1.1. Software for stress calculation and fracture simulation in arbitrary porous microstructures

*The program "PReMISe" for **P**o**R**ous **MI**crostructure **S**imulation and fracture modelling has been developed in Oxford University within the framework of the EDF sponsored project 'Microstructure-based modelling of crack nucleation and growth in nuclear graphite', 2013-2015. This software allows simulation of synthetic microstructures with spherical, ellipsoidal or arbitrary shaped pores, stress field calculation and fracture simulation within a porous microstructure on the basis of the presented algorithms. The interface has been developed in Delphi and examined for 32- and 64-bit Windows platforms. Codes for stress calculation and fracture simulations have been developed in Intel Fortran with 'OpenMP' technology.*

In order to run the program:

1. Intel redistributable library package 'w_fcompxe_2011.10.325' (Update 10 for 32-bit version) must be installed for correct working of the code's parallel part (https://software.intel.com/en-us/articles/redistributable-libraries-for-the-intel-c-and-visual-fortran-composer-xe-for-windows/)
2. Unpack 'PReMISe' zip-file saving the paths to the sub-folders.
3. Run PReMISe.exe.

The main window of the program contains four tabs: "Microstructure simulation", "Microstructure processing", "Stress calculation", and "Fracture simulation".

1.2. 'Microstructure simulation' tab

1. Chose the first tab 'Microstructure simulation' if you want to create a synthetic microstructure with the given porosity and filler fractions and chosen geometrical shape of the pores (Figure 1).
2. Menu 'Help' allows reading manual about using of this software, shows information about the program and a license file (MIT license is accepted for this case).
3. Indicate a lattice edge size in cells. An optimal size is 100 cells, which is considered as the maximum in order to avoid excessive memory and time consumption during the program run.

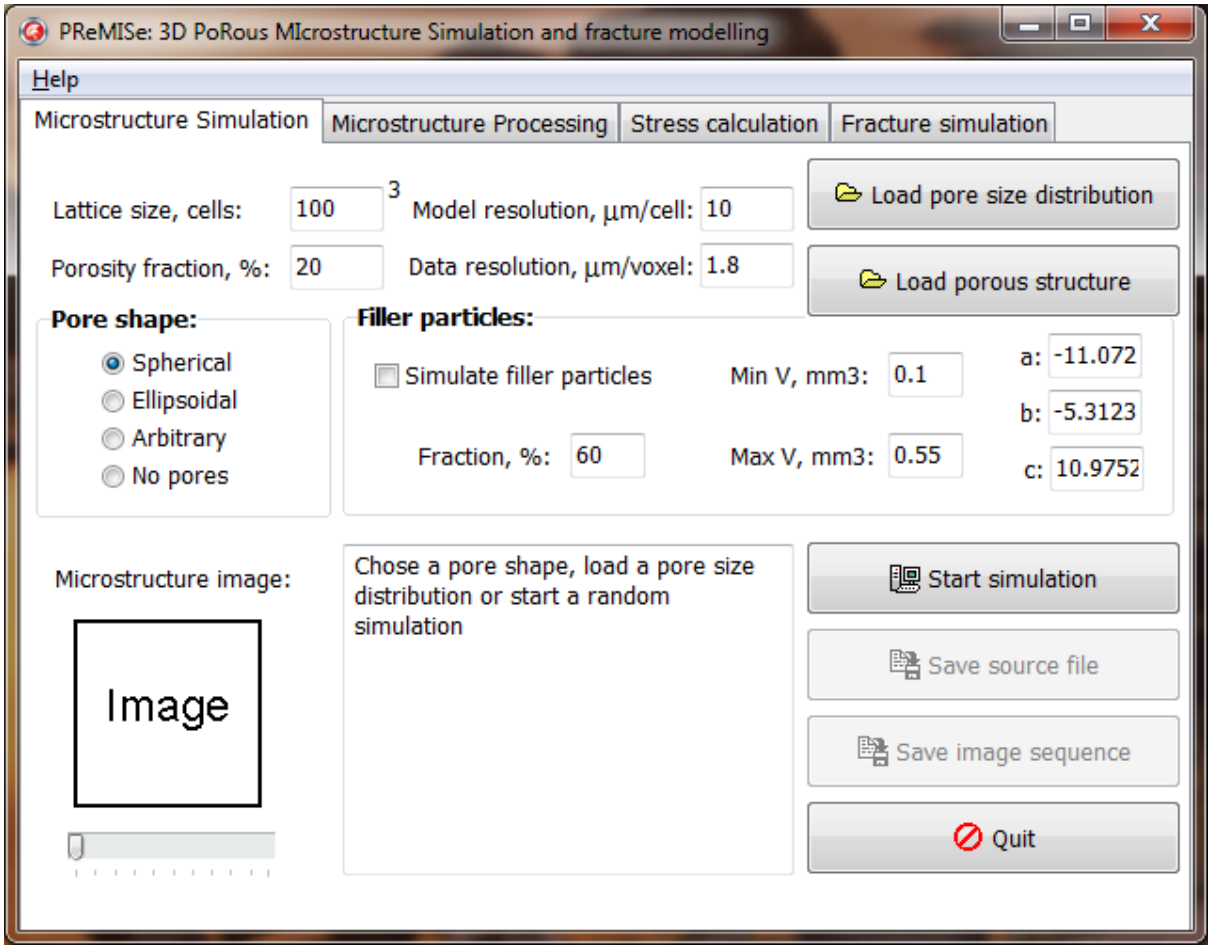

Figure 1 - The first tab of the program for microstructure simulation.

Three different work flows are possible further:

1. Creation of a synthetic porous microstructure without filler particles

- Indicate a desirable porosity fraction in percent. The final value of the porosity fraction obtained may slightly differ from the original value that is specified here; this depends on the chosen pore geometry and a presence of the filler particles in the microstructure. The final value will be shown in the same field after the simulation.
- Indicate a resolution of the model and experimental data in the corresponding fields (i.e. the size of the voxel). The resolution of the data is necessary to provide a correct scaling between the real data and the model.
- If you need to create the pores in the microstructures, first load a txt-file with a pore size distribution if you want to create a microstructure that is obtained according to a pre-defined pore volume distribution. Otherwise, random pore volumes will be used in the microstructure; the maximum possible pore diameter is limited in this case depending on the lattice size and porosity fraction. The file 'distribution.txt' that is located in the 'Files' folder with the program contains pore volumes in units of cubic micrometres with a corresponding cumulative distribution their frequency.
- Chose one of the pore shapes. The following geometrical shapes are available: spherical, ellipsoidal and arbitrary shapes. All pores will be allocated randomly inside the microstructure. Pore overlapping is allowed.

– To run the simulation of the synthetic microstructure with the indicated parameters, press ‘Start simulation’ button. A geometrical estimation of the bulk value of Young’s modulus for the porous synthetic microstructure is performed during the simulation. The value will be shown in the text window (Figure 2).
– The field ‘Microstructure image’ is empty before the program starts. After the simulation has been performed, browsing of the microstructure slice by slice is available using a slider in the bottom of the image stack. The total number of slices corresponds to the lattice size.

