Numerical Methods in Rock Mechanics – a short overview

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1 Introduction

There are different possibilities to classify numerical methods applied in geoengineering, for instance:

- in respect to the mesh: mesh-based and meshless methods
- in respect to the solution scheme: explicit and implicit methods
- in respect to the continuum: continuum / discontinuum and hybrid methods
- in respect to applications: general purpose and specific geotechnical programs
- in respect to physical component / coupling: mechanical / hydraulic / thermal simulation codes as well as coupled codes
- in respect to code assess: commercial codes and open source codes

The following short description does not follow the more restrict classification criteria given above, but follows a more practical way. Also: the already quite popular and widely used methods / approaches like classical FEM, FDM or BEM will not discussed here.

2 General purpose codes

General purpose codes like for instance Ansys, Abaqus, Nastran, Lsdyna, Pamcrash or Comsol are powerful tools, which include solver as well as pre- and post-processing. Most of them are continuum mechanical codes, but some of them have also discontinuum capabilities. They are highly verified and are used in nearly all fields of science and engineering. In general, they allow the simulation of arbitrary physical processes. They are also used in geosciences and geoengineering. However, the driving force for further development and application is not geo-related. This in turn means, that specific geo-related features are not available, like specific constitutive laws, specific couplings, specific structural elements, specific geo-related processes etc. Although it may be possible to install them via specific interfaces and programming, it makes the usage complicated. Also, validation of theses codes in respect to geo-related applications is limited.

3 Geo-related continuum codes

For geoengineering purposes several continuum based commercial codes like Plaxis or Flac among others are available. They were developed continuously over the last decades and are new very powerful tools. However, there are also open-source codes available like OGS, Code_Bright or Code_Aster which can be used together with open-source pre- and post-processors. Very popular for both - open source as well commercial codes - is the use of ParaView using the VTK format for post-processing and plotting. The underlying numerical solution schemes of classical continuum codes are well known, established and documented, therefore they are not discussed further here. Some valuable hints for practical applications are given in the ebook “Practical hints for using numerical methods in rock mechanics”.

4 Geo-related commercial codes versus open source codes

Commercial codes (geo-related):

- Advantages:
    - Highly verified
    - Excellent documentation
    - Huge professional user group
    - Professional service
    - Good handling
    - Many options
    - Excellent integrated pre- and post-processing
    - Standard interfaces and compatible with different formats
    - Excepted by authorities
    - Popular in industry
- Disadvantages:
    - Very expensive (service as well as leasing or purchase)
    - No access to the source code
    - No full insight into the numerical solution scheme
    - Extensions limited to the provided access capabilities

Open source codes (geo-related):

- Advantages:
    - Full access to the source code (full insight into the solution scheme)
    - Free of charge
    - No limitations in respect to extensions
    - Very active exchange via user groups in universities and research institutions
    - Widely used by universities and research organisations
- Disadvantages:
    - Difficult handling
    - Documentation limited
    - Functionalities limited
    - Pre- and post-processing limited
    - No professional service
    - Often higher error rate (bugs)
    - Not popular in industry

5 Special numerical techniques

5.1 Discrete element methods (DEM)

The DEM covers discontinuum-based methods based on angular as well as spherical basic elements. Methods based on spherical particles are also called particle methods (PM), and can be considered as a special version of the DEM. Both methods can be performed in an explicit (e.g. 3DEC) or implicit (e.g. DDA) manner. DEM allows elements of arbitrary shape (either stiff or deformable), whereas the PM is restricted to spherical non-deformable basic elements (for PM: please see our ebook "Particle Methods"). Both methods can simulate a continuum similar like the classical FEM or FDM, however they allow in addition desintegration (e.g. by fracturing, cracking etc.) and finally movement of fragments in the physical (e.g. gravitational) field. The basic calculation scheme applied in explicit DEM (also called distinct element method) is illustrated in Fig. 5.1.1 for both deformable and stiff basic elements. The calculation scheme considers block deformations, displacements and rotations and allows detachment and automatic contact detection. Fig. 5.1.2 to 5.1.4 show selected applications.

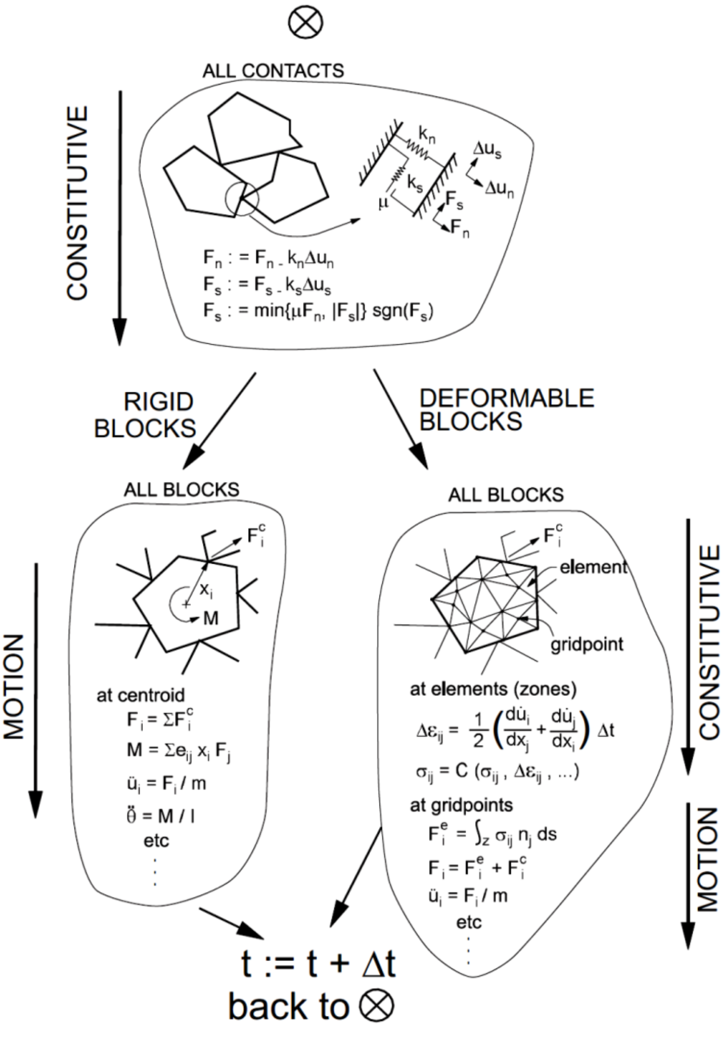


Fig. 5.1.2: Illustration of explicit calculation scheme for 2-dimensional DEM (Itasca, 2019)

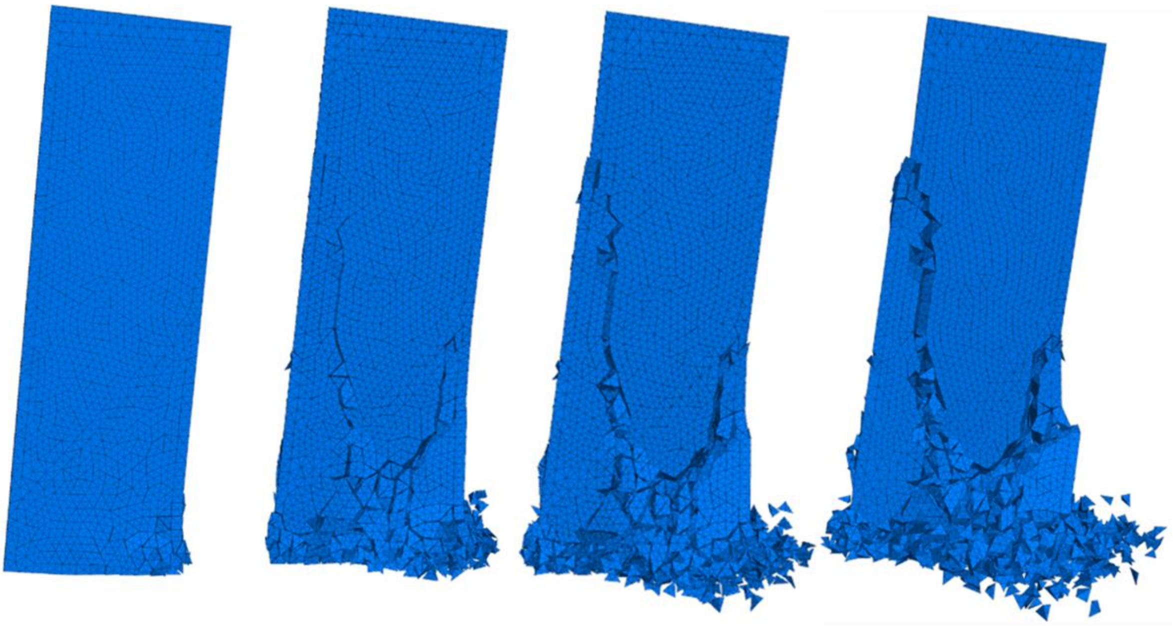


Fig. 5.1.2: Fracturing or nuclear waste canister due to dynamic impact simulated by DEM (Zhao et al., 2021)

