

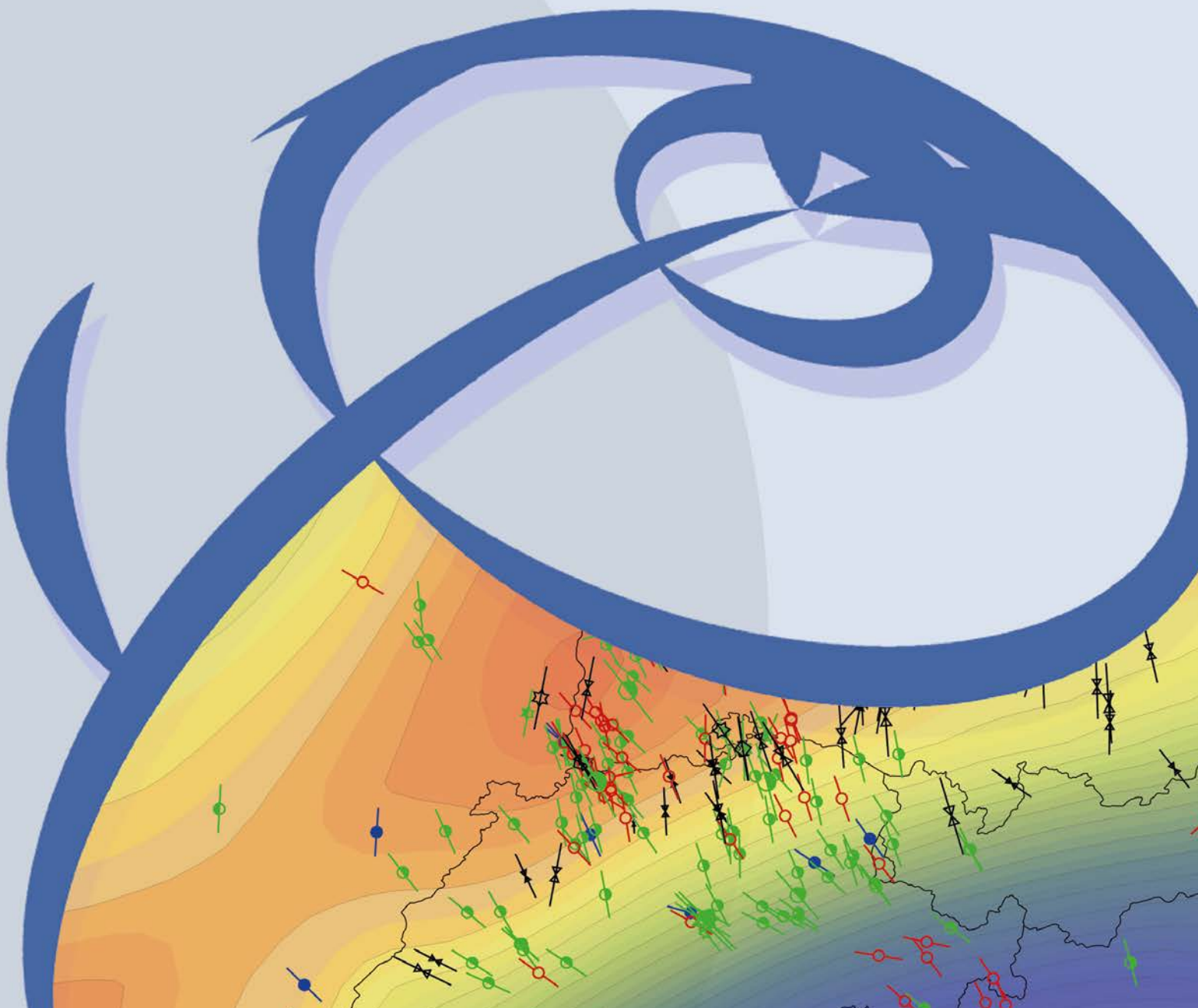


WSM WORLD STRESS MAP

WSM *Technical Report 21-02*

Manual of the Matlab Script FAST Calibration v2.0

Moritz O. Ziegler and Oliver Heidbach



Recommended citation of the report:

Ziegler, M. O. & Heidbach, O. (2021). Manual of the Matlab Script FAST Calibration v2.0. World Stress Map Technical Report 21-02, GFZ German Research Centre for Geosciences.
DOI: <https://doi.org/10.48440/wsm.2021.002>

The software described in this report, including data examples, is published as:

Ziegler, M. O. & Heidbach O. (2021). Matlab Script FAST Calibration v2.0. GFZ Data Services.
DOI: <https://doi.org/10.5880/wsm.2021.002>

The software is available for download on GitHub:

https://github.com/MorZieg/FAST_Calibration

Previous version of the report:

Ziegler, M. O. (2018). Manual of the Matlab Script FAST Calibration v1.0. World Stress Map Technical Report 18-01, GFZ German Research Centre for Geosciences.
DOI: <https://doi.org/10.2312/wsm.2018.003>

Previous versions of the software are published as:

Ziegler, M. O. (2018). Python Script FAST Calibration v1.0. GFZ Data Services.
DOI: <https://doi.org/10.5880/wsm.2018.003>

Imprint

World Stress Map Project
GFZ German Research Centre for Geosciences

Telegrafenberg
D-14473 Potsdam
Published in Potsdam, Germany
March 2021
<https://doi.org/10.48440/wsm.2021.002>



WSM Technical Report 21-02

Manual of the Matlab Script FAST Calibration v2.0

Moritz O. Ziegler and Oliver Heidbach

GFZ German Research Centre for Geosciences, Potsdam, Germany

Table of Contents

List of Tables	II
List of Figures	II
Abstract	1
Changelog v2.0	3
1 Introduction	5
2 Background of geomechanical modelling	6
3 Calibration data	8
3.1 Stress magnitude data	8
3.2 Stress magnitudes derived from assumptions	8
3.2.1 Observed seismicity	9
3.2.2 k-ratio	9
3.3 Quality checking the modelled stress state	10
3.3.1 Formation integrity test	10
3.3.2 Borehole breakouts	11
3.3.3 Drilling induced tensile fractures	12
3.3.4 k-ratio	13
3.3.5 Tectonic stress regime	13
4 Calibration of a model	15
4.1 Preparation	15
4.2 Implementation (FAST_calibration.m)	15
5 Multistage calibration	18
5.1 Conceptual background	18
5.2 Preparation	20
5.3 Implementation (branch_calibration.m)	21
6 Functions	24
6.1 Writing Tecplot 360 EX macro function (write_macro.m)	24
6.2 Difference between observation and model (model_deviation.m)	25
6.3 Estimation of best-fit displacement boundary conditions (calibrate.m)	26
6.4 Solve the calibrated stress state at individual locations (solve.m)	29
6.5 Additional S_{Hmax} calibration data (kratio.m)	30
6.6 Calibrate a critical S_{Hmax} stress state (critical_shmax.m)	30
6.7 Assess the accuracy of the calibrated stress state (accuracy.m)	33
6.8 Calibration point function (nodes2calibrationpoints.m)	34
7 Example	36
7.1 Model calibration	36
7.2 Multi-stage approach	38
Acknowledgements	39
References	40

List of Tables

Tab. 0-1	Structure of the GitHub repository.	1
Tab. 0-2	Content of the folder “calib_functions”.....	2
Tab. 0-3	Structure of the folder “examples”.	2
Tab. 3.3-1	Expected stress state depending on borehole breakouts	11
Tab. 3.3-2	Expected stress state depending on drilling induced tensile fractures	12
Tab. 4.2-1	Required input variables for FAST_calibration.m.....	16
Tab. 5.3-1	Required input variables for branch_calibration.m.....	22
Tab. 6.1-1	Required input variables for the function write_macro.m.	24
Tab. 6.2-1	Required input variables for model_deviation.m.....	26
Tab. 6.3-1	Example for the information required for the generation of the planes.....	26
Tab. 6.3-2	Required input variables for calibrate.m.....	26
Tab. 6.4-1	Required input variables for the function solve.m.	29
Tab. 6.5-1	Required input variables for the function kratio.m.	30
Tab. 6.6-1	Required input variables for the function critical_shmax.m.....	33
Tab. 6.7-1	Required input variables for the function accuracy.m.	33
Tab. 6.8-1	Required input variables for the function nodes2calibpoints.m.....	35
Tab. 7.1-1	Data used for calibration and evaluation.	36
Tab. 7.2-1	Extent and coordinates of the example models.....	38

List of Figures

Fig. 2-1	Map view of a model area (blue box) in a geographical coordinate system.....	6
Fig. 2-2	Basic workflow of the tool FAST Calibration.....	7
Fig. 4.2-1	Schematic chart of the script workflow	17
Fig. 5.1-1	Embedded, nesting and multistage approach.....	18
Fig. 5.1-2	Workflow of the FAST Calibration multistage branch calibration.....	19
Fig. 5.1-3	Distribution of calibration points.	20
Fig. 5.3-1	Schematic chart of the script workflow.	23
Fig. 6.3-1	Best-fit displacement boundary conditions as planes in 3D.	27
Fig. 6.3-2	Best-fit displacement boundary conditions.....	28
Fig. 6.6-1	Horizontal components of the reduced stress tensor and fault strike.....	32
Fig. 6.8-1	Different possibilities for calibration point positioning.....	35

Abstract

The 3D geomechanical-numerical modelling aims at a continuous description of the stress state in a subsurface volume. The model is fitted to the model-independent stress data records by adaptation of the displacement boundary conditions. This process is herein referred to as model calibration. Depending on the amount of available stress data records and the complexity of the model the calibration can be a lengthy process of trial-and-error to estimate the best-fit boundary conditions.

The tool FAST Calibration (Fast Automatic Stress Tensor Calibration) is a Matlab script that facilitates and speeds up this calibration process. By using a linear regression it requires only three test model scenarios with different displacement boundary conditions to calibrate a geomechanical-numerical model on available stress data records. The differences between the modelled and observed stresses are used for the linear regression that allows to compute the displacement boundary conditions required for the best-fit estimation.

The influence of observed stress data records on the best-fit displacement boundary conditions can be weighted. Furthermore, FAST Calibration provides a cross checking of the best-fit estimate against indirect stress information that cannot be used for the calibration process, such as the observation of borehole breakouts or drilling induced fractures.

The script files are provided for download at http://github.com/MorZieg/FAST_Calibration. Tab. 0-1 gives an overview of the folder structure and input files with a short explanation.

Tab. 0-1 Structure of the GitHub repository.

Folders and files in the GitHub repository http://github.com/MorZieg/FAST_Calibration.
Page numbers (if available) direct to the documentation in this manual.

File Name	Explanation	Page
FAST_calibration.m	Matlab script for the calibration of a geomechanical-numerical model on stress data records.	15
branch_calibration.m	Matlab script for the calibration of a geomechanical-numerical model on the stress state from another model.	18
CITATION.bib	The recommended citation for the software.	
LICENSE	The full GPL v3.0 license text.	
README.md	Readme file that contains relevant information on the usage of the software.	
calib_functions/	Folder that contains additionally required functions (Tab. 0-2).	24
Examples/	Folder that contains example files for a calibration and multi-stage approach (Tab. 0-3).	36

Tab. 0-2 Content of the folder “calib_functions”.

Short explanation of the additionally required functions. The page numbers direct to the documentation in this manual.

File Name	Explanation	Page
accuracy.m	Function that tests the validity of the modelled stress state based on k-ratio and regime stress ratio.	33
calibrate.m	This function is the heart of the FAST calibration tool and computes the boundary condition of the best-fit model.	26
critical_shmax.m	Function that computes the S_{Hmax} magnitude derived from the assumption of a critically high magnitude of S_{Hmax} .	30
kratio.m	Function that computes S_{Hmax} from k-ratio assumptions.	30
model_deviation.m	Function that computes the difference between the modelled and observed stress state.	25
nodes2calibrationpoints.m	Matlab function that controls the location of generic calibration points in a branch calibration approach.	34
solve.m	Function that computes the calibrated horizontal stress component from the difference between the modelled and observed stress state and the best-fit boundary conditions.	29
write_macro.m	Matlab function that writes a Tecplot 360 EX macro which extracts the stress state at the location of calibration data from models.	24

Tab. 0-3 Structure of the folder “examples”.

Short explanation of the files provided for an exemplified calibration and multi-stage approach.

File Name	Explanation
root.geom	Geometry of the geomechanical-numerical root model.
root_initial.inp root_initial.odb root_initial.plt	Initial lithostatic stress state for the root model. Abaqus® input file (.inp), output database (.odb), and binary Tecplot file (.plt).
root_test.inp root_test.odb root_test.plt	Three model scenarios with different boundary conditions. Abaqus® input file (.inp), output database (.odb), and binary Tecplot file (.plt).
root_final.inp root_final.odb root_final.plt	Calibrated root model. Abaqus® input file (.inp), output database (.odb), and binary Tecplot file (.plt).
root_nodes.csv	Nodes section from the root_test.geom input file.
branch.geom	Geometry of the geomechanical-numerical branch model.
branch_initial.inp branch_initial.odb branch_initial.plt	Initial lithostatic stress state for the branch model. Abaqus® input file (.inp), output database (.odb), and binary Tecplot file (.plt).
branch_test.inp branch_test.odb branch_test.plt	Three model scenarios with different boundary conditions. Abaqus® input file (.inp), output database (.odb), and binary Tecplot file (.plt).
branch_final.inp branch_final.odb branch_final.plt	Calibrated branch model. Abaqus® input file (.inp), output database (.odb), and binary Tecplot file (.plt).

Changelog v2.0

The following changes have been made in FAST Calibration v2.0 compared to the previous release FAST Calibration v1.0. The manual for v1.0 is available as Ziegler (2018). Both software versions are available on GitHub (Ziegler, 2018a; Ziegler & Heidbach, 2021).

- Additional stress information can now be used for the model calibration and cross checking the quality of the best-fit estimate. This additional information is:
 - Formation Integrity Tests (FITs) as lower boundary for the stress state
 - K-ratio and observed failure of fault planes to calibrate S_{Hmax}
 - K-ratio and Regime Stress ratio to test the quality of the modelled stress state
 - Occurrence of borehole breakouts and drilling induced tensile fractures to check accuracy of the modelled stress state
- To accommodate these new methods parts of the original code have been outsourced to functions, such as *calibrate.m* and *model_deviation.m*
- New functions that are required for the additional methods are: *critical_shmax.m*, *accuracy.m*, *kratio.m*, and *solve.m*.
- The scripts *FAST_calibration.m* and *branch_calibration.m* and the structure of the input variables have been changed in order to work with the new and outsourced functions.
- The function *write_macro.m* has been changed in order to accommodate the altered structure of variables. As a result, the structure and output of the Tecplot 360 EX macro has been changed. Files written by *write_macro.m* function v1.0 cannot be read by FAST Calibration v2.0.
- Due to the amount of changes, a compatibility of v1.0 and v2.0 is not provided. It is recommended to use v2.0 only.
- FAST Calibration v2.0 is compatible with Matlab 2020a, Tecplot 360 EX 2019 R1, the Tecplot Add-on GeoStress v2.0 (Stromeyer et al. 2020), and Abaqus 2019.

