned option (1) was tested only with links to the libraries: /usr/lib/libf77lapack.dylib, /usr/lib/libblas.dylib which come with OS X. Benchmark tests revealed that for option (1) the errors of calculated eigenvalues are larger if compared to the results which are derived with the aforementioned self-contained libraries according to option (a). The latter indicates that the calculated eigenvalues may be sensitive with respect to the versions of the libraries of BLAS and LAPACK. The aforementioned sensitivity is also in accordance with the following note in the "README" which is provided with the ARPACK-package: "\*\*\* NOTE \*\*\* Unless the LAPACK library on your system is version 2.0, we strongly recom-

mend that you install the LAPACK routines provided with ARPACK." Accordingly, for the present installation, the LAPACK and BLAS routines have been used which come with the ARPACK-package. Otherwise stated, calculated eigenvalues should be carefully tested against benchmark calculations if ARPACK is installed with links to BLAS and LAPACK according to options (1) to (2) above. Exception: link according to option (3) above.

- *Installation*. Steps a to f:
  - (a) Download GNU-zipped tar-files: "arpack96.tar.gz" and "patch.tar.gz" from site:

http://www.caam.rice.edu/software/ARPACK/

The tar-files will be downloaded on your Desktop.

(b) Install source files. Drag tar-files: "arpack96.tar.gz" and "patch.tar.gz" from Desktop to the installation directory according to your installation path: "calculix\_inst\_path". The tar-files, therefore, now should be located on the same directory level as directory "CalculiX" from Fig. 1.

Next, install files with Terminal commands (without comments):

\$ cd "calculix\_inst\_path" <return> # Set working directory.

\$ tar -xzf arpack96.tar.gz <return> # Creates directory "ARPACK" and installs # source files under directory "ARPACK".

\$ tar -xzf patch.tar.gz <return> # Installs patch of source code under # directory "ARPACK".

The source files of BLAS and LAPACK are installed in directories "BLAS" and "LAPACK" (cf. "calculix\_inst\_path"/ARPACK/BLAS and "calculix\_inst\_path"/ARPACK/LAPACK for the aforementioned source files).

- (c) Modify files second.f, ARmake.inc:
  - Backup files prior to modifications.
  - File "second.f" modify code. Location: "calculix\_inst\_path"/ARPACK/UTIL/second.f. Open file "second.f" with an editor of your choice and

replace the following two existing lines:

\* REAL ETIME EXTERNAL ETIME

with the following two lines:

Modified June, 2014 for gfortran 4.9.0
 external real etime

Save file and quit editor.

- File "ARmake.inc" – modify code. Location of file: "calculix\_inst\_path"/ ARPACK/ARmake.inc. Open file with an editor of your choice. Then replace red code to the left of arrows with green code to the right of arrows and in addition replace: "*calculix\_install\_path*" in the first line below with the full path to the chosen installation directory (cf. Section 4.2 for the installation path):

```
home = (HOME)/ARPACK \rightarrow home = "calculix_inst_path"/ARPACK

PLAT = SUN4 \rightarrow PLAT = MAC

LAPACKLIB = \rightarrow # LAPACKLIB =

BLASLIB = \rightarrow # BLASLIB =

ALIBS = (ARPACKLIB) (LAPACKLIB) (BLASLIB) \rightarrow ALIBS = (ARPACKLIB)

FC = f77 \rightarrow FC = gfortran

FFLAGS = -O -cg89 \rightarrow FFLAGS = -c -O -v### -dumpmachine

MAKE = /bin/make \rightarrow MAKE = make

SHELL = /bin/sh \rightarrow SHELL = /bin/bash
```

Save file and quit editor.

(d) Build serial library libarpack\_MAC.a. Use Terminal commands (without comments):

\$ cd "calculix\_inst\_path"/arpack <return> # Set directory.

Note. The last command generates several warnings which may be ignored.

(e) Remove object files. Use Terminal commands (without comments):

\$ cd calculix\_inst\_path/arpack <return> # Set working directory.

**\$ make clean <return>** # Removes object files.

- (f) Repeat installation of library. If you want to repeat the installation for some reason, first remove object files according to previous step (e).
- *Test installation*. The installation of ARPACK will be tested in Section 8.1 below (solver ARPACK invoked for solution of eigenvalue problems amongst test examples).