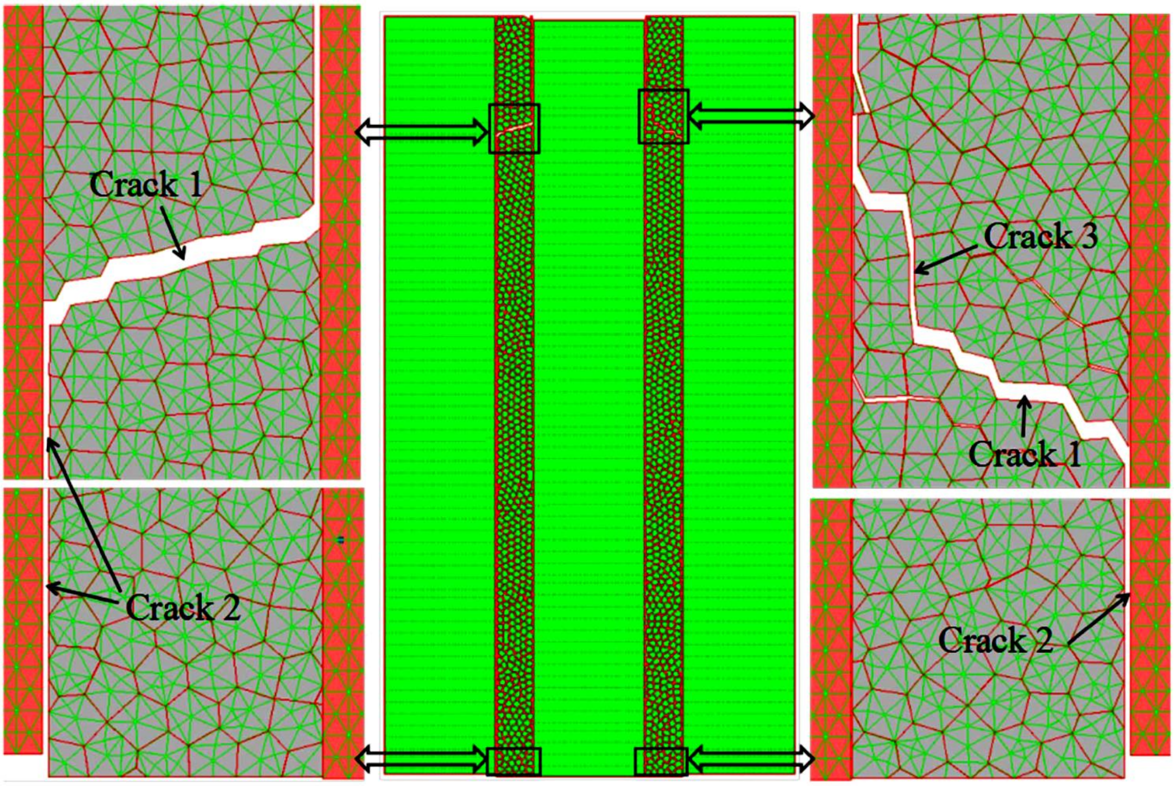


Fig. 5.1.3: Crack evolution in a special brick work simulated by DEM (Chen et al., 2021)

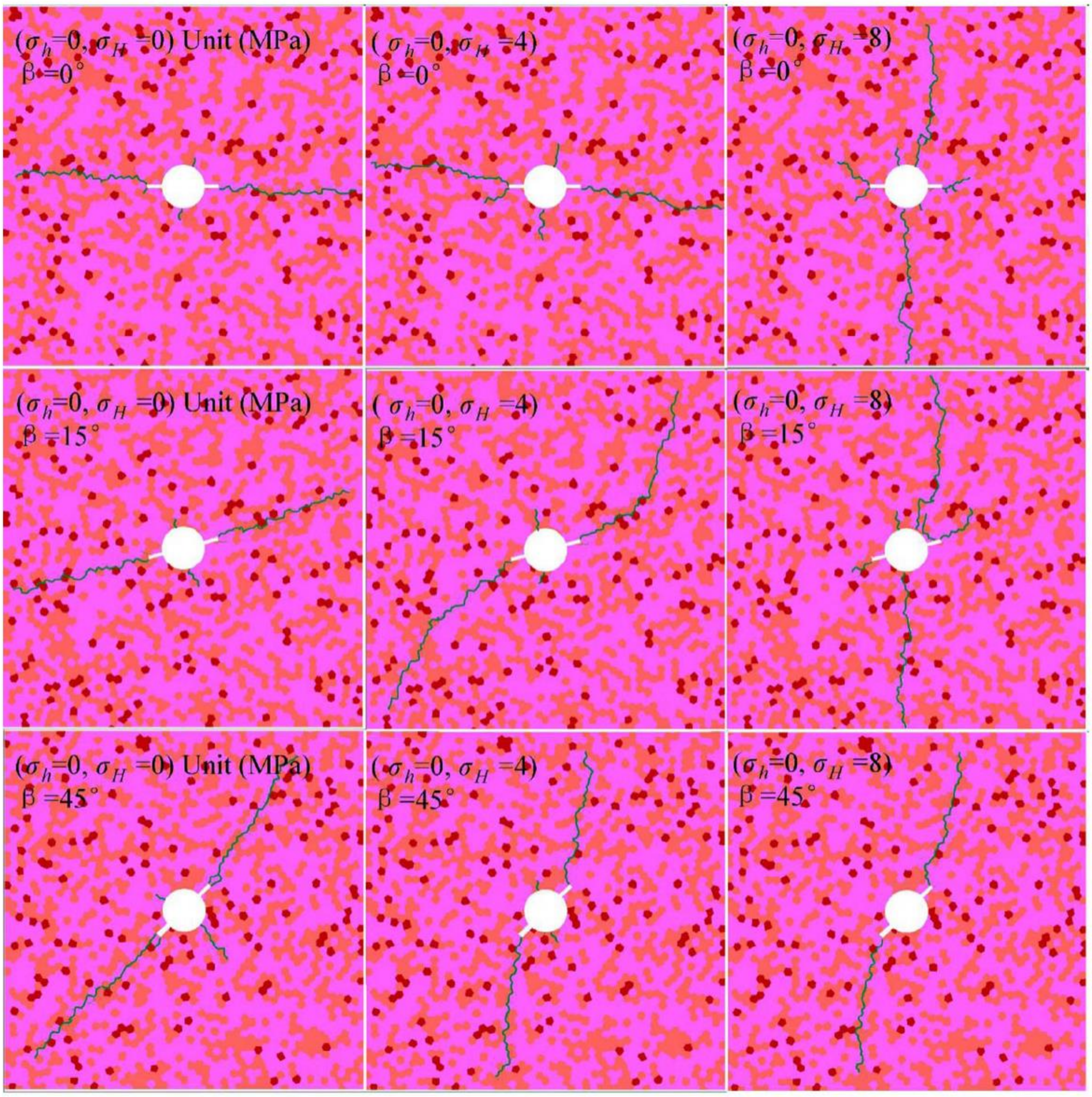


Fig. 5.1.4: Hydraulic fracture propagation simulated by DEM (Chen et al., 2018)

Selected further applications:

- Thermal cracking or rocks (e.g. Wang & Konietzky, 2022)
- Dynamic fracturing due to impact loading (Zhao et al. 2021)
- Modelling of tectonic processes (e.g. Liu & Konietzky, 2021)
- Modelling of brick structures (e.g. Chen et al., 2018)
- Rock damage evolution at the micro-scale (e.g. Konietzky, 2017)

5.2 Hybrid methods

Hybrid methods combine different numerical techniques. Typically a continuum-based approach is coupled with a discontinuum-based approach, like FDEM (a coupling between FEM and DEM). Typically, such techniques start with simulation of a continuum and later one in case failure states are detected the simulation switches toward a discontinuum approach. These codes can either handle both techniques internally by switching automatically between the two techniques or two codes are externally coupled (e.g. RPFA or IRAZU code). Exemplary, Fig. 5.2.1 shows a FDEM based simulation of hydraulic driven crack propagation and interaction (Bai et al., 2021). Fig. 5.2.2 and 5.2.3 illustrate possible coupling mechanisms between two separate codes (continuum code FLAC3D and particle code PFC3D), see also Purvance & Garza-Cruz (2020), Hu, W. et al. (2020), Jia et al. (2018) or Cai et al. (2007).

