

bringing discrete element modelling to your PC or laptop



- ▶ Many different fault, wall and displacement boundary conditions (extension, contraction)
- ▶ High (10s m) to ultra-high resolution (c. 1 m)
- ▶ Growth strata, erosion
- ▶ Inversion

RAM: 8GB minimum

- ▶ Repose and Biaxial tests
- ▶ Mechanical Stratigraphy
- ▶ Stress and Strain
- ▶ “Live” processing/visualisation of models
- ▶ OpenMP parallelised for maximum speed

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Introduction

cdem2Ddesktop is a Windows 10/11 standalone application for discrete element modeling of geological structures and their associated deformation in two dimensions (2D). The discrete element method (DEM) is a discontinuum method that is used here to simulate a cross-section of the upper crust. This cross-section is represented by an assembly (collection) of elements that respond to applied forces and displacement boundary conditions. The DEM as a numerical technique allows large deformations and complex, abrupt boundary conditions. In addition, the formation and linkage of faults and fractures is a natural part of any simulation.

In cdem2Ddesktop an assembly of scaled, circular elements of different radii is used to represent a cross-section of the upper crust. Different assemblies, model scalings, acting forces, element properties, and boundary conditions can be chosen within the application. After setting-up and starting a simulation, the progress of the simulation is displayed graphically as the deformation evolves. While the model is running, different components of displacement, strain, and stress can also be visualised as element attributes. A completed model can also be examined and displayed in a similar manner. The entire "Experiment" can be saved as an archive, ready to be re-loaded at a later date.

The DEM is a computationally (relatively) intensive numerical technique. It involves many hundreds of thousands, if not millions, of calculations that are repeatedly undertaken until a simulation is completed. In order to make a simulation observable and tractable in realistic timescales, cdem2Ddesktop makes use of all available CPUs and cores/threads, so the more powerful a machine is, and the more cores it has, the better. This documentation is intended to be a guide to the use of cdem2Ddesktop. It is *not* a detailed description of the theory behind cdem2Ddesktop or the DEM method in general. This can be found in the references/bibliography at the end of this manual.

Background

cdem2Ddesktop is the result of many years of research, coding and generally evangelising about discrete element modelling. In the end, after many years of requests, I gave in and finally decided to create a Windows version of my research code. I did this from "ground zero". I literally knew *nothing* about Windows 10/11 programming in 2023, but here we are now with a working application. I thank you very much for your support in this adventure.

I have tried, and hopefully partially succeeded, to make the application very much like an experimental platform or toolbox, almost creating a "**digital sandbox**". Your job is basically to design an experiment (within limits), decide on your geological parameters, and run the model. However, I did not want this to be a *static* experience. I wanted the user to be able to *drive* the experiment: observe its evolution, interrogate it, stop it, change something and perhaps start again. In the end, this is all about time and effort/efficiency, with the aim of avoiding checking the results of a simulation at the end of a run only to find out that you messed up at the start. Time wasted and never to be gotten back.

When I started out coding discrete element models, many years ago, runtimes were on the order of *days (!)* for even *very* simple models. All of that has since changed remarkably. Computing techniques, compilers and hardware have moved on enormously. cdem2Ddesktop

is parallelised, meaning that it can avail itself of all the compute power on your laptop, desktop computer or virtual machine. *Bottom line: the more up-to-date and faster your kit the better.*

Quick Overview & Workflow

Let's start right at the beginning of running a model/simulation using the application.... Open the folder into which you unzipped your cdem2Ddesktop package: you will be presented with something similar to the screenshot below (Fig. 1).

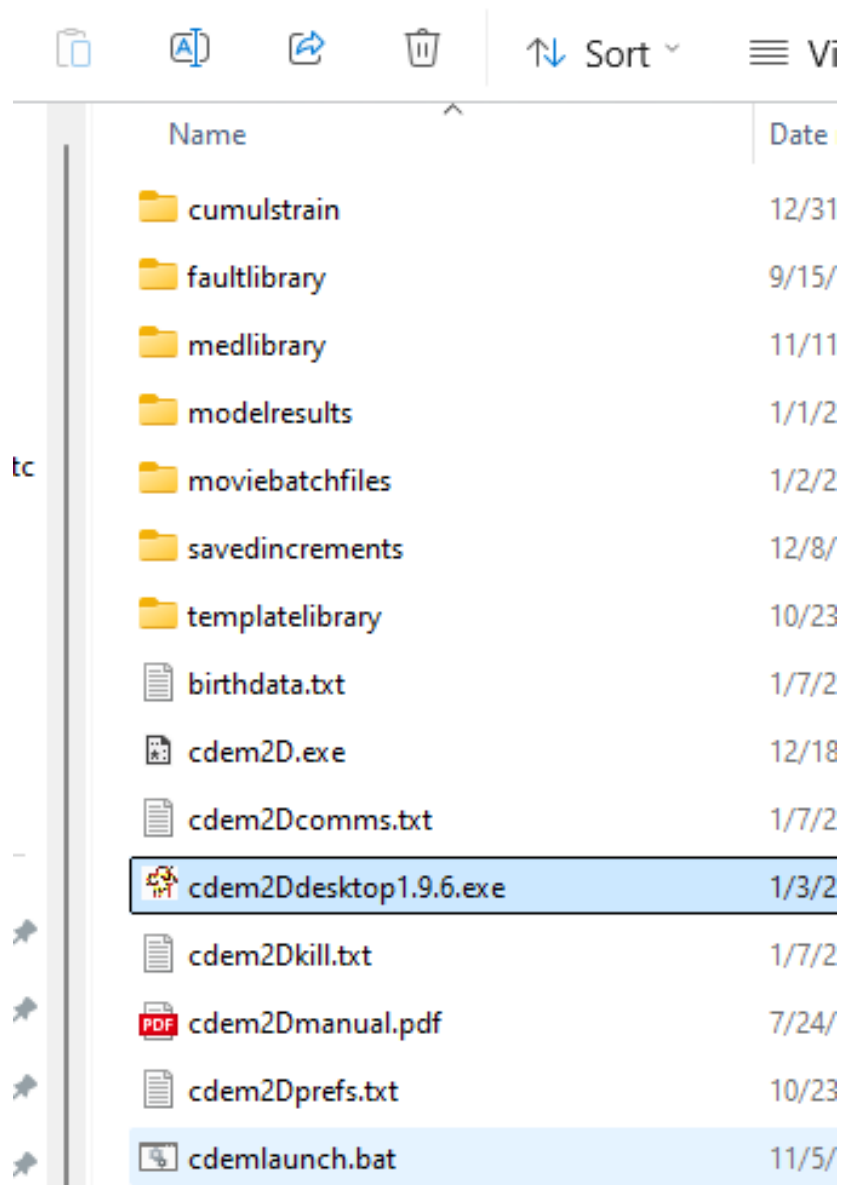


Figure 1. Screenshot of a typical installation folder.

In this folder you will see quite a few different items, files and sub-folders etc., but the only one you really need to bother about (at this stage) is the application...

cdem2Ddesktop1.9.6.exe

Double-click on this file and the application should launch, at this stage a black Windows terminal window may appear momentarily. Ignore it (*but do not close it!*), the application window will soon come to the front. You will be presented with a “default model”. This might be a caldera, a normal fault, a reverse fault or a slope-failure simulation. It doesn't matter, the “workflow” is the same regardless. Initially, and for about 5 seconds or so, in the Info Panel on the righthand side of the application window, a message “**Model is being configured**” will be displayed. Wait until that changes colour (to green) and displays “**Model is Ready**” (see Fig. 2 below). At this point the model is waiting for either a change in parameters values, boundary conditions, display attributes, or for you to start a model run/simulation. Nothing is being computed or calculated by the application.

N.B. cdem2Ddesktop works on a single document interface (SDI) model of interaction. This means that the model “view” and menu items, settings and parameters are singularly linked. You cannot have 2 separate model “views” up, or simulations running, at the same time.

You are now ready to run your first simulation. In order to do so select the following command from the Menu Bar: “**Run->Start Model Run**”.

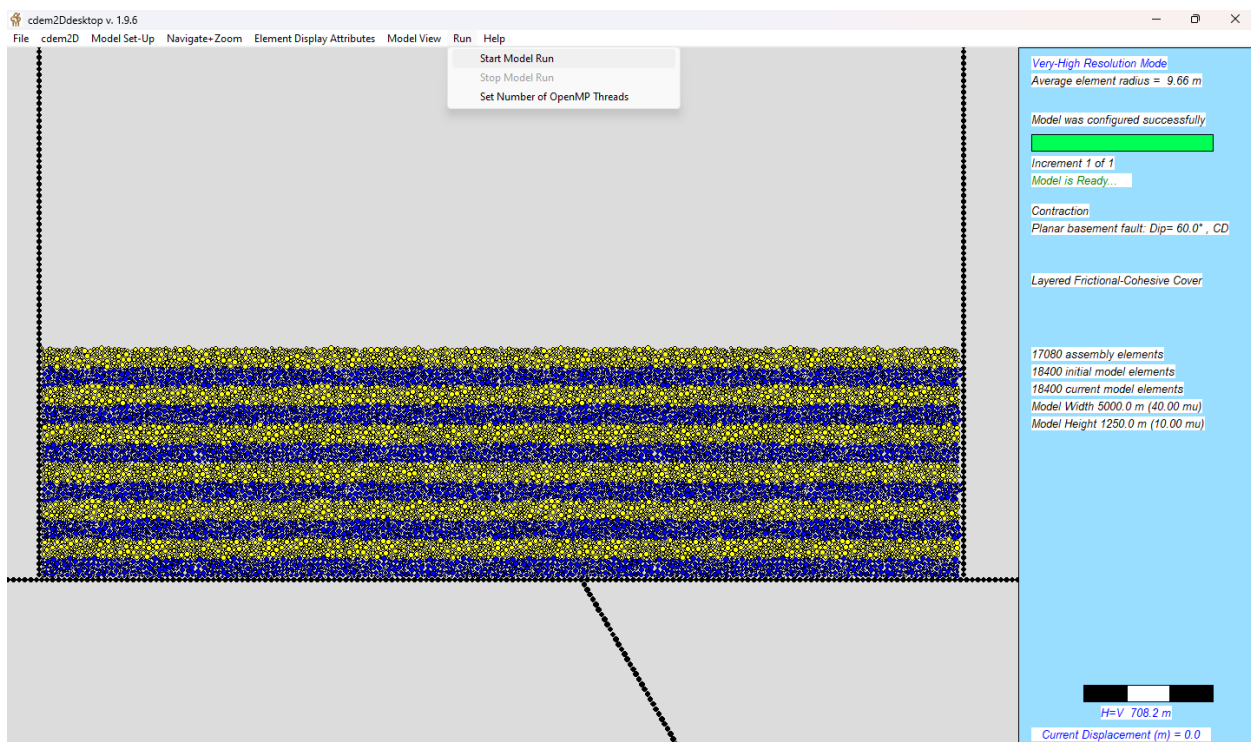


Figure 2. Screenshot of a successfully configured model ready to be run.

The simulation should start, and you will see various types information displayed in the information panel to the right (see Fig. 2 above): boundary conditions, the progression of the run, a scale-bar and assembly info. The model simulation will progress according to the parameters which it was given, and at a speed dependent upon your host machine. As with all things in life, please be patient and observe.

For your first model run it is probably best to just let this example *finish* - this will be indicated by the progress bar and info in the side panel. *While* the model is running, and hopefully the geometry is evolving and deforming, you will notice that a sub-set of the menus and menu items are greyed out, this is because their actions, or the changes they might induce, are not appropriate for a *running model*. There are, however, many ways in which a simulation can be examined, interrogated and attributes displayed whilst it is running. These will all be explained in the appropriate sections below.

If the model has not finished (or you get bored waiting) you can always stop it (at any time) by selecting the following command from the Menu Bar: **"Run->Stop Model Run"**. If you wish to quit the application select the following command from the Menu Bar: **"File->Exit"** in standard Windows fashion.

After this quick start and jump into running a model, it is maybe now appropriate to go back to basics a little and define/outline the manner in which we set up a model and all of its components, before we actually run a simulation.

Technical Note

cdem2Ddesktop.exe is actually an application (effectively the GUI) that drives the compute engine **cdem2D.exe**. Both exes reside in the same folder, however it is solely cdem2Ddesktop.exe that needs to be "double-clicked" to start the software. It launches and starts up the compute engine and checks that everything is in place and displays results. The other items in the installation folder are a series of folders which contain saved output files, template files and text files, and other files which are used to communicate with and drive the compute engine. It is strongly advised that you do not edit, alter the names of, or move any of these folders or files.

The basic model results are always saved in the folder "modelresults" as simple text files whose format is very straightforward (x, y ,radius, layerID), they can be copied and further processed with ease using Python and/or imported into other graphics programs. There are also a variety of other ways that model data can be saved/exported for further, external use.

Essential Components of a Model Run/Simulation

Any given model run/simulation is a collection of several *key components* which together make up the final experimental set-up. These components can be set/changed via various of the menus and sub-menus of cdem2Ddesktop. Here, these key components, and how they relate, are summarised and explained.

Size and resolution of the model assembly

The size (dimensions) of your model is controlled by the dimensions of the “assembly” that you are using or choose to use. There are 8 *built-in* assemblies spanning a variety of length:height aspect ratios, and very soon you will be able to design your own bespoke assembly within the application itself. The available assemblies, their dimensions in model units and number of elements are shown in the screenshot below (they are selected via the Model Set-Up menu). As an assembly is defined in terms of model units, these assemblies have to be scaled to real-world dimensions by setting the *resolution* of the model.

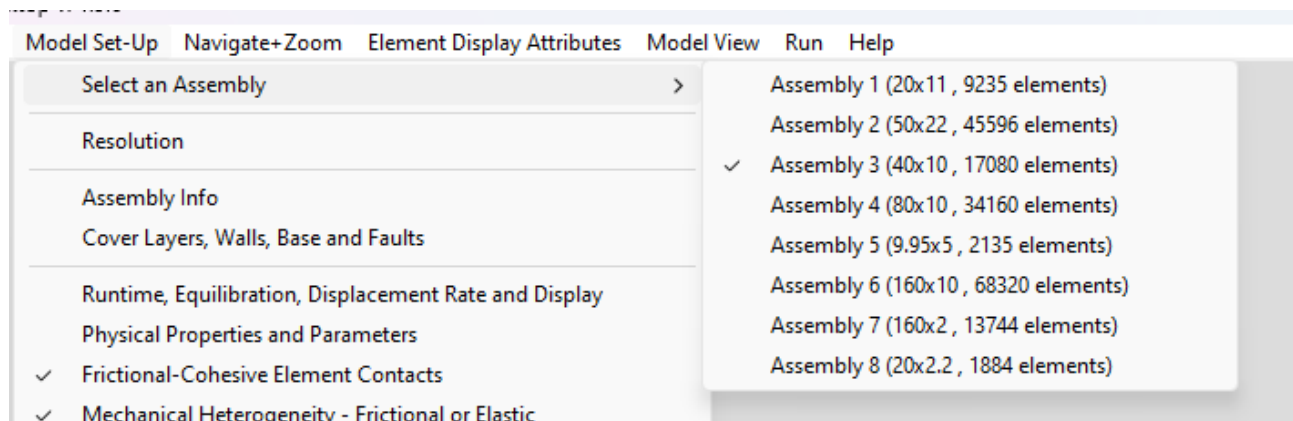
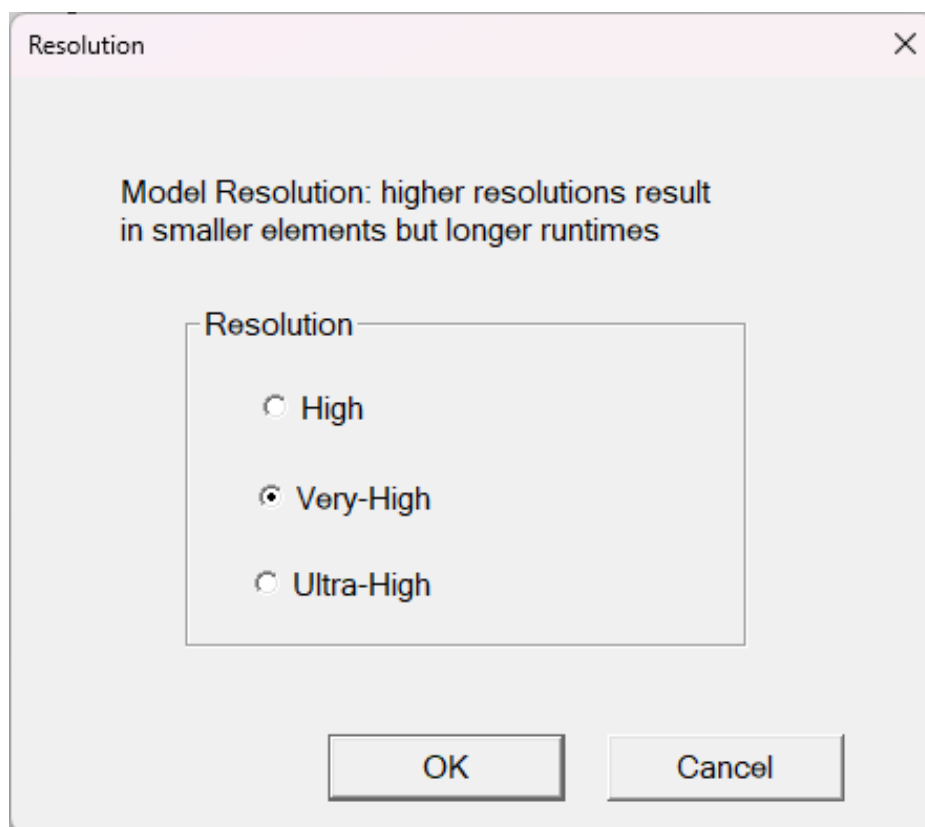


Figure 3. Screenshot of assembly selection.

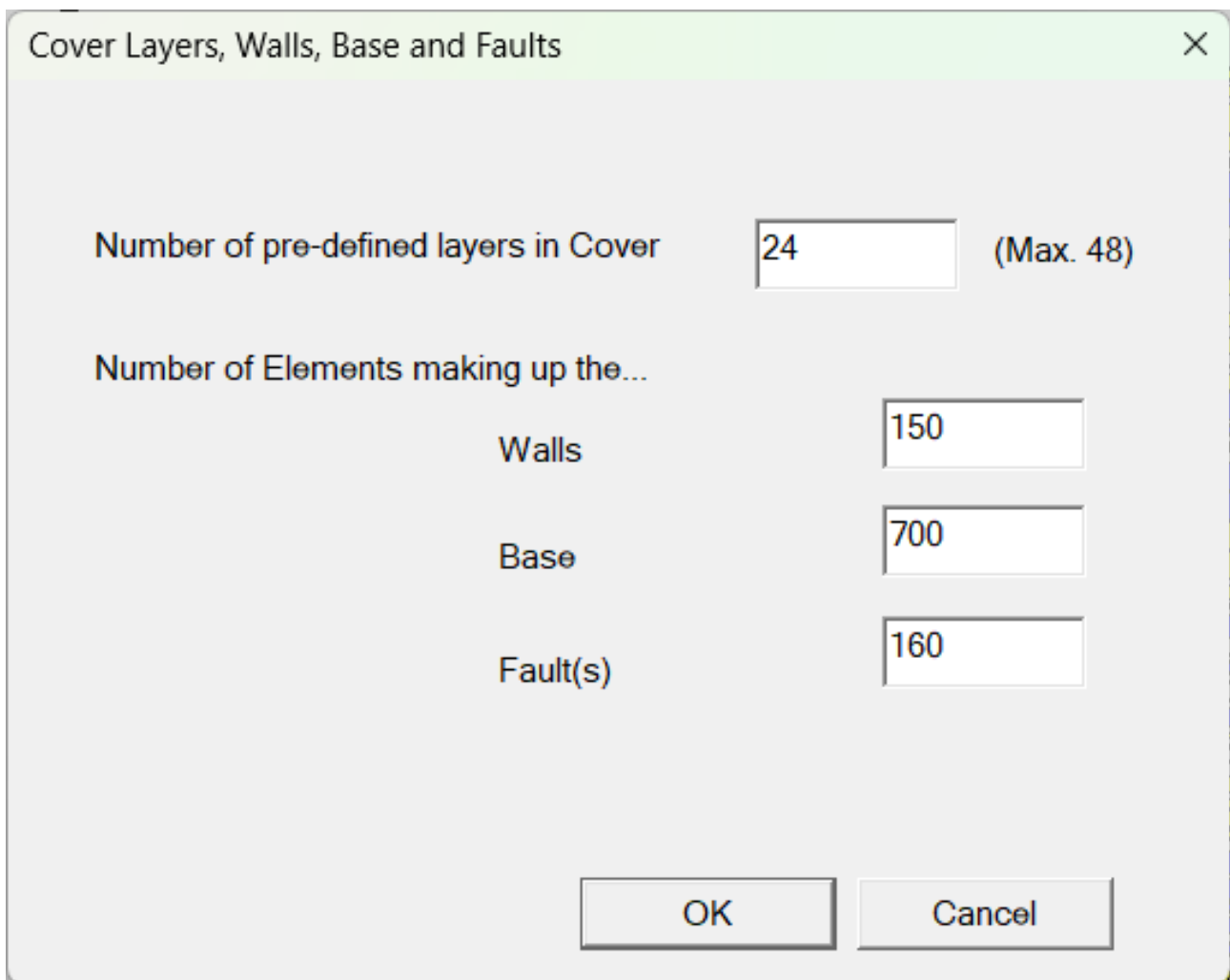


Currently, there are 3 model resolutions to choose from: *High*, *Very High* and *Ultra-High*. These give increasing resolutions for a given assembly. Typically, with the built-in assemblies, *High* gives an average element radius of c. 19 m, *Very-High* c. 9 m and *Ultra-High* c. 0.8 m.

Figure 4. The model resolution dialog box.

For the same resolution, assemblies with *more* elements have *slower* runtimes as a result of increased computation. Similarly, for a given assembly, *higher resolutions* have *longer runtimes* than lower resolutions as a result of the (necessary) smaller time-steps used to ensure numerical stability. The current limit to assembly size is **500,000** elements.

Each assembly can have up to **48** regularly-spaced layers or units defined within it (the coloured layers in the screenshots shown herein actually represent groups of 2 layers). In addition, each assembly has associated walls, base and fault(s) made up similarly of discrete elements. This results in the “final” assembly having more elements than just the “body” elements. The number of defined layers and the number of elements comprising the boundaries/faults can be adjusted by the user (Fig. 5). Sometimes these values need to be adjusted depending on the specific boundary conditions that are chosen.