# 7. INSTALL AND LAUNCH CCX, TEST INSTALLATION, GETTING STARTED AND TEST EXAMPLES

## 7.1 Install ccx

The source files of ccx as well as the libraries of the external solvers already have been installed in Section 4 and Section 6 for the installation path:

"calculix\_install\_path" (cf. Section 4.2 for details).

In the present section the basic installation of ccx according to Section 1.2 will be completed; i.e. the installation of ccx for multi-threading (MT) together with the additional external solvers SPOOLES (single- and multi-threading) and ARPACK (single threading). The installation first requires some minor modifications of files and finally to build and install ccx. The location of the external solver libraries is already set relative to the build-directory "src" of ccx with path (cf. Fig. 1): "calculix\_install\_path"/CalculiX/ ccx\_2.8/src. Furthermore, the binary "ccx\_2.8" of ccx will be copied to the default search path: /User/ local/bin for executables. Accordingly, no explicit path setting is required for the installlation of ccx.

Installation steps (1) to (4):

(1) *Modify file "calculix.h"*. Location: "calculix\_install\_path"/calculix/ccx\_2.8/ src/calculix.h. Open file with an editor of your choice. Then find line (located close top of file):

#define Linux 1

and insert the following two lines before existing line "#define Linux 1":

/\* mac include pthread\_t.h \*/

#include <pthread.h>

Save file and quit editor.

(2) *Modify file "Makefile"*. Location: "calculix\_install\_path"/calculix/ccx\_2.8/ src/Makefile. Open file with an editor of your choice. Then replace the following existing red code to the left of arrows with new green code to the right of arrows:

```
CFLAGS = -Wall -O3 -I ../.././SPOOLES.2.2 -DARCH="Linux" -DSPOOLES -DARPACK – DMATRIXSTORAGE
```

```
_
```

```
CFLAGS = -Wall -O3 -pthread -I ../../.SPOOLES.2.2 -DARCH="Linux" -DSPOOLES -DARPACK - DMATRIXSTORAGE -DUSE_MT
```

```
CC=cc \rightarrow CC=/usr/local/bin/g++
```

```
LIBS = \

$(DIR)/spooles.a \

../../ARPACK/libarpack_INTEL.a \

-lpthread -lm -lc

→

LIBS = \

$(DIR)/spooles.a \

../../ARPACK/libarpack_MAC.a
```

Save file and quit editor.

(3) *Build and install cgx*. Use below specified Terminal commands (without comments) and replace "calculix\_install\_path" in commands with full path specification according to Section 4.2:

\$ cd "calculix\_install\_path"/calculix/ccx\_2.8/src <return> # Change to directory with # source code and makefile.

\$ make <return> # Build binary "ccx\_2.8" of cxx. Some warnings will appear # which are not relevant for the functionality of ccx.

Command "make" builds the binary "ccx\_2.8" of ccx in directory "src" (cf. also the file system in Fig. 1): "calculix\_install\_path"/calculix/ccx\_2.8/src/ccx\_2.8.

Before re-build of ccx, remove object files with Terminal command: \$ rm \*.o <return> as already specified above.

(4) Install binary of ccx in: /usr/local/bin. First, check if: /usr/local/bin already exists with Terminal command: \$ cd /usr/local/bin <return>. If directory "bin" already exists, then continue with: "Further steps" below. Otherwise, i.e. if the screen message: "No such file or directory" appears, then create: /usr/local/bin now with Terminal command: \$ sudo mkdir /usr/local/bin <return>.

Further steps:

\$ cd "calculix\_install\_path"/calculix/ccx\_2.8/src <return> # Change to directory with # binary of ccx.

\$ sudo cp cgx\_2.8 /usr/local/bin <return> # Copy binary "ccx\_2.8" in /usr/local/bin.

The copy "ccx\_2.8" of the binary of ccx in /usr/local/bin/ccx\_2.8 enables to launch ccx from working directories. You also might change the protection with command: \$ sudo chmod ao+rx /usr/local/bin/ccx\_2.8 <return>.

Alternatively, instead of copying the binary of ccx in: /usr/local/bin as explained above, you may set the path: "calculix\_install\_path"/calculix/ccx\_2.8/src to the binary of "ccx" in your .bash\_profile (cf. Section 3.3 for instructions and examples).