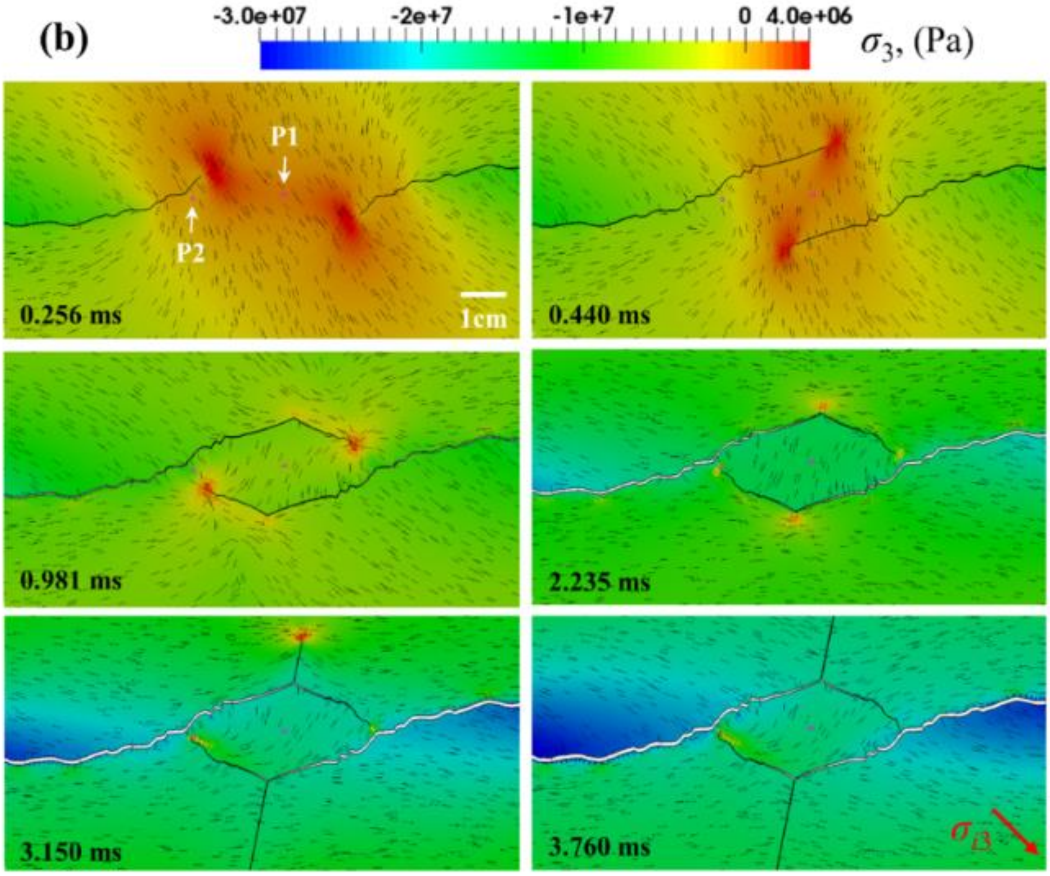


Fig. 5.2.1: Simulation of hydraulic driven crack propagation and interaction (Bai et al., 2021)

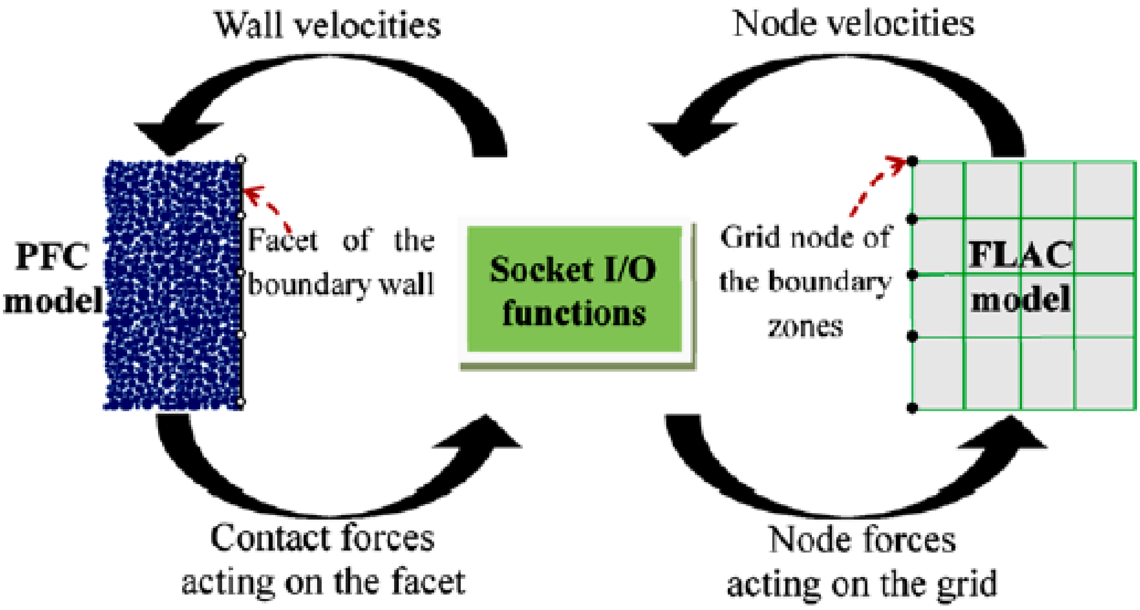


Fig. 5.2.2: Simulation scheme for hydraulic driven crack propagation and interaction using a coupling algorithm between FLAC and PFC (Jia et al., 2018)

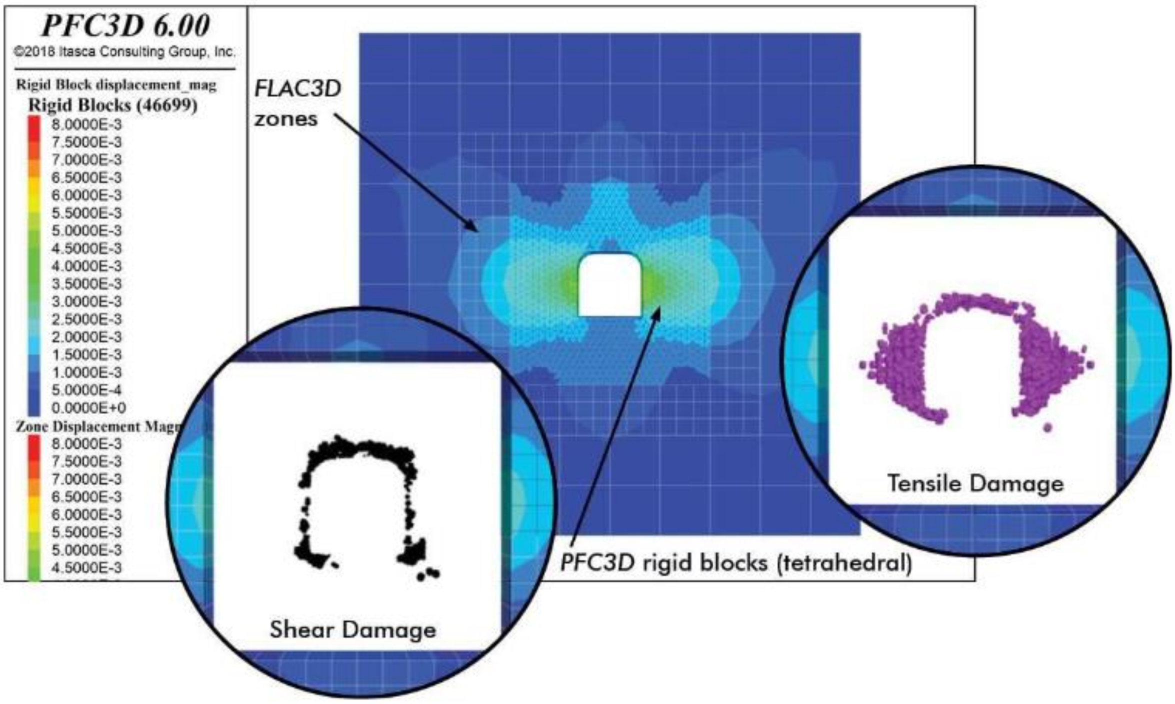


Fig. 5.2.3: Illustration of FLAC3D/PFC3D coupling (Itasca, 2022)

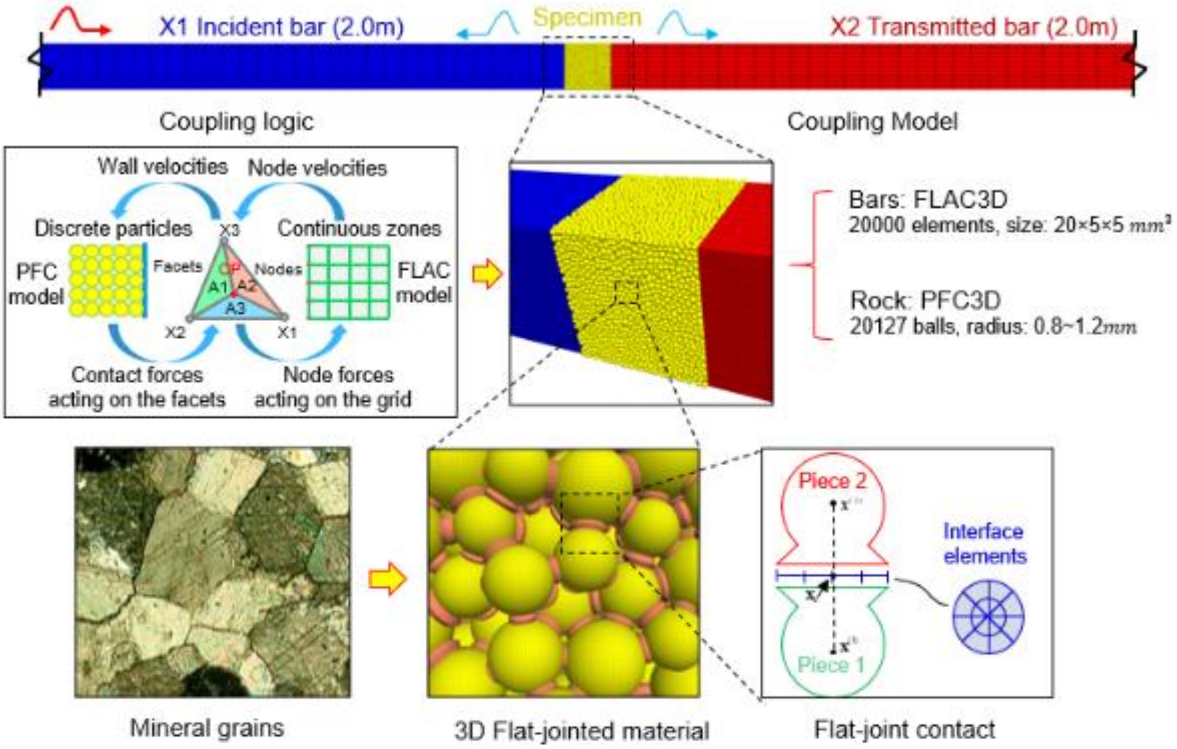


Fig. 5.2.4: Illustration of FLAC3D/PFC3D coupling for dynamic Hopkison bar simulation (Hu et al., 2020)

