Preparation of Gocad-Skua Models for Numerical Simulations

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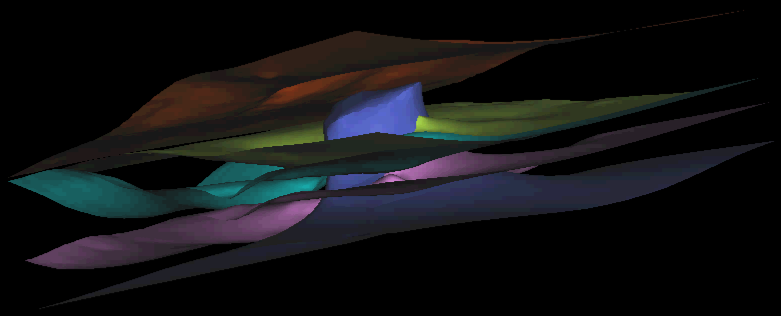
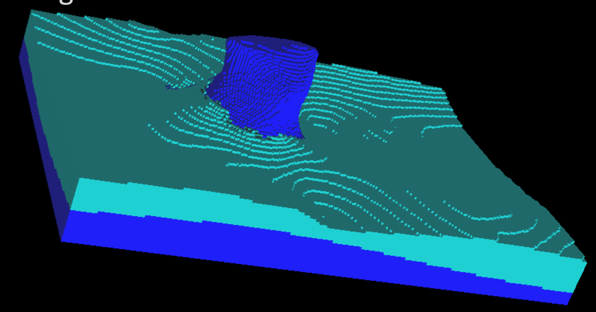
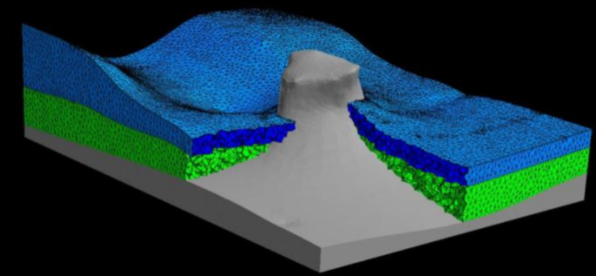


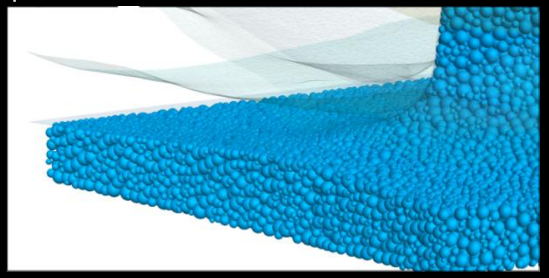
Regular Hexahedral Grid



Unstructured Tetrahedral Mesh



Spherical Distinct Particles



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Motivation

How can I use my 3D models?

Geometry modeling

- include all available information
- include geological concepts
- represent complex geometries

Process simulation

- include the best constrained geometry + material parameters

Where can I genereate the geometry?

- **Geomodeling software**
  - Geologic data → Subsurface geometry model
- **Meshing software**
  - Meshing Volume discretization
- **Simulation software**
  - Process model → Visualization of results

Simulation Methods

Solve partial differential equations

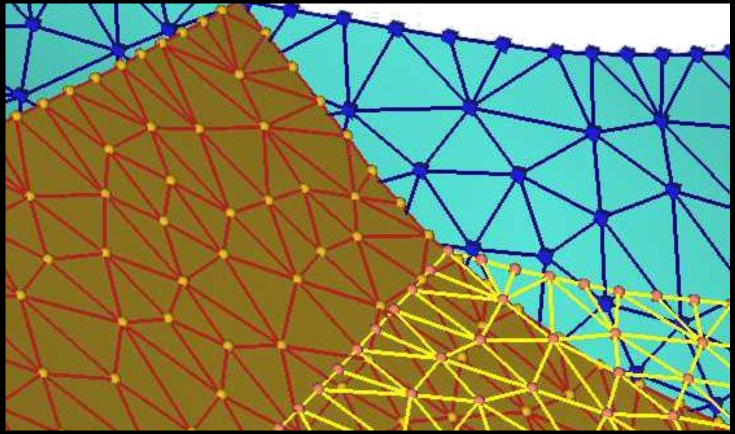
	Finite Difference Method	Distinct Element Method	Finite Element Method
Equation replaced by	differences	contact force-displacement and motion law	piecewise continuous basis functions
Solution is approxi-mated for	discrete points	discrete points	finite elements
Peculiarity	easily to implement on regular grids	break and decoupling of body parts	allows modeling on complex geometries
Discretization	**regular grid**	**unstructured set of particles**	**unstructured mesh**
Example	hexahedral grid	spherical particles	tetrahedral mesh

Is there an ideal mesh?

