

MacroPac Evaluation Manual

MacroPac runs on IBM compatible PC's with Windows 95, 98, NT or 2000. **MacroPac** obeys typical Windows conventions. It is mouse-driven using pull-down menus. Some of the functions can also be accessed using icons, which are arranged using a Toolbar across the top of the screen. You may prefer to use the toolbar rather than the pull-down menus. When a pull-down menu is in place, or the cursor is positioned over a toolbar icon, a message at the bottom of the window describes what the highlighted menu item does.

In all cases, 'mouse click' refers to the left-hand mouse button, unless specifically indicated otherwise. A single click positions the cursor, while a double click on a field highlights it and allows it to be overwritten; these are standard Windows conventions.

This evaluation version of **MacroPac** comes with four pre-set test examples, which are discussed in detail in Section 12. You will not be able to change the objects - their size, shape, or size distribution - or add new objects. Otherwise, this evaluation version contains much of the functionality of **MacroPac** version 4. You will be able to change the box size and boundary conditions, the number of particles, and the packing regime (within limits). And the visualization and analysis functions are all enabled.

There is online help available in **MacroPac**, which can be accessed at any point through the Help buttons on each screen.

To run the full version of **MacroPac**, the minimum information you need is (a) an estimate of the regular shape (plates, spheres, rods...) that best represents your particle and (b) an idea of the particle size distribution and range, although for simple simulations particles can be treated as monodisperse. The dimensions of the simulation box also need to be chosen appropriately to get the best results from your model. The boundary conditions will default to hard walls, unless you select soft or periodic boundaries for any of the walls.

1. Overview of MacroPac

Many technologically important systems require an insight into the way objects, most commonly small particles, pack together. The choice of particle size, shape and size distribution can significantly affect the packing density of a system, as can the size and boundaries of the container which holds them.

MacroPac models the packing of particulate materials by placing objects into a simulation box. The original algorithms were developed by Professor Ken Evans and Dr Mark Ferrar at the University of Liverpool, and have subsequently been extended by OxMat. **MacroPac** offers you the options of static packing (placing the particles anywhere in the box, and not allowing them to move), gravity packing (allowing them to move in one direction until they collide with a wall of the box, or with another object), or shake packing (when they can move in a random direction, provided they do not collide with another object or box wall). Overlap minimization, enabled in the full version, is not available in this evaluation.

Post-processing is also allowed, so that the box can be shaken, and the particles allowed to settle. Particles can also be translated in specified directions. By selecting appropriate packing algorithms, and post-processing options, a wide variety of packing situations can be simulated.

MacroPac allows several particle classes to be modelled in one system, with a choice of (regular) shapes and size distributions for each particle class. So, you can mix spheres, rods and plates in the same box, for example. In this evaluation version, you will be unable to add objects, or modify their shapes. These functions are available in the full version of the program, of course.

Simulations can be performed in two and three dimensions, with a choice of boundary conditions for the walls of the simulation box.

MacroPac generates objects that obey a user-specified shape and size distribution for each object class. In this evaluation, we have specified these for you, and you will not be able to change them.

Each object is then placed in the simulation box, and (if gravity or shake pack is used) allowed to move to its new position. The program checks for overlap with neighbouring particles as each object is packed. If an overlap is detected, the particle is placed again, in a new position. Once a user-specified end condition is reached, the simulation stops. Alternatively, you can pause the simulation at any stage of the packing so that 'snapshots' of the system can be taken.

Information on the packed system and simulation box can be saved - either for analysis at a later date or else as a starting point for further packing. Some parameters can be changed when simulations are paused. This allows you to build up layered systems, or to introduce new small particles into spaces in a box that has already been packed with larger particles.

When the packing is complete, various analysis tools provide further information on the system. The distribution (either weight or number distribution) of packed objects across each axis of the packing space can be displayed as a histogram. The orientation of particles in 2D systems can also be displayed in a histogram, with each bar representing an orientation range specified by the user. The number of inter-particle contacts between each object can also be analyzed. New in v4 is the Diffusion module, which lets you look at the effect of tortuosity of the packed box.

Analysis can be performed on the whole system or for individual object classes in a mixed system. The user specifies the 'active classes' for each particular analysis.

Visualization of the packed systems is an important feature of **MacroPac**. The packed system can be displayed in two or three-dimensional representations. Individual particle classes in a mixed system can be examined by 'turning off' the other particle classes from a visualization using the 'active classes' feature.

All the details of a simulation can also be output to a general report that can be pasted into your spreadsheet software.

2. Using MacroPac: General Aspects

2.1 Introduction to Menus

The pull down menus used by **MacroPac** aim to follow standard Windows conventions. Items shown in black on the menus are currently available; items which are greyed out are not, but may become available at different stages of the simulation. For example, results are not available before a simulation has been performed.

The first pull-down is the **File** menu. In this full version, this enables you to Open and Save files, and to set up New files - all options which are disabled here. Each file contains data about the simulation setup and any objects that may already be packed into the simulation box. In addition, the File pulldown has the Exit option, when you are finished with **MacroPac**.

In the full version, typically you would Open a file or set up a New file under the File menu, and then use the Parameters menu to change or set up the packing box and objects, together with information on the endpoints and any box growth steps. When you have run the simulation using the Process options, you can look at and analyze your results using the Results items.

In this evaluation version, the New, Open, Save and Save As options have been disabled, and a new item **Load Examples** has been added.

The **Parameters** menu allows access to all of the windows that you will need for data input for a simulation. The **Process** menu contains the options that monitor and run a simulation.

Once either the simulation has started running or a previously packed system has been loaded, the results will be available under the **Results** menu along with the analysis functions.

2.2 Starting and Stopping Simulations

The Pack Status command under the Process pulldown gives the Pack status window. Simulations can be launched using the Start Packing option, found in the Control pulldown. Simulations can also

be started using the Start icon on the main toolbar, which is marked with a green arrow or, if the status window is open, by pressing on the Start button. Once the simulation is running, the Start button changes into the Stop button.

To pause or stop a simulation, you can either use the Stop button on the status window or use the button on the main toolbar, which is marked with a red stop sign. The status window only displays the Stop button while a simulation is running. When the simulation is stopped or paused, this button is marked Resume. Press it when you want to continue packing.

The simulation will stop automatically when certain endpoint conditions are met. These end points are set in the simulation parameters window (using the Packing options) and will be discussed further in Section 7.

2.3 The Toolbar

The toolbar contains icons that allow you to control the simulation without recourse to the pull-down menus. Placing the mouse cursor above one of the icons causes a message to appear at the bottom of the window. This message tells you what action the icon will perform. From left to right across the tool bar, these are:

Message	Pull down equivalent	
Creates a new parameters file	File	New
Open an existing parameters file		Open
Saves this parameters file		Save
View/Edit packing parameters	Parameters	Packing
View/Edit box parameters		Box
View/Edit object classes		Objects
View/Edit steps parameters		Steps
Show packing status window	Process	PackStatus
Start/Resume packing simulation		Start Packing
Stop simulation		Stop
Translate Objects		Translate Objects
Settle Objects		Settle Objects
Abort and scrap existing packing data		Abort
Display objects in 3D	Results	3D Visualize
View 2D sphere representation of objects		2D Visualize

3. Scientific Background

3.1 Basis of the Packing Algorithm

3.1.1 Static Random Packing

The static packing randomly places objects into a simulation box to build up a packed system. They are therefore 'parked' rather than 'packed'. Objects are picked from the different particle classes defined by the user. When an object has been placed at a random position in the simulation box, a proximity check is initiated to determine whether the newly positioned object interacts with a neighbouring object. If there is an interaction, the computer attempts to place the object in another position and counts a failed packing attempt. If no interaction is detected, it is allowed to stay in position. The user can choose to terminate the packing process when a certain number of unsuccessful attempts to pack an object have been made.

