Practical hints for using numerical methods in rock mechanics

Author: Prof. Dr. habil. Heinz Konietzky (TU Bergakademie Freiberg, Geotechnical Institute)

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TU Bergakademie Freiberg, Institut für Geotechnik, Gustav-Zeuner-Straße 1, 09599 Freiberg • sekr_fm@ifgt.tu-freiberg.de

1 Introduction

Although numerical software products become more and more easy to handle and find broad acceptance and use in engineering practice (see for instance EUROCODE) as well as in geo-engineering sciences, careful choice and use of these powerful tools are necessary to avoid wrong calculation results. Quite a lot of aspects have to be considered, like:

- Choice of appropriate numerical technique and tool
- Initial and boundary conditions
- Appropriate model size
- Choice of appropriate constitutive models and parameters
- Meshing (structure, density, element type) and mesh-dependency
- 2D versus 3D
- Coupling (hydro-thermal-mechanical)
- Modelling sequence
- Continuum versus Discontinuum approach
- Calculation efficiency versus accuracy
- Static versus dynamic simulations
- Large strain vs. small strain calculation modus

Also, different solution schemes (implicit versus explicit), different element-types, different couplings etc. often need application of special simulation procedures.
Therefore, careful inspection of model set-up and in-depth analysis of simulation results is necessary. Comparison with other methods and experience or measurements is strongly recommended.

A good overview how numerical modelling has to be integrated into the rock engineering design and how the corresponding auditing should be organised is provided by Hudson & Feng (2010).

2 Initial- and boundary conditions

The solution of differential equations (both, analytical and numerical) requires the specification of initial and/or boundary conditions. Boundary conditions describe time-independent or time-dependent mechanical, thermal, hydraulic, chemical … conditions, which are applied to inner or outer boundaries. Initial conditions describe mechanical, thermal, hydraulic or chemical … conditions at the beginning of the simulation (at zero point in time) either at the boundaries and/or the inner model area.

<u>Boundary conditions (exemplary):</u>

- stresses
- forces
- velocities
- accelerations

- displacements
- water pressures
- temperatures

<u>Initial conditions (exemplary):</u>

- primary stress state
- primary deformation state
- primary pore water pressure / joint water pressure
- initial temperature distribution

Displacement boundary conditions are also called ‘Dirichlet’ conditions, force and stress conditions, however, are called ‘Neumann’ conditions.

For static calculations in geomechanics, depending on the application and modelling task, displacement and stress boundaries are applied. In most cases (not always!) displacement boundary conditions deliver too small deformations inside the model and stress boundary conditions over-predict deformations. However, if boundaries are far enough away from the interesting inner model area both types of boundary conditions deliver similar results (results converge with increasing model size).
If analytical rough estimates or practical experience are not available, a preceding parameter study shall be performed to investigate the influence of model size and boundary conditions on the results of the specific model.

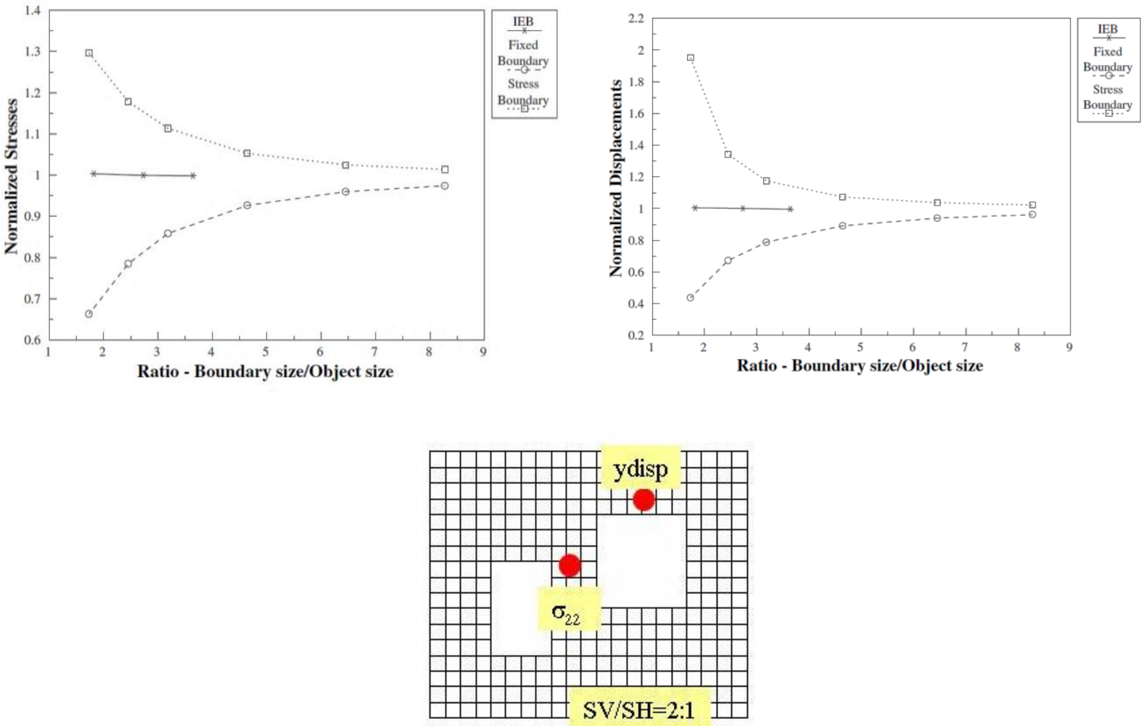


Fig. 2.1: Normalized stresses and displacements at two observation points in dependence of the type of boundary condition and the ratio of model size to excavation size [ITASCA 2011]

Exemplary, Fig. 2.1 demonstrates, how displacement and stress values inside the model with two excavations alter in relation to model size. Furthermore, this figure illustrates the influence of the displacement and stress boundary conditions on the results in comparison to the exact analytical solution. One recognizes, that with increasing distance between the boundaries and the inner model area both types of boundary conditions converge and come finally close to the analytical solution. Boundary conditions are normally applied in form of normal and/or tangential components or in Cartesian coordinates. Also, over different regions of the boundary different types of boundary conditions can be applied.

3 Meshing rules

For 2- and 3-dimensional discretization (meshing) of objects, three fundamental aspects should be considered:

- Choice of appropriate element type
- Appropriate mesh density
- Choice of appropriate meshing technique

In principle, it can be distinguished between the following element types:

- Volume elements (e. g. triangular or rectangular elements in 2D and tetrahedral or squared elements in 3D) – typical for rock mass or massive concrete
- Shell elements (planar 2D elements with negligible thickness, but explicit consideration of moments and membrane stresses) – typical for shotcrete and thin masonry or concrete walls
- Bar elements (1-dimensional elements) – typical for anchors, piles or struts

Furthermore, for one element type, different shape functions can be applied, which implies different interpolation functions and finally leads to different accuracy (non-linear interpolation).

Two competitive demands have to be considered in respect to mesh density (grid point distance):

> Mesh density ↑: this leads to improved resolution and higher accuracy, but: this leads, on the other side, to increasing calculation time and storage demand

For meshing the following general practical rules are guilty:

- Several elements of low order (linear shape function) give equivalent results compared to less number of elements of higher order (non-linear shape function)
- Refined meshing is necessary, whenever high stress and deformation gradients are expected, that means for instance at free surfaces, areas with high stiffness contrasts, areas with support elements or areas with load entry points
- Elements should be designed preferably equidistant, meaning the ratio of maximum edge length to minimum edge length should be smaller than about 10, also very small angles between edges should be avoided

- Elements should preferably aligned according to the expected stress trajectories
- Transition between coarse and fine meshed areas should be smooth (preferably without discrete jumps in element size)
- In general: Quad-elements gives more accurate results than triangular-shaped elements

4 Meshing techniques

In a broader sense, meshing comprises two phases: set up of geometrical model and subsequent filling with elements (meshing).

A distinction is made between:

- free meshing: delivers an unstructured mesh, which just satisfies a few general user defined criteria (e. g. max. edge length ≤ pre-defined value)
- mapped meshing: delivers a structured mesh, e. g. adjusted according to the model geometry and/or expected stress trajectories

The following conventional meshing techniques are used:

- Generation of geometry (e. g. CAD-based with Boolean Algebra) and subsequent automatic meshing via free or mapped meshing
- Generation via primitives (”Lego”-system): compilation via several basic bodies filled with elements (already meshed volumes)
- Deformation of a basic mesh and extension by copying / extrusion / mirroring
- Set-up of model (geometry + mesh) via imported point, edge and element data

Today, 2D meshing with different techniques is unproblematic, performed fast and nearly fully automatic. However, 3D meshing, especially with top-quality cuboidal elements and complicated geometry, like for example tunnel crossings, are still complicated to perform, quite time consuming and often manual interaction is necessary during the meshing process.

For 3D models in most cases the following procedure is applied (see also Fig. 4.4):

- Generation of geometrical model with a CAD-Program
- Export of CAD model data into a standard format (e.g. IGES, STEP, STL etc.)
- Import of CAD geometry into a meshing tool, execution of meshing and export of mesh into a format, which can be used as input for the numerical simulation tool (solver)
- Input of mesh into the numerical simulation tool and solving the problem

Several of the numerical simulation tools have already integrated CAD tools and meshers. The following Figures 4.1 – 4.7 illustrate exemplary some of the above mentioned meshing techniques. Please note, that surface remeshing allows excellent control over element size, including edges and points that need to be on the surface. Surface meshes can be used directly for volume meshers. The final solid elements composing the mesh (hexahedrons, tetrahedrons, prisms, pyramids etc.) have faces that coincide with the input surface mesh. Fig. 4.4 shows the workflow from CAD model to

3D volume mesh. Fig. 4.5 illustrates the difference between free and mapped meshing. Fig. 4.6 shows the so-called octree-meshing used to create local refinement with minimum number of elements (note, that this kind of meshing results in small errors). Remacle et al. (2010) proposed an interesting algorithm for creation of quadrilateral meshes based on prior triangulation (Fig. 4.8).

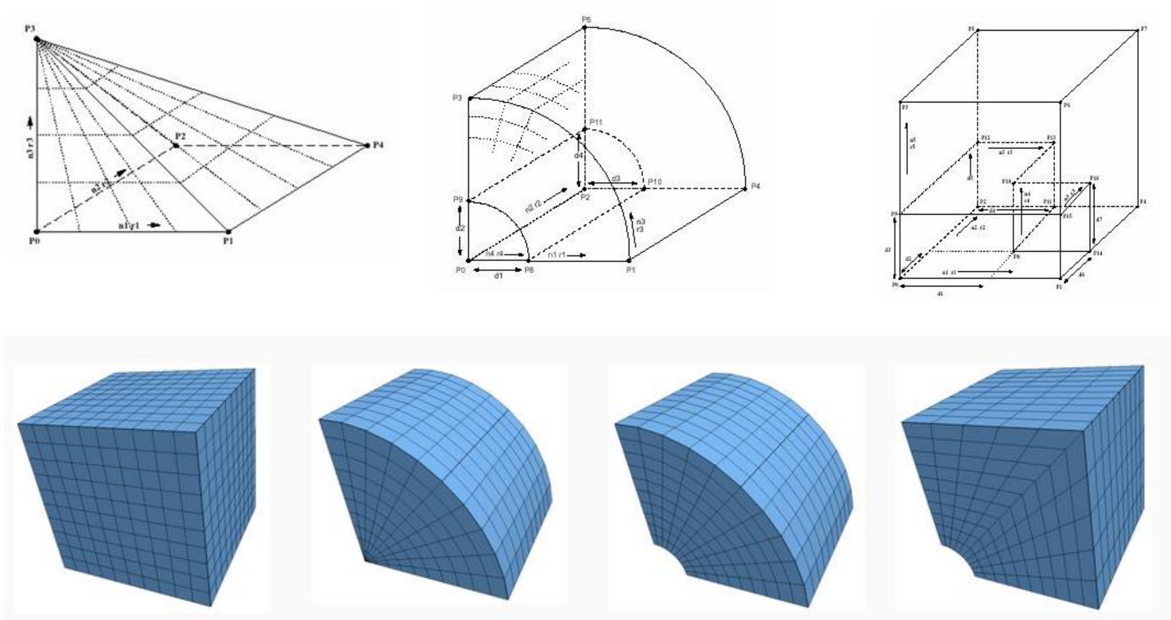


Fig. 4.1: Basic volumes filled with zones, which can be composed to a final model (‚LEGO-system‘), (ITASCA 2012)

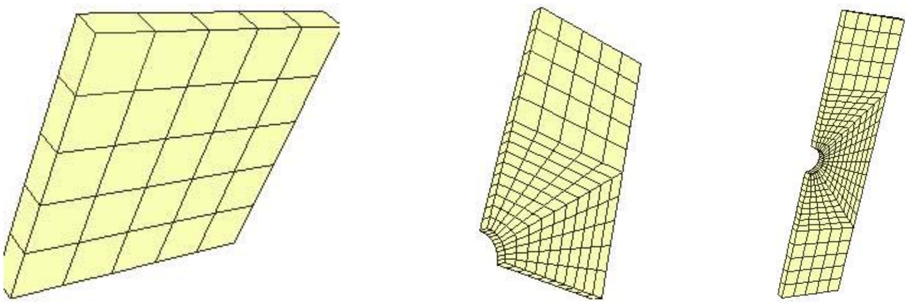


Fig. 4.2: Assemblage of subnets via docking and mirroring

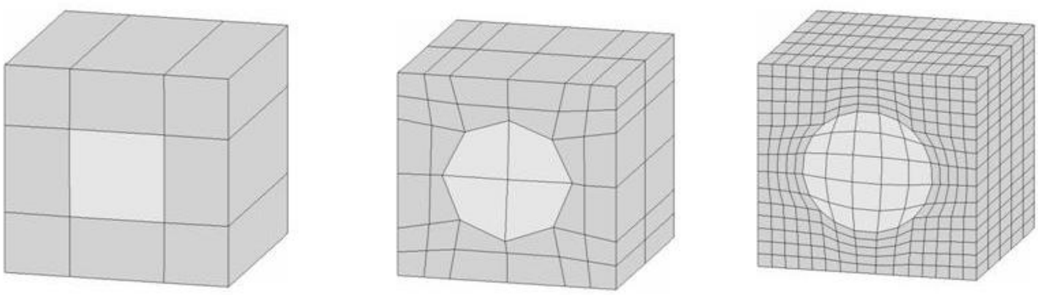


Fig. 4.3: Generation of final mesh by gradual geometrical adaption and mesh refinement

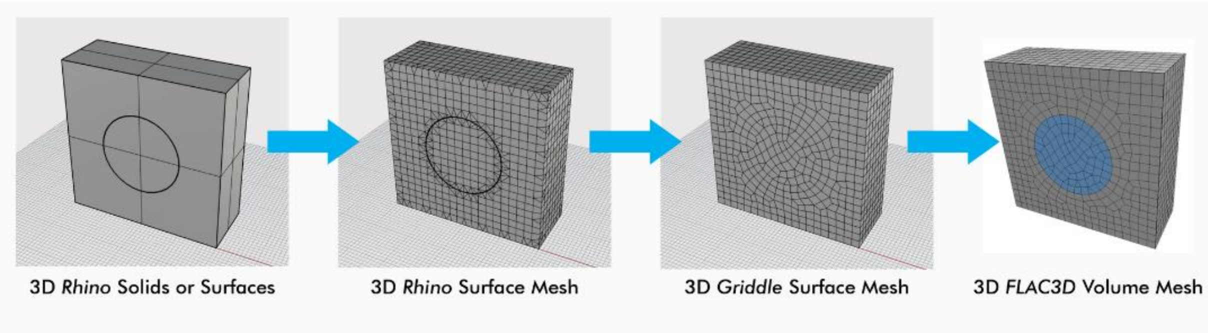


Fig. 4.4: Workflow from 3D CAD surface model to 3D volume mesh (Itasca, 2021)

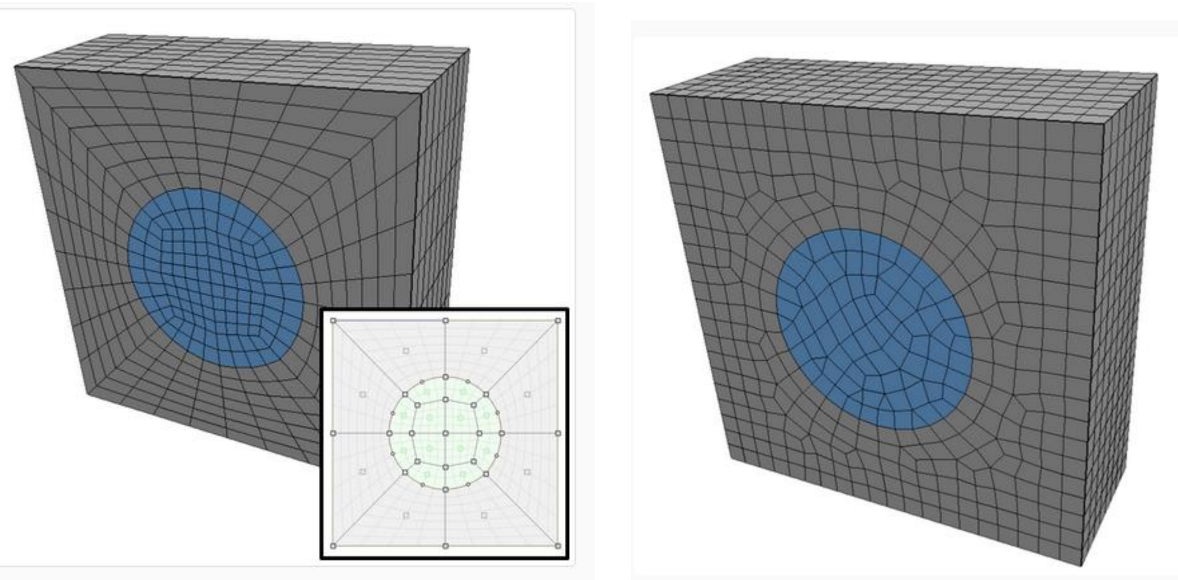


Fig. 4.5: Workflow from 3D CAD surface model to 3D volume mesh (Itasca, 2021)

