

A macOS application for discrete element modeling of geological structures and their associated deformation

Academic version (v. 4.9)

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Disclaimer

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This is a free of charge **Academic version** of cdem, which can only be used for non-profit purposes. The program can be obtained by contacting Nestor Cardozo at nestor.cardozo@uis.no. Please don't distribute it to others. We'd like to keep track of the users of cdem.

Referencing this program

The following paper describes in detail cdem and its application:

Cardozo, N. and Hardy, S. 2023. cdem: A macOS program for discrete element modeling of tectonic structures. *Geosphere*, <https://doi.org/10.1130/GES02647.1>.

Use the link above to access the paper. Please refer to this publication in any study or presentation that result from the use of the program.

Credits

cdem is based on the discrete element code **cdem2D** by Stuart Hardy. The core of **cdem** is a stripped-down version of **cdem2D**. **cdem** was written entirely in the Swift programming language. We translated the original **cdem2D** code from C to Swift, designed the interface following a Model-View-Controller pattern, and implemented parallelization, i.e., use of all available CPU's cores/threads, using Grand Central Dispatch (GCD). To compute percentiles, **cdem** uses the Swift statistics library by Alan James Salmoni (2016).

Introduction

cdem is a macOS 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 we use here to simulate a cross section of the upper crust. This cross section is represented by an assembly of elements that respond to applied forces and displacement boundary conditions. The DEM allows large deformations and complex, abrupt boundary conditions. In addition, the formation and linkage of faults and fractures is a natural part of the simulation.

In **cdem**, an assembly of circular elements of different radii represent a cross section of the upper crust. Different assemblies, model scaling, acting forces, element properties, and boundary conditions can be chosen. After initializing and starting the simulation, the progress of the simulation can be observed in real time. When the run is complete, any increment, displacement, strain, and stress can be visualized, or saved as an image. All increments can also be saved *together* as an animated gif or an album of images from which one can make a movie. Increments can also be exported as text files that can be imported in the program **SSPX** (Cardozo and Allmendinger, 2008) for computing strain.

cdem is a document-based application. Several documents corresponding to different simulations can be run and compared at the same time. This is a great way to explore the impact of different assemblies, model parameters, and boundary conditions. The DEM is a computationally intensive numerical technique. We have implemented **cdem** to make use of all available CPU's cores/threads, so the more powerful and the more cores the machine you are using has, the better. This documentation is a quick guide for the use of **cdem**. Although at the end we include a **Theory** section, this document is not a detailed description of the theory behind **cdem** or the DEM method.

Setting up a model

A **cdem** document consists of three views: The *Set-up* view, the *Summary* view, and the *Results* view. The *Set-up* view (Figure 1) is where the user can choose the model parameters and boundary conditions from the available options. These options are:

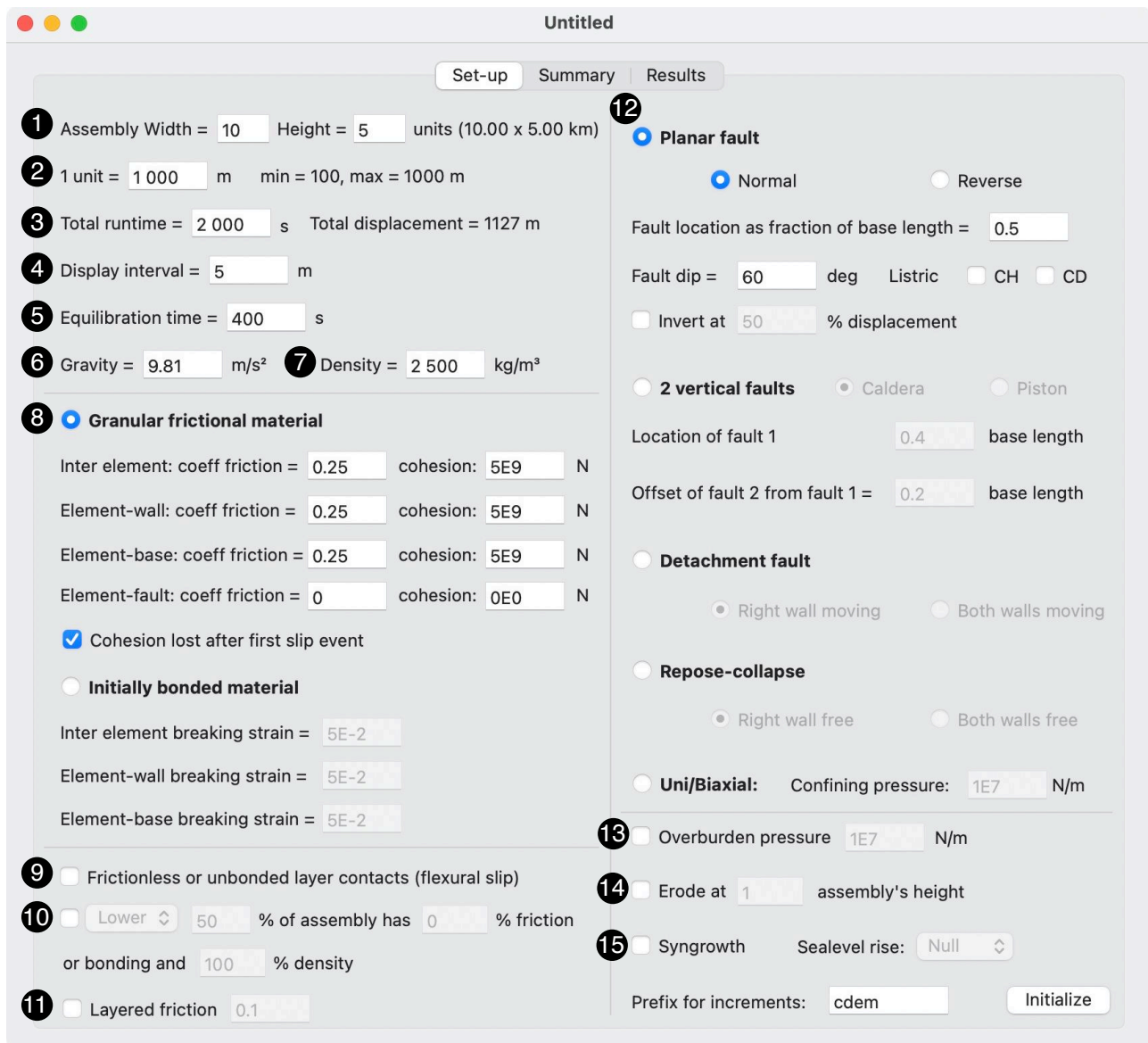


Figure 1. The Set-up view at start, showing default parameter values

1. The assembly. Here the user can set the width and height of the assembly in units. The width of the assembly can be between **10 and 100 units**, and the height between **2.5 and 7.5 units**. We restrict the thickness of the assembly to a maximum of 7.5 units because thicker assemblies may result in too much overlap of the bottom elements and unstable simulations. The assembly is made of elements of four different radii: 0.05, 0.075, 0.1, and 0.125 units¹. All the simulations in this document are made with an assembly of 10 by 5 units.

¹ It is possible to choose a denser assembly with elements of half these radii via [the Preferences panel](#).

2. The length scale of a model unit, which has a range between **100 and 1000 m**. By default the length scale is set to 1000 m, so that results in an assembly of 10 x 5 units being 10 by 5 km.
3. The total model runtime in seconds. The minimum value is **100 s** and the default value is 2000 s. Please notice that this is the simulation time, it has nothing to do with geologic time. The element behavior in **cdem** is time independent. For all but the repose-collapse simulation, the estimated total boundary displacement² is reported next to the model time.
4. The display interval, which has a range between **1 and 1000 m**. The default value is 5 m. For the repose-collapse simulation, this value is internally converted to seconds.
5. The equilibration time in seconds. This is the time for equilibration of the assembly before any boundary displacement begins. This value should be lower than the total runtime. The minimum value is **100 s** and the default value is 400 s, although for biaxial tests we recommend a minimum value of 800 s. The equilibrium phase is necessary because “a priori” the assembly does not know what its properties will be. Thus, after choosing the preferred set-up and starting the run, the model needs to “feel” the new conditions and equilibrate to a static state that is appropriate to the run. Please notice that the initial layering of the assembly is updated in the first increment after the equilibration.
6. Gravity, which has a range between **0.5 and 25 m/s²**. By default this value is set to the gravity of the Earth, 9.81 m/s².
7. The density of the elements, which has a range between **1500 and 3500 kg/m³**. The default value is 2500 kg/m³.
8. The elements’ properties. Here the user can choose between two types of models: A granular friction material defined by an inter-element coefficient of friction and cohesion force in Newtons, or an initially elastic bonded material defined by an inter-element breaking strain. The granular frictional material gives the characteristic Mohr-Coulomb behavior of rocks in the frictional regime. Setting the inter-element cohesion to zero results in a purely frictional material. The initially bonded material uses elements that are bonded by elastic springs that break when the separation between the elements exceeds the defined breaking strain times the sum of the elements radii. Notice that these parameters can be defined between the internal elements, and also

² This is a first-order estimation. The total displacement may vary depending on if there are growth strata (numeral 15), or if the assembly is not homogeneous in density (numeral 10).

between the internal elements, the walls and any fault. For the granular frictional material, there is one button that when checked, it indicates 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. In general we find that “first slip” (the checkbox on) works well in contraction, whilst “first separation” (the checkbox off) works better in extension. By default, this checkbox is on.