1 Introduction

The knowledge of the contemporary stress state in a rock volume is required for many geotechnical and scientific applications such as hydrocarbon and geothermal reservoir management or underground storage of energy or waste (Cornet, 2015; Henk, 2008; Fjaer et al., 2008). However, the available orientation and magnitude data on the stress state is quite sparse and in general not sufficient for a robust assessment of the local stress state (Heidbach et al., 2018; Morawietz et al., 2020). Therefore, geomechanical-numerical modelling is used to predict the 3D stress state in a confined volume. Such a modelling approach is based on the knowledge of the subsurface structure (geological layers, faults), rock density distribution and the elastic rock properties (e.g. Reiter & Heidbach, 2014; Hergert et al., 2015).

Besides the volume forces due to gravity, the surface forces due to plate tectonics are introduced by Dirichlet displacement boundary conditions which are altered until the observed stress data at discrete points are fitted. Herein, this fitting process is referred to as model calibration. Once the displacement boundary conditions are found with which the model is best fitted to the stress data records the model is calibrated.

FAST Calibration (Fast Automatic Stress Tensor Calibration) is a Matlab tool that controls the statistical calibration of a 3D geomechanical-numerical model of the stress state following the approach described by Reiter and Heidbach (2014), Hergert et al. (2015), Ziegler et al. (2016), and Ziegler & Heidbach (2020). Mainly it is used for the calibration of a single geomechanical-numerical model. However, it also supports the multi-stage modelling procedure presented by Ziegler et al. (2016), see Section 5. The tool runs in Matlab 2020a and higher and is meant to work with the visualization software Tecplot 360 EX 2019 R1 and higher in conjunction with the Tecplot 360 Add-on GeoStress v2.0 (Heidbach et al., 2020). The user should be familiar with 3D geomechanical-numerical modelling, Matlab, Tecplot 360 EX, including a basic knowledge of Tecplot 360 EX macro functions, and the Tecplot 360 EX Add-on GeoStress v2.0 provided by Heidbach et al. (2020). This FAST Calibration manual provides an overview of the scripts and is designed to help the user to adapt the scripts for their own needs.

FAST Calibrations main script *FAST_calibration.m* controls the calibration of 3D geomechanical-numerical models that use the Finite Element method. In addition, it provides the possibility for first order cross checking of the modelled stress state against other stress information that cannot be used for the calibration process, such as formation integrity tests, borehole breakout or the occurrence of seismicity. FAST Calibration evaluates if the model results are in agreement with these observations. The additional script (*branch_calibration.m*) is only required if a multistage-modelling approach is used. It controls the calibration of 3D geomechanical-numerical models using the stress state retrieved from a larger stress model following the multi-stage procedure described by Ziegler et al. (2016).

This manual contains basic technical information on 3D geomechanical-numerical modelling (Section 2). The required and optional input data and the syntax are presented in Section 3. It also includes the underlying concepts of the first order sanity-checks and quality assessment. The execution of the script *FAST_calibration.m* is explained in detail in Section 4. This is followed by a theoretical treatment of the multistage procedure and a detailed explanation of the execution of the *branch_calibration.m* script (Section 5). Section 6 provides information on the individual Matlab functions that come with FAST Calibration. This is mainly dedicated to advanced users. Eventually, two examples are provided in Section 7 – a basic geomechanical-numerical model calibration and an example for the application of the multistage approach.

2 Background of geomechanical modelling

3D geomechanical-numerical modelling requires a static geological model that describes the geometry of the geologic units and faults, the density distribution and the elastic rock properties. For the calibration process stress data records are needed at individual points within the model volume. To solve the partial differential equation of the equilibrium of forces the model volume is discretized into finite elements. The discretized geometry is populated with rock properties, i.e. the density, Young's module, and Poisson ratio. Fitting the magnitude of the vertical stress S_V is easy as the density distribution is relatively well known. In contrast fitting the magnitudes of maximum and minimum horizontal stress, S_{Hmax} and S_{Hmin} respectively, is challenging as stress data of these two components is sparse (we assume here for simplicity that S_V and thus S_{Hmax} and S_{Hmin} are principal stresses). Information on the orientation of the stress tensor by means of the orientation of S_{Hmax} is provided by the World Stress Map (WSM) database (Heidbach et al., 2016). However, stress orientations are helpful for the model calibration any differential displacement boundary condition will lead to an instantaneous adjustment of the stress tensor orientation parallel and perpendicular to the model boundary regardless the amount of displacement. In contrast, information on the magnitudes of principal horizontal stresses is generally sparse and incomplete (Morawietz et al., 2020).

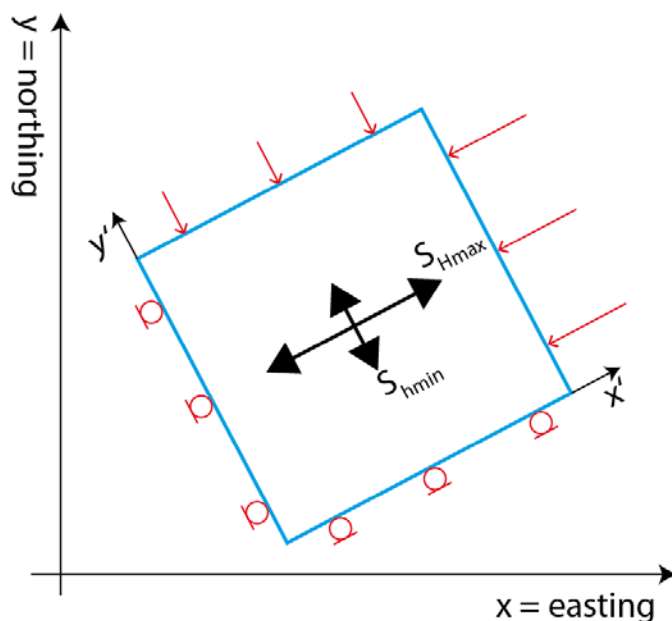


Fig. 2-1 Map view of a model area (blue box) in a geographical coordinate system.

The boundary conditions (red) are applied in a rotated coordinate system (x' and y') parallel to the model boundaries which are oriented parallel to the prevailing orientations of the principal horizontal stress axes. Information on the orientation is available from data of the World Stress Map database (Heidbach et al., 2016). The application of even small displacement boundary conditions (Dirichlet type) perpendicular to the model boundaries are usually sufficient to achieve a good fit of the overall stress orientation.

To calibrate the geomechanical-numerical model information on the S_{Hmax} and S_{Hmin} magnitudes is essential. The model calibration is achieved by a comparison of the modelled stress to the observed S_{Hmax} and S_{Hmin} magnitudes in dependence of the Dirichlet displacement boundary condition (Fig. 2-1). Their values are altered until a good fit of the modelled stress

state to the observed stress information at the calibration points is achieved. Thus, the models calibration depends on only two displacements which facilitates the calibration process as the best-fit boundary conditions can be found by a system of linear equations. The automated setup and solving of this linear equation system is the core of the FAST-Calibration tool. Note that two implicit assumption are that 1) the rheology is linear elastic and 2) that the stress state is controlled by a lateral displacement that is not changing with depth

The calibration procedure is illustrated in Fig. 2-2. Three different test model scenarios with different arbitrary, but reasonable displacement boundary conditions are solved (Fig. 2-2a). At several locations within the model volume stress data records are available (Fig. 2-2b). For each test model scenarios the modelled stress state is compared with these stress data records. Each comparison provides a mean deviation for S_{Hmax} and S_{Hmin} , respectively (Fig. 2-2c). A system of linear equations is set up in the domain of the displacement boundary conditions (x and y) and the deviations of observed and modelled data (z) (Fig. 2-2d). For the smallest deviation of each, S_{Hmax} or S_{Hmin} , an infinite number of corresponding displacement boundary conditions exist. However, only one set satisfies both the requirements for the smallest deviation in observed and modelled S_{Hmax} and S_{Hmin} (see Section 6.3). This set of displacement boundary conditions is applied to compute the best-fit model (see Ziegler et al., 2016).

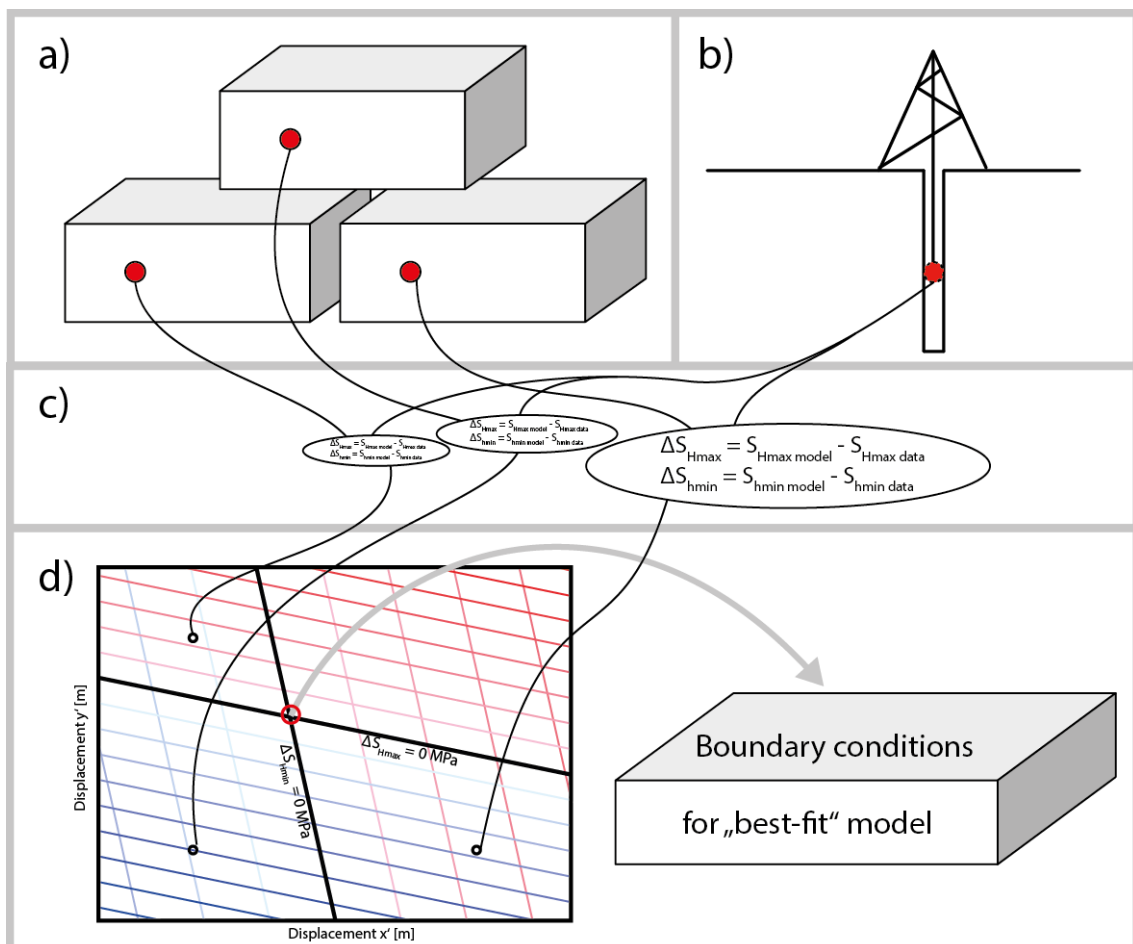


Fig. 2-2 Basic workflow of the tool FAST Calibration.

The stress state from three test model scenarios with arbitrary displacement boundary conditions (a) and observed stress data records (b) are compared (c). A set of linear equations is set up that provide the best-fit boundary conditions (d).

3 Calibration data

There are different types of stress data that can be used in FAST Calibration and they are classified in three groups. The first group contains direct estimates of the S_{Hmax} and S_{Hmin} magnitudes that result e.g. from mini-hydro-fracs, hydro-fracs on pre-existing faults, sleeve fracturing or overcoring methods (e.g. Amadei and Stephansson, 1997; Cornet and Burel, 1992; Morawietz et al., 2020). Details are given in section 3.1. The second group of stress information contains stress magnitudes that are determined using specific assumptions. The two types of information used here are using (1) the slip tendency formulation (Morris et al., 1996) when seismicity is observed or (2) assumptions on the k-ratio which is the ratio of the mean horizontal stress and S_V as a function of depth (see section 3.2). To use the tool FAST Calibration at least one data record of the S_{Hmax} and S_{Hmin} magnitude is needed from the first or second group.

The third group contains upper or lower limits of the S_{Hmax} and S_{Hmin} magnitudes e.g. derived from the occurrence of borehole breakouts, drilling induced tensile fractures or the results from formation integrity tests (see section 3.3). Even though this additional information cannot be used to calibrate the model, their agreement or disagreement with the modelled stress can be used as a quality check of the model. When running FAST Calibration results of this cross check are printed to the screen.

3.1 Stress magnitude data

At least one S_{Hmax} and S_{Hmin} magnitude data record are required for a successful calibration. S_{Hmax} may also be calibrated using only assumption based magnitudes, e.g. k-ratio or observed seismicity. Ideally, several data records of both stress components S_{Hmax} and S_{Hmin} are available throughout the model in different lithologies. S_{Hmin} magnitude data records usually originate from hydro-fracs, mini-fracs, or leak-off-tests (Morawietz et al., 2020). S_{Hmax} magnitude data records are very rare and may be derived according to the frictional limit (Jaeger & Cook, 1969, Zoback et al., 2003) or from sophisticated overcoring measurement campaigns (Cornet, 2015).

Each data record consists of a location defined in the model coordinate system (x, y, z), a magnitude (in MPa), and is assigned a confidence between 0 (low) and 1 (high). The syntax for a leak-off test (low confidence) and a hydro-frac (high confidence) used for S_{Hmin} calibration is presented in the following as an example.

```
stress_data = {  
  
  "shmin"...  
  [5050 -3500 -800 12.7 0.5;  
   5100 -3450 -2745 41.9 1.0];  
};
```

3.2 Stress magnitudes derived from assumptions

S_{Hmax} magnitudes are often not available and if they are they are subject to large uncertainties. Often assumptions are made to derive the magnitude of S_{Hmax} . Since these assumptions are also dependent on the other stress components, the manual usage within the FAST Calibration workflow would be cumbersome. Thus, FAST Calibration includes the automatized usage of two possible approaches to calibrate S_{Hmax} based on assumptions.

3.2.1 Observed seismicity

Even though seismic events do not provide any data records on S_{Hmax} already their mere occurrence provides the information that the stress state was critical and the rock failed. Therefore, a critically high value for S_{Hmax} i.e. an S_{Hmax} magnitude that brings a certain fault or fault population to fail is assumed. FAST Calibration v2.0 uses this critically high S_{Hmax} as a way to estimate and calibrate S_{Hmax} .