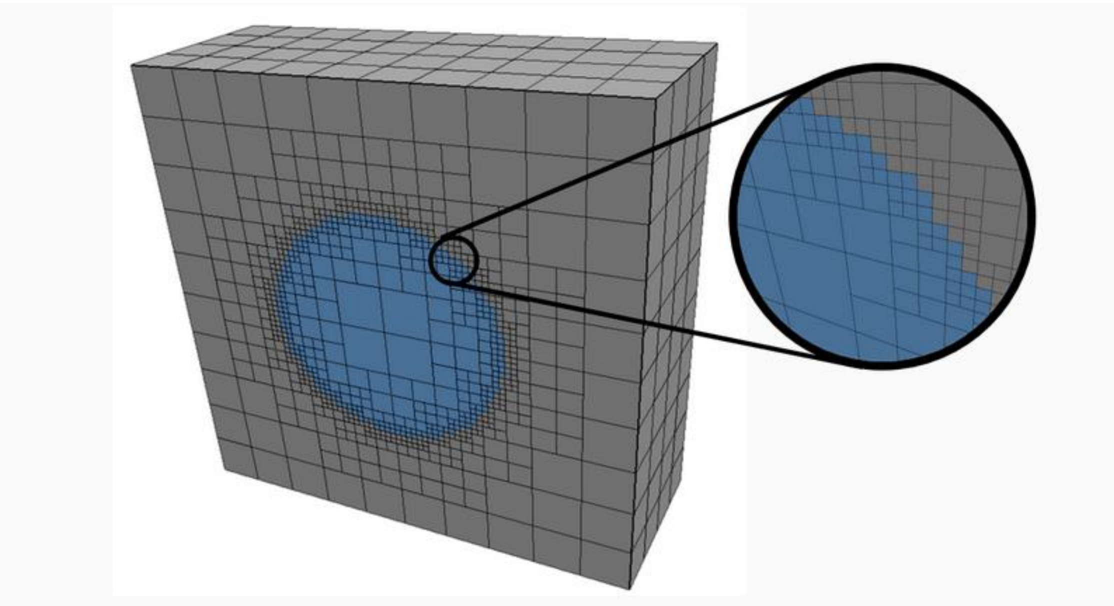


Fig. 4.6: Octree meshing (Itasca, 2021)

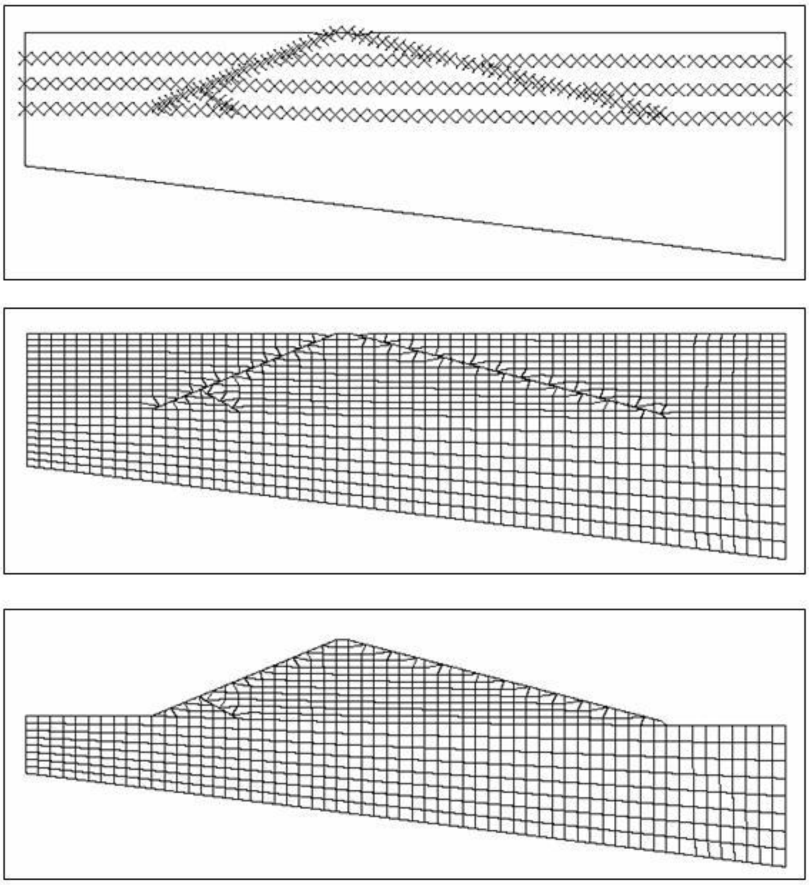


Fig. 4.7: Generation of final mesh via trimming, deformation and partial deletion of virigin (initial) mesh

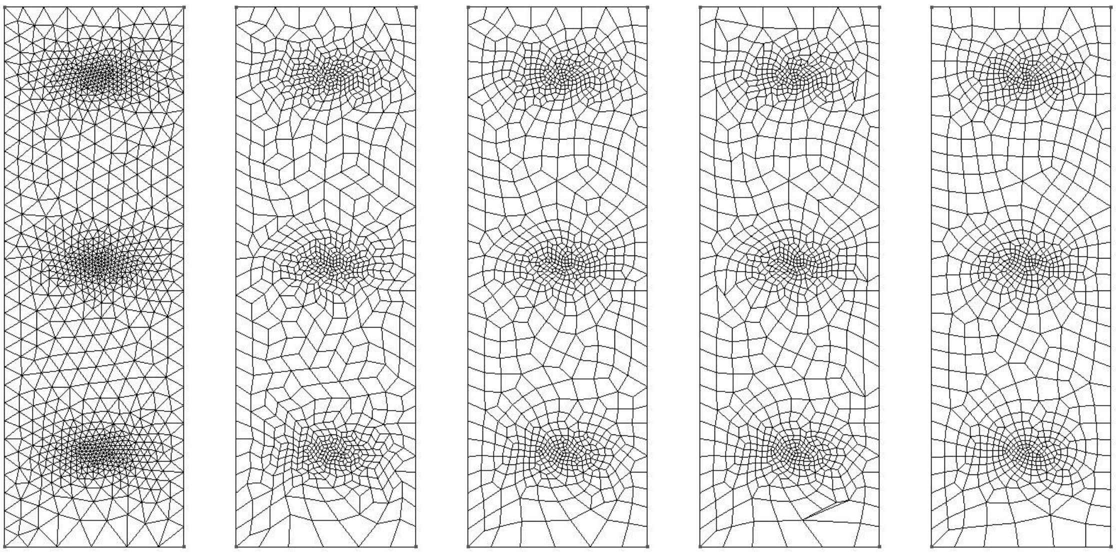


Fig. 4.8: Illustration of Blossom-Quad algorithm: transition from triangulation to quad-mesh (Remacle et al. 2010)

5 Mesh quality

Shape, structure and size of the elements (zones) of the mesh have tremendous influence on the quality of the simulation results. There are several geometric properties which influence the element quality, like:

- Aspect ratio: ration of maximum edge length to minimum edge length
- Volume ratio: ratio of volumes of adjacent zones
- Non-orthogonality: deviation from orthogonal internal angles of elements
- Skewness: deviation of optimum zone size to existing zone size
- Element type: brick, wedge etc.

Please note, the absolute and relative error is also depending on applied numerical simulation technique and shape functions. Exemplary, Fig. 5.1 documents absolute and relative errors of radial stresses for a circular opening in an elasto-plastic material for different degree of mesh resolution and different element shapes by using a finite difference code.
The ‘perfect’ element is a cube (right angles, equal zone edge size).

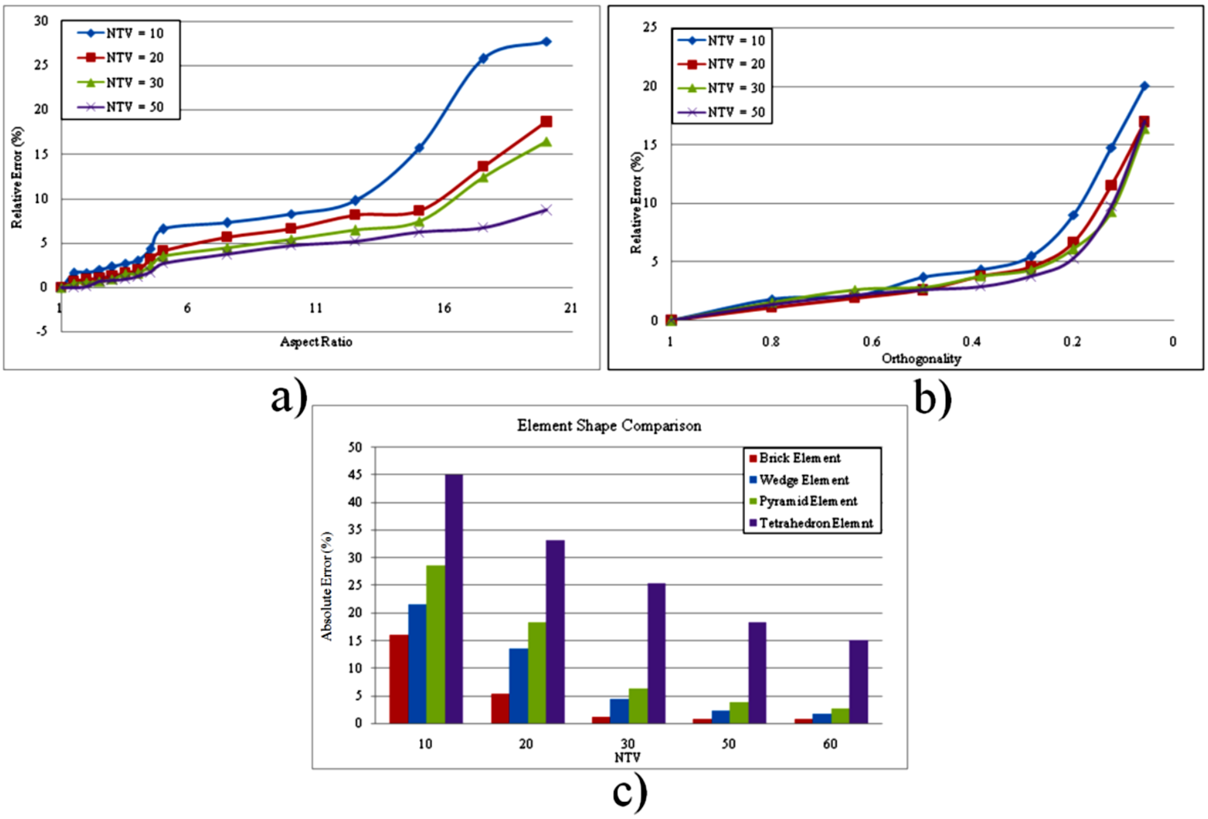


Fig. 5.1: Calculation error (radial stress) in respect to mesh parameters: (a) realtiv error vs. aspect ratio, (b) relativ error vs. orthogonality, (c) alsolute error vs. NTV (= mesh density) for different element types (Abbasi et al. 2013)

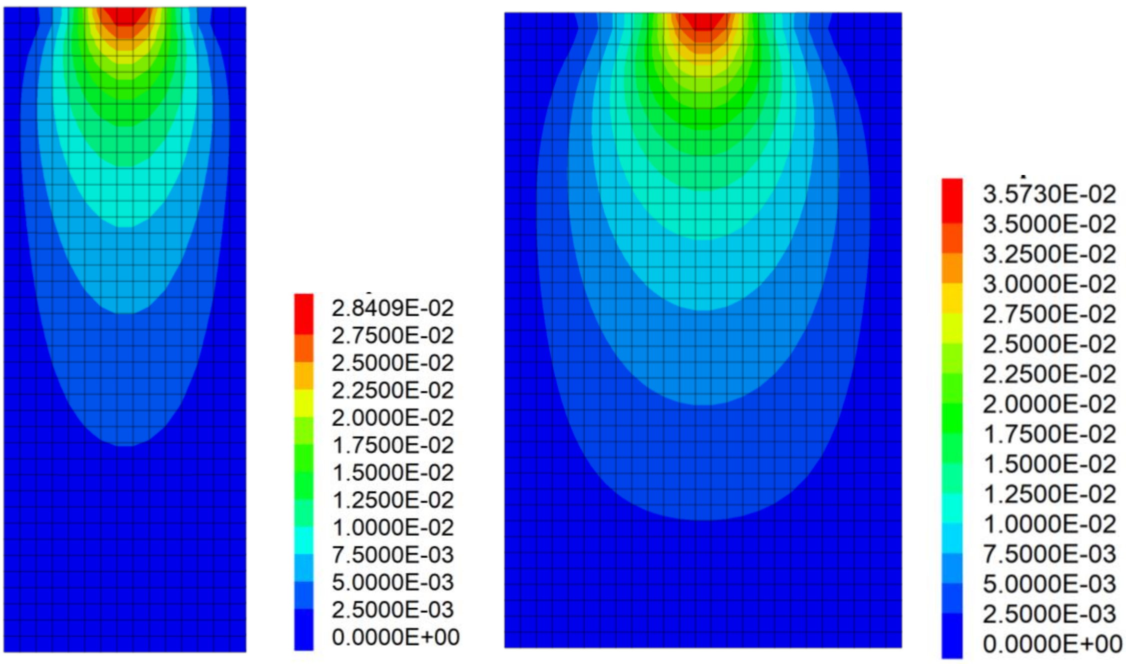
6 Model Size

The ratio between model size (overall dimension of numerical mesh) and object size (e.g. dimension of excavation, pillar, slope etc.) plays an important role in respect to correct simulations (see also DGGT 2014). An optimum of two competitive requirements have to be found (see also chapter 'Meshing rules'):

- Preferably large ratio of model size / object size to minimize boundary influence
- Preferably small ratio of model size / object size to minimize calculation time and memory space

A second aspect, especially important for settlement and uplift prediction, is the problem, that overall model size (especially in the vertical direction) has a non-vanishing influence of these deformation values. In case of large overall model dimension elastic or simple elasto-plastic models would lead to unrealistic high deformation values. To avoid these problems either depth-dependent stiffness values or so-called 'small-strain stiffness' has to be included.

The following two extremely simple examples illustrate the problem of appropriate model size (in combination with boundary conditions). Fig. 6.1 illustrates how horizontal model extension influences the displacement field. At vertical load is centrically applied at the model top. Pure isotropic elastic material behaviour is assumed. Bottom and vertical boundaries are fixed. As Fig. 6.1 documents: the displacements increase with increasing horizontal model extension. Fig. 6.2 documents a similar pattern: displacements increase with increasing model height. Of course boundary conditions have significant influence and we should be aware, that for geomechanical problems neither fixed nor free nor stress boundary conditions represent the reality in a perfect manner. Therefore: depending on the problem and the modelling task model size (extension) and boundary conditions should be selected carefully.