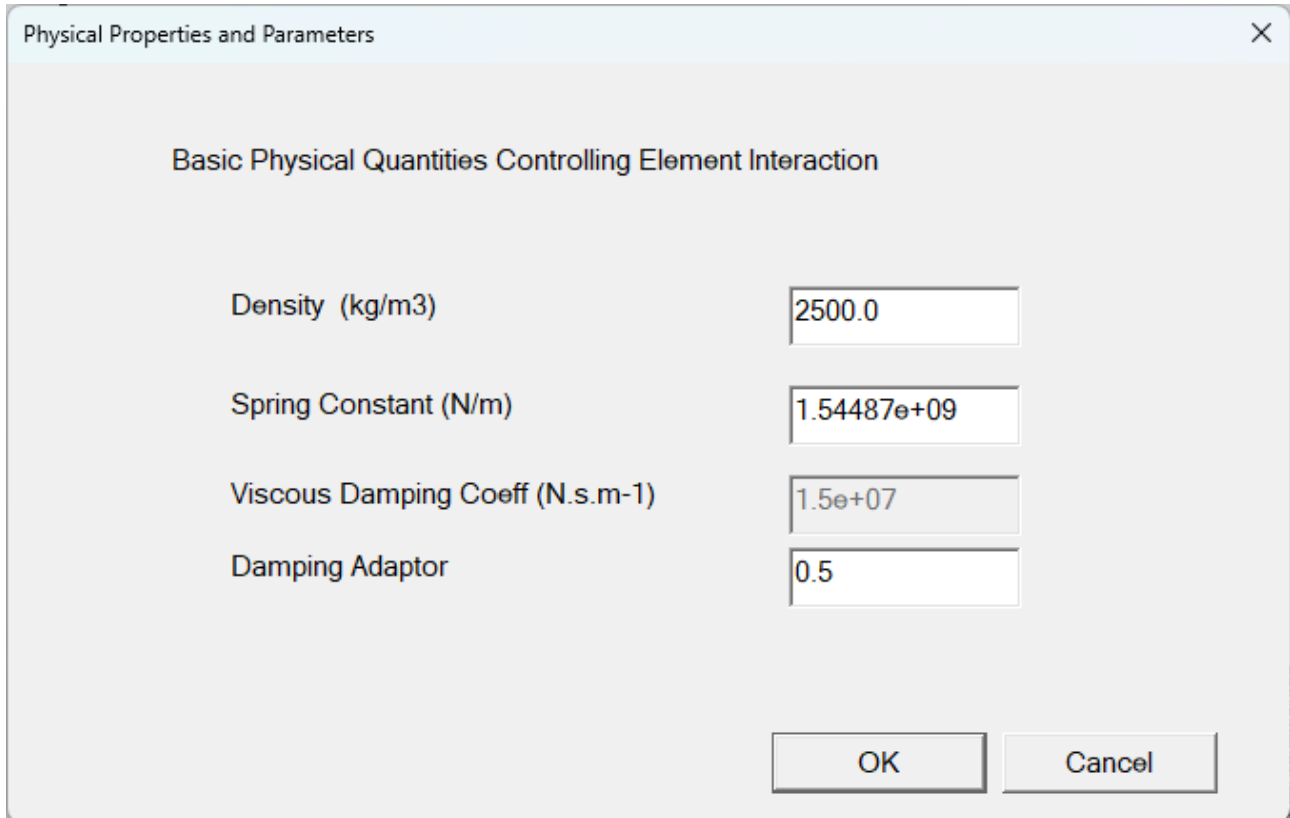
Cover Layers, Walls, Base and Faults	
Number of pre-defined layers in Cover	24 (Max. 48)
Number of Elements making up the...	
Walls	150
Base	700
Fault(s)	160
OK Cancel	

Figure 5. The Cover Layers, Walls, Base and Faults dialog box.

Physical Properties and Parameters

There are only a few fundamental physical parameters that control model behaviour, these are:

*The Spring Constant "**K**" (N/m)* - This defines the basic elastic interaction between elements and thus controls the bulk strength and behaviour of an assembly (see Theory Section). The default value of **K** used in the application is c. $1.54\text{e}9$, and this gives a Young's Modulus of c. 1-2 GPa. The value of **K** can be changed, however in an upcoming version of the application changing its value will be better integrated into the code and will be directly reflected in the choice of time-step.



Basic Physical Quantities Controlling Element Interaction	
Density (kg/m3)	2500.0
Spring Constant (N/m)	1.54487e+09
Viscous Damping Coeff (N.s.m-1)	1.5e+07
Damping Adaptor	0.5

OK Cancel

Figure 6. The Physical Properties and Parameters dialog box.

Density - this value defines the density of individual elements (not the bulk density) of the assembly, the default value is 2500 kg/m³, any variations will soon feed directly into the time-step calculation.

Damping Viscosity - this not a fundamental property but is used to ensure numerical stability (see Theory section), this can be changed (but in general should be left alone) via the Damping Adaptor. The value changes automatically when the resolution is changed.

Element-Element Contact Laws

In cdem2Ddesktop there are 2 basic element-element contact interactions that are possible: Frictional-Cohesive or Bonded-Elastic. For both, the default condition is that the assembly is homogenous internally, but it may have different properties when interacting with

the wall, base and fault boundary elements. In more complex simulations the assembly can be layered/heterogeneous - this is controlled via the Mechanical Heterogeneity Menu item (see later).

Boundary Conditions

A wide variety of boundary conditions are possible ranging from simple basement faulting, through paired synthetic faults, caldera collapse and user-defined fault geometries. Lateral boundaries can also be displaced, angle of repose simulations undertaken and caverns, tunnels created within an assembly. For boundary conditions that involve moving boundaries and/or faults, simulations can be run in both extension or contraction.

Model Runtime and Equilibration

Given a model assembly, element contact law and boundary conditions, the simulation needs to be “run” or allowed to evolve for a certain amount of time (or time-steps).

Runtime, Equilibration and Display Interval

Total Runtime (incl. equilibration) model seconds 4160.0

Equilibration time (no displacement) model seconds 200.0

☒ Equilibrate without bonding or friction

Display or recording interval - equivalent metres of boundary displacement 2.0

The default (high-resolution) displacement rate on boundaries and faults is 0.25 m/s, for very high-resolution it is 0.1 m/s, and for ultra-high resolution it is 0.005 m/s

☐ Override default displacement rate, use: 0.025 (m/s)

OK Cancel

Figure 7.The Runtime, Equilibration and Display Interval dialog box.

Such a runtime usually includes an initial period of *equilibration* when the assembly is not subject to any boundary displacement, and elements are often considered to be un-bonded and frictionless (see Fig. 7). The total model runtime, including equilibration, is measured in seconds. Please note that this is the simulation time, it has nothing to do with geologic time. The element behaviour is time-independent. For boundary conditions involving moving walls or faults, a displacement rate is also explicitly (and necessary) part of the model “condition” and implies an incremental displacement and total, final displacement that is measured in metres. This displacement rate depends on the resolution of the model. For all but the simulations involving no boundary displacements, the total boundary displacement is reported at the bottom of the information panel.

A crucial concept is the **Display or Recording Interval** during a simulation (see Fig. 7 above). In the example shown above this is 2 m, and given that this example is “High Resolution” this translates, via the default displacement rate of 0.25 m/s to 8 seconds of model run-time, meaning that display increments 0 to 25 will encompass equilibration (200s), followed by a further 495 display increments to finish the model run (4160s).

To summarise then, an experiment consists of a selected assembly, with given dimensions and resolution and with specified material properties subject to a subset of possible boundary conditions. The experiment typically starts with a period of equilibration during which the assembly adjusts to these chosen parameters before undergoing a typically much longer “runtime” during which the assembly is deformed in response to the applied/specified boundary conditions. Model runtimes are measured in model seconds, outputs however are typically recorded at intervals related to amounts of incremental displacement of boundaries (metres).

Viewing a Model & Displaying Attributes

As explained previously, to run the model, and start a simulation, choose the following command from the Menu Bar **"Run->Start Model Run"**. This will update the current "view" and it will show the evolution of the assembly as it is subject to the boundary conditions. At any time during the run, you can terminate the simulation by choosing this command from the Menu Bar **"Run->Stop Model Run"**. The normal cycle of cdem2Ddesktop is thus: i. Set-up the set of model parameters, ii. Run the model. iii. Analyse/examine model while it is running or has finished. In general, parameters/boundary conditions are changed via the Model Set-Up menu, and the model is viewed and "interrogated" via either the Navigate+Zoom, Element Display Attributes or Model View menus. In this section I will focus on viewing and "interrogating" a model. These three menus will be dealt with in turn below.

Navigate+Zoom

The Navigate+Zoom Menu provides commands to move around and zoom in and out of the current model "view". It can be accessed both during and after a model run. Included are the usual navigation functionalities together with their keyboard shortcuts (Fig. 7).

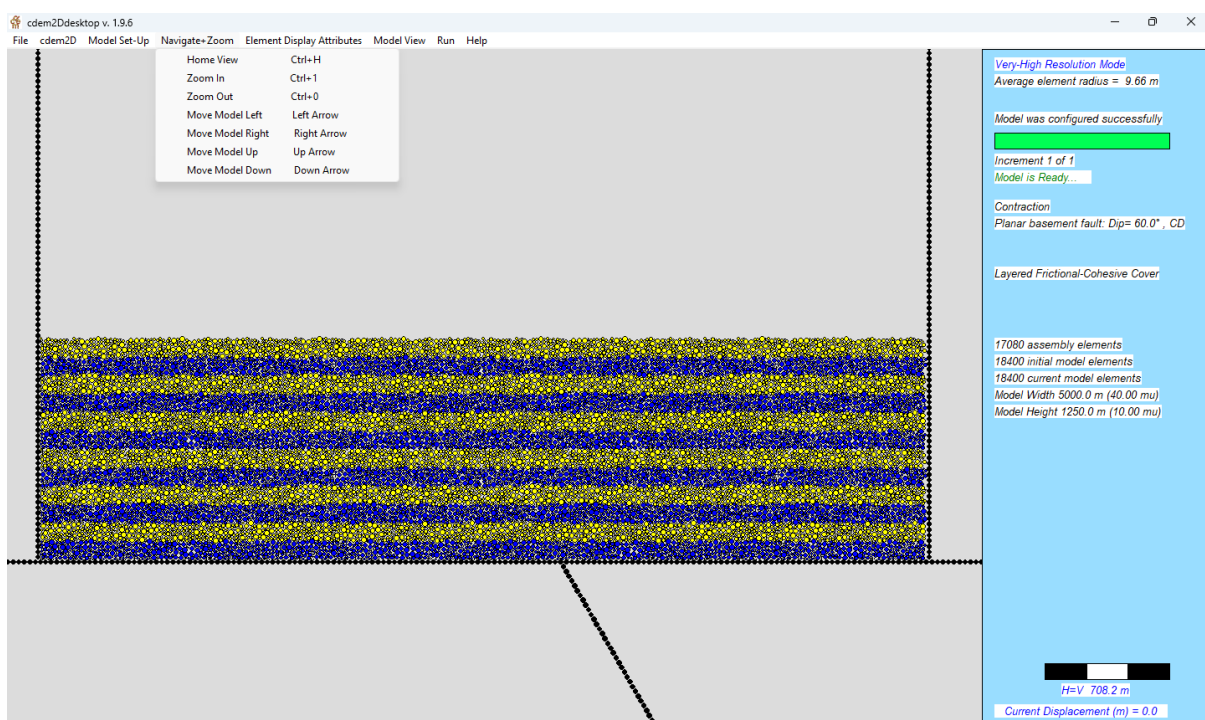


Figure 8. Screenshot showing Navigate+Zoom menu items.

N.B. If you ever get "lost" while panning around and zooming in/out of model results, you can always use the "Home View" command (Ctrl+H) to return your view to the global, default setting.

Element Display Attributes

Either during a model run or after a run is completed, the elements in any displayed model increment can be coloured according to the following attributes: displacement, strain or stress. Individual components of these attributes (where appropriate) can also be displayed. The display of such attributes is controlled via the Element Display Attributes menu (shown below).

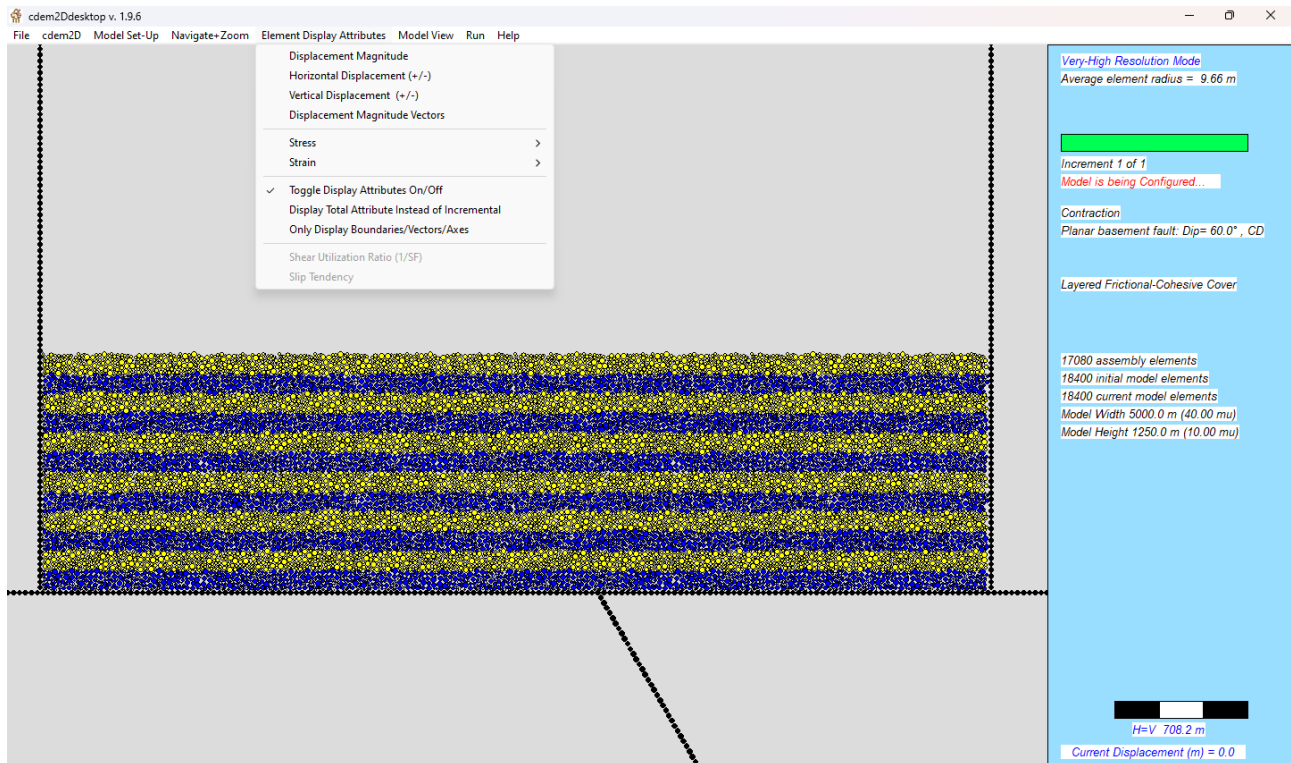


Figure 9. Screenshot showing Element Display Attributes menu items.

The basic premise is that any element, in addition to being coloured according to the simple geometric layering scheme (e.g. that seen in Fig. 9), can also be coloured according to an “attribute” that can be calculated and carried along with that element during deformation. Attribute display can be toggled On/Off via the Toggle Display Attributes On/Off menu command.

Either *incremental* or *total* displacement or strain can be visualised. Total displacement and strain are calculated *from the end* of the equilibration phase, i.e., the equilibration increments will not display any (or zero) total displacement or strain. On the other hand, incremental displacements and strains are displayed throughout the entire simulation, including the equilibration stage. These attributes are actually a great way to check that an assembly is stable after the equilibration phase. Incremental displacement or strain is calculated between the *current* model increment and the *previous* increment. Total displacement or strain is calculated between the current increment and the increment at the end of the equilibration phase.

For displacement, elements can be coloured according to the horizontal component, the vertical component or the magnitude of the incremental or total displacement (see Fig. 10 below). Displacement vectors (incremental or total) can also be displayed.

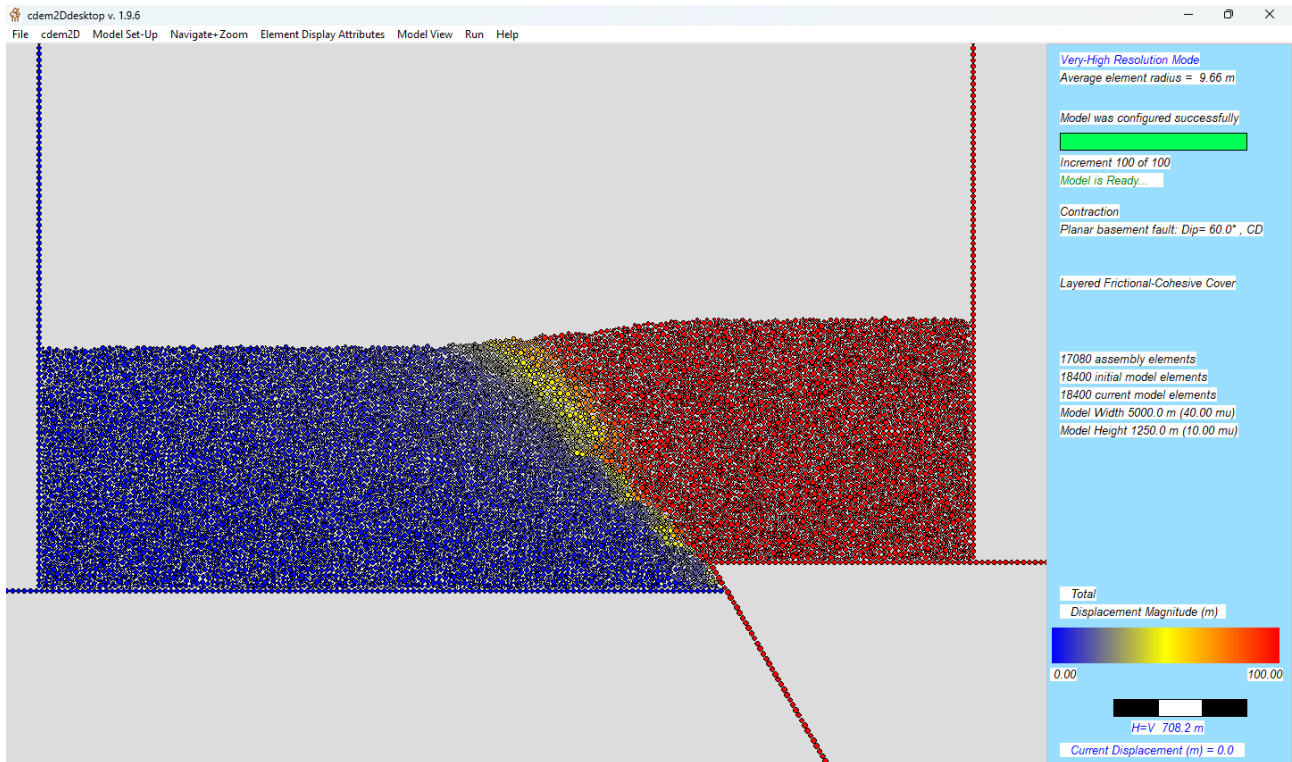
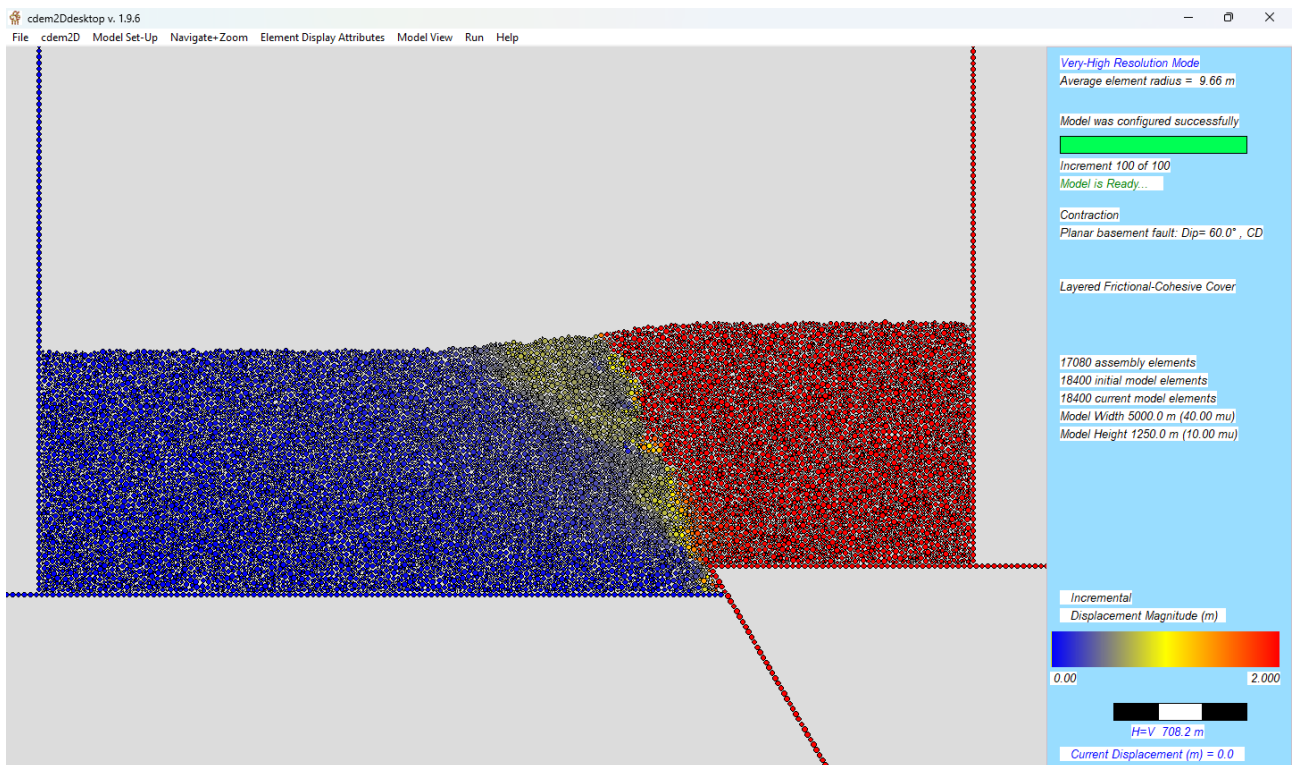


Figure 10. Screenshots of Incremental and Total Displacement being displayed as an element attribute.