9. A check button to set the layer contacts frictionless and cohesionless (if granular material) or unbonded (if bonded material). This simulates slip between the layers, i.e., flexural slip. This option is not available for the uni/biaxial test.
10. A check button to make the friction and cohesion (if granular material) or breaking strain (if bonded material) of a lower or upper percentage (0-100%) of the assembly, a percentage (0-100%) of the user-specified values in the material model (numeral 8). Entering 0% results in a frictionless and cohesionless (if granular material) or unbonded (if bonded material) interval. In addition, it is possible to set the density of this interval to be 50 to 100% the user-specified density (numeral 7). This creates a lighter interval. The “weaker” and/or “lighter” interval is highlighted as semi-transparent. This option is not available for the uni/biaxial test.
11. The number of pre-growth layers is 24. Toggling on this check button makes the friction of layers 5-8, 13-16 and 21-24 equal to the value entered in the text field. This is useful to simulate a sequence of competent (e.g., friction = 0.25) and incompetent (e.g., friction = 0.1) layers of equal thickness. This option is not available for bonded material, or for the uni/biaxial test.
12. The boundary/faulting conditions. Five types can be chosen: Planar fault, 2 vertical faults, detachment fault, repose-collapse test, and uni/biaxial test (Figure 2). If choosing a planar fault, the user can select normal or reverse displacement, fault location as a fraction (**0 to 1**) of the base length, and fault dip in degrees (Figure 2a-b). In addition, fault inversion can be toggled on 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.

For the planar fault case, there are two buttons next to the *Fault dip* field to move along a listric (the default) or irregular fault. If the fault is listric, it increases in dip from its input value to a maximum of 90°. An irregular fault can be chosen by selecting the *Model -> Irregular fault* menu. In this case, you will be asked to choose a text file with

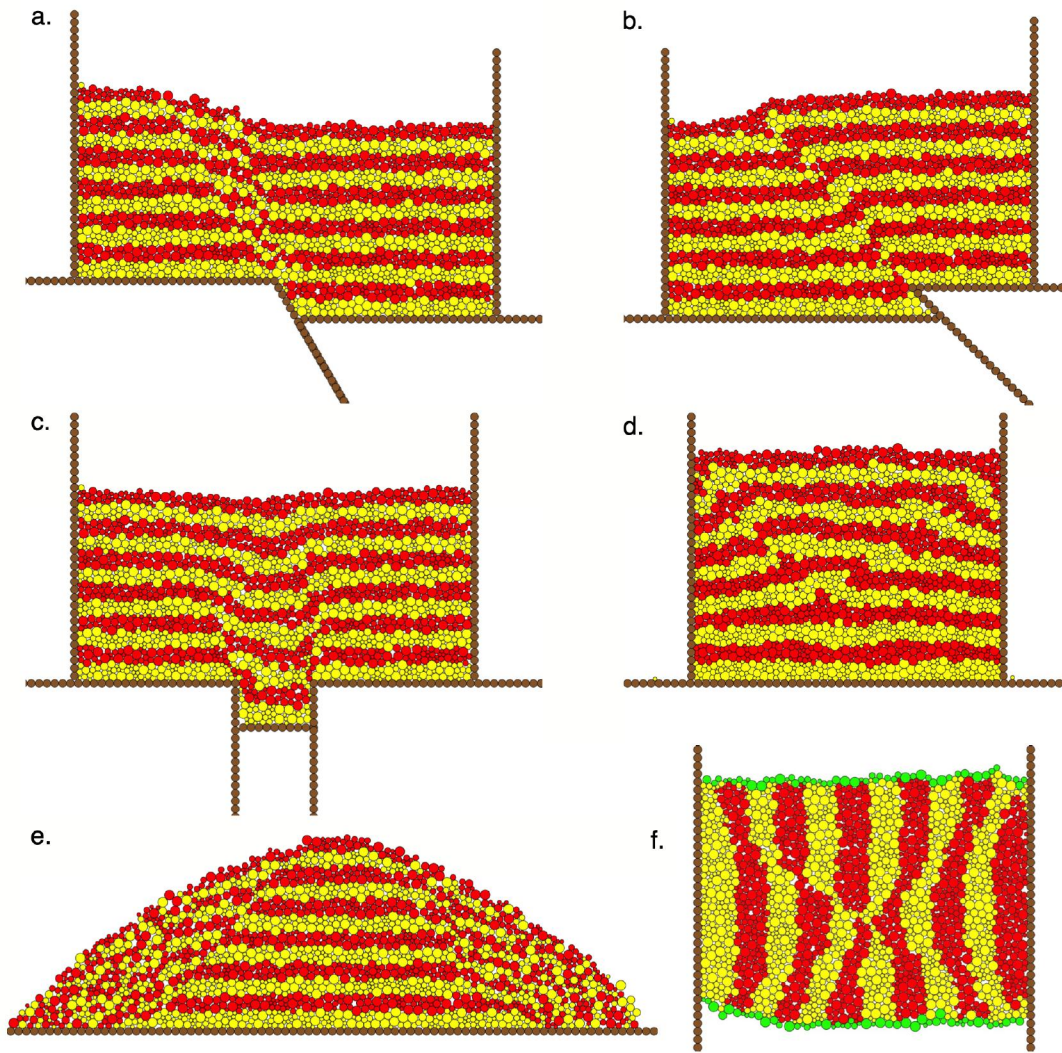


Figure 2. The five main fault types in **cdem**. **a** and **b**. Planar normal and reverse faults, **c**. 2 vertical faults in caldera mode, **d**. Detachment fault, both walls moving, **e**. Repose-collapse, both walls removed, **f**. Biaxial simulation with 20 MPa confining pressure.

the x and y coordinates of the fault. These coordinates should be defined from the base of the fault and up-dip. The first coordinate should be at $x = \text{the fault location}$, and $y = 0$ (e.g., $x = 5000$ and $y = 0$ for the setup of Figure 1). Also since the fault dips to the right, subsequent points should have lower x and higher y. If these conditions are not satisfied in the txt file, **cdem** will throw an error. To make the fault listric again, select the *Model -> Listric fault* menu.

For both, the listric or irregular fault, the elements in the footwall are removed. If the CH (constant heave) 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) 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. In both cases and if doing extension, the first slip button should be off (numeral 8).

For the two vertical faults case, the location of the first fault and the distance from the first to the second fault, are defined as a fraction (**0 to 1**) of the base length. The vertical faults can act either in extension (caldera, Figure 2c) or compression (piston). For the detachment fault, the user can select either only the right wall moving, or both walls moving (Figure 2d). For the repose-collapse simulation, the user can choose either to remove only the right wall or both end-walls after equilibration (Figure 2e).

Finally, the uni/biaxial simulation allows modeling of a biaxial test at a user-specified confining pressure in N/m (Pa in 3D, Figure 2f). The “edge” elements on which these pressure is applied are marked with a different color. This simulation only works with an assembly of 10 by 5 units, since in a way this assembly is a sample of the other assemblies.

13. Apply a user-specified vertical overburden pressure to the top of the assembly. This option is not available for the repose-collapse or uni/biaxial test, nor for erosion or syn-tectonic sedimentation (numerals 14 and 15).
14. Erosion of elements above a user-specified base level which can be equal (**1.0**) or higher (**max. 10.0**) than the assembly's height. This option is not available for the repose-collapse or uni/biaxial test.
15. Sedimentation of elements below a user-specified sea level. Sea level is initially defined by the height of the assembly after equilibration, and it can be static (null sea level rise), or rise at a low, mid, high, or very high rate. The growth elements have the same strength than the uppermost pre-growth elements. This option is not available for the repose-collapse or uni/biaxial test. This [section](#) explains syn-sedimentation.

Initializing a model

After defining the model parameters and boundary conditions, the model can be initialized by pressing the **Initialize** button (or using the *Model -> Initialize* menu, ⌘I). This writes the model parameters and boundary conditions to the *Summary* view, as shown in Figure 3³. The text in the *Summary* view is important. Here, the number of elements, the

³ Initialization will not work if the decimal separator in your system is not a full stop (.). Use the System Preferences -> Language and Region panel to set the decimal separator to a full stop.