In order to estimate the criticality of the fault slip tendency (Morris et al., 1996) is employed as

$$ST = \frac{\tau - C}{\sigma_n} \mu^{-1}$$

with the fault orientation specific shear stress τ and normal stress σ_n , the cohesion C , and the friction coefficient μ . If slip tendency is smaller than 1 the fault is stable. Failure occurs at values larger than 1. A critically high value for S_{Hmax} is defined by $ST = 1$. With the assumption of known and calibrated S_{hmin} and S_v as well as known fault parameters the only unknown in the equation for slip tendency is the magnitude of S_{Hmax} . Transformation of the equation allows computing the value of S_{Hmax} at a given location that is required for a failure (Section 6.6).

The fault properties and orientation are often only estimates with a certain variability. In order to accommodate this, FAST Calibration tests the fault orientations and properties within a user-defined range of uncertainties. The minimum magnitude of S_{Hmax} estimated from the provided range of parameters that leads to failure is used to calibrate the model, i.e. the most optimally oriented fault in this stress state is chosen. The user needs to be aware that this calibration method for S_{Hmax} is a first order approximation and should only be used as such.

The syntax for the critical S_{Hmax} calibration approach consists of a location defined in the model coordinate system (x, y, z), the strike and dip of the (assumed) fault plane in degree, the cohesion (in MPa), and the coefficient of friction. It is followed by the variability of the four values. If no variability is known or should be regarded, zeros are appended instead.

```
stress_data = {  
  "critical_shmax"...  
  [5000 4000 -3000 310 30 10 0.6 10 7 2 0.1;  
   5000 4000 -3000 120 10 5 0.6 0 0 0 0;  
   5000 4000 -3000 90 60 10 0.6 8 7 0 0]  
};
```

3.2.2 k-ratio

The k-ratio is a depth and material dependent relation coefficient between the vertical and two horizontal stress magnitudes. It is defined as

$$k = \frac{S_{Hmax} + S_{hmin}}{2 S_v}$$

and takes values between 3-4 at the surface to usually around 1 in greater depth (Reiter & Heidbach, 2014). There are a number of publications that derive k-ratio as a function of depth based on stress magnitude data (McCutchen, 1982; Brown and Hoek, 1978) or semi-analytical

models (Sheorey, 1994). These assumptions on the k-ratio can be used by FAST Calibration in order to calibrate S_{Hmax} . Therefore, S_{hmin} and S_v (indeed the density as the driver for the overburden) need to be sufficiently well known. If these two stress components are assumed to be represented in the model with enough certainty, the S_{Hmax} magnitude at a location is computed by

$$S_{Hmax} = 2 k S_v - S_{hmin}$$

and can then be used for calibration.

The syntax for the k-ratio calibration approach consists of a location defined in the model coordinate system (x, y, z), the k-ratio, and a confidence between 0 (low) and 1 (high).

```
stress_data = {
    "k_shmax"...
    [4000 4000 -800 1.1 1.0;
     800 2000 -4500 0.9 0.4];
};
```

3.3 Quality checking the modelled stress state

A range of observables exist which do not provide any direct information on the stress magnitudes. These observables cannot be used for calibration of the stress state. But their agreement with a modelled stress state supports the estimated boundary conditions. If such data is available, FAST Calibration provides the user a feedback on the quality of the modelled stress state via messages printed to the screen. However, the evaluation of these observables resort to the estimation of the stress state from within Matlab based only on the test model scenarios (see function *solve.m* in Section 6.4). Thus the evaluation of observables from within FAST Calibration should be limited to a first order assessment. In the following the implemented methods are presented.

3.3.1 Formation integrity test

A common test carried out in boreholes during drilling operations is the so called formation integrity test (FIT). For an FIT a section of the well is isolated and the (drill) fluid pressure within this part of the well is increased up to a certain pre-defined level. If fluid is lost into the formation a so called leak-off occurred. Then, the recorded pressure can be even used for calibration under certain assumptions. However, if no fluid is lost into the formation the test is successful. Since no fracturing occurred, the fluid pressure was lower than the least principal stress component S_3 , (i.e. S_{hmin} or S_v assuming that the S_v is a principal stress depending on the tectonic stress regime; White et al., 2002). Hence, an FIT provides a lower boundary for the S_3 magnitude. FAST Calibration checks if the modelled stress state is in agreement with the observed FIT magnitude or not. If the modelled stress is lower than the FIT value, FAST Calibration reports this disagreement.

The syntax for FITs or lower boundaries of S_3 in general consists of a location defined in the model coordinate system (x, y, z), the lower boundary magnitude (in MPa), and a confidence between 0 (low) and 1 (high). The standard output provides only the percentage of FITs that are in disagreement with the modelled stress state. The confidence level for the FIT is used as

a weight. If “_detail” is appended to the data type description, a more detailed output that contains information on each defined location is printed to the screen.

```
stress_data = {
  "fit_detail"...
  [5000 7000 -3100 55.0 0.6;
   2000 2000 -800 8.1 1];
};
```

3.3.2 Borehole breakouts

Borehole breakouts (BOs) occur when the maximum circumferential stress $\sigma_{\phi\phi}^{max}$ exceeds the compressive strength of the rock. The borehole wall spalls off at two opposite sections indicating the orientation of S_{hmin} (Bell and Gough, 1979). Neglecting temperature, chemical and poroelastic effects (Amadei and Stephansson, 1997; Schmitt et al., 2012) the Kirsch equations (Kirsch, 1898) can be used to compute $\sigma_{\phi\phi}^{max}$ as

$$\sigma_{\phi\phi}^{max} = 3 S_{Hmax} - S_{hmin} - \Delta P$$

with ΔP as the difference between the formation fluid pressure and the fluid pressure in the borehole (Amadei and Stephansson, 1997). Thus, if borehole breakouts occur (or not) this expression also provides a lower (upper) boundary of the stress magnitudes. If $\sigma_{\phi\phi}^{max}$ is larger than the compressive strength C_0 of the rock BOs form if

$$\sigma_{\phi\phi}^{max} > C_0 - \Delta P$$

This is used in FAST Calibration to test if the modelled stress state is in agreement with the occurrence of BOs or not. Their locations and depths or intact sections of the borehole wall are included in the input data. The compressive strength of the rock (with subtracted ΔP value if applicable) is appended. Then FAST Calibration evaluates whether BOs would occur in the modelled stress state or not. This information is then compared with the observations by the user (Tab. 3.3-1). Note that FAST Calibration only evaluates points in the borehole. If a continuous section of long BOs is to be evaluated multiple instances of BOs or intact borehole sections should be included, e.g. in a spacing of 1 metre.

Tab. 3.3-1 Expected stress state depending on borehole breakouts

Matrix indicates if the modelled stress state is in agreement (green) or disagreement (red) to the observed occurrence of borehole breakouts or the intact borehole.

	$\sigma_{\phi\phi}^{max} > C_0$	$\sigma_{\phi\phi}^{max} < C_0$
Observed borehole breakouts		
No observed borehole breakouts		

The syntax for initiation varies depending whether BOs are observed (bbo) or the borehole wall is intact (nbo). The standard output provides only the number of locations that are in agreement with the modelled stress state and the observations of BOs or intact borehole

walls. If “_detail” is appended to the data type description, a more detailed output that contains information on each defined location is printed to the screen.

The syntax for the evaluation of BOs occurrence consists of a location defined in the model coordinate system (x, y, z) and the compressive strength of the rock.

```
stress_data = {
  "bbo_detail"...
  [3000 3000 -430 20];

  "nbo"...
  [3000 3000 -750 40];
};
```

3.3.3 Drilling induced tensile fractures

Drilling induced tensile fractures (DITFs) occur when the minimum circumferential stress $\sigma_{\phi\phi}^{min}$ around a borehole wall is smaller than the tensile strength of the rock formation. Small vertical (A-type) or en-echelon (E-type) fractures appear that indicate the orientation of S_{Hmax} (Aadnoy, 1990). Comparable to the computation of the maximum circumferential stress required for breakouts the $\sigma_{\phi\phi}^{max}$ can be computed as

$$\sigma_{\phi\phi}^{min} = 3 S_{hmin} - S_{Hmax} - \Delta P$$

If $\sigma_{\phi\phi}^{min}$ is smaller than the tensile strength T_0 of the rock DITFs form if

$$\sigma_{\phi\phi}^{min} < T_0 - \Delta P$$

This is used in FAST Calibration to test if the modelled stress state is agreement with the observation of DITFs or not. Their locations and depths of intact sections of the borehole wall are included in the input data. The tensile strength of the rock (with subtracted ΔP value if applicable) is appended. Then, FAST Calibration evaluates whether DITFs can occur or not. The user compares this to the actual observations and can thereby assess the quality of the modelled stress state (Tab. 3.3-2). Note that FAST Calibration only evaluates points in the borehole. If a continuous section of long DITFs is to be evaluated multiple instances of DITFs or intact borehole sections should be included, e.g. in a spacing of 1 metre.

Tab. 3.3-2 Expected stress state depending on drilling induced tensile fractures

Matrix that indicates if the modelled stress state is in agreement (green) or in contradiction (red) to the observed occurrence of drilling induced tensile fractures or the intact borehole.

	$\sigma_{\phi\phi}^{min} > T_0$	$\sigma_{\phi\phi}^{min} < T_0$
Observed DITF		
No observed DITF		

The syntax for initiation varies depending on whether DITFs are observed (dif) or the borehole wall is intact (nif). The standard output provides only the number of locations that are in agreement with the occurrence of DITFs or intact sections. If “_detail” is appended to the data type description, a more detailed output that contains information on each defined location is printed to the screen.

The syntax for the DITFs consists of a location defined in the model coordinate system (x, y, z) and the tensile strength of the rock.

```
stress_data = {
  "dif"...
  [5000 6500 -800 24];

  "nif_detail"...
  [5000 6500 -1500 30];
};
```

3.3.4 k-ratio

Previously, the k-ratio was introduced as a way to estimate the S_{Hmax} magnitude. Alternatively, the k-ratio is used as a very rough tool to assess accuracy of the models calibration. Therefore, the modelled k-ratio is compared against the expected values. A mean value of deviation of the expected from the modelled k-ratios and a standard deviation is provided. The confidence is used as a weight. The standard output prints information on the general agreement only. If “_detail” is appended to the data type description, a more detailed output that contains information on each defined location is printed to the screen.

The syntax for the k-ratio consists of a location defined in the model coordinate system (x, y, z), the k-ratio, and a confidence between 0 (low) and 1 (high).

```
stress_data = {
  "k-ratio"...
  [4000 4000 -800 1.1 1.0;
   800 2000 -4500 0.9 0.4];
};
```

3.3.5 Tectonic stress regime

Observed seismic events for which a focal mechanism solution is available provide information on the type of failure, i.e. whether the seismic event had a normal, strike slip or thrust faulting mechanism. Simpson (1997) uses these three faulting regimes to derive a continuous scale for the Regime Stress Ratio (RSR). The RSR takes on values between 0 and 3. 0.5 being normal faulting ($S_v > S_{Hmax} > S_{hmin}$), 1.5 strike slip ($S_{Hmax} > S_v > S_{hmin}$), and 2.5 thrust faulting ($S_{Hmax} > S_{hmin} > S_v$). Expectations of the tectonic stress regime are formulated as a RSR value at a certain depth and location. According to Simpson (1997) the RSR is computed as

$$RSR = (n + 0.5) + (-1)^n(SR - 0.5)$$

with the stress ratio

$$SR = \frac{(S2 - S3)}{(S1 - S3)}$$

and

$$n = \begin{cases} n = 1 & \text{if } S_{hmin} \leq S_v \leq S_{Hmax} \\ n = 2 & \text{if } S_v \leq S_{hmin} \leq S_{Hmax} \\ n = 0 & \text{otherwise} \end{cases}$$

In FAST Calibration this value is compared against the modelled stress state. A combined mean deviation between the modelled and observed RSR value from all locations and the corresponding standard deviation is provided. If “_detail” is appended to the data type description, a more detailed output that contains information on each defined location is printed to the screen. This information can then be used to assess the validity and quality of the modelled stress state. The syntax for the RSR evaluation consists of a location defined in the model coordinate system (x, y, z), the RSR value, and a confidence between 0 (low) and 1 (high).

```
stress_data = {
  "rsr_detail"...
  [2500 2000 -3000 0.8 1.0;
   4500 4000 -800 1 0.9];
};
```

4 Calibration of a model

4.1 Preparation

FAST Calibration can be downloaded from http://github.com/MorZieg/FAST_Calibration. The following preparations are required in order to successfully use the FAST Calibration tool.

1. Create a directory with the following files and subfolders:
 - *FAST_calibration.m*
 - empty subfolder *data*
 - subfolder *calib_functions* containing the following files:
 - *accuracy.m*
 - *calibrate.m*
 - *critical_shmax.m*
 - *kratio.m*
 - *model_deviation.m*
 - *solve.m*
 - *write_macro.m*
2. At least one data record for each the S_{Hmax} and S_{Hmin} magnitude is required. The data records are assigned in the variable *stress_data* in the file *FAST_calibration.m*.
3. Three test model scenarios with arbitrary but different displacement boundary conditions are required. These test model scenarios should be loaded in Tecplot 360 EX and at least S_{Hmax} , S_{Hmin} , S_v , and the azimuth of S_{Hmax} need to be computed. This is most easily done by the Tecplot 360 EX Add-on GeoStress (Heidbach et al., 2020). If these variables are derived by another tool it is imperative that they are named “SHmax”, “Shmin”, “Sv”, and “SHazi” (not case sensitive).

4.2 Implementation (FAST_calibration.m)

The calibration of a model on horizontal stress magnitude information is conducted with help of the script *FAST_calibration.m*. A schematic overview of the procedure is provided in Fig. 4.2-1. The script is divided into two parts. In the first part the calibration data records and additional information are defined in variables. At least one S_{Hmin} and one S_{Hmax} magnitude is required and additional observables may be defined. If no S_{Hmax} magnitude information is available, alternatively a critically stressed crust assumption or an assumption on the k-ratio can be used to calibrate S_{Hmax} . Tab. 4.2-1 lists the required input. In the provided script file, exemplified variables are defined that can be used for the calibration of the example files (Section 7.1).

Once the variables are defined the first section of the script can be run. A Tecplot 360 EX macro file of the specified name is created and written to the current working directory of Matlab (it is encouraged to use the folder specified in the variable *folder*). The macro exports the modelled stress tensor at each location of a calibration data record for each of the three test model scenarios. Therefore, load the geomechanical model with displacement boundary conditions, derive S_{Hmax} , S_{Hmin} , S_v , and the azimuth of S_{Hmax} with GeoStress, and execute the macro in Tecplot 360 EX. The variables are now written to a data file in the subfolder *data* that is accessible for Matlab. Now proceed to the second part of the script.

Tab. 4.2-1 Required input variables for FAST_calibration.m.

Examples are provided in the script file.