Strain is calculated at the centre of each element using the neighbouring elements (see Cardozo and Allmendinger, 2009). In calculating total strain, we don't keep track of the path of the deformation (the cumulative history of incremental strains), but just the current and initial states (e.g. Fig. 11). This may result in the total strain locally being "reduced" with time, for example during tectonic inversion, which of course is not realistic. In such cases, it is recommended to use the "Cumulative Total Max. Shear Strain" calculations. This basically calculates the cumulative total of the incremental shear strain from the end of the equilibration phase. Cumulative strain is better than total strain in some cases since it captures the path of

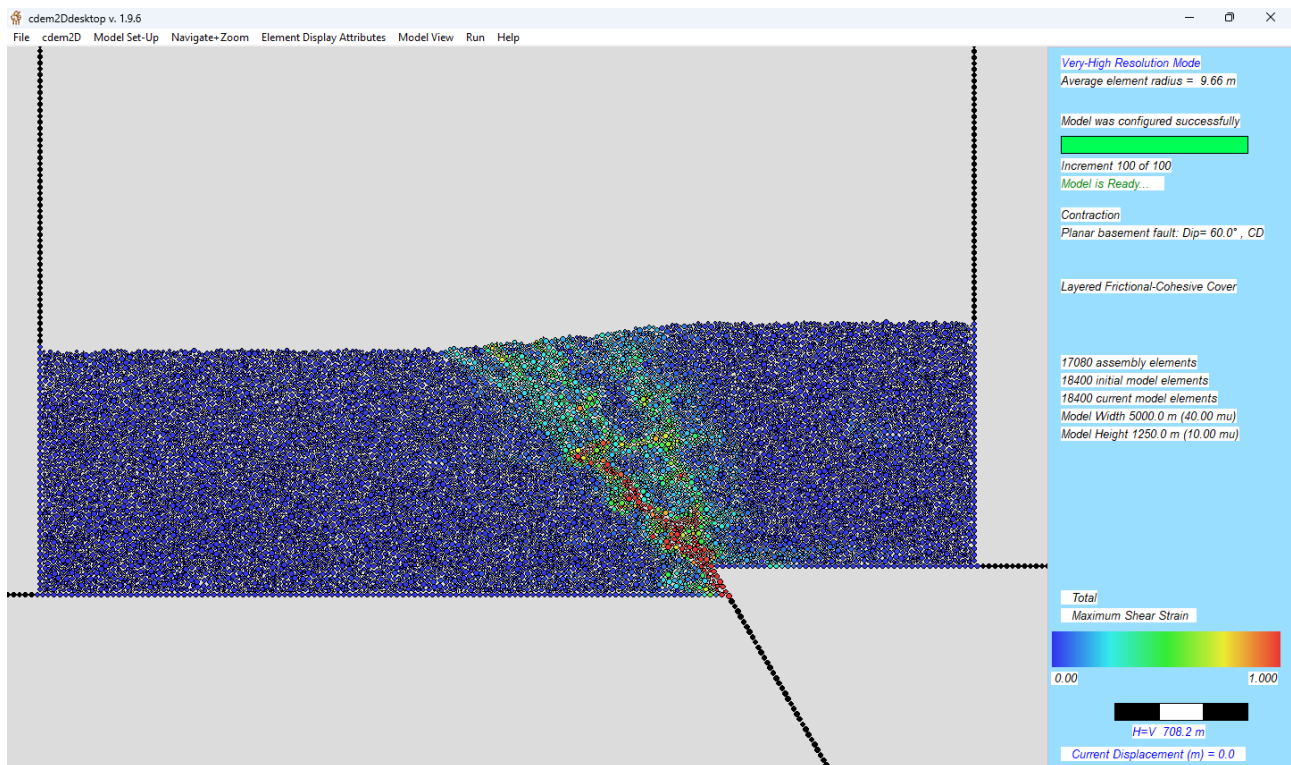


Figure 11. Screenshot of total Max. Shear Strain being displayed as an element attribute.

deformation. However, cumulative strain takes time to compute, since the program must calculate and sum all the incremental strains from the end of the equilibration to the current increment.

For strain, elements can be coloured by incremental or total extension (e_1), shortening ($-e_3$), maximum shear strain and dilation. Rotation is strictly only valid for instantaneous strains, so is not available for "total" calculations. Elements where strain cannot be calculated, because of fewer than three neighbours, are shown in black.

N.B. Calculation and display of total strain components in *growth* strata is still somewhat problematic and experimental, whilst incremental strain works normally as does cumulative maximum shear strain.

For stress, elements can be coloured by horizontal or vertical stress (σ_{xx} or σ_{yy}), shear stress (τ_{xy}), maximum or minimum principal stress (σ_1 or σ_3), maximum shear stress ($(\sigma_1 - \sigma_3)/2$), slip tendency (τ/σ) on a plane, and 1/safety factor. *Please note that to have access to the stress menu items you need to toggle on the Calculate Stress option in the Model Set-Up menu.*

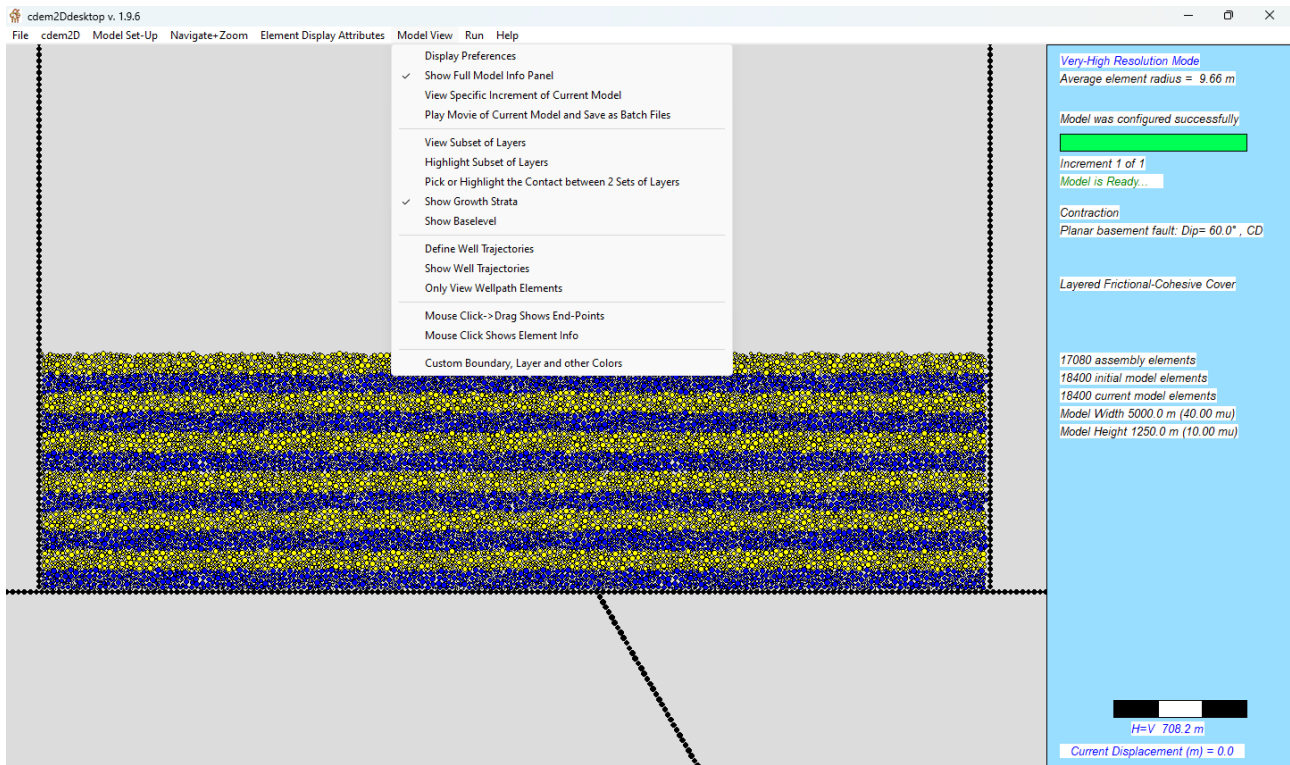


Figure 12. Screenshot showing the Model View menu items.

Model View

The Model View menu provides the user with a variety of different methods for viewing the model results, creating and viewing well trajectories, viewing specific increments of a model and changing a wide variety of display parameters and colours (see Fig. 12). *From top to bottom these menu items are:*

The **Display Preferences** menu item brings up a dialog with many key display properties for the simulation that is either running or has been run. It takes a bit of navigation to get familiar with all these settings but usually you are just changing one to two (Fig. 13).

Most of the editable fields are the numeric values of upper limits used in the colour scheme/bar for that attribute. In natural groupings these are:

- Total Displacement Colour Bar: **Max. Value** in metres
- Incremental Displacement Colour Bar: **Max. Value** in metres
- Movie Display Increment Stride: Display every **number** of increments
- Displacement Vector Exaggeration: **Value** by which vectors are exaggerated
- Stress Color Bar: **Max. Value** in MPa
- tmax and stress_xy Max. Values: **Max. Values** in MPa

- Slip Tendency on Plane: **Angle** of calculation plane in degrees
- Safety Factor (SF): - Mohr Coulomb **Failure Envelope Parameters**

Display Preferences

Total Displacement Colour Bar
0.0 Max. Value (m)

Incremental Displacement Colour Bar
0.0 Max. Value (m)

Movie Display Increment Stride

Displacement Vector Exaggeration (x)

Stress Colour Bar
0.0 Max. Value (MPa)

tmax and stress_xy Max. Values (MPa)

Slip Tendency on Plane "P"
Angle between P and horizontal
0-180 degrees, < 90 right-dipping

Safety Factor (SF)
MC Angle MC Cohesion MPa

Total or Cumulative Strain - Max. Colour Bar Value

Incremental Strain - Max. Colour Bar Value

Rotational Strain - Max./Min. Colour Bar Value (degrees)

Strain Attribute Mask
Strain mask, cutoff, value below
which an element is not drawn
☐ Display Mask Active
☒ Display Background Stratigraphy
☐ Show Background Strat on Strain Mask

Uniaxial-Biaxial Stress-Strain Graph
Strain X-Axis, Max. Value
Stress Y-Axis, Max. Value

Growth Sequence 1 ends at layer
[inclusive]

OK Cancel

Figure 13. The Display Preferences dialog box.

- Total or Cumulative Strain - Max. Color Bar: **Value**
- Incremental Strain - Max. Color Bar: **Value**
- Rotational Strain Max-Min Value: in **degrees**
- Strain Attribute Mask: Strain values can be masked (i.e. only values above threshold displayed), in this group box we have:
 - A cutoff **value** which defines the threshold
 - A **Checkbox** to activate the display mask
 - A **Checkbox** to activate the background stratigraphy (on by default)
 - A **Checkbox** to show only the background stratigraphy in the display mask (off by default)

- Stress-Strain Graph: the X and Y axis **limits** for the thumbnail stress-strain graph in Uniaxial-Biaxial Simulations
- Growth Sequence 1 ends at Layer: An integer **value** that acts to define and thus separate 2 growth sequences for display purposes.

The **Show Full Model Info Panel** menu item allows the side information panel to be toggled in and out of the view, this results in a view with a minimal side panel as shown below (Fig. 14):

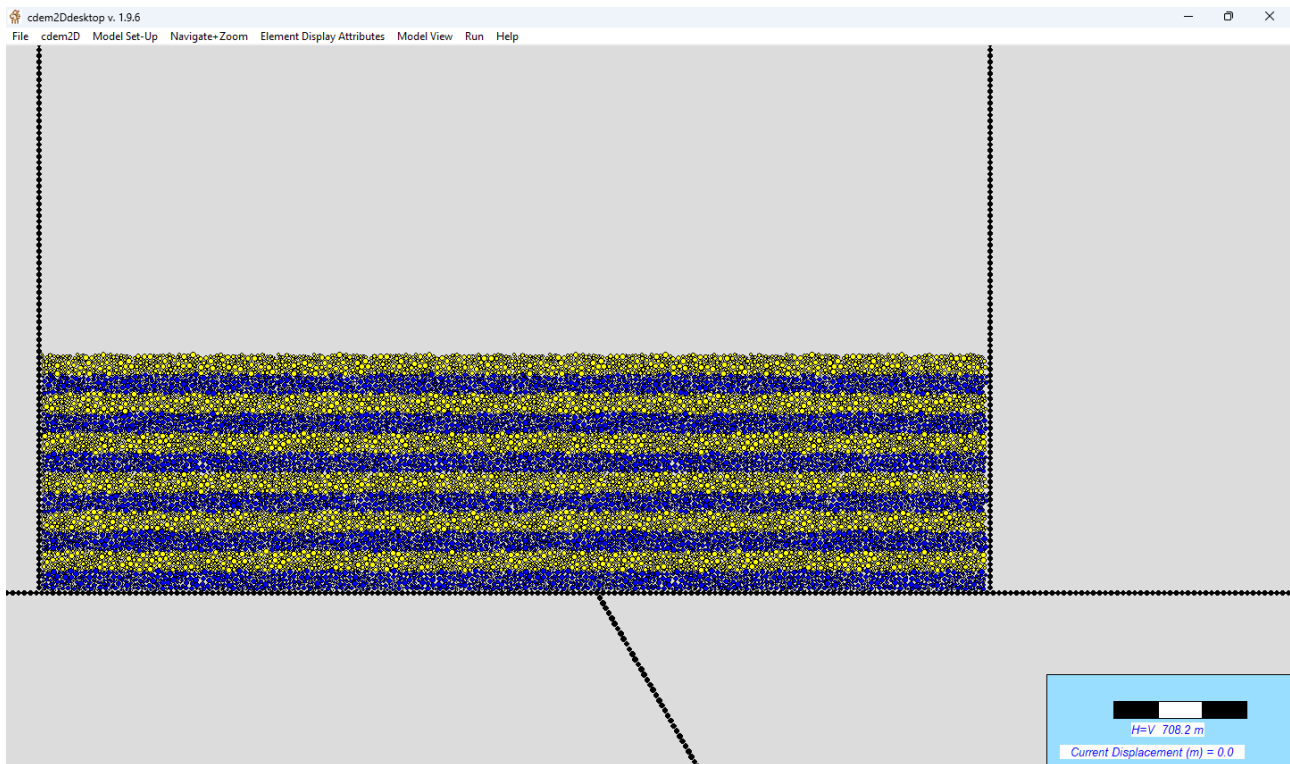


Figure 14. Screenshot of a model view with a minimal side panel.

The **View Specific Increment of Current Model** menu command brings up the dialog box shown in Figure 15 below.

This command allows the user to select/view an increment of the current (or loaded) model, within the limits given for the available increment indices.

A second function of this dialog is to set the “window” over which the Cumulative Max. Shear Strain attribute is calculated. The default value is 10 model increments, allowing a “running”

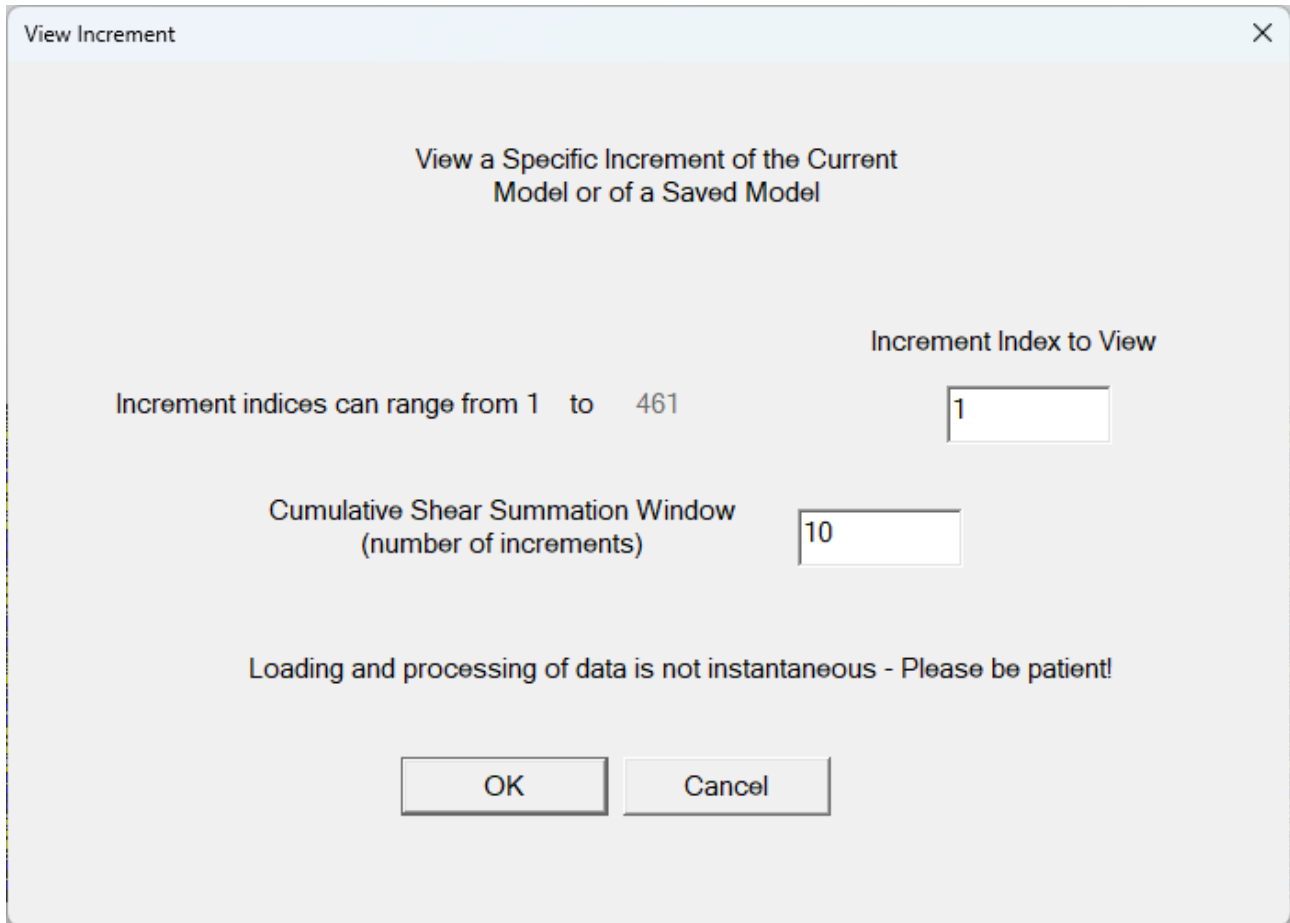


Figure 15. The View Specific Increment of Current Model dialog box.

average type view of cumulative strain, however in order to examine this attribute over *all* increments you should set this value to be the upper index limit - e.g. 461 in the example above.

The ***Play Movie of Current Model and Save as Batch Files*** menu item does exactly what it says: a movie/animation of the simulation is played, and at the same time a set of batch files (simple text format) for external use are saved in the folder "moviebatchfiles" in the application folder. These batch files contain *both* the elements' geometry and the displayed attribute,

The next "set" of menu items (Fig. 16) allow highlighting, selection and display of subsets of assembly layers, and the toggling On/Off of the baselevel and growth strata display.

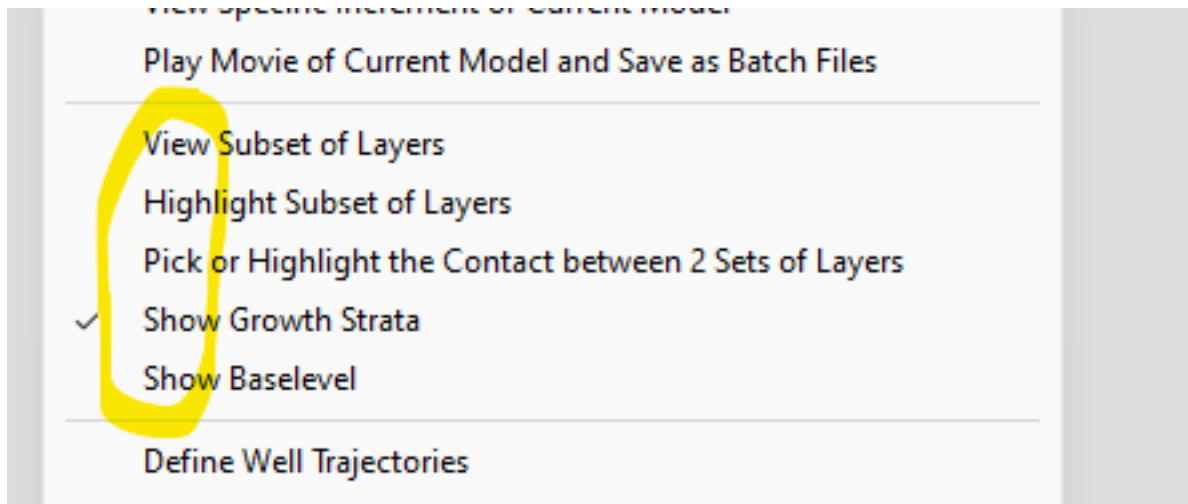


Figure 16. Screenshot of highlighting, selection of layers etc. menu items.

This is followed by another “set” of menu items which allow the definition, and display, of a set of wells through the current model (Fig. 17). [A detailed explanation of their use will follow in the next version of this manual.](#)

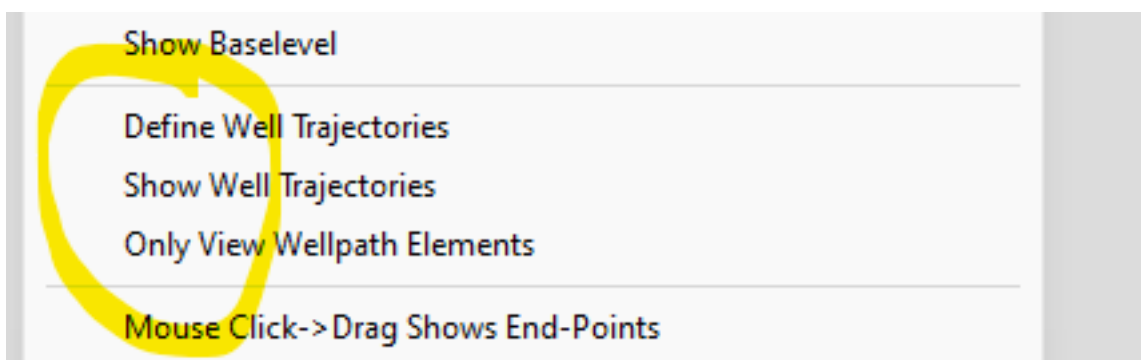


Figure 17. Screenshot of well-definition and viewing menu items.