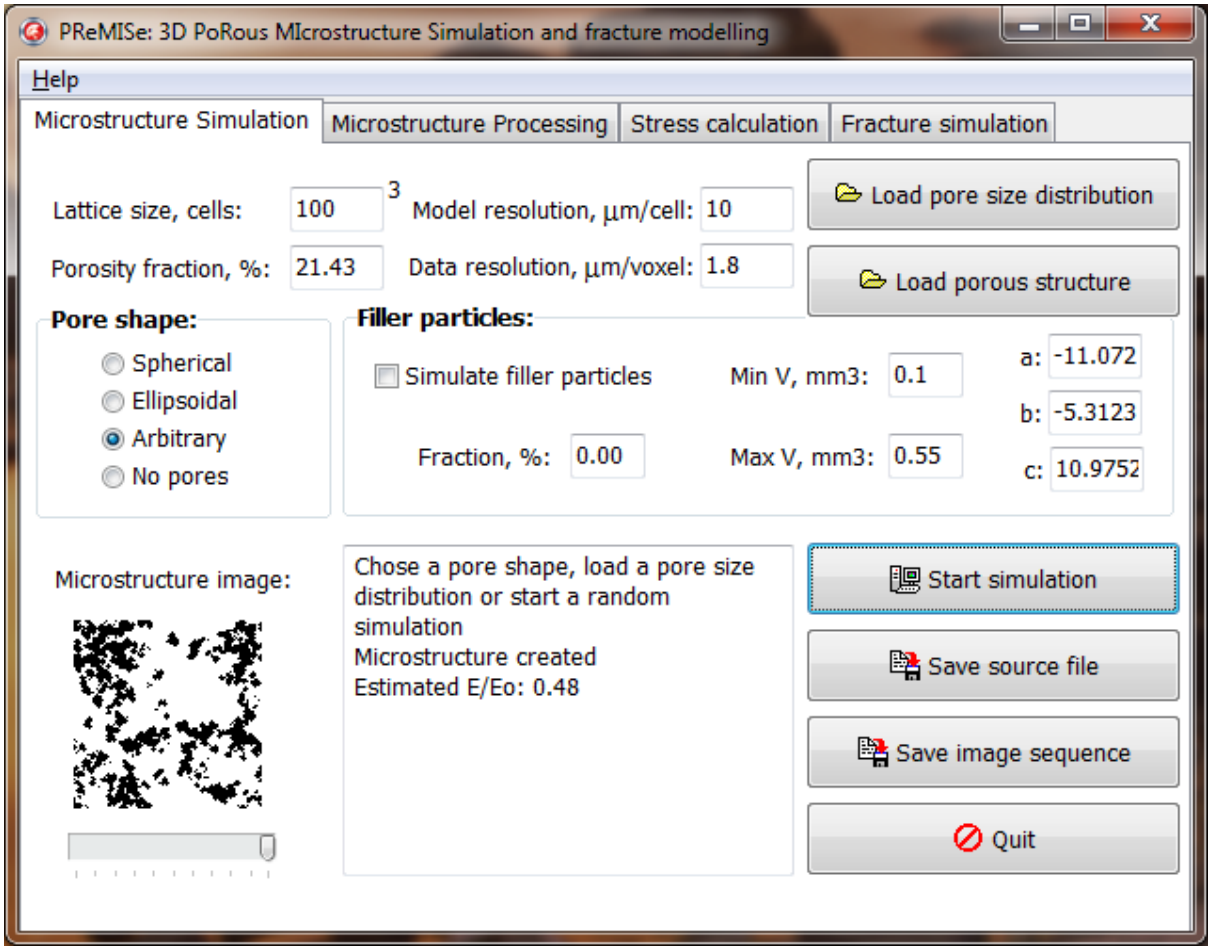

Figure 2 - A view of the first tab after the simulation performed.

– When the simulation has been performed, the buttons ‘Save source file’ and ‘Save image sequence’ are enabled. Press ‘Save source file’ button in order to save a txt-file for further processing and stress field computation. A source file contains one column with the length equal to the total number of cells in the CA lattice, where each symbol corresponds to a certain element of microstructure with the following codes: 0 is the pore element, 1 is the matrix element, 2 is the damaged cell, 3 is the filler particle element.
– Press ‘Save image sequence’ button, create a folder and type sequence name in order to save a series of bmp-images of the simulated microstructure, which can be open in ImageJ/Avizo or other software for further processing.

2. Creation of a synthetic porous microstructure with filler particles

- Make all setting as prescribed for porous microstructure simulation before the use of 'Start simulation' button.
- Check the box ‘Simulate filler particles’, if a large scale model must be simulated. Then indicate a desired filler fraction in the microstructure. NOTE: the final value of the filler fraction may slightly differ from the original due to the filler overlapping. The final fraction of the filler particles will be shown in the corresponding field. Filler particles are simulated as spheres according to the following distribution:

$$P = a \exp\left(\frac{V}{b}\right) + c,$$

where V is the volume of the particle, P is the probability to find a particle of the volume V within the microstructure. The initial parameters a, b and c of the distribution are given in the program's window for virgin graphite (Heysham II). All parameters for the microstructures simulated are shown in Table 1. The user can correct the distribution alongside with the maximum and minimum volumes of the particles, which will be allocated in the microstructure.

Table 1 - Parameters of the filler particle size distributions for virgin HYB and oxidised HPB graphite.

	State	Minimum volume (mm^3)	Maximum volume (mm^3)	a	b (mm^3)	c
1	Virgin (HYB)	0.10	0.55	-11.072	-5.312	10.975
2	Oxidised (8.1%)	0.05	0.25	-2.331	-0.062	1.058
3	Oxidised (11.2%)	0.04	0.26	-1.568	-0.128	1.221
4	Oxidised (12.2%)	0.07	0.31	-1.773	-0.122	1.093
5	Oxidised (14.2%)	0.07	0.33	-2.223	-0.100	1.126
6	Oxidised (27.5%)	0.04	0.24	-1.469	-0.086	1.036
7	Oxidised (34.7%)	0.02	0.19	-1.952	-0.173	1.741
8	Oxidised (41.5%)	0.05	0.23	-1.923	-0.127	1.297
9	Oxidised (53.0%)	0.08	0.20	-3.722	-0.060	1.064
10	Oxidised (61.2%)	0.02	0.24	15.439	3.204	-15.557
11	Oxidised (68.2%)	0.03	0.25	-30.211	-6.118	30.079

- To run the simulation of the synthetic microstructure with the indicated parameters, press ‘Start simulation’ button. A geometrical estimation of the bulk value of Young’s modulus for the porous synthetic microstructure is performed during the simulation. The value will be shown in the text window (Figure 2). It is important to note that this calculation considers only the calculated porosity and assumes the filler particles have the same modulus as the solid material. The filler particles are coloured in green in the image stack, pores are black (Figure 3).
- When the simulation has been performed, the buttons ‘Save source file’ and ‘Save image sequence’ are enabled. Press ‘Save source file’ button in order to save a txt-file for further processing and stress field computation. Since a simulated microstructure contains filler particles, three files will be saved in the same directory: ‘*name_pores.txt*’ with pores only, ‘*name_filler.txt*’ with filler particles only and ‘*name.txt*’ with the full microstructure, where ‘*name*’ is the file name given.

– Press ‘Save image sequence’ button, create a folder and type sequence name in order to save a series of bmp-images of the simulated microstructure, which can be open in ImageJ/Avizo or other software for further processing.