5.3 *Numerical Manifold Method (NMM)*

The main characteristic of the NMM is the use of two cover systems: i.e. the physical cover (PC) and the mathematical cover (MC), which is illustrated in Fig. 5.3.1 and 5.3.2. The manifold element is the common area of several physical patches and is the basic unit for integrating the weak formulation of the problem. The local approximation on each physical patch is defined as:

$$u_i(x) = \sum_{i=1}^{n} N_i(x) d_i$$

where:

u_i	value of local approximation on patch i
n	degree of freedom (DOF)
N_i	basis of cover function
d_i	vector of DOF

The global field value U(x) for each manifold element is obtained by multiplying the local approximation functions with weight functions φ_i (m is the number of physical patches inside a manifold element):

$$U(x) = \sum_{i=1}^{m} \varphi_i(x) u_i(x)$$

The weight function value varies between 0 and 1.

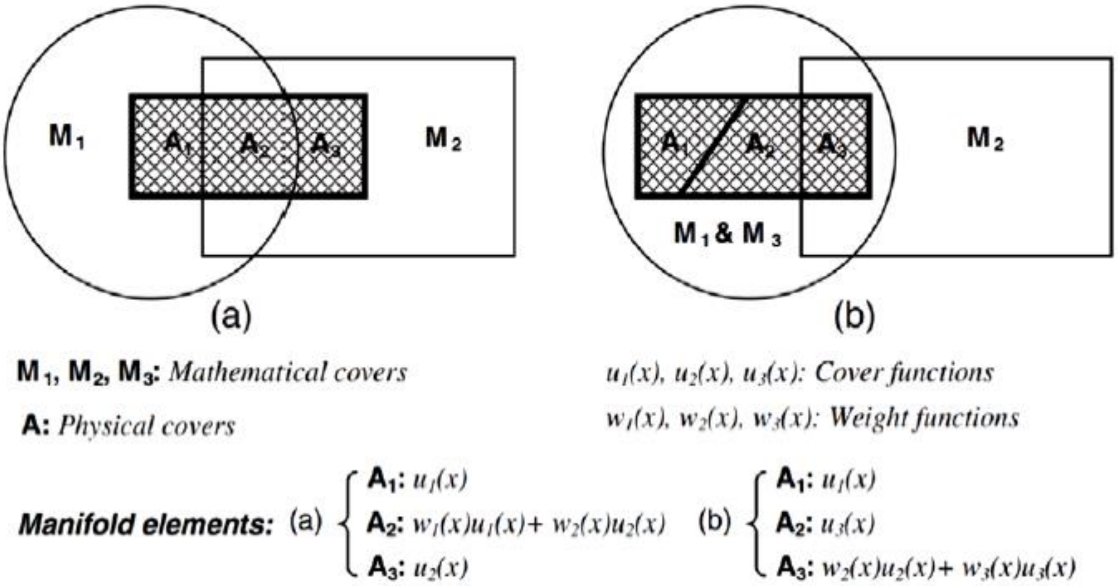


Fig. 5.3.1: Illustration of physical and mathematical cover within the NMM method (Sun et al., 2013)

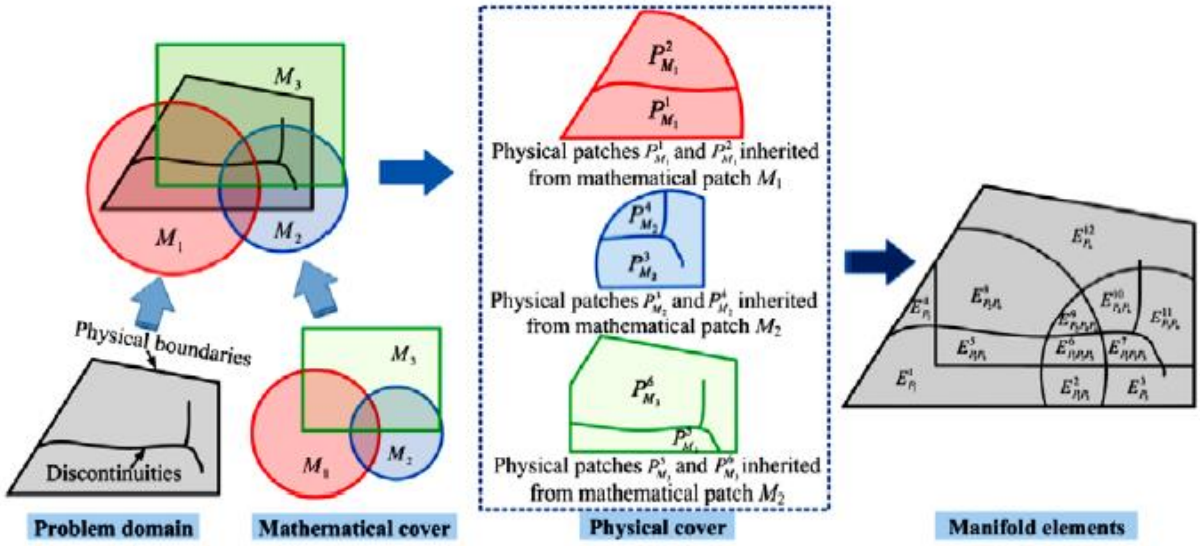


Fig. 5.3.2: Illustration of physical and mathematical cover within the NMM method (Zhou et al., 2022)

NMM has some similarities with DEM (explicit method) and DDA (implicit method), however NMM (implicit method) allows to subdivide each block into several covers which allows a more precise description of the field values. Techniques developed for the implicit FEM are applied also for NMM.

NMM offers all the capabilities of the discrete element method and is therefore also used to simulate crack propagation processes, mass flow, block interaction etc. (see exemplary Fig. 5.3.3 to 5.3.5).

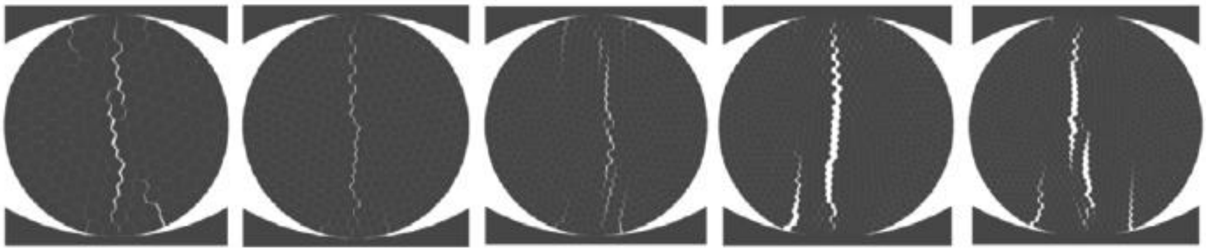


Fig. 5.3.3: Simulation of Brazilian tests using NMM with different number for Voronoi cells (Zhou et al., 2022)