Next, there are 2 Mouse Click/Drag menu items (Fig. 18), these commands *do not* function whilst a model is running. The default behaviour of a single mouse click is to do nothing. The default behaviour of a mouse click and drag/release (with neither option below toggled on) is to show distances and angles (Fig. 19). Toggling the first menu item "On" changes that behaviour to showing end-points, and toggling the second menu item "On" shows model info in response to a single mouse click (Fig. 20).

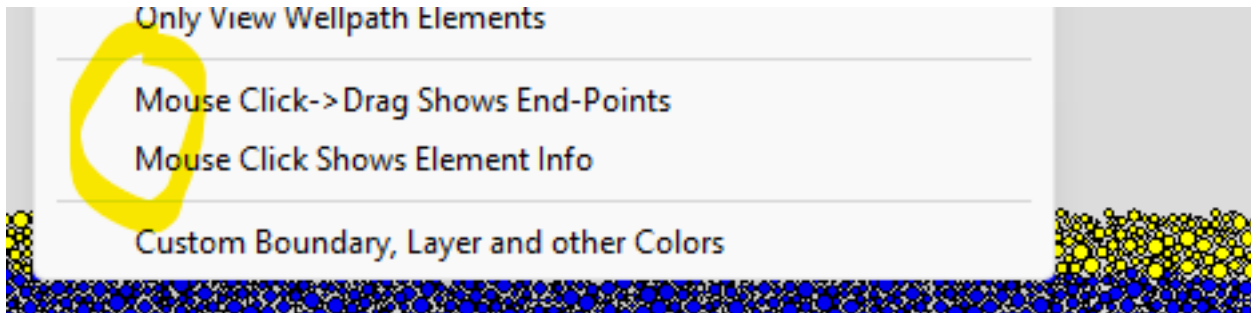


Figure 18. Screenshot of the mouse click/drag menu options

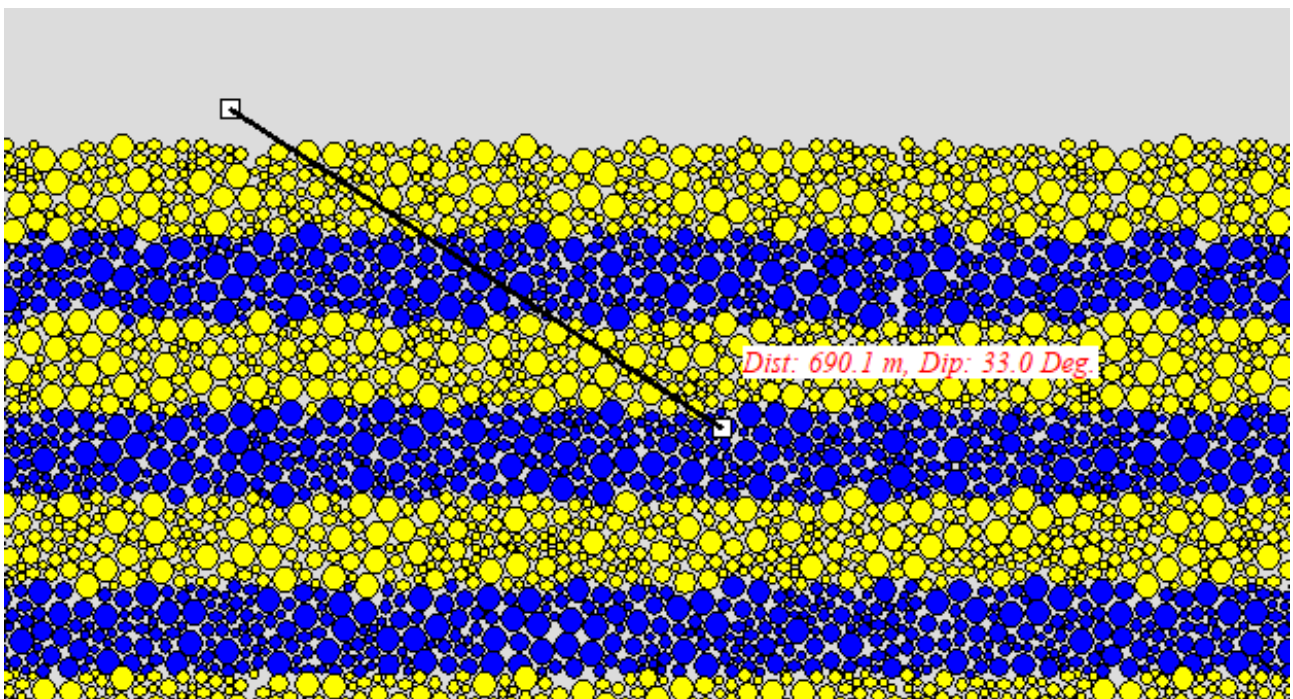


Figure 19. Screenshot of a mouse click and drag, showing distance and angle between end points.

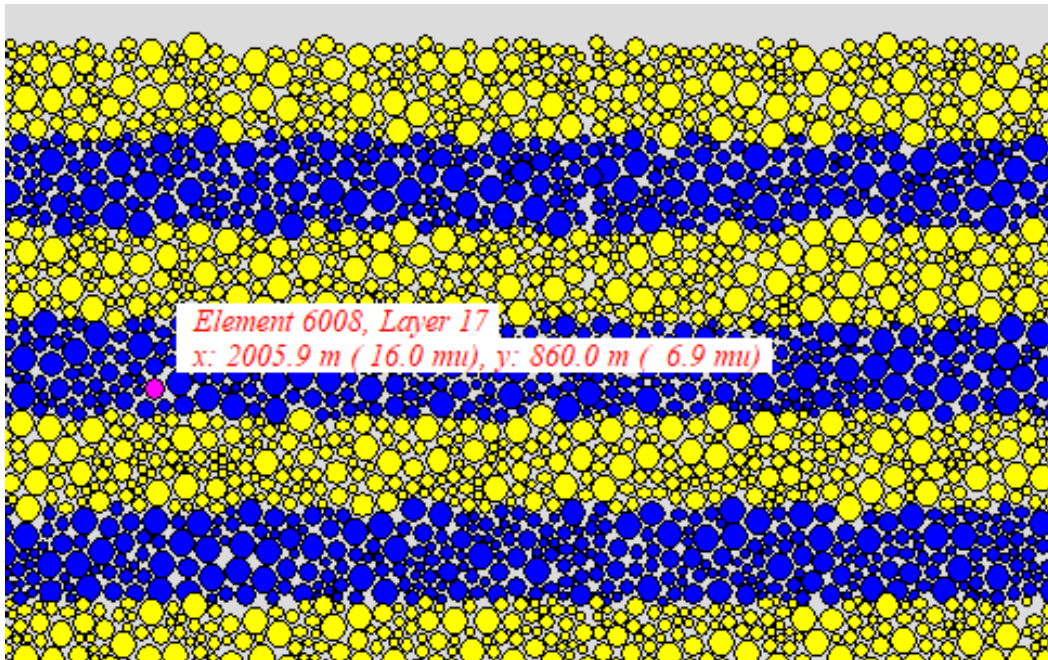


Figure 20. Screenshot of a single mouse click, Model Info toggled on, showing element information.

The final menu item **Custom Boundary, Layer and other Colours** brings up a dialog box which enables you to change a wide range of items to the colour of your choice (Fig. 21 below). You can use the "Edit" buttons to set the colours of the boundary elements, pre-growth elements, elements in growth sequences 1 and 2 amongst others things. The "Apply" button (as normal) allows you to try out these colours without committing to the changes.

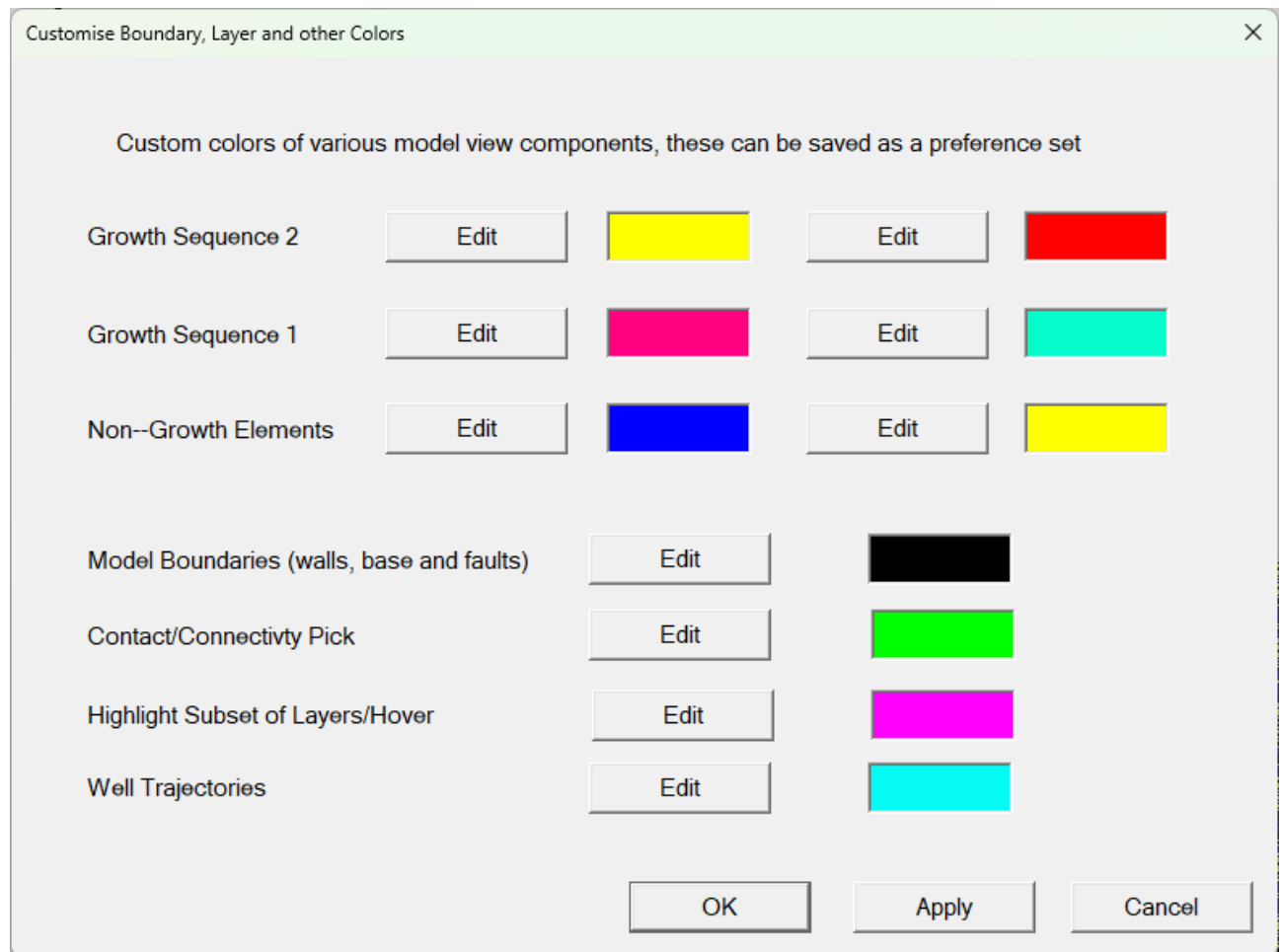


Figure 21. The Customise Boundary, Layer and other Colors dialog box.

Setting Up a Model: Assembly Properties and Boundary Conditions

As explained previously, to run a model/start a simulation choose this command from the Menu Bar **"Run->Start Model Run"**. This will update the current "view" which will show the evolution of the assembly as it is subject to the chosen boundary conditions. At any time during the run, you can terminate the simulation by choosing this command from the Menu Bar "Run->Stop Model Run". In this section I will focus on Setting-Up a Model via Assembly Properties and Boundary Conditions (Fig. 22 below),

Assembly Properties

The discrete elements' properties are fundamental to the behaviour of an assembly. In cdem2Ddesktop the user can choose between two different types of assemblies/materials: A granular friction material characterised by an inter-element coefficient of friction and cohesion, or an elastic-bonded material characterised by an inter-element breaking strain (Fig. 22). Notice that these material parameters can be defined between the internal elements, and also between the internal elements, the walls and any fault. *These two materials are mutually exclusive.*

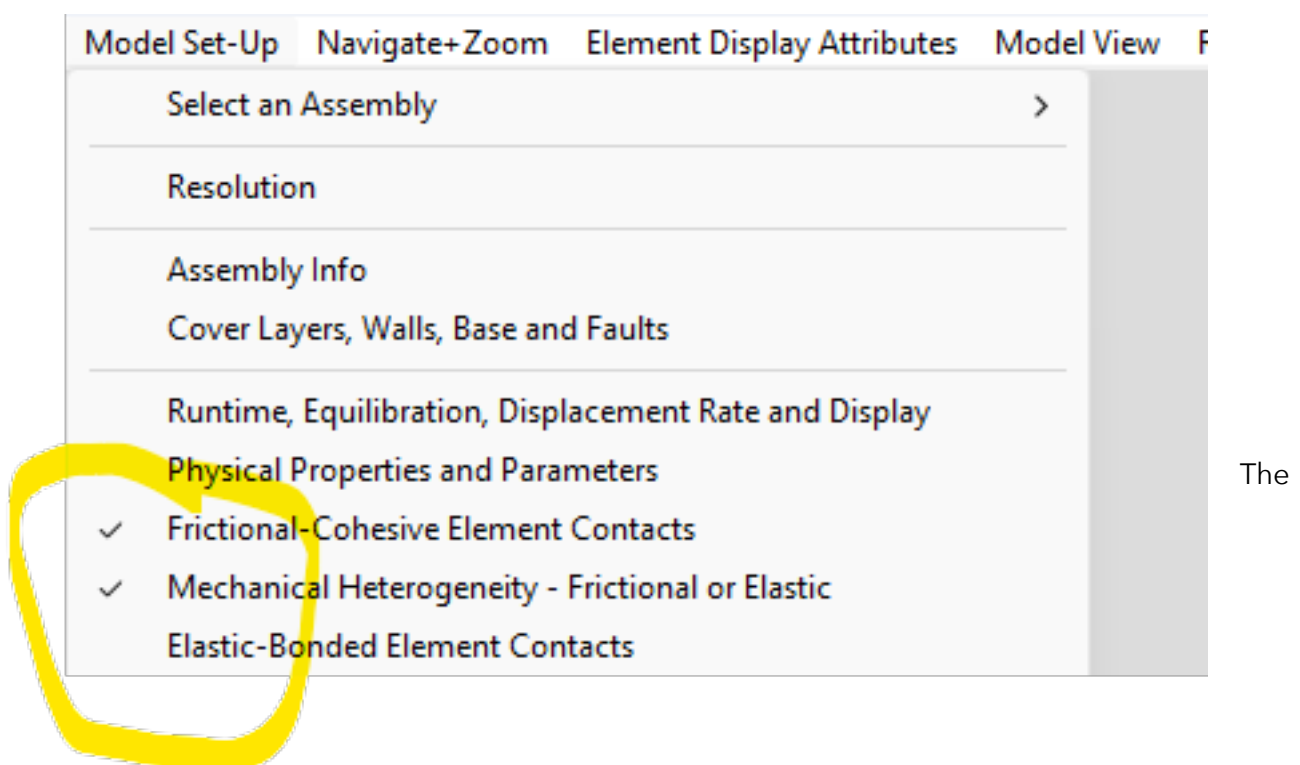
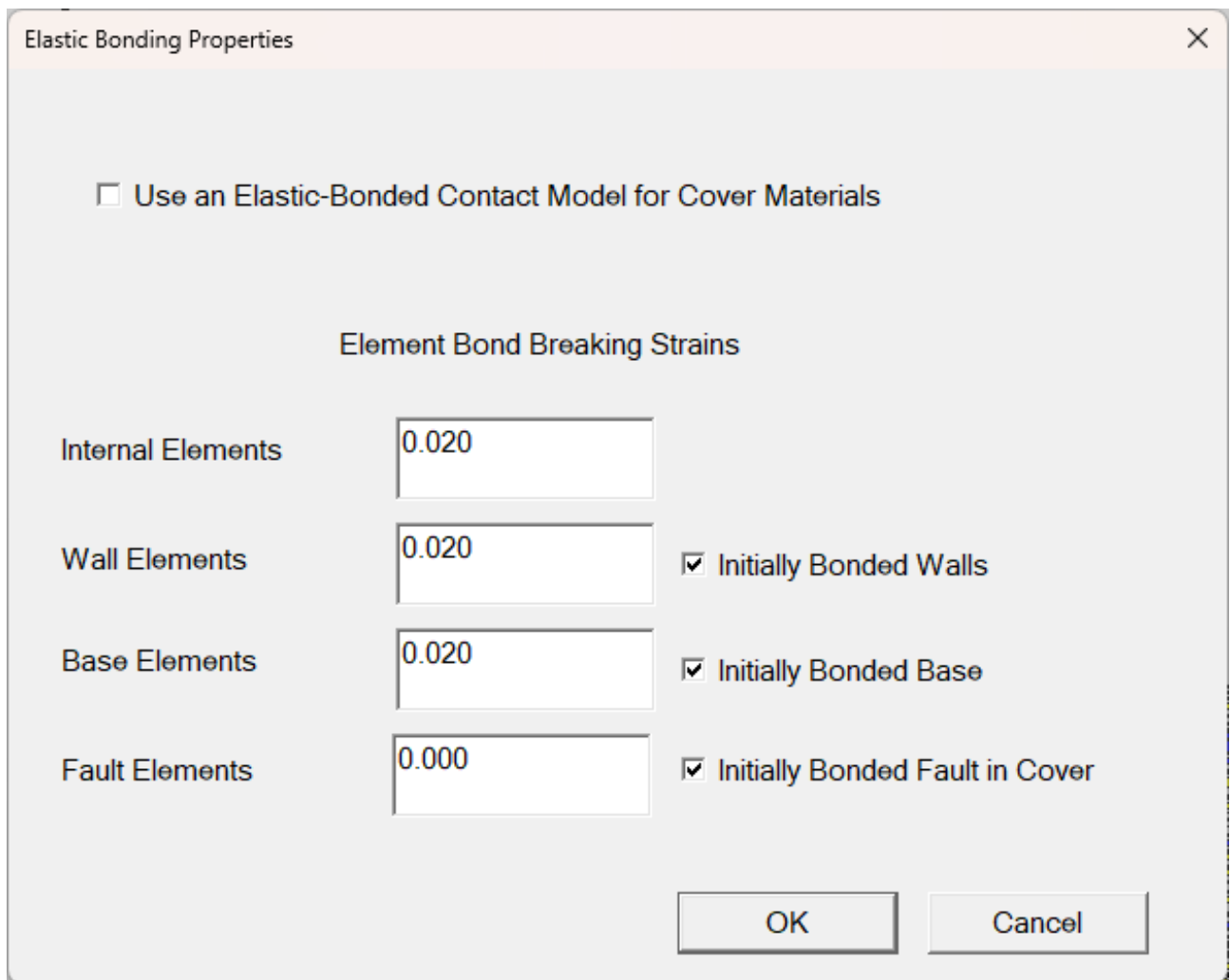


Figure 22. Screenshot of available assembly contact laws in the Model Set-Up menu.

elastic-bonded material uses discrete elements that are initially bonded by elastic springs. These springs break when the separation between the elements exceeds the defined breaking strain times the sum of the elements radii (see Theory section).

This type of material behaviour is activated by selecting the menu command **"Model Set-Up->Elastic-Bonded Element Contacts"** which brings up a dialog (Fig. 23) and then by checking

the topmost “Check Box” in this Dialog. Breaking strains can be assigned to both/between



The dialog box is titled "Elastic Bonding Properties" and has a close button (X) in the top right corner. It contains a checkbox labeled "Use an Elastic-Bonded Contact Model for Cover Materials" which is currently unchecked. Below this is a section titled "Element Bond Breaking Strains". This section contains four rows of input fields and checkboxes:

Element Type	Bond Breaking Strain	Initially Bonded
Internal Elements	0.020	
Wall Elements	0.020	<input checked="" type="checkbox"/> Initially Bonded Walls
Base Elements	0.020	<input checked="" type="checkbox"/> Initially Bonded Base
Fault Elements	0.000	<input checked="" type="checkbox"/> Initially Bonded Fault in Cover

At the bottom right of the dialog are two buttons: "OK" and "Cancel".

internal and boundary elements. Boundary elements may also be set to bonded or un-bonded initially via a set of three check-boxes next to their breaking strain fields.

Figure 23. The Elastic Bonding Properties dialog box.

In contrast, the granular frictional material exhibits the characteristic Mohr-Coulomb behaviour of rocks in the frictional regime. This type of material behaviour is activated by selecting the menu command "**Model Set-Up->Frictional-Cohesive Element Contacts**" which brings up a dialog and by checking the Check-Box at the top (Fig. 24). Internal and boundary elements can have distinct coefficients of friction, and boundary elements can be initially set to be frictionless via a set of checkboxes to the right of their coeff. of friction fields. Setting the inter-element cohesion to zero results in a purely frictional material. When the check-box "Cohesion lost after first slip between elements" is checked, it indicates that the cohesion is lost after the first slip event at any element-element contact; when unchecked cohesion is lost after 2 elements initially in contact physically separate. The final parameter in this dialog box allows strain weakening via a reduction (by a fraction) of original coefficients of friction after the loss of cohesion (*this is a somewhat experimental feature*).

Frictional Properties

☒ Use a Frictional-Cohesive Contact Model for Cover Materials

Coefficients of Friction

Internal Elements (overridden by mechanical stratigraphy)	0.20	
Wall Elements	0.20	<input type="checkbox"/> Frictionless Walls
Base Elements	0.20	<input type="checkbox"/> Frictionless Base
Fault Elements	0.00	<input type="checkbox"/> Frictionless Fault
Inter-Element Cohesion (Pa) (by default, cohesion is lost after elements separate)	3e+07	<input type="checkbox"/> Cohesion lost after first slip between elements
After loss of cohesion, coefficients of friction are reduced to this fraction of their original value (min 0.0, max 1.0)	1	

OK
Cancel

Figure 24. The Frictional Properties dialog box.

A more “advanced”, and perhaps more geologically realistic, option is also available when setting up the chosen assembly: This is to have an initially layered, mechanically-heterogeneous, assembly, whose parameters are set by choosing the “**Mechanical Heterogeneity - Frictional or Elastic**” menu item, which brings up the dialog box shown below:

Mechanical Heterogeneity

Use this table to define Frictional or Elastic Mechanical Stratigraphy

Cover Top	from	Layer	to	Layer	Element Coeff. of Friction	Element Elastic Bond Breaking Strain
Layer Group16		40		40	0.2	0.02
Layer Group15		36		39	0	0.02
Layer Group14		35		35	0.2	0.02
Layer Group13		25		34	0	0.02
Layer Group12		23		24	0.2	0.02
Layer Group11		21		22	0	0.02
Layer Group10		19		20	0.2	0.02
Layer Group9		17		18	0	0.02
Layer Group8		15		16	0.2	0.02
Layer Group7		13		14	0	0.02
Layer Group6		11		12	0.2	0.02
Layer Group5		9		10	0	0.02
Layer Group4		7		8	0.2	0.02
Layer Group3		5		6	0	0.02
Layer Group2		3		4	0.2	0.02
Layer Group1		1		2	0	0.02

Cover Base

OK

Cancel

Figure 25. The Mechanical Heterogeneity dialog box.