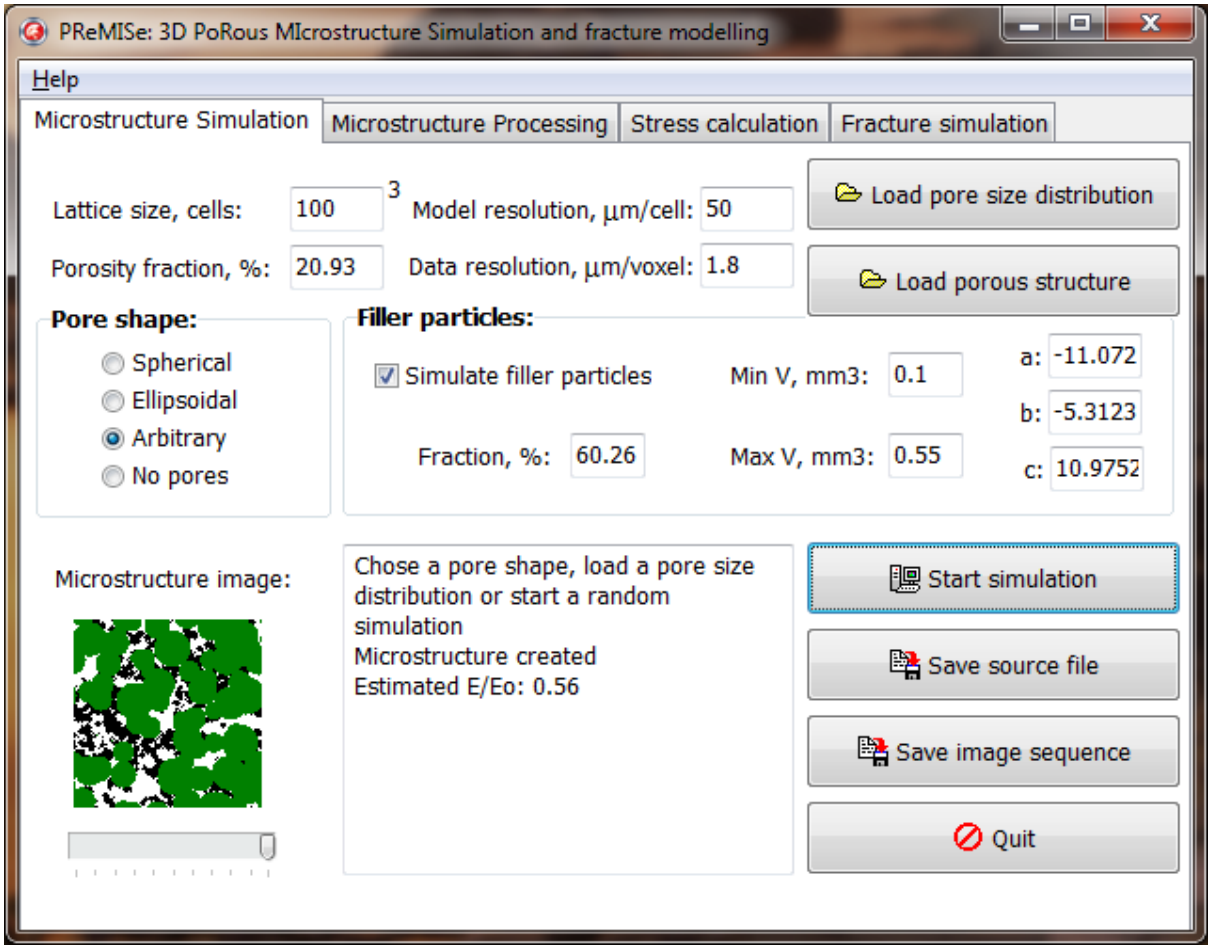

Figure 3 - Simulation of a large scale microstructure with filler particles.

3. Creation of artificial filler particles embedded into the loaded porous structure

– If you already have a porous microstructure (e.g. segmented experimental data) and want to simulate filler particles between which the pores should be distributed, then press ‘Load porous structure’ button to load a source file with porous microstructure.
– The indicator in ‘Pore shape’ field should be set as ‘No pores’ in order to prevent additional porosity simulation.
– Indicate lattice size, model and data resolutions.
– Check 'Simulate filler particles' box and indicate filler fraction, maximum and minimum sizes and parameters of the distribution from Table 1.
– To run the simulation of the synthetic microstructure with the indicated parameters, press ‘Start simulation’ button.
– You can also save the created microstructure using the corresponding buttons as described in the previous paragraphs.

1.3. 'Microstructure processing' tab

1. Activate the second tab 'Microstructure processing', if you want to perform additional operations with the simulated microstructures.

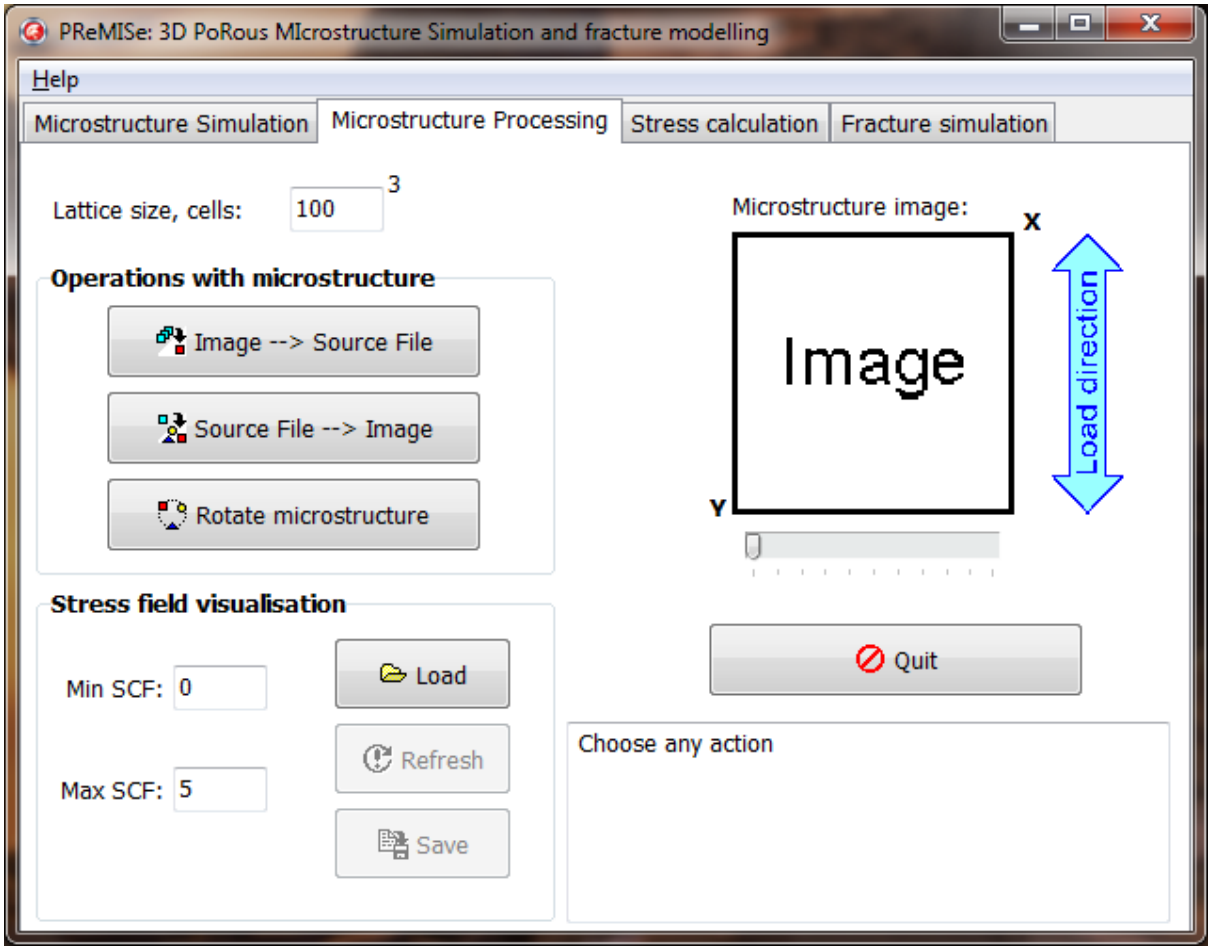

Figure 4 – An overview of 'Microstructure processing' tab.

2. Indicate the lattice edge size in cells in the corresponding field. This is usually 100 cells, as the usual lattice modelled is 100 x 100 x 100 cells.
3. Use 'Image -> Source file' button, if you want to convert binary images of microstructure (e.g. tomography or microscopy data) into the file format that is compatible with the programs for stress computation and fracture modelling (tabs 3 and 4). The source image must be binary: pores and other stress concentrators (e.g. notch, crack) must be coloured in black, matrix must be white. In order to upload an image sequence, click on the first file of the sequence, then hold SHIFT and click on the last file so that all files are selected. The image stack will be uploaded into the field for microstructure image, where it will be available for browsing using a slider in the bottom of the image. 'X' and 'Y' indicators show the directions of the corresponding axes. As soon as the image sequence is processed, a message will be shown inviting you to save a source file (Figure 5). Press OK, chose the destination folder for the file, type a file name and save it. The path to the saved file will be shown in the text window.

