

Documentation of elastic-plastic-diffusion-fracture simulation code

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This documentation accompanies the elastic-plastic phase field fracture simulation code for hydrogen embrittlement, which can be coupled to the results of the welding process model, consisting of ABAQUS user subroutines, of the pipeline structural integrity framework described in

”J. Wijnen, J. Parker, M. Gagliano, E. Martínez-Pañeda. A computational framework to predict weld integrity and microstructural heterogeneity: Application to hydrogen transmission. *Materials & Design* 2025.”

The model can be used with and without results of the welding model, of which the code can also be obtained from <https://mechmat.web.ox.ac.uk/codes..> In the latter case, homogeneous properties are specified. The model setup in ABAQUS CAE is the same in both scenarios. The reading of weld model results is done in the user-subroutine, which can be specified in the additional parameter file. In addition the fracture model can be run with hydrogen diffusion or without.

This documentation is accompanied with input files (including .cae file) of a pipeline weld containing a crack.

In addition, a video tutorial on how to setup a fracture simulation that is coupled to weld model results is available on Youtube:

<https://youtu.be/1AR920VhQn0>

Note that this video is the third part of three video tutorials, in which the full model (welding simulation, residual stress simulation, and fracture simulation) is setup for a pipeline weld.

1 Software requirements

This documentation assumes that ABAQUS is setup properly such that the `abaqus` command can be used in the Command Prompt or Terminal. Additionally, the intel fortran compiler needs to be setup to be able to run user-subroutines.

Some python pre-/postprocessing scripts are provided that make use of the ABAQUS python scripting language. They can be run with the `abaqus python` command.

ABAQUS version 2022 is used in the accompanying .cae files, and can only be opened with this or later version. Nevertheless, the code itself should be able to run with any ABAQUS version, but this is not tested.

2 Abaqus CAE setup

Large part of the simulation can be setup in the ABAQUS CAE environment. The most important steps in the setup are explained below.

2.1 Geometry, crack, assembly and mesh

A geometry can be created in the ABAQUS CAE environment. If the fracture simulation is based on a welding simulation, a copy of the thermal model can be made so that the same geometry is used. The crack can be inserted into the geometry as a partition of the sketch. As usual with ABAQUS geometries, an instance of the part is created under **Assembly**. Quadrilateral elements of quadratic order with reduced integration have to be used:

```
Element Type > Family: Plane Strain, Geometric order: Quadratic, Reduced integration
```

2.2 Material

The assigned material needs to have the following material behaviors assigned:

- General > User Material
- General > Depvar.
Number of solution-dependent state variables: 11.

2.3 Steps

Create a loading step

Step, Static

Note that if hydrogen diffusion is modeled, the real world time period should be described.

Convergence with the quasi-Newton solver might be better than the conventional Newton-Raphson solver, even when the fracture simulation is coupled to hydrogen diffusion. This can be set as follows in the step definition window: **Other > Solution technique: Quasi-newton** The default number of iterations after which a kernel is reformed (8) usually works. If convergence problems are encountered, changing this number can sometimes improve convergence.

In increments where crack propagation occurs it is not uncommon that several hundred iterations are needed to reach convergence. To ensure that ABAQUS does not abort the solution process and reduces the time increment, we need to change the solution controls. In **Module: Step**, in the menu bar at the top:

Other > General solution controls > Edit > Step-1

The following settings are usually sufficient

Time Incrementation > IO: 2000, IR: 2000

More > Ip: 2000, IC: 2000, IL: 2000, IG: 50

Finally, better convergence is usually achieved when the line search method is enabled. In the same **General solution controls** window:

Line search > N: 10-20 range

2.4 Boundary conditions

Displacement boundary conditions can be described as usual in ABAQUS. For pipelines, a radial displacement needs to be applied to represent a pressure, following the theory for thin-walled cylinders

$$u_r^* = \frac{pR^3}{bE} \left(1 - \frac{\nu}{2}\right) \quad (1)$$

where p is the pressure, R is the radius, b is the wall thickness, E is the Young's modulus, and ν is the Poisson's ratio. To prescribe a radial displacements, a radial CSYS needs to be created and selected. In the boundary condition definition window

Create Datum CSYS > Cylindrical > Origin: 0 0 0 (center pipeline)
> Point on R-axis: 1 0 0 > Point on R-Theta plane: 0 1 0

When this CSYS is selected, displacement U1 is the radial displacement. Make sure that the **Amplitude** is set to **Ramp** or create a amplitude that describes the displacements over time.

The phase field crack cannot be directly prescribed as dof. This also depends on which dof the user-element is using as phase field dof, which will be described later. A python script is provided to prepare the input files. This script assumes that the crack is initially prescribed as dof **UR3**, under **Type: Displacement/Rotation**.

