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Particle Analytics Manual

This is the summary of the documentation.

- Installation
- Pre-Processing
- Post-Processing
- Licensing

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Installation

For the installation of GiD, please download and follow the instructions in the GiD web page: http://www.gidhome.com/download.

- Extract the compressed file of P4 into GiD problemtypes folder, located in the GiD installation folder. (The folder location can change depending of the GiD installation)
 - Linux: /usr/local/lib/GiDx64/11.0.5/problemtypes
 - Windows: C:\ProgramFiles\GiD\11.0.5\problemtypes
- Open GID and get the machine information appearing at Register Problem Type window (Help > Register Problem Type)
- Ones you have received your P4 licence, enter the password in the Register dialog box.
- Restart GiD and select P4 problemtype in the GiD menu (Data > Problem Type > P4) to Start to work with P4.

Note:

If you have an USB compatible with GiD connected to the computer, you must choose "Local machine" sysinfo - Choose the P4 problemtype and use the information displayed to request your P4 licence. The password will be sent to the email address provided in the form.

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P4 Pre-processor - User Manual

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Introduction

In most cases where DEM is used, it is necessary to carry out some averaging of the data to a more representative scale of what is required. As such it is quite common for spatial averaging, temporal averaging or both to be applied to the DEM data. To aid the process, a toolbox for the processing of DEM data both temporally and spatially has been implemented in the University of Edinburgh. The toolbox has been developed to support many codes such as EDEM, PFC, DEMPack and LAMMPS and provides a simple interface for the averaging process for the large datasets that DEM simulations produce. The toolbox provides both a coarse graining method for projecting the results on to a continuum field and a binning method. A study of the effect of both temporal and spatial averaging using this toolbox is presented in [4] and some of the results are shown in Figure 1.1. Full details of the methods implemented in the toolbox are available in several papers [1, 2, 3, 5]. The coarse-grained density ρ is provided by equation:

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where r is a point in space where the values are to be evaluated, $r(t)_i$ is the vector of the centres of mass of the particles at a given timestep t , and ϕ is the coarse graining function which is subject to the condition of its integral over space being unity.
The coarse-grained velocity V is provided from equation
where ${\bf p}$ is the coarse-grained momentum density.
The stress tensor is given by equation
where $f_{-ij\alpha}$ is the interaction force between two particles, $r_{-ij\beta}$ is the branch vector, s is the integral of the branch vector and v' is the fluctuating velocity of the particle.
Figure 1.1. P4 toolbox in use - Post-processing on a fluidised bed [4]. a) Particles visualization. b) Spatial averaged density. c) Spatial and temporal averaged density over 20 sec.

The P4 Toolbox is implemented within GiD, which is a pre and post-processor software package for numerical simulations. Detailed manuals for GiD are located at http://www.gidhome.com/support/manuals while some tutorials are available at http://www.gidhome.com/support/tutorials. GiD is available on a selection of computers but a trial version of the software can be downloaded and used for a three month period on any computer.

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Introduction

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$$\rho(\mathbf{r},t) = \sum_{i} m_{i}\phi(\mathbf{r} - \mathbf{r}_{i}(t))$$

where r is a point in space where the values are to be evaluated, r(t) is the vector of the centres of mass of the particles at a given timestep t, and ϕ is the coarse graining function which is subject to the condition of its integral over space being unity.

The coarse-grained velocity V is provided from equation

$$V(\mathbf{r},t) \equiv \mathbf{p}(\mathbf{r},t)/\rho(\mathbf{r},t)$$

where \mathbf{p} is the coarse-grained momentum density.

The stress tensor is given by equation

$$\sigma_{\alpha\beta} = \frac{1}{2} \sum_{i,j} f_{ij\alpha} r_{ij\beta} \int_0^1 ds \phi(\mathbf{r} - \mathbf{r}_i + s \mathbf{r}_{ij}) - \sum_i m_i v'_{i\alpha} v'_{i\beta} \phi(\mathbf{r} - \mathbf{r}_i)$$

where $f_{-ij\alpha}$ is the interaction force between two particles, $r_{-ij\beta}$ is the branch vector, s is the integral of the branch vector and v' is the fluctuating velocity of the particle.

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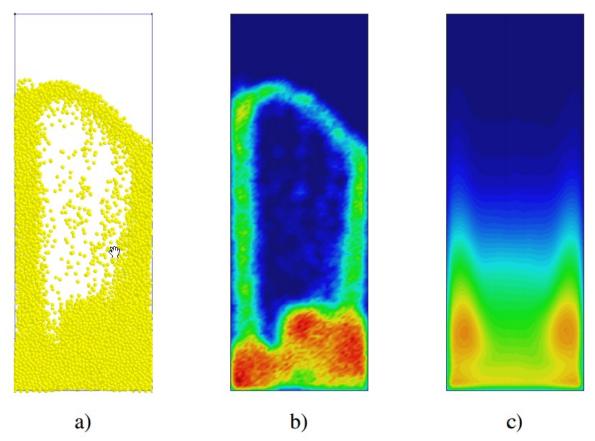


Figure 1.1. P4 toolbox in use - Post-processing on a fluidised bed [4]. a) Particles visualization. b) Spatial averaged density. c) Spatial and temporal averaged density over 20 sec.