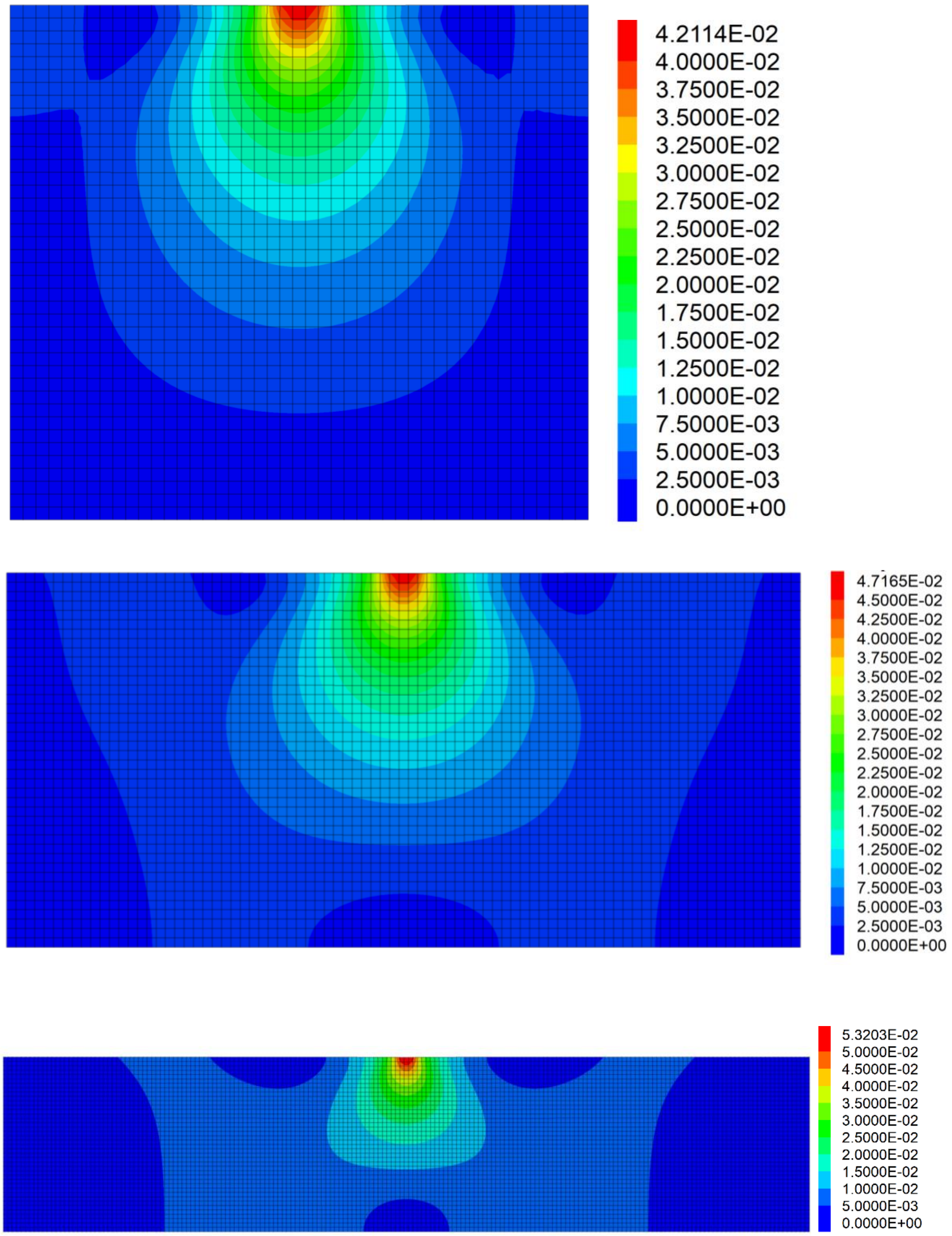


Fig. 6.1: Example: Influence of horizontal model extension on the displacement magnitude (bottom and vertical boundaries are fixed, load is applied in central position at the top over 5 m in each model. Grid size is 1 x 1 m. Horizontal dimensions are: 15, 25, 45, 85 and 185 m; vertical heigth is always 40 m)

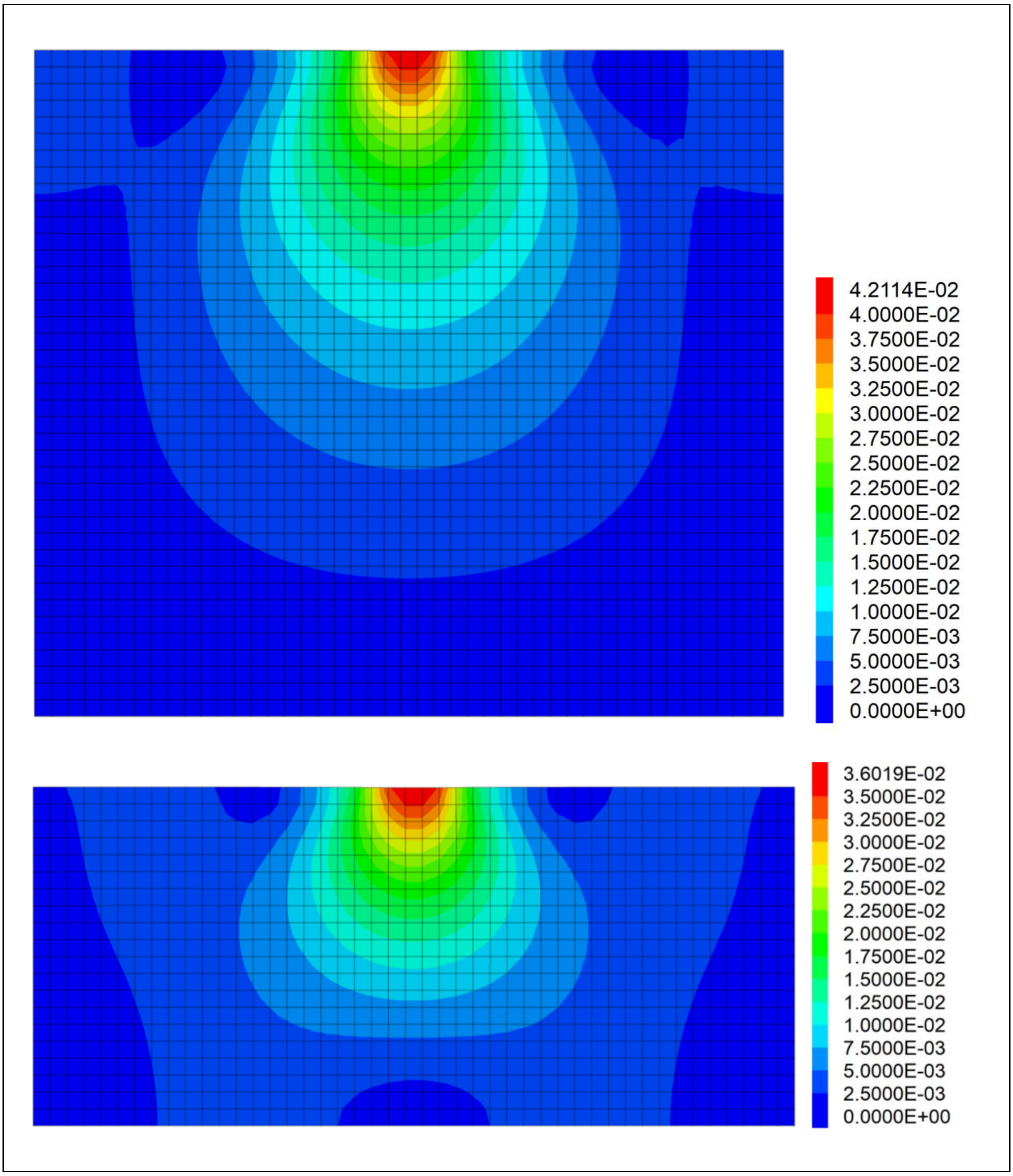


Fig. 6.2: Example: Influence of vertical model extension on the displacement magnitude (same conditions as documented in Fig. 6.1; horizontal extension is 45 m, vertical dimensions are: 40 and 20 m)

7 Continuum versus Discontinuum – Scale Effects

At a certain scale all geomaterials and construction materials should be considered as discontinua, e.g. sand in form of grains or a fractured rock mass in form of rock blocks as well as composite constructions like tunnel lining / rock mass, anchor / rock mass, geotextile / ballast or pile / wall.

Whether discontinuum modelling shall be applied or not, depends on three factors:

- Ratio of representative elementary volume (REV) to total volume
- Modelling task (interesting phenomena)
- Availability of parameters
- Availability of software

REV is defined as the smallest volume, from which measurements, parameters and object reactions, respectively, can be obtained and which are representative for the whole rock mass. That means: the REV is the smallest continuum mechanical volume, which is statistical equivalent to the in-situ discontinuum.

Fig. 7.1 shows the history of the two quantities n_{pm} and n_{fr} as function of considered volume. One recognizes, that the spread of the quantity decreases with increasing volume (e.g. strength values, deformation module, permeability etc.) und finally the quantity converges and reaches a nearly constant value.

Beyond a specific volume V_{min}, which represents the REV, the quantity does not change any more significantly even over a bigger volume towards V_{max}. Like Fig. 7.1 also shows, the area of V_{min} - V_{max} can be quite different for different physical quantities. If several quantities have to be considered simultaneously the common intersection (overlap) has to be considered. In such a case R_{fp} hast to be considered as REV.

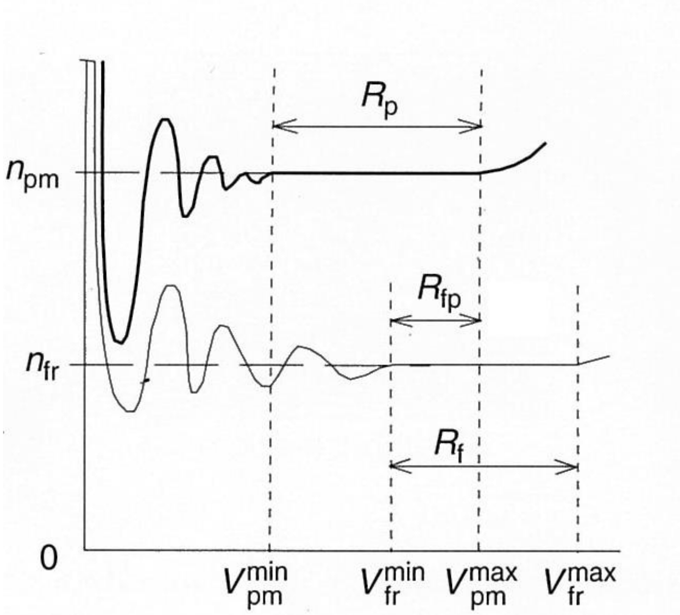


Fig. 7.1: Parameter history as function of considered volume (scale effect).

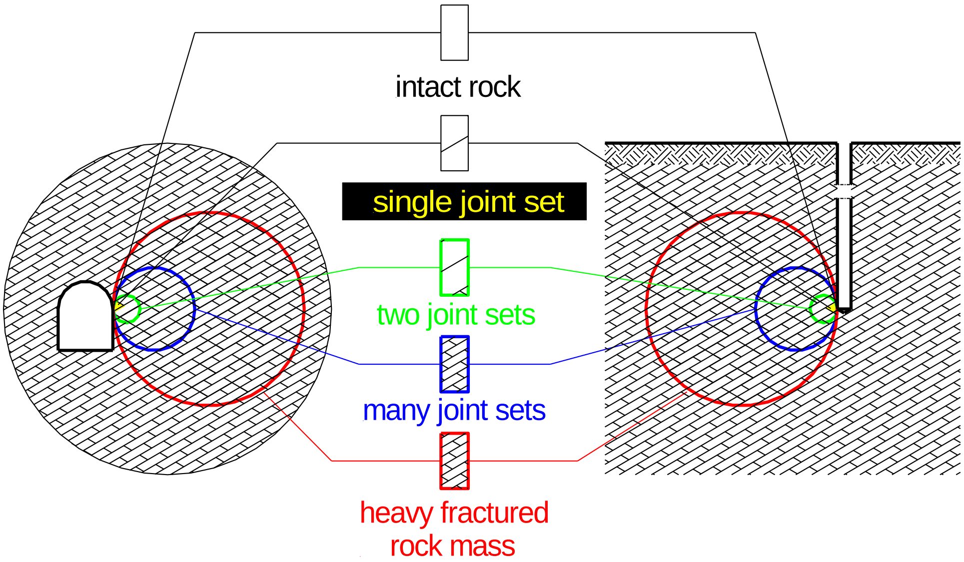


Fig. 7.2: Relation between structure and considered volume using the example of a rock mass (scale effect).

Depending on the considered volume the rock mass structure shall be modelled in different ways (see Fig. 7.2). In case of very small volumes, it is possible that only intact rock exist and therefore a classical continuum mechanical approach with rock mechanical parameters is recommended. At bigger volumes several single joints or joint sets are observed, which can be handled best with a discontinuum mechanical approach (e.g. Discrete Element Method), where different material laws and parameters are assigned to rock matrix and discontinuities in an explicit manner. If a huge number of joints or joint sets exist (highly fractured rock mass), it make sense, to go back to a continuum mechanical approach, where the effect of the discontinuities is not directly (discrete) considered, but in a smeared manner by reduced strength and stiffness parameters. But, due to increased computer power today even complex DFN's can be modelled via DEM-techniques (e.g. Sainsbury 2015).
The scale effect is highly important for rock masses and has to be considered carefully whenever constitutive laws and corresponding parameters are chosen. Rock mass classification schemes can be used to deduce appropriate rock mass parameters based on rock mechanical lab data and engineering-geological investigations according to the following scheme:

- Determination of rock mechanical parameters in the lab
- Engineering-geological inspection (core analysis, joint-set statistics etc.)
- Rock mass classification (e.g. RMR, Q, GSI, RQD) on the basis of the engineering-geological inspection and the rock mechanical lab data
- Deduction of rock mass parameters for suitable constitutive laws (e.g. Hoek-Brown, Mohr-Coulomb etc.) on the basis of the rock mass classification

8 2D versus 3D

In the forefront of any numerical model set-up the following key questions should be answered:

- Is a 3-dimensional modelling necessary or is a 2-dimensional consideration acceptable?
- Are there symmetry lines or planes which would allow to reduce the model size?

A complete 3-dimensional modelling is necessary, if:

- the strike of the geological elements (layer, joint, fault, bedding plane …) does not coincide with the long axis of the geotechnical construction
- the axes material anisotropy do not coincide with the axes of the geotechnical construction
- the directions of principal stresses are neither parallel nor perpendicular to the axes of the geotechnical construction
- the dimensions of the geotechnical constructions and the geological bodies, respectively, are nearly equal in the three spatial directions
- several structural components intersect each other (e.g. tunnel crossings)
- applied boundary conditions (forces, velocities, stresses ….) have components in all 3 spatial directions

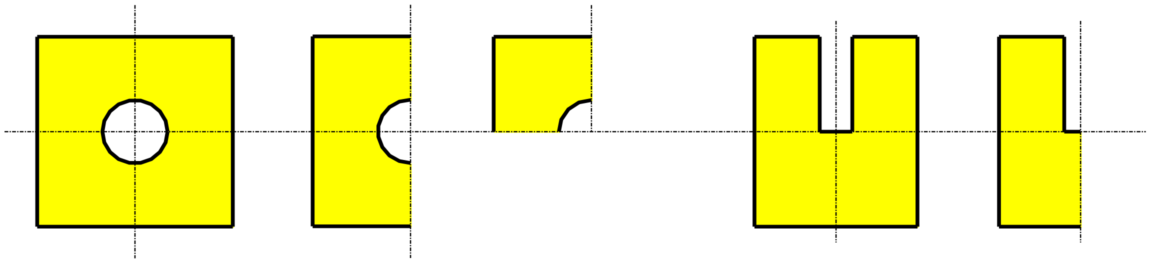


Fig. 8.1: Examples for model reduction on the basis of the consideration of pure geometrical symmetry conditions (full model, half model and quarter model)

If symmetry conditions are met, models may be reduced (simplified) to half or quarter models or even reduced from 3D to 2D (axisymmetric). However, one has to take into account, that symmetry conditions have to be referred to several aspects, which have to be met simultaneously:

- in respect to the geometry
- in respect to the stress field
- in respect to the constitutive law (planes of anisotropy, orientation of joints etc.)
- in respect to the modelling sequence (construction process, excavation phases, support measures etc.)
- in respect to boundary conditions
- in respect to support installation- and preservation measures (anchors, shotcrete, piles, struts etc.)
- in respect to couplings (hydraulic, thermal etc.)

Fig. 8.1 illustrates potential model reductions on the basis of pure geometrical considerations, like used to simulate shaft- , tunnel- and borehole problems or building excavations.

9 Specifics for Simulation of Dynamic Processes

The simulation of dynamic processes involves wave propagation and requires the consideration of four important aspects:

- The correct representation of movement of waves requires that the maximum grid point distance $h_{p,s}$ has to be considerable smaller than the shortest wave length $\lambda_{p,s}$:

$$h_P \approx 10 \cdot \lambda_P = 10 \cdot \frac{c_S}{f} = \frac{\sqrt{\frac{E}{\rho} \frac{1-\nu}{(1+\nu)(1-\nu)}}}{f} \tag{9.1}$$

$$h_S \approx 10 \cdot \lambda_S = 10 \cdot \frac{c_S}{f} = \frac{\sqrt{\frac{G}{\rho}}}{f} \tag{9.2}$$

h_P: maximum grid point distance for P-wave (longitudinal wave / compression wave)
h_S: maximum grid point distance for S-wave (transverse wave / shear wave)
c_P: P-wave velocity
c_S: S-wave velocity
f: Frequency
E: Young's modulus
ν: Poisson's ratio

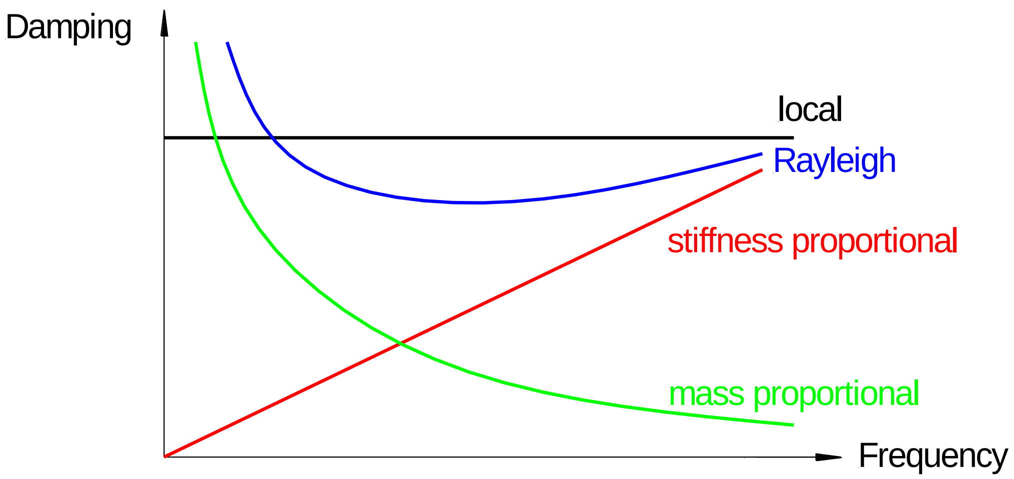


Fig. 8.1: Damping vs. frequency for different damping procedure

- Model boundaries shall be designed in such a way, that reflections are avoided to a large extent (application of anechoic boundary conditions).
- As a general rule, dynamic strength parameters are higher than static values (e.g. factor of app. 1.5). Therefore, strength parameters have to be adjusted for the dynamic calculation part.