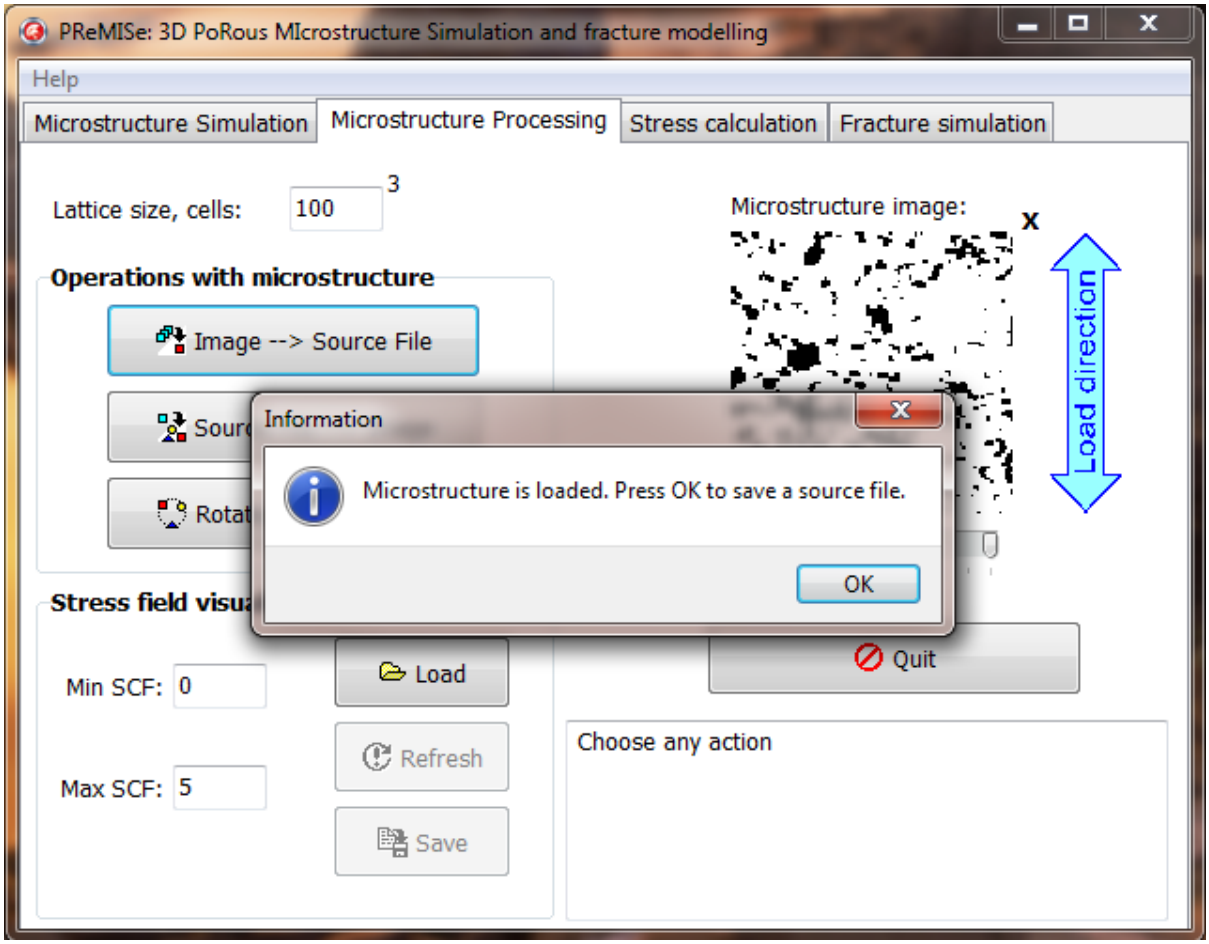

Figure 5 - Image -> Source file conversion.

4. Use ‘Source File -> Image’ button, if you want to visualise a txt-file of a microstructure. The microstructure will be uploaded into the image stack; the stack will be saved automatically in ‘*name_image*’ sub-folder of the same folder, where the source file titled ‘*name’* is.
5. Use ‘Rotate microstructure’ button, if you want to produce a microstructure from the source files for the same microstructure, which is rotated around the x and y axes. This option is useful for computation of the stress field under uniaxial tension that is applied to the same microstructure in three orthogonal directions. The source files named as ‘*name_RotateX*’ and ‘*name_RotateY*’, where a source file titled as ‘*name’*, will be saved automatically in the same folder as the original file. The original microstructure will be uploaded into the image stack for browsing.
6. ‘Stress field visualisation’ - Use this option when you already have a computed stress state for a microstructure (obtained using the 'Stress Calculation' tab) and want to look at the regions of the highest stress within this microstructure. This option requires the selection of two parameters: minimal and maximal stress concentration factors. Press ‘Load’ button in order to open the txt-file with the computed stress state. The stress field in the microstructure will be uploaded into the image stack as a coloured image sequence with blue colour for the lowest stress values and red colour for the highest stress values. A rainbow gradient is used for intermediate values. Changes in the maximal and minimal SCF values can be seen by using the ‘Refresh’ button to update. Press the ‘Save’ button, if you want to save the bmp-image sequence (i.e. stack) for further use.

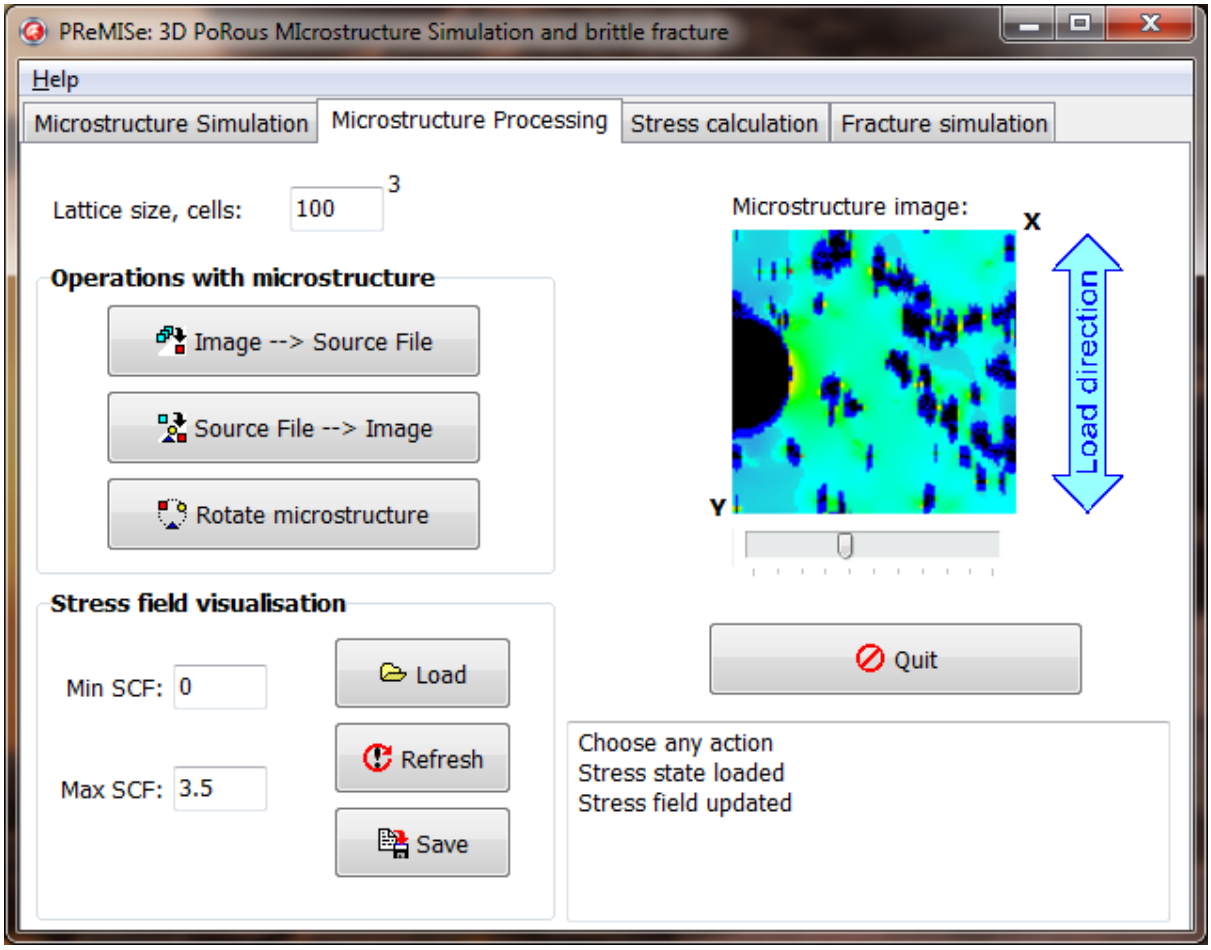

Figure 6 - Stress field visualisation.

