**User Manual for MATLAB toolbox to predict compressibility using Digital Rock**

Digital Rock workflow has been developed to predict compressibility at 1500 psi and maximum compressibility corresponding to the compressibility curve from laboratory experiments. Details of the workflow can be found in manuscript.

This User Manual is prepared to guide the users through the codes developed for compressibility prediction. The different MATLAB functions used for running the workflow are described below.

The code requires segmented image for calculations. The segmented image is assigned code for different mineralogy according to the following table

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Name in CAP summary** | **Code** | **Bulk Modulus (GPa)** | **Shear Modulus (GPa)** | **Density (kg/m3)** |
| QuartzMono | 0 | 36.6 | 45 | 2650 |
| Intergranular | 1 | 0.000001 | 0.000001 | 0.000001 |
| Shale/Claystone | 2 | 15 | 7 | 2400 |
| BrittleMRFs | 3 | 30 | 20 | 2600 |
| AlkaliFeldspar | 4 | 35 | 25 | 2650 |
| Heavy/OpaqueMinerals | 5 | 36 | 45 | 3000 |
| DuctileMRFs | 6 | 15 | 7 | 2400 |
| QuartzPoly | 7 | 36 | 45 | 2650 |
| Biotite | 8 | 50 | 25 | 3050 |
| Carbonate | 9 | 70 | 30 | 2750 |
| Muscovite | 10 | 50 | 25 | 2750 |
| Clay(Pore-Filling) | 11 | 15 | 7 | 2400 |
| Undiferentiated | 12 | 36 | 45 | 2650 |
| CalciteOvergrowth | 13 | 70 | 30 | 2750 |
| Grain-Fracture | 14 | 0.000001 | 0.000001 | 0.000001 |
| Clay(Pore-Lining) | 15 | 15 | 7 | 2400 |
| K-FeldsparOvergrowth | 16 | 35 | 25 | 2630 |
| VisiblePorosity | 17 | 0.000001 | 0.000001 | 0.000001 |
| VisibleMicroporosity | 18 | 0.000001 | 0.000001 | 0.000001 |
| QuartzOvergrowth | 19 | 36.6 | 45 | 2650 |
| Intragranular | 20 | 0.000001 | 0.000001 | 0.000001 |
| Unclassified | 21 | 36 | 45 | 2650 |
| PyriteCement | 22 | 140 | 100 | 4810 |
| Bitumen | 23 | 4 | 1 | 1000 |
| Lamin | 24 | 15 | 7 | 2400 |
| Burrow | 25 | 36 | 45 | 2650 |
| Undif.Clay | 26 | 15 | 7 | 2400 |
| DrillingMud | 27 | 15 | 7 | 2400 |
| Plagioclase | 28 | 75 | 25 | 2630 |
| Chert | 29 | 36 | 45 | 2650 |
| Undif.Sandstone | 30 | 36 | 45 | 2650 |
| SilicicGlass | 31 | 25 | 30 | 2500 |
| Undif.VRFs | 32 | 15 | 7 | 2400 |
| Undif.PRFs | 33 | 36 | 45 | 2650 |
| Glauconite | 34 | 10 | 5 | 2300 |
| CarbonateFossils | 35 | 70 | 30 | 2750 |
| PlantFragments | 36 | 4 | 1 | 1000 |
| Calcite | 37 | 70 | 30 | 2750 |
| Dolomite | 38 | 90 | 45 | 2900 |
| Pyrite | 39 | 140 | 100 | 4810 |
| DolomiteOvergrowth | 40 | 90 | 45 | 2900 |
| Siderite | 41 | 120 | 50 | 4000 |
| Ankerite | 42 | 90 | 45 | 2900 |
| Illite | 43 | 30 | 15 | 2700 |
| Chlorite | 44 | 50 | 25 | 2900 |
| Kaolinite | 45 | 15 | 7 | 2400 |
| Undif.Carbonate | 46 | 70 | 30 | 2750 |
| Sulfate | 47 | 55 | 30 | 3000 |
| Albite-FeldsparOvergrowth | 48 | 35 | 25 | 2630 |
| Zeolite | 49 | 46 | 28 | 2250 |
| CCReplacement | 50 | 36 | 45 | 2650 |
| Grain-moldic | 51 | 0.000001 | 0.000001 | 0.000001 |
| VisibleJunk | 52 | 4 | 1 | 1000 |
| VisibleMacroporosity | 53 | 0.000001 | 0.000001 | 0.000001 |
| Vuggy | 54 | 0.000001 | 0.000001 | 0.000001 |
| Throats | 55 | 0.000001 | 0.000001 | 0.000001 |
| Undif.MRFs | 56 | 30 | 20 | 2600 |
| Other | 57 | 0.000001 | 0.000001 | 0.000001 |
| Throat | 58 | 0.000001 | 0.000001 | 0.000001 |