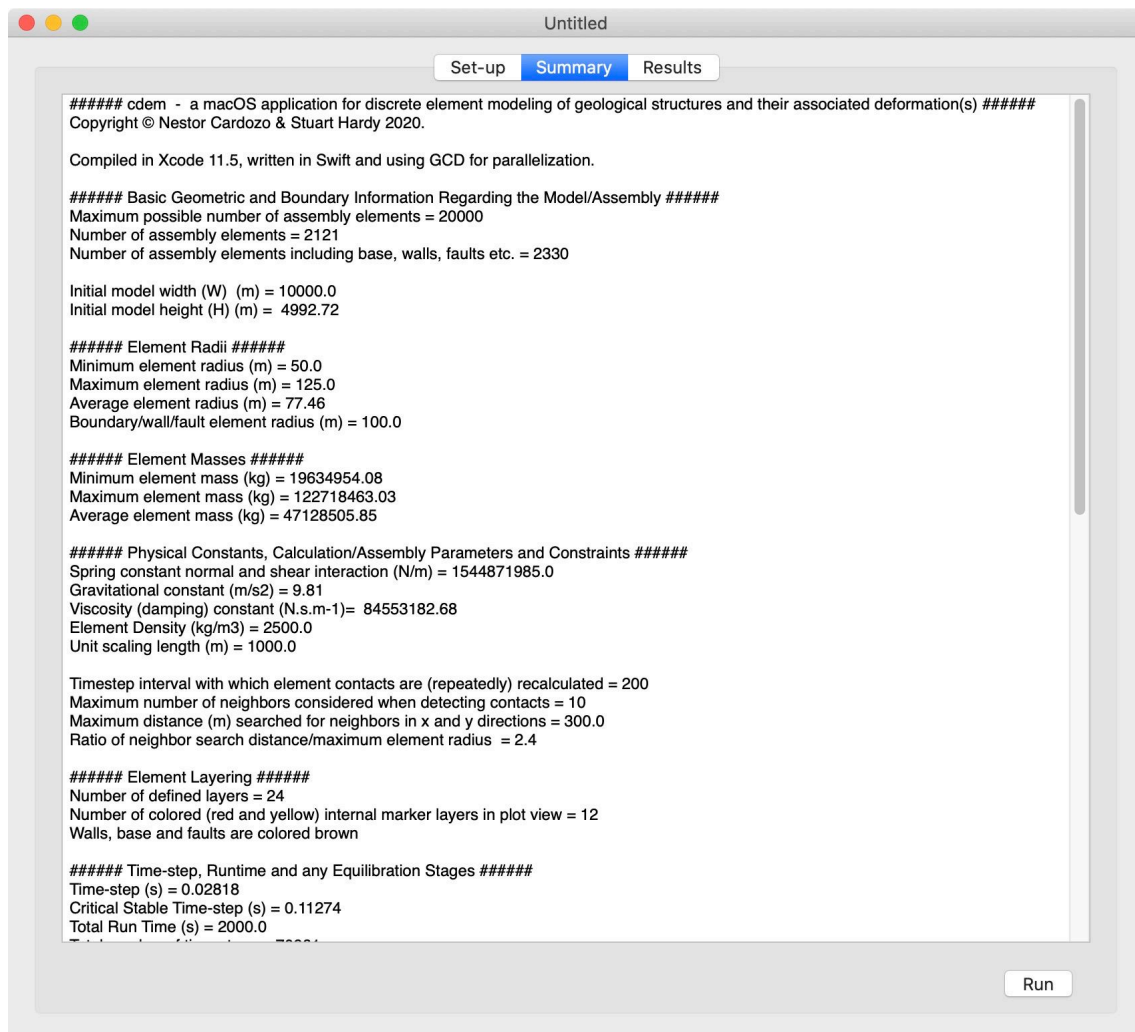


Figure 3. The Summary view after initializing the model

model dimensions, element radii and masses, physical constants, calculation parameters and constraints, time step and runtime details, boundary displacements, display increments, fault configuration, material properties, and growth sedimentation details are all reported. Reading this text is an effective way to check any possible inconsistencies in the simulation (are you doing what you intended to do?) and provides a definitive record of what you are simulating.

Running a model

To run the model, just press the **Run** button in the *Summary* view (Figure 3, or use the *Model -> Run* menu, ⌘R). This will take you to the *Results* view (Figure 4) and it will show the evolution of the assembly as it is deformed. A counter in the lower left corner of the *Results* view will show the current/total number of display increments, and the net displacement for faulting simulations, or time for the repose-collapse simulation. Notice

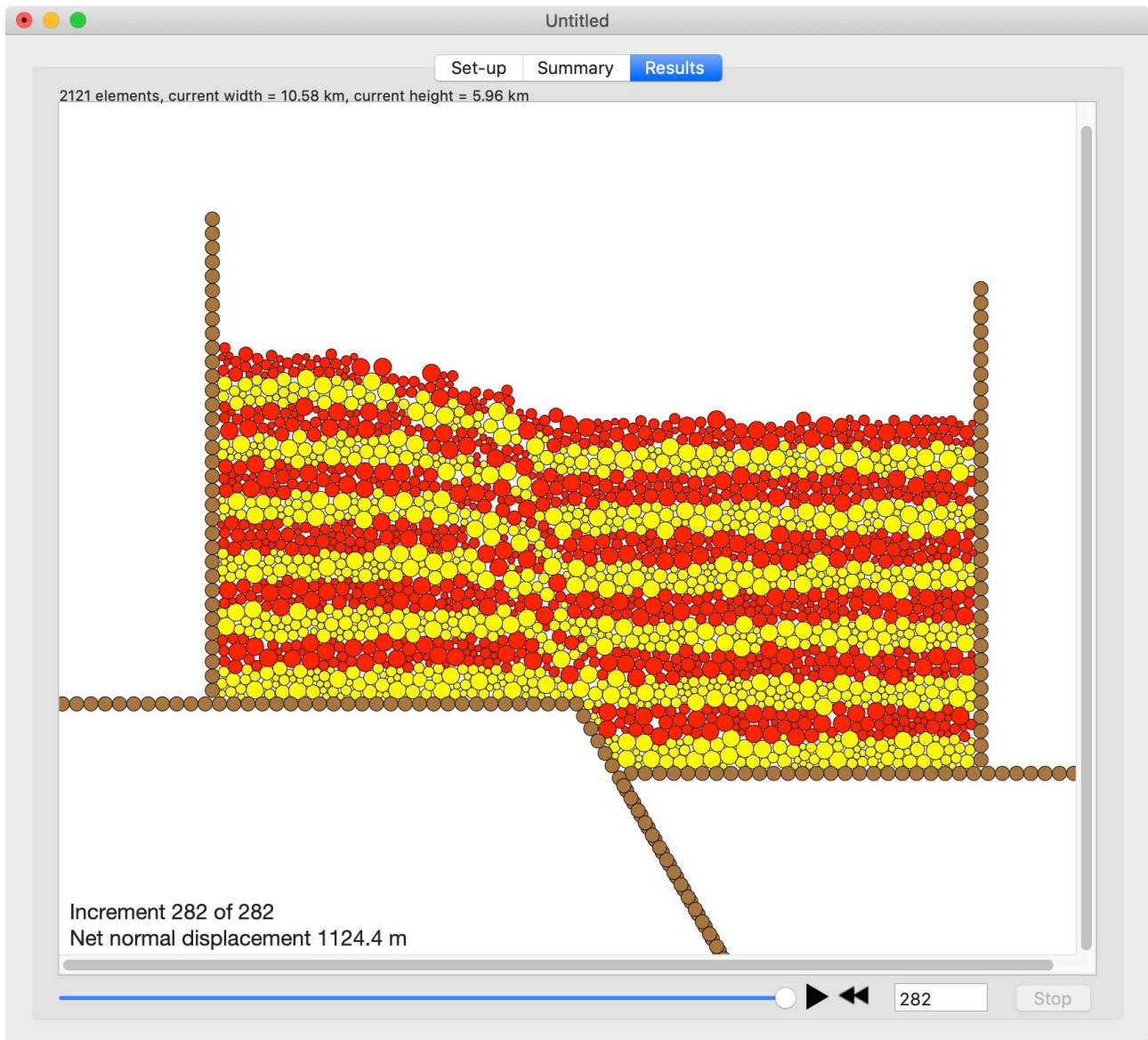


Figure 4. The Results view after running the model

that at any time during the run, you can terminate the simulation by pressing the **Stop** button (Figure 4, or use the *Model* -> *Stop* menu, ⌘T).

By default, the wall elements are colored brown, and the internal elements in yellow and red layers. These colors can be changed using the Preferences panel (*cdem* -> *Preferences* menu, ⌘,). In the Preferences panel, it is also possible to select a range of layers to be highlighted⁴. The normal cycle of **cdem** is thus: i. Set model parameters, ii. Initialize model, and iii. Run model. After running or stopping a simulation, the model

⁴ If you do so, this will not highlight the lower zero-friction or unbonded part of the assembly in case this option is selected.

parameters can be changed via the *Set-up* view, the new model can be initialized using the **Initialize** button, and then run using the **Run** button.

Visualizing a model

After the run is completed, any increment can be chosen using the slider at the base of the *Results* view or the text field next to it (Figure 4). Pressing the play/pause button next to the slider (or pressing the space bar) plays/pauses the simulation. Pressing the rewind button (or ⌘0) rewinds the simulation to its initial step⁵. The menus under the Assembly menu allow zooming the assembly (menus under the *Zoom* menu), displaying a scale bar (*Scale bar* menu), displaying displacement vectors (menus under the *Displ. Vectors* menu), displaying principal strain and stress and maximum shear strain axes (menus under the *Axes* menu), coloring the elements by displacement, strain or stress (menus under the *Color by* menu), toggling vectors, axes and colors (*Toggle attributes* menu, ⌘K), toggle coloring by attribute only those elements whose attribute value is greater than 10% the maximum value (*Toggle > 0.1 * max. value* menu), and toggle the elements (*Toggle elements* menu, ⌘E). [Please notice that to have access to the stress menus, you need to toggle on the **Calculate stress** option in the Preferences panel \(*cdem* -> *Preferences* menu, ⌘,\).](#) Either incremental or total displacement or strain can be visualized. Total displacement and strain are displayed from the end of the equilibration phase, i.e., the equilibration steps will not display any total displacement or strain. On the other hand, incremental displacements and strains, and stress are displayed throughout the whole simulation, including the equilibration steps. These are a great way to check the assembly is stable after the equilibration phase.