- The numerical algorithm has to include physical correct damping for wave propagation. Often applied algorithms are:
    - mass-proportional damping
    - stiffness-proportional damping
    - local damping
    - Viscous damping
    - Rayleigh damping
    - Intrinsic damping (damping due to plastification)

The damping behaviour can be described by the seismic quality factor Q. The seismic quality factor is frequency independent and effects increasing damping with increasing frequency, which is characteristic for geomaterials. This requirement is satisfied by the local damping scheme and, for a broader frequency range, also for the popular Rayleigh damping (Fig. 9.1).

$$Q = \frac{\pi f}{\alpha c} \tag{9.3}$$

where:
f: frequency [Hz]
c: wave speed [m/s]
α: damping coefficient [m^{-1}]

The logical consequence is, that normally dynamic meshes shall have much higher resolution (much smaller grid point distances). This results in larger computation times. Also, often it is necessary to filter the dynamic input signal to suppress higher frequencies and to perform baseline-correction.

An important parameter for solving dynamic problems, but also for other non-stationary processes like fluid flow, is the so-called Courant-Friedrichs-Lewy condition (sometimes also called Courant number C):

$$C = \frac{c \cdot \Delta t}{\Delta x} < 1 \tag{9.4}$$

where:

c	velocity of physical quantity (wave speed, fluid flow velocity etc.)
Δt	time step
Δx	gridpoint distance

C should be smaller than 1, may be 0.7 from the practical point of view. This is a necessary, but not sufficient condition to obtain stable and correct results.

10 Mesh dependency in the post-failure region

The post-failure behaviour is characterized by so-called 'localization'. Localization means the progressive accumulation (concentration) of microcracks within a small macroscopic fracture plane (zone, band). This process is numerically represented by the so-called strain softening, which is dependent on the grid structure (Fig. 10.1). That means, that the stress-deformation behaviour inside the post-failure region is heavily dependent on the mesh resolution. In principal, there are three different solutions to overcome this problem:

- Calibration on a fixed grid structure (mesh resolution should be constant for any model using one calibrated data set)
- Adaptive re-meshing inside the localization (mesh refinement)
- Extension of the constitutive model by internal scaling parameter (regularization)
- Using of Cosserat theory

Similar behaviour is sometimes observed, when static problems with pronounced plastification are calculated by using explicit methods and loading or unloading occurs instantaneously. Therefore, in such cases properties, loads or geometrical changes should be performed gradually. Exemplary, Fig. 10.3 shows displacement magnitudes along the tunnel contour for a model according to Fig. 10.2 with isotropic virgin stress field, but anisotropic material behaviour with complex plastification pattern. As Fig. 10.3 illustrates, coarse mesh (here: 900 zones) does not deliver correct values, but meshes with number of zones around 14000 or bigger give nearly identical results. Also, without soft relaxation of boundary stresses at the tunnel contour (see dashed line in Fig. 10.3) wrong displacements are obtained. That statement, that appropriate choice of elements and mesh density is essential to obtain reasonable results is supported by a lot of studies, e.g. Batoz et al. (1980), Jovanovic et al. (2010), Ljustina et al. (2014) or Veyhl et al. (2010).

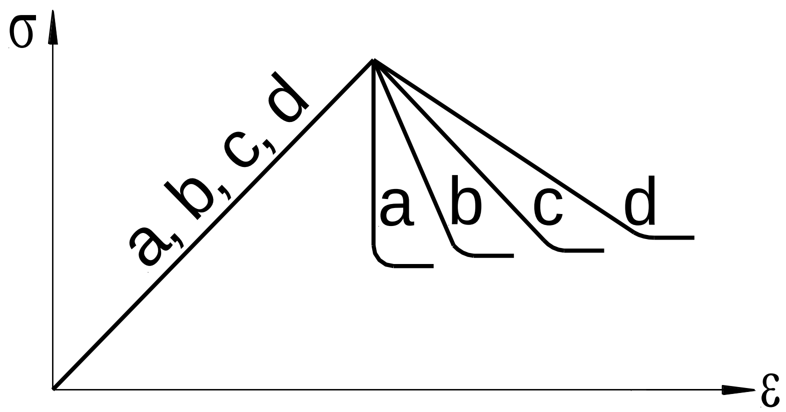


Fig. 10.1: Stress-strain behavior with strain-softening and different mesh refinement a,b,c and d without any procedure to avoid influence of mesh dependency

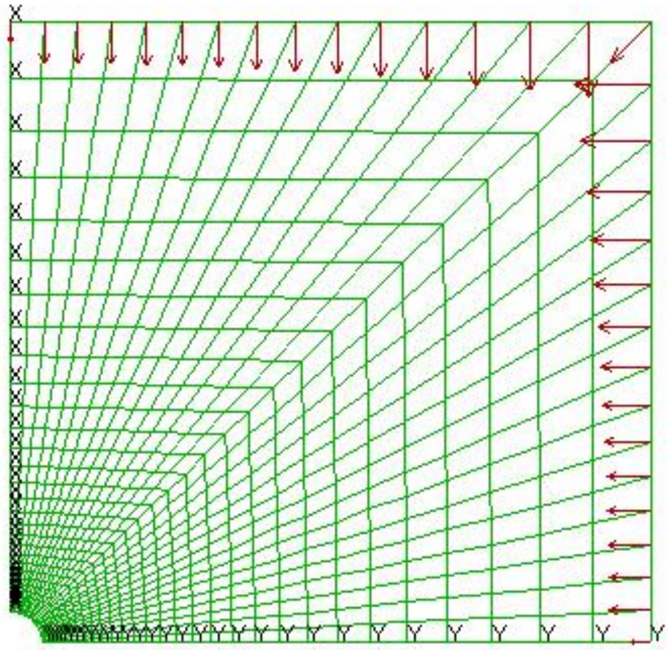


Fig. 10.2: Mesh for ¼-symmetric tunnel including boundary conditions (900 zones)

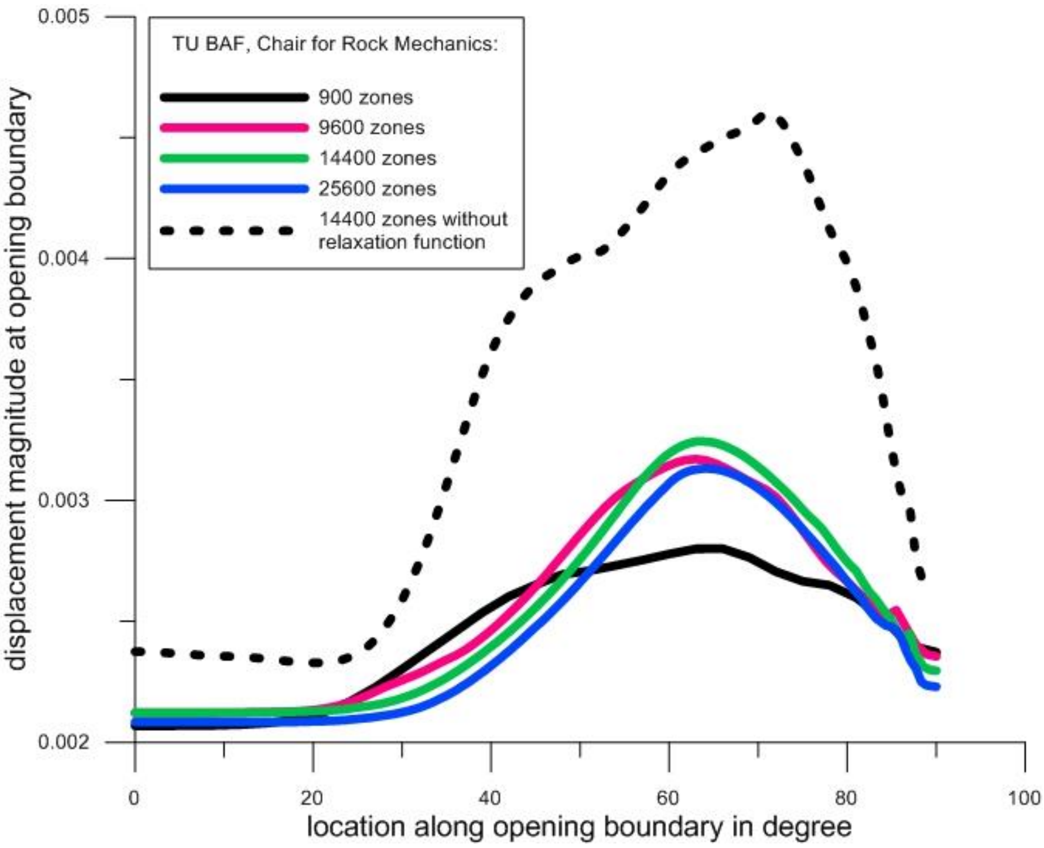


Fig. 10.3: Displacement magnitudes along tunnel contour vs. location of observation point

As mentioned above, one possibility to overcome the problem of mesh dependency is to use the Cosserat theory, which implies not only deformations, but also rotations and corresponding moment stresses. It also implies, that the stress tensor is not any more symmetric. As Fig. 10.4 exemplary documents, inside the shear bands - besides shear deformations - also significant rotations occur.

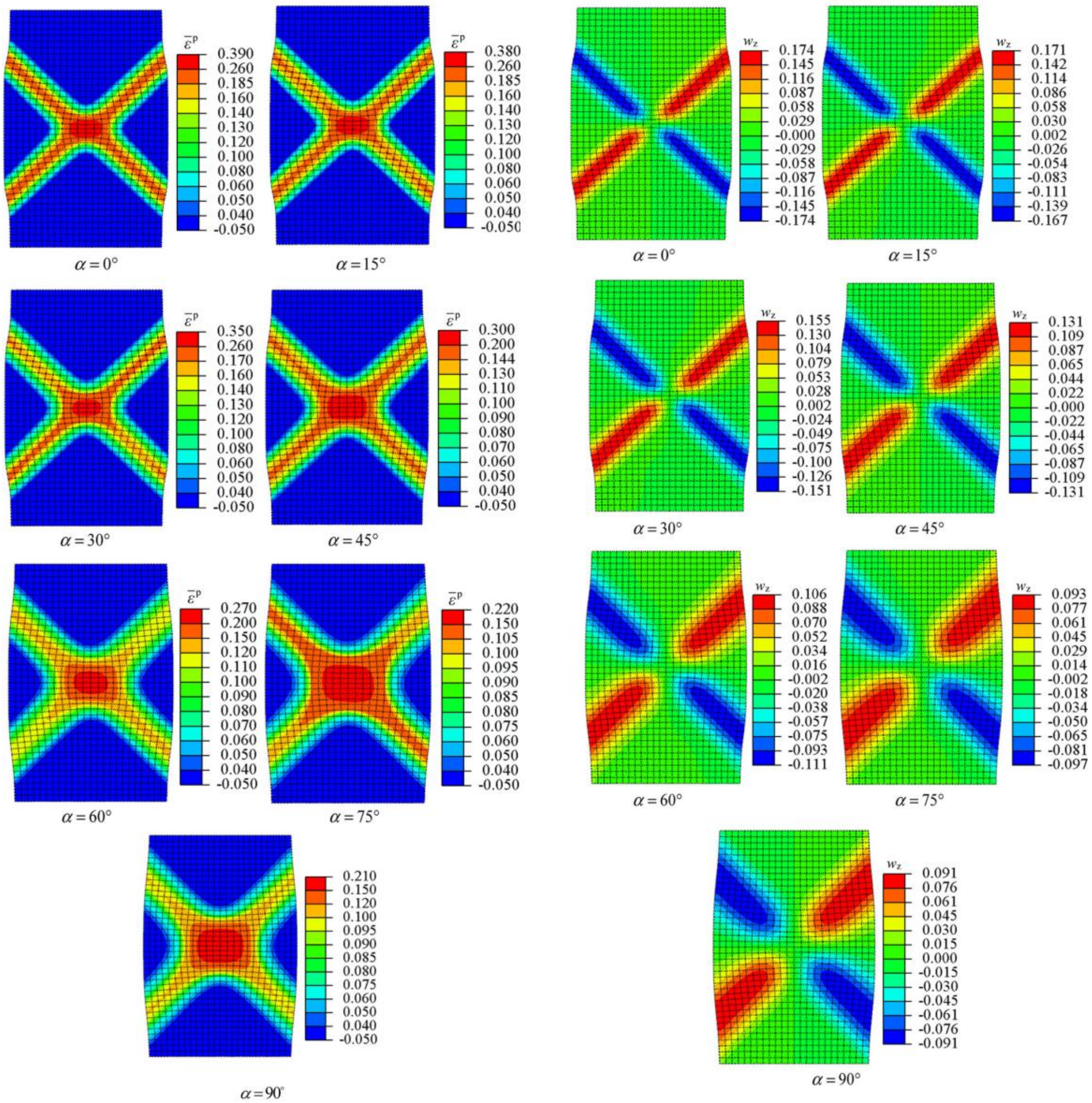


Fig. 10.4: Plastic strain (left) and rotations (right, in radians) for a biaxial loaded sample (transverse isotropic MC model) with different angle of weak plane α in the post-failure region at 6% vertical strain (Wei et al. 2025).

Fig. 10.5 documents the mesh-independency of the simulation results using meshes of difference size in comparison with the classical mesh-dependent approach.

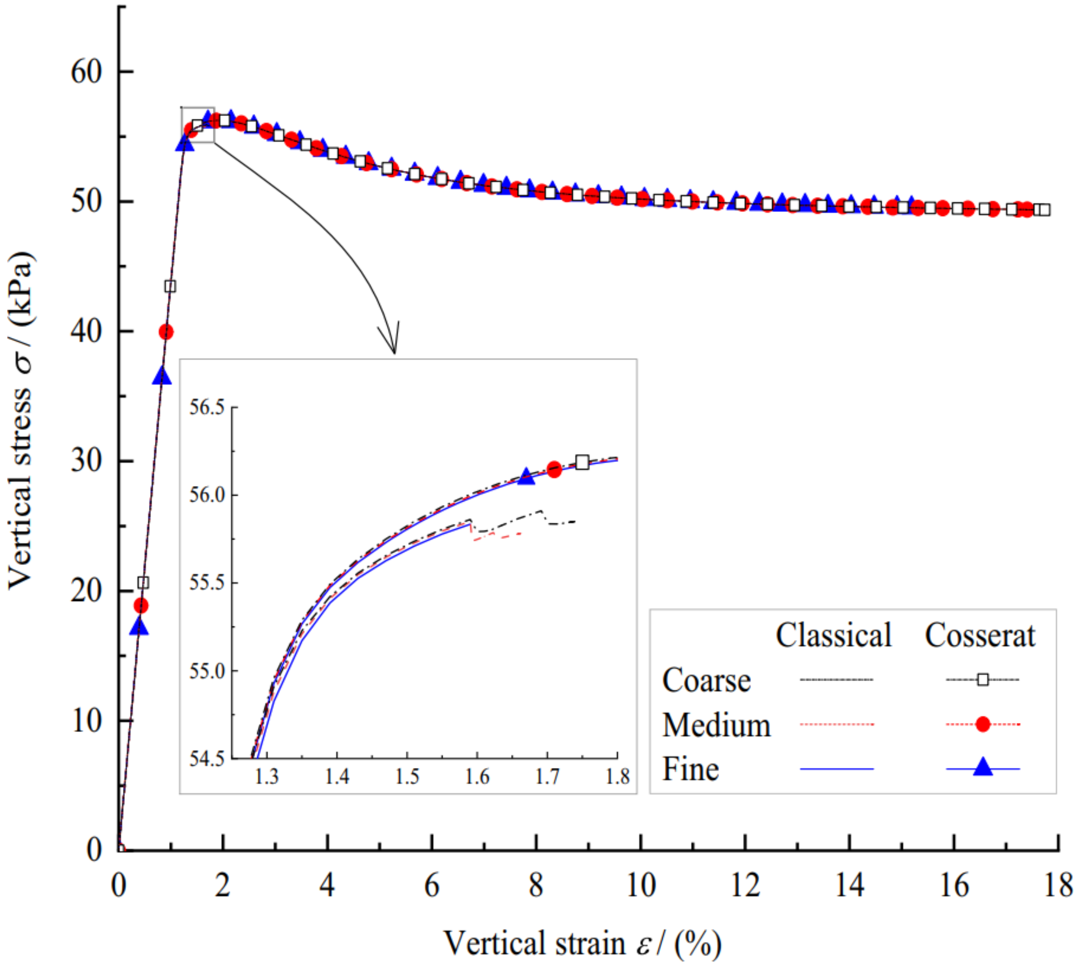


Fig. 10.5: Stress-strain curve for model with inclination angle of weak plane of 45° (Wei et al. 2025). The edge length of the meshes are as follows: coarse mesh: 3.5 mm, medium mesh: 2.5 mm, fine mesh: 1 mm.

11 Parallel Computing

Huge numerical models (huge number of elements, zones, blocks, grid points etc.) demand very long runtimes (days up to weeks). Therefore, parallelizing also called high performance computing (= usage of several processors in parallel) is suggestive. Parallelization can be realized in different ways: e.g. by hyper- and multi-threading (shared memory computing) or physical partitioning of the model to several processors (at best this could be several processors at one board, but also several computers within a network or cluster – distributed memory computing). Shared memory computer reach maximum speed, if all processors on board are used. Further speed increase can be reached if hybrid parallel computing is applied (combination of shared and distributed memory methods). However, the calculation speed does not linearly increase with number of processors, but the calculation speed follows Amdahl's law:

$$S_m = \frac{1}{f_s + \frac{f_p}{N}} \tag{11.1}$$

where:

S_m factor of speed increase
N number of processors
f_p share of parallelized code
f_s share of serialized code

It holds $f_s + f_p = 1$, where $f_p < 1$, because at least the communication between processors has to be performed in a serial manner. Fig. 11.1 illustrates Amdahl's law.