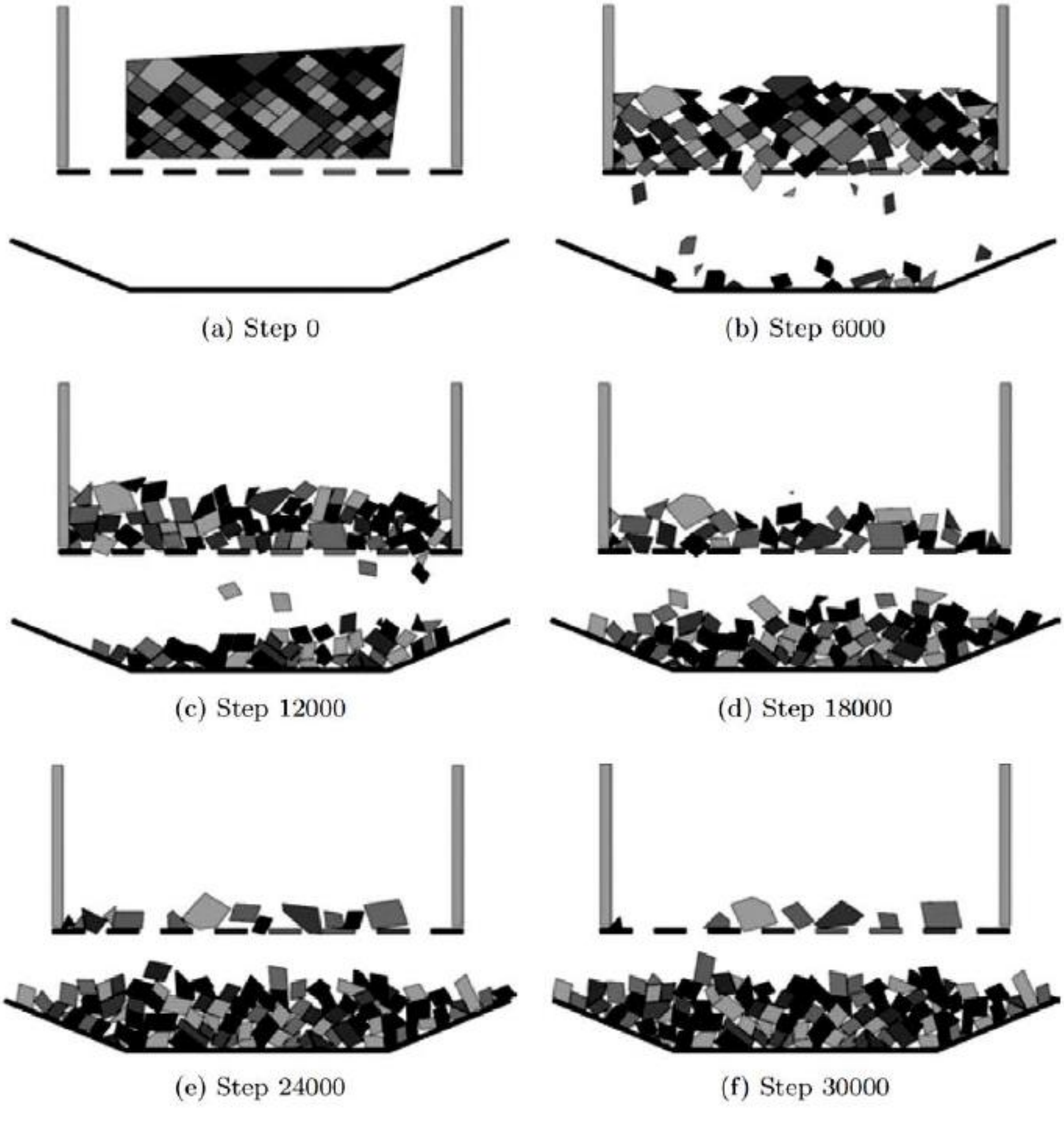


Fig. 5.3.4: Simulation of particle movement with a vibrating screen via NMM (An & Fu, 2012)

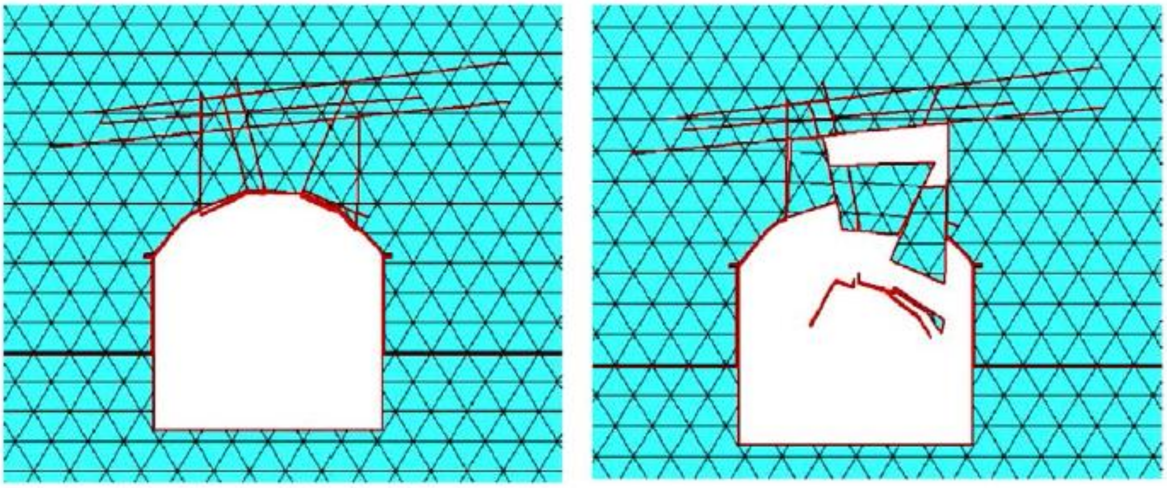


Fig. 5.3.5: Simulation of failure in a shotcrete supported roof via NMM (Wu & Wong, 2014)

5.4 Smooth Particle Hydrodynamics (SPH) / Peridynamics (PD)

Both methods are meshless. If nodal integration is used both methods are equivalent (Zhou et al., 2021). More details - especially related to SPH - can be found in our ebook called “Particle Methods”.

PD can be state-based (use of classical geomechanical parameters) or bond-based (use of parameters connected with particle-based contact laws)

Feng & Zhou (2021) used PD to simulate Mode-I and Mode-II crack propagation in granite samples exposed to uniaxial loading and compared the obtained fracture pattern with those obtained by CT analysis (see Fig. 5.4.1).

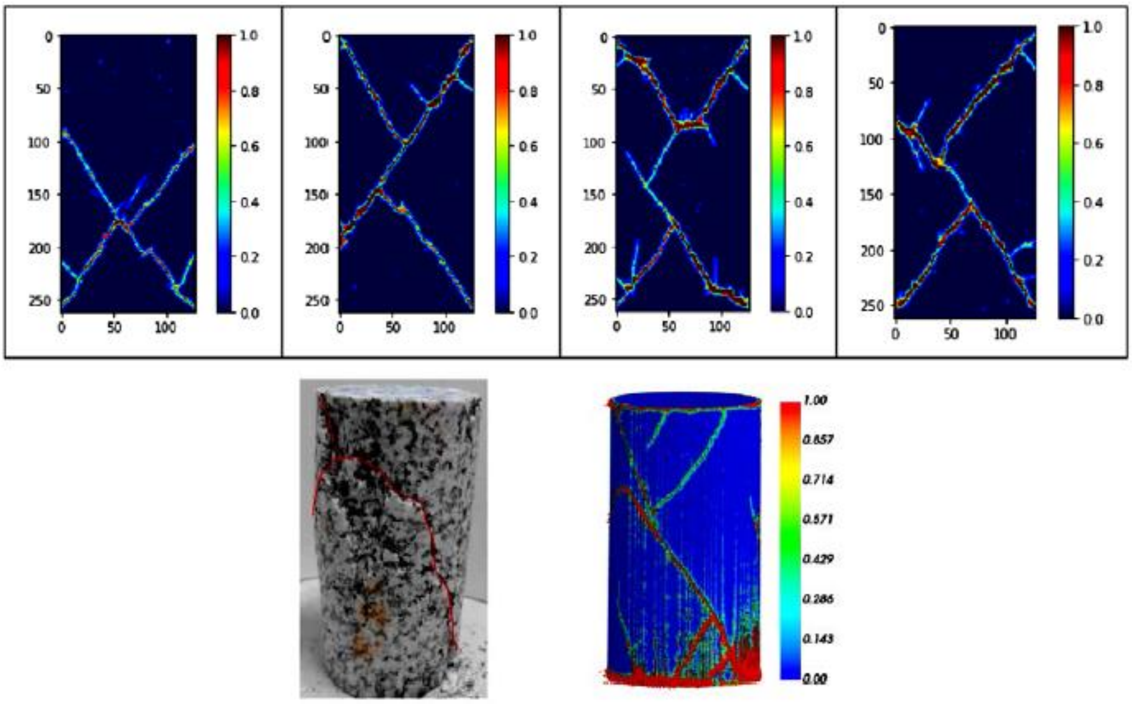


Fig. 5.4.1: Simulation of failure pattern in granite samples exposed to uniaxial compressive loading via Peridynamics (Feng & Zhou, 2021)

5.5 Enhanced Finite Element Methods

The classical FEM or FDM cannot handle singularities and discontinuous problems like crack propagation, fracturing and discrete fracture networks in a proper manner. Therefore, several extended version of FEM were developed, like XFEM (extended finite element method), GFEM (generalized finite element method), MFEM (mixed finite element method) or PFM (phase field method) besides other not so popular methods.

XFEM and GFEM use the “partition of unity method”. The main characteristic is the introduction of discontinuous enrichment functions for the nodes to describe discontinuities (cracks etc.):

$$u(x) = \sum_{i=1}^{n} N_i(x)\left(u_i + \sum_{j=1}^{nc(i)} a_{ji} F_j(r,\varphi) \right)$$

where:

r,φ	parameters of polar coordinate system
$u(x)$	displacement at location x
a_{ji}	node enrichment coefficient
$N_i(x)$	standard FEM shape function at crack tip
$nc(i)$	number of coefficients for node i
F_j	enrichment function

Fig. 5.5.1 shows the most popular crack models. XFEM and GFEM uses the imbedded strong (sharp) crack model whereas MFEM applies the smeared or crack band model (see Fig. 5.5.1 and 5.5.2). PFM uses regularized models (see Fig. 5.5.1 and 5.5.2). Exemplary, Fig. 5.5.3 documents the application of the enrichment functions to the corresponding nodes for the case of 3 crossing cracks.