3.1.2 Gravity Packing

In this mode, you need to specify the axis to which gravity should apply, and you have the option to pick the opposite direction using reverse axis. When an object is placed into the box, it 'drops' along the given axis, stopping only when it hits another object or a boundary wall.

The object drops using simplified hard sphere dynamics. The simplification arises because only one object is dropped at a time, and this object is the only moving object in the simulation. Thus the collisions between the dropped object and other (previously placed) objects result only in a change in velocity to the dropped object, and when it comes to rest it is fixed in position.

The exception to this happens if BLP (bottom layer penetration) is toggled on. In this case, if the dropped object hits an object in the bottom layer (i.e. which touches the bottom boundary) then the objects in the bottom layer are dynamically moved until the dropped object succeeds in penetrating the bottom layer, or else all attempts fail.

If objects stick is toggled on, then the dropped object is translated along the gravity axis, stopping as soon as it comes into contact with another object or wall. This models particles which stick on impact with other particles or a wall.

In gravity mode, non-spherical particles do not rotate into a different orientation. Therefore, this provides only a crude model of gravitational effects for non-spherical objects. Also, non-spherical objects do not slide past each other realistically, because they are made of spheres which can interact. For these reasons, it is recommended that you use gravity model for spherical objects only, unless you do not wish the objects to rotate.

Gravity packing mode can not be used along an axis which has periodic boundary conditions, since it could fall through the wall. Because of the dynamics calculations, gravity model can take considerable time to execute, especially if BLP is selected.

3.1.3 Shake Packing

In shake pack mode, the objects that have been packed are 'shaken' every so often, using a Monte Carlo algorithm. Like in the gravity mode, a force (for example, gravity) can be applied along an axis in the box, and you should select X, Y, Z or none as appropriate. If an axis is selected, then movement that results in an increased potential energy ('up' an axis) is not allowed. If **none** is selected, there is no preferred axis for movement. Therefore, objects can move in any direction in the box. The direction of the movement along an axis can be reversed, by clicking on the Reverse axis toggle.

The DRMax value is the maximum starting distance which an object can be moved in the box. This value is automatically adjusted by the shake algorithm. However, the simulation will be more efficient if a reasonable value is entered at the start.

If you start packing objects using shake model, then either when the simulation ends or when it is paused, the value of DRMax will be set to the value last used by shake. It is reset to the default value of 1 when the simulation is aborted.

The Every (attempts) value is the number of attempts which are made before the objects are shaken again. It is only implemented after a certain point in the simulation, specified by After (fails). For example, using the default values, a shake will take place every 100 attempts at picking an object. But, this will only be applied after 1000 failed attempts to place that object in the box. The shake takes considerably longer to process than each attempt at placing a new object in the box. The Every(attempts) and After(fails) can be adjusted for maximum efficiency.

This mode leads to higher packing fractions than static pack, because the shake opens up gaps between objects, allowing more particles to be packed in the box.

The shake uses a simplified version of the Monte Carlo Settle simulation. As well as randomly moving previously packed objects, non-spherical particles are randomly rotated. Thus this mode can be used to model systems where non-spherical objects are subject to gravity or some other force along an axis. It should be used instead of gravity mode for such systems.

3.2 Effect of Changing Maximum Misses

The packing method relies on objects being packed into spaces between previously placed objects. The probability of a particular object finding an appropriately sized space reduces as the simulation

box fills with particles. The number of unsuccessful attempts to pack an object therefore increases as the filling takes place hence the rate of filling decreases.

After a while there will be no more space in the box for particles to be placed into and the box can be considered "full". The program detects this situation when the number of unsuccessful packing attempts reaches a set value. This value is called the Maximum misses value and is set by the user.

The work of Evans and Ferrar shows how the volume fraction of a filled box increases with the Maximum misses value. The volume fraction does however reach a plateau above which no appreciable increase in volume fraction can be achieved by raising the Maximum misses value.

3.3 Shape Representation

MacroPac uses clusters of spheres to represent the various shapes it models. The use of spheres to define an object reduces the computation power required to define an object and the proximity checks required to detect particle interactions are made very simple.

Using spheres to represent particles can potentially produce inconsistencies between the shape of the particle defined and the shape of the particle that is packed. **MacroPac** minimizes the effect of these inconsistencies on packing results in the following ways.

3.4 Volume Correction

MacroPac ensures that the volume of a sphere representation is equal to the volume of the defined object by accounting for the interstice volume between the spheres into which other particles cannot pack and the fact that sphere represented objects have bumpy edges.

4 Specifying Objects

Although you will not be able to add, delete or modify objects in the evaluation, this section will indicate what is possible with the full version of **MacroPac** v4.0.

4.1 Defining Object Classes

MacroPac can pack several different types of shape in a simulation. Up to twenty object classes can be defined in each data file. An object class can be considered to be an ingredient in a packing formulation. Each object class consists of information about the particle shape, its size distribution and the amount that is to be packed. This amount is represented as a number ratio relative to the other ingredients.

For an example, an equal mix of spheres and fibres could be represented with two object classes each with packing ratios of 0.5 and separate size and shape information.

In some cases it may be necessary to represent a particle type with several classes in order to achieve a skew distribution. One particular skew distribution - the log normal distribution - is handled automatically in **MacroPac**.

Object information is entered into **MacroPac** by selecting the Objects option from the Parameters pull-down menu. New objects are added by clicking Add in the Object class window - this opens the Object class parameters window. Existing object classes can be deleted by highlighting the unwanted classes, and pressing the Delete button. You can open the Object class parameters window for an existing object class, in order to edit the parameters, by double-clicking on the class in the Object classes window.

4.2 Object Shapes

You can represent your materials from a choice of several standard shapes. The simulation builds these shapes up using an organized cluster of spheres. The user defines the shapes by specifying the dimensions of the object and, for plates, an angle. Trapezoids require you to specify the top and bottom lengths, since specifying an angle might result in an X-shaped particle. Triangles can be approximated using trapezoids with a short 'top side'.

4.2.1 Building Specific Shapes

Spheres

Simple spheres can be packed by selecting the Sphere radio button when the Object class parameters window is opened. The diameter must then be entered in the relevant field. You must then specify the type of size distribution that will represent particles between these limits. For Gaussian (Normal) or log normal distributions, you need to enter the mean sphere diameter, and the variance. For Uniform distributions you need to enter lower and upper sphere diameters. If the spheres are all of the same size, the distribution can simply be left at None, and a single diameter is specified.

Flat shapes

Selecting the Plate radio button when the Object class parameters window is opened can generate flat shapes, including rods and cubes. For Uniform size distributions, the window has fields that allow the upper and lower dimensions for length, width and thickness to be specified. An upper and lower limit for the primary angle should also be entered. To produce a flat particle, the thickness should be small compared to the other dimensions.

For the other size distributions - Gaussian and log normal - you will need to specify the mean value and the standard deviation in the fields provided.

If you want the Plates (rods, cubes) to be all the same size and shape, leave the distribution at None. You will then only need to enter a single value for length, width, thickness and angle. For Gaussian and log normal distributions, you will need to specify the mean value for each dimension and in the angle, and the variance in each.

Thick objects

Blocks and chunks can be built up in the same way as flat objects. The object is again based on a plate but this time the thickness can be extended to similar proportions to the length and width.

Rods

Plates can be elongated into rods by defining a large length to width ratio.

Definition of Angles

The angle specified represents the primary plate angle, distinguishing square plates from parallelograms. Extending the thickness rather than length can specify rods and blocks with a parallelogram cross-section.

4.2.2 Keeping a Fixed Shape

If the objects are specified without activating the fixed shape button, then each dimension and the angle for the object is selected randomly (within the distributions), and objects with variable shapes will be generated.

Selecting the Fixed shape option will ensure that the objects generated have the same shape but different sizes. **MacroPac** does this by selecting the length from the given distribution, but then choosing the remaining values in the same proportion, between their limits. For example, if you specify plates with length and width between 1 and 3, you will only generate squares if Fixed shape is selected, rather than generating 1x3 rods and the like.