## 7.2 Launch ccx and Test Installation

For the launch and test of the installation of ccx the example: "beamp.inp" will be considered. The input file "beamp.inp" is provided in directory "test": "calculix\_install\_path"/calculix/ccx\_2.8/test/beamp.inp.

Use Terminal commands (without comments):

\$ cd calculix\_inst\_path/calculix/ccx\_2.8/test <return> # Set working directory "test".

\$ ccx\_2.8 beamp <return> # Run ccx with input file "beamp.inp".

The installation basically works, if after the last command the message: "Job finished" is displayed on your screen and if in directory "test" the files "beam.dat" (contains user-directed output) and "beam.frd" (contains plot data for cgx) have been created (cf. also the ccx User's Guide [2] for further explanation of the file types: .inp, .dat and .frd). The tests are continued in Section 8 below.

See the ccx manual [2] and also the subsequent Section 7.3 below how to get started with ccx.

## 7.3 Getting Started With ccx

Consider the html-help files of cxx which are provided by cgx (cf. cgx installation guide [4] for details) and references:

- User's guide [2].

- Tutorial [3]: "Getting Started With CalculiX".

## 7.4 Test Examples

Test examples are provided in the ccx manual [2]. Furthermore, the functionality of ccx will be tested for several test examples in Section 8 below.

# 8. TESTS - TEST EXAMPLES, NUMERICAL ACCURACY AND MULTI-THREADING

## 8.1 Test Examples and Numerical Accuracy

The test examples in directory "test": "calculix\_install\_path"/calculix/ccx\_2.8/test will be considered (cf. also [2], Section 10 for details). For the aforementioned examples the following files are provided in directory "test": (cf. also the ccx manual [2] for the file extensions: .inp, .dat, .frd):

<filename>.inp: input files for ccx.

<filename>.dat.ref: files with reference data for user-directed output.

<filename>.frd.ref: files with reference data for cgx-directed plot data.

If you run one of the test examples, ccx provides the output files: <filename>.dat and <filename>.frd which may be compared with aforementioned reference output files.

In directory "test" the script: "compare" is provided which automatically runs all examples and also automatically compares the computational results with the aforementioned reference data. Run script "compare" with Terminal commands (without comments):

\$ cd "calculix\_inst\_path"/calculix/ccx\_2.8/test # Set working directory test.

\$ ./compare # Run script "compare".

During runtime of "compare" screen output is provided with a brief list of executed examples and general error messages. If for the aforementioned comparison errors exceed prespecified values, then a message is written to file (cf. example below): error.<random number> in directory "test". Accordingly, file error.<random number> is empty, if all errors are within the pre-specified ranges. Otherwise, follow the instructions given in references [1], [2].

For the present installation the execution of "compare" finished with the following three lines of screen output:

check the existence of file error.22856 if this file does not exist, the present results agree with the reference results

and in file error.22856 the following errors are reported:

deviation in file beamptied6.dat line: 14 reference value: 2.339439e+06 value: 2.086567e+06 absolute error: 2.528720e+05 largest value within same block: 3.164432e+06 relative error w.r.t. largest value within same block: 7.991071 %

beamread.dat and beamread.dat.ref do not have the same size !!!!!!!!!!	
deviation in file cubef2f1.frd line: 7502 reference value: 3.947900e+01 value: 3.981660e+01 absolute error: 3.376000e-01 largest value within same block: 3.360410e+02 relative error w.r.t. largest value within same block: 0.100464 %	
deviation in file cubef2f2.frd line: 7468 reference value: -1.882140e+01 value: -3.039420e+06 absolute error: 3.039401e+06 largest value within same block: 3.374260e+02 relative error w.r.t. largest value within same block: 900760.812326 %	
deviation in file segment.frd line: 182049 reference value: 2.110000e+04 value: -2.029550e+04 absolute error: 4.139550e+04 largest value within same block: 1.488060e+05 relative error w.r.t. largest value within same block: 27.818435 %	
deviation in file simplebeampipe3.dat line: 50 reference value: -8.419138e+03 value: -1.496024e+04 absolute error: 6.541102e+03 largest value within same block: 8.748470e+04 relative error w.r.t. largest value within same block: 7.476853 %	

For totally six test examples, therefore, the errors exceed the pre-specified values. The reported errors are currently subject of further investigations.