Variable	Description
folder	Provide the directions to the folder in your system which contains the script data. It is important to include the full path since this information is not required for Matlab (which supports relative paths) but for Tecplot 360 EX (which does <i>not</i> support relative paths).
name	Provide a name for the macro file and data files the macro will create. Note that if such a file already exists it will be overwritten by Matlab.
x	Enter the displacements in x' (S_{hmin} or S_{Hmax}) direction that are prescribed at the three different test model scenarios. Make sure to assign the values in the correct order.
y	Enter the displacements in y' (S_{Hmax} or S_{hmin}) direction that are prescribed at the three different test model scenarios. Make sure to assign the values in the correct order.
stress_data	<p>$N \times 2$ cell variable. In the first column define the types and order of stress indicators defined in stress_data. The following keywords are allowed for definition of stress magnitudes:</p> <ul style="list-style-type: none"> shmax: An S_{Hmax} magnitude data record. shmin: An S_{hmin} magnitude data record. k_shmax: The k-ratio used as a method to estimate S_{Hmax}. seism_shmax: The assumption of a critically high S_{Hmax} magnitude in order to estimate S_{Hmax}. <p>Additional stress information to test the accuracy of the modelled stress state:</p> <ul style="list-style-type: none"> fit: Formation integrity test or another type of lower boundary for the least principal stress. rsr: Regime stress ratio as an indication for the accuracy of the stress state. k-ratio: The k-ratio used as an indication for the accuracy of the stress state. bbo: Observed BOs as a test for accuracy of the modelled stress state. nbo: Intact borehole walls (no BOs) as a test for the accuracy of the modelled stress state. dif: Observed DITFs as test for the accuracy of the modelled stress state. nif: Intact borehole walls (no DITFs) as a test for the accuracy of the modelled stress state. <p>The second column defines the x, y, and z coordinates of data records for calibration. Then, the data values such as the magnitude (in MPa) and if applicable the confidence between 0 (low) and 1 (high) is specified. Please make sure that the coordinate system is the same as in the model. Note that z is not the True Vertical Depth (TVD) but the actual z-coordinate from the models coordinate system. In case of a critical S_{Hmax} calibration following the coordinates are the strike, dip, cohesion, and friction coefficient.</p>

The second part of the script reads the data that was exported from Tecplot 360 EX. In the function *model_deviation.m* the modelled S_{hmin} and (if available) S_{Hmax} data is compared to the actual stress data records. This allows the calibration of S_{hmin} and (if available) S_{Hmax} .

The alternative calibration methods for S_{Hmax} (critical stress/slip tendency or k-ratio) and the quality checks require information on the expected magnitudes of S_{hmin} and S_v at the calibration points. However, at these locations only the stress state computed from the arbitrary displacement boundary condition for the three test model scenarios are available. The magnitude of S_v does not change in between these model scenarios since it is defined by the overburden and can be extracted from either one of the arbitrary scenarios. The

magnitude of S_{hmin} , however, depends on the displacement boundary conditions and thus cannot be extracted directly from the test model scenarios. It is estimated by the function *solve.m*.

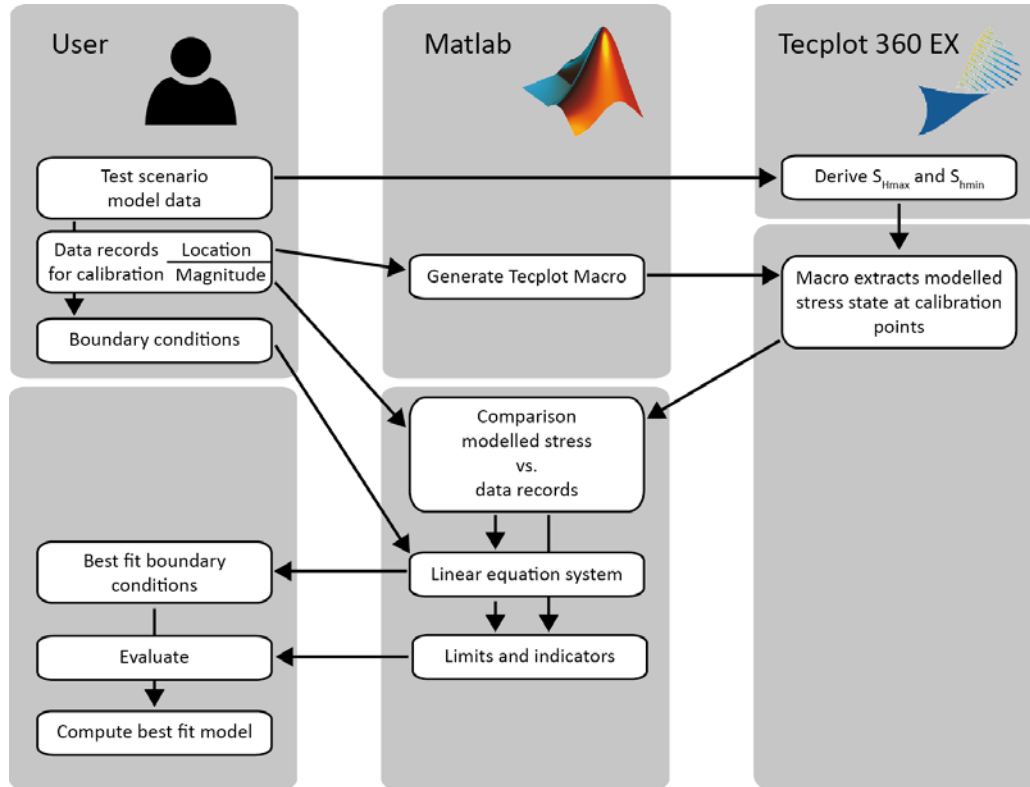


Fig. 4.2-1 Schematic chart of the script workflow

Workflow of the calibration of a model on stress data records in two steps.

The different methods of S_{Hmax} calibration are considered and the according functions are called. An S_{Hmax} calibration according to critical S_{Hmax} necessarily has to be the only mean of S_{Hmax} calibration. No other calibration points for S_{Hmax} are allowed then and are thus disregarded. In contrast, the k-ratio method can be used together with magnitude calibration data records and each data point can be weighted accordingly. These additional calibrations of S_{Hmax} are under the assumption of a well calibrated S_{hmin} and S_v magnitude.

Afterwards, a check of the stress state is performed to assess the quality of the model calibration. The additional indirect stress information may be data on the regime stress ratio, the k-ratio or the occurrence intervals of borehole breakouts or drilling induced tensile fractures as well as intact sections of the borehole wall. Furthermore, formation integrity tests serve as a lower boundary for the least principal stress component. The additional indirect stress information are evaluated in the function *accuracy.m*. The results are printed to the screen.

Eventually, the best-fit boundary conditions are computed by the function *calibrate.m* and printed to the screen. The best-fit displacement boundary conditions are then included by the user in the (Abaqus®) solver deck and the best-fit stress state can be computed.

5 Multistage calibration

Please note that this section is only relevant for the application of a multistage-modelling approach as described in Ziegler et al. (2016).

5.1 Conceptual background

A typical problem that occurs during geomechanical reservoir modelling is that stress magnitude data are not available within the model volume which prevents a meaningful calibration. To overcome this problem Ziegler et al. (2016) presented a multi-stage approach that uses two differently sized models. A large scale model called *root model* has a low resolution but within its volume stress data records for calibration are available. A small-scale, high resolution model, called *branch model* is geographically located within the root model volume and uses the modelled stress state from the root model for its calibration despite the lack of actual stress data within the branch models volume. Fig. 5.1-1c displays the consecutive steps of this multi-stage approach which is beneficiary in terms of the simplified mesh generation and faster computation time in comparison to approaches that use embedding (Fig. 5.1-1a) or nesting (Fig. 5.1-1b). Furthermore, the multi-stage approach allows to use the root model stress state to be used for several small scale reservoir models within its volume (Fig. 5.1-1c).

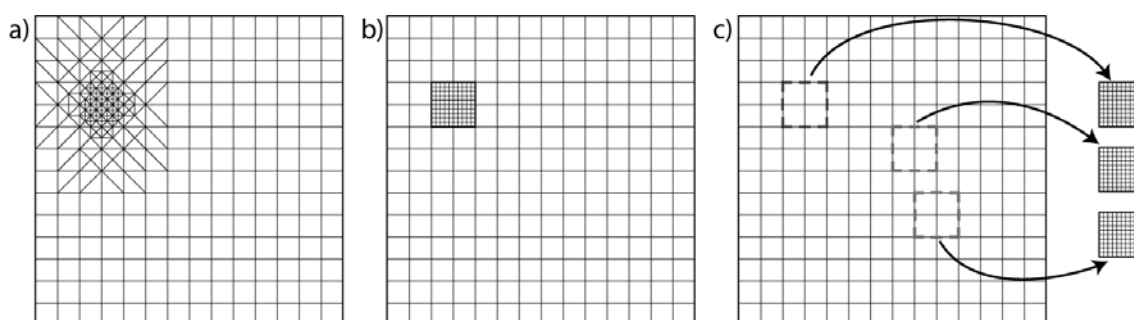


Fig. 5.1-1 Embedded, nesting and multistage approach.

Different approaches to cope with a large scale model area with only a small area with a high resolution. a) A gradient in element size. b) A nested modelling approach. c) The multi-stage approach that uses two or more models (Ziegler et al. 2016).

The concept of model calibration is the same, whether a large-scale root model is calibrated or a small-scale branch model. The only difference is that a root model is calibrated on “real” stress data records while a branch model is calibrated on synthetic stress data records provided by the larger root model.

Three branch model scenarios with arbitrary but reasonable Dirichlet displacement boundary conditions are computed (Fig. 5.1-2a). At defined locations within the best-fit root model which also lie within the branch models extent the modelled stress state is collected (Fig. 5.1-2b). These synthetic stress data records need to be chosen with care (Ziegler et al, 2016). It is important to (1) only choose calibration points which are nodes in the model that provides the reference calibration points. Otherwise the interpolation of the visualization software from nodes into the volume may result in erroneous deviations. (2) The points used for calibration should be located at the border of the branch model. Otherwise the stress field from the larger and less detailed root model is imposed everywhere in the branch model. Thereby no stress

variations due to features that are only present in the branch model would be allowed (Fig. 5.1-3). Suitable calibration points that adhere to these two rules are provided via subroutine *nodes2calibrationpoints.m* (for details see the corresponding section on the function). In addition, a third restriction concerns the material properties. Due to the modelling approach that uses displacement Dirichlet boundary conditions it is imperative that the synthetic data records locations in both models are in volumes characterized by the same material properties. The adherence of this rule needs to be enforced by the user, e.g. by using the root model geometry and rock materials at the boundaries of the branch model where synthetic data records are collected.

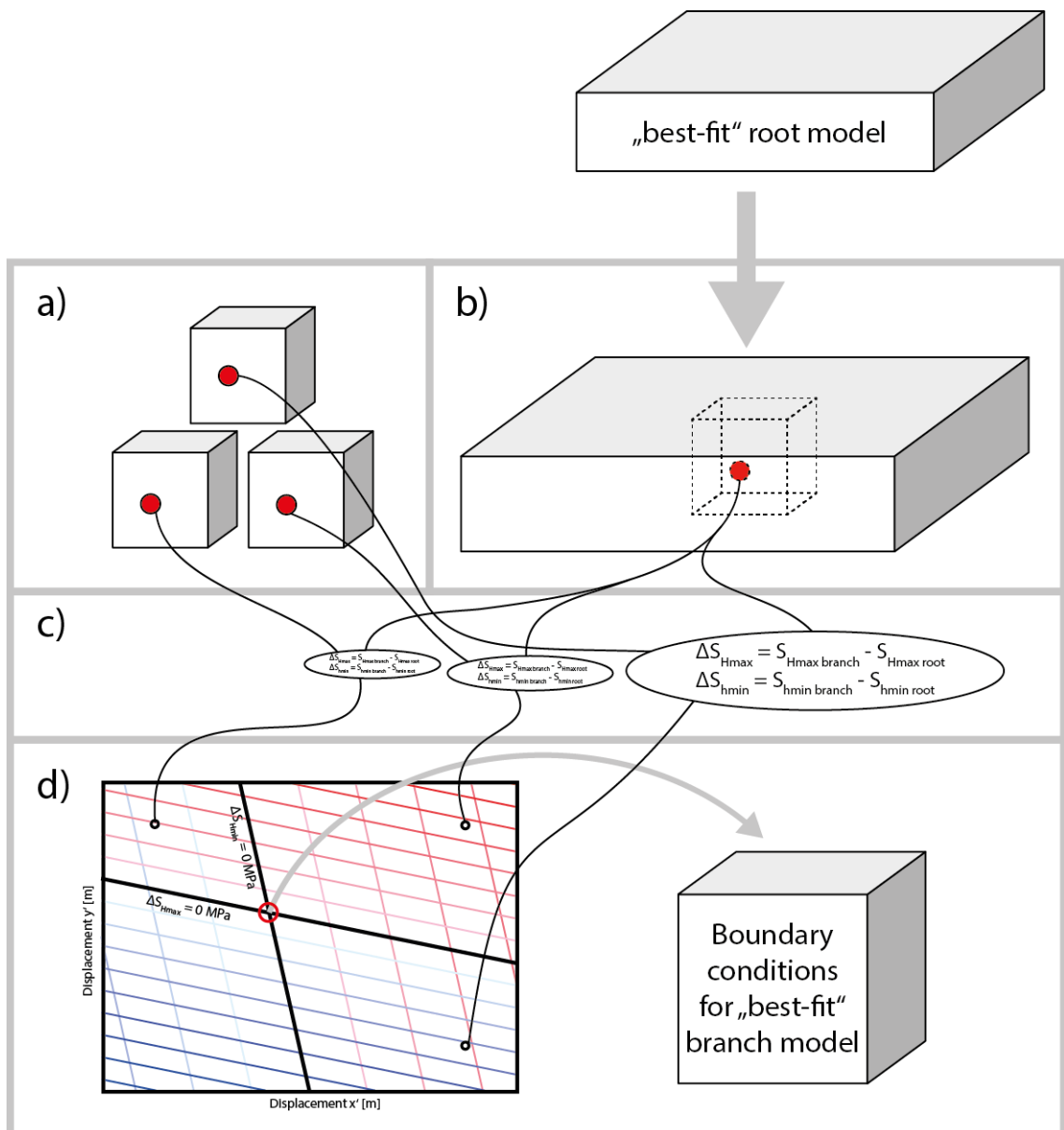


Fig. 5.1-2 Workflow of the FAST Calibration multistage branch calibration

The stress state from three branch model scenarios with arbitrary boundary conditions (a) and the modelled stress state from the root model (b) are compared (c). A set of linear equations is set up that provide the best-fit boundary conditions for the branch model (d).