Mechanical heterogeneity is activated by checking the “Check Box” at the top of this dialog (Fig. 25). This contains a table with 16 rows where you can set up “packages” or units with variable frictional or elastic properties within the assembly. The Layer Group numbers “link” back to the number of layers that are defined for the assembly: e.g. if there are 24 layers you must ensure that all layers between 1 and 24 are dealt with in the dialog in a similar way to the dialog shown above. Layer numbers greater than the total defined for the assembly, e.g. 24 in this instance, are ignored.

Boundary Conditions

There are a wide variety of boundary conditions that can be selected to “condition” your model and then run your simulation. These are accessed mainly through the lower half of the “Model Set-Up” menu (see below).

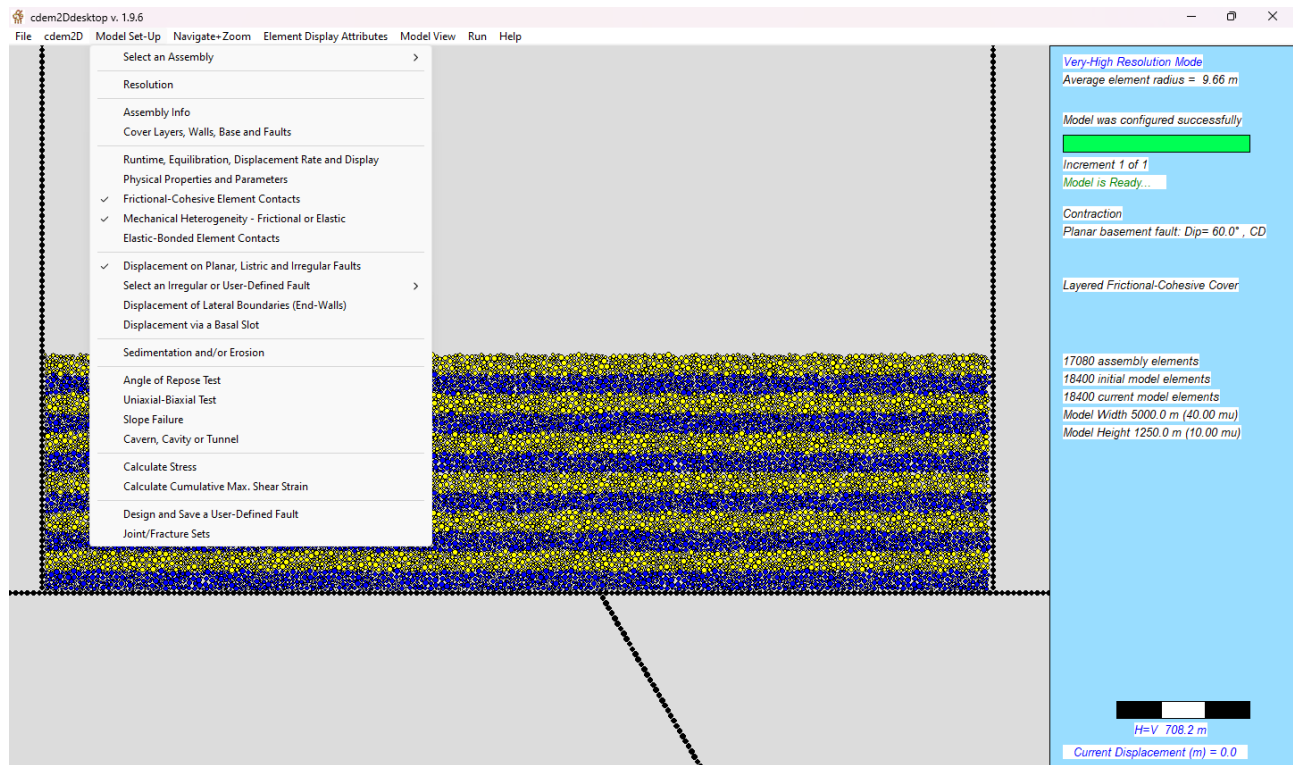


Figure 26. Screenshot of the Model Set-Up menu and its items.

The boundary conditions are available via selection of the appropriate menu items. These typically bring up a dialog containing controlling parameters (e.g. Fig. 27, see below), *these boundary conditions are mutually exclusive*. Reading down the lower half of the menu the following boundary condition are available:

Displacement on Planar, Listric and Irregular Faults:

This menu command selects boundary displacement controlled by faulting: such faults can be either Planar, Listric or Irregular (by irregular we mean an arbitrary geometry made up of line segments). The menu command brings up the dialog shown in Figure 27. The *default* sense of movement on all faults is extensional, but the user can change this to contraction easily via a checkbox at the top of the window. Planar fault parameters are on the left of the dialog, listric and irregular faults are on the right. The default set-up is a planar basement fault geometry.

Faulting Parameters and Configuration

The Default Configuration of displacement is to the right and down producing extension on right-dipping faults and the right endwall

☐ Inversion occurs after 60.0 percent of model run

☒ Change to Displacement Sense to Contraction

Displacement is applied as

- ☒ Constant along fault (CD)
- ☐ Constant Heave (CH)

Planar Basement Fault

Fault Position (model units) 23.6

Fault Dip (degrees) 60.0

Paired Fault Offset (model units) 4.0

☐ Sculpted or Irregular Fault in Cover

Default Geometry is Listric

Maximum Dip of this Listric Fault in Cover 75.0

☐ Use an, imported, user-defined fault shape

Paired Basement Faults

- ☐ Caldera-Piston
- ☐ Keystone
- ☒ Synthetic

0.0 2nd Fault Disp. Ratio

OK Cancel

Figure 27. The Faulting Parameters dialog box.

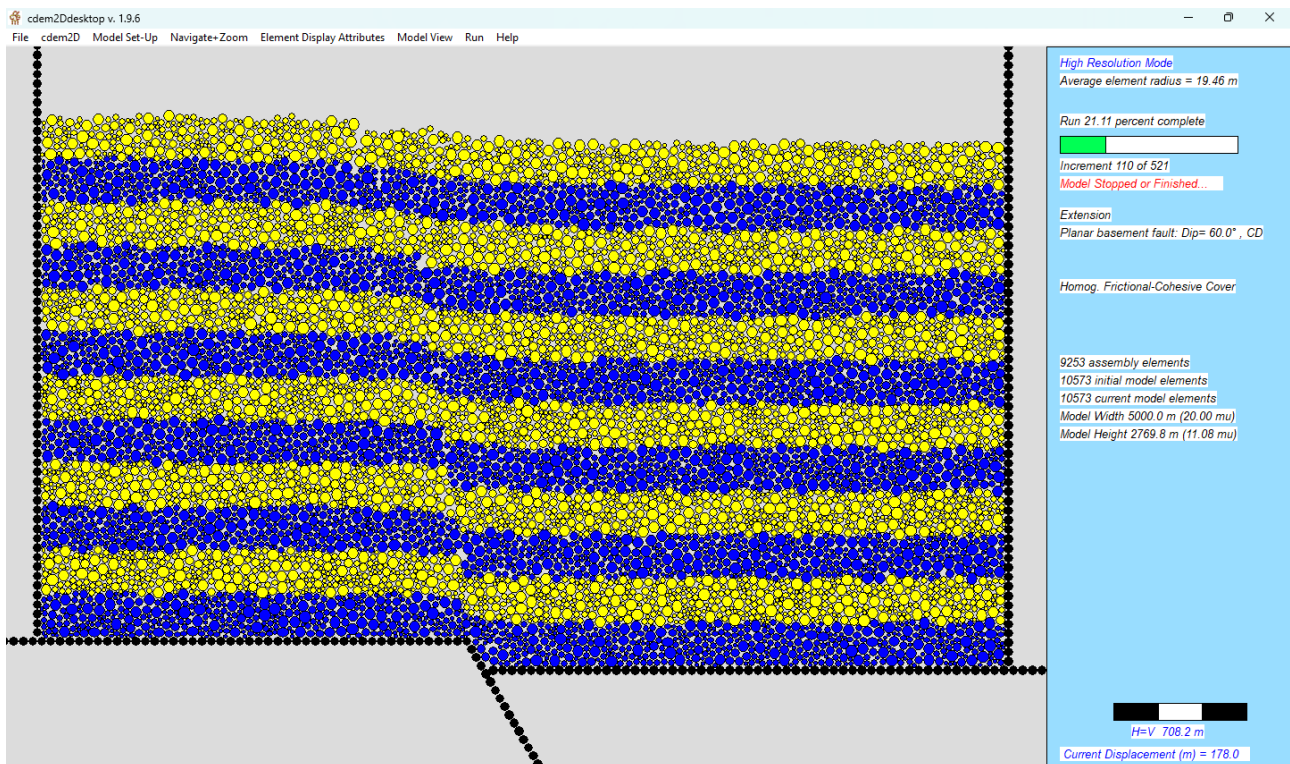


Figure 28. Screenshot of a planar fault in basement, constant displacement simulation.

For the planar basement fault, there are 2 essential text/value fields which “place” the fault within the model assembly:

- the Fault Position in *models units* from the left boundary of the assembly
- the Fault Dip in *degrees* (dipping to the right).

Planar basement faults can also be “paired” with a second fault, whose offset from the first is specified in the next text/value field:

- Paired Fault Offset (model units)

Such paired basement faults can take 3 forms (selected via Radio Buttons):

- a Caldera-Piston (fault dip must be set to 90 degrees),
- a Keystone configuration with 2 opposing, but identical, faults
- a Paired Synthetic Fault.

The 2nd fault in the Synthetic Fault case has a displacement rate that is a ratio of that on the 1st fault; when this field set to zero, the 2nd fault does not exist conceptually and is not displayed.

In addition, fault inversion can be activated via a check-box at the top right of the dialog. This will occur at a percentage of the total fault displacement. For example, if the fault is normal and fault inversion is toggled on at 50% displacement, the first half of the fault displacement will be normal and the second half will be reverse.

If the CH (constant heave) radio button is on, fault movement is simulated by moving the hanging wall vertically and the fault horizontally to fit the displacement of the lower planar fault segment. In this case, it is important to have the element-fault friction and/or cohesion equal to zero. If the CD (constant displacement) radio button is on, fault movement is simulated by moving the fault elements parallel to the fault. In this case, it is important to have friction and/or cohesion along the fault.

Finally, if a simple planar basement fault geometry is not desired, there is a check-box to the right of the Fault Position field to move along either a Sculpted listric (the default) or an Irregular Fault. If the fault is listric, it increases in dip from its input value to the specified maximum value. An “irregular” or piecemeal fault can be used instead by *also* checking the **“Use an imported user-defined fault shape”** check-box. In this case, the application will use the fault (previously) selected in the menu **“Select an Irregular or User-Defined Fault”** (see below).

For either the listric or the irregular fault selection, the elements in the footwall are removed from the computation and do not interact mechanically with the fault or the hanging-wall.

Select an Irregular or User-Defined Fault

This next menu item allows the user to choose an irregular or user-defined fault. Irregular, or user-defined, faults are geometries which are piecemeal, i.e. composed of multiple linear segments, and are thus not some analytical function or simple planar fault. They can be introduced into the application in one of two ways: either externally, following a fault text file format, or internally, via a dialog box. The menu **“Select an Irregular or User-Defined Fault”**,

allows the user to choose between 3 built-in example faults, a User-Defined *External* fault and a User-Defined *Internal* fault. All these fault definition text files are stored in the **faultlibrary** folder in the installation directory.

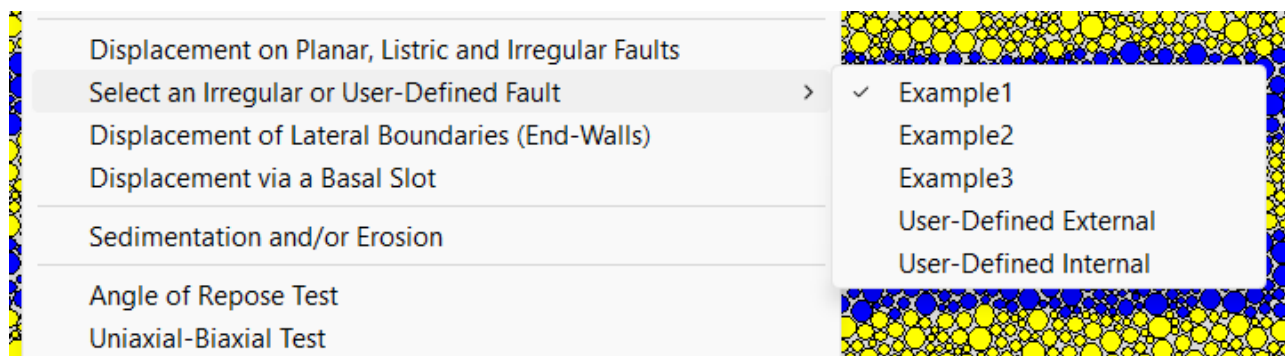


Figure 29. Screenshot of a the Select an Irregular or User-Defined Fault menu.

These text files must contain the number of coordinates followed by the x and y coordinates (in metres) of the piecemeal fault. These coordinates should be defined from the base of the fault and up-dip. The first coordinate should be at x = the fault location, and y = 0 (e.g., x = 2250 and y = 0 in the example shown below). Also since the faults dip to the right, subsequent points should have lower x and higher y coordinates in metres

```
7
2250    0
1479    24.6
1381    759.6
531     1382.6
474     1289.6
266     2080.6
99      2620.6
```

Figure 30. Screenshot of an irregular fault text definition file.

N.B. The User-Defined External Fault text file is located in the **faultlibrary** directory and must be named **itsmyfault.txt** if it is to be replaced by a different set of coordinates or file.

Displacement of lateral boundaries

Displacement of lateral boundaries (walls) is activated by firstly selecting the appropriate menu item, and then checking a combination of check-boxes in the dialog which appears (Fig. 31 below). Either the Left or the Right Wall can be active singly or together. Their sense of movement can be changed as well to produce contraction or extension. The final check-box, at the bottom, allows rotation of the model (clockwise) by a set amount after model equilibration.

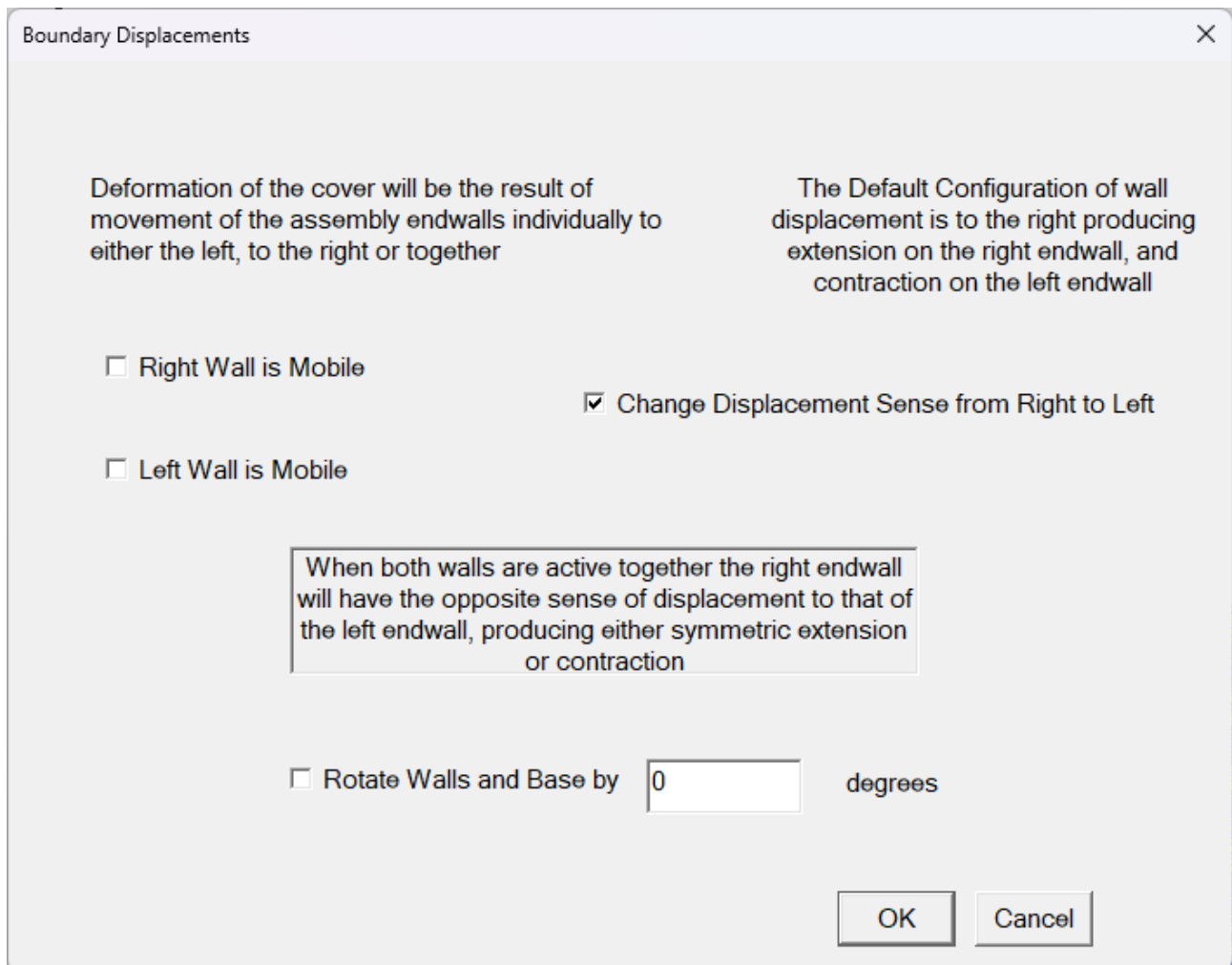


Figure 31. The Boundary Displacements dialog box.

An example of a simulation undergoing contraction via movement of only the right end-wall is shown in Figure 32. In this example elements are coloured according to the Total Max. Shear Strain and show both localisation within the model and along the base.

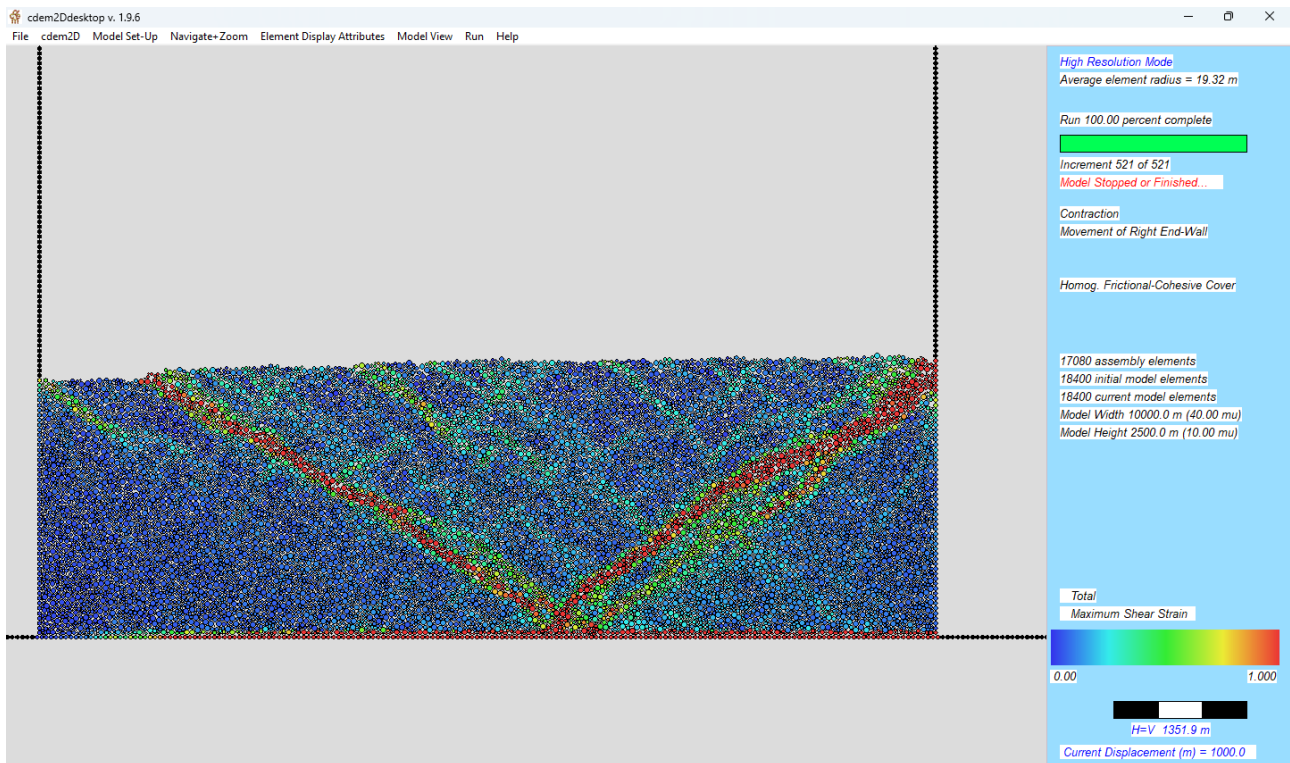


Figure 32. Screenshot of a simulation of model where there is contraction via the right end-wall, elements are coloured according to total max. Shear strain.

Displacement via a Basal Slot

Displacement via a basal slot is a set of boundary movements which produce either contraction or extension via slot with a given location and slot dip. The Dialog in Figure 33 is shown after selection of the Displacement via a Basal Slot menu item. The boundary condition is activated by checking the "Displacement...." Checkbox in the Dialog. The text fields allow the slot position and dip to be specified. Figure 34 shows a screenshot of a simulation where there is extension via the basal slot.