- appropriate to physics
- efficient and stable during simulation
- desired resolution

Problems

No ideal mesh in general ⟷ One ideal mesh for each application

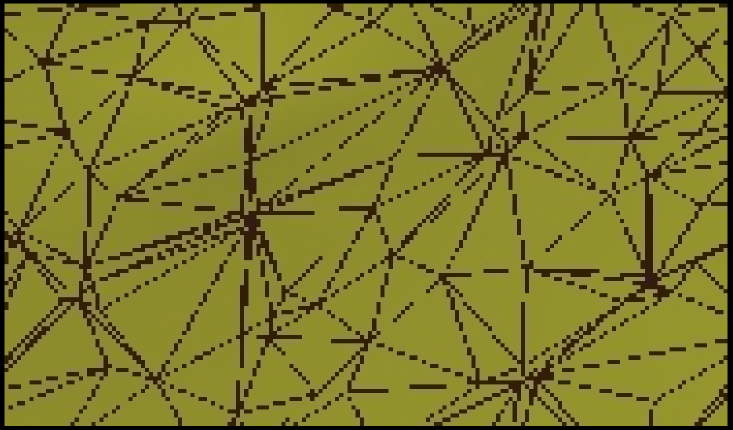


What do we need?

Different kinds of discretization

Good quality of discretization

Flexible import /export of models



Main problems:

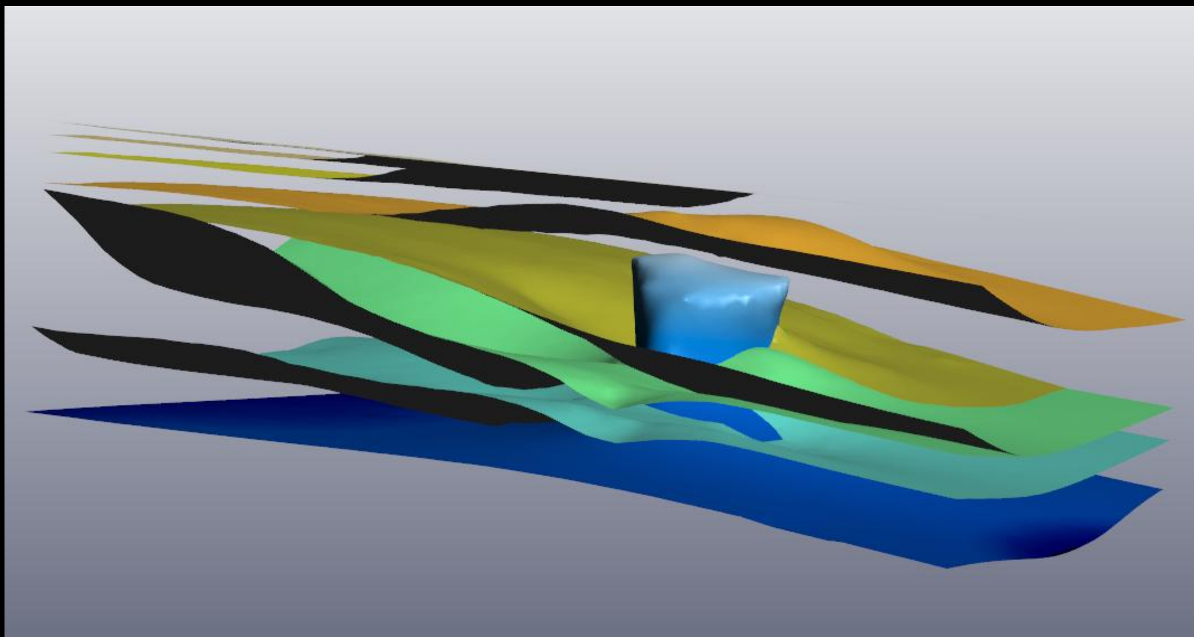
Unconformable triangulation (Gocad)

Bad triangles (SKUA)

Missing export functions

Example: Salt Diapir With Deformed Host Rocks

Geology



Stratigraphy

Cenozoic	Sand
	Clay
	Clay+Sand
	Marl
Mesococic	Claystone
	Limestone
	Sandstone
	Saltstone