This however relies on the angle ω for the particle being fixed. If a range of angles is specified, then the particles can never really have a fixed shape.

4.3 Object Size Distributions

Size distributions offer four options. If all the particles are the same size (monodisperse), there is no 'distribution', so you can select None. In this case, just the parameters to specify the particle size are required.

If particles have a uniform distribution over a size range, then the Uniform option shows that the upper and lower limits need to be specified. The program picks dimension values that are evenly spread between your upper and lower limits. The inputs must be positive values.

Gaussian (normal) distributions will prompt you for the mean value, and the variance. The program will generate the distribution according to this specification. Select the Gaussian option.

Many real particulate systems have a Log Normal distribution. Again, you will need to provide log normal mean values and variances for each of the parameters.

For both spheres and plates, if you change from one distribution type to another, **MacroPac** will convert your parameters for the current distribution into equivalent parameters for the new distribution. For example, changing from a uniform distribution, with low of 1.0 and high of 2.0, to a gaussian distribution, will generate a Gaussian mean 1.5 and variance 0.1667. Changing back to Uniform will convert the Gaussian parameters into the uniform distribution by representing the low and high as three standard deviations either side of the mean value. The exception to this is the log normal distribution, which is not converted sensibly to the other distributions.

Note that it is possible that the distribution may be truncated if your low value is below zero. For example if you entered a gaussian mean of 5.0 with variance of 2.0, then the uniform low value is -1, and the distribution will be truncated as you can not produce objects with size parameters below zero.

Pressing OK will accept any changes to the object class parameters you have made. Cancel will ignore any changes made.

4.4 Object Densities (Mass)

Your system might involve particles with different densities. If you want to undertake settling, or if you are looking at a density analysis, it might be important to know about these. In the Object class parameters window, there is a field for the density of each object. By default it is 1.0, but you can enter an appropriate value into the field. This value is specific to each object class.

4.5 Specifying Packing Ratios

When you have entered the size and shape details of your required object classes, closing the Object class parameters window enters the new object as a new line in the Object classes window. Now, you need to specify the ratios in which you want the objects to be packed. This is done in the Object classes window, where you enter the appropriate value into the Target Fraction field. Note that in this window, some of the items are given in blue. These are not editable here.

The target fraction values are normalized (to sum to 1) by **MacroPac** when the packing is started, so you can specify your ratios in any way you wish. If you leave all the values at zero (the default value), then equal proportions will be assumed. However, if you specify one value to be zero, while others are non-zero, the objects with zero proportion will never be packed.

Note that these proportions relate to relative numbers or relative volumes, depending on the toggle you select for the Target Fraction, in the lower right hand side of the window.

5. Specifying the packing box

Within this evaluation version, you can change the packing box from 2D to 3D, and change the boundary conditions if you wish. The following section gives you more information on this.

5.1 General Considerations

You need to specify a packing box that best represents the system you are modelling. Boundary conditions and dimensions should be chosen according to the physical nature of the real system and relative to the size of the objects you are packing. The box dimensions must be big enough to provide a good sample of a system but not so big that a large number of particles is needed to fill the box - this could lead to memory problems with the PC. There are no predefined rules as to how box size is determined.

It is best to generate, analyze and make use of results from small components of a system rather than modelling an entire system with a large number of particles.

The parameters for the packing box are entered in the Box parameters window. This is opened by selecting Box from the Parameters pull-down menu.

5.2 2D & 3 D Packing

When the Box parameters window is open you can select whether the packing box is in two or three dimensions by clicking on the 2D or 3D radio button. Selecting 2D greys out the parameter field for the z-axis of the box. 2D packing only allows objects to be packed flat. It is useful for simplifying otherwise complex systems, and generally achieves higher packing fractions since one of the dimensions is constrained to a plane. Otherwise three 3D simulations can be performed for a more realistic representation of the system.

5.3 Box Dimensions

The box dimensions are specified using three Cartesian lengths. The box dimensions should be chosen so that enough particles can be packed to perform sensible analysis. However, it should not be so large that huge numbers of particles need to be packed, since then simulation times become unnecessarily large. There is no definitive way of determining the best box length to particle size ratio, but you rapidly gain experience of what suits your problem.

5.4 Simulating Settled Systems by 'Growing' the Box

To simulate settled systems, it can be useful to 'grow' the simulation box. A simulation box is packed, and then allowed to 'grow' in one dimension. Packing then recommences to pack the unfilled part of the box. This feature is less useful now that the gravity and shake pack options are available, but can still be useful in looking at settled systems.

If you plan to use the step option to grow the box, then the box dimensions specified at the beginning of the simulation give the starting point for the growing steps. The growth step should also be specified. By controlling the size of the box compared to the particles, and the growth step, it is possible to simulate higher packing fractions than are obtained from a simple random packing. See Section 8 for more details.

5.5 Boundary Conditions

There is a choice of boundary condition that can be applied to each wall. If a hard boundary is specified, objects will be rejected if any part of the object crosses a wall. Hard boundaries can represent a mould or container wall.

If a soft boundary is selected, objects are allowed to cross the boundary as long as the centre of mass of that particle lies inside the boundary. This option can be used to represent an air interface, such as the surface of a coating.

Periodic boundary conditions allow particles to cross the box wall, but the portion of the particle that leaves the box re-enters from the other side of that box. For this reason it is necessary for periodic conditions to be specified on both opposing walls. **MacroPac** ensures this by updating the boundary condition field for the opposite wall automatically if periodic boundary conditions are specified.

Periodic boundary conditions represent packing in the bulk of a system where wall effects can be neglected.

6. Specifying the General Simulation ('Packing') Parameters

The simulation parameters determine the packing procedure by setting the termination or endpoint conditions, and the packing algorithm to be used. Parameters are entered in the Packing parameters window which is opened by selecting the Packing option from the Parameters pull-down menu.

You can change these parameters in the evaluation version.

6.1 Termination Conditions

Number to pack

The number to pack is the target number of objects that the program will try to pack before stopping. If any other terminating conditions are met before this value is reached, the number to pack value will not be attained.

Maximum misses

The Maximum misses value is the number of attempts that will be made to place a certain particle before either the packing is terminated or else the object class which the particle belongs to is switched off. Object classes are only switched off if the Maximum packing option is activated, as it is in the screen above. If Maximum packing is activated, then once **MacroPac** can no longer pack big objects, it will continue to try to pack smaller ones, as discussed below.

6.2 Packing Conditions

6.2.1 Random seed

This value provides a start point for the random number generator. Selecting a new random seed allows different simulations to be run with the same data without producing identical results each time. A random seed of zero results in random results being generated each time the simulation is run. Ticking the Randomize box will automatically set the random seed to zero.

6.2.2 Maximum packing

The Maximum packing option can be activated by toggling on the button at the bottom of the Packing parameters window. Activating Maximum packing permits continued packing of remaining object classes even though the Maximum misses value has been reached for a particular object.

6.2.3 Pack Type: Packing Algorithms

Static

The first pack mode simply places objects in the box at random. They stay fixed in the position they have been placed. There are no extra parameters associated with this mode of packing.

Gravity

As described earlier (section 4.1.2) objects are packed one at a time, and stops when it hits another object or a boundary wall. The drop involves simplified hard sphere dynamics, in which the new dropping object is the only one which can move.

You need to select the direction for gravity, i.e. whether it is the x, y or z axis. You can reverse the direction of the axis if you want using the Reverse axis toggle.

BLP stands for Bottom Layer Penetration. If this is toggled on, then if the dropped object hits an object in the bottom layer (an object which touches the bottom boundary) then the objects in the bottom layer are moved to try to let the new object in. This option is quite time consuming, so it is not advisable to use it unless you have a fast computer, and a relatively small simulation box.

Gravity can not be applied along an axis having periodic boundary conditions, since a particle could 'fall' out of the box. Therefore, in this case, the option to apply gravity along that axis is disabled. If you select Gravity pack along an axis, then try to set the corresponding walls as periodic, you will be warned that the walls are being reset as hard boundaries.