Because of similar reasons, the hydrogen boundary condition needs to be prescribed as an **Electric potential** dof. The prescribed hydrogen concentration can be related to the hydrogen pressure following Sievert's law

$$C = S\sqrt{p}, \quad (2)$$

where S is the hydrogen solubility in steel. Since C does not increase linearly when p is prescribed linearly, an **Amplitude** needs to be used to prescribe the hydrogen concentration as a function of time.

2.5 Job

Create a job. Here we named it thermal. To write the simulation input file of the job:

Right-click on the job in the tree > Write Input

3 Additional input files

3.1 set_parameters_fracture.f90

The material properties need to be specified in a file *set_parameters_fracture.f90* in the working directory of the simulation. An example of *set_parameters_thermal.f90* is:

```
! Elastic
param%ee = 2.1d5 ! (Youngs modulus)
param%enu = .3d0 ! (Poissons ratio)

! Plastic
param%sy0 = 500.d0 ! (yield strength)
param%n = 0.1 ! (hardening exponent)

! Damage
param%strainsplit = 1 !(0: no split, 1: hydrostatic-deviatoric split)
param%Gc0 = 50.0 ! (crititcal energy release rate)
param%lc = 0.4d0 ! (phase field length scale)
param%beta = 0.1d0 ! (fraction of plastic energy contribution to damage)

! Hydrogen degradation
param%D = 4.5d-4 ! (Hydrogen diffusivity)
param%Hdeg_flag = 1 ! (0: no degradation, 1: degradation law)
param%Hdeg_fmin = 0.1d0 ! (degradation law paremeter, see paper)
param%Hdeg_q1 = 25.0d0 ! (degradation law parameter, see papaer)
param%Hdeg_q2 = 1.8d0 ! (degradation law parameter, see paper)

! Abort simulation when average stress falls below fraction of
! maximum (over time) average stress.
param%maxloaddrop = 0.3d0
```

3.2 Using welding model results as input

The results of the welding model (properties, residual stress), can be used as initial conditions for the fracture simulation. A python script *fracture_initial.py* is provided that prepares the input file. The script can be run with

```
abaqus python fracture_initial.py database.odb fracture.inp toughness_data.txt
```

where the following files are included

- **database.odb**: the path to the output file of the welding simulation (residual stress simulation).
- **fracture.inp**: the input file of the fracture simulation created following this document. The mesh does not have to coincide with the mesh of the odb file. The results are interpolated to the new mesh.
- **toughness_data.txt** (Optional, can be removed from the script command): This file contains phase-dependent fracture properties, which are properties that cannot be read in from the welding simulation. The file has the following format:

```
*Gc0, 80., 80.
*lc, 0.37, 0.31
*fmin, 0.15, 0.08
*q1, 25., 20.
*q2, 1.8, 1.
*n, 0.1, 0.05
*D, 4.5e-4, 3.0e-4
```

The first column of each property defines the value for ferrite/pearlite. The second row defines the value for bainite/martensite.

The script creates a new file `fracture-initial.inp`, which has the following format:

```
10, 64483, 4
*q1
1, 1, 24.999999
1, 2, 24.999999
...
```

The first line defines the number of input properties, number of elements, and number of integration points per element, respectively. The second line specifies which property is specified. The following $64483 \cdot 4$ rows specify the element number, integration point number and value of the property.

To use this file, the following line needs to be added to `set_parameters_fracture.f90`:

```
param%propfile = '~/path/to/folder/fracture-initial.inp'
```

The properties that are specified in this file overwrite the properties specified in `set_parameters_fracture.f90`.

3.3 Prepare the .inp file

The simulation code makes use of user-elements. These need to be inserted in the `fracture.inp` file. A python script `fracture_input.py` is provided which automates this process. It can be used with the following command

```
abaqus python fracture_input.py fracture.inp 1
```

Here, the `fracture.inp` file is the input file created following this document. The 1 specifies that the simulation includes hydrogen diffusion. Alternatively, a 0 can be used, which specifies that no hydrogen diffusion is modeled. A new file `fracture_mesh.inp` is created in which the following is changed

- The user element is defined, with dof number 3 for the phase field dof and dof number 7 for the hydrogen dof. These dof numbers work with a static analysis.
- User elements are inserted in the file.
- The initial plane strain elements are inserted after the user elements. These are needed to show the results in ABAQUS.
- The element sets are changed to the new element ordering so that the material defined following this document is assigned to the initial plane strain elements.
- The names of the state-dependent variables are inserted to create a readable output.
- Boundary conditions prescribed to `UR3` (dof number 6) are changed to dof number 3. Boundary conditions prescribed to `Electric potential` (dof number 9) are changed to dof number 7.

4 Running the simulation

To run the model, the `sim_fracture.f90` file needs to be linked to ABAQUS. This can be done by running the following command:

```
abaqus job=fracture input=fracture_mesh.inp user=sim_fracture.f90 cpus=1 interactive
```