Geometry/Topology

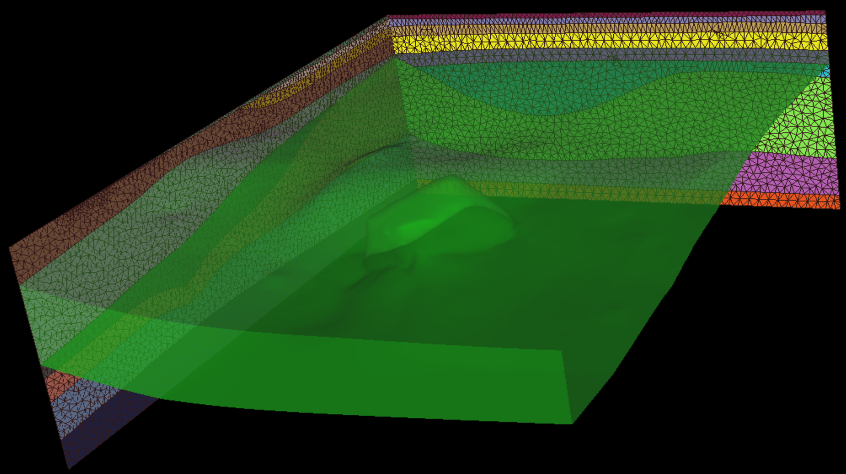
Multiple Z-Values
Polyhedra with holes
Horizons end in the model

Petrophysical Parameters

Density
Specific heat conduction
Specific heat capacity
Heat production
Spec. electrical resistivity
Friction coefficient
Normal and shear stiffness

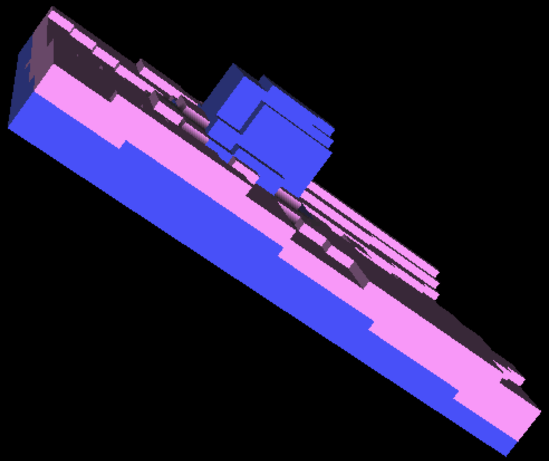
Temperature Simulation with the Finite Difference Method

Discretization



Merge parts of the boundary representation to closed volumes

Regular Hexahedral Grid



Constant step width
Constant volume

Simulated Process

Heat conservation equation with heat production

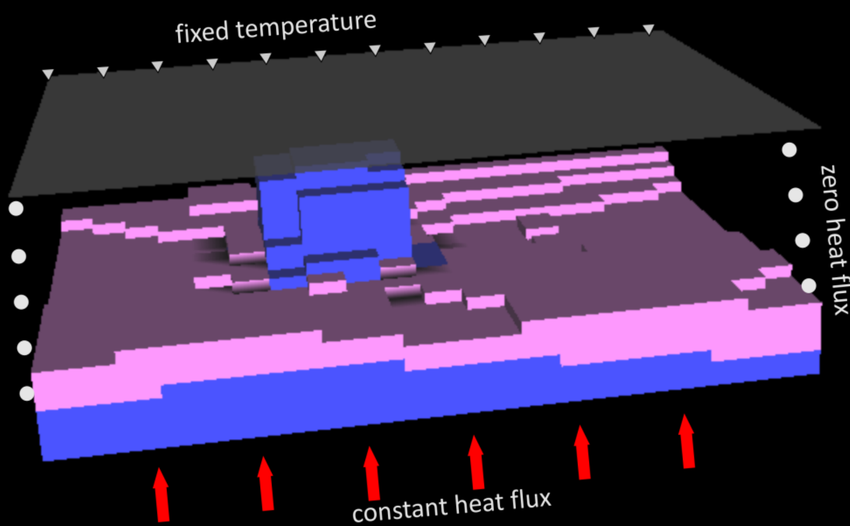
$$\rho \cdot c \cdot \frac{\partial T}{\partial t} = \frac{\partial k \partial T}{\partial x^2} + \frac{\partial k \partial T}{\partial y^2} + \frac{\partial k \partial T}{\partial z^2} + H$$

ρ … Density
c … Specific heat capacity
t … Time
T … Temperature
k … Specific heat conductivity
H … Heat production

Gerya (2010)