Shake

The algorithms underlying Shake pack mode were described in section 3.1.3. In Shake pack, the objects which are already packed are shaken every so often using a Monte Carlo algorithm. In shaking, the objects are moved each time a certain number of attempts has been made at packing the objects (including successful as well as unsuccessful attempts in this number). The Every (attempts) value is the number of attempts which are made before the objects are shaken again. The After (fails) value is the number of fails for the current object which are required before the shake starts. For example with the default values the box is shaken every 100 attempts at packing the object, but this only starts after 1000 fails have occurred for the current object.

The DRMax value gives the maximum starting distance which each object can move. If this value is too large, then most of the move attempts will be unsuccessful, giving a low efficiency. Therefore, it is adjusted during the simulation, as described in section 3.1.3.

The shake takes considerably longer to process than each attempt at placing a new object in the box. You can adjust the Every (attempts) and the After (fails) to try to find maximum efficiency. The simulation may take a long while to complete, especially if plates are being packed.

OM (Overlap Minimization) is disabled in the evaluation version. The on-line Help gives details on how it works.

7. The Step Function: Growing the Simulation Box

The step function allows the simulation box to grow as the packing progresses. The purpose of this to constrain the placement of particles into settled layers. It can also be used to constrain particles to near-horizontal orientations if necessary.

If no step information is entered into the Step parameters window then packing commences into the fixed box as specified in the Box parameters window.

If growth steps are required then they must be set up by opening the Step parameters window which is opened via the Parameters pull-down menu.

7.1 The Step Parameters Window

MacroPac assumes that the packing box grows in the y direction. It is therefore necessary to specify the starting box dimension with a smaller y value than the 'finished' box.

Step size

The width of each growth increment or step is entered in the Step size field. You should specify an appropriate size relative to the particle and box size to achieve the desired effect. The increase in the box is made in the y direction, and can be thought of as moving the y1 boundary out by 'step size' each step. For this to work, the y boundary can not be periodic.

Number of steps

The number of steps that are required should be entered in the Number of Steps field.

Step misses

The Step misses value serves a similar role to the Maximum misses value in the Simulation parameters. In this case, it marks the number of unsuccessful packing attempts that must be made before a step increment is made. The higher the value, the more densely packed each layer is likely to be. The Step misses value should always be set lower than the Maximum misses value to ensure that all step increments are made before the program terminates.

8. Running a Simulation

8.1 Starting a Simulation

Once you have entered the parameters, or loaded a simulation file, **MacroPac** is ready to run.

MacroPac simulations can be started by clicking on the green arrow icon on the top tool bar or by pressing Start in the Process pull-down menu or the Pack status window, if it is already open.

8.2 Monitoring the Progress of a Simulation

Starting a simulation automatically opens the Pack status window, if it is not open already. The Pack status window, shown below, displays the progress of the packing. The simulation status is the first item shown. While the simulation is running, it is shown as Packing. Other information is given on the following topics.

Objects packed

This displays the number of objects that have been successfully packed. It is also displayed as fraction of the number to pack in a bar format.

Pack attempts (total)

This is the total number of attempts successful and unsuccessful that have taken place during the simulation. It is a good indication of how long the simulation has been running.

Fails (current object)

Displays the number of failed attempts to pack the current object. When this value reaches the Maximum misses value the packing terminates or switches off that object class depending on whether Maximum pack is activated. The display is enhanced by a bar representing the fraction of the Maximum misses value that has been reached.

Packing fraction

The packing fraction is represented as the total volume of particles packed as a fraction of the simulation box volume expressed as a percentage. A histogram style bar also displays this percentage as it grows during a simulation.

Efficiency

The packing efficiency is determined by the number of fails per packing. It is expressed as a percentage, both numerically and in bar format.

As soon as packing commences, the Start button on the Pack status window changes to display Stop.

8.3 Pausing and Resuming Simulations

You may want to pause the simulation during the packing in order to analyze intermediate results or alter the packing setup in some way, or to save it to continue at a future date. The simulation can be paused by pressing either the Stop button on the Pack status window or the red Stop icon on the main tool bar.

When you stop a simulation, the label on the Stop button changes to Resume. When you are ready to resume packing, either press the Resume button in the Status window or select Resume from the Process pull-down menu. Alternatively, you can use the Start button on the main tool bar.

8.4 Moving Packed Objects

Once objects have been packed, some of the Process options allow them to be moved. The two options that are available are:

8.4.1 Translate Objects

The objects are translated - moved in a straight line - with no rotation. This is not a reversible operation; the position of the objects is changed and cannot be restored. Objects can be translated along the X, Y or Z axes, or the reverse axis for these directions. Alternatively, each object can be moved along a Random vector. The translation distance is the target distance which the objects are moved. By varying this distance, different degrees of 'shrinkage' can be modelled.

The objects do not slide or rotate around the contact objects, or rotate into different orientations. The translation algorithm works by attempting to move each object by the translation distance along the required direction. If the object hits a hard or soft wall, the object cannot move further. If it hits another object, it stops temporarily until all the other objects have been moved. Another attempt is then made to move the object, until either it moves the target distance, or it has failed to move at all for 10 iterations in which all the other objects have been moved. In this latter case, it is assumed that the objects are sufficiently closely packed that this object cannot move further in the required direction.

Note that you can specify the Translation distance, the maximum distance which objects can move. If you want to model 'shrinkage' of a box, rather than maximum packing, this can often be achieved by judicious selection of the Translation distance.

8.4.2 Settle Objects

The objects can also be 'settled' once the simulation is stopped, using a Monte Carlo simulation. The results of settling the system are not reversible. The simulation alters the position and orientation of each object, and the original configuration cannot be restored.

The Settle objects dialog is designed to work alongside the Pack status screen, which can be open at the same time. When Settle Objects is selected from the Process menu, the Settle objects dialog is displayed. As the figure below shows, this screen is split into two. The top half allows you to input

parameters which control the simulation; the bottom half contains information returned by the simulation.

You can select the axis along which to settle the system, and reverse the direction if you wish. The selected axis determines the direction of the force on the objects, e.g. gravity, which is causing the objects to settle.

You cannot settle objects along an axis with periodic boundary conditions.

Initial DRMax is the starting maximum distance by which an object can be translated in the simulation. This value will be adjusted during the simulation, and the value of DRMax in the lower half of the screen shows the current value.

The Kinetic factor determines the probability that an object will move against the direction of the settle axis. Its value depends on a number of factors (described below) but in general the higher the value, the less likely it is that objects will move against the direction of the applied force. If the value is set to zero, then objects are as likely to move 'up' as 'down', i.e. they can move in any direction.

Lifts and drops

The parameter Number of drops determines how many times the objects in the simulation are lifted to the top (defined by the direction of the axis) of the box. The default value of zero means that if you run the simulation, it will simply settle the objects once. If a higher value is chosen, the simulation will settle the objects, lift them to the top of the box, and re-settle them Number of drops times. Lifting and settling objects several times can be used to give size segregation effects that might not be seen with just one 'settle'.

Number of tries, in the bottom half of the screen, gives the maximum number of Monte Carlo steps (movement tries), both successful and unsuccessful, which are made before the simulation stops. The simulation finishes when the total number of tries equals the sum of the stage 1 tries and the stage 2 tries.

In stage 1, the value of DRMax is not changed. Stage 1 is used to move objects across larger distances, preventing the simulation from getting stuck in a particular configuration. However, stage 1 can become very inefficient, since many more moves may be rejected than are accepted.

In stage 2, the Efficiency tries to adjust itself to 50%, by changing the current value of DRMax. If most of the moves are being rejected, and efficiency is below 50%, the value of DRMax is progressively reduced until efficiency reaches 50%. Similarly, if the efficiency is above 50%, then the value of DRMax will be increased until the efficiency decreases to 50%.