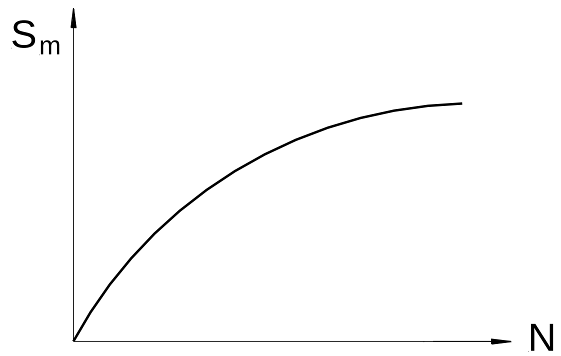


Fig. 11.1: Amdahl's law: Increase in claculation speed S_m as fuction of number of processors N

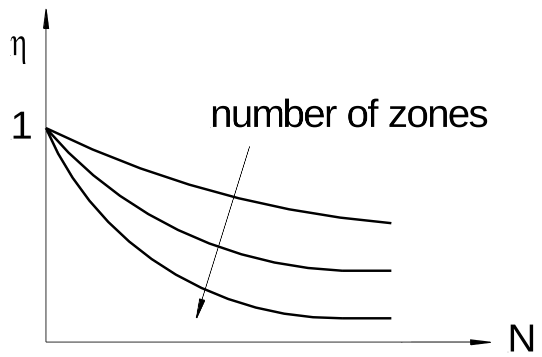


Fig. 11.2: Calculation efficiency η as function of number of processors N and number of zones

To evaluate the efficiency of parallelization, a measure of efficiency η can be defined (Fig. 11.2):

$$\eta = \frac{T_S}{N \cdot T_N} \tag{11.2}$$

where:
T_S calculation time using one processor
T_n calculation time using N processors
N number of processors

The efficiency of parallelization increases with increasing number of zones and decreases with rising number of processors.

Exemplary, Fig. 11.3 and 11.4 show results in respect to efficiency by parallel computing of CFD problems using a HPC cluster.

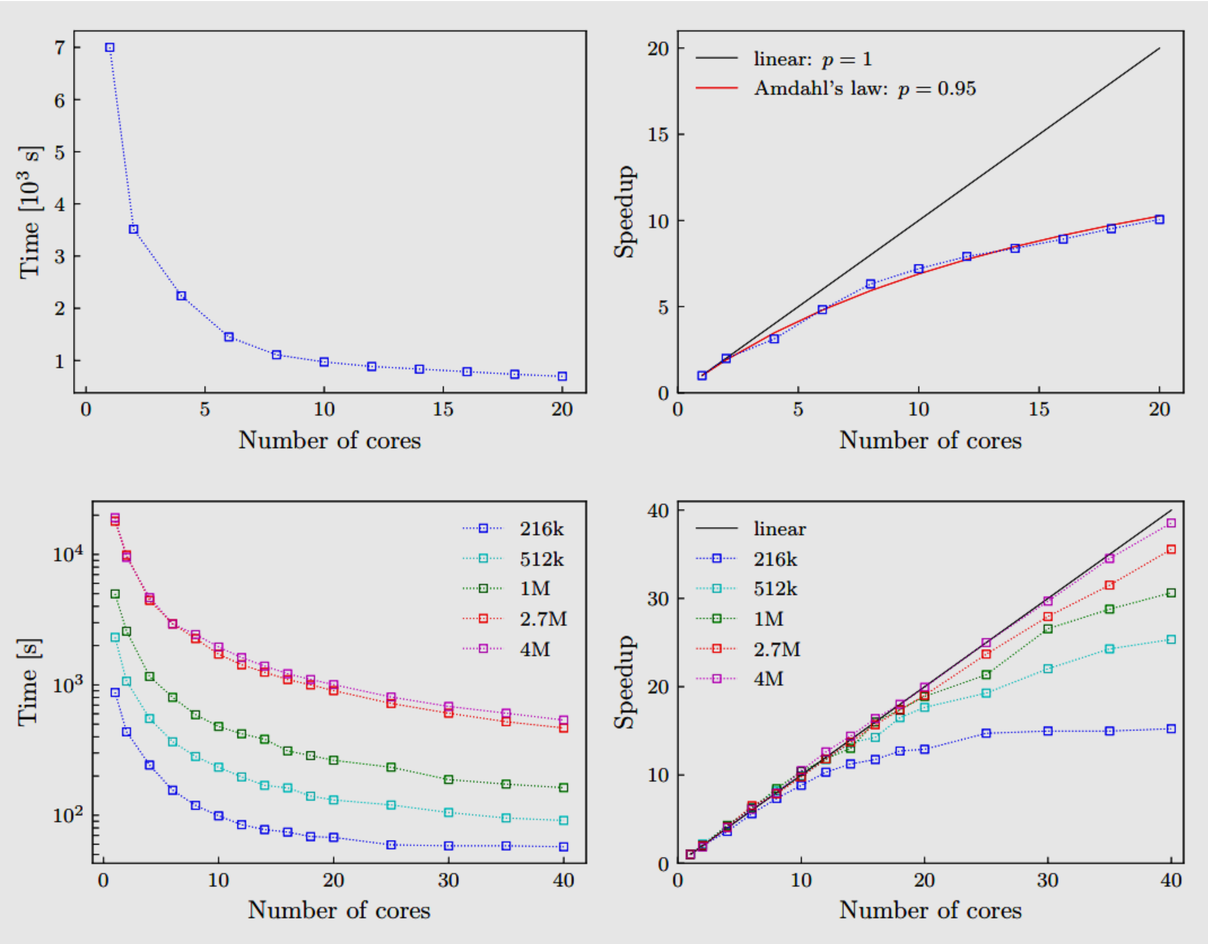


Fig. 11.3: Calculation performance on an HPC cluster for a fixed problem, top: calculation time and speed-up for a 2D mesh with 100.000 zones using different number of cores (note: p=f_p), bottom: calculation time and speed-up for a 3D mesh with 216.000 to 4.000.000 zones using different number of cores (Finenko, 2022)

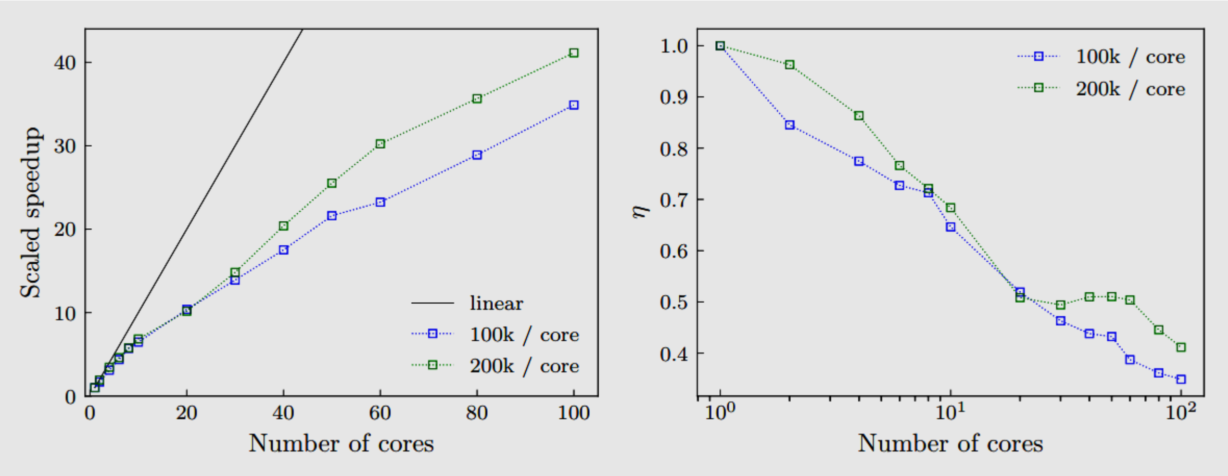


Fig. 11.4: Performance scaling on a HPC cluster for growing problem size, left: speed-up vs. number of cores for mesh with 100.000 or 200.000 zones per core, right: corresponding efficiency (Finenko, 2022)

12 Large strain vs. small strain modus

Meshless (mesh-free) methods always update coordinates of their elements during the calculation. However, mesh-based methods like FEM or FDM can be run either in small strain mode (no updating of zone/node coordinates during deformation) or large strain mode (permanent updating of zone/node coordinates). Often the small strain mode is used as standard, also some codes are not able to handle the large strain mode. As long as deformation of elements are negligible small compared to element and edge length, respectively, the small strain mode can be applied. However, especially in geomechanics (rock as well as soil mechanics) large deformations often (typically) occur and application of the small strain mode can induce large errors.

The following simple elastic example demonstrates the problem (see Fig. 12.1 and 12.2): a soft cubic rock block with 1 m edge length is loaded by an extremely stiff and heavy rock block of 2 x 2 x 1 m. The problem is run using the small and large strain modus. The gravitational force of the upper block is 10 MN. Using the small strain modus delivers – as expected – a vertical stress of 10 MPa (10 MN / 1 m^2) in the lower soft block. Using the large strain modus delivers a vertical stress of only 6.6 MPa because the cross section is significantly extended from 1 m^2 to about 1.5 m^2. Therefore, the same load produced by the stiff upper block will produce a lower vertical stress in the deformed lower block. The large strain modus delivers the correct solution, the small strain modus shows a significant error of about 50%. Comparing Fig. 12.1 and 12.2 also reveals, that not only stresses, but also deformations are wrong using the small strain modus (for instance: 15 cm versus 12 cm for horizontal displacement).

Large strain has to be expected for instance whenever:

- Creep is considered
- Plastification occurs
- Soft material under high load is considered
- Fracturing / failure occurs
- Impact is considered

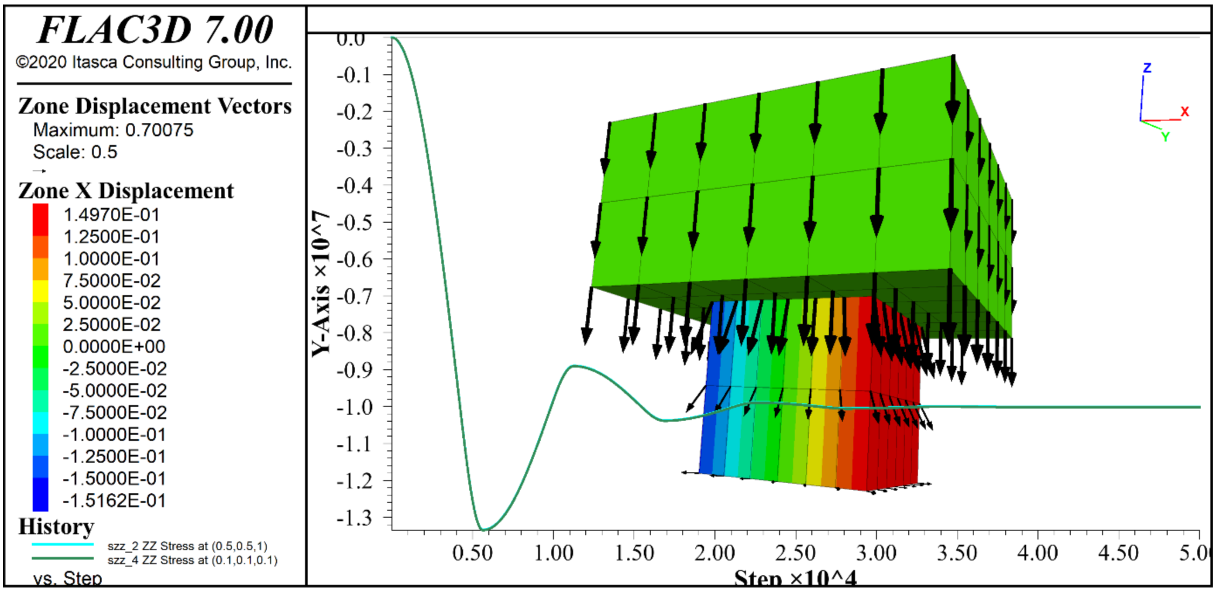


Fig. 12.1: Displacement vectors [m], horizontal displacement contours [m] and vertical stress evolution [Pa] in lower block using **small strain modus**

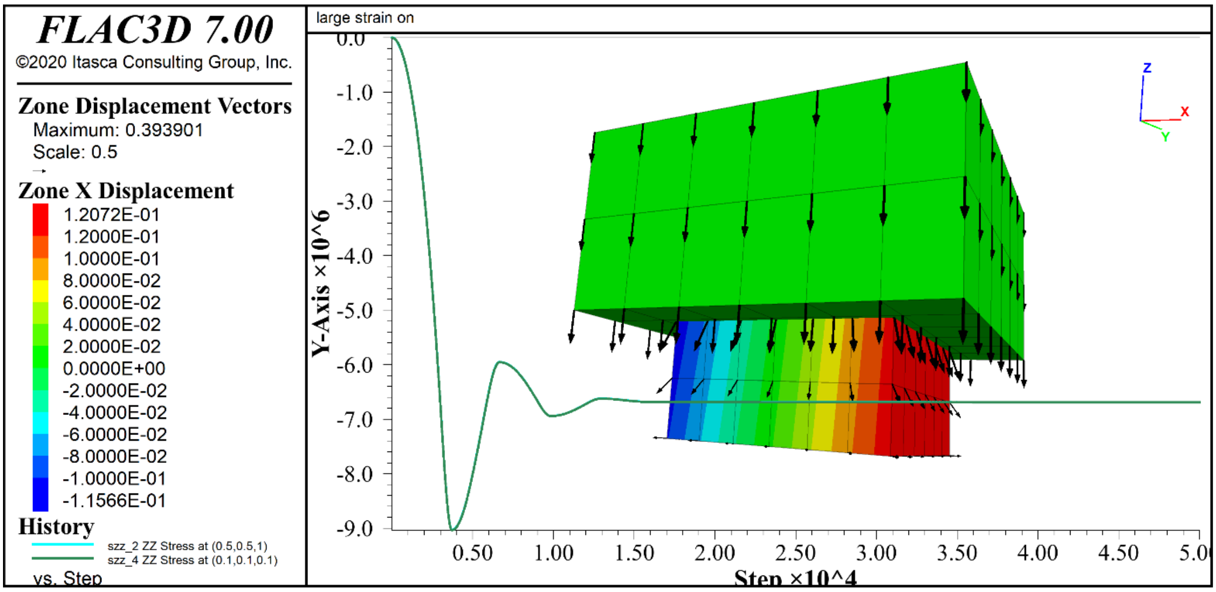
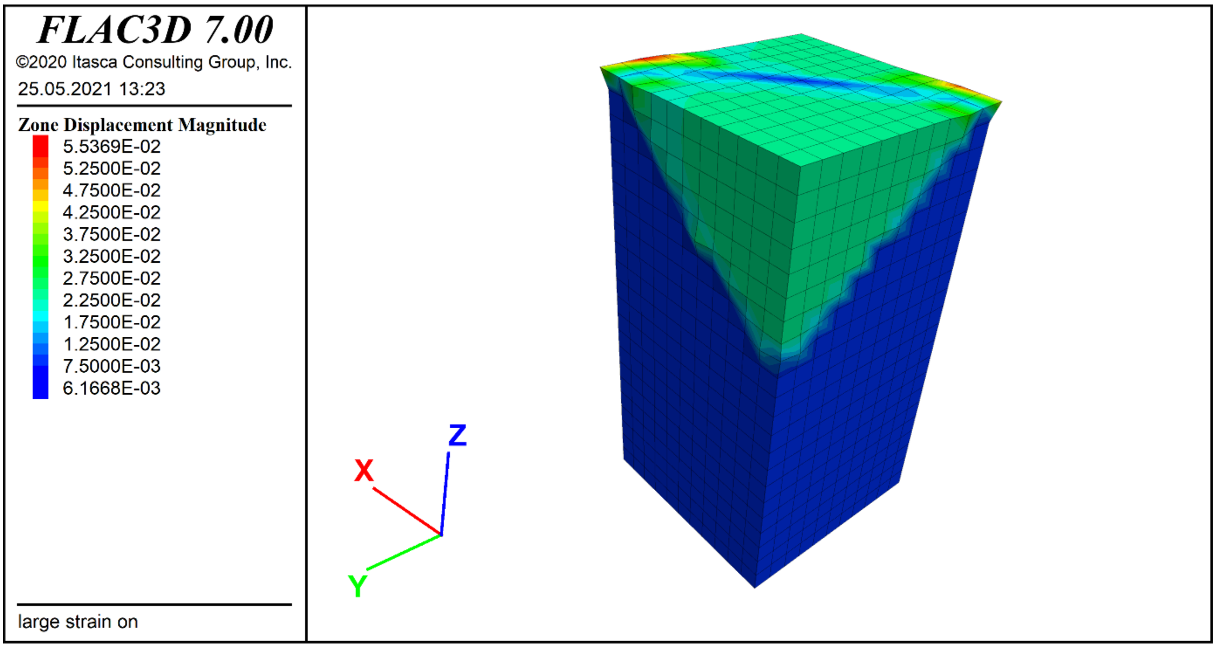


Fig. 12.2: Displacement vectors [m], horizontal displacement contours [m] and vertical stress evolution [Pa] in lower block using **large strain modus**

The following example shows the simulation of an UCS test (sample size: 1 x 1 x 2 m) with Mohr-Coulomb plasticity and strain softening applying a constant loading velocity at top and bottom of the sample. Provided pictures represent point in time when vertical displacements at bottom and top of the model have reached 9e-3 m. In general both procedures show a physical plausible result with strain localization (shear banding). However, the magnitudes in terms of displacement and deformation are quite different (see Fig. 12.3 and 12.4). Also the shear band development is different (see Fig. 12.5).