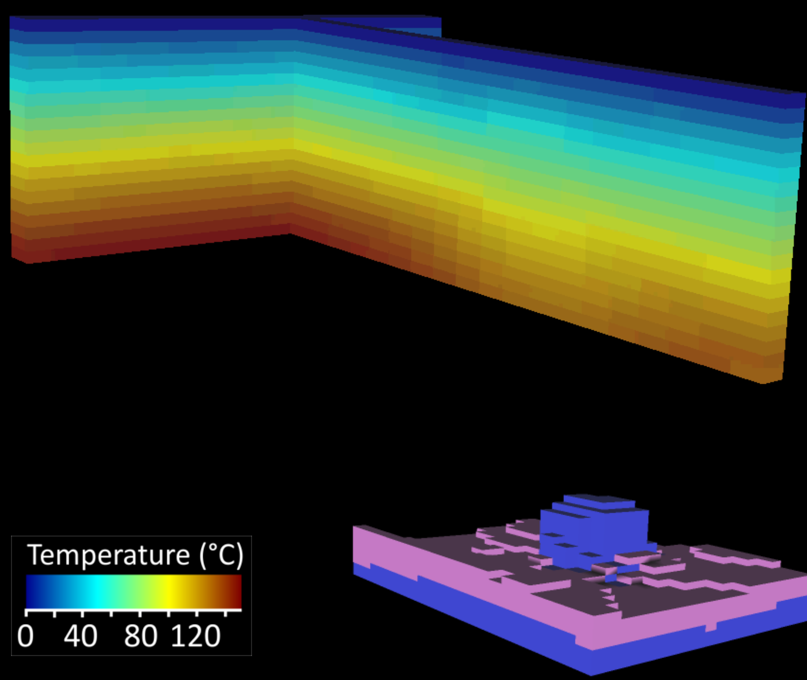
Temperature Simulation with the Finite Difference Method

Modeling setup



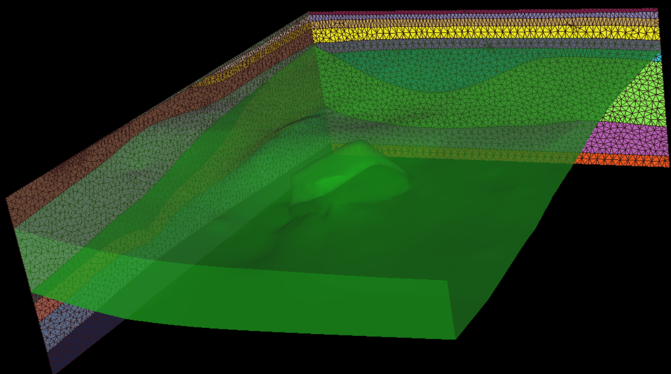
Material parameters:
Density,
Specific heat capacity,
Specific heat conductivity,
Heat production

Preliminary Simulation Results

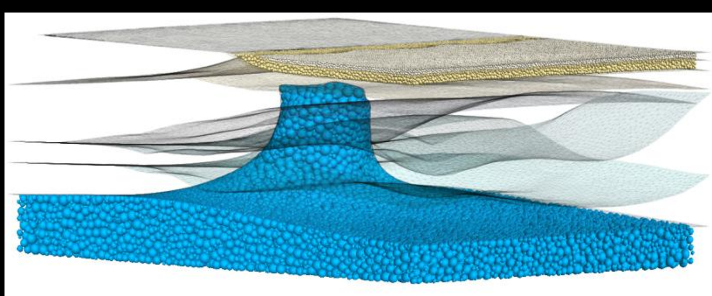


Displacement Simulation with the Distinct Particle Method

Discretization

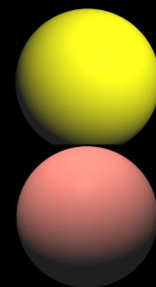


Merge parts of the boundary representation to closed volumes

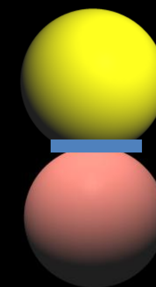


Spherical Particle Assembly

PFC3D 5.0



Contact stiffness
Contact overlap
Contact force
↓
Ball motion



Contact bond
Bond strength
Fracture force
↓
Delete bond

Variable ball radii
Radius distribution
Porosity

Simulated Process

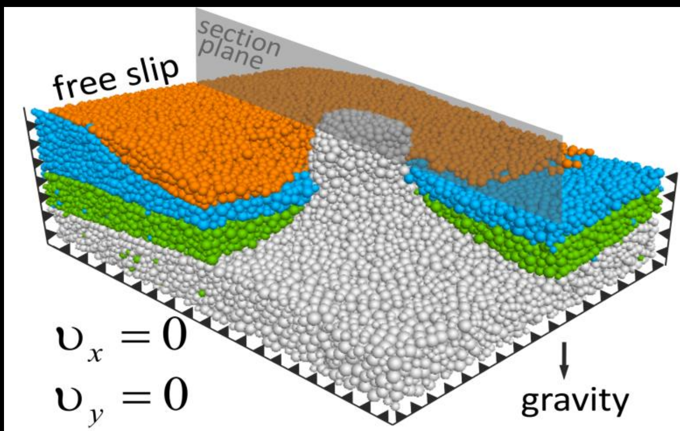
Force-displacement law for a linear contact model