Incremental displacement or strain is calculated between the current increment and five (5) increments before. Total displacement or strain is calculated between the current increment and the increment at the end of the equilibration phase⁶. Strain is calculated at the center of each element using the neighboring elements within a radius

⁵ You can also use the *Play in slow-motion* menu under the *Model* menus to play the simulation slowly.

⁶ 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. This may result in the total strain being "reduced" with time, for example during tectonic inversion. To track the path of deformation, use cumulative strain.

equal to twice the maximum radius of the elements. For incremental displacement or strain, notice that the first four initial increments have their values calculated from the start of the simulation (less than 5 increments). Thus, their values may seem lower. In addition, it is possible to color the elements by “Cumulative” strain (*Assembly -> Color by -> Cum. Strain* menus). This is basically the cumulative of the incremental strains from the end of the equilibration phase, i.e. the equilibration steps will not display any cumulative strain. Cumulative strain is better than total strain since it captures the path of 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.

Incremental displacement vectors are exaggerated five (5) times, while total displacement vectors are not exaggerated. Axes are displayed on a grid of points spaced in the horizontal and vertical twice the maximum radius of elements. Axes are not displayed on wall elements. Notice that the axes just show orientation, i.e., their length is constant and is not scaled by the value of the parameter.

For displacement, elements can be colored by horizontal, vertical, or magnitude of the incremental or total displacement. In addition, elements can be colored by uplift and subsidence. For strain, elements can be colored by incremental or total extension (e_1), shortening ($-e_3$), maximum shear strain, or dilation⁷. In addition, for incremental strain, elements can be colored by rotation (positive rotation is clockwise and vice versa)⁸. For stress, elements can be colored by horizontal or vertical stress (σ_{xx} or σ_{yy}), shear stress (τ_{xy}), maximum or minimum principal stress (σ_1 or σ_3), or maximum shear stress ($(\sigma_1 - \sigma_3)/2$). With the exception of uplift-subsidence, dilation, and rotation, elements are colored using a blue-green-red color bar, where blue are low, and red are high values. For uplift-subsidence, the color bar is blue (subsidence) and red (uplift). For dilation and rotation, the color bar is blue (negative value) and red (positive value).

For incremental displacement, the limits of the color bar are the minimum and maximum incremental displacement at the current increment. For total displacement, the limits of the color bar are the minimum and maximum total displacement at the last increment of the simulation. As such, the limits of the color bar for total displacement

⁷ Dilation or volumetric strain is equal to the product of the principal stretches minus 1.0. Since the deformation is plane strain, this is equal to $S_1 * S_3 - 1.0$.

⁸ Notice that rotation only works for infinitesimal strain.

don't vary with increment, while those for incremental displacement do. For strain, the limits of the color bar are fixed. For incremental strain, they are 0 and 0.1, and for total strain, they are 0 and 2.0. For stress, the limits of the color bar are calculated based on all increments, and they are set to a maximum magnitude of 200e6 N/m (200 MPa in 3D).

Figure 5a shows the model of Figure 4 with the elements colored by total displacement magnitude, while Figure 5b shows the same model colored by total maximum shear strain. The color bar is shown in the plot, and the displayed property is listed in the text field above the plot.

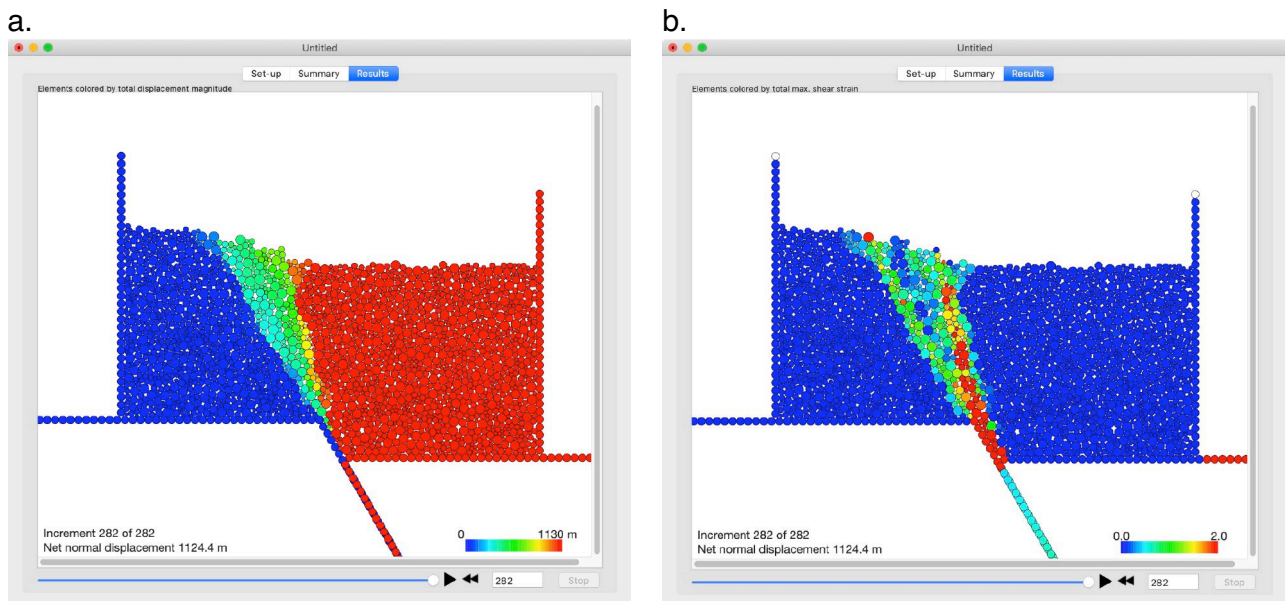


Figure 5. The model in Figure 4 with the elements colored by **a.** Total displacement magnitude, and **b.** Total maximum shear strain.

Distances and angles can be queried in the assembly by left-clicking (first point) and dragging (second point) the mouse in the plot. Option-clicking an element provides information about the element's coordinates and displayed values (displacement, strain or stress). All this information is displayed in the text field above the plot.

Saving a model

Under the *File* menu, there are menus to save the simulation as a file with **cdem** extension (*Save, ⌘S*), the current increment in the plot view as a pdf (*Save increment as PDF, ⌘P*) or png (*Save increment as PNG*), all increments as png (*Save all increments as PNG*), all or some increments as an animated gif played forward or backwards

(submenus under the *Save increments as animated GIF* menu), the current increment as a text file (^⌘S), all increments as text files (^⇧⌘S), or biaxial (strain- stress) data as a text file (*Save Uni/Biaxial data as text*).

cdem files store all increments in the simulation, and therefore they are large (the **cdem** file for the simulation in Figure 4 is 10.1 MB). Please notice that if you calculate stress (i.e., have the **Calculate stress** option in the [Preferences panel](#) on), the **cdem** file will be bigger (27.4 MB for the default simulation in Figure 4). **cdem** files can take some time to save and open, so be patient, but remember they are a *complete* record of your simulation. When saving all increments as either png images or text, the program will ask for a directory to save the files. All files will be named with a prefix plus the increment number (e.g., cdem282.txt). This prefix can be changed in the *Set-up* view, *Prefix for all increments* field (Figure 1). Saving increments as an animated gif produces a movie. However, this file can be large; the default window size and default simulation produces a gif of 48.4 MB. You can reduce the gif size by reducing its resolution or saving just the odd increments via [the Preferences panel](#). High resolution and using all increments is the default. Increments saved as text files can be imported to **SSPX**, a macOS application by Cardozo and Allmendinger (2009), which offers more options for computing strain. The section [Computing strain in SSPX](#) explains how to do this.

Finally, biaxial data exported as text can be used to plot strain-stress curves in other programs, and data from several tests at different confining pressures can be used to determine the failure envelope of the assembly. The section [Calibrating the assembly](#), explains how to do this.

The Preferences panel

The Preferences panel (*cdem* -> *Preferences* menu, ⌘,) is a great way to set some key properties for all **cdem** Documents. Figure 6 shows this panel:

You can use the color boxes to set the colors of the wall elements, pre-growth elements, and elements in growth sequences 1 and 2. The text field below can be used to set the number of layers in growth sequence 1, and the button and text fields below to highlight a range of layers.