Without stage 1 (i.e. if only stage 2 tries are made) there is a danger that the simulation might become stuck in a particular non-equilibrium condition. DRMax may be decreased so much that objects that have not yet settled will not move very far when they are selected for a move. In a visualization of such a system, it will look like the particles have been caught 'mid fall'.

Generally, stage 1 is useful for getting objects settled, but not to a highly packed state. Stage 2 is best for bedding particles down to achieve maximum packing of objects. The values to enter for the number of 'tries' for stage 1 and stage 2 depends on several factors. Both parameters depend on the number of objects in the system, and the more objects you have, the higher the stage 1 tries and stage 2 tries values should be. If you are packing a box using the static packing option, then settling it, or if you are using lifts and drops, then you should enter roughly the same number for the number of stage 1 tries and stage 2 tries. If the box is already more or less settled, then stage 1 tries are not needed, and you can set this value to zero.

Once the initial parameters have been entered, you can start the simulation by clicking the Start button. Once the simulation has started, this button is labelled Pause; if you press it to pause the simulation, it will change to Resume. The simulation state displays whether the simulation is Ready to start, or whether it is Paused or Settling (i.e. the simulation is running). While the simulation is

running, the input parameters are greyed out and cannot be altered. The simulation output values are continually updated.

The results that are shown are:

Number of tries	the total number of attempts so far. The simulation finished when the total number of tries equals the Max tries value
Efficiency	shows the percentage of attempted moves that are currently being accepted. This relates to the value of DRMax.
DRMax	is the current maximum distance which an object can be translated in the simulation. It starts at the value Initial DRMax, but is then adjusted in the simulation.

If you want to terminate a simulation before it has finished settling, press the End button. This will stop the simulation and allow you to change the parameters.

8.4.3 The Monte Carlo Simulation for Settling

For each Monte Carlo step, an object is randomly selected, and it is moved in a random direction by a random distance between zero and DRMax. Non-spherical objects are also randomly rotated, from zero to +/- 0.5 degree. If there is a collision with another object, the move is rejected. It is accepted if the potential energy decreases i.e. if the centre of mass moves in the direction of the force. It may or may not be accepted if the potential energy increases, depending on the value specified for the Kinetic factor.

The probability that an object moves 'up' (against the direction of the force) is given by the expression

$$\text{Prob} = \exp(-\Delta E/RT)$$

where ΔE is the change in potential energy when the object moves against the downwards force.

$$\Delta E = g.m.\Delta h$$

where g is gravity or other force constant, m is the mass of the object, and Δh is the change in height between the new state and the old one.

In the simulation, we define the probability that an object moves against the force direction as

$$\text{Prob} = \exp(M.\Delta h.Kf)$$

where M and Δh are the relative mass and distance, defined by the object's mass (density x volume) and box dimension parameters. These are not necessarily 'real' units. Kf is the Kinetic factor

$$Kf = mf.hf.g/RT$$

where mf and hf are factors which convert the relative units used in the simulation to 'real' units. Thus, the kinetic factor depends on the real units of mass, the real units of distance, the gravity (force) constant, and the temperature of the system. It also relates to the input of external energy into the system, provided by the degree of shaking. For a system that is vigorously shaken, the value of the kinetic factor will be decreased, since more particles can move against the force direction because of the shake.

9. Looking at Results

You can look at results either once the simulation has stopped - either because you paused it manually or after it has reached a predefined end point. The general packing results are already displayed on the status window. Details of each class are displayed in the Object classes window. Analysis, report and visualization options are available in the Results pull down menu.

Total packing fraction

The total packing fraction of particles in the simulation will be displayed on the Pack status window during packing and at the end of the simulation.

Partial packing fractions (by number and volume)

The partial volume of each object class as a percentage of the total volume of packed objects is shown in the Object classes window. This window also displays the number fraction of particles of each class relative to the total number in the packed box (packing fraction) and the number of particles packed for each class.

9.1 Generating a Report

In addition to the data that can be read from the Pack status and Object classes windows, you can generate a report that displays all of the packing information. This is done by selecting Report from the Results pulldown. It is worth noting that these reports generate data on each individual particle that has been packed and hence can contain a lot of information.

The report contains position orientation and dimensional details of each particle that has been successfully packed in the simulation, as well as information on the particles packed. Once the report is on screen, the top menu displays a new item, Spreadsheet. Under this menu item you will find options to let you copy the information to the Clipboard, and to save it as a text file. You can also set up your printer, preview the print, and send the information to be printed. The Save Text button allows you to save the information to a file, whose name you can specify; it is given the .txt file extension unless you have specified something different.

9.2 Making Classes Active

In some cases, you may wish to look only at specific classes of objects, rather than the whole packed box. In this case, you will need to specify which classes are 'active' for the analysis, or visualization, which you plan to carry out. This is done by selective the Active classes option from the results pulldown.

10. Visualization

There are visualization capabilities built into **MacroPac** to help you understand the packed system better. Selecting 2D Visualize or 3D Visualize from the Results menu at any stage during packing will open the visualizer. The visualizer will then display all the objects that have been selected as Active.

10.1 Visualizing Objects

Each time you select Visualize from the Results menu (whether 2D Visualize or 3D Visualize), a new visualizer window will open, displaying the objects currently active at the time. You can have more than one visualizer window open at a time in case you want to compare visualizations, for example, with and without a particular object class active. To keep the **MacroPac** desktop tidy, you can minimize visualization windows by clicking on the 'underscore' key in the top right hand corner of the visualization window. (This is similar to other Windows applications.) Windows can then be enlarged again by clicking on the maximize button on the top right hand corner of the display bar. If a visualization is no longer needed, clicking on the top right hand button, which is marked with a cross, will close it.

When either 2D or 3D Visualization is selected, an additional menu item (2D or 3D) will appear in the list of pull-down menus at the top. These give additional options for the display, and are discussed in more detail below.

If you require a print out of a **MacroPac** visualization, press the Alt key and print screen key on your keyboard at the same time. An image of the screen display will be saved to the Windows clipboard and can then be pasted into a word processor or presentation file. There is no direct printing capability for the 2D and 3D visualizations.

10.1.2 The 2D Visualizer

The 2D Visualizer can display 3D simulation boxes, as well as 2D ones. However, only the constituent spheres which make up each object will be shown, and each sphere will be rendered simply as a flat circle. To get an image which you can rotate, you will need to use the 3D Visualizer. You can change colours of the circle which outlines the objects, as discussed in Section 11.2. The interior of the objects will be the background colour.

10.1.3 The 3D Visualizer

The 3D Visualizer has three different display modes. These are accessed under the 3D pull-down menu, and allow you to show the shapes themselves, or to show the constituent spheres which make up the shapes, or to show both together. When both are displayed, you will see that the spheres protrude a little bit beyond the sides. This is because of the volume correction for the particles.

The axes and scale bar are toggled on by default. If you do not want them to be displayed, toggle them off using the relevant items under the 3D menu.

Note that you can display 2D simulations with the 3D Visualizer. The objects will be displayed in 3D, but all the objects will lie in the plane.

Rotation is carried out by holding down the left mouse button and moving the mouse.

Within the 3D Visualizer, the sphere resolution for the display is governed by the window size, so for smoother sphere representations, maximize the window.

10.2 Changing Colours

Once you have selected 2D Visualize or 3D Visualize, and the 2D View or 3D View is on screen, the top menu will show a new item, 2D or 3D, whichever is relevant. An item under these is Colour. If you select this, you will get the Colour chooser. By picking the radio button, and using the down-arrow to select the right object, you can determine whether you wish to change the background colour, or the colour of one of the objects. Use the slider bars (one for each of red, green and blue) to give the colour that you want for the object, or for the background. In this way, you can customize the picture to have the colours you want.

10.3 Rotation and Zooming in 3D Plots

You can rotate the 3D plot by positioning the mouse above the graphic, then holding down the left mouse button and dragging the mouse. However, if you wish a more controlled rotation, specific keys can be used to rotate about specific axes.