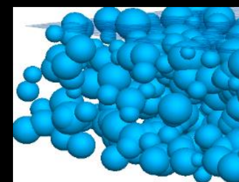
$$\boldsymbol{F}_{\mathrm{i}} = \boldsymbol{F}_{\mathrm{i}}^{N} + \boldsymbol{F}_{\mathrm{i}}^{S} = K_{\mathrm{i}}^{N} \cdot U_{\mathrm{i}}^{N} \cdot \boldsymbol{n}_{\mathrm{i}} + K_{\mathrm{i}}^{S} \cdot \Delta U_{\mathrm{i}}^{S} \cdot \boldsymbol{t}_{\mathrm{i}} = m_{\mathrm{i}} \cdot (\ddot{\boldsymbol{x}}_{\mathrm{i}} - \boldsymbol{g})$$

$\boldsymbol{F_i}$ … Resultant particle force
$\boldsymbol{F_c}$ … Contact force
N … Normal component
$\boldsymbol{n}$ … Normal unit vector
$\boldsymbol{t}$ … Tangential unit vector
S … Shear component
K… Contact stiffness
U … Overlap at contacts
$\boldsymbol{\ddot{x}}$ … Particle accelaration
$\boldsymbol{g}$ … Gravity acceleration

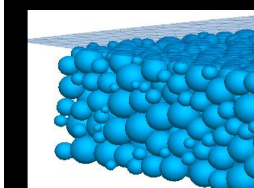
Displacement Simulation with the Distinct Particle Method

Modeling setup

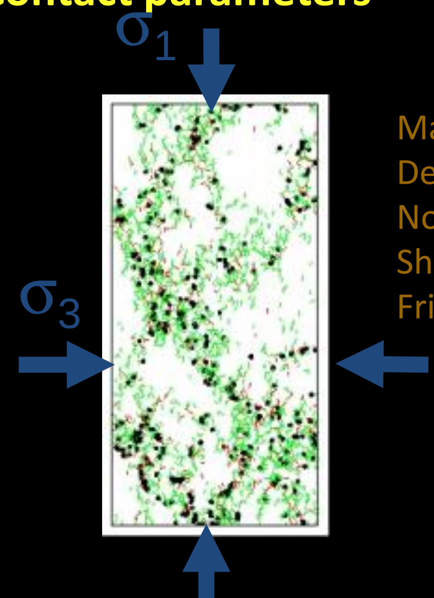




Minimize overlap

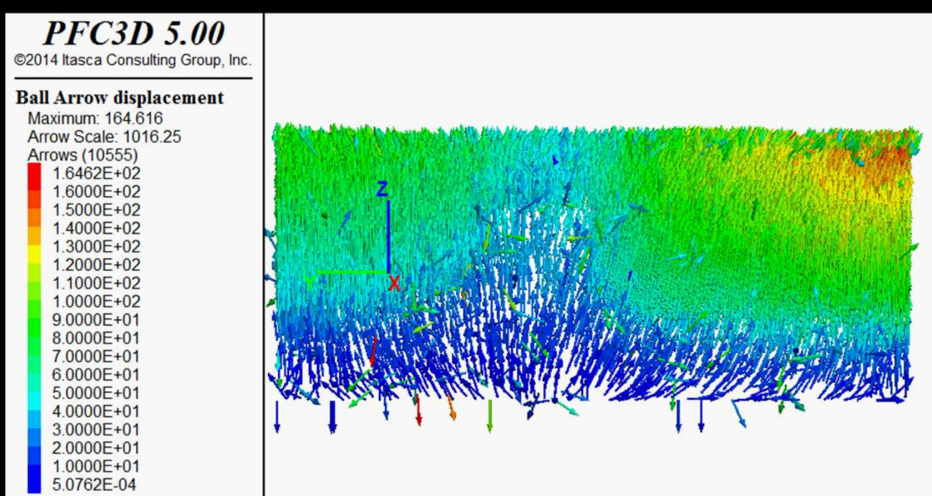


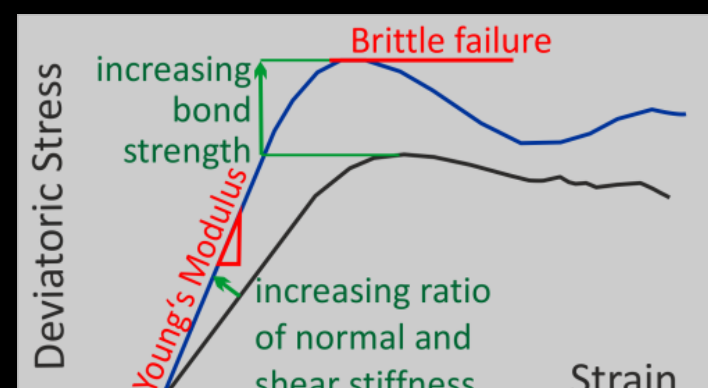
Contact parameters



Material parameters:
Density,
Normal contact stiffness,
Shear contact stiffness,
Friction coefficient