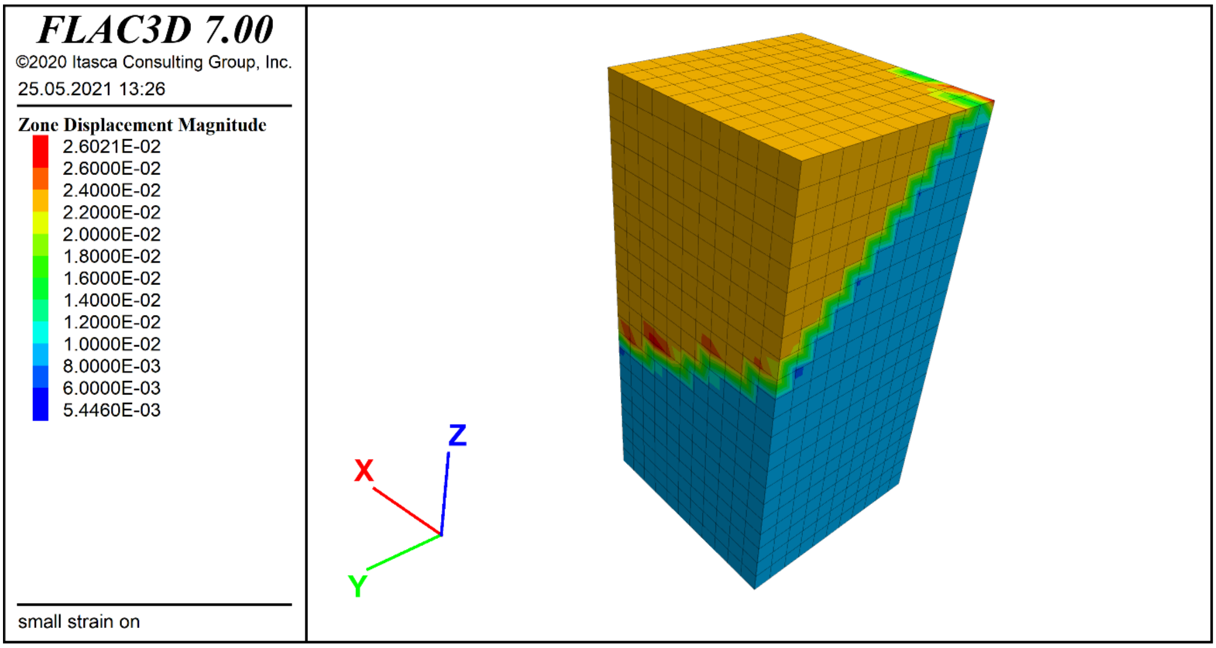


Fig. 12.3: UCS test: displacement magnitudes [m] for **large strain modus** (above) **and small strain modus** (below) for identical vertical displacement at sample top and sample bottom of 9e-3 m

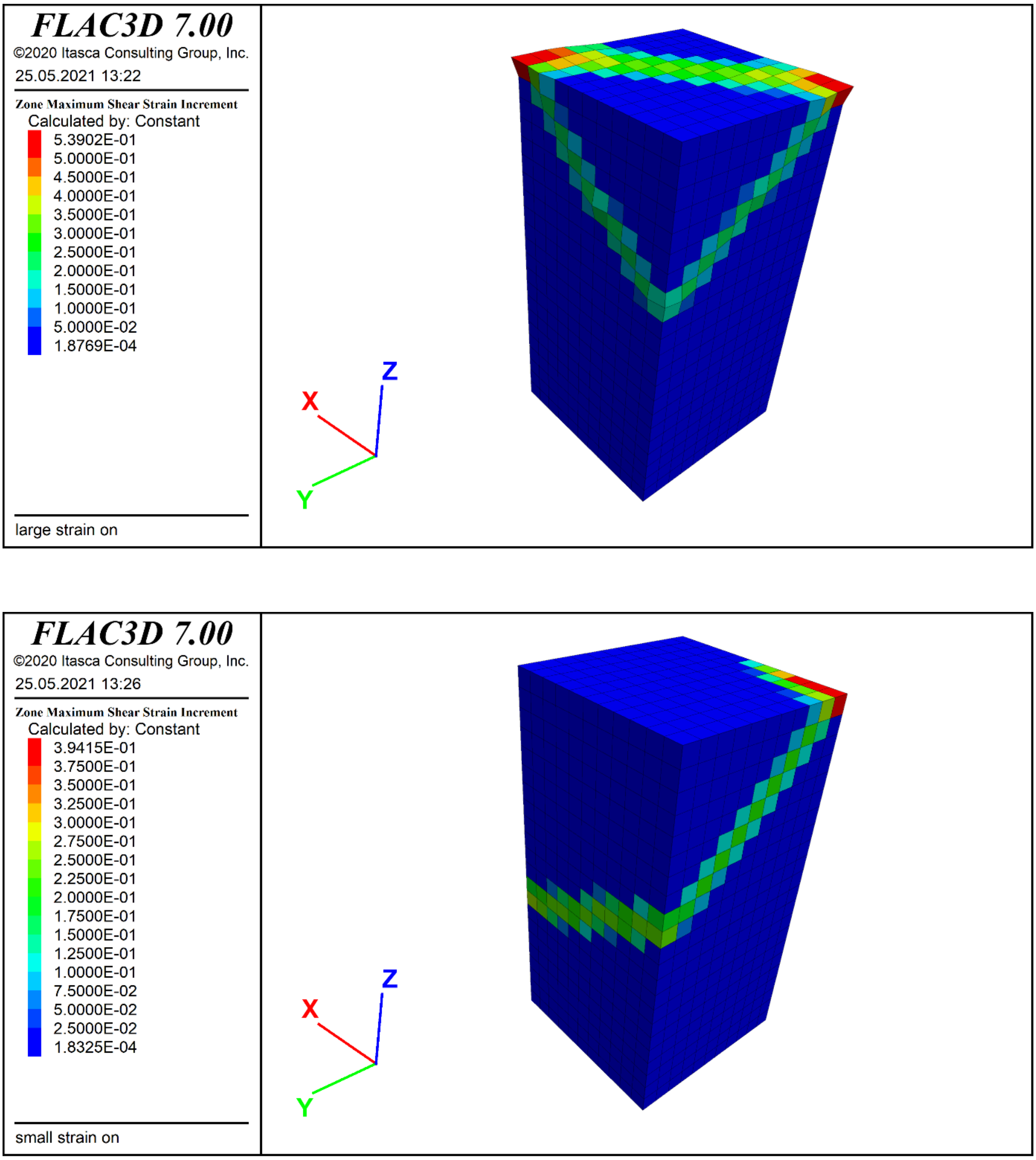
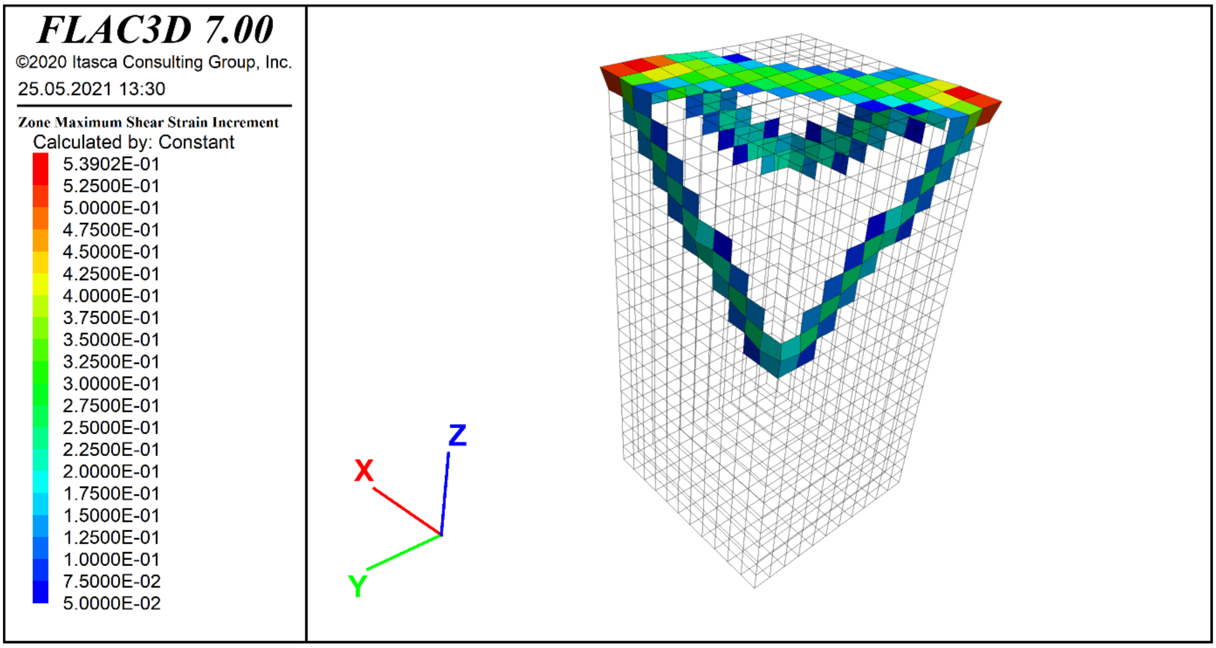


Fig. 12.4: UCS test: Accumulated shear strain for **large strain modus** (above) **and small strain modus** (below) for identical vertical displacement at sample top and sample bottom of 9e-3 m



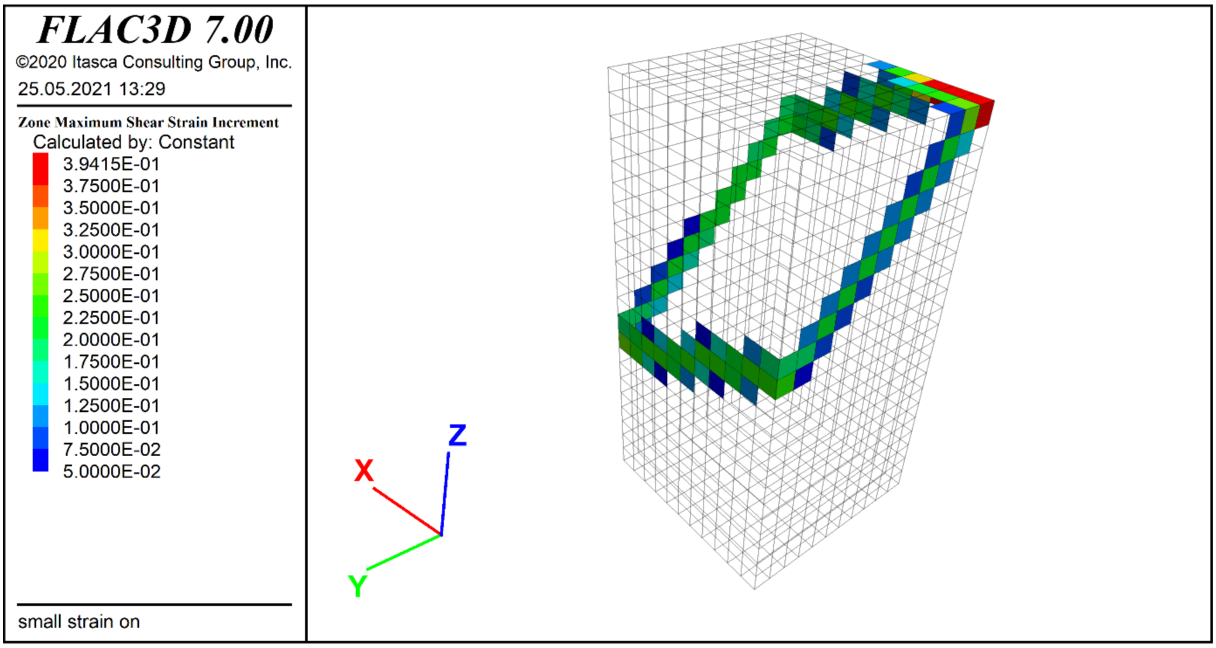


Fig. 12.5: UCS test: indication of shear plane (strain localization) by accumulated shear strain for **large strain modus** (above) **and small strain modus** (below) for identical vertical displacement at sample top and sample bottom of 9e-3 m

The last simple example documents that the small strain modus might be sufficient to detect the onset of failure, but cannot be applied to simulate the deformation and stress redistribution process afterwards.

13 Choice of numerical method and code

Numerical simulation techniques can be distinguished in the following two ways:

- temporal discretization into explicit and implicit methods
- spatial discretization into mesh-based and meshless methods

Whereas implicit methods are faster than explicit methods in case of elastic simulations, explicit methods are better suited whenever large deformations, strong non-linearities or physical instabilities occur (e.g. crash or impact simulations, blasting, rock cutting or drilling, rockfall etc.)

In respect to spatial discretization of mesh-based methods one can further distinguish Finite Element (FE, XFE), Finite Difference (FD), Volume Element (VE) and Boundary Element (BE) methods. The most popular representatives of meshless methods are the Discrete Element Methods (DEM) based on spheres or polyhedra and the Smooth Particle Hydrodynamics (SPH) method. Other methods like the Numerical Manifold Method (NMM) distinguish between physical and mathematical cover making the approach flexible (e.g. Li & Zhao, 2019; Ma et al. 2010; Zhou et al. 2020)

Mesh-based methods can be distinguished into integral (BEM) and differential (FEM, FDM, XFEM, VEM) methods. Integral methods have the following general characteristics:

- simple meshing (only at surfaces)
- exact far-field solution
- minimized discretization error
- no problems with singularities
- small demand of computational power
- ***but:*** problems to handle anisotropies, inhomogeneities, couplings, non-linearities

Differential methods have the following general characteristics:

- ability to depict any kind of anisotropies, inhomogeneities, couplings, non-linearities
- tremendous flexibility to solve continuum mechanical problems
- higher demand for computational power
- sometimes complicated meshing procedure
- problems to simulate disintegration and mixture of material

Compared to classical integral or differential methods, meshless methods including DEM are characterized by several additional features:

- discrete elements should be able to follow all kinematic possible movements (displacements and rotations)
- automatic contact detection and elimination of contacts (e.g. via cell-space or Verlet algorithm)
- contact laws, which act, whenever a contact (direct touch or long-ranging interaction) exist

Due to this additional features, especially the automatic contact detection algorithms, these approaches are quite computational intensive, but offer unique simulation possibilities whenever disintegration, mixture or flow of material, mass movement, blasting, rock cutting and drilling, rockfall or micro-mechanical problems at the grain size level are of interest (e.g. Stahl & Konietzky 2011, Lunow & Konietzky 2009, Groh et al. 2011, Wang & Konietzky 2009, Lisjak & Grasselli 2014). Fig. 13.1 gives an impression about the power of DEM methods to simulate disintegration processes.

All of the above mentioned techniques have advantages and disadvantages considering a specific modelling tasks. Also, a lot of problems can be solved with different techniques with nearly same quality and efficiency. Currently under development are hybrid codes, which combine mesh-based and meshless approaches. Besides general purpose programs (e.g. Ansys, Abaqus, Nastran, Comsol etc.) special designed codes for rock- and soil-mechanical simulations were developed, which have the advantage, that appropriate constitutive models and structural elements (for simulating anchors, piles, walls etc.) are already included. These codes have participated in a lot of benchmarks and validation procedures (e.g. DECOVALEX).

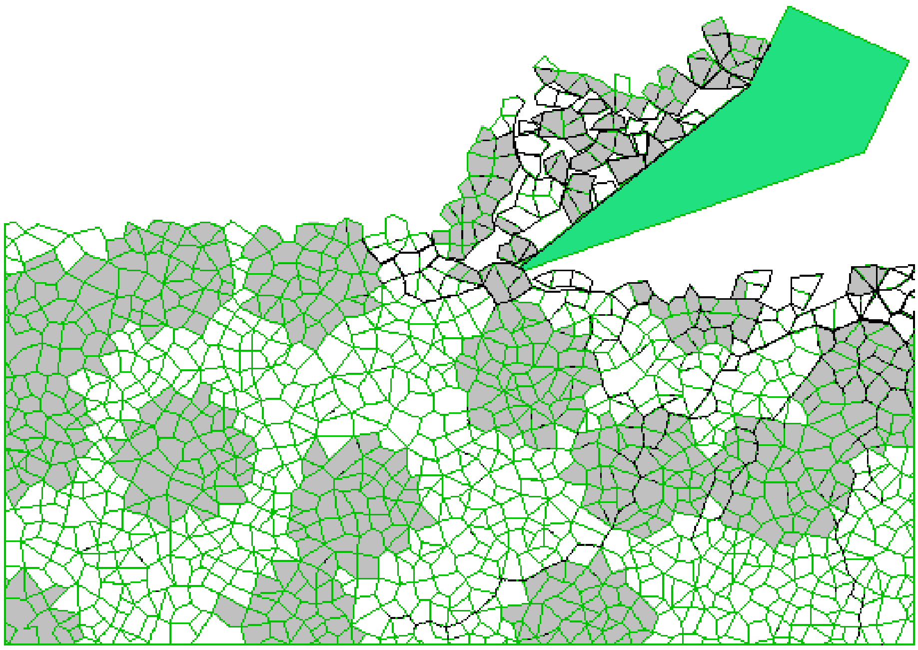


Fig. 13.1: DEM Simulation of cutting process for brittle rock (Lunow & Konietzky 2009)

14 Conceptual and numerical model

Each numerical modelling should be separated into 2 successive phases:

- 1. Phase: Conceptual model
- 2. Phase: Numerical model

The first phase comprises the development of the general modelling strategy and includes some more general decisions about simulation tools and approaches.