1 and 2 rotate about the X axis.

3 and 4 rotate about the Y axis.

5 and 6 rotate about the Z axis. 5 rotates in a clockwise direction, while 6 is counter-clockwise.

To zoom out or in, use the keys 9 and 0. 9 will zoom out (make the image smaller) while 0 zooms in (makes the images bigger).

11. Analysis

11.1 Number and Mass Density Analysis

MacroPac's density analysis function displays a histogram of the number density or the mass density distribution across the packing box. If either Number Density or Mass Density is selected from the Results menu, then a display of density distributions along the axes of the packing box are displayed overlapping each other - they can of course be moved around like normal windows, so that you can view them all. (There will be 2 windows for the x and y directions in the case of 2D boxes, and 3 windows, for x, y and z directions, when a 3D box is used.) The density plots can be enlarged, compressed or closed by clicking on the appropriate buttons in the top right hand corner of the display. The Tile option under the Window pull-down menu lets you display all three figures side by side.

The histograms show the variation of number of particles in arbitrary units, across the length of the box. The width of the box or bin sizes that each histogram bar represents is set to one unit of the packing box length dimension. For spheres and plates, all of the density is assumed to lie at the centre.

Classes can be selected as Active or Inactive, so that each object class can be examined separately, or in combination with selected others.

When either a Density Analysis or Orientation Analysis is on screen, the top menu displays a new item, Plot, which lets you copy the plot to the Windows clipboard. There are also options to Print the plot, Print Preview and use Print Setup to set up the printer.

11.2 Orientation Analysis

The orientation analysis function works in much the same way as the density analysis. It is available for any 2D packing, and displays a histogram showing the number of particles at each angle (relative to the x-axis) between 0 and 180 degrees.

Note that if you try to carry out an orientation analysis for a 3D box, you will be warned that this facility is not available. Orientation in three dimensions is too complex for an easy representation.

Selecting Orientation from the results menu calls up a dialogue box which asks for a value for the Number of sampling bins. This value determines the range of orientations represented by each histogram bar. If 180 is specified, then each bar represents one degree of orientation. If 18 is specified, each bar represents ten degrees - so that objects which are between 30 and 40 degrees from the x-axis will be in the same bin.

As with the density analysis, individual object classes or mixes of object classes can be included in an analysis. Just select the classes which you wish to be Active.

11.3 Contacts Analysis

The contacts analysis determines the number of neighbouring particles within a certain distance of any object. When the Contacts option is selected from the results menu, the Contacts analysis dialogue box is opened.

The cutoff value specifies how close neighbouring particles must be, if they are considered to be in contact. If the cutoff value is set equal to a very small number, then the contact analysis records the number of objects actually in direct contact with a particular particle. The output file contains information on each active particle and the number of particles within the specified contact distance of the object.

The results of a contacts analysis can be output to a spreadsheet-enabled report on the screen. Alternatively, selecting Contacts web graphic gives a 3D 'spider web' showing the contacts between the active objects as lines, connecting their centres. The contacts web can be coloured according to the number of contacts, by toggling on Use Colour Coding on Graphic. The following list shows the colour coding that is used.

Colour	Number of Contacts
bright red	1
bright green	2
bright blue	3
bright yellow	4
bright purple	5
bright cyan	6
grey	7
dark red	8
dark green	9
dark blue	10
dark yellow	11
dark purple	12

dark cyan 13
black 14+

11.4 Radial Distribution

This option (selected from the **Results** menu) generates a plot of the radial distribution function $G(r)$ for the system. 100 sampling bins are used automatically, and the distribution is analyzed to a distance (r) of half the shortest box length. The distance from the central position of each object to every other object is calculated, and the number of objects within each sampling bin is summed. The bins are then normalized with respect to a perfectly randomized system. If the system is behaving as if it is an ideal system, then the distribution will be around 1.0 for all the sampling bins.

The radial distribution function can be useful (especially when you have packed spheres) to see how much order or disorder exists in the system.

11.5 Pore Size Analysis

Selecting **Pore Size Analysis** from the **Results** menu gives the **Pore Size Analysis** window. There are two options for generating the grid. Low resolution produces up to 100 cubic grid points. High resolution analyses are made of slabs (each of thickness 10) of up to 1000 square grid points.

The low resolution grid is a maximum of 2MB in size. The high resolution grid is generated from slabs, because each slab uses up to 20MB of memory. Consequently, high resolution grids require a reasonably high performance computer.

For both low and high resolution cases, the results can be output to a spreadsheet-enabled table. This table displays the box dimensions in terms of grid points, a table of 2 times the logarithm of the size of pore (in grid points) versus the number of pores with that size, the porosity fraction, the number of pores and the size of largest pore (measured in grid points). Underneath that, the size of each grid point in cubic units (of box dimension) is displayed. Note that changing the box dimensions will change the grid point size, so the tables of number of grid point numbers can be directly compared only in systems where the same box dimensions are used. So that you can compare different box sizes, the maximum and minimum pore size in cubic units is displayed, together with a histogram table of \log_{10} the pore sizes in cubic units versus the number of pores with that size.

The **Graphic** can be displayed only for the low resolution grids.

Note that if you view the entire box the analysis will be very slow, and may result in your computer freezing up!

11.6 Packing Fractions

Selecting **Packing Fractions** from the **Results** pulldown gives a window that allows you analyze the packing fraction across the simulation box.

In the **Packing Fractions** analysis, the current system is converted into a grid of lattice points; each lattice point is either inside or outside an object. Summing up grid points contained within objects then generates the packing fraction for slices of the box, taken along a given axis. There are two options for the resolution of this grid, **Low** and **High**.

The **Low** resolution option generates a grid which is 100 units along the longest box dimension. For a 2D system, the maximum number of points is 100 x 100. For 3D systems, the maximum number of points is 100 x 100 x 100. This option should only be used when the smallest object is greater than 1/100th of the longest box length.

You can choose which axes, (**x**, **y** and/or **z**) are used to display the histogram chart. For each of these axis you also enter the **Low** and **High** value of the box dimension you wish to display on the plot. Each time you click on or off the **x**, **y**, or **z** axis buttons the range is set to the full (default) dimension for that axis.

The **High** resolution option should be used if any of the packed objects are less than 1/100 the size of the longest box length. In this mode, the grid is 1000 units along the axis to be cut. The grid is then analyzed in slabs of 10 grid units, due to memory constraints.

You can only choose one axis at a time (x, y or z) for which to display a histogram, and you can not enter **Low** and **High** values of the box dimension - they are disabled.

A high resolution plot will take very much longer time to be generated than a low resolution plot. If the low resolution is high enough to analyze your objects, then there is no advantage to using high resolution - the plots will look the same. High resolution should only be used if low resolution is not good enough for your data.

Plots of Packing Fraction compared to Simulation Packing Fraction

When you look at the full range of the plots, the displayed packing fraction may be significantly different from the value given in the **Simulation status** screen. If this is the case, then the grid resolution is not high enough to model your system accurately. The **Simulation status** packing fraction is always correct, whereas the values shown in the plot title show the result after the system is converted to a grid of lattice points.

11.7 Options for 2D plots

11.7.1 Graph zooming

To magnify a portion of the plot use the following procedure:

- Move the mouse pointer to the start of the area that you wish to expand.
- Press and hold down the left mouse button.
- With the button held down, move the mouse to the end of the area that you wish to expand.
- Release the button.

As you move the mouse, the area to be magnified is displayed against a black background. If you move outside the plot, the zoom rectangle is not displayed (the background will revert to white), but it re-appears when you move back into the plot area with the button still held down.

To cancel zooming, move outside the plot display area (until the zoom rectangle is no longer displayed), and release the mouse button.

If you attempt to zoom into an area of a graph beyond the resolution of the data, you will be given a message, and asked if you wish to reset to the default range.