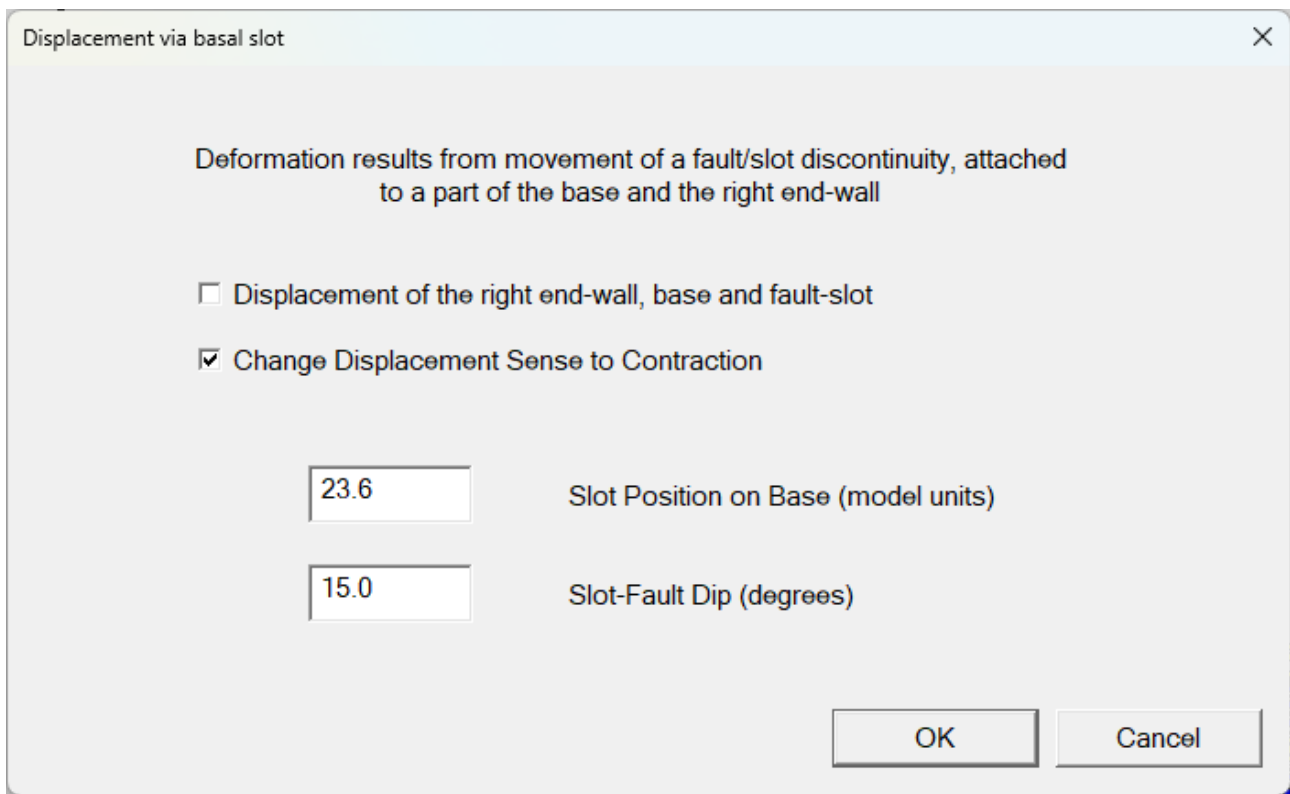


Figure 33. The Displacement via Basal Slot dialog box.

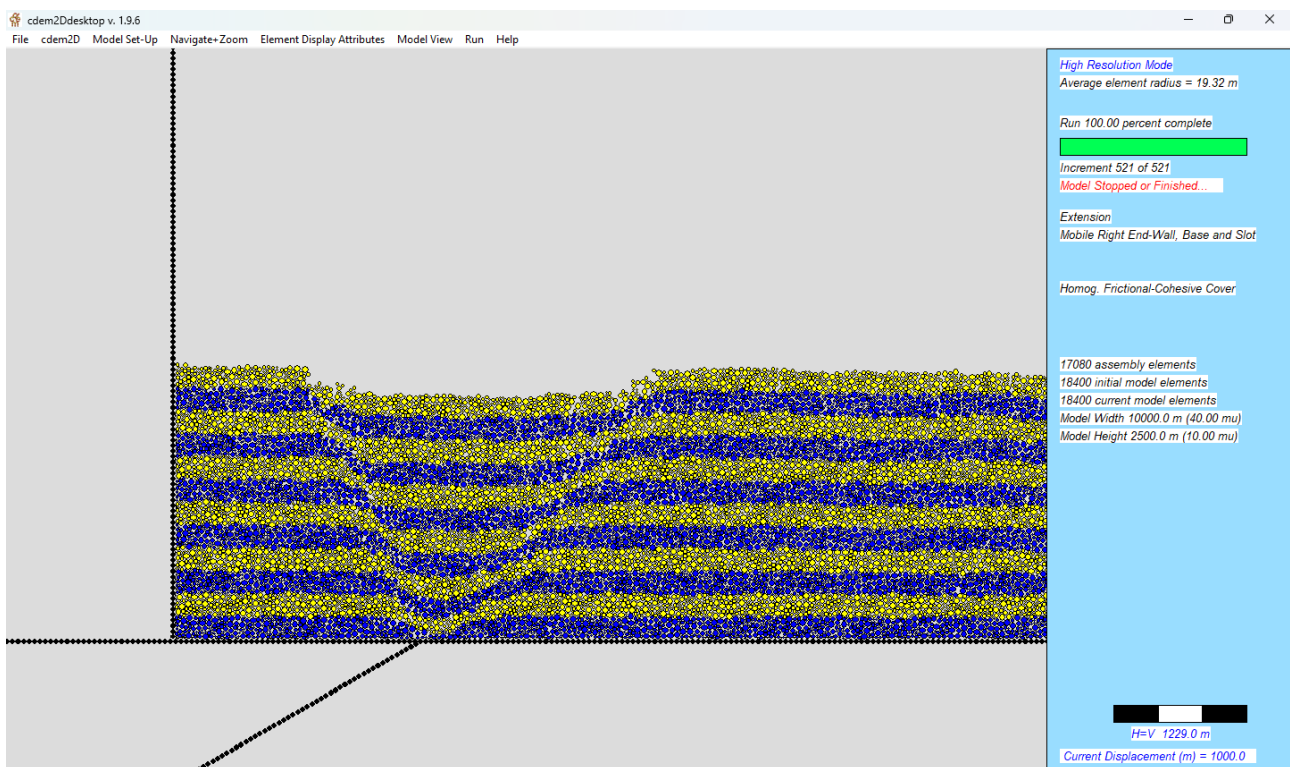


Figure 34. Screenshot of a simulation of model where there is extension via a basal slot.

Angle of repose test

The angle of repose test works by removing either the right wall, or both right and left walls after equilibration, and letting the assembly collapse under its own weight. In addition, the whole of the model can be tilted (to the right) at this stage. This test is a very good way to test the behaviour of, and calibrate, your assembly given the material properties that you have chosen. One of the most challenging aspects of the discrete element technique is the calibration of the micro-element properties so that the bulk behaviour of the assembly is mechanically, geologically, realistic. This repose-collapse simulation provides a quick assessment of the assembly's bulk behaviour in terms of its angle of repose. Upon selection of the Angle of Repose menu item the dialog in Figure 35 is brought up. The checkboxes allow 1) activation of the repose test, 2) selection of both walls, whilst the numeric field allows tilt specification.

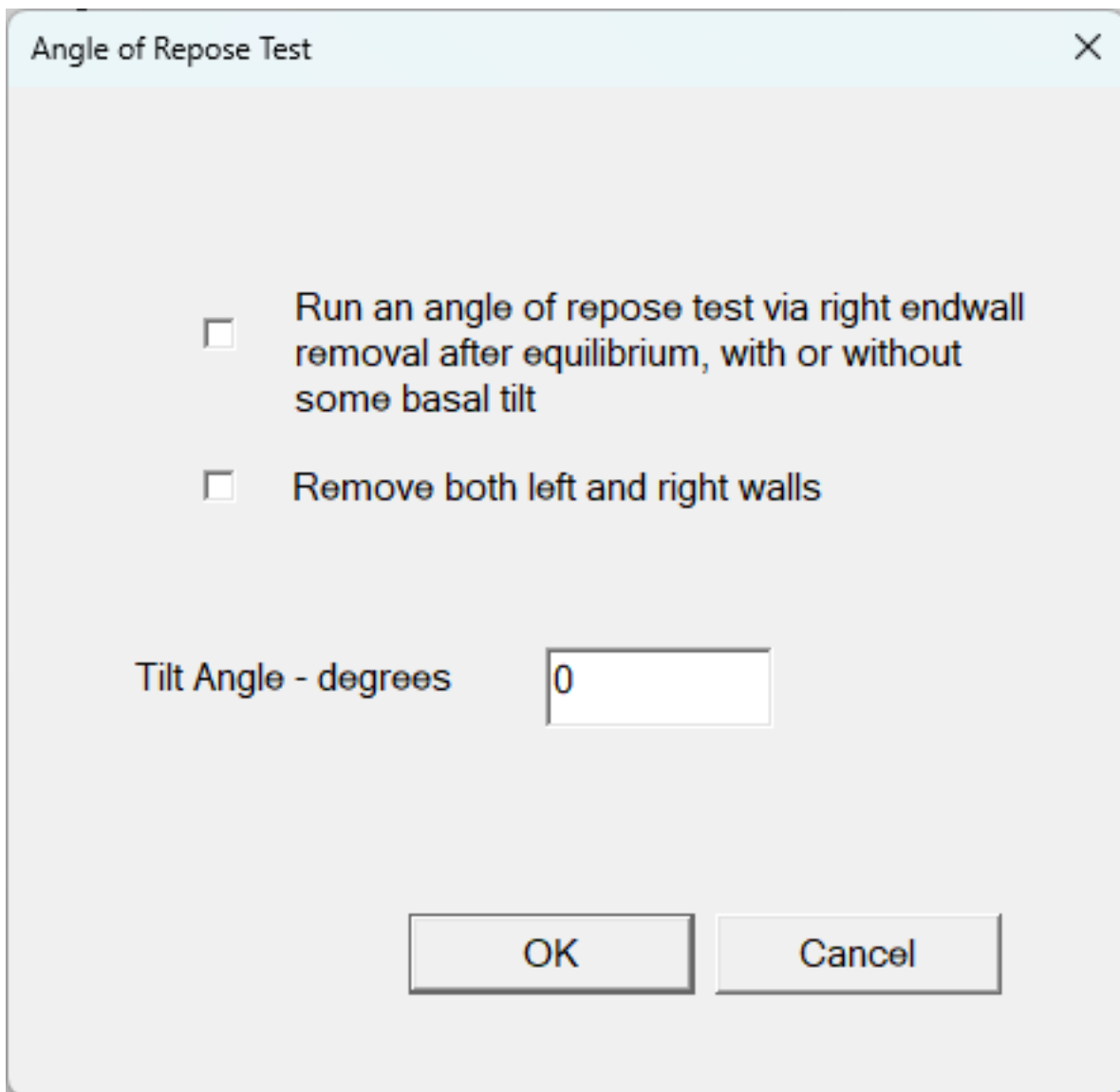


Figure 35. The Angle of Repose test dialog box.

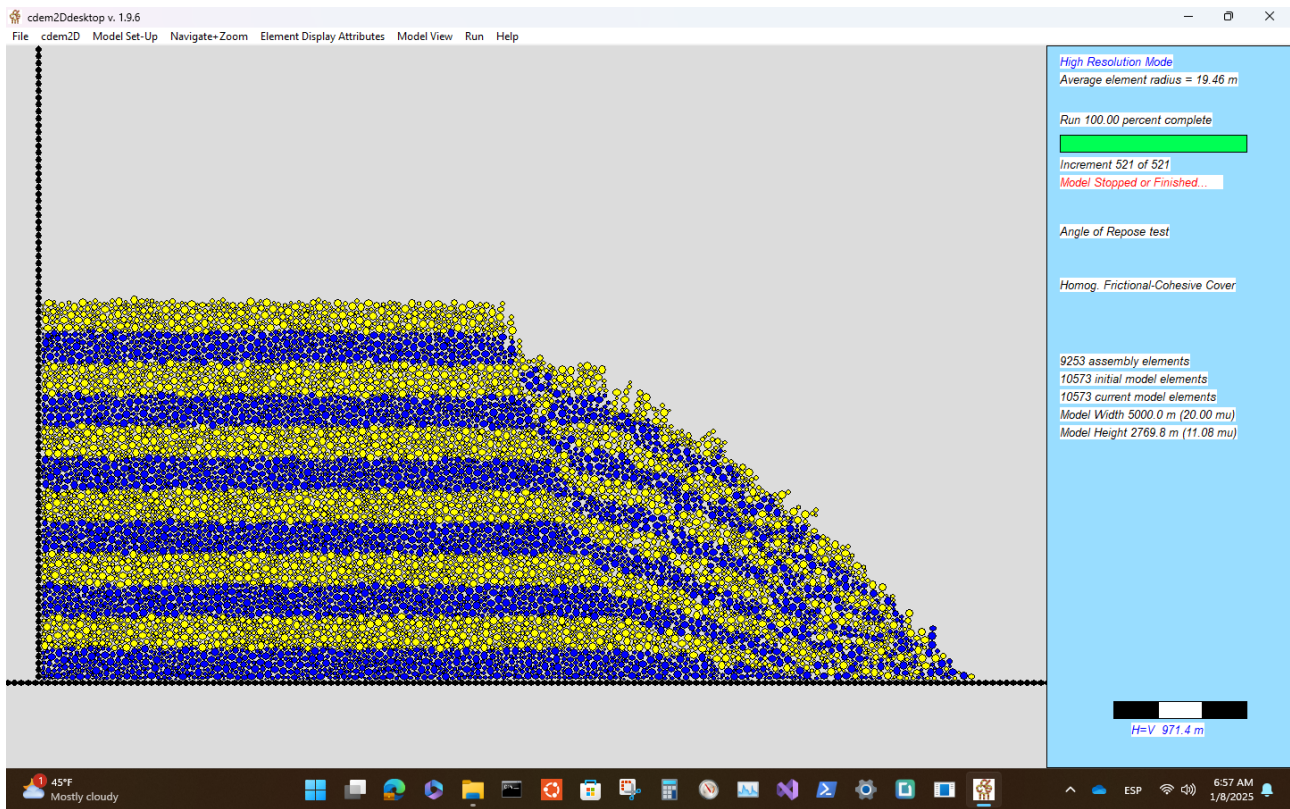


Figure 36. Screenshot of an angle of repose simulation via right-wall removal.

Uniaxial-Biaxial test

One of the most challenging aspects of the discrete element technique is the calibration of the micro-element properties so that the bulk behaviour of the assembly is mechanically realistic. This can be done by performing biaxial tests on the assembly at different confining pressures. From these tests axial strain vs. differential stress can be extracted/derived. These data can then be plotted (using an appropriate graphing program) in a Mohr circle diagram, where each circle would represent the state of stress at failure in each test. From a Mohr circle diagram, it is possible to determine the failure envelope of the assembly. The Uniaxial-Biaxial Test menu item allows simulation of a uniaxial or a biaxial test at a user-specified confining pressure in Pa (Fig. 37). The “edge” elements on which this pressure is applied are marked with a different colour (Fig. 38). The Uniaxial-Biaxial test command brings up the dialog box shown below, where the Uniaxial-Biaxial Test check-box activates this mode, the Tensile Test check-box is experimental, and the Confining pressure to be applied is specified in the editable value field. An example simulation is shown in Figure 38.

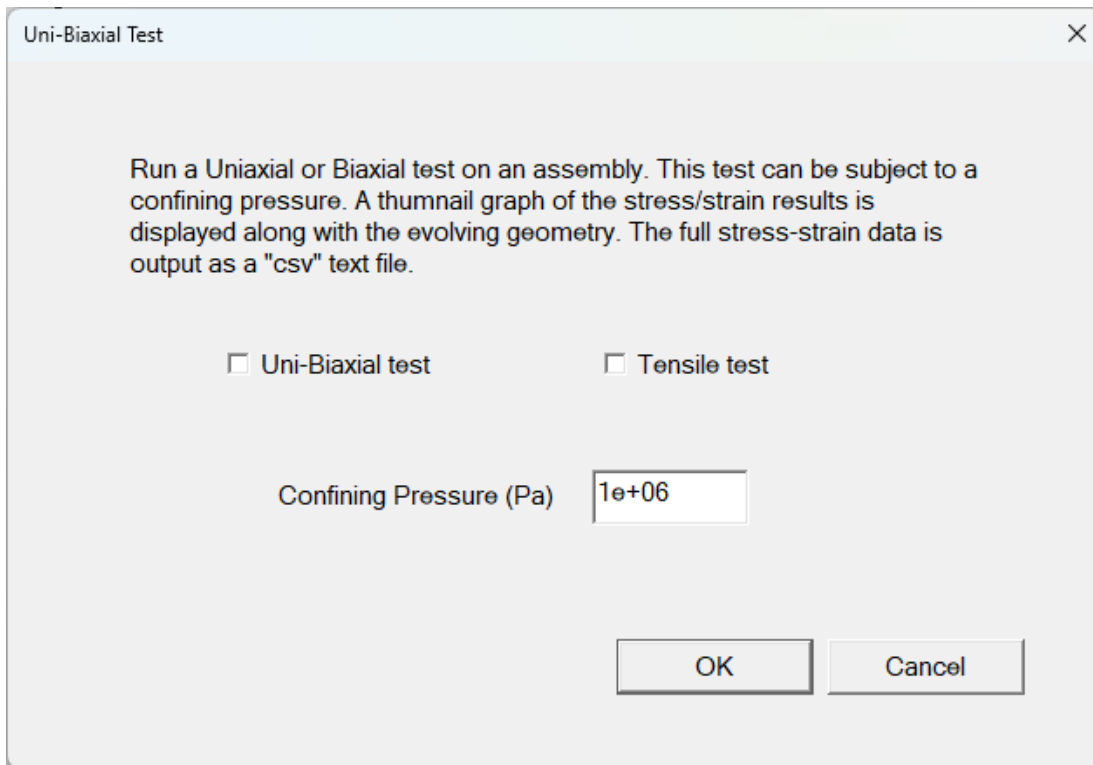


Figure 37. The Uni-Biaxial Test dialog box.

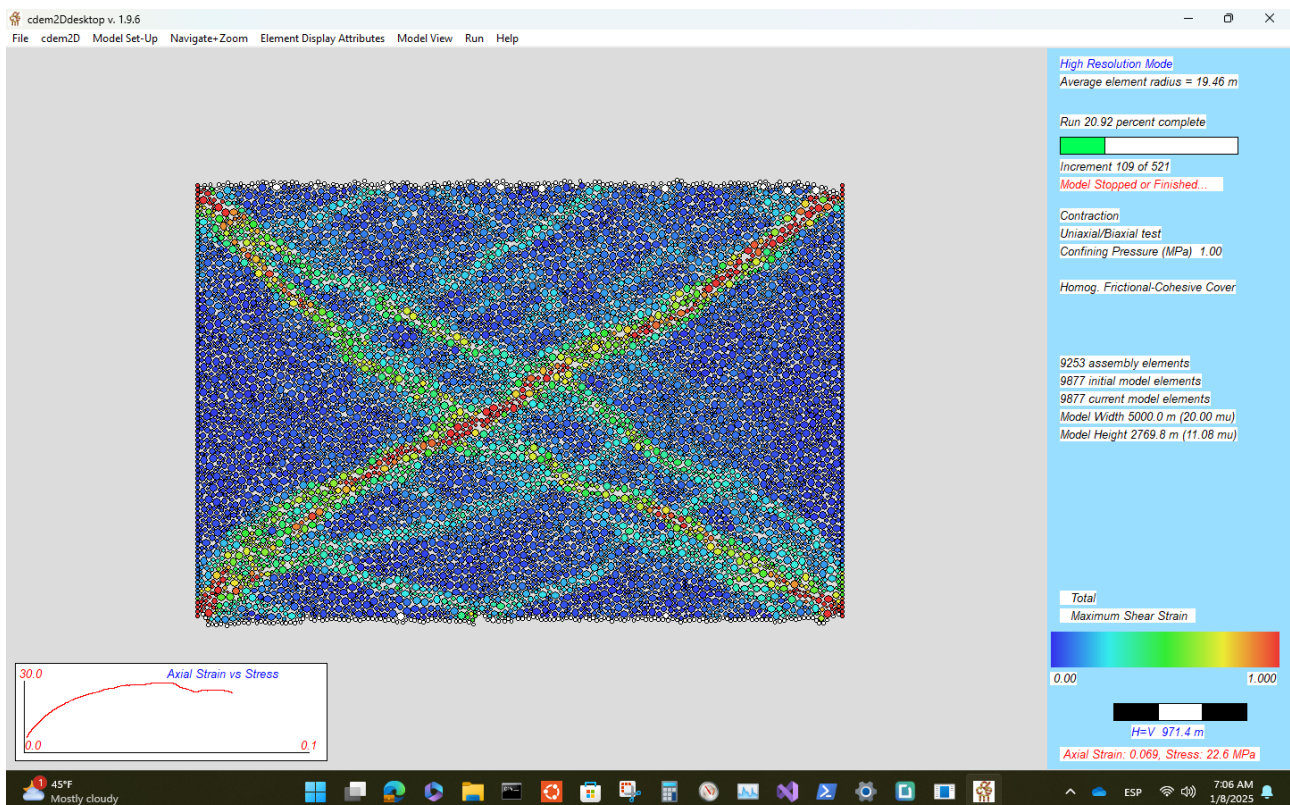
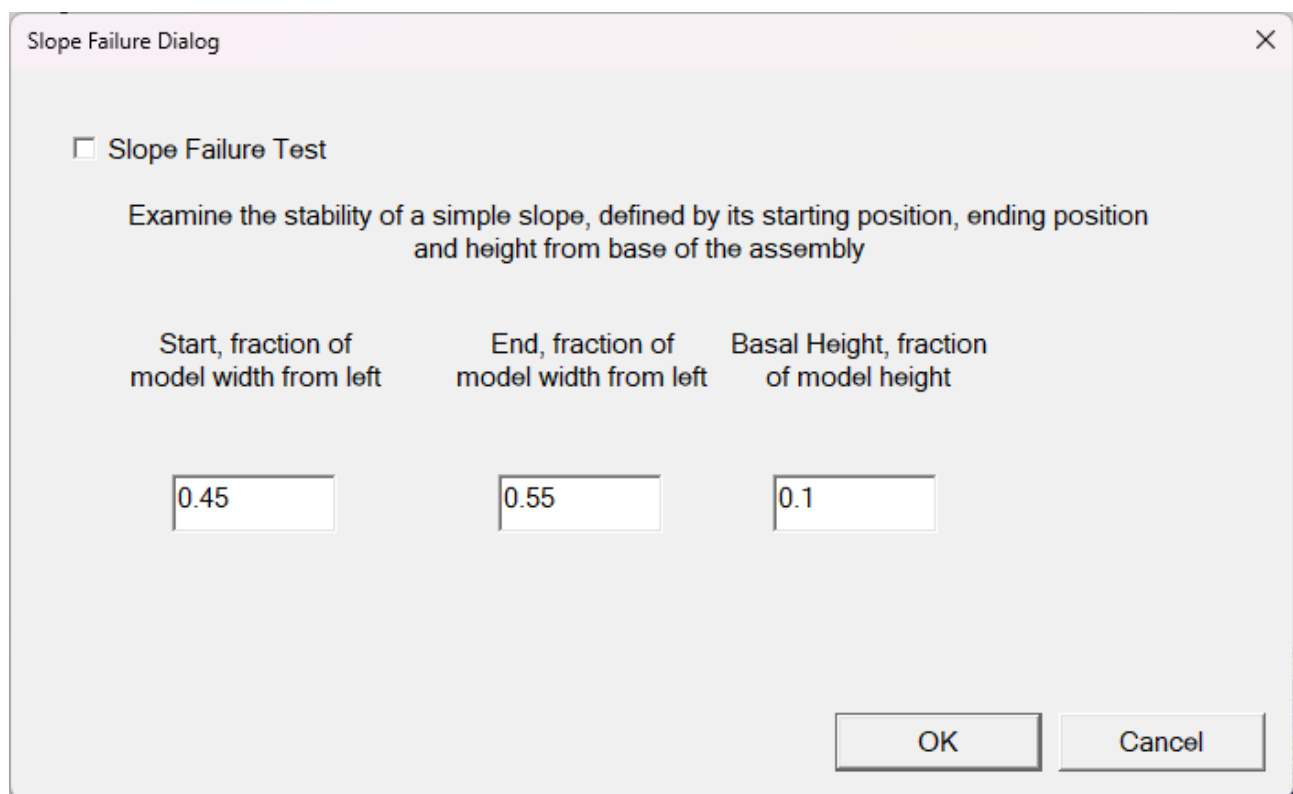


Figure 38. Screenshot of a simulation of biaxial test model.