1.4.'Stress calculation' tab

1. Activate 'Stress calculation' tab when you want to calculate the stress field in a microstructure. A general view of the tab is presented in Figure 7.
2. Indicate the edge size of the lattice, on the basis of which your microstructure was created. NOTE: the stress computation is limited by a lattice edge size of 100 cells, because a larger lattice might require a very long computational time.
3. Indicate the number of parallel threads needed for the simulations. NOTE: this number must be indicated by taking into account the number of CPU for the work station that is to be used for the simulation. The optimal number of 10 threads provides the fastest computation. If a chosen work station has fewer than 12 cores, then it is recommended to decrease the number of threads as (*core_number – 1*).
4. Indicate Poisson's ratio for the chosen material.
5. Press 'Load a source file of microstructure' button and open a txt-file with a microstructure. This must be either a source file, which was created with the help of 'Microstructure simulation' tabs or a source file converted from the image dataset using 'Microstructure processing' tab.

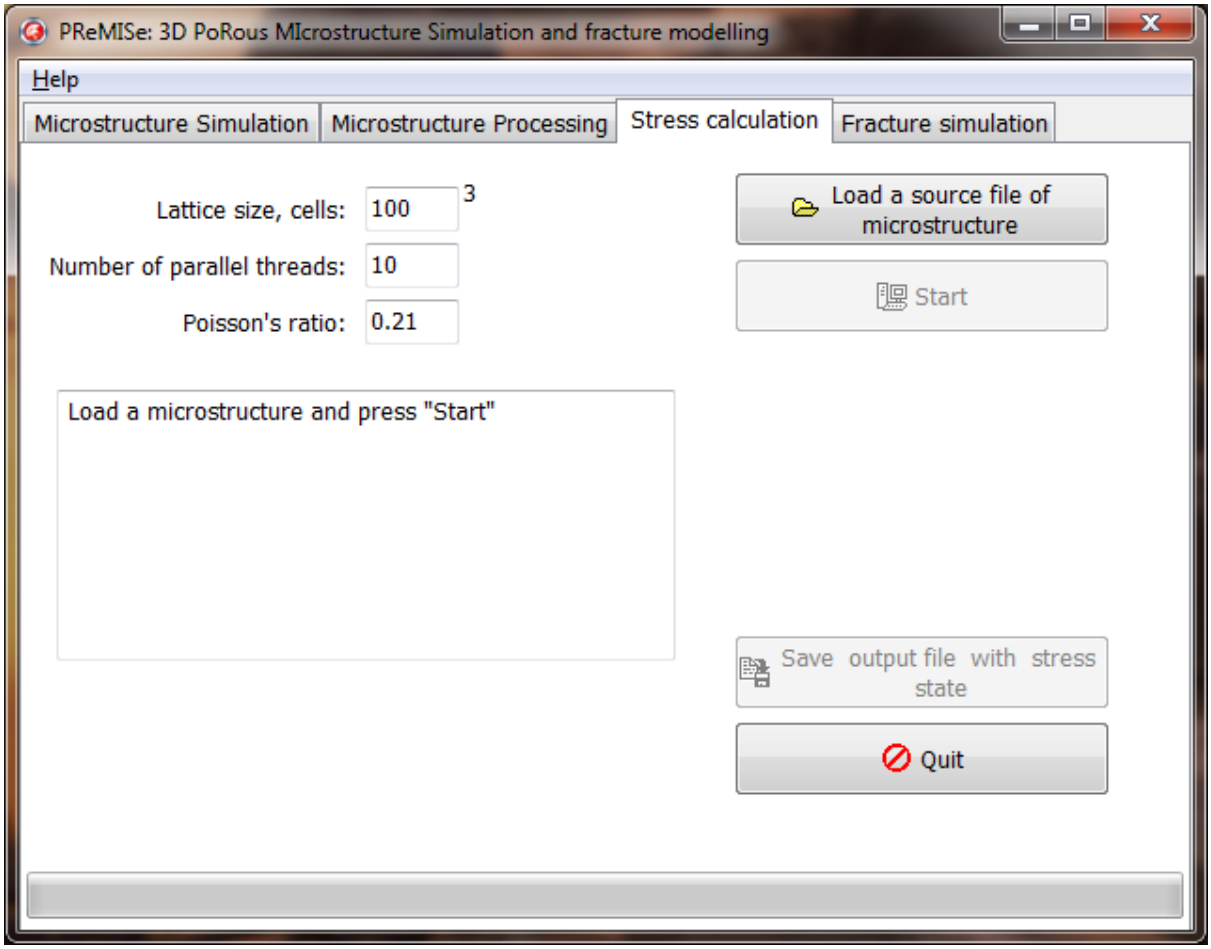

Figure 7 - An overview of 'Stress calculation' tab.

6. Brief information about the loaded microstructure will be shown in the text window of the tab (Figure 8). The estimated computational time is based on the lattice size, porosity of the microstructure and number of the threads; it also depends on the computer's performance. This parameter is rough and may be considered as an approximation only. A middle slice of the microstructure will be also shown.

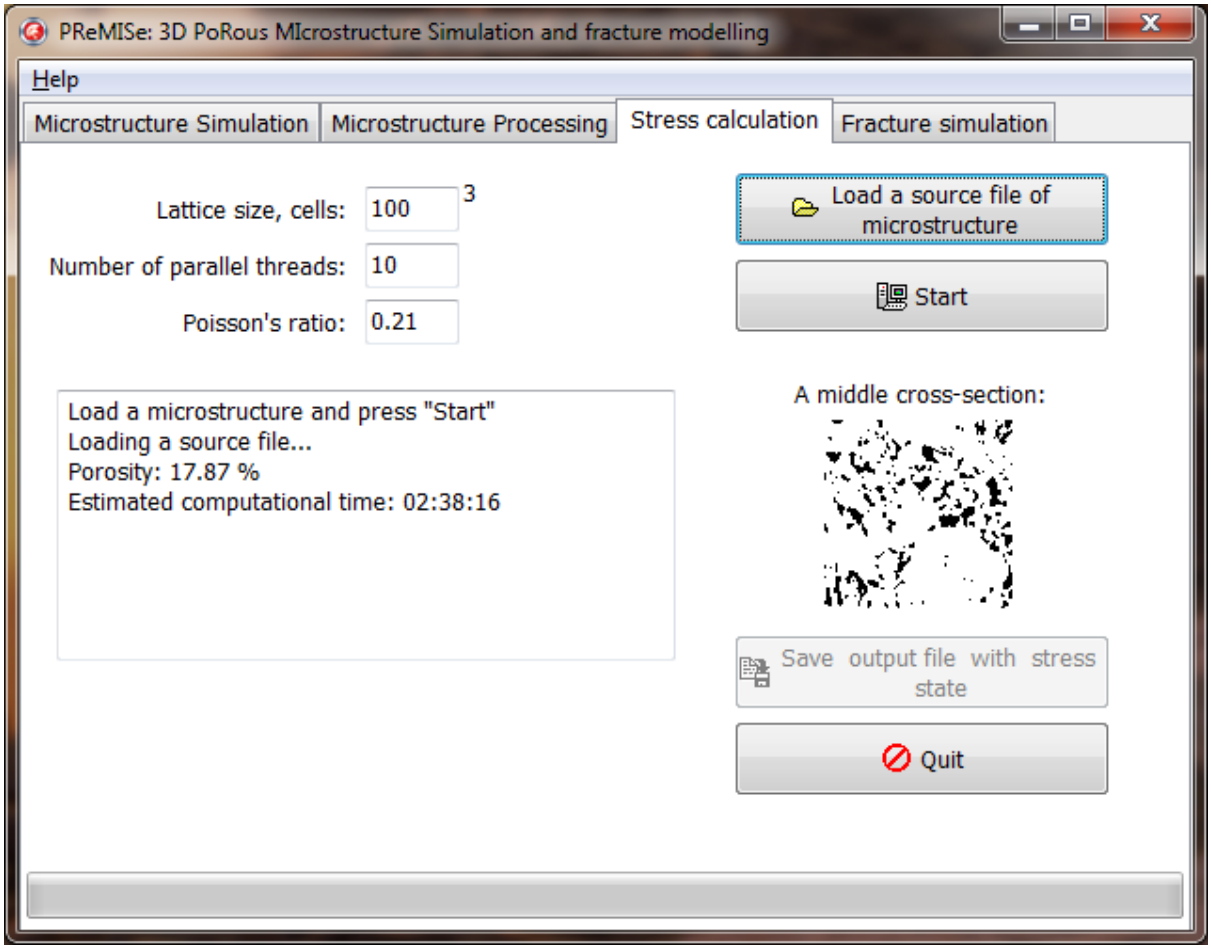

Figure 8 - 'Stress calculation' tab with the loaded microstructure.