There are two forms of zooming, that restricted to the x axis, or that in which a box can be zoomed into on the x and y axis (see below, free zoom). Free zoom does not work for histograms.

12.7.2 Customizing the Plot Display

Pressing the right mouse button in a plot window pops up the plot options menu. Click with the left mouse button on the option you wish to use.

Replot	Redisplays the whole plot range.
Grid	Toggles on or off a grid displayed on the plot extending the ticks displayed on the x and y axis.
Symbols	By default symbols are displayed on the plot. These can be toggled on or off using this option.
Free Zoom	This option allows you to toggle between using restricted x axis only zoom (the default) or free zoom (x and y axis). Note that with x-axis-only zoom the x axis is automatically scaled to start and end at a data point.

Time Stamp Stamps the plot with the current time and date.

The **Copy**, and **Print**, **Printer Setup** and **Print Preview** options are available in the **Plot** pull-down menu window, which is available when a plot is on screen.

Copy copies the plot to the Windows clipboard. This can then be pasted into a graphics package or word processor.

Print prints the plot using the currently selected printer.

Printer Setup allows you to select and setup your printer.

Print Preview gives a view of the plot as it will be printed.

12. The Examples

Four examples are shown, which illustrate the range of object types which can be included. These are loaded in by selecting Examples under the File menu - you will then be offered the four choices.

You can try out different things for these - we have given some suggestions below. Note that you may have to abort an existing simulation to allow some of the changes we have mentioned e.g. to the packing box. You can change the number of particles, or the packing regime, without needing to abort the previous simulation.

12.1 Spheres

In this example, we have set up a Gaussian distribution of spheres of diameter of 1 and standard deviation 0.2. (If you double-click on the Spheres line, you will get the Object class parameters window which shows you this.) We have chosen to pack 60 objects into a 2D box which is 10 units long in each of the x and y directions. The 'gravity'pack option has been selected.

Running this example will give a packing fraction of about 46%. If you Visualize the system (use either the 2D or 3D visualiser) then you will see that the particles are at the bottom of the box, randomly packed.

Some interesting things to try included the following:

(a) Select the Process options and pick Settle Objects. Set the Number of drops to 5 and settle along the y axis. Start the settling process with the Start button. In the first 'settle', nothing much will happen, since the gravity packing will have ensured everything is at the bottom) and they will then be thrown to the top of the box, and settled again, five times.

Pick the Start option, and let **MacroPac** carry out the five 'drop and settle' steps. Now, if you visualize again, you will see that, in general, the larger particles have segregated to the top.

(b) Change the Box parameters to look at a 3D box. Toggle 3D on, and you will see that the z-direction parameters become active. Leave the size at 10, and make the z boundary conditions periodic. (You will see that when you change one of the z parameters to periodic, the other changes automatically.)

The 60 objects we packed are not many in a 3D box, so go into the General parameters and increase this to about 600.

Then, carry out the packing, visualisation, and processing (Settle Objects with 5 drops) as before.

You might also want to try to changing the box size, changing the boundary conditions, or changing the packing regime from 'gravity' to 'shake' or 'static'.

12.2 Cereal

This case has two plate-like species 'cereal1' and 'cereal2' and one spherical object- the 'raisins'. We have chosen them to be packed in equal numbers, but you can change this Target Fraction if you wish.

The 3D packing box has dimensions 7.5, 10 and 7.5, and the walls were chosen to be hard boundaries in each case. The Packing parameters show that 200 particles are being randomly packed.

200 particles gives a volume fraction of 12%. The Visualization (3D Visualization is best here) will show that the box is pretty evenly packed by this random packing.

Some interesting things to try include:

(a) taking the packed box, and choosing Settle Objects under the Process menu. Make sure the Number of drops is set to 0 (if you have set it to a different value for the Spheres example, or another case, **MacroPac** will have retained this value) and Settle along the y directions, then press the Start button. Once the process is complete, then visualize again. You should see that the particles are now occupying the bottom of the box.

At this stage a number of options are open to you. For example, you can shake the box (see Example 12.1) to see the segregation effects. You can go back to the Packing menu to increase the number of particles, and continue packing. Explore for yourself some of these possibilities, or try out some new ones of your own.

If you do decide to look at segregation, you might want to look at the distribution of each particular type of class. At the bottom of the Results menu, you can look at Active Classes. By making each of the classes active separately, you should see more clearly that the larger particles are at the top.

(b) without settling, just go into the packing menu and increase the number of particles, to some large number. Then Resume the simulation. A few more particles will be packed, but packing fractions will rise only to about 15%. You can of course settle or translate the objects, as described in (a) above.

12.3 Fibres

Fibres are set up as long thin plates, as you can see by double-clicking on one of the blue items in this line, to get the Object class parameters window. Here, we have set up fibres which are all the same length.

The simulation box has been set up to be two-dimensional, 5 units in the x direction and 20 units in the y direction. Hard walls have been chosen in each case - you can change this if you want to. We have set this example up with static packing, with 50 fibres to be packed.

If you run the simulation, you will see that about 23 particles are packed before the program stops because the Number of misses reaches 10,000. If you simply hit Resume at this point, you should find that one or two more particles is packed. Packing fractions are about 35-38%.

If you visualize the system, you will see that the fibres show local orientation. You can perform an orientation analysis (since this is a 2D box). This should show that most of the particles are reasonably well aligned. You can also perform a density analysis, which will probably show a reduced density near the walls of the box.

Some interesting things to try:

(a) Increase the number of particles, and make the simulation box a 3D box. You will probably see a significant decrease in the volume fraction of packed particles, since the fibres are no longer restricted to packing in a plane.

(b) Translate the particles, or settle them, in a particular direction, and compare this with the case when they are not settled.

(c) Change the packing regime to 'shake' pack, with a force along either the x or y axes.

12.4 Diamonds

This example shows how some more unusual shapes can be represented. The 'diamonds' are plates with a non-perpendicular internal angle.

Our starting box is a simple 2D box, with hard walls, and dimension 10 in each direction. The object we use is a plate with omega angle 60 degrees. We use uniform distribution of object size between 0.5 and 1.5, with fixed aspect ratio.

Once again, changing the box and boundary conditions can be an interesting thing to try. So can settling or translating the objects, as described above.

13. The Diffusion Module

MacroPac-Diffusion is *not* a standalone package, and it can only be launched from **MacroPac** itself. However, because it is a separate module, **MacroPac-Diffusion** has its own menu items, described in more detail below.

Note that displaying the box grid slows the simulation significantly, since it takes quite a bit of system resource. Therefore, it is recommended that the window is closed (click on **x** at the top right hand corner) while running a simulation. You can get the box grid back again by selecting **Display Box Grid** from the **Parameters** menu.

13.1 The File Menu

The **File** menu has only one item, **Exit**. Use this when you wish to close down the **Diffusion** module.

13.2 The Parameters Menu

The **Parameters** Menu has two items. The second of these, **Display Box Grid**, is used to get the box grid back on screen if you have dismissed it to speed up the running of the simulation (see above).

The second menu item is **Simulation**. Selecting this gives the **Simulation parameters** window. Within this window you are given options on how you want to handle the simulation, as well as information on the box which was set up in **MacroPac**. Once you have set up the parameters you want, clicking on **OK** will make them take effect.

The box lengths are taken directly from the **MacroPac** input, and are not adjustable. Note that you can change the box boundary conditions, though.

Simulation Parameters

Number of runs describes the number of times that you wish to run the simulation. Typically, to get meaningful results on diffusion, this value should be set on the order of several hundreds. If the number of runs is greater than one, then each run will be given a different starting point (random seed) and the results will be run-averaged automatically.

Number of steps per run determines how long each simulation will run. A step occurs each time a particle (or a head or tail, if the diffusing particle is a chain) attempts to move, regardless of whether the move is successful. Therefore, the number of steps can be regarded to be proportional to the time for which the particle has been diffusing.