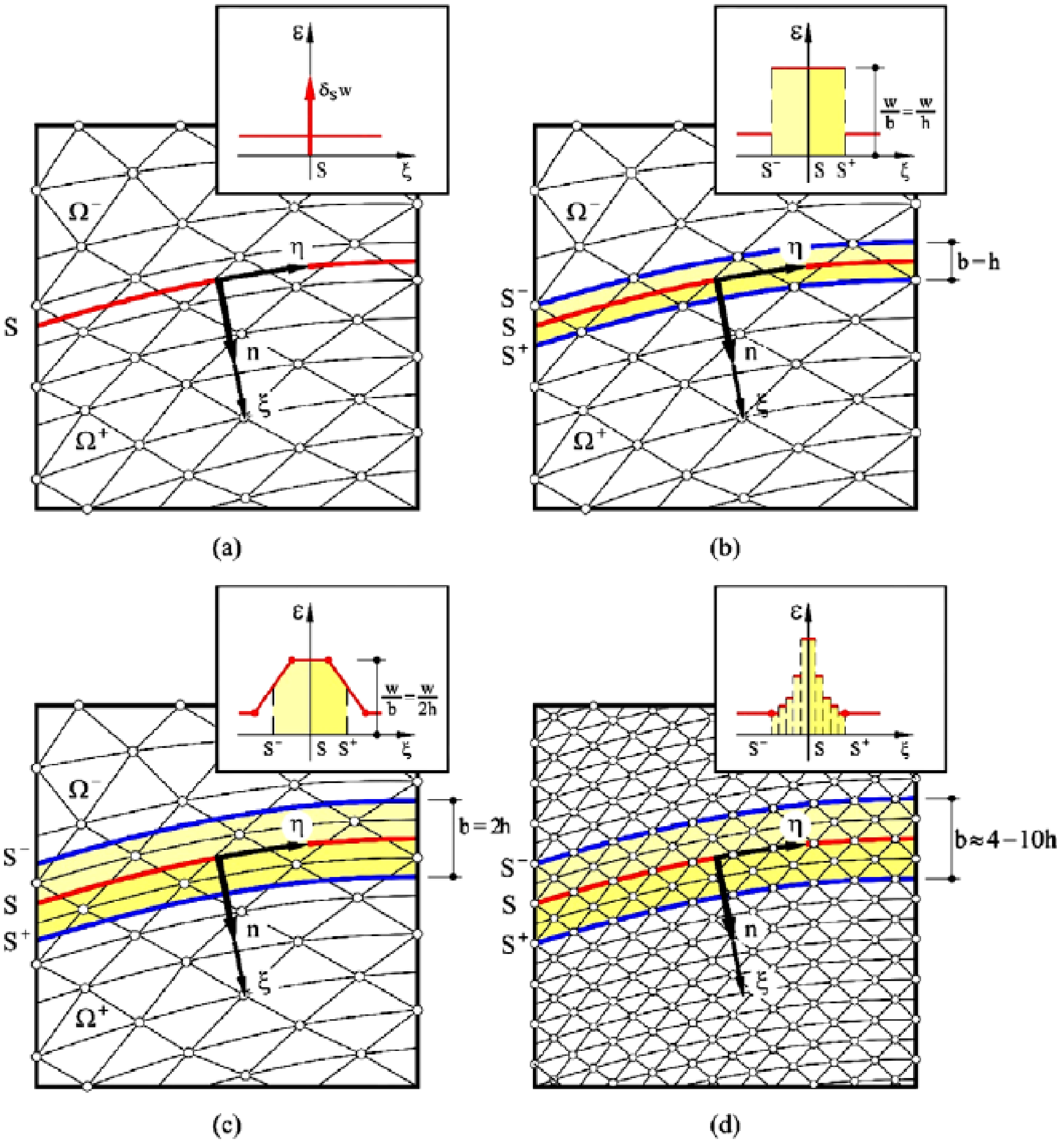


Fig. 5.5.1: Discrete crack representation for (a) embedded, (b) standard crack band, (c) mixed crack band and (d) regularized model (Cervera et al., 2021)

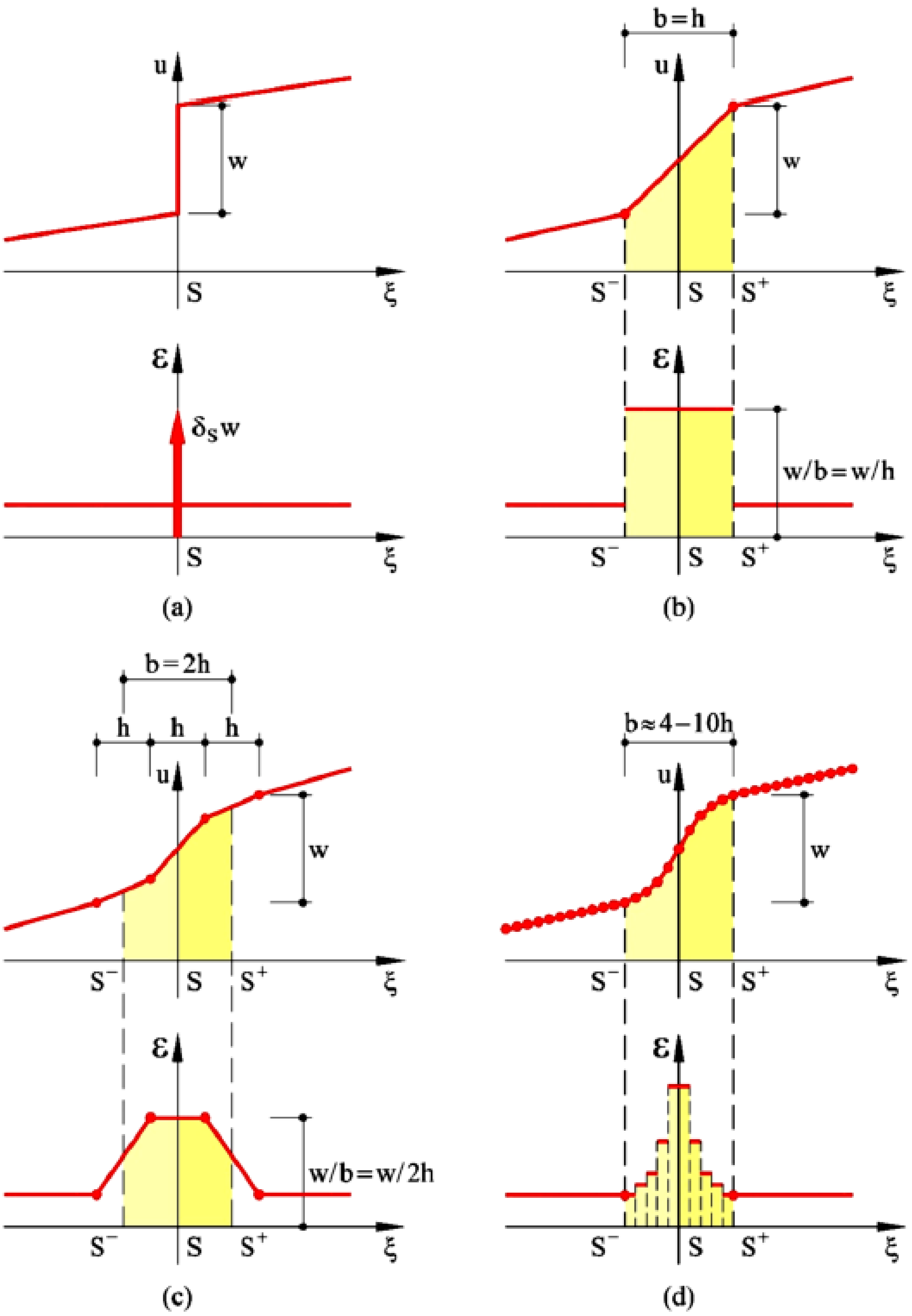


Fig. 5.5.2: Discrete crack representation for (a) embedded, (b) standard crack band, (c) mixed crack band and (d) regularized model in terms of displacements and strains (Cervera et al., 2021)