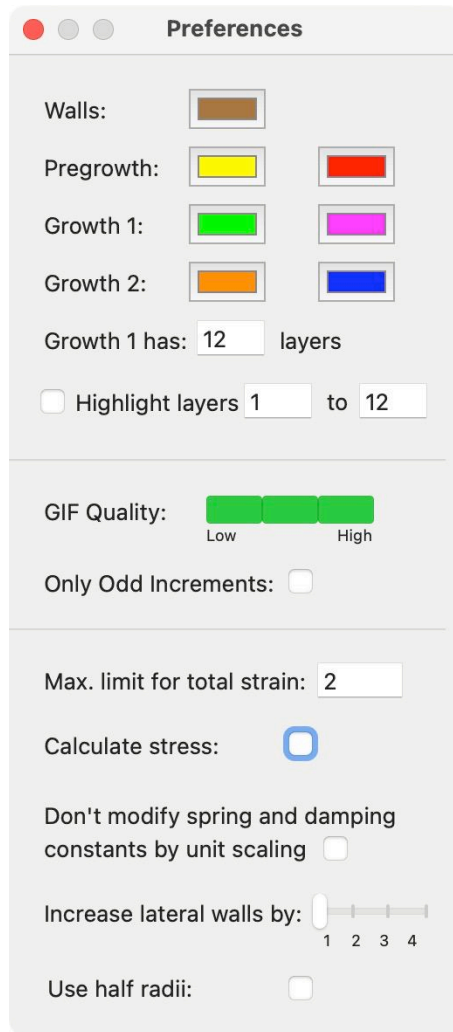


Figure 6. The Preferences panel.

The middle field allows setting the quality, and number of increments (every increment or only odd increments) of animated gifs. Finally, the bottom field allows setting the maximum limit for coloring total strain, toggling stress calculation, toggling the scaling of the spring and damping constants (see the [Theory](#) section), increasing the height of the lateral walls, which is useful for simulations where the assembly thickens a lot (e.g., detachment simulations), and using a denser assembly with half radii elements (0.025, 0.0375, 0.05, 0.0625 units).

Importing cdem2D simulations

cdem2D is a discrete element code by Stuart Hardy. **cdem2D** is a command based program that is written in C and uses OpenMP (Windows and Linux) or GCD (macOS) for parallelization. As such, it is more powerful than **cdem**. It can handle more

elements, and it has functionalities not yet implemented in **cdem**, such as salt deformation. Also, **cdem2D** runs on Windows, macOS and Linux.⁹

cdem can import **cdem2D** simulations (Figure 7). To do this just choose the *File -> Import cdem2D simulation* menu, and choose the folder where the simulation files are. All files from the **cdem2D** simulation including the `modelparameters.txt` and `modelresults_n.txt` files should be in the folder¹⁰. **cdem** will import the increments and

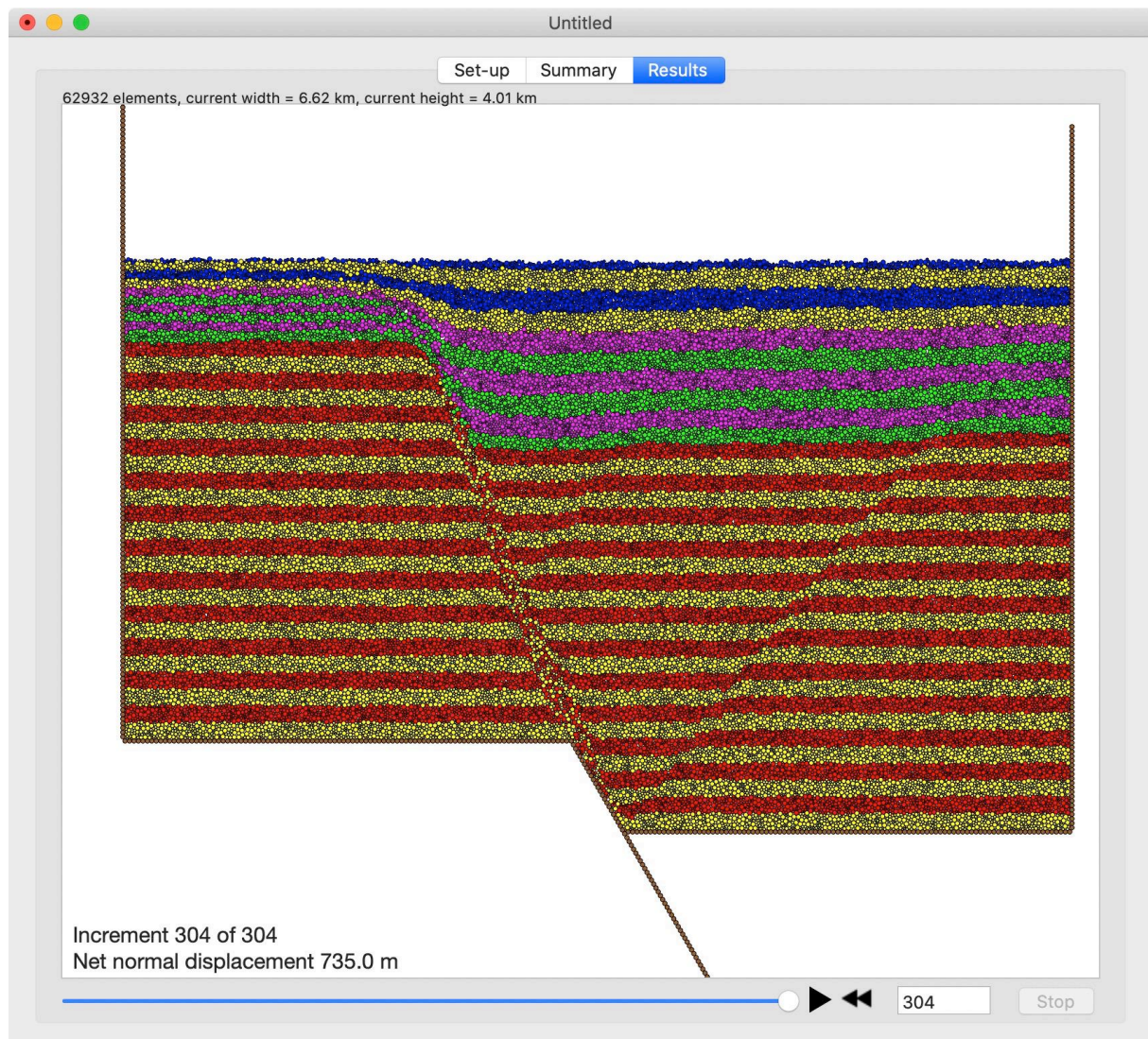


Figure 7. **cdem2D** simulation imported into **cdem**. Normal fault with growth strata. The simulation can be played back and forth, and elements can be colored by displacement or strain.

⁹ From **cdem** v. 4.5, **cdem2D** and a set of simulations as well as instructions are included with the program.

¹⁰ From v. 4.3 `modelforces_n.txt` files can be imported using the *File -> Import cdem2D simulation with forces* menu. This imports in addition stress. Note that for this to work, the *Calculate stress* option in the *Preferences* panel (Figure 6) must be on.

display them in the *Results* view. In addition, it will write the `modelparameters.txt` file (which is a record of the simulation) to the *Summary* view¹¹. Once the files are imported, they behave exactly as **cdem** increments: The simulation can be played and paused, and increments can be colored by displacement or strain. Also, the simulation can be saved as a **cdem** file. Be careful though, **cdem2D** simulations can contain tens of thousands of elements and the resultant **cdem** files can be very large.

Computing strain in SSPX

To compute strain in an increment of a **cdem** simulation using **SSPX**, you will need to export the increment and a previous increment as text files. For example, to compute the total strain in Figure 4, you will need to export the last increment (increment 282), and the increment at the end of the equilibration (increment 56). Import the first increment (56) into **SSPX** using the program's *Load Stations from cdem* menu. Then import the last increment (282) using the same menu. In the displayed warning panel, select the *Subtract* option. This subtracts the element coordinates of the last increment from those in the first increment, thus providing the total element displacements. From here, it is just a matter of navigating **SSPX** to:

- Display the model in the deformed configuration.
- Apply an algorithm to compute strain.
- Choose the parameter to plot, for example maximum shear strain, as well as set the color scale bar and its maximum and minimum values.
- Toggle off the elements.
- Display the color scale bar.

Figure 8 shows the result of these steps in **SSPX**.

After computing strain in one increment, you may want to visualize the evolution of strain throughout the simulation. This is easy. In **cdem** export the increments 56 to 282 as text files. In **SSPX**, choose the *Batch process cdem files/Total* menu if computing total strain, or the *Batch process cdem files/Incremental* menu if computing incremental strain.

¹¹ From v. 4.4 the *Set-up* view is disabled after importing a **cdem2D** simulation.