7. Press 'Start' button to start the stress calculation for the loaded microstructure. During the stress calculation the program will be disabled for any user action. You can minimise the window during this time; the progress bar in the bottom of the window will show the approximate remained time. If the computation is interrupted for some reason that closes the main form of the program, you should call Windows Task Manager and make sure that the companion process titled 'stress.exe' was finished together with the main program. If it is still running, click the process and chose 'End process' action.
8. When the stress calculation is finished, the main program will be enabled again. Press 'Save output file with stress state' button to save the result of the computations. Chose a destination folder and type the name of the file. Two txt-files will be saved in the folder: a file with '_scf' indicator that contains the calibrated stress concentration factor data (this can be visualised with the help of the "Microstructure Processing" tab; the second file contains uncalibrated data, which is to be used as input of the stress state for fracture simulation using the Fracture Simulation tab. The reserved copies of these files are automatically saved in *'stress'* sub-folder with the names of *'scf.txt'* for the calibrated stress field and *'Vx_unc.txt'* for the uncalibrated source file; they will be replaced by new versions of the files after the next computation.

1.5.'Fracture simulation' tab

1. Activate 'Fracture simulation' tab. A general view of the tab is presented in Figure 9.

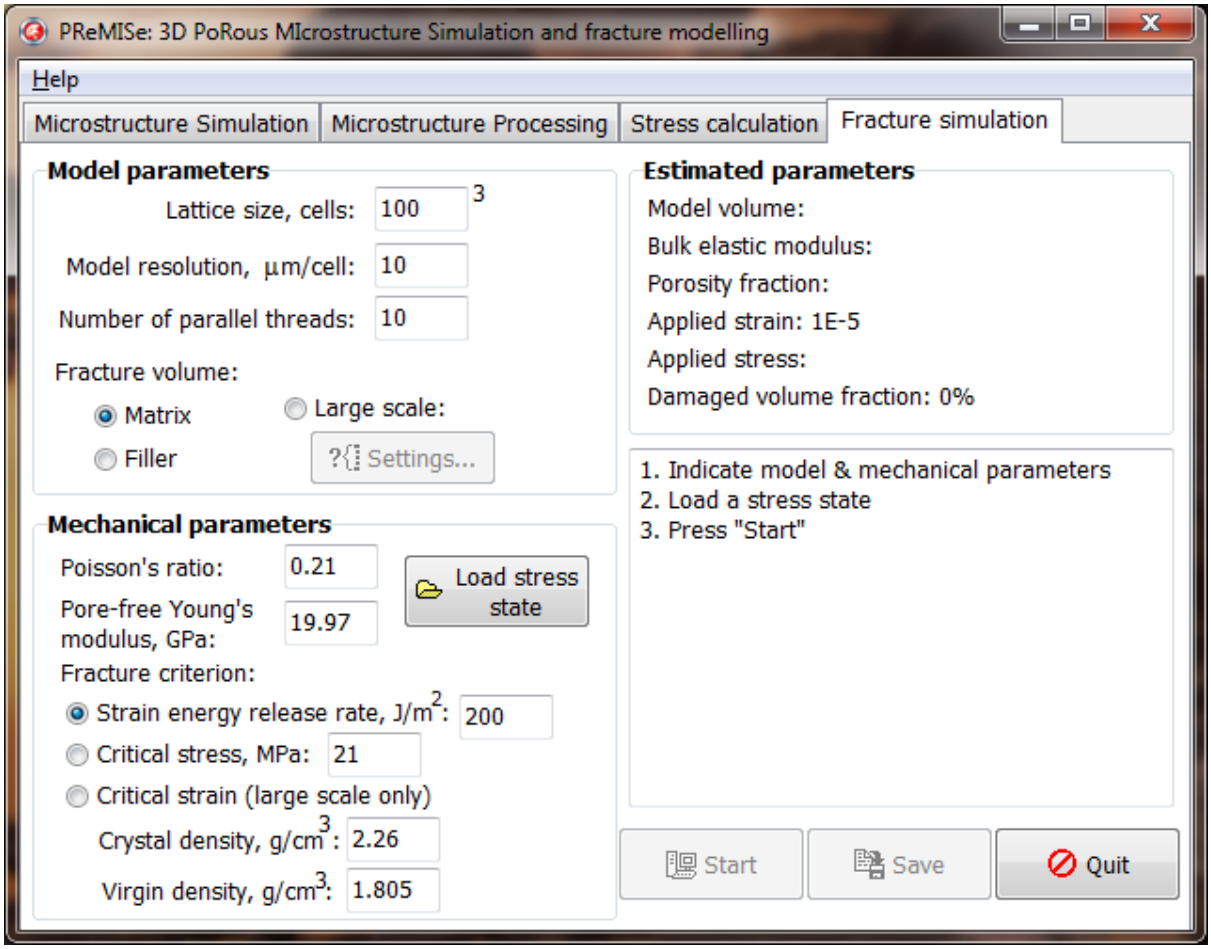

Figure 9 - An overview of 'Fracture simulation' tab.

2. Indicate the edge size of the lattice, on the basis of which your microstructure was created.
3. Indicate the model resolution.
4. Indicate the number of parallel threads needed for the simulations. NOTE: this number must be indicated by taking into account the number of CPU for the work station that is to be used for the simulation. The optimal number of 10 threads provides the fastest computation. If a chosen work station has fewer than 12 cores, then it is recommended to decrease the number of threads as (*core_number – 1*). Computational time estimation is impossible in this case, since the fracture process is a step-by-step simulation.
5. Depending on the application of the model, chose the volume within which fracture will be simulated. Three indicators are available for choice. To simulate fracture of a matrix sub-volume, choose “matrix” volume; fracture will be able to develop anywhere within the full lattice. To simulate fracture of a filler particle, choose “filler”; fracture will develop within the ellipsoidal volume, which boundaries will be defined automatically according to the loaded microstructure. To simulate fracture in a microstructure that contains filler and matrix, then select “large scale”; the Young’s modulus estimation will be performed on the basis of the total porosity fraction only without consideration of the pore geometry. The porosity fraction is calculated from the weight loss. Weight loss of 0% corresponds to the virgin state of HYB material. Crystal density and virgin density of the porous material must be indicated for the simulation of a large scale mode. Press 'Settings…' button to give individual parameters of the critical strain distributions for matrix and filler during the large scale simulation (Figure 10).

According to the performed analysis, two types of critical strain distribution is observed, which can be fitted by either Weibull distribution function:

$$y = A\left(1 - e^{-(k(x-xc))^d}\right)$$

or exponential growth function:

$$y = y_0 + Ae^{x/t}$$

Further parameters of both types of distributions are shown in Table 2.