Preliminary Simulation Results

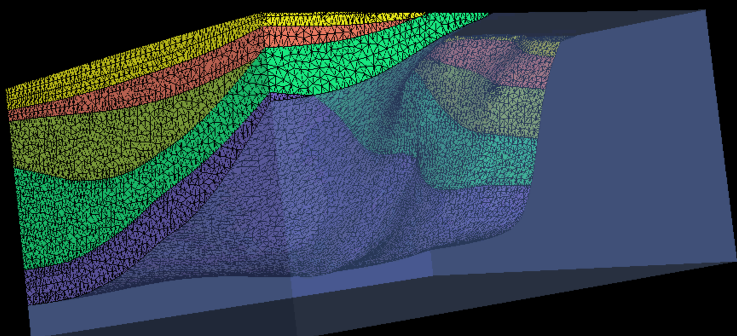




Cundall (1987),
Cundall and Strack (1979)

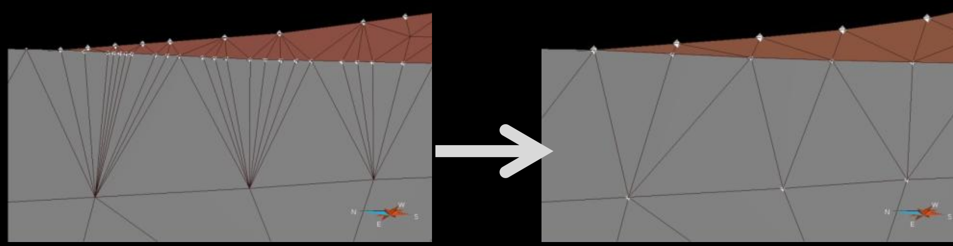
Electromagnetic Simulation with the Finite Element Method