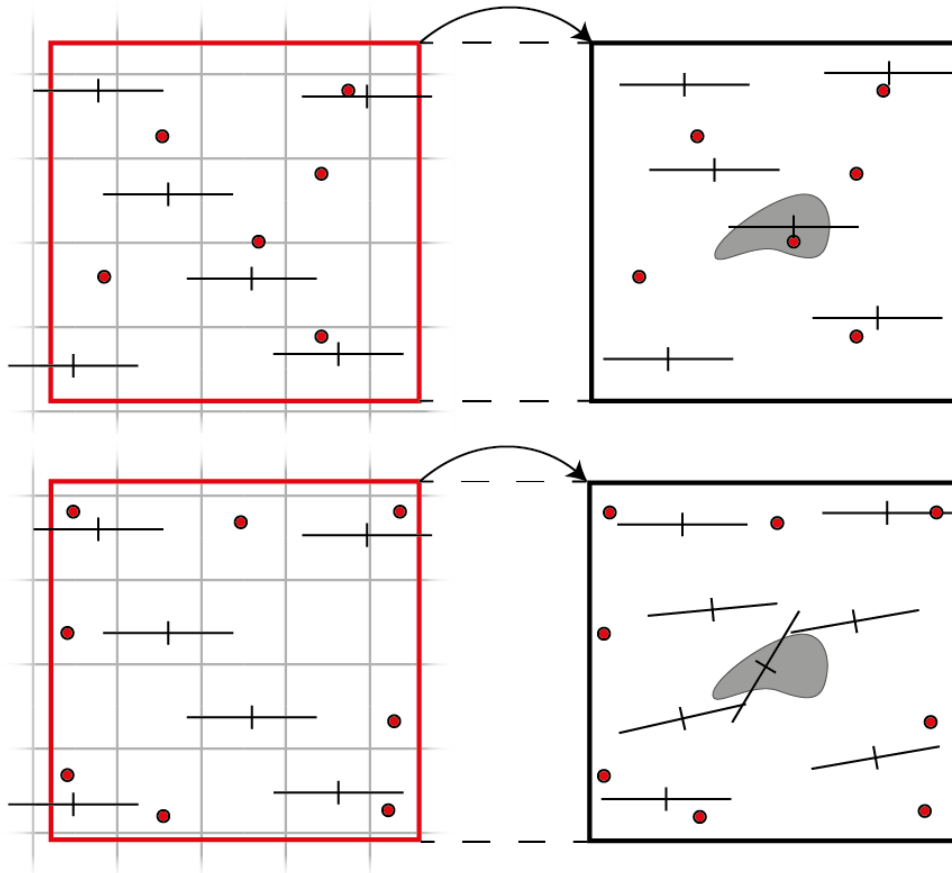


Fig. 5.1-3 Distribution of calibration points.

Red dots are the calibration points that are randomly distributed (top) versus calibration points at the borders of the branch model (bottom) in the root model (left) and branch model (right). Lines indicate the orientation of S_{Hmax} (long line) and S_{Hmin} (short line). A calibration point from the root model (top left) that is located within different rock properties in the centre of the branch model (right) imposes an erroneous stress state on the branch model (top). If the calibration points are at the borders of the branch model material contrasts only present in the branch model are free to influence the stress state (bottom right).

In the next step the stress state from the three branch test model scenarios is compared with the chosen calibration points from the best-fit root model and the deviation is computed for the S_{Hmax} and S_{Hmin} magnitudes in each test model scenario (Fig. 5.1-2c). A linear equation system is setup in the domain of the displacement boundary conditions (x' and y') and the deviations between the calibration points derived from the root stress state and the branch test model stress states (Fig. 5.1-2d). In Fig. 5.1-2 this is indicated by the intersection of the two bold lines of zero deviation. The boundary conditions at this point are used to compute the best-fit branch model.

5.2 Preparation

The following preparations are required in order to successfully use the FAST Calibration tool for a multi-stage calibration approach.

1. Create a directory with the following files and subdirectories:
 - *FAST_calibration.m*
 - *branch_calibration.m*
 - empty subfolder *data*
 - subfolder *calib_functions* that contains the following files:
 - *accuracy.m*
 - *calibrate.m*
 - *critical_shmax.m*
 - *kratio.m*
 - *model_deviation.m*
 - *nodes2calibrationpoints.m*
 - *solve.m*
 - *write_macro.m*
2. At least one data record for the S_{Hmax} and S_{hmin} magnitude is required. The data records are assigned in the variable *stress_data* in *FAST_calibration.m*.
3. Three test model scenarios with arbitrary but different displacement boundary conditions are required. These test model scenarios should be loaded in Tecplot 360 EX and at least S_{Hmax} , S_{hmin} , S_v , and the azimuth of S_{Hmax} need to be computed. This is most easily done by the Tecplot 360 EX Add-on GeoStress (Heidbach et al., 2020). If these variables are derived by another tool it is imperative that they are named "SHmax", "Shmin", "Sv", and "Shazi" (not case sensitive). It is required that the differently sized models are in the same coordinate system and the smaller models extent is covered by the larger model.
4. A *.csv file is required which contains all root model nodes and their location. Four columns are required: Node number, X coordinate, Y coordinate, Z coordinate (see the example file). The *NODES section of an Abaqus® input file is suitable.
5. The best-fit root model is required to be loaded in Tecplot 360 EX and at least S_{Hmax} , S_{hmin} , S_v , and the azimuth of S_{Hmax} need to be computed by the Tecplot 360 EX Add-on GeoStress. If these variables are derived by another tool it is imperative that they are named "SHmax", "Shmin", "Sv", and "Shazi" (not case sensitive).

5.3 Implementation (branch_calibration.m)

The calibration of a branch model on stress data provided by another (larger) root model is achieved by the script *branch_calibration.m*. Basically the script works in the same way as the script to calibrate the root model (*FAST_calibration.m*). A schematic overview of the scripts functions and steps is displayed in Fig. 5.3-1.

In the first part of the script the user needs to define several variables to enable the script to run. Tab. 5.3-1 lists the required input. In the provided script file exemplified variables are defined that can also be used for the example files. Once the variables are set, the function *nodes2calibrationpoints.m* is called and provides the desired amount of calibration points at nodes in the root model. A 3D visualization with the derived calibration points is displayed. Please note that the subroutine may take some time to compute, in particular for large models. Furthermore, the function *write_macro.m* is called twice and generates two Tecplot 360 EX macros which are written to Matlabs current working directory. The first macro is used to extract the best-fit stress state at the calibration points from the root model. The second macro extracts the comparison stress data from the three branch test model scenarios.

Tab. 5.3-1 Required input variables for branch_calibration.m.

Variable	Description
folder	Provide the directions to the folder in your system which contains the script data. It is important to include the full path since this information is not used in Matlab but for the Tecplot 360 EX macro which does not support relative paths.
branch_corner	Define the corners of the branch model in the model coordinate system in a clockwise manner. Make sure that both models are in the same coordinate system.
root_nodes	Provide the filename and location of the *.csv file that contains the nodes of the root model.
type	Specify where the calibration points should be located in the branch model. The three options are: 'border': The calibration points are distributed at the sidewalls of the model. 'corner': The calibration points are mostly located in the corners of the model. 'random': The calibration points are randomly distributed within the entire model (not recommended in a classical multistage application). 'user': User-defined calibration node coordinates are read from the file user_defined_branch_calibration_nodes.csv.
num	Define the desired number of calibration points. Depending on the type of algorithm the number of output calibration points may vary slightly and the variable indicates only the rough order of magnitude.
distrib	This variable defines the density of the calibration points in the corners. A value between 10 and 30 is recommended. (Only for type <i>corner</i> .)
minelem	This variable defines the distance between the boundary of the model and the closest calibration point.
Zmax	The minimum topographic elevation in the entire branch model. No calibration points are situated above this value.
Zmin	The bottom of the branch model. This is especially important if the branch model does not extend as deep as the root model. No calibration points are situated below this value.
x	Enter the displacements in x' (S_{Hmin} or S_{Hmax}) direction that are prescribed in the different branch test scenarios. Make sure to assign the values in the correct order.
y	Enter the displacements in y' (S_{Hmax} or S_{Hmin}) direction that are prescribed in the different branch test scenarios. Make sure to assign the values in the correct order.

The best-fit root model and the three branch test models scenarios need to be loaded in Tecplot 360 EX and the S_{Hmin} and S_{Hmax} magnitudes are derived by the Tecplot 360 EX Add-on GeoStress. Then, the macros are called in order to export the modelled stress state at the designated calibration points.

The second part of the Matlab script reads the data that was exported from Tecplot 360 EX. The modelled stress data from the three branch test model scenarios is compared to the calibration data derived from the root model and the deviation of the S_{Hmax} and S_{Hmin} magnitudes between these is computed for each calibration point as well as the mean deviation. Then, the system of linear equations is setup and solved (for details see previous section). Finally, the best-fit displacement boundary conditions are presented. They are used to compute the best-fit branch model.

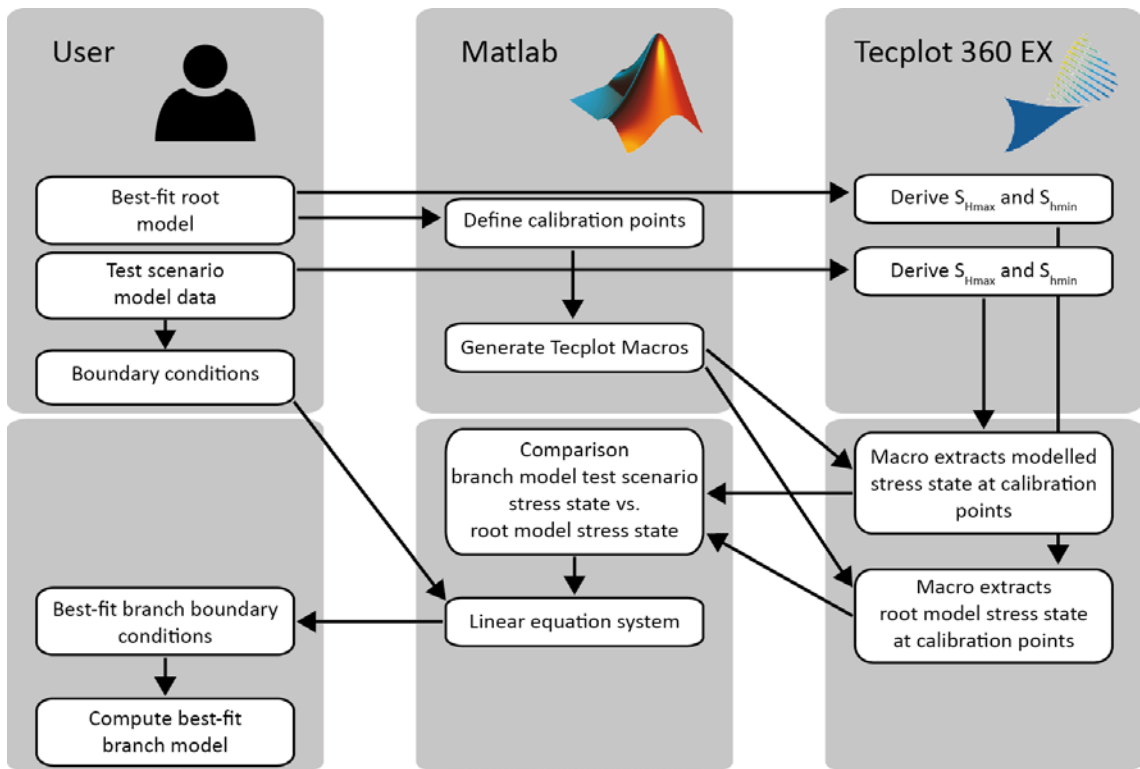


Fig. 5.3-1 Schematic chart of the script workflow.
 Workflow for the calibration of a model on a modelled stress state in two steps.

6 Functions

The FAST Calibration scripts *FAST_calibration.m* and *branch_calibration.m* call several functions. In the following these functions are described.

6.1 Writing Tecplot 360 EX macro function (write_macro.m)

The function *write_macro.m* generates a Tecplot 360 EX macro that exports the modelled stress state from given locations in the model, usually at calibration points. Since the calibration points are not necessarily at nodes the variables are interpolated from the nodes to the exact coordinates in the volume. The function requires four input variables (Tab. 6.1-1) which are automatically provided and transmitted by the root and branch calibration scripts.

Tab. 6.1-1 Required input variables for the function write_macro.m.

Variable	Description
stress	An $n \times 2$ cell-variable in which the data records for calibration and their coordinates are stored and sorted according to types of stress information.
name	The desired name of the macro without the file type extension ".mcr".
mod	The number of modelled stress states (steps) from which data should be exported. For each stress state the data is exported at all locations specified in the variable stress_data.
folder	Provide the directions to the folder in your system which contains the script data. It is important to include the full path since this information is not used in Matlab but for the Tecplot 360 EX macro which does not support relative paths.

With these variables the function creates a Tecplot 360 EX macro with the following structure.

1. The Tecplot macro header is written.
2. The internal number of the variables S_{Hmax} , S_{hmin} , S_v , and azimuth of S_{Hmax} in Tecplot 360 EX are sought and stored in the macro variable SHMAX, SHMIN, SV, and SHAZI.

```

$!GETVARNUMBYNAME |SHMAX|
NAME = "SHmax"

```

3. For each data record location specified in the variable stress an individual 1D zone (point) is created. The number of zones created per data record location depends on the number of model scenarios, usually three. The following syntax is repeated accordingly often.

```

$!CREATERECTANGULARZONE
IMAX = 1
JMAX = 1
KMAX = 1
X1 = 6.621267e+05
Y1 = 5.300777e+06
Z1 = -1.259692e+02
X2 = 6.621267e+05
Y2 = 5.300777e+06
Z2 = -1.259692e+02

```

- The four variables are linearly interpolated from the source zones (i.e. one of the model steps) to the zones defined in step 1. The following code is repeated accordingly often.

```

$!LINEARINTERPOLATE
SOURCEZONES = [1]
DESTINATIONZONE = 4
VARLIST = [|SHMAX|,|SHMIN|,|SV|,|SHAZI|]
LINEARINTERPCONST = 0
LINEARINTERPMODE = DONTCHANGE

```

- The variable values in the 1D zones are exported to four comma-separated data files. Each file contains all instances of one of the four variables.

```

$!EXTENDEDCOMMAND
COMMANDPROCESSORID = 'excsv'
COMMAND = 'FrOp=1:ZnCount=6:ZnList=[4-9]:VarCount=1:VarList=[SHMAX]:ValSep=",":FNAME="C:\Documents\Geom-Num-Model\Calibration\data\root_shmax.csv"'

```

- The 1D zones created in step 3 are deleted from the Tecplot 360 EX file.

```

$!DELETEZONES [4-34]

```

Once the macro is written to the current output directory of Matlab the text message “Macro file created” is returned to the caller.