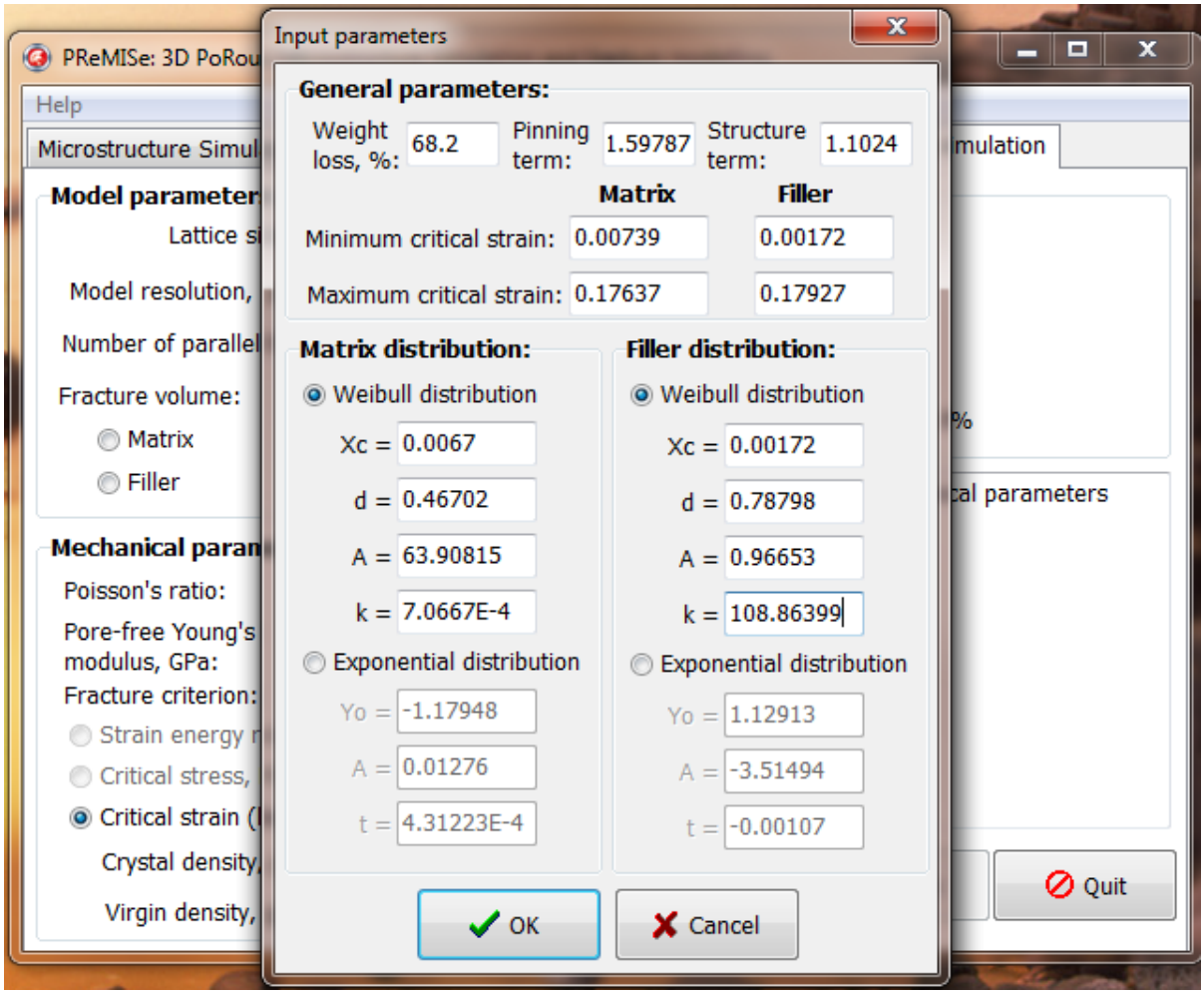

Figure 10 - An example of input parameters for large scale fracture simulation of an irradiated sample.

Table 2 - Parameters of the critical strain distributions for a large scale model containing both matrix and filler at certain weight loss values.

	Weight loss (%)	Minimum critical strain	Maximum critical strain	Parameters of the distribution	
				Matrix	Filler
1	0 (Virgin)	0.00222 (M) 0.00192 (F)	0.00529 (M) 0.00956 (F)	(W) xc=0.0022 d=0.49957 A=45.18485 k=0.14756	(W) xc=0.00192 d=1.45173 A=0.9382 k=724.81151
2	8.1	0.00185 (M) 8.36826E-4 (F)	0.00227 (M) 0.00237 (F)	(W) xc=0.00183 d=1.76325 A=0.97713 k=4900.25076	(W) xc=6.35669E-5 d=5.68646 A=0.95252 k=691.16815
3	11.3	0.00171 (M) 0.00102 (F)	0.00216 (M) 0.00429 (F)	(W) xc=0.00164 d=1.29946 A=44.04801 k=104.55558	(E) y0=1.12913 A=-3.51494 t=-0.00107
4	12.2	0.00196 (M) 6.89063E-4 (F)	0.00225 (M) 0.00898 (F)	(E) y0=-1.17948 A=0.01276 t=4.31223E-4	(E) y0=1.08158 A=-3.00195 t=-9.12831E-4
5	14.2	0.0018 (M) 8.40049E-4 (F)	0.00338 (M) 0.00285 (F)	(W) xc=0.0018 d=1.03089 A=1.17309 k=1412.79327	(W) xc=8.40049E-4 d=5.13851 A=0.89097 k=1455.21308
6	27.5	0.0022 (M) 0.00189 (F)	0.00322 (M) 0.14584 (F)	(W) xc=0.0022 d=0.84617 A=3.40858 k=325.37845	(W) xc=0.00187 d=1.02905 A=0.92668 k=496.58734
7	34.7	0.00216 (M) 7.71432E-4 (F)	0.0039 (M) 0.01262 (F)	(W) xc=0.00168 d=2.3112 A=1.34993 k=518.92905	(W) xc=7.71432E-4 d=1.53512 A=0.94375 k=484.90338
8	41.5	0.00395 (M) 0.00149 (F)	0.00957 (M) 0.00566 (F)	(W) xc=0.00193 d=3.69572 A=0.98727 k=215.2026	(W) xc=0.00148 d=1.28239 A=0.97758 k=1214.02659
9	53.0	0.00465 (M) 0.00165 (F)	0.02093 (M) 0.048 (F)	(W) xc=0.00465 d=1.26972 A=0.96524 k=269.05792	(W) xc=0.00164 d=0.724 A=0.94658 k=373.08225
10	61.2	0.01678 (M) 0.00229 (F)	0.46997 (M) 0.03496 (F)	(W) xc=0.01527 d=0.99778 A=0.96967 k=24.88006	(W) xc=0.0018 d=1.18298 A=0.93987 k=196.73093
11	68.2	0.00739 (M) 0.00172 (F)	0.17637 (M) 0.17927 (F)	(W) xc=0.0067 d=0.46702 A=63.90815 k=7.0667E-4	(W) xc=0.00172 d=0.78798 A=0.96653 k=108.86399

Notations in the table: (M) = matrix, (F) = filler, (W) = Weibull distribution, (E) = Exponential distribution.

6. Indicate Poisson's ratio and pore-free Young's modulus. Calculated pore-free elastic moduli for two grades of graphite are presented in Table 3.

Table 3 - Estimated pore-free elastic moduli for two grades of graphite.

	E_0 (GPa) Hinkley Point B (HPB)	E_0 (GPa) Heysham II (HYB)
Virgin state	19.97	24.33
Irradiated state	57	73

7. Chose a fracture criterion. Two criteria are available for the small scale simulation: on the basis of critical strain energy release rate or critical stress value. Critical strain fracture criterion is enabled for large scale only, since it is estimated with the use of the coupled stress and elastic modulus distributions.
8. Press 'Load stress state' button and open the txt-file with the uncalibrated stress state, calculated previously with the use of the 'Stress calculation' tab. Some parameters of the model such as model volume, bulk elastic modulus and porosity fraction will be shown in 'Estimated parameters' section (Figure 11).