Geometry



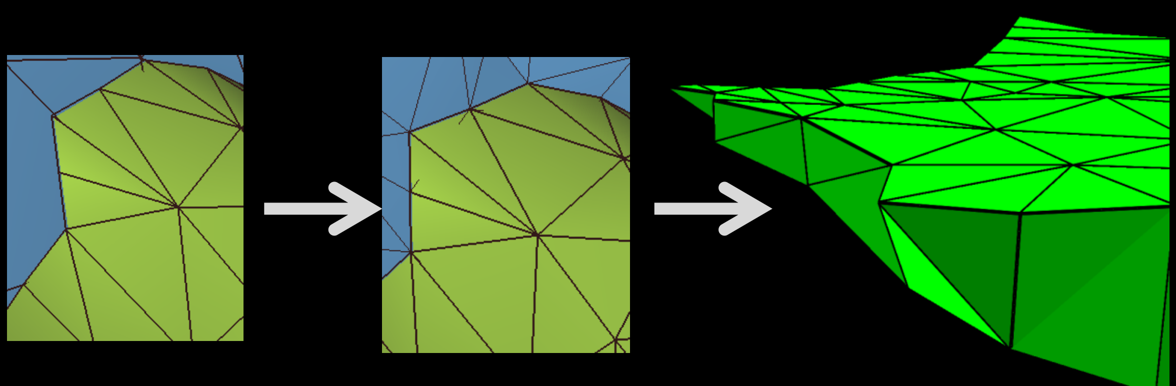
Improve mesh quality

Gocad CompGeom Plugin extract contact lines
Gocad Tweedle Plugin Voronoi diagram



Discretization

Unstructured tetrahedral mesh



Watertight boundary representation

For complicated geometries

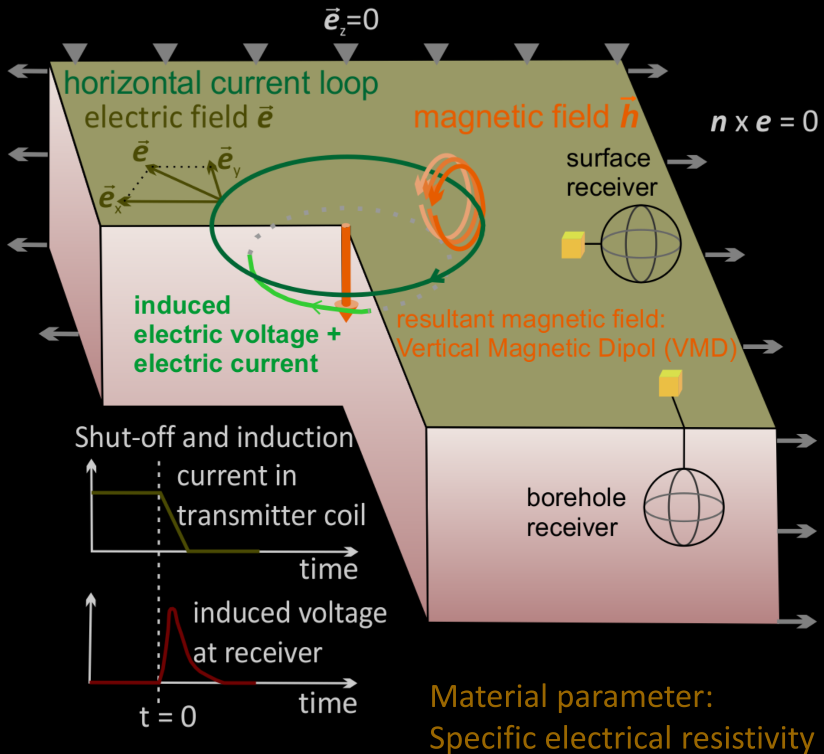
Simple topological model

Pellerin et al. (2014),
Zehner et al.(2015)

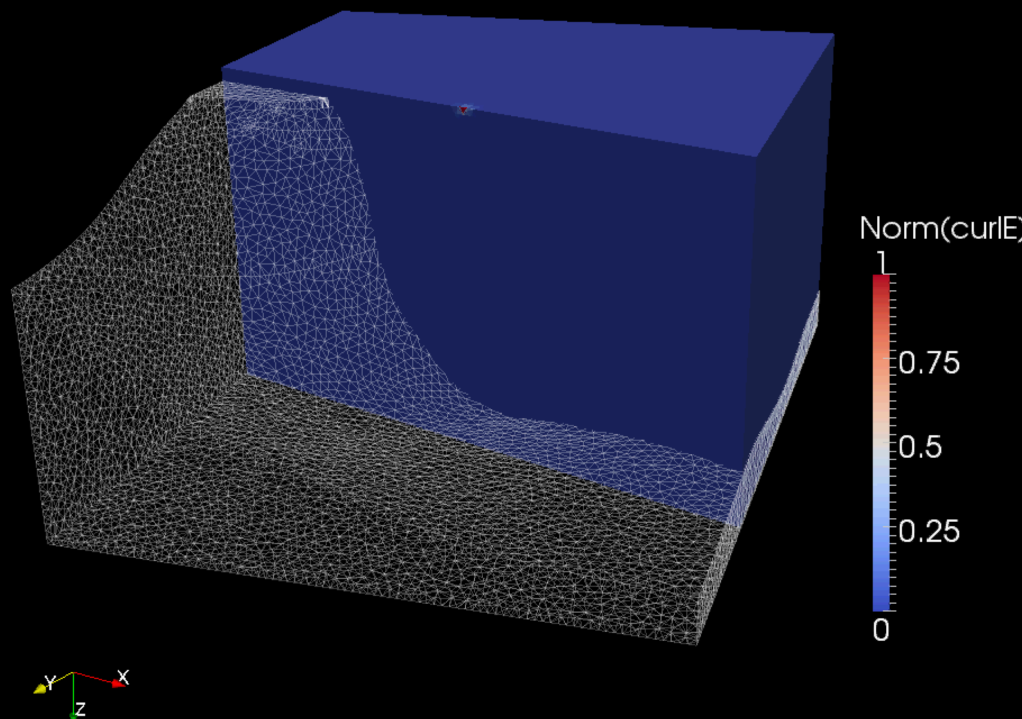
Simulation of a Transient Electromagnetic Experiment