Slope failure



The image shows a software dialog box titled "Slope Failure Dialog". It contains a checkbox labeled "Slope Failure Test". Below the checkbox is a descriptive text: "Examine the stability of a simple slope, defined by its starting position, ending position and height from base of the assembly". There are three input fields: "Start, fraction of model width from left" with the value 0.45, "End, fraction of model width from left" with the value 0.55, and "Basal Height, fraction of model height" with the value 0.1. At the bottom right are "OK" and "Cancel" buttons.

Start, fraction of model width from left	End, fraction of model width from left	Basal Height, fraction of model height
0.45	0.55	0.1

Figure 39. The Slope Failure test dialog.

A Slope Failure Test is activated by checking the Check-Box in the Dialog Box which appears after selecting the **Slope Failure** menu item (Fig. 39). An initial, quite basic, slope profile is defined here by 3 control parameters: the start of the slope from the left edge of the model, the end of the slope from the left edge of the model, and the height of the lowest part of the slope as a fraction of the model height. This profile is "cut out" and removed from the chosen assembly after equilibration. The removed assembly elements play no further part in the simulation and the model can collapse under its own weight if mechanically appropriate. A typical, ultra-high resolution, slope failure simulation is shown in Figure 40.

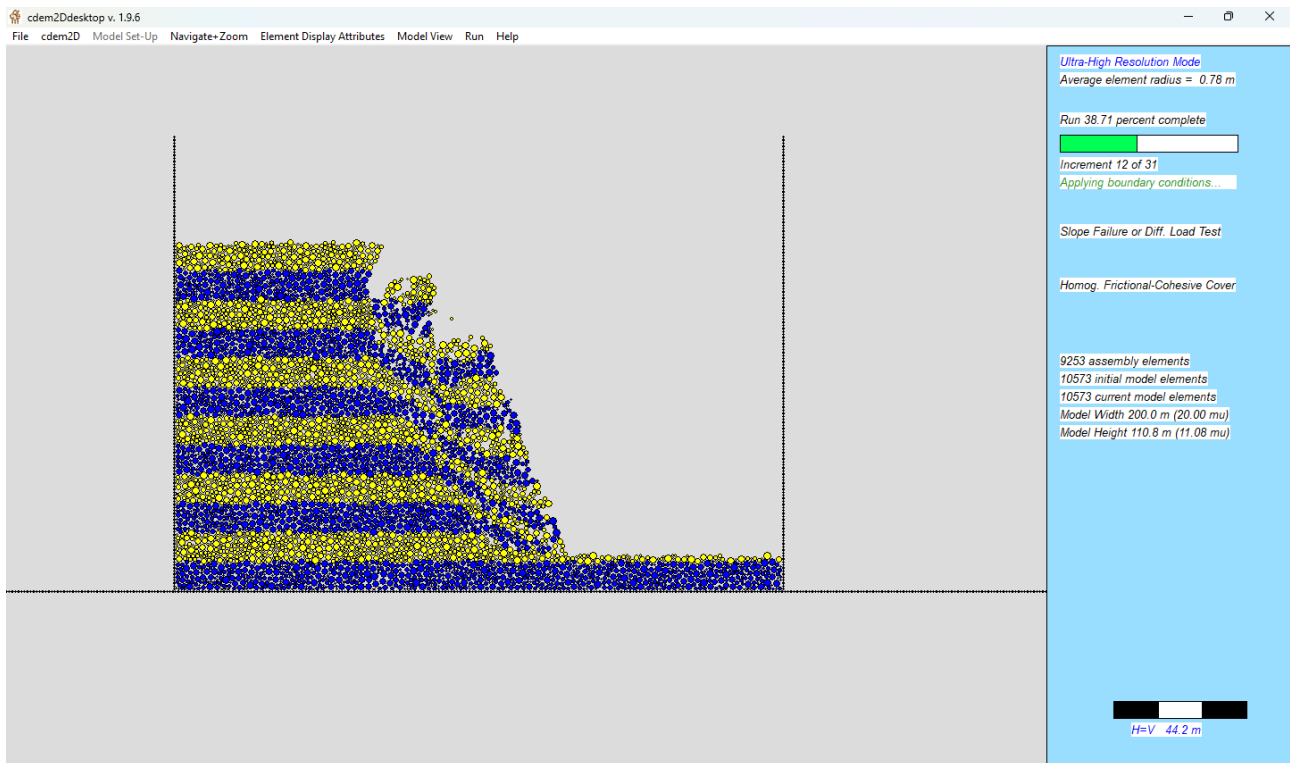


Figure 40. Screenshot of a typical slope failure model, ultra-high resolution.

Cavity, Cavern or Tunnel

A variety of different types of “voids” can be created within (excavated or carved out of) the assembly after model equilibration. Their configuration, and activation, is done via the **Cavity, Cavern or Tunnel** menu item. This brings up the dialog box shown below (Fig. 41). There are currently 4 different styles of voids available, each can have their simplified geometry specified. An additional, experimental, feature is also included: an outwards-directed wall pressure which is applied (at this stage) after twice the equilibration time. The “excavated” elements play no further part in the simulation.

Cavern, Cavity or Tunnel

☐ Create a Cavern, Cavity or Tunnel within the Assembly

Wall Pressure Pa

Geometric Style

☐ Sphere

☐ Ellipse

☐ Tunnel

☒ Rectangle

Dimensions (m)

Radius

X Axis Z Axis

Width Height

OK Cancel

Figure 41. The Cavity, Cavern or Tunnel dialog box.

This mode is activated by checking the check-box at the top-left of the dialog-box. The different types of excavated voids are as follows (chose via radio buttons), all are centred within the assembly:

- Sphere: defined by a radius
- Ellipse: defined by an X and a Z axis
- Tunnel: defined identically to the ellipse but is only the upper half
- Rectangle: defined by a width and a height

For those interested in experimenting with the the Wall Pressure the value can be changed in the edit field, for "normal" use this should be set to 0.0.

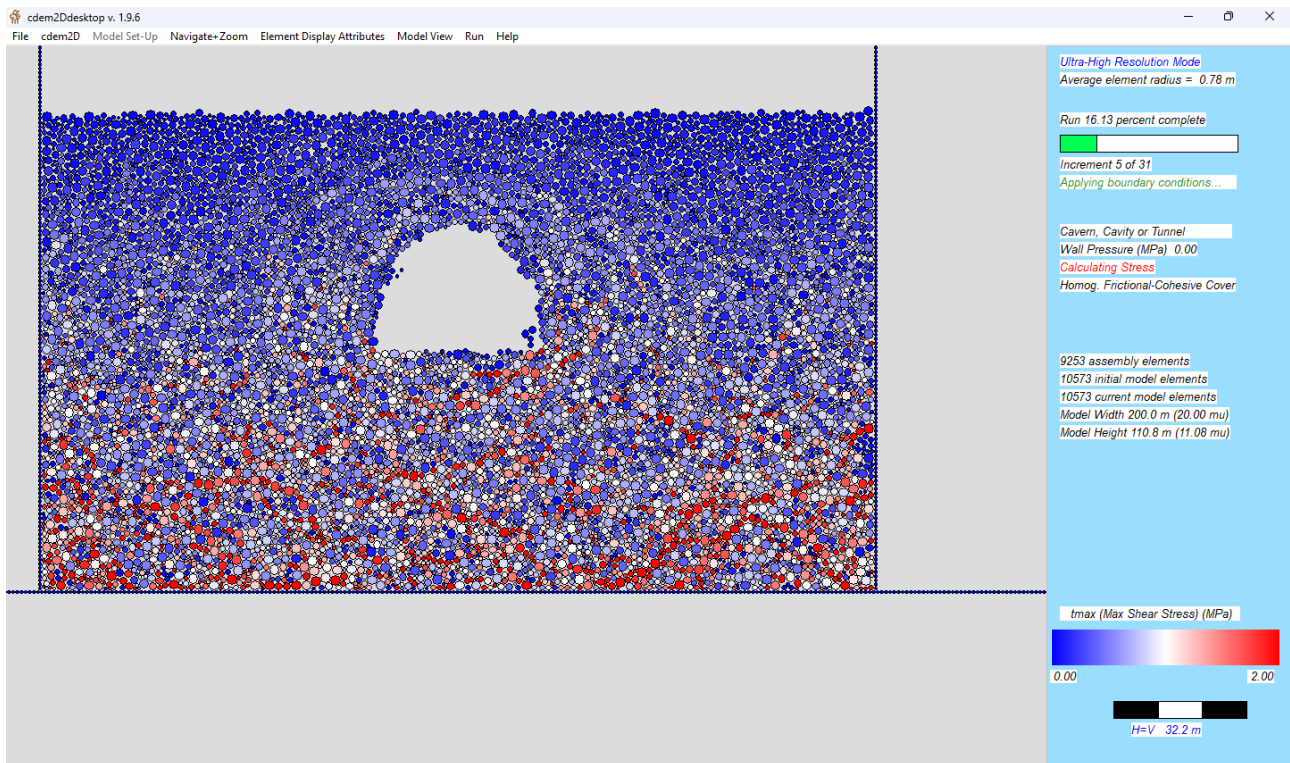


Figure 42. Ultra-high resolution model of a tunnel, coloured by maximum shear stress in MPa.

Additional “features” or functionality can be added to these driving boundary conditions above, but are not actually boundary conditions in themselves:

Sedimentation and Erosion

Sedimentation is activated by toggling on the Sedimentation and Erosion menu item in the Model Set-Up menu (see above) and then checking the Growth Sedimentation check-box. This results in the addition of elements at a given sediment interval, and the equilibration of these elements during a settling time. Notice that when the elements are settling, boundary walls are not displaced. The choice of sediment interval and settling time is not trivial. Sediments are added at intervals equal to the equilibration time and are first deposited at the start of deformation. The upper boundary of the space available for sedimentation (the accommodation space) is defined by a baselevel. Initially, the baselevel is equal to the maximum height of the assembly after equilibration. Baselevel can be static, or rise throughout the simulation. Notice that the growth elements have the same strength as the pre-growth elements.

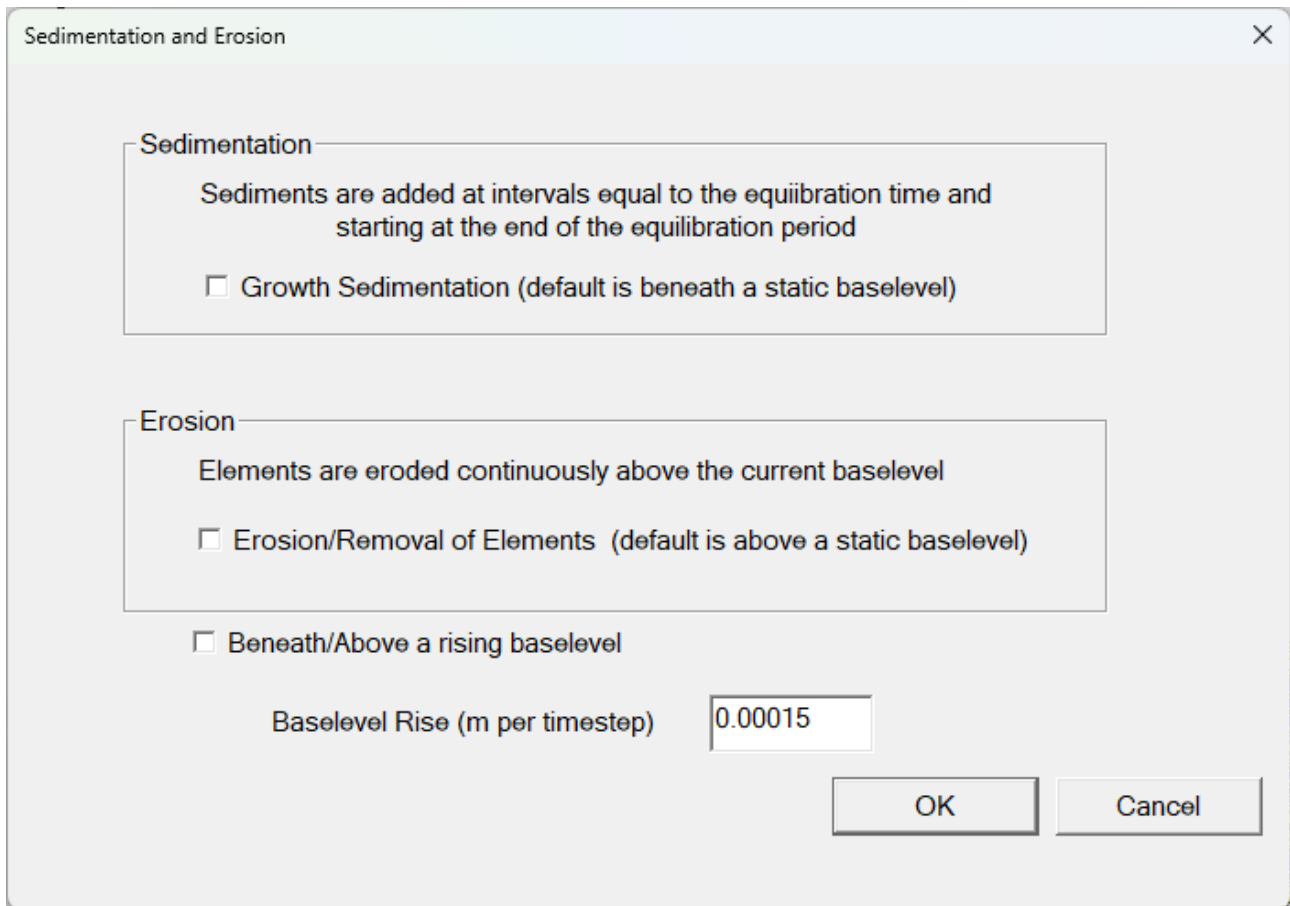


Figure 43. Sedimentation and Erosion dialog box.

Erosion of elements works in a similar fashion to sedimentation in that elements are eroded continuously above the current baselevel.

The sedimentation and erosion options are not available for the repose-collapse or uniaxial-biaxial tests.

Calculate Stress

Selecting this menu item activates the calculation of stress during a model run. It also activates the display of stress components as model "attributes". Calculating stress has a slight, but not excessive, computational "hit" such that runs may take a little longer.

Calculate Cumulative Max. Shear Strain

Selecting this menu item activates the calculation of cumulative maximum shear strain during a model run. It also permits its display as another strain component "attribute". Calculating cumulative max. shear strain has a slight, but not excessive, computational "hit", i.e. model runs take a little longer as a result.

Joint/Fracture Sets

	Dip (0-90, degrees)	Spacing (m)	Coeff. of Friction	<input type="checkbox"/> Dips to Right
Set 1	60	300	0	<input type="checkbox"/>
Set 2	30	300	0	<input type="checkbox"/>

Figure 44. Joint or Fracture Sets dialog box.

Two sets of joints or fractures can be introduced into the model assembly, however they only become a mechanical part of the assembly after equilibration has completed. Each set of joints/fractures can have its own dip, sense of dip, spacing and coefficient of friction (see Fig. 44 above). This is a relatively recent feature which is actively being improved.

Design and Save a User-Defined fault

Defining, or designing, faults via a set of (x,y) points is always a little tricky. However... here is an explanation of how I have *provisionally* tackled this issue in cdem2Ddesktop.

Essentially, in cdem2Ddesktop, there are 2 ways to define a set of fault vertices: either *externally*, via a text file (as discussed in the previous section above), or *internally* via a dialog box. In this section, I will focus on the "Internal" method but nearly everything that is described here also applies to the "External" method.

When you use the Displacement on Planar, Listric and Irregular Faults dialog you can choose to use a User-Defined Irregular Fault, this implies that you are choosing from one of the five preset faults. For our purposes here let us assume you are using the "User-Defined Internal" fault. It conceptually links to the **Design and Save a User-Defined Fault** menu item (see below).

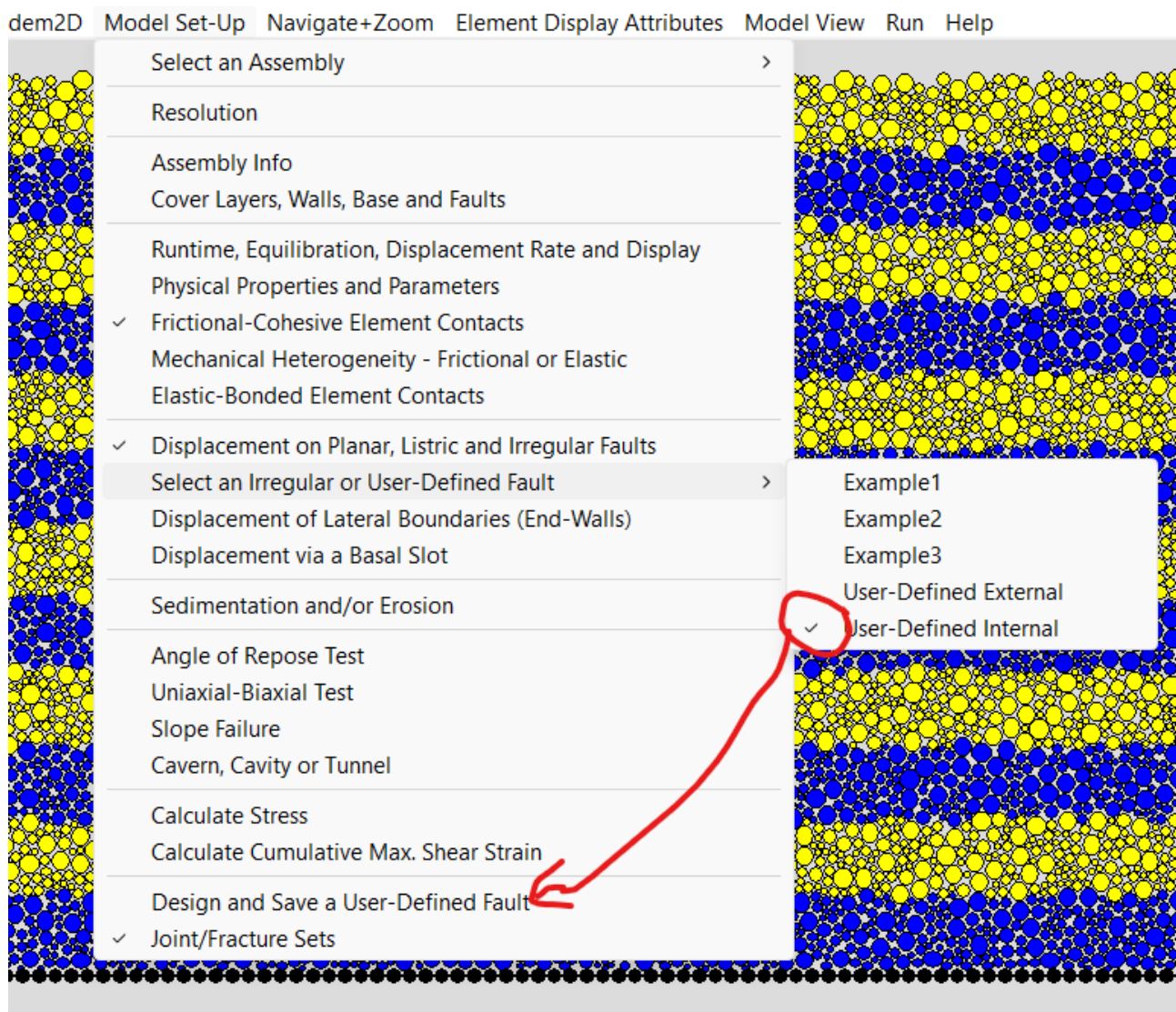


Figure 45. Screenshot of how the User-Defined Internal fault selection links to the Design and Save... menu item.

If we select the **Design and Save a User-Defined Fault** menu item it will bring up the User Fault Definition dialog box. There are several key points to notice about this dialog box.

The fault is defined by this sequence of x,y control points which change toward the anchor point, both x and y must decrease consistently in this direction

Point	x (m)	y (m)
(1)	0.00	2950.00
(2)	350.00	1950.00
(3)	400.00	1900.00
(4)	600.00	1850.00
(5)	900.00	1750.00
(6)	1000.00	1700.00
(7)	2000.00	1000.00
(8)	2650.00	200.00
Basement Anchor Point	2950.00	0.00

OK Cancel

Figure 46. Internal User-Defined Fault Definition dialog box.

- It contains 9 sets of (x,y) vertices which define the piecemeal fault.
- The x coordinates of these vertices increase consistently, but not uniformly, to the value of 2950 m, this is the "basement Anchor Point" where the fault meets the lower bound of the model (with 0.0 m height).
- The y coordinates of these vertices decrease consistently towards 0.0, in this instance from 2950 to 0.0 m
- The basement anchor point is the point at which the cover fault meets or links with the fault in the basement.

The end result is a fault which looks rather arbitrary (Fig. 47), but is consistent with the model dimensions and basement fault position (Fig. 48) - it is saved as the default internal fault definition.