6.2 Difference between observation and model (model_deviation.m)

FAST Calibration uses the deviations of the three modelled stress states (the test model scenarios) to the observed stress state in order to set up a system of linear equations. The function *model_deviation.m* provides the according data. The deviation of the modelled stress state and observed data record for each displacement boundary condition scenario (bc) at each location (x, y, z) with available observed stress data records is computed by

$$\Delta S_{Hmax}(x, y, z, bc) = S_{Hmax,modelled}(x, y, z, bc) - S_{Hmax,observed}(x, y, z)$$

exemplified here for S_{Hmax} . The weighted mean deviation of the modelled and observed S_{Hmax} and S_{hmin} magnitudes are computed for each displacement boundary condition scenario by

$$\widetilde{\Delta S}_{Hmax}(bc) = \frac{\sum_i w_i \Delta S_{Hmax}(x_i, y_i, z_i, bc)}{\sum_i w_i}$$

with i the number of data records and w_i the individual weighting of each data record. Now for each displacement boundary condition scenario a mean deviation of S_{Hmax} and S_{hmin} exists. If no S_{Hmax} data records are available the corresponding deviations $\widetilde{\Delta S}_{Hmax}(bc)$ are temporarily assigned zeros. The function *model_deviation.m* requires the input variables

specified in Tab. 6.2-1. The output is a vector that contains the mean deviation of observed and modelled stress states for each displacement boundary condition scenario (usually three).

Tab. 6.2-1 Required input variables for `model_deviation.m`.

Variable	Description
stress_data	An $n \times 2$ cell-variable in which the data records for calibration are stored according to the different types of stress indicators.
calib_data	A $1 \times n$ cell-variable in which the test model scenario stress states (magnitudes of S_{Hmax} , S_{hmin} , and S_v , as well as the orientation of S_{Hmax}) at each calibration point are stored.
type	The type of stress component considered. Either "shmax" or "shmin".

6.3 Estimation of best-fit displacement boundary conditions (`calibrate.m`)

The core of FAST Calibration is the function `calibrate.m` that sets up a system of linear equations which are used to estimate the best-fit displacement boundary conditions. Therefore, the prescribed displacements of at least three different combinations of boundary conditions is required. In addition, the mean deviation of modelled and observed S_{Hmax} and S_{hmin} magnitudes in the different boundary condition combinations are required. An example of this information that is provided by `model_deviation.m` is shown in Tab.6.3-1. This information is used to derive the boundary conditions that fulfil the requirement of no deviation between the observed and modelled $\overline{\Delta S}_{Hmax}$ and $\overline{\Delta S}_{hmin}$ magnitudes. The function `calibrate.m` requires the variables indicated in Tab. 6.3-2 in order to setup and solve a system of linear equations that can be visualised as two intersecting planes (Fig.6.3-1).

Tab. 6.3-1 Example for the information required for the generation of the planes.

Three different displacement boundary condition scenarios are required. For each scenario the displacement in x' and y' and $\overline{\Delta S}_{Hmax}$ and $\overline{\Delta S}_{hmin}$ are available.

Bc	x' displ.	y' displ.	$\overline{\Delta S}_{Hmax}$	$\overline{\Delta S}_{hmin}$
1	-10	5	-12.3	8.7
2	-30	25	2.5	-3.2
3	-30	5	-14.4	-4.8

Tab. 6.3-2 Required input variables for `calibrate.m`.

Variable	Description
dshmin	Difference between the modelled stress scenarios and the actual stress data records for S_{hmin} . Output of <code>model_deviation.m</code>
dshmax	Difference between the modelled stress scenarios and the actual stress data records for S_{Hmax} . Output of <code>model_deviation.m</code>
x	Displacement in x' direction prescribed at different test model scenarios.
y	Displacement in y' direction prescribed at different test model scenarios.

For each S_{Hmax} and S_{hmin} in each of the three test model scenarios a vector is available in the form

$$\vec{v} = \begin{pmatrix} x \\ y \\ \overline{\Delta S}_{Hmax} \end{pmatrix}$$

with the displacement boundary displacement x in x' direction and y in y' direction as well as $\widehat{\Delta S}_{Hmax}$ the resulting difference of the modelled and expected stress state in the corresponding component S_{Hmax} .

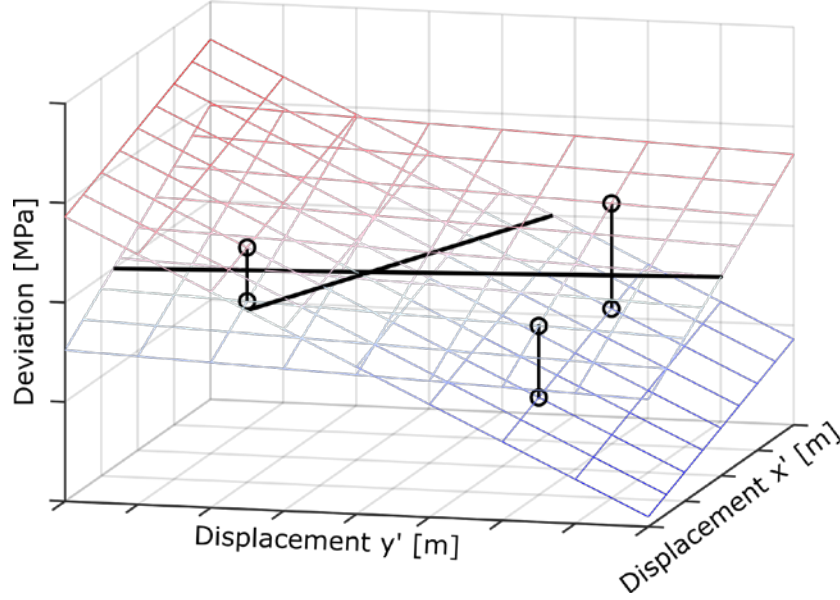


Fig. 6.3-1 Best-fit displacement boundary conditions as planes in 3D.

Three test model scenarios (vertically connected black circles) provide mean deviations of modelled and observed S_{Hmax} and S_{Hmin} magnitudes for specific displacement boundary conditions. For both, S_{Hmax} and S_{Hmin} , the plane spanned by the displacement boundary conditions and the deviations in $\mathbb{R}^3(x', y', \widehat{\Delta S}_{Hmax})$ and $\mathbb{R}^3(x', y', \widehat{\Delta S}_{Hmin})$, respectively, are sought. They are colour coded with blue as a negative deviation and red as a positive deviation. The best-fit displacement boundary conditions are found where the isolines $z=0$ (black lines) of the two planes intersect.

For each S_{Hmax} and S_{Hmin} from the calibration data record this information is used to set up the equation of the plane that is defined by the displacement boundary conditions in x' and y' direction and the mean deviation of S_{Hmax} and S_{Hmin} , respectively. Hence, the planes are set up in $\mathbb{R}^3(x', y', \widehat{\Delta S}_{Hmax})$ and $\mathbb{R}^3(x', y', \widehat{\Delta S}_{Hmin})$, respectively (Fig. 6.3-2). The planes equation in parameter form is

$$\vec{x} = \vec{p} + s \vec{r}_1 + t \vec{r}_2$$

with the position vector $\vec{p} = \vec{v}_1$, the parameters s and t , and the direction vectors \vec{r}_1 and \vec{r}_2 which are computed by

$$\begin{aligned} \vec{r}_1 &= \vec{v}_2 - \vec{v}_1 \\ \vec{r}_2 &= \vec{v}_3 - \vec{v}_1 \end{aligned}$$

Then the parameter form is transferred to the coordinate form of the planes equation which is defined as

$$n_1 x' + n_2 y' + n_3 \widehat{\Delta S}_{Hmax} = d$$

with \vec{n} as the normal vector of the plane derived by

$$\vec{n} = \vec{r}_1 \times \vec{r}_2$$

and d as

$$d = \vec{p} \cdot \vec{n}$$

with \vec{p} the planes position vector.

Then $\widetilde{\Delta S}_{H_{\max}}$ is set to $\widetilde{\Delta S}_{H_{\max}} = 0$ which represents the line with no deviation between observed and modelled stress state (black solid lines in Fig. 6.3-2). The coordinate form of the equation now reads

$$n_1 x' + n_2 y' = d$$

Then the equation is transformed to represent this line in $\mathbb{R}^2(x', y')$.

$$y' = \frac{d - n_1 x'}{n_2}$$

The same equation is setup for $S_{h_{\min}}$. Then, $\widetilde{\Delta S}_{h_{\min}}$ is set to $\widetilde{\Delta S}_{h_{\min}} = 0$ which defines the according line of zero deviation of modelled from observed $\widetilde{\Delta S}_{h_{\min}}$ magnitude. Both lines of zero deviation are now defined in $\mathbb{R}^2(x', y')$. At their intersection both, $\widetilde{\Delta S}_{H_{\max}}$ and $\widetilde{\Delta S}_{h_{\min}}$, are zero and hence x' and y' at the intersection define the best-fit displacement boundary conditions (indicated by the red circle and dashed red lines in Fig. 6.3-2).

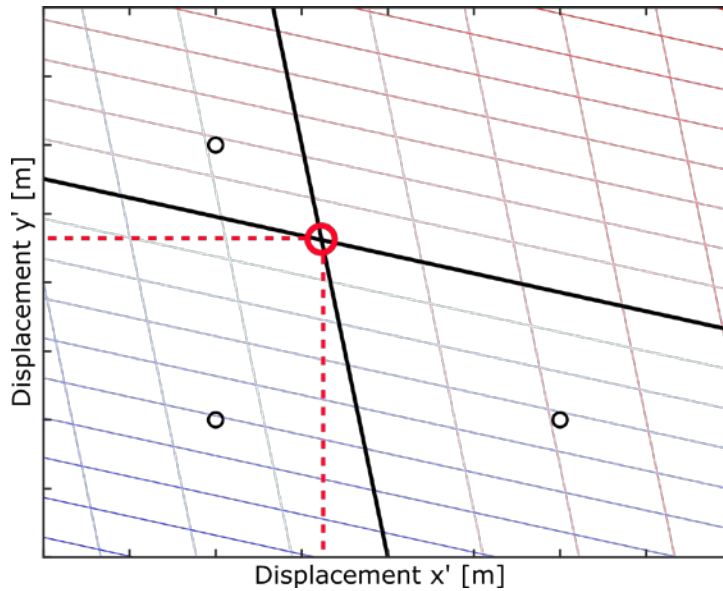


Fig. 6.3-2 Best-fit displacement boundary conditions.

Red dashed line and red circle are displayed in $\mathbb{R}^2(x', y')$. Three test model scenarios (black circles) provide mean deviations of modelled and observed $S_{H_{\max}}$ and $S_{h_{\min}}$ magnitudes for specific displacement boundary conditions. For both, $S_{H_{\max}}$ and $S_{h_{\min}}$, the plane spanned by the boundary conditions and the deviations in $\mathbb{R}^3(x', y', \widetilde{\Delta S}_{H_{\max}})$ and $\mathbb{R}^3(x', y', \widetilde{\Delta S}_{h_{\min}})$, respectively, are sought. They are represented here by the colour coded isolines with blue as a negative deviation and red as a positive deviation. The best-fit displacement boundary conditions are found where the isolines $z=0$ of the two planes intersect.

6.4 Solve the calibrated stress state at individual locations (solve.m)

Some functions such as *critical_shmax.m*, *accuracy.m*, or *kratio.m* require the best-fit stress state for one or both of the horizontal stress components. The best-fit stress state is not yet known in contrast to the displacement boundary conditions that are required to estimate the best-fit stress state. In order to quickly provide a preliminary stress state of a horizontal stress component at a certain location *solve.m* computes the expected stress magnitudes in Matlab according to the (preliminary) best-fit displacement boundary conditions.

In order to estimate the magnitude of S_{hmin} at a given location in the model first the best-fit displacement boundary conditions are computed using $\widetilde{\Delta S}_{hmin}(bc)$. If available, S_{Hmax} data records are also taken into account. If no S_{Hmax} data records are available $\widetilde{\Delta S}_{Hmax}(bc) = 0$ is used. Then, the best-fit displacement boundary conditions only satisfy the S_{hmin} magnitudes. At the given location these preliminary partial displacement boundary conditions are used to compute the resulting first order S_{hmin} magnitude using the function *solve.m* that requires the input variables specified in Tab. 6.4-1.

Tab. 6.4-1 Required input variables for the function solve.m.

Variable	Description
stress_scenario	Excerpt from calib_data for the stress component that is to be solved at the corresponding location.
X	Displacements in x' direction prescribed at different test model scenarios.
Y	Displacements in y' direction prescribed at different test model scenarios.
Bcx	Preliminary best-fit displacement boundary displacement in x' direction.
Bcy	Preliminary best-fit displacement boundary displacement in y' direction.

Comparable to *calibrate.m* the function *solve.m* founds on the equation for a linear plane to estimate the best-fit stress state at a certain location. This plane is constituted by three points in $\mathbb{R}^3(x', y', S_{hmin})$. For each of the (at least) three test model scenarios arbitrary displacement boundary conditions (x' , y') and the resulting stress state (S_{hmin}) are available. Note that in contrast to *calibrate.m* *solve.m* uses the stress magnitude at the calibration location. The vectors constructed from the model scenarios available for each S_{hmin} and S_{Hmax} are therefore in the form of

$$\vec{v} = \begin{pmatrix} x \\ y \\ \widetilde{\Delta S}_{hmin} \end{pmatrix}$$

with the boundary displacement x and y in the directions of x' and y' and the resulting magnitude S_{hmin} (or S_{Hmax}). Recall the derivation of the planes equation from these vectors as presented earlier on. That leads to the equation

$$n_1 x' + n_2 y' + n_3 S_{hmin} = d$$

with the normal vector n and the scalar component d that are derived from the three points in which all three variables are known. Here, the best-fit boundary conditions x' and y' are inserted in the equation and it is transferred to solve for S_{hmin} (or S_{Hmax}) as

$$S_{hmin} = \frac{d - n_1 x' - n_2 y'}{n_3}$$

Due to the linear elastic behaviour of the model the resulting stress component is used as a first order approximation of the numerical results.

6.5 Additional S_{Hmax} calibration data (*kratio.m*)

In addition to or instead of actual stress data records of the magnitude of S_{Hmax} , another methods can be employed. FAST Calibration v2.0 allows to calibrate S_{Hmax} on the k-ratio which is defined as

$$k = \frac{S_{Hmax} + S_{hmin}}{2 S_v}$$

If the k-ratio is provided for a certain depths and S_{hmin} is already preliminarily calibrated (see above or *solve.m*) the magnitude of S_{Hmax} that is required to generate the provided k-ratio can be derived by

$$S_{Hmax} = 2 k S_v - S_{hmin}$$

Therefore, *kratio.m* calls the function *solve.m* to estimate the magnitude of S_{hmin} . S_v is extracted from the test scenarios. Then, the magnitudes of S_{Hmax} derived from k-ratios are used for calibration corresponding to the actually observed S_{Hmax} magnitude data records. The variables specified in Tab. 6.5-1 are required for the execution of this part of the script.

Tab. 6.5-1 Required input variables for the function *kratio.m*.