MathWorks

Modeling setup



Simulation Results



Simulated Process

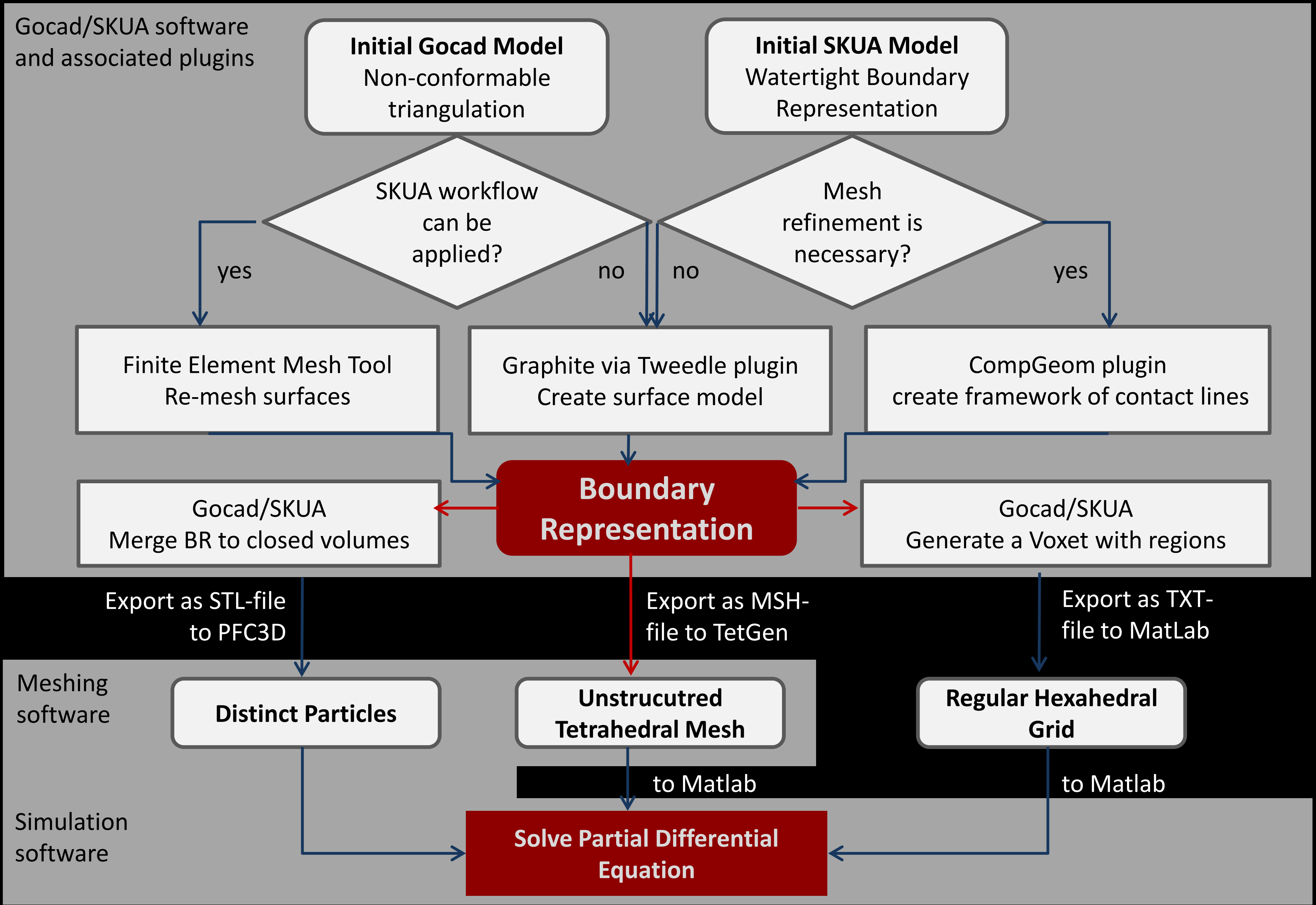
Curl–curl equation of the electric field describing the inductive response in the time domain

$$\nabla \times (\mu^{-1} \nabla \times \boldsymbol{e}) + \partial_t \sigma \boldsymbol{e} = -\partial_t \boldsymbol{j}^e$$

e ... Time-dependent electrical field
t ... Time
μ ... Magnetic permeability
je ... Electric source current density
σ ... Electrical conductivity

Börner et al. (2015)
Afanasjew et al. (2013)

Workflow



Gocad/SKUA software and associated plugins
Initial Gocad Model
Non-conformable triangulation
Initial SKUA Model
Watertight Boundary Representation
SKUA workflow can be applied?
Mesh refinement is necessary?
yes
no
no
yes
Finite Element Mesh Tool
Re-mesh surfaces
Graphite via Tweedle plugin
Create surface model
CompGeom plugin
create framework of contact lines
Gocad/SKUA
Merge BR to closed volumes
Boundary Representation
Gocad/SKUA
Generate a Voxet with regions
Export as STL-file to PFC3D
Export as MSH-file to TetGen
Export as TXT-file to MatLab
Meshing software
Distinct Particles
Unstrucutred Tetrahedral Mesh
Regular Hexahedral Grid
to Matlab
to Matlab
Simulation software
Solve Partial Differential Equation

Conclusions

The examples show:

Simulation results reflect the geometry of the domain
It‘s worth to use complex geometry models for process simulation!

How can we prepare the 3D models for a flexible use?

Provide models as conformable boundary representations
Generate a good mesh quality

Software developments:

Flexible export functions
Preserve boundary representation during model update
Algortithms for model simplification