The second phase comprises the programming, specific allocation of constitutive laws, initial and boundary conditions, parameters etc. and the corresponding model runs including evaluation.

Phase 1: Conceptual model:

Phase 1 starts with an analysis of the modelling task and the available data base followed by the allocation to the corresponding project phase and finally the detailed analysis of all aspects according to Fig. 14.1. Each geotechnical task can be subdivided into several stages, like:

- Pre-planning
- Dimensioning
- Construction
- Monitoring
- Back analysis

Besides typical geotechnical project work, applied or fundamental geotechnical research work exist. Depending on the project phase, tasks, demands and applications, numerical simulations will be quite different.

In the pre-planning phase quite often only a very limited data base exists, the budget is limited and the expectations about precision in prediction are lower. Therefore, in this phase numerical modelling is restricted to simplified geometries, coarser meshes, simple constitutive laws and consideration of less construction stages. This phase also includes the comparison of different concepts. The aim of this phase is to detect the main geomechanical features, characteristics, pitfalls etc. of the project, to get the correct order of magnitude in terms of stresses and deformations and to obtain a deeper understanding of the geomechanical processes. Also different construction methods can be compared and evaluated.

The phase of dimensioning and detailed planning requires a valuable and comprehensive data base. Material behaviour and interaction between rock mass and structure have to be described by appropriate constitutive laws in detail.

The construction phase is characterized by application of numerical modelling in parallel to the in-situ construction steps. During that phase the model has to be updated, corrected, improved etc. based on actual in-situ measurements and observations. The model is used to explain and interpret observations and can be used to predict the effect of short-termed changes during the construction or to perform back analysis in case of any disaster (failure).

The phases of monitoring and back analysis normally starts, when the construction is finished and characterized by the fact, that in-situ measurement data and observations in respect to the interacting rock mass – construction are available. The aim of modelling during these phases is the back-calculation of parameters or to analyse failure situations. The approach to perform fundamental or applied research can be quite different and is highly dependent on the modelling task (often innovative approaches).

If one has defined the corresponding phase, several aspects according to Fig. 14.1 have to be considered. Especially, the following questions have to be discussed:

- Should the problem be modelled 3-dimensional or is a 2-dimensional approach sufficient or is the assumption of axisymmetric (quasi-3D) acceptable? If so, how can symmetry lines / planes be defined? Please note, that in respect to symmetry not only geometry has to be considered, but also other factors like stress state, anisotropy of material etc.
- What is the most appropriate way to solve the modelling task: a continuum approach or a discontinuum approach? This is decisive for the choice of corresponding software tools.
- What type of constitutive model is appropriate (elastic, elasto-plastic, visco-elasto-plastic, fracture mechanical, damage mechanical or others)?
- Can the simulation be performed as a pure mechanical one or should couplings be considered, e.g. hydro-mechanical, thermo-mechanical, hydro-thermo-mechanical, hydro-thermal-mechanical-chemical and others?
- Do we have a pure static incl. quasi-static problem or is it necessary to include dynamic effects like wave propagation etc.?
- Which construction stages (excavation stages, installation of support measures etc.) have to be considered to take the stress path dependency of the material behaviour and structural engineering requirements into account?
- What are the principal initial and boundary conditions (initial stresses, pore water pressures, stress and / or displacement boundary conditions, static vs. dynamic boundary conditions etc.)?

To answer these questions and consider the aspects according to Fig. 14.1 allows to formulate the “Conceptual Model”.

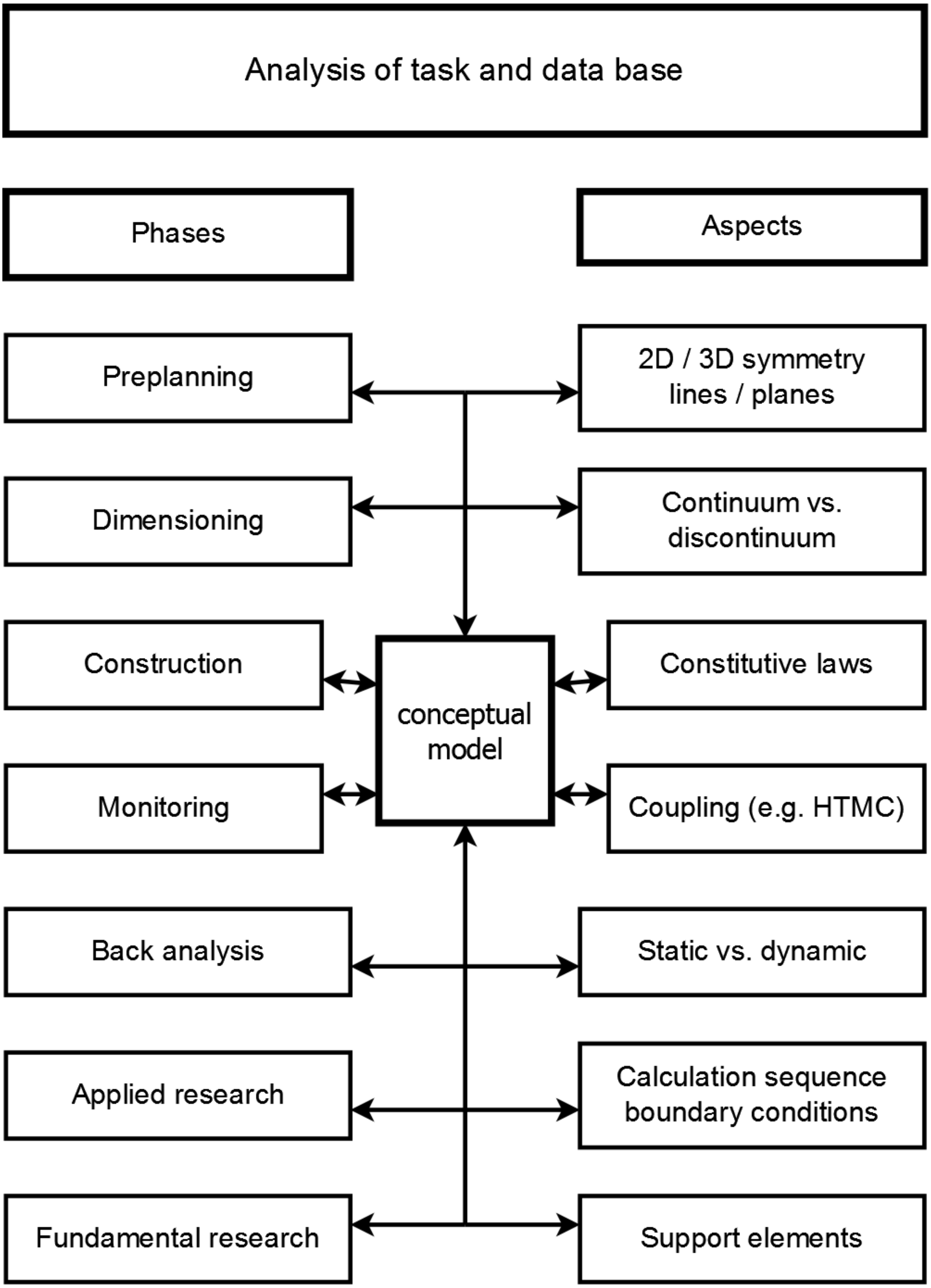


Fig. 14.1: Conceptual model workflow

Phase 2: Numerical model:

In a second step the ‚Numerical Model' (Fig. 14.2) has to be set-up, which means to perform the detailed programming including specification of initial and boundary conditions, meshing, parameter specification etc.

The second phase starts with a detailed analysis of the data base and demands also thinking ahead, how and which model results should be obtained and documented. After that analysis, the model set-up starts with definition of the mesh, the initial and boundary conditions, the calculation sequence, the specification of constitutive laws und their parameters etc. in form of an input script or a menu-driven dialog. In case of any ambiguity or problem or to test the behaviour, it is helpful to set up small models (in an extreme case a 1-zone-model) and to perform test simulations until the problem is exhausted. Then, the numerical simulation will be started and the model results will be stored for further evaluation. However, before reporting is started, the modelling results have to be checked carefully. Considering that, the following methods are available:

- Plausibility check: That means to check, whether the calculated physical values are generally feasible (Are they within a plausible range? Is the general deformation, stress and failure pattern logical?).
- Comparison with experience: That means, are the model results located inside the field of experience and if not, can they be explained logical on a physical basis?
- Direct comparison with measurements / observations in situ: This approach is always the best choice and should be always used.
- Comparison with other calculation methods: either alternative numerical simulation approaches or semi-analytical solutions. This is often a demand at least for projects of special importance.

If the check of modelling results is successful and positive, either the project can be finished by writing a report or further simulations follow, e.g. in form of a parameter study, sensitivity analysis, robustness analysis, optimization, comparison between variants, etc.

If the check of the modelling results is negative, one has to check if it is a more principal conceptual error (e.g. effect of water not considered, continuum approach not able to duplicate significant discontinuum effects, etc.) or a more detailed error inside the numerical model (e.g. wrong parameter, wrong initial condition, etc.) Depending on this evaluation one has to jump back inside the scheme, has to make corrections and then execute all subsequent steps again.

It is strongly recommended to perform geotechnical simulations always in parallel to the construction (project in-situ), that means starting already with the preplanning phase until the phase of monitoring and back analysis. Finally, this leads to more economic design, allows optimisation and the chance to react short-termed to problematic situations like collapses. If such a strategy is applied, the numerical model will be modified step-by-step and improved by adjustments according to the actual observations and measurement results. This allows improvement towards more precise predictions.

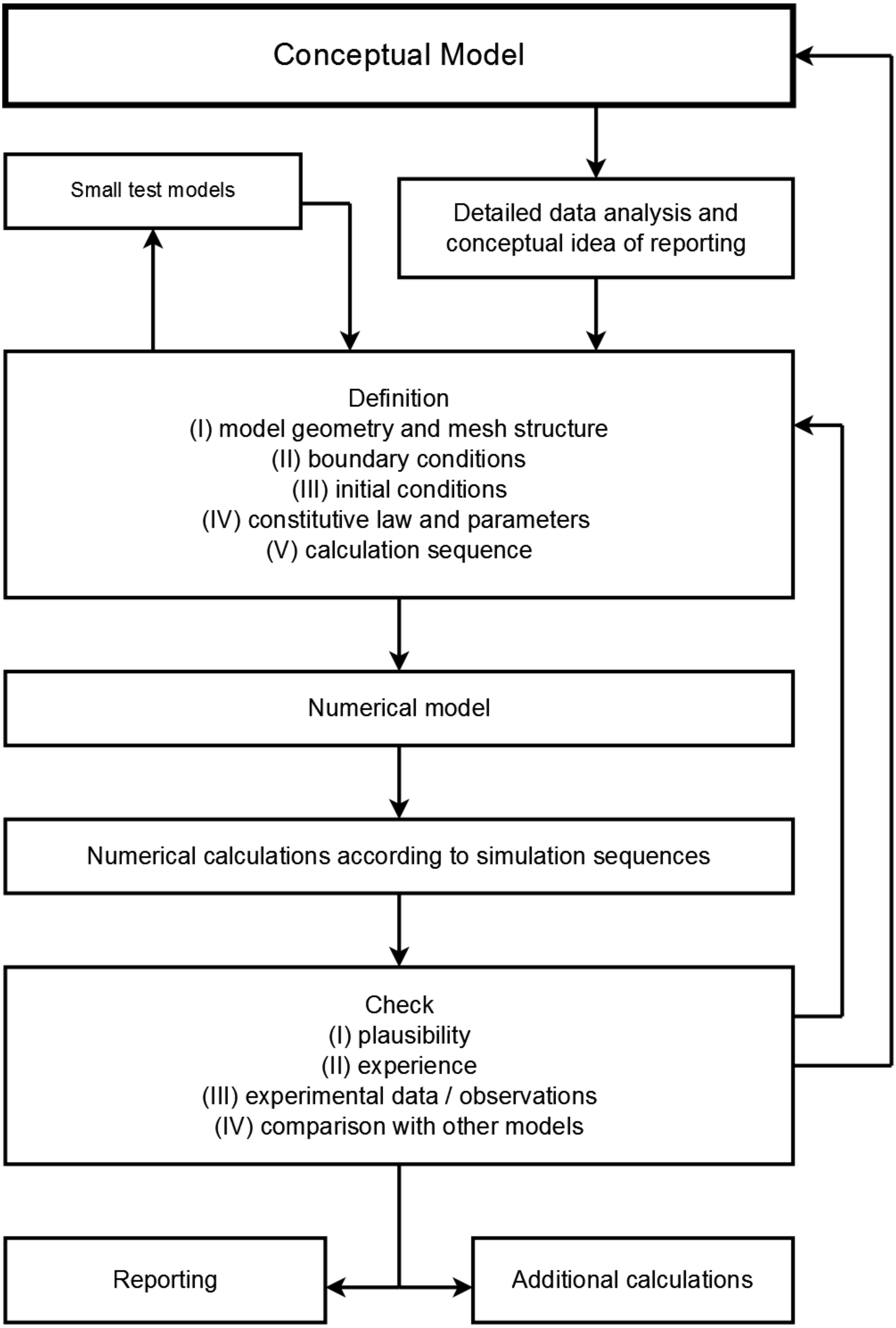


Fig. 14.2: Numerical model workflow

15 Important terms

- **Verification (verify = make good)**

  Process to proof the correct mathematical-physical implementation of the desired algorithms and models etc. In most cases this is done by comparison with analytical solutions or proofed numerical solutions – often called 'Benchmarks'.

- **Validation (validate = become valid)**

  Process to determine, to what degree the underlying model represents reality in a correct manner under chosen perspective. In most cases this is performed by comparison with observations and measurements - in situ or in the lab.

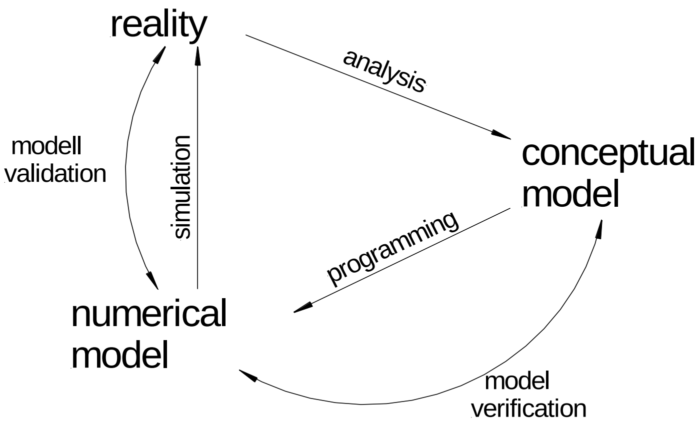


Fig.15.1: Role of verification and validation within the framework of simulation and software development

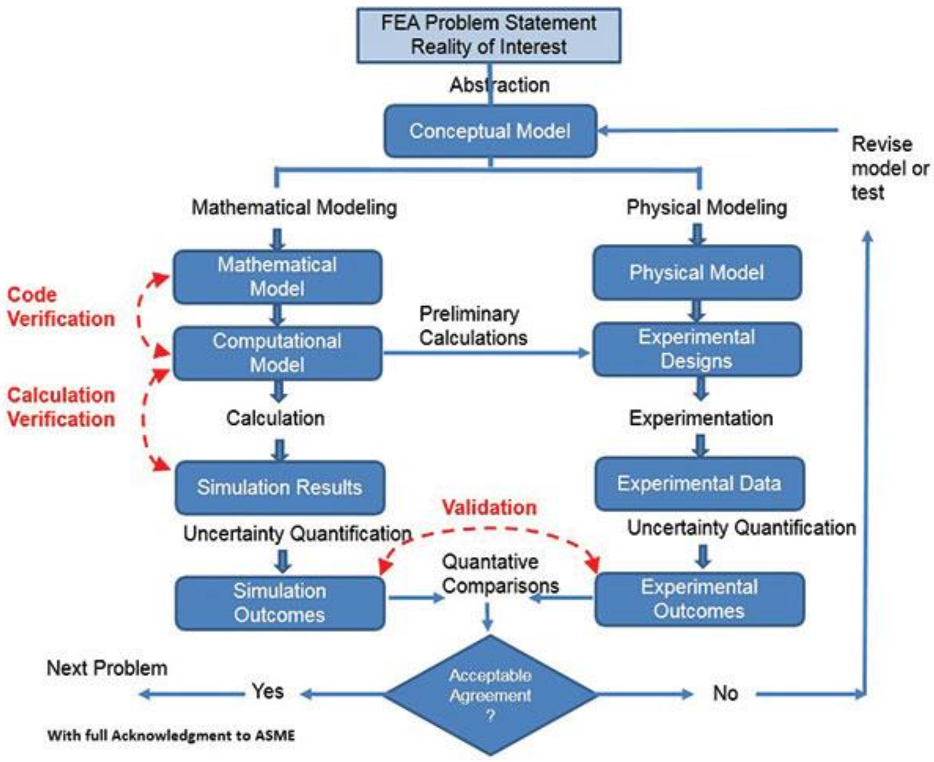


Fig. 15.2: Illustration of verification and validation (ASTM)