Variable	Description
stress_data	An $n \times 2$ cell-variable in which the data records for calibration are stored according to the different types of stress information.
calib_data	A $1 \times n$ cell-variable in which the test model scenarios stress states (magnitudes of S_{Hmax} , S_{hmin} , and S_v , as well as the orientation of S_{Hmax}) at each calibration point are stored.
x	Displacement in x' direction prescribed at different test model scenarios.
y	Displacement in y' direction prescribed at different test model scenarios.
bcx	Preliminary boundary displacement in x' direction.
bcy	Preliminary boundary displacement in y' direction.

6.6 Calibrate a critical S_{Hmax} stress state (*critical_shmax.m*)

FAST Calibration v2.0 offers the possibility to use observed seismicity as an assumption for a critically high S_{Hmax} magnitude as a way to estimate and calibrate S_{Hmax} . Therefore, for one or several locations one or more fault orientations and properties are provided by the user. In order to estimate the criticality of the fault the scalar value slip tendency (Morris et al., 1996) is employed and computed as

$$ST = \frac{\tau_{max} - C}{\sigma_n} \mu^{-1}$$

with the fault orientation specific shear stress τ and normal stress σ_n , as well as the fault specific properties cohesion C and the friction coefficient μ . If slip tendency is smaller than 1

the fault is stable. Failure occurs at values larger than 1. A critically high magnitude of S_{Hmax} is defined by $ST = 1$.

In general, slip tendency is computed as follows. The shear and normal stress are derived from the traction vector

$$\mathbf{T}^{(n)} = \sigma_{ij} \mathbf{n}$$

with the stress tensor σ_{ij} and the normal vector of the fault plane \mathbf{n} . Then the normal stress is derived from the traction vector by

$$\sigma_n = \mathbf{T}_i^{(n)} \mathbf{n}_i$$

The magnitude R of the traction vector is computed by

$$R = \sqrt{\sum_{i=1}^3 \mathbf{T}_i^{(n)2}}$$

and the magnitude of the shear component is then derived according to the Pythagorean theorem by

$$\tau_{max} = \sqrt{R^2 - \sigma_n^2}$$

Here, ST is set to 1, which corresponds to a critically high S_{Hmax} magnitude. In order to be able to use the critical S_{Hmax} assumption to calibrate S_{Hmax} $\mathbf{T}^{(n)}$ is not estimated from the full stress tensor but only from the three principal stresses under the assumption of one of them being vertical. Hence, the derivation of $\mathbf{T}^{(n)}$ is reduced to

$$T_1 = S_{hmin} n_1$$

$$T_2 = S_{Hmax} n_2$$

$$T_3 = S_v n_3$$

The orientation of the reduced stress tensor is now only defined by the orientation of S_{Hmax} . In order to simplify computations, both, the strike of the fault β and the orientation of S_{Hmax} are rotated in a way that the orientation of S_{Hmax} $\theta' = 0^\circ$ (parallel to the y -axis). The traction vector on the fault does not change by this operation since the angle ω of the orientation of S_{Hmax} on the fault does not change (Fig. 6.6-1).

$$\theta' = \theta - \theta$$

$$\beta' = \beta - \theta$$

With S_v known and S_{hmin} calibrated the only unknown in the equation for slip tendency remains the magnitude of S_{Hmax} . The known equation for slip tendency

$$ST = 1 = \frac{\tau_{max} - C}{\sigma_n} \mu^{-1}$$

is transformed to compute the required value of S_{Hmax} at a given location, fault orientation and properties, and S_{hmin} and S_v magnitudes. With

$$\tau_{max} = \sqrt{R^2 - \sigma_n^2}$$

the equation for slip tendency takes the form of a quadratic equation as

$$\sigma_n^2 + \sigma_n^2 \mu^2 + 2\mu C \sigma_n + C^2 - R^2 = 0$$

Recall σ_n and R^2 defined by the known normal vector of the fault plane and stress magnitudes of S_v (known) and S_{hmin} (calibrated). Thus, the only unknown remains the magnitude of S_{Hmax} . The normal stress is simplified to

$$\sigma_n = S_{hmin} n_1^2 + S_{Hmax} n_2^2 + S_v n_3^2 = S_{Hmax} n_2^2 + N$$

and the shear stress magnitude is simplified to

$$R^2 = S_{hmin}^2 n_1^2 + S_{Hmax}^2 n_2^2 + S_v^2 n_3^2 = S_{Hmax}^2 n_2^2 + S$$

and hence the quadratic equation is rewritten as

$$S_{Hmax}^2 [n_2^4 + \mu^2 n_2^4 - n_2^2] + S_{Hmax} 2n_2^2 [N + \mu^2 N + 2\mu C] + [N^2 + \mu^2 N^2 + 2\mu CN + C^2 - S] = 0$$

The equation is then solved for S_{Hmax} and the positive result is used as the value of S_{Hmax} that is required for a critically high S_{Hmax} magnitude.

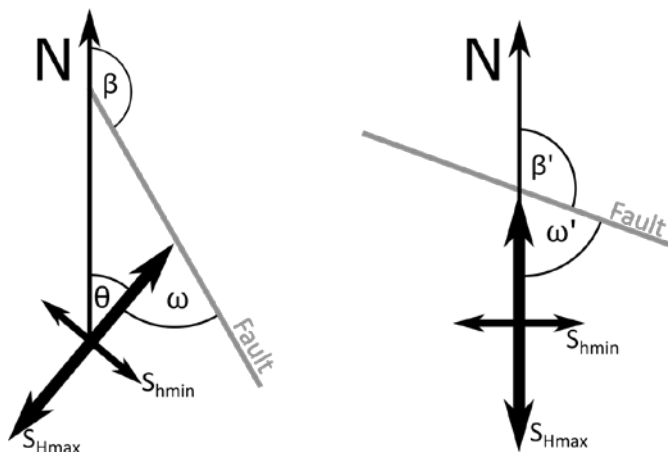


Fig. 6.6-1 Horizontal components of the reduced stress tensor and fault strike.

The traction vector that acts on a fault does not change if both strike direction β and S_{Hmax} orientation θ are rotated by the same angle. The angle ω between the faults strike and the orientation of S_{Hmax} θ remains the same.

Tab. 6.6-1 Required input variables for the function `critical_shmax.m`.

Variable	Description
stress_data	An $n \times 2$ cell-variable in which the data records for calibration are stored according to the different types of stress information.
calib_data	A $1 \times n$ cell-variable in which the test model scenario stress states (magnitudes of S_{Hmax} , S_{hmin} , and S_v , as well as the orientation of S_{Hmax}) at each calibration point are stored.
x	Displacement in x' direction prescribed at different test model scenarios.
y	Displacement in y' direction prescribed at different test model scenarios.
bcx	Preliminary boundary displacement in x' direction.
bcy	Preliminary boundary displacement in y' direction.

The function `critical_shmax.m` allows the evaluation of various fault orientations at various locations. In addition, several possible orientations per fault may be evaluated in case of uncertainties in the fault parameter. At each location and for each orientation the critical magnitude of S_{Hmax} is expected to be different. Thus, from the ensemble of many different magnitudes of S_{Hmax} , the smallest is used for calibration. If different locations with different depths are provided in the input data a bias towards the shallower data is introduced. Hence, it is recommended to only use one location or locations in the same depth. The principle caveat emptor is emphasized here since it is only a first order approximation.

The variables specified in Tab. 6.6-1 are required for the execution of the function. It returns the variable `dshmax`. For certain constellations of fault orientation and stress state a failure may even occur due to the magnitudes of S_{hmin} and S_v alone. If this is detected a message is printed to the screen.

6.7 Assess the accuracy of the calibrated stress state (accuracy.m)

The function `accuracy.m` evaluates if any information or limits of the stress state are provided by the user. Then they are evaluated individually and for each specified location with additional information on the stress state it is tested whether and how accurate the calibrated stress state satisfies the provided constraints. The calibration procedure and best-fit displacement boundary conditions are not influenced. The required input variables are indicated in Tab. 6.7-1 and the different information and limits and their assessment is presented in the following.

Tab. 6.7-1 Required input variables for the function `accuracy.m`.

Variable	Description
stress_data	An $n \times 2$ cell-variable in which the data records for calibration are stored according to the different types of stress information.
calib_data	A $1 \times n$ cell-variable in which the test model scenario stress states (magnitudes of S_{Hmax} , S_{hmin} , and S_v , as well as the orientation of S_{Hmax}) at each calibration point are stored.
X	Displacement in x' direction prescribed at different test model scenarios.
Y	Displacement in y' direction prescribed at different test model scenarios.
Bcx	Preliminary boundary displacement in x' direction.
Bcy	Preliminary boundary displacement in y' direction.

The results from formation integrity test (FIT) are compared to the modelled S_{hmin} and S_v magnitudes. Both can be the least principal stress, depending on the tectonic stress regime

(S_{hmin} in normal faulting and strike slip faulting and S_v in thrust faulting regimes). Using the function *solve.m* the calibrated modelled magnitude of S_{hmin} at the calibration point with an FIT data record is computed. The magnitude of S_v is provided directly by the test model scenarios. If an observed FIT magnitude is larger than the modelled S3 magnitude (either S_{hmin} or S_v) a message is displayed to the user. Eventually, a summary of the percentage and number of location at which the FIT magnitude and the modelled stress state are in disagreement is provided. Note that a percentage of more than 100% is possible if both the S_{hmin} and S_v magnitudes are below the threshold.

Information on the modelled regime stress ratio (RSR) or the k-ratio is assessed for accuracy by a computation of both S_{hmin} and S_{Hmax} at the data record location using the function *solve.m*. S_v is extracted from the test model scenarios. Then either the RSR according to Simpson (1994) or the k-ratio is calculated for each data record location. The resulting value is compared to the expected value. The mean difference between the expected and modelled value is printed to the screen. Furthermore, the standard deviation is displayed in a message to the user. By appending “_detail” to the data type in the *stress_data* variable individual information are displayed for each location.

To test whether borehole breakouts or drilling induced tensile fractures are expected to occur in vertical boreholes in the modelled stress state or not both S_{hmin} and S_{Hmax} at the data record location are computed using the function *solve.m*. Then the maximum and minimum circumferential stress is computed and compared to the compressive strength of the rock and the tensile strength of the rock, respectively. Then information is printed on the screen whether borehole breakouts or drilling induced tensile fractures are expected or not. By appending “_detail” to the data type in the *stress_data* variable individual information are displayed for each location. This is especially useful when locations with and without borehole failures are to be compared.

6.8 Calibration point function (nodes2calibrationpoints.m)

The function *nodes2calibrationpoints.m* is only required for a multi-stage approach as it provides suitable points for the calibration of a geomechanical-numerical branch model on the stress state provided by a root model. Therefore, a user-defined number of calibration points is selected out of all nodes from the root model that are geographical located within the boundaries of the branch model. The coordinates are transferred to the caller function and written to the file *branch_calibration_nodes.csv*.

The function provides three different possibilities for the lateral distribution of calibration points (Fig. 6.8-1). The nodes for calibration can be located (1) equally distributed at the borders of the branch models, (2) in the corners of the branch model, and (3) randomly distributed in the entire branch model (which is not recommended in a classical multi-stage application). The depth distribution of the calibration points is random. The minimum distance of the calibration nodes from the border of the branch model can be specified in order to mitigate boundary effects. Furthermore, if the nodes are sought in the corners the density of the nodes can be controlled (Fig. 6.8-1a, b). The subroutine uses the Matlab function *inpolygon* in order to determine whether a node is within the specified boundaries of the branch model. Therefore, the model boundaries can be arbitrarily oriented and are not required to be parallel to the model coordinate systems axes. The function requires the input information specified in Tab. 6.8-1.

Tab. 6.8-1 Required input variables for the function nodes2calibpoints.m.

Variable	Description
corner	Clockwise X and Y coordinates of the four corners of the branch model.
filename	Name of the file that contains the nodes of the root model.
num	Number of desired calibration points.
distrib	This variable defines how close the calibration points should be in the corners. A value between 10 and 30 is recommended. (Only for type corner.)
type	The type of distribution for the calibration points, 'border', 'corner', 'random', or user
minelem	This variable defines the distance between the boundary of the model and the closest calibration point.
Zmax	The minimum topographic elevation in the entire branch model. This is at the same time the highest topographic isoline that is present in the entire model. No calibration points are situated above this value.
Zmin	The bottom of the branch model. This is especially important if the branch model does not extend as deep as the root model. No calibration points are situated below this value.

The function returns a $num \times 3$ shaped Matlab variable with the coordinates of the derived calibration points. Please note that depending on the chosen type of calibration point distribution the number of calibration points may vary slightly (approx. 10%) for technical reasons. The function provides the coordinates of calibration nodes as comma separated values in an exported file. Furthermore, user-defined coordinates of calibration points can be imported from a comma separated file.

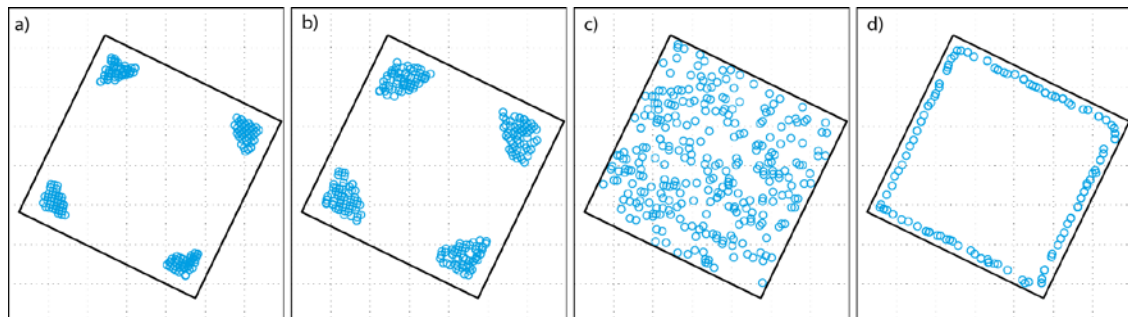


Fig. 6.8-1 Different possibilities for calibration point positioning.

Calibration points at the corner with $distrib = 20$ (a) and $distrib = 50$ (b) and $minelem = 2000$.
 c) Randomly distributed calibration points with $minelem = 500$. d) Calibration points at the borders of the model with $minelem = 1000$.

7 Example

In the following, two examples are presented. The first shows the calibration of a single geomechanical-numerical model and the second example describes a multi-stage approach with a branch model that uses the model results from the first example or calibration.

All models are available in the examples folder as Abaqus® solver input file (.inp), output file (.odb), and Tecplot binary file (.plt). An initial stress state, three test model scenarios with arbitrary displacement boundary conditions and a final model are presented. The geometry is provided in a separate file (.geom). The exemplary parameters that are provided in the Matlab scripts match these examples.