## 8.2 Invoke and Test Multi-Threading (MT) for Spooles

• *General*. According to Section 2 in the ccx manual [2] several MT-capabilities are available for ccx and external solvers.

According to Section 2 in [2] MT may be invoked with the help of user defined ENVs (environment variables), whereas prior to the execution of ccx one or more ENVs may be set with Terminal command: \$ export ENV=value <return>.

General procedure to invoke MT according to the following steps 1 - 3 (cf. also Section 2 in [2] for details):

(1) If required, set number of available logical cores for MT. The notation "logical cores", respectively "logical CPUs" is explained in subsection: "*Physical Cores and Logical Cores*" below. Use: NUMBER\_OF\_CPUS=ncpu to set number ncpu of logical CPUs which are available for MT.

For the present Mac-installation ccx detects the number ncpu automatically. Accordingly, for the present Mac-version of ccx the ENV: NUMBER\_OF\_CPUS is not required.

- (2) Set optional global switch for MT. The ENV: OMP\_NUM\_THREADS=nthreads invokes all MT-capabilities which are available for ccx and the considered external solvers (cf. Section 2 in [2] for details), whereas the number nthreads sets the number of threads for MT. Additional ENVs may be necessary for fine-tuning of specific MT-capabilities, for example if user subroutines for materials are used (cf. Section 2 in [2] for details).
- (3) Set optional switches for specific MT-capability. For example the ENV: CCX\_NPROC\_EQUATION\_SOLVEROMP\_NUM\_THREADS=nthreads invokes MT for solvers only, whereas the number nthreads sets the number of threads for MT. Further ENVs for specific MT-capabilities are available (cf. Section 2 in [2] for details).

The further explanations are restricted on the above introduced ENVs which may be set to invoke MT for Spooles:

- NUMBER\_OF\_CPUS,
- OMP\_NUM\_THREADS,
- CCX\_NPROC\_EQUATION\_SOLVEROMP\_NUM\_THREADS.

Furthermore, according to steps 1 – 3 above for the present Mac-version of ccx basically the ENV: CCX\_NPROC\_EQUATION\_SOLVEROMP\_NUM\_THREADS is sufficient to invoke MT for solvers, respectively for Spooles.

• *Physical Cores and Logical Cores*. The CPU on your Mac (for OS X) has a certain number of physical cores, respectively physical CPUs. The number of available logical cores (addressable from OS and, therefore, relevant for parallel-processing), however, in general is different from the number of physical cores if hyper-threading is supported. Use Terminal commands (without comments) to display the number of available physical and logical cores:

**\$ sysctl hw.physicalcpu <return>** # Display number of physical cores.

\$ sysctl hw.ncpu <return> # Display number of logical cores.

For the further explanation of MT the number: ncpu of available logical cores is relevant.

- *Default Threading-Mode*. If none of the below specified environment variables is set, single-threading for Spooles (and ccx) is invoked.
- MT for Spooles. For MT (parallel-processing) the max number: nthreads of threads for MT may be set as explained below. The upper bound for nthreads is determined by the number: ncpu of available logical cores: 0 < nthread ≤ ncpu; display ncpu with previously explained Terminal command: \$ sysctl hw.ncpu <return>.

As already outlined in subsection "General" above, MT may be invoked by setting one or more of the following environment variables ENVs:

- *NUMBER\_OF\_CPUS=ncpu*. With the ENV: NUMBER\_OF\_CPUS the number: ncpu of available logical CPUs may be set manually. For the considered installation of ccx on Mac OS X, however, NUMBER\_OF\_CPUS is not required because ccx determines the number of available logical CPUs automatically (cf. also Section 2 in [2]).
- *OMP\_NUM\_THREADS=nthreads*. The ENV: OMP\_NUM\_THREADS invokes MT for both Spooles and ccx. The number: nthreads for max number of threads may be set. MT for ccx may be controlled with further environment variables as explained in Section 2 in [2].
- *CCX\_NPROC\_EQUATION\_SOLVER=nthreads*. The ENV: CCX\_NPROC\_EQUATION\_SOLVER invokes MT for Spooles only. The number: nthreads for max number of threads may be set.
- *OMP\_NUM\_THREADS and CCX\_NPROC\_EQUATION\_SOLVER*. If both of the latter ENVs are set, ENV: CCX\_NPROC\_EQUATION\_SOLVER is relevant for MT. Accordingly, MT will be invoked for Spooles only as already explained above.