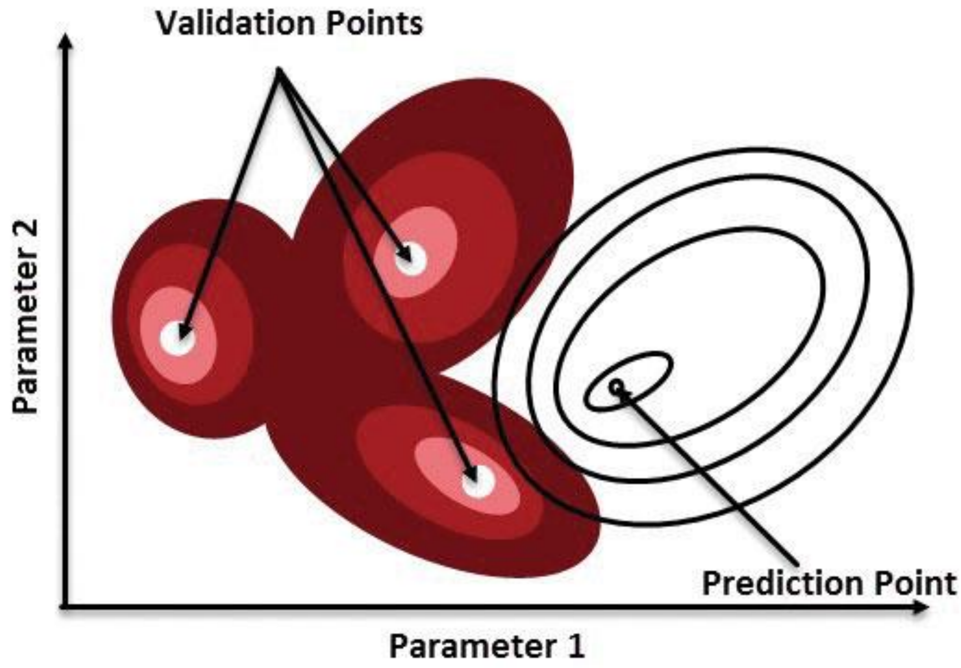
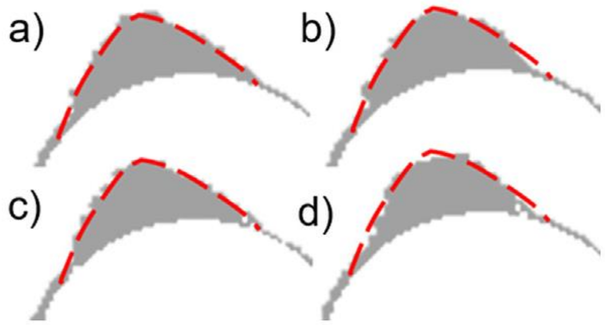


Fig. 15.3: Uncertainty in validation (LANL)

If the performed prediction is outside of the validation area the uncertainty is increasing and the prediction may be even questionable (see Fig. 15.3). More detailed information about verification and validation in general can be found in Trucano et al (2002), Oberkampf et al. (2003), Thacker et al. (2004) and Schwer (2005).

One should be careful with the term ‚validation' in respect to models and numerical models in particular because any scientific model is provisional based on the current scientific state-of-the-art. Furthermore, models inherently involve always some uncertainties based on non-uniqueness, divergence in time and space, subjectivity of model assessment as well as limited data base. As discussed for instance already by Oreste et al. (1994), the agreement between measurements and model results does not mean, that the ‚reality' is preproduced. At the best a specific behaviour or pattern of the ‚reality' can be reproduced and used for predictions.

Non-uniqueness means that several different models may produce identical or nearly identical results. Walton & Sinha (2022) provide an example: the simulation of breakouts at an URL in Canada (granite) using the same initial and boundary conditions as well as the same constitutive model provided nearly identical results although quite different parameter constellations were used (see Fig. 15.4). The higher the model complexity the higher the likelihood of non-uniqueness. Moreover, even different model concepts can lead to same or very similar results.



Case	Peak cohesion, c_{peak} (MPa)	Peak friction angle, ϕ_{peak} (°)	Plastic shear strain for cohesion evolution, ε_c^{ps}	Plastic shear strain for friction evolution, ε_ϕ^{ps}	Residual cohesion, c_{res} (MPa)	Residual friction angle, ϕ_{res} (°)	Dilation angle, ψ (°)
a	50	0	2×10^{-3}	5×10^{-3}	15	48	30
b	35	12	2×10^{-3}	3×10^{-3}	2.8	60	20
c	50	0	2×10^{-3}	3×10^{-3}	4.4	60	30
d	45	10	0	0	4.5	45	30

Fig. 15.4: Breakout shape simulated with same model but four (a-d) different parameter constellations (Walton & Sinha, 2022)

Divergence in time and space means that predictions over long periods of time and/or larger areas show increasing uncertainty. This is based on the fact, that observations and data used for model development and calibration are often based on time- and space-restricted data. Typical observation time spans are years or decades, but predictions may be requested for thousends or even million of years. For instance, Konikov & Bredehoeft (1992) have shown that two quite different geohydraulic models (no flow through confining layers vs. transient flow through confining layer) gave same fit to applied pump tests. Descrimination of the two models would need about 1000 years of pumping test. Consequently, at least two different models have to be considered for predictive modelling. Fig. 15.5 illustrates examplary the problem of increasing uncertainty in data for increasing model size considering an open pit.

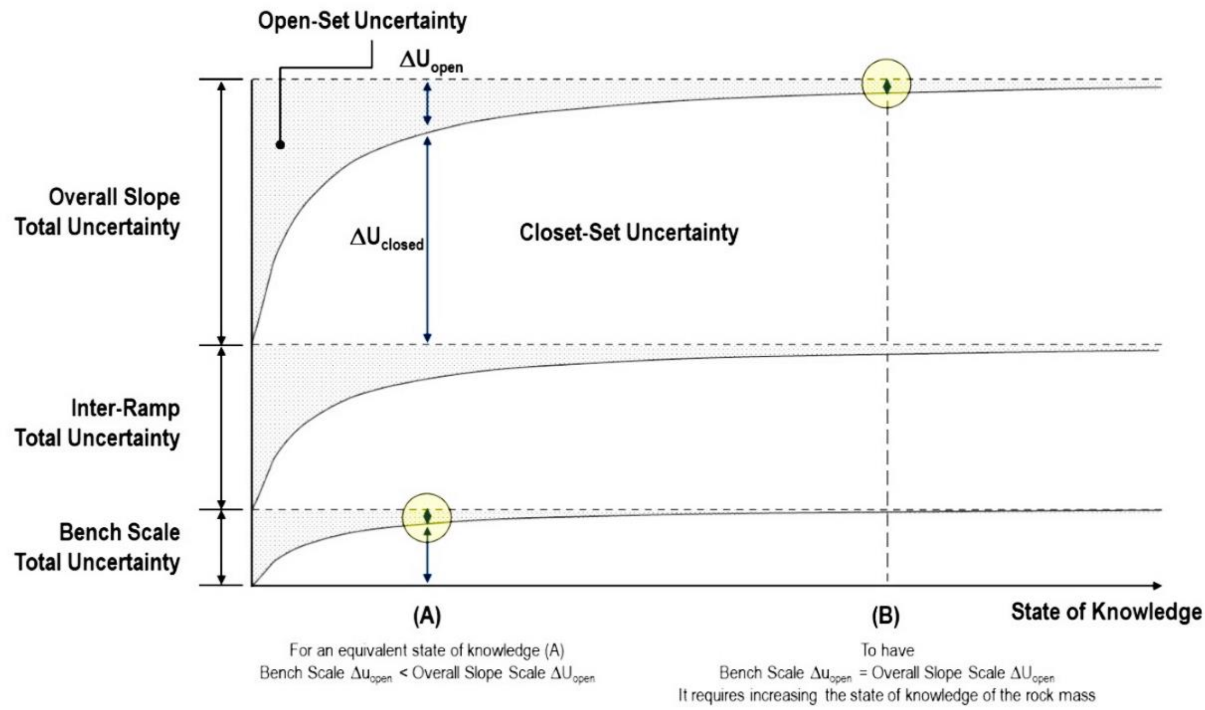


Fig. 15.5: Uncertainty in data at different scale for a given slope rockmass (Shapka-Fels & Elmo, 2022)

Subjectivity of model assumptions means the subjectivity to what extend (quality) the model duplicates the reality (measurements, observations etc.). There is no unique definition of exceptable errors (misfit). Li (2017) desribes different measures for assessing the accuracy of predictive models (pros and cons). Model quality assessment as well as numerical backanalysis demand to compare model response with measurement data / observations. How strong in terms of their weight the individual parameters are included is subjective. Also quality (reliability, error) as well as importance of different data is quite different. All this can be quantified only to some extend and therefore remains to some extend subjective.

Limited data base means that the number of unknown model parameters is often smaller than available field or lab dat for model validation and calibration, respectively. The consequence is, that several assumptions have to be made without proof of correctness. The higher the model complexity (e.g. produced by couplings, non-linearities etc.) the more parameters and functional relations are incorporated, and consequently more data are necessary for calibration/validation. Fig. 15.6 illustrates this dilemma, which will lead to increasing overall data misfit.

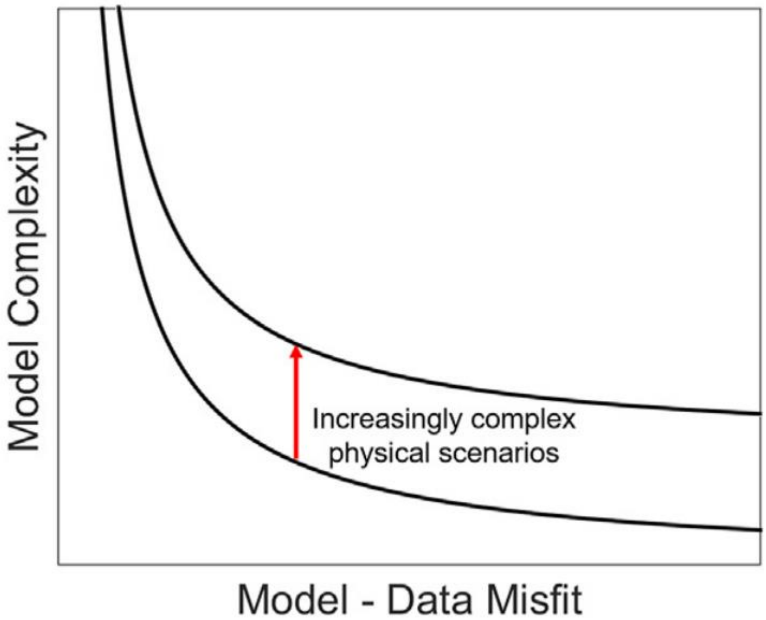


Fig. 15.6: Relation between model complexity and model data misfit (Walton & Sinha, 2022)

Wiles (2006) provides a interesting practical example about predictive modelling in mining. He documents also, that typical coefficient of variation for mining problems is in the order of 30% to 40% incorporating both: uncertainty in stress and strength.

Important terms for numerical simulations:

- **Calibration:**
  Process of adjusting model parameters in such a way, that measured values are reproduced in a satisfying manner. The prerequisite is successful verification and validation. Calibration can be achieved by trial-and-error procedure, by mathematical based back analysis on the basis of special in-situ or lab tests or by mathematical based optimisation.

- **Parameter studies:**
  The model is systematically tested with different parameter sets. The model output is evaluated as function of input parameters.

- **Sensitivity analysis:**
  This analysis investigates the sensitivity of the model output as function of varying input parameters. This can be performed by a parameter study or in a more sophisticated and effective manner by stochastic sampling with statistical evaluation.

- **Uncertainty analysis:**
  Probabilistic modelling to determine the influence of the fuzziness (range of variation) of input parameters on the model response.

- **Robustness analysis:**
  Probabilistic modelling to determine the robustness (stability) of the model response as function of varying (fluctuating) input values.

- **Reliability analysis:**
  This analysis investigates border violations (limit state violations) of the system behaviour. The probability of failure is the quotient of the number of model runs with failure to total number of model run

16 Modelling Documentation

Numerical calculations and simulations, respectively, have to be carefully documented. Such documentations should contain the following elements:

(a) General description:

- Name of used numerical code including version (and sub-version) number
- References in respect to the code (e.g. manuals, homepage/link to producer, papers etc.)
- Underlying numerical method (e.g. FEM, DDA, DEM, VEM, SPH, BEM, NMM etc.) and used calculation scheme (explicit vs. implicit, large strain vs. small strain etc.)

(b) Specific model description:

- Information about model size (outer extension in all directions as well as extension/coordinates of relevant geometrical features, e.g. layer boundaries, interfaces, internal boundaries etc.)
- Information about meshing (e.g. type of elements, size of elements, total number of zones/nodes, applied meshing procedure: free or mapped meshing etc.)
- Information about calculation time (run time) considering used hardware
- Used constitutive models and parameters incl. their deduction or corresponding references
- Initial and boundary conditions
- Calculation sequence (construction stages etc.)
- Usage of small or large strain calculation scheme

(c) Graphical presentation of simulation results:

- Any plot should contain a coordinate system
- For each presented physical quantity the corresponding units must be given (use only SI units)
- Clear explanation of sign (+ vs. -) for physical quantities like stresses or volumetric strain etc. has to be given (e.g. dilation/tension vs. compression or inflow vs. outflow)
- Depending on the purpose specific physical quantities (mechanical, hydraulic or thermal) may be plotted in form of vectors or tensors or magnitudes (filled colour plots or isoline plots) for single components, results or own defined (deduced) quantities. For specific purposes animations or picture sequences are helpful.
- Documentation of initial state (e.g. virgin stress state, initial pore water pressure distribution etc.) as well as all relevant subsequent modelling stages
- Often not only total (accumulated) values, but also differences between different stages (e.g. construction stages) should be illustrated

- In case of failure, damage and plasticity, respectively: the failure pattern has to be illustrated (e.g. by shear or tension failure indicators, velocity fields, plasticity states, accumulated plastic shear strain etc.).
- The state of equilibrium or disequilibrium (failure) has to be documented. It has to be distinguished between local and global failure (disequilibrium).
- In case of time-dependent simulations (creep, fluid flow, heat transfer etc.) the time-dependent process has to be illustrated (e.g. series of plots for different points in time or histories of physical quantities vs. time for interesting observation points).

(d) Evaluation / Interpretation of simulation results:

- Simulation results have to be interpreted according to the modelling task (verbal description + figures + diagrams + tables). This includes also, that simulation results have to be checked using different other available techniques, like comparison with practical experience, in-situ measurements, analytical solutions, calculations with other methods etc.
- More comprehensive projects should include sensitivity, uncertainty and robustness analysis.
- The potential problem of mesh-dependency should be discussed.
- Choice and calibration of parameters has to be discussed.
- Model simplifications and their potential impact on modelling results should be discussed.
- Chosen initial and boundary conditions should be justified.

To achieve a smooth workflow, contractual agreements between client and contractor should contain the following regulations:

- Should the final report be send only in electronic format or does the client demand paper printed versions?
- The contractor should specify the necessary input data incl. format, which the client should provide.
- Should the contractor store the numerical simulation results? If yes: how long and which data. Also: does the client demand the hand-over of input or save-files or data in VTK/VTU format?
- Can the contractor use the data for other purposes (e.g. publications) or are they confidential?
- Is the client free to choose the numerical simulation tool or should he use a predefined one?
- The modelling task incl. the content of expected reporting has to be specified in detail.
- In case of complex (comprehensive) modelling tasks, it is recommended to specify milestones with interim reports and/or meetings.

17 Auditing

Hudson & Feng (2010) provide an overview about the integration of numerical modelling into rock engineering and focus on auditing of numerical simulations. The following defined questions should be answered within an auditing process:

(1) Modelling objective

a. Has the modelling objective been clearly established ?
b. ow will it be known when the modelling work is completed?

(2) Modelling concept and technique

a. What rock mass systems are being considered ?
b. What are the main physical processes being involved ?
c. What is the changing independent variable ?
d. How is the system perturbed so that the mechanisms are initiated ?
e. Listing of physical variables / parameters and THM couplings
f. Is the model 1D, 2D or 3D ?
g. Continuum or discontinuum modelling ?
h. Specification of boundary and initial conditions
i. How is final condition established ?
j. What is required model output ?
k. Does the model match the modelling objectives ?
l. Are quality control checks in place ?
m. Which code is used and why ?
n. Where does the code from and what about is verification / validation ?
o. Have the input data justified ?
p. What about sensitivity / robustness of output in respect to input ?
q. How are the modelling results presented ?

(3) Modelling adequacy

a. List of potential errors; errors are corrected ?
b. Is model adequate to the purpose ?
c. Are corrective actions are required ?

18 Current and future trends

There is an ongoing development of numerical simulation techniques. Some of the very active current research fields are listed below:

- Multi-scale modelling
- Coupling of different codes (e.g. codes with strengths in geomechanics with CFD-tools to perform efficient HM-coupled simulations)
- High performance computing
- Automatic coupling of mesh based and mesh free methods
- 3D-visualization within caves, via holograms etc.
- Integration of numerical models into GIS and BIM
- Coupling with optimisation tools
- Integration of time-dependent and time-independent damage and fracture mechanical approaches into classical elasto-plastic ones
- Sophisticated HTMCB-coupling
- Scientific programming
- Use of failure probability for geoengineering projects instead of classical factor-of-safety
- Implementation of EUROCODE-conform analysis in practical rock engineering based on further development of the EUROCODE itself

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