The .odb files can be imported in Tecplot 360 EX and the FAST Calibration tool can hence be tested without using Abaqus®. Note that we used Abaqus® 2019 and that the binary output files from this version can only be read from Tecplot 360 EX 2019 R1 onwards. For compatibility with older Tecplot 360 EX versions or in order to experience the entire workflow the input files can be rerun in an according Abaqus® version (Abaqus 6.11 output is read by Tecplot 360 EX versions up to 2017, Abaqus® 6.14 output is read by Tecplot 360 EX 2018).

7.1 Model calibration

The first example is a 3D geomechanical-numerical model that has an extent of $10 \times 10 \times 5 \text{ km}^3$. The calibration data provided in Tab. 7.1-1 or already in FAST Calibration syntax in the *FAST_calibration.m* file should be used for calibration of the model and evaluation of the results. Furthermore, a fault ($310 \pm 10 | 30 \pm 10$) with associated friction of 0.6 ± 0.2 and cohesion of $10 \pm 5 \text{ MPa}$ can be used for a critical S_{Hmax} calibration. The critical S_{Hmax} calibration is per default commented out in the file *FAST_calibration.m*.

Tab. 7.1-1 Data used for calibration and evaluation.

Method	Location (X,Y,Z)	Value	Confidence
S_{Hmax}	3000 3000 -800	17.16	1.0
	5000 6500 -1800	36.0	0.6
S_{hmin}	3000 3000 -800	11.6	1.0
	5000 6500 -3000	53.0	0.9
S_{Hmax} by k-ratio	5000 5000 -4000	1.0	0.3
FITs	3000 3000 -400	5	1.0
	3000 3000 -700	14	1.0
	5000 6500 -1000	12	1.0
	5000 6500 -3000	45	0.1
Regime Stress Ratio	8500 9200 -4500	0.9	0.8
	8400 8900 -4800	1.5	0.8
k-ratio	5000 5000 -4000	0.9	1.0
	5000 5000 -3000	1.0	1.0
Borehole breakouts	3000 3000 -750	40	1.0
	3000 3000 -430	20	1.0
Drilling induced tensile fractures	5000 6500 -800	24	1.0
	5000 6500 -1500	30	1.0
No observed borehole breakouts	3000 3000 -750	40	1.0
	3000 3000 -430	20	1.0
No observed drilling induced tensile fractures	5000 6500 -800	24	1.0
	5000 6500 -1500	30	1.0

The following steps are required for implementation:

1. Abaqus®: Run *root_initial.inp* and *root_calibration.inp*.
2. Matlab: Execute the first part of *FAST_calibration.m*. A Tecplot 360 EX macro file is written to the current Matlab directory.
3. Tecplot 360 EX: Load *root_calibration.odb*, compute S_{Hmax} , S_{hmin} , S_v and the azimuth of S_{Hmax} with the Add-on GeoStress, and execute the macro *root.mcr* that was generated by Matlab in 2. The four variables at the calibration points are written to files in the *data* subdirectory.
4. Matlab: Execute the second part of *FAST_calibration.m*. Matlab provides the best-fit displacement boundary conditions for the root model and the following output is printed to the screen.

RESULTS:

FIT #1 is 0.93795 MPa larger than S_{hmin} .

FIT #2 is 4.2902 MPa larger than S_{hmin} .

FIT #2 is 0.2842 MPa larger than S_v .

Summary:

97% of the weighted lower boundary constraints (FITs) failed.

2 of 4 lower boundary constraints failed for S_{hmin} .

1 of 4 lower boundary constraints failed for S_v .

No breakout at observed borehole position #1.

Breakout at observed borehole position #2.

Summary: 1 breakouts out of 2 observed locations.

No breakout at intact borehole section #1.

Breakout at intact borehole section #2.

Summary: 1 intact borehole walls out of 2 observed intact locations.

Drilling induced fracture at observed position #1.

No drilling induced fracture at observed position #2.

Summary: 1 drilling induced fractures out of 2 possible locations.

Drilling induced fracture at observed intact section #1.

No drilling induced fracture at observed intact section #2.

Summary: 1 intact borehole walls out of 2 observed intact locations.

Position #1: modelled k-ratio is 0.95506. Difference in k-ratio: 0.055057.

Position #2: modelled k-ratio is 0.95314. Difference in k-ratio: -0.046857.

Summary: Mean deviation of k is 0.0040999 Standard Deviation 0.072064.

Position #1: Difference in RSR: 0.22827.

Position #2: Difference in RSR: -0.34366.

Summary: Mean deviation of RSR is -0.057691 Standard Deviation 0.40441.

BOUNDARY CONDITIONS:

Root model boundary condition X: -4.135

Root model boundary condition Y: 3.471

5. Open a text editor and set the displacement boundary conditions in *root_final.inp* according to the output of Matlab from step 4.
6. Abaqus®: Run *root_final.inp*. Now, the model is successfully calibrated on stress data records and a best-fit stress state is provided.

If the critical S_{Hmax} calibration approach is followed the output includes the following message.

Orientation #1 (303|40) with a cohesion of 5 MPa and a friction coefficient of 0.4 fails for $S_{Hmax} = 140.8751$ MPa.

7.2 Multi-stage approach

In order to test the FAST Calibration multi-stage approach another example is provided. It uses the model results from the previous section as a root model. The additional branch model has an extent of $4 \times 4 \times 4$ km³ and is situated within the root model. Detailed coordinates are listed in Tab. 7.2-1. Additionally, the nodes of the root model are represented in a .csv file. The exemplary parameters that are provided in the Matlab scripts match these examples.

Tab. 7.2-1 Extent and coordinates of the example models.

Model	Coordinates	Min [m]	Max [m]
Root	X	0	10,000
	Y	0	10,000
	Z	-5,000	0
Branch	X	2,000	6,000
	Y	2,000	6,000
	Z	-4,000	0

Once the root model is successfully calibrated on stress data records the branch model calibration can be started as described in the following:

1. Abaqus®: Run *branch_initial.inp* and *branch_calibration.inp*.
2. Matlab: Execute the first part of *branch_calibration.m*. Two Tecplot 360 EX macros files are written in the current Matlab directory.
3. Tecplot 360 EX: Load *branch_calibration.odb*, compute S_{Hmax} , S_{hmin} , S_v and the azimuth of S_{Hmax} with the GeoStress Add-on, and execute the *branch_calib.mcr* macro that was generated by Matlab in 2. The four variables at the calibration points are written to files in the *data* subdirectory.
4. Tecplot 360 EX: Load *root_final.odb* compute S_{Hmax} , S_{hmin} , S_v and the azimuth of S_{Hmax} with the GeoStress Add-on, and execute the macro *root_branch_calib.mcr* that was generated by Matlab in 2. The four variables at the calibration points are written to files in the *data* subdirectory.
5. Matlab: Execute the second part of *branch_calibration.m*. Matlab provides the best-fit displacement boundary conditions for the branch model.
6. Open a text editor and set the boundary conditions in *branch_final.inp* according to the output of Matlab in 5.
7. Abaqus®: Run *branch_final.inp*.

Now, the multi-stage approach has been successfully conducted and a best-fit local branch stress state is provided.

Acknowledgements

The authors would like to thank Karsten Reiter and Tobias Hergert who contributed to the script, Robin Seithel for initial testing, and Solveig Strutzke and Kirsten Elger for typesetting, final checks and supporting the publication.

The work leading to these results has received funding from the Initiative and Networking Fund of the Helmholtz Association through the project “Integrity of nuclear waste repository systems - Cross-scale system understanding and analysis (iCross)” project by the Federal Ministry of Education and Research (project number 02NUK053D), the Helmholtz Association and the Helmholtz Centre Potsdam - Deutsches GeoForschungsZentrum GFZ.

References

- Aadnoy, B.S. 1990. In-situ stress directions from borehole fracture traces. *Journal of Petroleum Science and Engineering*, 4(2), 143-153. [https://doi.org/10.1016/0920-4105\(90\)90022-U](https://doi.org/10.1016/0920-4105(90)90022-U)
- Amadei, B., and O. Stephansson 1997. *Rock Stress and its Measurements*, 1st ed., Chapman and Hall, New York.
- Bell, J.S. and Gough, D.I. 1979. Northeast-southwest compressive stress in Alberta - evidence from oil wells. *Earth and Planetary Science Letters*, 45(2), 475-482. [https://doi.org/10.1016/0012-821X\(79\)90146-8](https://doi.org/10.1016/0012-821X(79)90146-8)
- Brown, E. T., and E. Hoek 1978. Trends in Relationships between Measured In-Situ Stresses and Depth, *International Journal of Rock Mechanics and Mining Sciences and Geomechanical Abstracts*, 15, 211-215. [https://doi.org/10.1016/0148-9062\(78\)91227-5](https://doi.org/10.1016/0148-9062(78)91227-5)
- Cornet, F. H., and D. Burllet 1992. Stress Field Determinations in France by Hydraulic Tests in Boreholes, *J. Geophys. Res.*, 97. <https://doi.org/10.1029/90JB02638>
- Cornet, F.H. 2015. *Elements of Crustal Geomechanics*. Cambridge University Press. <https://doi.org/10.1007/s40948-015-0016-9>
- Fjaer, E., R. Holt, P. Horsrud, A. Raaen, and R. Risnes 2008. *Petroleum Related Rock Mechanics*, 2nd ed., Elsevier, Amsterdam.
- Heidbach, O., Rajabi, M., Reiter, K., Ziegler, M., & the WSM Team. 2016. World Stress Map Database Release 2016. GFZ Data Services. <https://doi.org/10.5880/WSM.2016.001>
- Heidbach, O., Rajabi, M., Cui, X., Fuchs, K., Müller, B., Reinecker, J., Reiter, K., Tingay, M., Wenzel, F., Xie, F., Ziegler, M., Zoback, M.-L., & Zoback, M. 2018. The World Stress Map database release 2016: Crustal stress pattern across scales. *Tectonophysics*, 744, 484-498. <https://doi.org/10.1016/j.tecto.2018.07.007>
- Heidbach, O., Stromeyer, D. & Ziegler, M.O. 2020. Manual of the Tecplot 360 Add-on GeoStress v2.0. World Stress Map Technical Report 20-01, GFZ Data Services. <https://doi.org/10.2312/wsm.2020.001>
- Henk, A. 2008. Perspectives of Geomechanical Reservoir Models - Why Stress is Important, *European Magazine*, 4, 1-5.
- Hergert, T., Heidbach, O., Reiter, K., Giger, S. B., & Marschall, P. 2015. Stress field sensitivity analysis in a sedimentary sequence of the Alpine foreland, northern Switzerland. *Solid Earth*, 6(2), 533–552. <https://doi.org/10.5194/se-6-533-2015>
- Jaeger, J. C. & Cook, N.G.W. 1969. *Fundamentals of Rock Mechanics*. Chapman and Hall. 513p.
- Kirsch, E.G. 1898. Die Theorie der Elastizität und die Bedürfnisse der Festigkeitslehre. *Zeitschrift des Vereines Deutscher Ingenieure*, 42, 797-807.

- McCutchen 1982. Some elements of a theory of in situ stress, *International Journal of Rock Mechanics and Mining Sciences and Geomechanical Abstracts*, 19, 201-203. [https://doi.org/10.1016/0148-9062\(82\)90890-7](https://doi.org/10.1016/0148-9062(82)90890-7)
- Morawietz, S.; Heidbach, O.; Reiter, K.; Ziegler, M.; Rajabi, M.; Zimmermann, G.; Müller, B. & Tingay, M. 2020. An open-access stress magnitude database for Germany and adjacent regions. *Geothermal Energy*. 8. <https://doi.org/10.1186/s40517-020-00178-5>
- 41 Morris, A., Ferrill, D. A., & Henderson, D. B. 1996. Slip-tendency analysis and fault reactivation. *Geology*, 24(7), 275-278. [https://doi.org/10.1130/0091-7613\(1996\)024<0275:STAAFR>2.3.CO;2](https://doi.org/10.1130/0091-7613(1996)024<0275:STAAFR>2.3.CO;2)
- Reiter, K., & Heidbach, O. 2014. 3-D geomechanical-numerical model of the contemporary crustal stress state in the Alberta Basin (Canada). *Solid Earth*, 5(2), 1123–1149. <https://doi.org/10.5194/se-5-1123-2014>
- Schmitt, D. R., C. A. Currie, and L. Zhang 2012. Crustal stress determination from boreholes and rock cores: Fundamental principles *Tectonophysics*, 580, 1-26, <https://doi.org/10.1016/j.tecto.2012.08.029>
- Sheorey, P. R. 1994. A Theory for In Situ Stresses in Isotropic and Transversely Isotropic Rocks, *International Journal of Rock Mechanics and Mining Sciences and Geomechanical Abstracts*, 31(1), 23-34. [https://doi.org/10.1016/0148-9062\(94\)92312-4](https://doi.org/10.1016/0148-9062(94)92312-4)
- Simpson, R. W. 1997. Quantifying Anderson's fault types. *Journal of Geophysical Research: Solid Earth*, 102(B8), 17909-17919. <https://doi.org/10.1029/97JB01274>
- Stromeyer, D.; Heidbach, O.; Ziegler, M. 2020. Tecplot 360 Add-on GeoStress v2.0. V. 2.0. GFZ Data Services. <https://doi.org/10.5880/wsm.2020.001>
- White, Adrian J., Traugott, Martin O., & Swarbrick, Richard E. 2002. The use of leak-off tests as means of predicting minimum in-situ stress. *Petroleum Geoscience*, 8(2), 189–193. <https://doi.org/10.1144/petgeo.8.2.189>
- Ziegler, M. O., Heidbach, O., Reinecker, J., Przybycin, A. M., & Scheck-Wenderoth, M.. 2016. A multi-stage 3-D stress field modelling approach exemplified in the Bavarian Molasse Basin. *Solid Earth*, 7(5), 1365–1382. <https://doi.org/10.5194/se-7-1365-2016>
- Ziegler, M. O. 2018. Manual of the Matlab Script FAST Calibration v1.0. World Stress Map Technical Report 18-01, GFZ German Research Centre for Geosciences. <https://doi.org/10.2312/wsm.2018.003>
- Ziegler, Moritz O. 2018a. Matlab Script FAST Calibration v1.0. GFZ Data Services. <https://doi.org/10.5880/wsm.2018.003>
- Ziegler, M. O., & Heidbach, O. 2020. The 3D stress state from geomechanical–numerical modelling and its uncertainties: a case study in the Bavarian Molasse Basin. *Geothermal Energy*. 8. <https://doi.org/10.1186/s40517-020-00162-z>

Ziegler, M. O.; Heidbach, O. 2021. Matlab Script FAST Calibration v.2.0. GFZ German Research Center for Geosciences. <https://doi.org/10.5880/wsm.2021.002>

Zoback, M.D., Barton, C.A., Brudy, M., Castillo, D.A., Finkbeiner, T., Grollimund, B.R., Moos, D.B., Peška, P., Ward, C.D. & Wiprut, D.J. 2003. Determination of stress orientation and magnitude in deep wells, *International Journal of Rock Mechanics and Mining Sciences*, 40(7-8), 1049-1076. <https://doi.org/10.1016/j.ijrmms.2003.07.001>