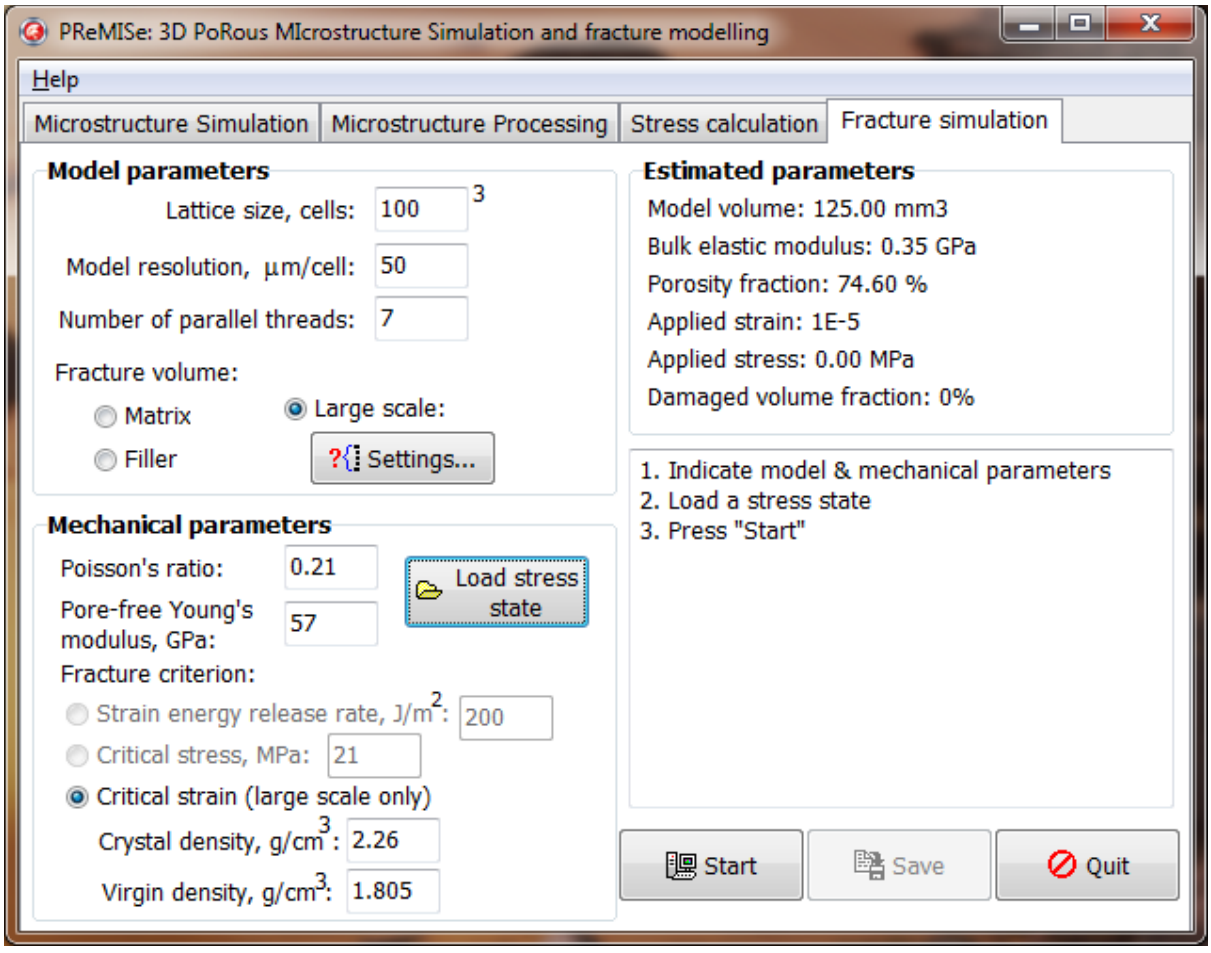

Figure 11 – Preliminary estimated parameters for large scale fracture simulation of an irradiated sample.

9. Press 'Start' button to run fracture simulation. The program will be disabled for any user action during the simulation. If the computation is interrupted for some reason that closes the main form of the program, call Windows Task Manager and make sure that the companion process

titled either ‘fracture.exe’ or ‘fracture_large.exe’ was finished together with the main program. If it is still running, click the process and chose ‘End process’ action.

10. When the fracture simulation is finished, the main program will be enabled again (Figure 12). A stress-strain diagram will be shown; peak stress and strain values will be indicated in ‘Estimated parameters’ section together with the damaged volume fraction.

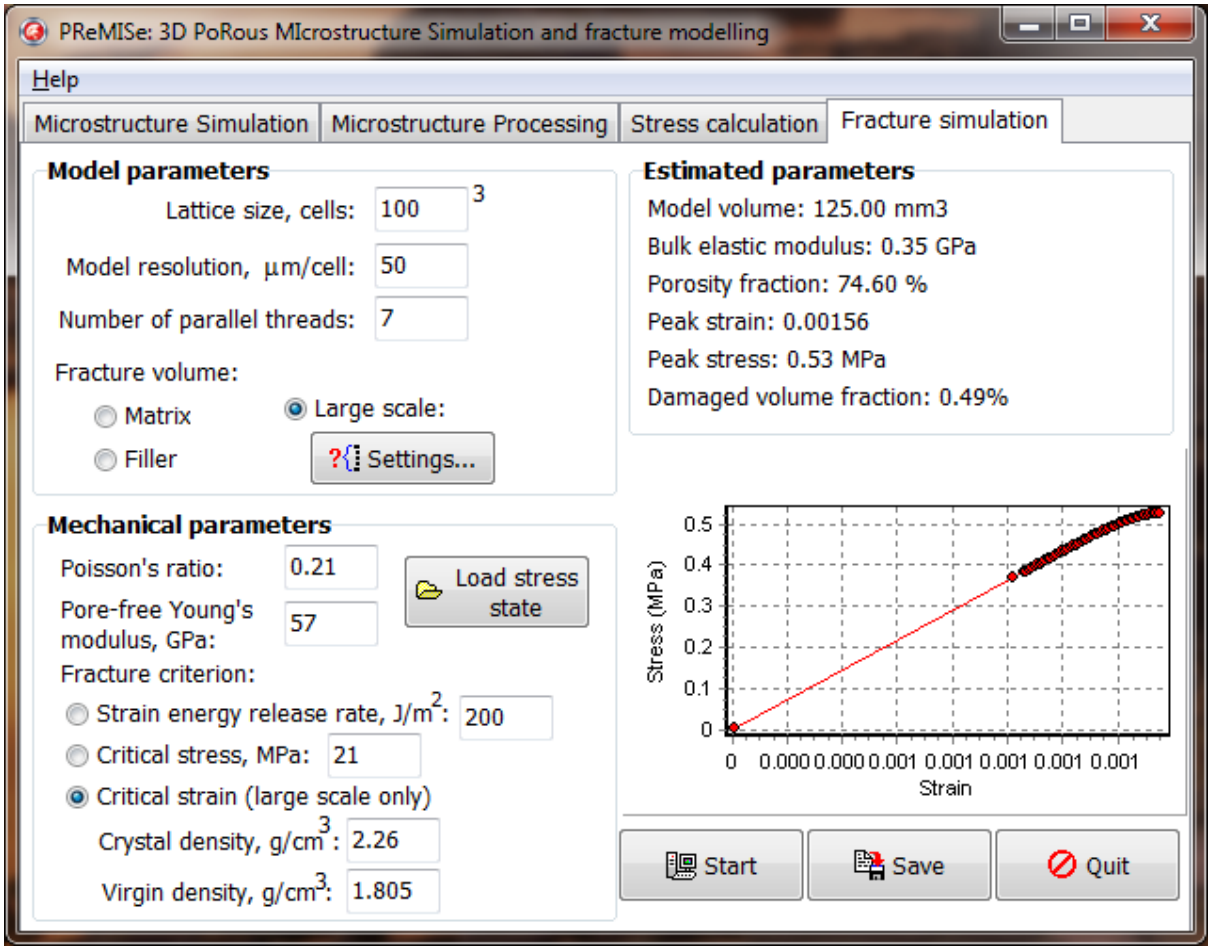

Figure 12 - Result of the large scale fracture simulation of an irradiated sample.

11. Press ‘Save’ button to save the results of fracture simulation. Two files will be saved. The first txt-file contains the first line as a caption; 4 columns with strain, stress, bulk Young’s modulus and porosity values. The number of lines in the file may be different for different microstructures and depends on the number of steps during fracture simulation. The second file named ‘*final_scf.txt*’ contains the SCF-map for the damaged microstructure at the end of the simulation; it will be saved in the same folder automatically. The reserved copies of these files are automatically saved in *'fracture'* sub-folder with the names of *'fracture.txt'* for the fracture simulation results and *'final_stress.txt'* for the stress field in a damaged microstructure; they will be replaced by new versions of the files after the next computation.

1.6.Simulation with the real microstructure image data

There are some tips, which will help to perform a proper fracture simulation on the basis of the datasets with real microstructures.

1. Before the simulation a microstructure dataset must be segmented. The program works with binary files only, where black regions correspond to the pores, white regions are the solid material.
2. A high resolution dataset may be rescaled to the appropriate resolution of the model. When downscaling is performed, it worth checking the total pore volume fraction. It should be close to the pore fraction of original sample.
3. A prepared image dataset must be saved as a bmp-image sequence.
4. It worth checking the direction of loading before the simulation. The default loading is in the Y-direction as shown in Figure 6. In some cases a sample rotation might be needed.
5. If a series of microstructures is simulated, then all microstructures in a series must have identical resolutions and volumes.