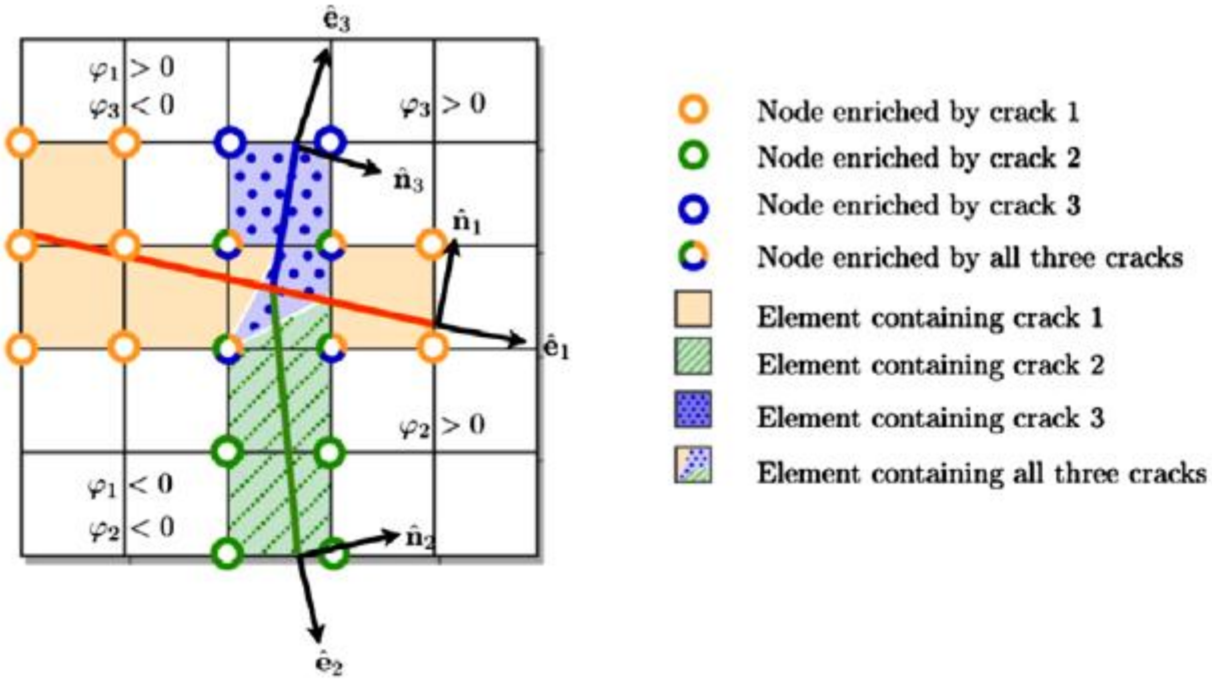


Fig. 5.5.3: Enriched nodes for 3 crossing cracks (Rivas et al., 2018)

The PFM belongs to the regularized methods. They avoid sharp crack models, but replace them by a continuous phase transition (e.g. from intact to completely separated). The scalar phase field (between 0 and 1) is similar to the damage variable in damage mechanics. The underlying solution scheme is based on the FEM. Fig. 5.5.4 illustrates the difference between sharp and diffuse crack models.

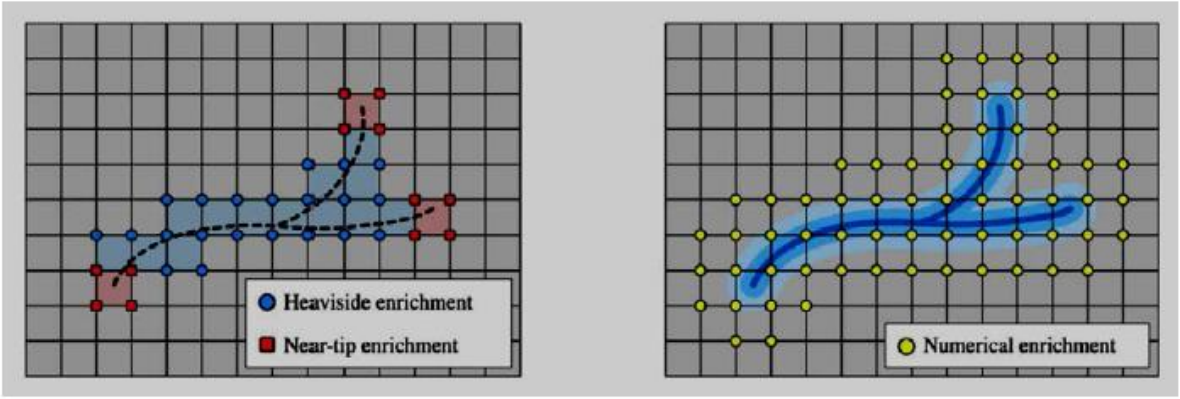


Fig. 5.5.4: Left: Standard XFEM approach, Right: PFM approach (Geelen et al. 2020)

XFEM can be applied to solve discontinuum-based problems in geo-engineering. Rivas et al. (2018) document the application of XFEM to simulate discrete fracture networks; Maulianda et al. (2020) document the application of XFEM for enhanced geothermal systems, geological carbon sequestration and block cave mining; Yu (2011) describes the application of XFEM for blocky rock masses and Lisjak et al. (2014, 2016) show applications about rock mass fracturing.

XFEM is based on cohesive elements between the basic finite elements as shown in Fig. 5.5.5a. The cohesive elements represent potential cracks, which can grow according to mode-I or mode-II as illustrated in Fig. 5.5.5b. Fig. 5.5.6 shows the simulation of the EDZ evolution induced by buckling effects (anisotropic rockmass). It demonstrates the transition from a continuum to a discontinuum.

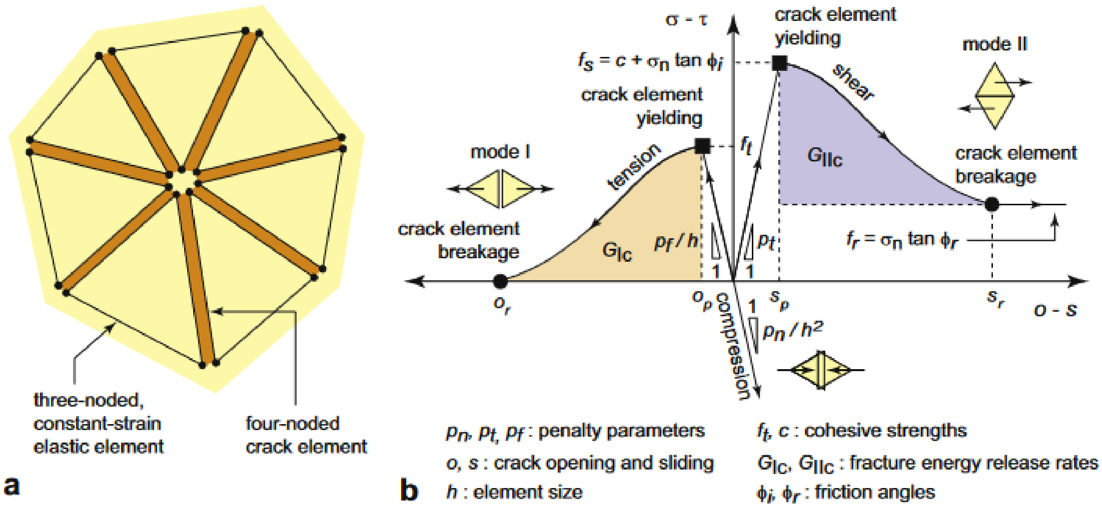


Fig. 5.5.5: Principle of FDEM simulation scheme (Lisjak & Graselli, 2014)

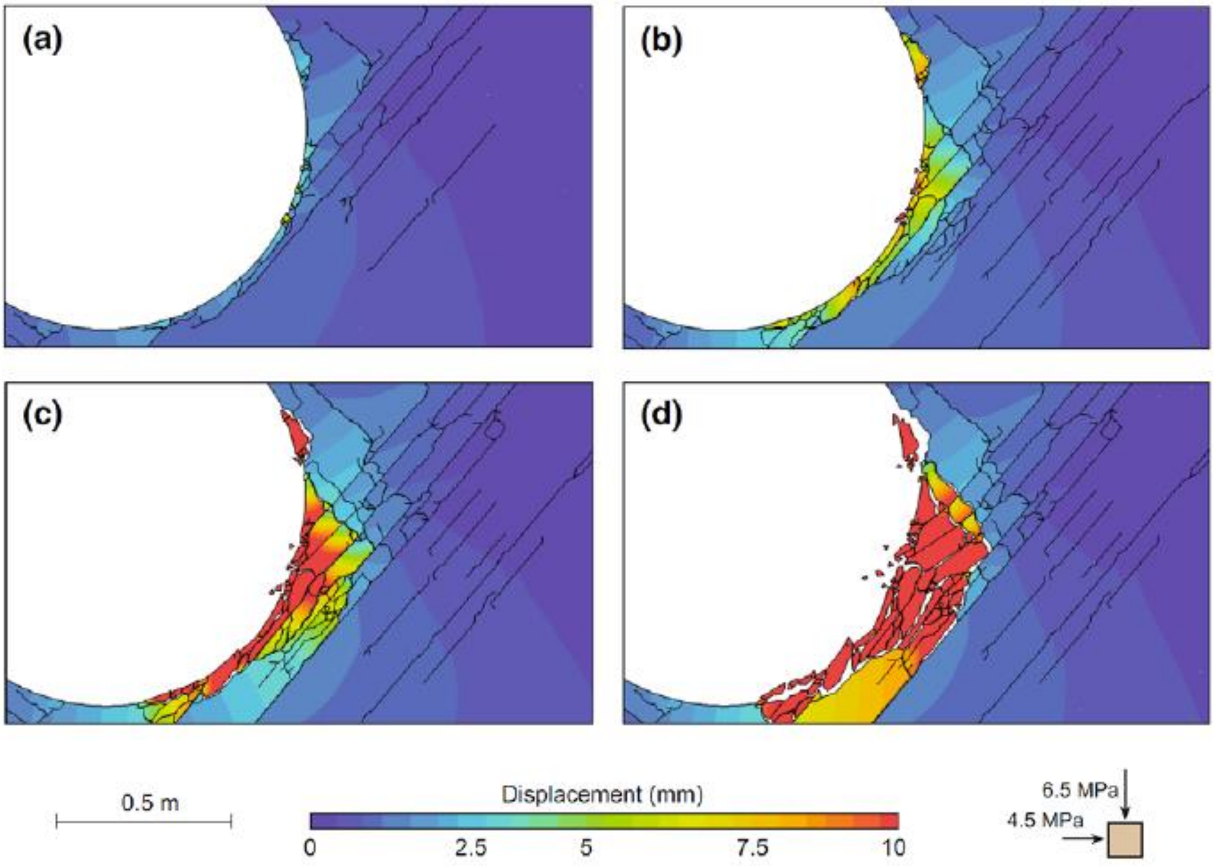


Fig. 5.5.6: Simulation of EDZ buckling of a tunnel in Opalinus Clay using FDEM (Lisjak et al., 2016)