Particle length (grid units) is the length of the chain used in the simulation. If you are simulating diffusion of a single particle (for example, for small molecules, or for thermal or electrical diffusion) then this value should be one. However, if you are modelling diffusion of a polymer, then enter the size of the polymer in grid units. (The grid units are specified in the **Fixed parameters** box.)

Starting random seed determines whether the results are randomized. If the starting random seed has the same value in two runs, then the simulation will start in the same place, and will give identical

results. If you want the simulation to be random, then set this value to zero. Note that if you are doing multiple runs, then run-averaging will be implemented and the random seed will be randomized for every run following the first.

Box parameters

These parameters are given in the box at the top right of the **Simulation parameters** screen. Some of these parameters are fixed - i.e. they are determined by the data passed to the **Diffusion** module from **MacroPac**, and are not editable within the **Diffusion** module. The box dimensions and **Mode** (whether it is a 2D or 3D box) are the values specified in **MacroPac**. The grid unit size is found by dividing the longest box dimension by 100, the number of grid points on this side.

The initial boundary conditions are defined by the conditions set up in **MacroPac**, but they can be changed by the user.

Matrix-Object Properties

By definition, the particles are defined as the Objects and the rest of the space in the simulation box is the Matrix. Therefore, matrix points are the void grid points that fall outside the packed objects. Object points are filled points that fall inside the packed objects. The **Matrix-Object Properties** determine how the simulated particle reacts to collisions with filled or void grid points.

In **Conductor-Insulator** mode, a particle starts at a void point, and can only move to other void points. That is, the matrix behaves as a conductor, and the objects are perfect insulators.

In **Conductor-Conductor** mode, a particle starts in either a void or a filled point, and can move to other void and filled points. Both the objects and matrix are conductors, and in this version of the program they are assumed to have the same conductivity.

In **Insulator-Conductor** mode, a particle starts in a filled point, and can only move to other filled points. This mode is useful in highly packed systems where many packed objects are touching, since then particles can diffuse from one object to another. The objects are conducting, and the matrix is a perfect insulator.

In **Conductor-SuperConductor** mode, a particle starts in a void point and can move to another void point. When it hits a filled point (one in an object) it accelerates along a random vector, and is placed at the next void point along that vector. The matrix is a conductor, and the objects are super-conductors.

13.3 The Walk Menu

The items under the **Walk** pull-down control the starting and stopping of the simulation. The first item, **Status**, produces the **Walk status** window. There is also a Toolbar icon that has the same effect.

The **Simulation status** will be one of **Ready**, **Running** or **Stopped**. While the simulation is running, the **Start** button will display **Stop** instead. If you stop the simulation, the button's display will change to **Resume**.

Run, in the form M/N, tells you that the simulation is currently the Mth run of the N requested runs (as set up in the **Simulation parameters**).

Number of steps tells you the number of movement steps (both successful and unsuccessful) which have been undertaken in this run.

Efficiency shows the percentage of successful moves compared to the total number of steps taken.

The second item under the **Walk** menu is **Start**. Selecting this produces the **Walk status** window described above, and starts the simulation running. Again, there is a Toolbar icon (with large green arrow) which performs the same job.

Finally under the **Walk** menu, you can **Abort** the simulation. This option is greyed out unless a simulation is running, of course. There is also a Toolbar icon for **Abort** - the small skull-and-crossbones. Aborting the simulation will cause all the results to be lost, so should only be done when

you are finished with a particular run. If you have produced reports or plots from this simulation, they will not be lost, but the results that generated them will be.

13.4 Results

The **Results** menu gives access to three plots, and to the **Report** generated in spreadsheet form. This **Report** recaps on the information used for the simulation, and then includes the calculated results - run-averaged, if multiple simulations were performed. Reports can be kept available after you abort a simulation, although of course they cannot be regenerated since aborting the simulation leads to the loss of the necessary information.

While the **Report** is on-screen, you will have access to a **Spreadsheet** pull-down menu, described below.

The **Average end to end distance** is only relevant if you have a diffusing chain, rather than a point. In that case, it is averaged over the course of the simulation and over the number of runs that have been used. That is, it is effectively the average of the **End to End Distance** plot.

Two values of the **Effective Diffusion Coefficient** are displayed. The first is obtained from the **Diffusion Coefficient** plot - in this plot, at each point the diffusion coefficient is calculated as:

$$D_{\text{eff}} = R^2 / (2dN)$$

where R^2 is the squared offset, N is the number of steps at this point (i.e. related to time) and d is the number of dimensions of movement (2 for a 2D box and 3 for a 3D box). The average of the Diffusion Coefficient plot is therefore the average value of the diffusion coefficient over the course of the simulation, and over the number of simulations which have been run.

The second value is obtained from fitting a line to the Squared Offset plot. The gradient of the line is

$$G = \langle R^2 \rangle / N$$

and the diffusion coefficient is

$$D_{\text{eff}} = G / (2d)$$

In general, this second value should give a better value. Provided the simulation is averaged over many runs, the two values should be very similar. As our single-run result above shows, they can be quite different unless many runs are averaged. However, over many runs, the values should converge.

Plots include the **End to End Distance**, the **Squared Offset** and the **Diffusion Coefficient**. For the **Squared Offset**, eight lines are plotted, including the overall squared offset, and the squared offset for each of the x, y and z directions, and the line fits for each of the previous four lines. For the **Diffusion Coefficient**, four lines are plotted: the overall effective diffusion coefficient, and the value in each of the x, y and z directions. The values are those averaged for that many steps in the simulation and for the number of runs done. While a plot is on-screen, you will have access to a **Plot** pulldown menu, described below.

You have options for controlling the plots. Holding the left-hand mouse button down and dragging across the plot, within the plot area, will highlight a selection of the plot. When you release the mouse button, the plot will zoom to show this area. So, to zoom to a particular portion, move the mouse pointer to the start of the region you wish to examine, press the left mouse button and hold it down as you drag across to the end of your desired region. If you try to zoom beyond the resolution of the data, you will be informed of this, and asked if you wish to reset to the default range.

By holding down the right mouse button in the plot area, you will get access to several options:

Replot returns the plot to its original form, before any zoom

- Grid** superimposes a grid on the plot. This is toggled on whenever there is a small tick beside Grid. To remove the grid, simply untick it by selecting it following a right-button mouse click.
- Symbols** by default are switched on. If you wish to toggle them off, select this item to remove the small tick.
- Free Zoom** allows you to zoom in both x and y directions. If you want to return to the default x-axis-only zoom, toggle this item off.
- Time Stamp** puts a note of the date and time at the top right-hand corner of the plot.

Plots remain available after you have aborted a simulation, although of course they cannot be regenerated since the relevant information is lost when **Abort** is executed. If you have two plots which you wish to view side by side, the **Tile** option of the **Windows** menu can do this.

13.5 The Box Grid Menu

This menu is only active while the box grid is displayed. It lets you **Copy** the box grid into the Windows Clipboard, as an alternative to using the *Alt-PrtScr* keys. It also allows you to choose whether to display the box grid as points (the default) or as cubes. Display with cubes can take quite a while to generate.

13.6 The Spreadsheet Menu

As discussed previously for **Reports**, this menu is only active when a spreadsheet-enabled **Report** is displayed. It lets you **Copy** the report into the Windows Clipboard (from where it can be pasted into a standard spreadsheet package), or save the text to a file. It also allows you setup your printer (**Printer Setup**), **Print Preview** and **Print** the report.

13.7 The Plot Menu

This menu, which is only active while you have a plot on-screen, allows you to **Copy** the plot to the Windows Clipboard, and to set up your printer, preview the printed results, and print.

13.8 Exiting from *MacroPac-Diffusion*

You must specifically execute from *MacroPac-Diffusion* using the **Exit** command under the **File** menu. Exiting from the main *MacroPac* program will not close the **Diffusion** module.

We hope that the above information and examples will allow you to experience some of the power of **MacroPac**, to see how it can be applied for some of your own applications. If you have comments or questions, please send them to sales@oxmat.co.uk.