1. **MATLAB function – calcm**

This function takes in properly segmented image in raw format and performs Digital Rock calculations and predicts the compressibility at 1500 psi and the maximum compressibility corresponding to the compressibility curve obtained using laboratory measurements. This function uses finite element code elas3d.exe (<https://www.nist.gov/services-resources/software/finite-elementfinite-difference-programs>) for elastic calculations of stresses corresponding to a uniaxial strain experiment. The direction of application of strain can be specified using the mode keyword in the function. After calculating the stresses, the function calculates the compressional modulus for the image. It then uses the following empirical equations to predict compressibility.

where, Cm = predicted compressibility, = compressibility calculated using Digital Rock, = mineral compressibility for the segmented image calculated using Hashin-Shtrikman upper and lower bounds, and n = exponent that has been obtained using calibration with laboratory measurements. The value of exponent used in the function for various cases are listed in the following table

|  |  |  |
| --- | --- | --- |
| Type of experiment | Predicted measurement | Exponent (n) value |
| Uniaxial – X direction | Cm @ 1500 psi depletion stress | 0.98 |
| Uniaxial – X direction | Maximum Cm | 1.26 |
| Uniaxial – Y direction | Cm @ 1500 psi depletion stress | 1.1 |
| Uniaxial – Y direction | Maximum Cm | 1.42 |

The inputs to this function are:

1. image\_name = name of the segmented image file (ASCII format)
2. row = length of the image (pixels)
3. col = width of the image (pixels)
4. mode = type of uniaxial experiment (1 = X direction, 2 = Y direction)
5. K\_HS = Hashin-Shtrikman average mineral bulk modulus (GPa)
6. U\_HS = Hashin-Shtrikman average mineral shear modulus (GPa)

The outputs from the function are:

1. Folder named <image\_name>\_simulations – This folder contains all numerical results. The files in this folder are the input raw image file, the input parameter file, stress files outputted from the numerical calculations, outputfile.out that contains the details of the numerical calculation.
2. Cmin = Predicted compressibility at 1500 psi (microsips) calculated using equation 1
3. Cmax = Predicted maximum compressibility (microsips) calculated using equation 1
4. **MATLAB script – mainscript**

This script contains an example case for running the compressibility toolbox. The inputs for running the script are kept in the Example folder and are as follows

1. test.raw – Input segmented image in binary format

All the required inputs can be found in the folder with the toolbox. The script executes and outputs the predicted compressibility at 1500 psi and maximum compressibility in the variables Cmin and Cmax respectively in MATLAB Workspace.

**Note:**

1. The codes in the toolbox should be kept in the same folder along with Dependencies folder
2. The codes assume that the image size is 480 x 512. In case of a different image size, change the nx and ny parameters corresponding to the new image size in the parameter files elas3d-uniaxial\_x.pam and elas3d-uniaxial\_y.pam in the Dependencies folder.

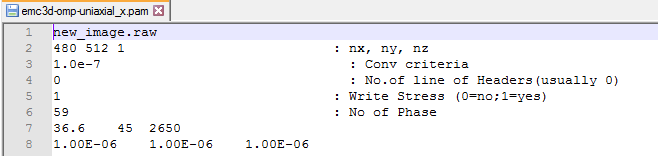


Figure: First few lines of emc3d-omp\_uniaxial\_x.pam file with the line corresponding to the image size highlighted.

**System requirements:**

1. Code developed and tested on MATLAB 2017b