5.6 Material Point Method (MPM)

The Material Point Method (MPM) combines the advantage of mesh-based and point-based approaches and is suitable especially for simulation of physical instabilities and large deformations. The continuum body is represented by Lagrangian points (material points), which move through an Eulerian mesh. The material points carry all material parameters and physical quantities (stresses, strains, velocities etc.). The computation consists or two parts: the moving material points and a finite element mesh. The finite element mesh has to cover the complete area of investigation. Boundary and initial conditions can be applied either to the mesh nodes or the material points. The classical calculation algorithm contains the following steps:

(1) Map information from material points to nodes

(2) Solve balance equations

(3) Map velocity field to material points

(4) Update positions of material points

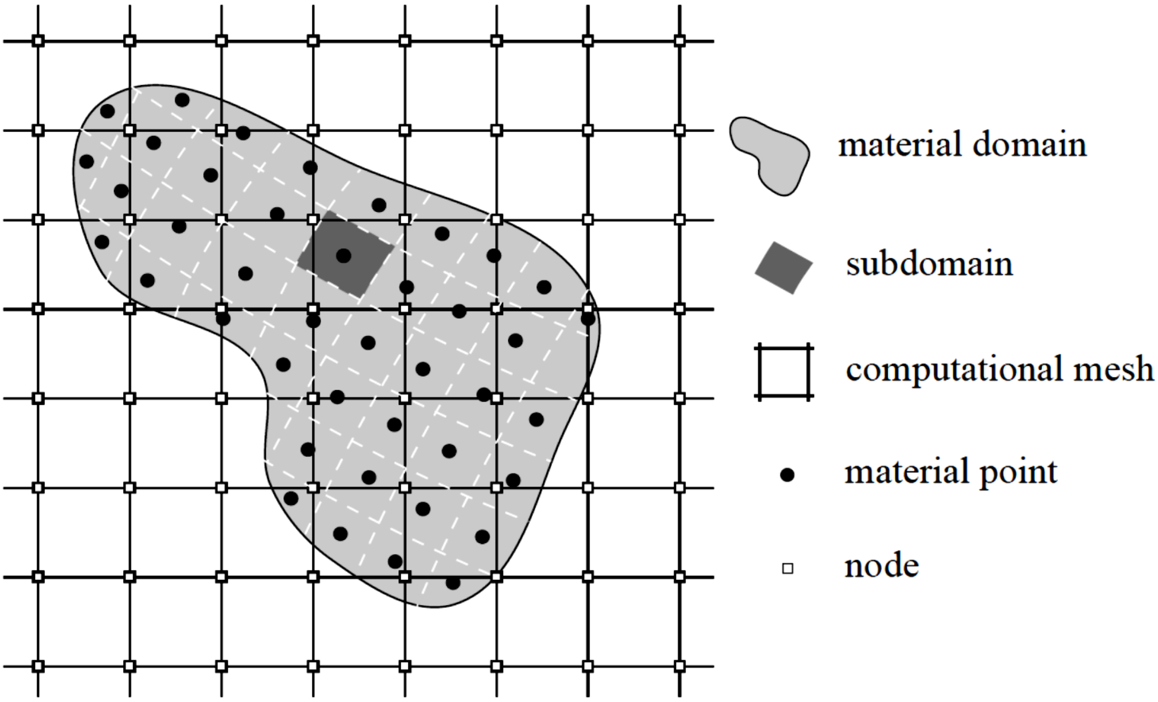
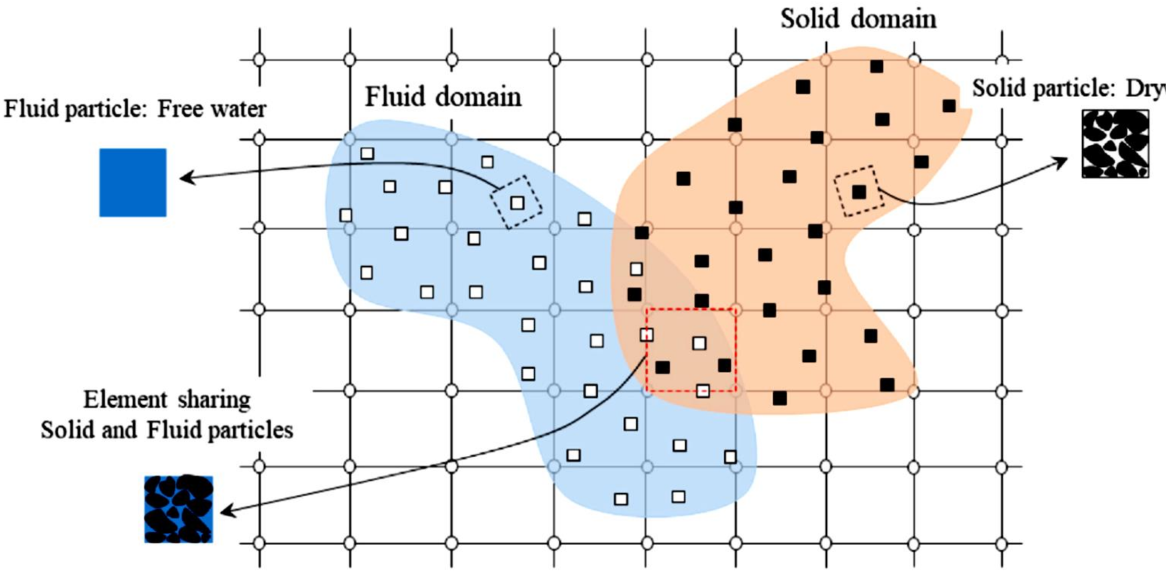


Fig. 5.6.1: Finite element mesh with material points and indication of the considered continuum (material domain) (Fern et al., 2019)

This technique allows also to simulate coupled processes, for instance THM-coupling. Du et al. (2022) applied this technique to simulate a complex landslide problem (see Fig. 5.6.2). They applied the double-point method. An alternative is the single-point method, where one point covers the two elements (solid and liquid).



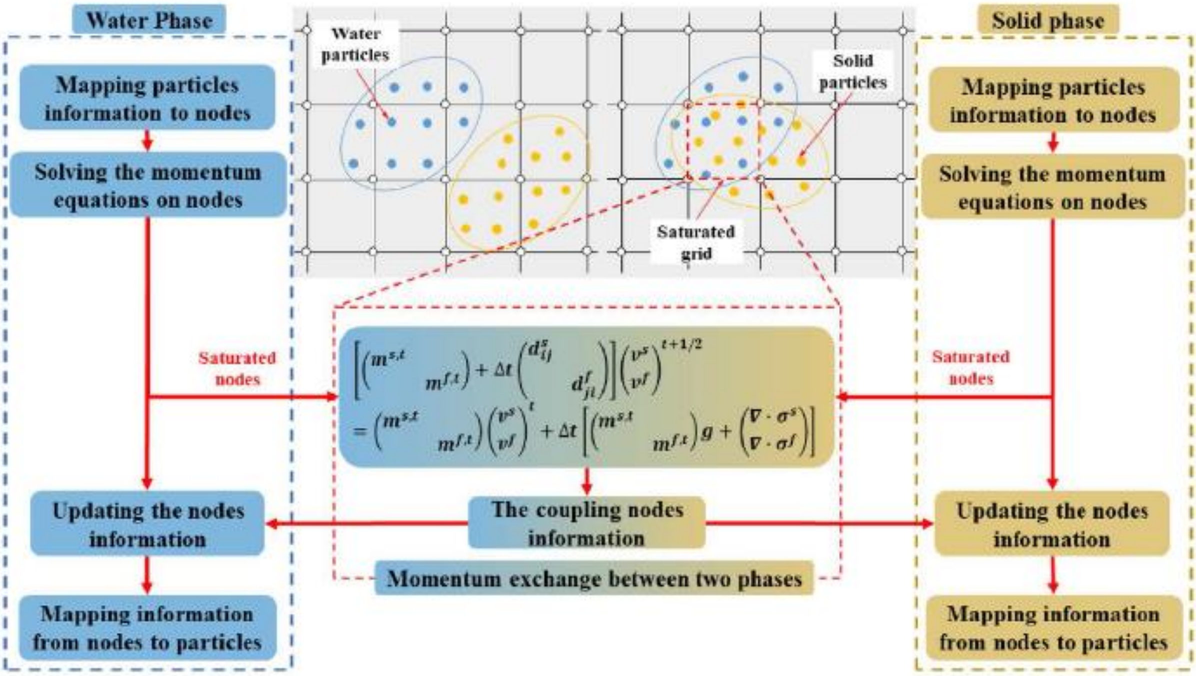


Fig. 5.6.2: HM-coupled MPM for simulation of a landslide problem (Du et al., 2022)

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