If in the above statements the number: nthreads is set larger than the number: ncpu of available logical CPUs, then ccx automatically resets nthreads to ncpu.

MT for Spooles only, therefore, may be invoked by setting the environment variable: CCX\_NPROC\_EQUATION\_SOLVER=nthreads and MT for both Spooles and ccx by setting the variable: OMP\_NUM\_THREADS=nthreads (cf. also example below).

The ENVs may be set with the following Terminal command:

\$ export <name environment variable>=nthreads <return>

with:

- <name environment variable>= OMP\_NUM\_THREADS,
- <name environment variable>= CCX\_NPROC\_EQUATION\_SOLVER,

nthreads: max number of threads for MT.

From Spooles output is provided for the actually used number of threads (which may differ from nthreads) in file spooles.out (cf. example below). For single-threading the file spools.out is empty.

• *Test of MT for ccx and Spooles*. MT for ccx and Spooles will be tested for the test example: "rotor" from directory "test" of ccx, a CPU with ncpu = 4 logical CPUs, OMP\_NUM\_THREADS=10, and, therefore, for nthread = 10 > ncpu=4. As already explained above, the ENV: OMP\_NUM\_THREADS invokes MT for both Spooles and ccx (to invoke MT for Spooles only use ENV: CCX\_NPROC\_EQUATION\_SOLVER).

Run test with Terminal commands (without comments):

\$ cd calculix\_inst\_path/claculix/ccx\_2.8/test <return> # Set working directory test.

\$ export OMP\_NUM\_THREADS=10 <return> # Set environment variable.

\$ ccx\_2.8 rotor <return> # Run example "rotor".

Extract of screen output:

Using up to 4 cpu(s) for spooles.

Using up to 4 cpu(s) for the stress calculation.

According to the screen output above up to 4 CPUs, respectively threads are used for MT of Spooles and ccx. The input nthread=10, therefore, has been reset to nthread=4=ncpu and, therefore, (correct) to the number ncpu=4 of available logical CPUs. Output for the number of threads which Spooles actually has used for MT is provided in file spools.out. For the present example file spools.out contains the output: "Using 4 threads". Spooles, therefore, actually has used 4 threads. The number of threads given in file spools.out may be less than nthreads (according to [1], actually used number of threads set by optimization routines which are implemented in Spooles). Furthermore, the above screen output reveals that ccx used up to 4 threads (CPUs) for the stress calculation. As already mentioned above, MT of ccx may be controlled with further environment variables as explained in Section 2 in [2].

If CCX\_NPROC\_EQUATION\_SOLVER=10 is used for the aforementioned test example, then MT is invoked for Spooles only. For ccx, then single-threading is invoked (Terminal output now: "Using up to 1 cpu(s) for the stress calculation"), whereas MT for Spooles is the same as explained above for the usage of ENV: OMP\_NUM\_THREADS=10.

Tests with various other settings for the above specified environment variables also revealed that MT works.

# 9. HINTS AND MAC-SPECIFIC PROBLEMS

## 9.1 Hints

Provided for later use.

# 9.2 Mac-Specific Problems

Provided for later use.

## REFERENCES

- [1] README.INSTALL. G. Dhondt, February 3, 2015. Short overview of installation of ccx 2.8 for Unix/Linux. Download: <u>http://www.dhondt.de/ccx\_2.8.README.INSTALL</u>.
- [2] CalculiX CrunchiX USERS'S MANUAL version 2.8. G. Dhondt, January 17, 2015. Download of PDF: <u>http://www.dhondt.de/ccx\_2.8.pdf</u>.
- [3] Getting Started With CalculiX. Tutorial. J. Baylor. Download of PDF: http://www.bconverged.com/content/calculix/doc/GettingStarted.pdf
- [4] Installation Guide CalculiX cgx 2.8 Graphical Pre- and Postprocessor on Mac OS X Mavericks. B. Graf, February 10, 2015.