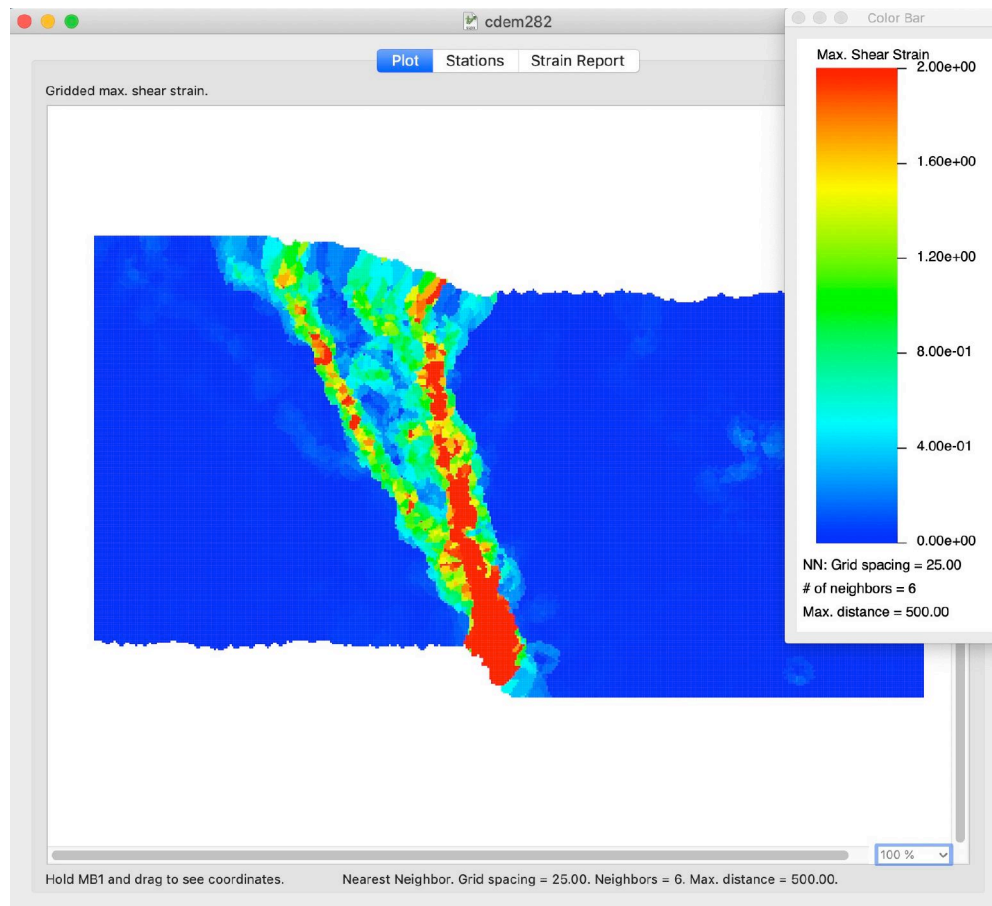


Figure 8. Maximum shear strain at the end of the simulation in Figure 4. Strain was computed in **SSPX**. This can be compared to Figure 5b.

Select the increments 56 to 282. Press Okay, and see how for each increment **SSPX** computes the strain and saves an image of it in your ~/Pictures folder. At the end of the batch, these images can be used to make a movie showing the evolution of strain in the simulation.

Calibrating the assembly

One of the most challenging aspects of the discrete element technique is the calibration of the micro, element properties (Figure 1) so that the bulk behavior of the assembly is mechanically realistic. This can be done by performing biaxial tests on the assembly at different confining pressures. Also, the repose-collapse simulation (Figure 2e) provides a quick assessment of the assembly's bulk behavior in terms of its angle of repose.

As an example, for the default element properties in Figure 1, we run five biaxial tests at different confining pressures: 0, 5, 10, 15, and 20 MPa (1 MPa = $1\text{e}6$ N/m in

cdem). In all five tests, an equilibration time of 800 s was used and the maximum axial strain is 0.2. For each test, we exported the data using the *Save Uni/Biaxial data as text* menu. This saves a text file with three columns: timestep (column 1), axial strain (column 2), and differential stress ($\sigma_1 - \sigma_3$) (column 3). We then plotted these data in another program. Figure 9a shows an axial strain vs. differential stress plot of the five tests.

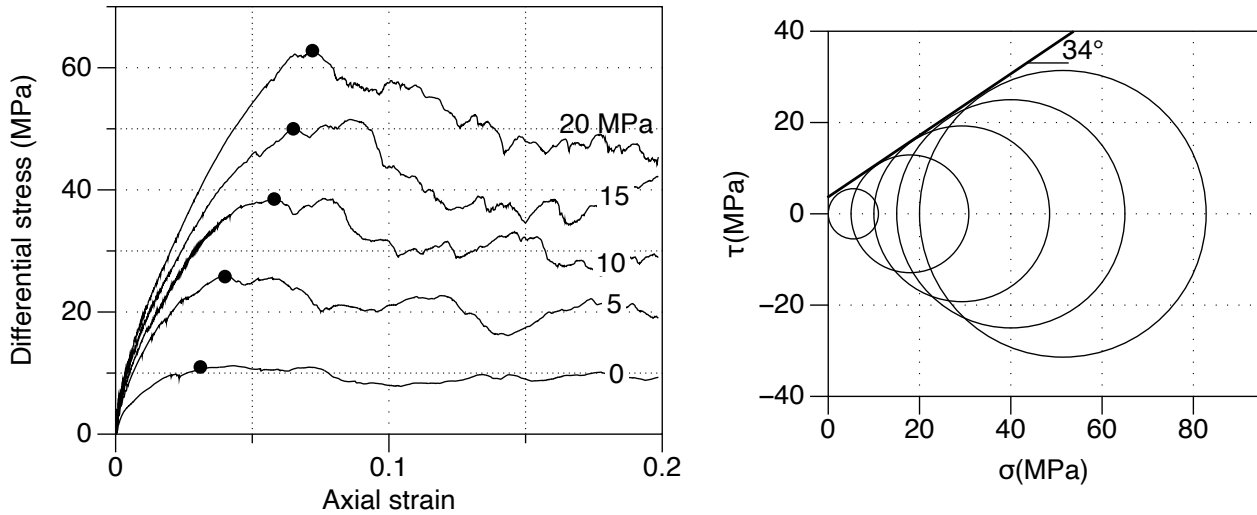


Figure 9. a. Uniaxial strain versus differential stress of biaxial tests at confining pressures of 0, 5, 10, 15 and 20 MPa, using the default element properties of Figure 1. b. Mohr circle diagram of the tests. The plots were made using the program **DataGraph** by David Adalsteinsson.

These data can also be plotted in a Mohr circle diagram, where each circle represents the state of stress at failure in each test (Figure 9b). $(\sigma_1 - \sigma_3)$ is the differential stress at failure (dots in Figure 9a), σ_3 is the confining pressure, $(\sigma_1 + \sigma_3)/2$ is the center of the circle, and $(\sigma_1 - \sigma_3)/2$ is the radius of the circle. From the Mohr circle diagram, it is possible to determine the failure envelope of the assembly. The default granular frictional material (Figure 1) gives an assembly with a bulk cohesion of ~ 4 MPa and a friction angle of $\sim 34^\circ$. Though the assembly is not purely frictional, this is consistent with the repose angle of the assembly in Figure 2e.

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 neighboring 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 parallelization 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 behavior 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:

$$\begin{aligned}
 F_n &= K_n(r - R) & (r - R) < r_0 * R & \text{intact bond} \\
 F_n &= K_n(r - R) & r < R & \text{broken bond} \\
 F_n &= 0 & r \geq R & \text{broken bond}
 \end{aligned}
 \tag{1}$$

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. For the default unit scaling (1 unit = 1000 m), K_n in **cdem** is 1.545e9 N/m. Elements within the assembly are bonded until the separation ($r - R$) between them exceeds the breaking strain times the equilibrium distance ($r_0 * R$), 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 modeled as a threshold-limited elastic spring with a cohesive force term (C_0) in parallel with that used to calculate the normal force (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:

$$\begin{aligned} F_s &= K_s X_s + C_0 \\ F_{s \max} &= \mu F_n \\ F_s &= F_{s \max} \text{ if } (F_s > F_{s \max}) \end{aligned} \tag{2}$$

where K_s is the elastic constant (shear spring stiffness) of the contact, $F_{s \max}$ is the maximum (limiting) shear (frictional) force, F_n is the normal force at a contact, and μ is the inter-element coefficient of friction. K_s in **cdem** is equal to K_n (1.545e9 N/m for the default unit scaling; 1 unit = 1000 m). 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 neighbors, calculated by:

$$F_{i,\alpha} = \sum_{j=1,\alpha} f_{i,j} \tag{3}$$

where $f_{i,j}$ is the elastic force (normal and shear) experienced by element i from its neighboring element j . However, we 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:

$$F = F_{i,\alpha} - v\dot{x} + F_g \quad (4)$$

where v 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).

Scaling, spring and damping constants

In **cdem**, for the default unit scaling of 1 unit = 1000 m, the spring and damping constants are defined by:

$$\begin{aligned} \text{springConstant} &= 1544871985.0 \text{ N/m} \\ dt &= 0.25 * \text{sqrt}(\text{minMass}/\text{springConstant}) \text{ s} \\ \text{dampingConstant} &= dt * 3000000000.0 \text{ Ns/m} \end{aligned} \quad (5)$$

where dt is the time step in seconds and minMass is the minimum mass of the elements. If the unit scaling is less than 1000 m, these constants are by default defined as:

$$\begin{aligned} \text{springConstant} &= \text{averageRadius} * 19944125.80 \text{ N/m} \\ \text{dampingConstant} &= \text{averageRadius} * 1091596.58430158 \text{ Ns/m} \end{aligned} \quad (6)$$

where averageRadius is the average radius of the elements. For unit scalings less than 1000 m, this provides reasonable and stable run-times. Please notice that if using the granular frictional material, the cohesion must be scaled as well to obtain a realistic result.