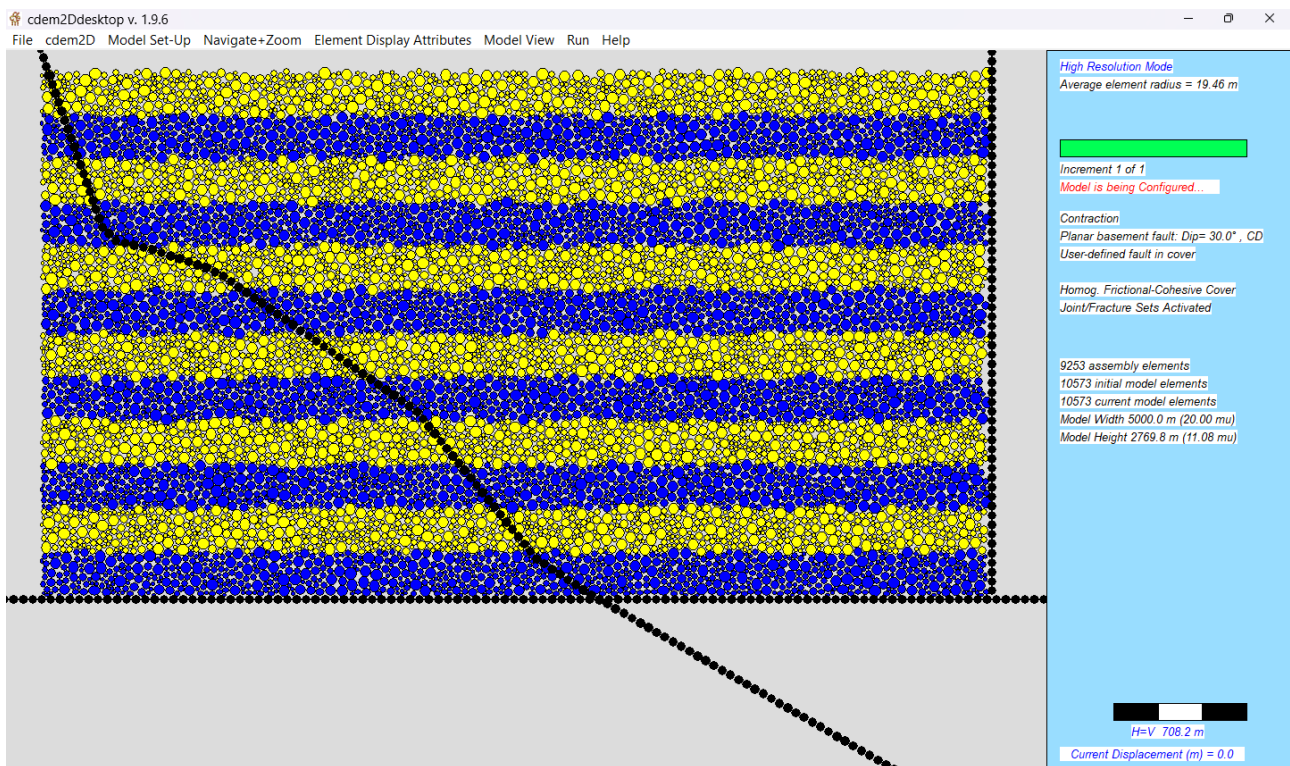


Figure 47. The User-Defined Fault produced by the dialog box in Fig. 46.

Figure 48. The Faulting Parameters dialog box, annotated to show the manner in which the user-defined fault is specified.

Model Templates

As can be seen below selecting the menu item "**File->Load Model Template**" brings up a list of **8** pre-defined model "templates" which cover a wide range of possible simulation scenarios, and illustrate to breadth of use of the code. The templates themselves have self-explanatory names. They are actually a great way to find your way around the different capabilities of the application. The **last** template "**Users_Template**" is a bespoke template that you can create to save, e.g. a frequently used starting scenario. This template is created via the menu command "**File->Save Parameter Set as Users_Template**", to save a working set of typical parameters that you use (Fig. 49).

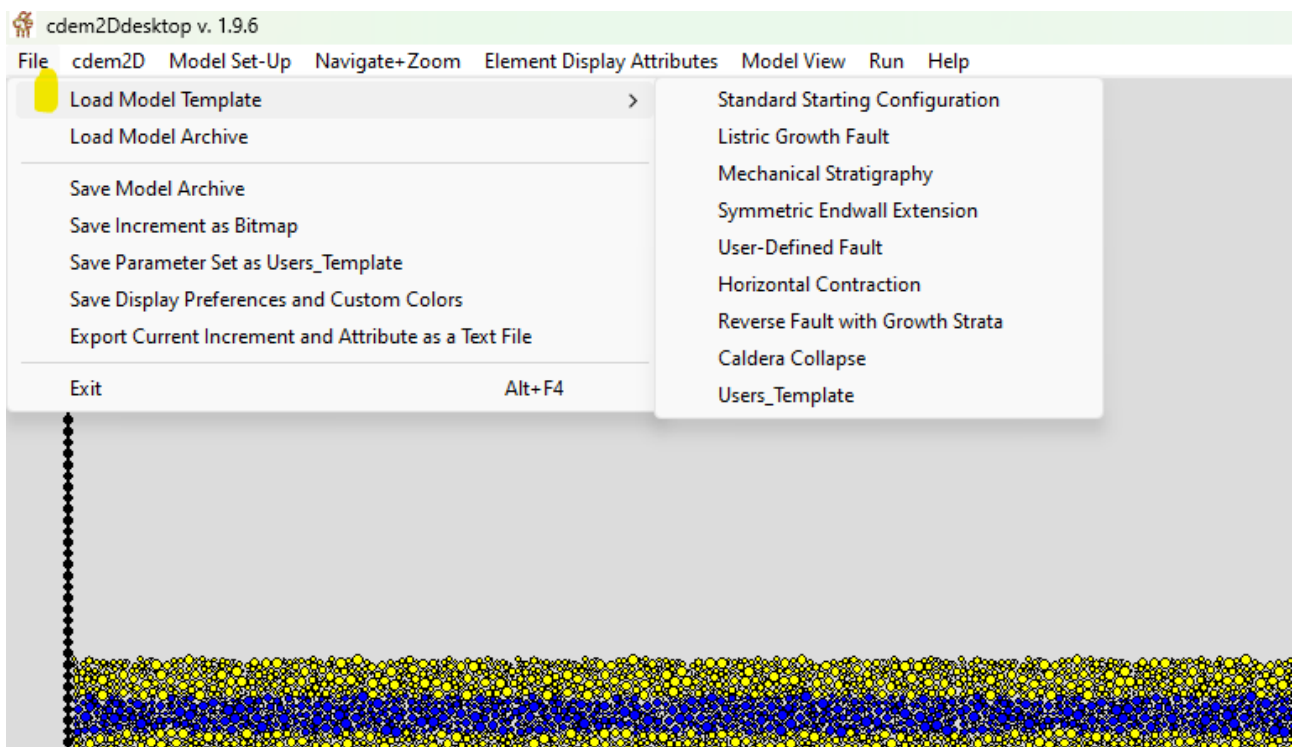


Figure 49. The Load Model Template menu item.

Saving Model Data: Increments, Batch files or an Entire Experiment

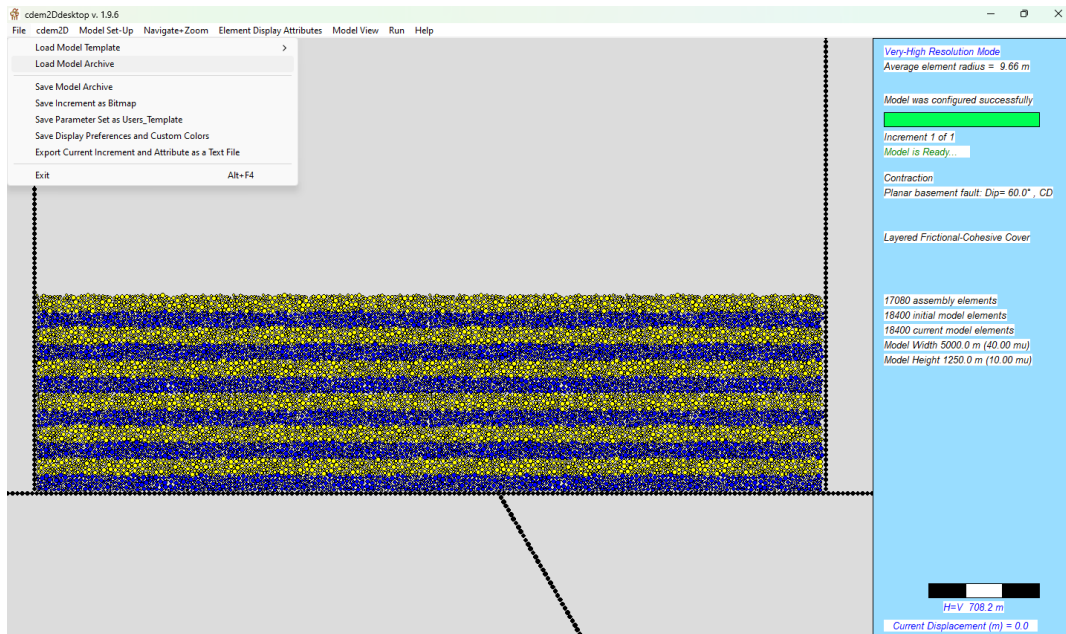


Figure 50. The various Save/Export menu items.

Under the **File** menu, there are menu items/commands to save the current increment in the plot view as a bmp file (**Save Increment as Bitmap**), to **Export Current Increment and Attribute as a Text File**, and one can also save the entire Experiment as an “archive” (**Save Model Archive**) which can also be subsequently loaded via this Menu (**Load Model Archive**).

Two additional “Saving” menu items are also available: the ability to **Save Display Preferences and Custom Colors**, and the ability to Save your current model as the “**Users_Template**” whereby it will appear as one of the “Templates” that can be loaded.

Miscellaneous Commands/Topics

Setting the number of OpenMP threads

As stated previously, cdem2Ddesktop makes use of all available cores/threads on your computer when performing numerical calculations. This is a *great* use of resources and enables rapid calculation of simulations results. It can, *however*, swamp your system, making it difficult to perform other, more routine, tasks on the machine. Therefore, there is a means by which to reduce the “hit” cdem2Ddesktop has on your system. This is achieved by selecting the following command from the Menu Bar: “**Run->Set Number of OpenMP threads**” which will bring up the dialog below (Fig. 51). In this manner you can limit the threads to, say, 50% of available threads. This command does require you to have prior knowledge of how many threads/cores your machine can utilise.

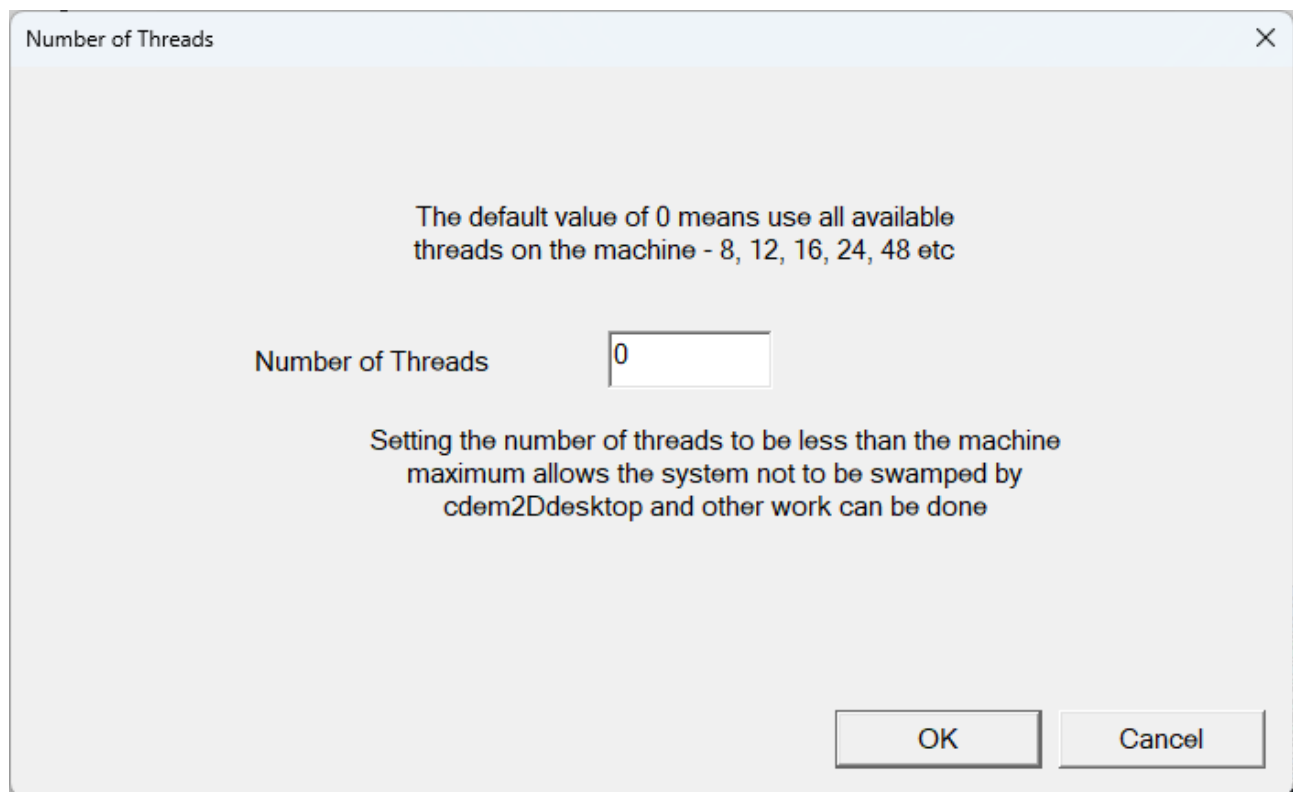


Figure 51. The OpenMP Number of Threads dialog box.

Assembly Info

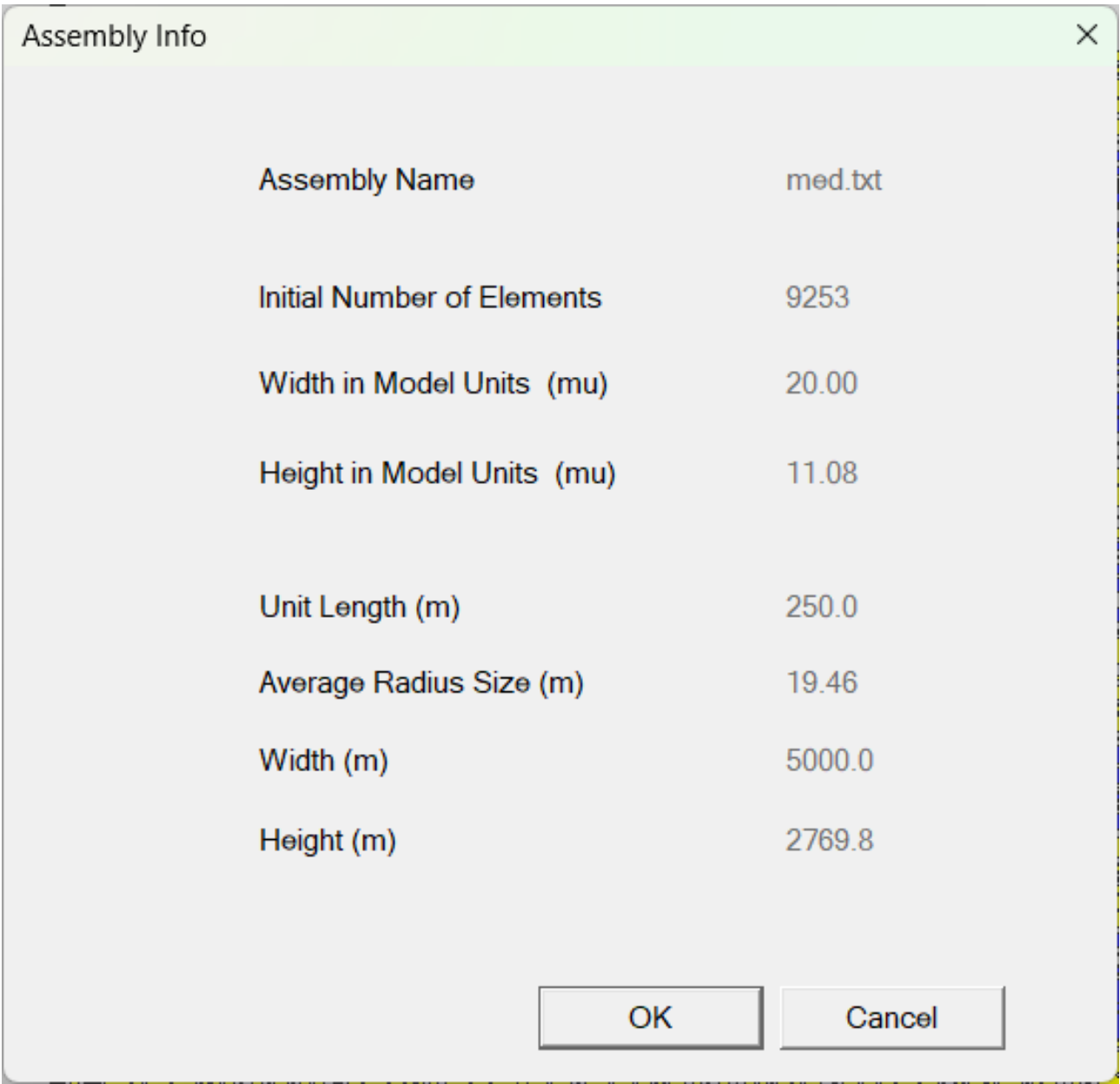


Figure 52. The Assembly Info dialog box.

The Assembly Info menu command brings up the simple dialog above (Fig. 52) which gives an overview of the assembly currently selected/in use. No parameters can be altered or changed.

Theory

The discrete element technique, in common with other numerical techniques, has both advantages and disadvantages when considering its application to any geological problem. Modeling of deformation to high strain is an ideal candidate for its use as it is well-suited to studying problems in which discontinuities (shear-zones, faults, fractures, etc.) are important. It also allows deformation involving unlimited relative motions of individual elements and complex, abrupt and changing boundary conditions (Cundall & Strack, 1979; Finch et al., 2004; Egholm et al., 2007; Hardy, 2008, 2011; Thompson et al., 2010). However, one disadvantage of the technique lies in the necessary, but time-consuming, calibration of micro-element parameters to physical properties (cf. Egholm et al., 2007; Botter et al., 2014). The interactions of many tens of thousands of elements, both locally and globally, also leads to situations wherein our ability to explain precisely why a particular fault or fracture grew at the expense of a neighbouring one is limited. Computational limitations on element size and/or model resolution, whilst important previously, are now no longer a particular concern due to recent rapid advances in computational power and the parallelisation of many discrete element codes.

The discrete-element model described here is a variant/development of the lattice solid model (LSM) (Mora and Place, 1993, 1994; Place et al., 2002). A rock, or sedimentary, mass is treated as an assembly of circular elements, which interact as if connected by breakable elastic springs (bonds) and that undergo motion relative to one another. The behaviour of the elements assumes that they interact through a 'repulsive-attractive' force (Mora and Place, 1993) in which the resultant (normal) force, F_n , is given by:

$$F_n = K_n(r-R) \quad (r-R) < (r_0 \cdot R) \quad \text{for an intact bond}$$

$$F_n = K_n(r-R) \quad r < R \quad \text{for a compressional broken bond}$$

$$F_n = 0 \quad r \geq R \quad \text{for a tensional broken bond}$$

Here, K_n is the elastic constant (normal spring stiffness) of the bond, r is the current distance between the element pair, R is the equilibrium distance between the elements (sum of elements radii), and r_0 is the breaking strain. Elements within the assembly are bonded until the separation ($r - R$) between them exceeds the breaking strain times the equilibrium distance ($r_0 \cdot R$), at which time the bond breaks. The force acting on a bond at this stage represents the force necessary for a bond to fail or yield, or, alternatively, can be cast as the stress acting on an element's bond at failure. After this breaking threshold, the element pair experiences no further attractive force and the bond is irreversibly broken. However, if the two elements return to a compressive contact ($r < R$), a repulsive force still acts between them.

For a frictional-cohesive material, all elastic bonds are initially broken and, in addition to treating the normal force (F_n) between elements, we also calculate the tangential (shear) force, F_s , as a result of displacement (X_s) perpendicular to the vector connecting the elements centroids. This frictional force acts in a direction opposite to that of the relative tangential velocity and is modelled as a threshold-limited elastic spring (cf. Cundall and Strack, 1979; Mora and Place, 1994). The magnitude of this force is limited to be less than or equal to the shear force allowed by Coulomb friction:

$$F_s = K_s X_s$$

$$F_{smax} = \mu F_n + C_0$$

$$F_s = F_{smax} \text{ if } (F_s > F_{smax})$$

where K_s is the elastic constant (shear spring stiffness) of the contact, F_{smax} is the maximum (limiting) shear (frictional) force, F_n is the normal force at a contact, μ is the inter-element coefficient of friction and C_0 is the cohesion force. If a contact is “lost” between two touching elements (i.e., they separate), then all the forces between the elements are set to zero. The total elastic force, $F_{i,\alpha}$ exerted on an element is thus obtained by summing the normal and tangential forces on each contact/bond that links a specific element to its neighbours, calculated by:

$$F_{i,\alpha} = \sum_j f_{i,j} \quad j=1,\alpha$$

where $f_{i,j}$ is the elastic force (normal and shear) experienced by element i from its neighbouring element j . However, we also include a viscous damping term (proportional to element velocity) that acts to dampen reflected waves from the rigid edges/boundaries of our model, preventing a build-up of kinetic energy within the closed system, a standard technique to ensure numerical stability (cf. Mora and Place, 1994; Place et al., 2002).

Finally, gravitational forces, F_g , acting on each element are calculated in the vertical direction, increasing the vertical stress with depth. Therefore, the total force (F) on any element is given by:

$$F = F_{i,\alpha} - \eta \dot{X} + F_g$$

where η represents the dynamic viscosity and \dot{X} is the velocity of the element.

At each discrete time step, the elements are advanced to their new positions within the model by integrating their equations of motion using Newtonian physics and a velocity-Verlet-based scheme (Allen and Tildesley, 1987).

The time-step (dt) used in a simulation is calculated as:

$$dt = 0.40 * \sqrt{\text{minimum_mass}/\text{spring_constant}}$$

So therefore the time-step depends on both the density and the spring constant, 0.4 is just a “safety factor” used to ensure numerical stability. At the moment these values are automatically calculated for the High, Very-High and Ultra-High resolution simulations across all assemblies.

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