If regardless of the unit scaling, you still want to use the values of the spring and damping constants as given by Equation 5, you can toggle on the “Don’t modify spring and damping constants by unit scaling” in the Preferences panel (Fig. 6). For a unit scaling

less than 1000 m, this will give a stiffer material and will prevent the overlap of elements. However, it will result in longer runtimes.

Syn-sedimentation:

Syn-sedimentation is triggered by toggling on the *Syngrowth* button in the Set-up view (item 13 in Figure 1). 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. In **cdem** is as follows:

$$\begin{aligned} \text{sedimentInterval} &= \text{displayInterval} * 30.0 \\ \text{settlingTime} &= \text{equilibrationTime} * 0.20 \end{aligned} \quad (7)$$

So, the sediment interval is 30 times the display interval, and the settling time is 1/5 of the equilibration time. Notice that the display interval and equilibration time are set up in the *Set-up* view (items 4 and 5 in Figure 1). Therefore, when including syn-growth strata, it is important to carefully choose the display interval and the equilibration time. You don't want to syn-sediment too often so that there is no accommodation space for the sediments, or too seldom so that the accommodation space to fill is huge. Likewise, you don't want to settle the elements too short so that they don't reach equilibrium, or too long so that they unnecessarily slow down the simulation. Also, notice that you may end up with the time between sediment steps being shorter than the time for settling the sediments. This of course is wrong. If this is the case, the program will report an error: "settling > displacement". To correct this error, you should either increase the display interval or reduce the equilibration time.

The upper boundary of the space available for syn-sedimentation (the accommodation space) is defined by sea level. Initially, sea level is equal to the maximum height of the assembly after equilibration (y_{max}). Sea level can be static (*Sea level rise = Null* in Figure 1), or rise throughout the simulation (*Sea level rise = Low, Mid, High, or Very high* in Figure 1). At any time step, sea level is calculated as:

$$\text{seaLevel} = y_{max} + (\text{timeStep} - \text{equilSteps}) * |\dot{u}| * \text{factor} \quad (8)$$

where \dot{u} is the displacement rate (displacement per step), and factor is 0.0 for null, 0.25 for low, 0.50 for mid, 0.75 for high, or 1.0 for very high sea level rise. Notice that the growth elements have the same strength than the uppermost pre-growth elements.

Future work

This is version 4.9 of **cdem**. We have concentrated on implementing a functional discrete element code for geologic deformation. Of course, there are more things we would like to implement in **cdem** depending on interest, time, and the support of the users. These include:

- Adding layers with user defined thickness and properties (a sequence of high and low friction layers of equal thickness can be already modeled).
- Modeling a viscous, time-dependent substrate such as salt (Hardy, 2018) (a zero-friction or unbonded and lighter substrate can be already modeled).
- Modeling several faults that are active at the same time or at different times

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Versions

v. 1.0: Released on April 12, 2020

v. 1.1: Released on May 4, 2020. Fixed the display of the Preference panel and the Documentation window.

v. 1.2: Released on May 27, 2020. i. Added fault inversion for planar faults. ii. Added erosion of elements above a user-specified horizontal base-level, which can be equal or higher than the assembly's height. iii. Added three more assemblies with a width/height ratio of 4. iv. Organize the list of assemblies in a more systematic way.

v. 1.3: Released on June 2, 2020. i. Output net displacement instead of total displacement for inverted faults, ii. Add text field to choose percentage of lower assembly that can be frictionless, iii. If a percentage of the lower part of the assembly is frictionless, make it semitransparent, iv. Disable Set-up and Summary views when saving all increments as images or animated gif, v. Use more consistent rounding of doubles.

v. 1.4: Released on June 30, 2020. i. Cleaner Set-up view, ii. Caldera or piston for two vertical faults, iii. "Lower part of the assembly" applies to both granular frictional and bonded materials, iii. Lower frictionless or unbonded part is also semi-transparent when coloring by displacement or strain, iv. In Preferences panel, highlight elements between user-specified bottom and top layers.

v. 1.5: Released on July 10, 2020: Add an option to set the density of the lower frictionless or unbonded interval of the assembly, as 50 to 100% the user-specified density. This makes this lower interval lighter.

v. 1.6: Released on August 31, 2020: i. Calculate and color elements by stress. ii. Incremental displacement and strain, and stress are displayed in the equilibration stage. This is a nice way to check the assembly is stable after the equilibration phase. iii. Option clicking an element provides information about the element's coordinates and displayed values (displacement, strain or stress), iv. Add an option in the Preference panel to not modify the spring and damping constants (Eq. 5) by the unit scaling.

v. 1.7: Released on September 25, 2020: i. Fix vertical position of scale bar before equilibration. ii. In the case of different element densities, fix density of lower and upper assembly in the Summary view. iii. Fix display of vectors, axes, strain and stress when the Results view is Zoomed. Updates occur now on the entire view and not only in the clipped, visible rectangle of the view. iv. Fix some minor bugs when computing strain and stress. v. Add menus to display principal strain and stress, and maximum shear strain axes. vi. Add a menu to toggle off the elements. This allows visualizing better displacement vectors and axes. vii. Compiled in Xcode 12.0.

v. 1.8: Released on October 2, 2020: i. Toggle elements toggles only the fill of the elements, leaving their outline. ii. Introduce a more general way to specify the Width and Height of the assembly via text fields. The Width can be between 10 and 100 units, and the Height between 2.5 and 7.5 units. iii. Limit the height of the assembly to 7.5 units. This prevents too much overlap of basal elements and “explosion” of the assembly.

v. 1.9: Released on November 2, 2020: i. Fix several issues with the resizing of the document window and the scale and zoom of the Results view. Now the behavior of the program is much more consistent. ii. Restrict zoom values from 1.0 to 64 x. This guarantees correct scaling of the Results view and its image. iii. Remove the Zoom -> Fit In menu; it was the same than the Zoom -> Actual menu. iv. Labels, color bar and scale bar show at the bottom of the Results view regardless of window size, zoom value or scrolled area. v. Fix number of elements in text info above the Results view. vi. Improve the appearance of the Results view in Dark mode. There is still a minor glitch in Dark mode. When creating an image from the Results view, text labels, displacement vectors colors, and element outline which are white, turn black because the image is transparent. This is the right output, but it produces a “strange” behavior when dragging the mouse over the Results view in Dark mode.

v. 2.0: Released on November 18, 2020: i. Flexural slip (zero friction or not bonding) between layers, ii. Fix some minor interface issues.

v. 2.1: Released on December 16, 2020: i. Disable menus for saving images from the Results view, when not in this view. This prevents a crash. ii. Reported assembly dimensions are now the current ones instead of the initial ones. iii. Playing the slider after a run, writes down just the increment and net displacement. iv. For faulting simulations, the net displacement reported in the Results view has been corrected and it is the maximum displacement of the wall elements . v. Optimize strain computation. vi. **cdem** can now import **cdem2D** simulations. Once a **cdem2D** simulation is imported, it behaves

exactly as a **cdem** simulation, it can be played and paused, and displacement and strain can be visualized. This feature is only available in the licensed version.

v. 2.2: Released on January 11, 2021: i. Add an option in the Preferences panel to increase the height of the lateral walls 1, 2, 3, or 4 times. This is useful for simulations where the assembly thickens a lot (e.g., detachment simulations). ii. Prevent initializing a simulation when a text field under editing has a wrong parameter value. If that is the case, the user will get an error message. iii. Add tool tips to the text fields in the Set-up view describing their minimum and maximum values.

v. 2.3: Released on January 22, 2021: i. Display a warning when importing a cdem2D simulation and there is already a simulation that may be overwritten. ii. Change the animated GIF menu to contain four submenus for saving all increments forward, all increments backwards, some increments forward, and some increments backwards. iii. Fixed a bug that made the program crash for high display interval values for which there were no increments during equilibration (thanks to Hasan Ozer and Jonny Wu for pointing out this bug). In addition, set the display interval to be between 1 and 1000 m.

v. 2.4: Released on March 10, 2021: i. Add an option in the Preferences panel to include elements of half radii, namely 0.025, 0.0375, 0.05 and 0.0625 units. This results in denser assemblies, which display richer behavior, but of course the simulations take longer. This option is only for the licensed version.

v. 2.5: Released on April 12, 2021: i. Modify the program to read stress from cdem2D simulations, ii. Fix a bug when colouring growth sequences from imported cdem2D simulations, iii. Change the default red layers in growth sequence 1 to magenta, iv. Fix scale and color bar for very small scale cdem2D simulations, v. Fix a bug when reading caldera or piston mode from cdem files, vi. Improve the behavior of the program when playing simulations, vii. Double the value of the spring constant for half radii and unit scaling < 1000 m. This gives the right scaling. Please notice that the first four changes apply to imported cdem2D simulations.

v. 2.6: Released on May 3, 2021: i. For half radii and unit scaling < 1000 m, the value of the spring constant as stated in Equation 6 is not doubled anymore (sorry for changing this in the previous version), ii. Improve biaxial simulation by averaging the platten length and axial stress over 20 increments, applying confining pressure linearly in a ramp (previously, it was applied at once), and correcting for non-zero differential stress right after equilibration, iii. Fix value of total displacement for detachment-both walls moving and biaxial simulations. For biaxial simulation, axial strain instead of total displacement is

reported, iv. For faults, caldera or detachment simulations, the limits of the scale bar for total displacement are computed from the walls elements. Also for the case of tectonic inversion, these limits are computed from the increment of maximum displacement.

v. 2.7: Released on August 25, 2021: i. Add a menu to color elements by uplift (red) and subsidence (blue), this is useful for tectonic inversion, ii. Update information text field while saving all or some increments as png or gif, iii. Speed up the processing machine (cdemBrain) by using array subscript syntax with a range operator, iv. Remove escaping elements that have move beyond the end walls, and base wall in detachment simulations, v. Added a menu under the Model menus to play the simulation slowly, vi. For the licensed version and cdem2D simulations, increase the number of growth layers to 200, vii. Zoom at a slower rate; Zoom In zooms the model 125%, while Zoom Out zooms the model 80%.

v. 2.8: Released on October 25, 2021: i. For imported cdem2D simulations, read the number of pre-growth layers from the modelparameters.txt file. Thus, cdem2D simulations are not limited to 48 pre-growth layers, ii. For the planar fault case, add two buttons to make the fault listric. These buttons are available for basal fault dip $\leq 30^\circ$. Checking either one of the buttons makes the fault increase in dip from its input value to a maximum dip $= 70^\circ$. It also removes the footwall elements. Fault movement is simulated by constant heave (CH button on), which involves moving the hanging wall elements vertically and the footwall elements horizontally to fit the displacement of the lower planar fault segment; or constant displacement (CD button on), which involves moving the fault elements along the fault. This is similar to analogue models where a mylar sheet drags the sand along the fault. In the first case (CH), the user should set the fault frictionless, while in the second case (CD) the fault should be frictional.

v. 2.9: Released on November 30, 2021: i. Change the listric function to work for any given fault dip angle, and set the maximum fault dip for the listric fault to 90° . ii. Add two menus to set the left fault to either listric or irregular. For an irregular fault, the user defines the fault's geometry from a text file with x and y coordinates of points along the fault, starting at the base of the fault and moving up-dip. So it is now possible to run either listric or irregular faults using either constant heave (CH) or constant displacement (CD), iii. Remove membrane elements in biaxial tests. They do not help much and introduce artefacts.

v. 3.0: Released on January 14, 2022: i. Syn-sedimentation. I finally managed to implement this important functionality following Stuart's cdem2D code. Please notice that syn-sedimentation is not trivial, it will probably require fine-tuning in future versions. Read

the new *Theory* -> *Syn-sedimentation* section in the *Documentation* of the program to understand how syn-sedimentation works. ii. Add menus to color the elements by incremental or total dilation. iii. Several bugs corrected.

v. 3.1: Released on February 4, 2022: Changes to the biaxial test: i. Color the edge elements differently if a confining pressure is applied to them, ii. Average axial stress and platten length over less increments (5 instead of 20).

v. 3.2: Released on February 18, 2022: Fixes to syn-sedimentation: i. Fix a bug in detachment simulation where the boundary walls were moving while new elements were settling. This is not anymore the case. The lateral walls are fixed while the new elements settle. ii. Catch and report an error if the settling time is larger than the time interval between sediment steps. If this is the case, the user must either increase the display interval or reduce the equilibration time to fix the error. iii. Change the way sea level rise is defined, now sea level rise is a fraction of the boundary displacement per step.

v. 3.3: Released on March 25, 2022: Add more options for layered anisotropy: i. Lower or upper percentage of the assembly can have a percentage of friction or bonding, and a percentage of density. ii. Layered friction: layers 5-8, 13-16, and 21-24 can have a different friction. This is useful to simulate a sequence of competent-incompetent layers of equal thickness. iii. For imported cdem2D simulations that have a weaker frictional or ductile interval, display that interval semi-transparent. iv. Add an option for applying a vertical overburden pressure to the top of the assembly.

v. 3.4: Released on May 2, 2022: Correct a bug when doing inversion on an irregular fault and CD boundary condition. Now, similar to the boundary walls, the mylar sheet is dragged up (if initial normal faulting) or down (if initial reverse faulting) during inversion.

v. 3.5: Released on May 12, 2022: i. Fix a bug when reading increments from cdem2D. Escaping elements which are “removed” during the simulation are now properly accounted for. ii. Implement a much better strategy to colour growth elements by total strain. Input displacements are estimated from the increment the element was deposited.

v. 3.6: Released on Sept 30, 2022: cdem is not anymore commercial and it does not rely on a license server. Instead, this academic version is provided free of charge for non-profit use.

v. 3.7: Released on February 1, 2023: 1. Fixed a bug where cdem could not save or open cdem documents. 2. Fixed Equation 1 and its explanation in the documentation.

v. 3.8: Released on March 13, 2023: 1. Fixed net fault displacement and equilibration steps for cdem2D models with sudden tilting. 2. Fixed a bug when fault inversion and the

amount of inversion is greater than the first phase of deformation. 3. Add a very high sea level rise for growth strata.

v. 3.9: Released on March 20, 2023: There were still bugs in tectonic inversion simulations in the previous version. In this new version, tectonic inversion seems to be working fine for both positive and negative inversion, with or without growth strata. Tectonic inversion is tricky though, so I suspect there are still some glitches.

V. 4.0: Released on April 10, 2023: 1. Significant changes to the CD algorithm on listric or irregular fault. On listric or irregular fault, for reverse fault or tectonic inversion, there is now a second set of elements acting as the “mylar sheet”. 2. Significant reduction of GCD calls which can cause overhead.

v. 4.1: Released on April 24, 2023: Changes to the listric/irregular fault algorithm: 1. For CD (mylar sheet), change mobility of the fault elements in extension, 2. For either CH or CD, remove the base elements in footwall. 3. Optimize the code by not computing the calculating force and neighbour routines on non-active elements. 4. Change flexural slip to make layers 4, 8, 12, 16 and 20 of zero strength. 5. Reduce minimum value of display increment to 0.1 m. This can be necessary for low unit scaling, e.g. 100 m. 6. Listric/irregular fault now have the same shape for simulations without and with growth strata.

v.4.2: Released on May 15, 2023: Improvements to the CD (mylar sheet) algorithm for listric or irregular fault.

v. 4.3: Released on July 3, 2023: 1. For the bonded model and intact bonds, multFact in calcForce and calcNewForce functions was changed to 0.0. This makes the scaleForce = 1.0. That is, there is no progressive weakening of the bond with stretch. 2. Add a menu to import modelforces_n.txt files from cdem2D. This imports stress as well. However, for this to work, the Calculate stress option in the Preferences panel must be on. 3. Change flexural slip back to zero strength layer contacts. This works better for extension.

v. 4.4: Released on July 10, 2023: 1. Change menu name to “Import cdem2D simulation with forces”. 2. Fix a bug where elements were not coloured by total displacement in imported cdem2D repose-collapse, or biaxial simulations. Now, when importing the simulation, cdem sets the faulting mode to either planar, caldera, detachment, repose, or biaxial. This takes care of this bug. 3. Disable Set-up view upon importing a cdem2D simulation. This makes sense since the Set-up view has no relation to the imported cdem2D simulation. 4. Fix a nasty bug when calculating total displacement. 5. Use 1 and 99 percentile for maximum and minimum displacement or stress, respectively.

v. 4.5: Released on September 13, 2023: 1. Fixed several issues with coloring of elements by displacement and the limits of the color scale bar. 2. Fixed issues with blue-white-red color scale bar. 3. Disable all menus under the Model menu, except Play in slow-motion, after importing a cdem2D simulation. 4. Change the main reference to the program to our Geosphere paper. 5. Fixed force calculations routines so that simulations with growth strata are reproducible. 6. Include in the distribution the program cdem2D (macOS), together with a library of simulations.

v. 4.6: Released on September 28, 2023: 1. Add the maximum limit for coloring total strain to the Preferences panel. The minimum value is 0.1, the maximum value is 5.0. 2. Allow reading files produced by cdem2D in Windows. 3. Change cdem2DPro to cdem2D. This is more consistent. 4. Add to the cdem2D runtime.txt file, additional lines to define mechanical stratigraphy. Update examples to the new format of runtime.txt. 5. Add a new cdem2D example illustrating mechanical stratigraphy.

v. 4.7: Released on January 2, 2024: 1. Imported biaxial test from cdem2D now behaves as the native biaxial test in cdem: axial strain is displayed at each increment, edge elements at which pressure is applied are highlighted by a different color, and attributes are correctly colored.

v. 4.8: Released on February 7, 2024: 1. Add incremental rotation to the coloring of elements. 2. Changed the blue-white-red color bar to have smoother gradients towards the end values.

v. 4.9: Released on June 1, 2024: 1. Display elements in the footwall of listric or irregular faults. These elements are fixed and are just for visualisation purposes. 2. Add a “Toggle > 0.1 max. value” menu. This menu toggles coloring by attribute only those elements whose attribute value is greater than 10% the maximum value. 3. Add Cumulative strain menus. This color the elements by cumulative strain: The sum of the incremental strains from the end of the equilibration stage to the current increment. Cumulative strain captures the path of deformation.