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Preparing post-processing

Once the P4 problemtype is started, GiD will display a new toolbar at the left (or top) of your GiD main screen, as shown in Fig 3.1.

Geometry Data Meshing Files View

Postprocess

x=6.6323 y=-0.15947

Quit escape

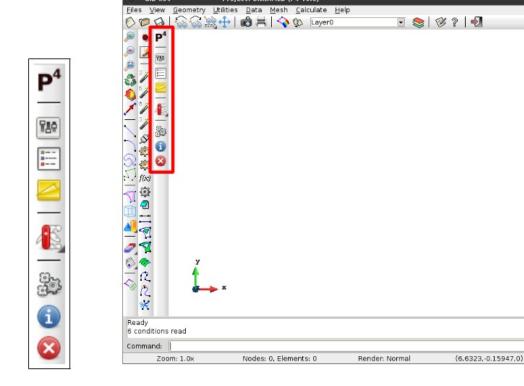
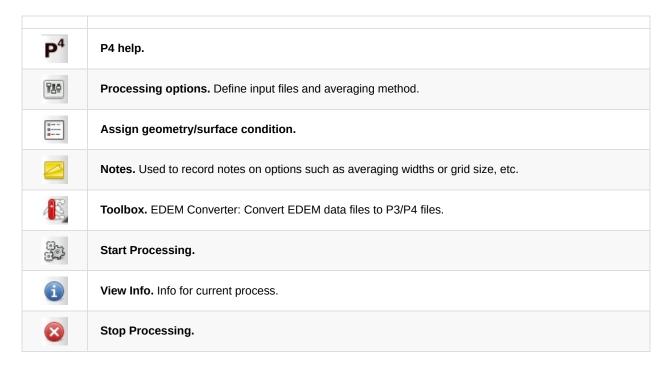


Figure 3.1. Example of P4 Toolbox within GiD.

The description of the different commands in the toolbar is presented below:



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- Generating a model
- Processing options
- Assign geometry/surface condition
- Notes
- Toolbox
- Processing control

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Generating a model

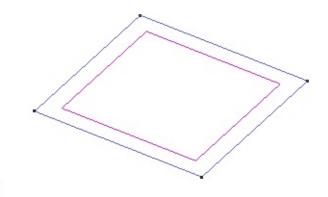
The GiD preprocessing capabilities allows the user to generate and import the geometry and/or mesh to be used for the analysis.

To import a geometry or mesh, different format are accepted. The most common format for geometry are *IGES*, *PARASOLID* and *DXF*. A detailed explanation of the import procedure can be found in: Menu > Help > Tutorials > Importing Files > Importing in GiD.

To generate a geometry from the scratch on GiD, the toolbar *Geometry & View*, located at the left of the screen can be used, or through the menu: Menu > Geometry . The detail of all available geometrical operations (generating, manipulating and deleting entities) can be found in: Help > Preprocessing > Geometry Menu . A useful command for simple geometries is the generation of geometrical objects, where the most common objects can be created in a simple way: Menu > Geometry > Create > Object .

Below, an examples of the required command to generate a cube (2.0 x 2.0 x 2.0) is presented:

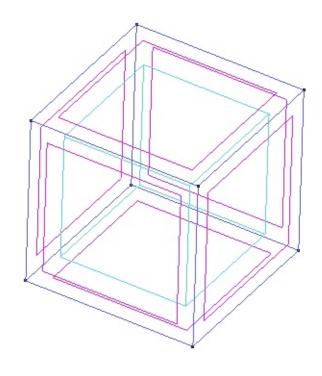
- Select the basic geometry: Geometry > Create > Object > Rectangle
- First corner point: (0.0 0.0 0.0). Second corner point: (2.0 2.0 0.0). Press ESC keyword to finish.



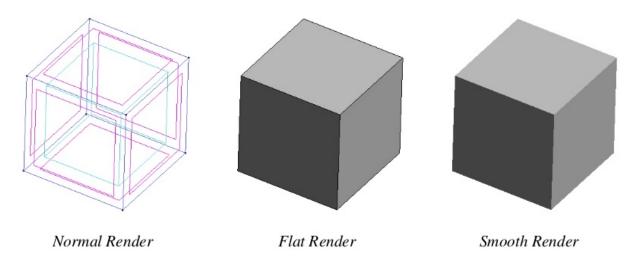


- Extrude the square to generate a cubic volume: Menu > Utilities > Copy .
- In the *Copy* windows, select: Entity = Surface, Tansformation = Translation, Do_Extrude = Volumes, First point = (0.0 0.0 0.0), Second point = (0.0 0.0 2.0).
- Press Select and with the mouse click over the surface in the screen. Press Finish to finish or ESC.

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• To change the render of the geometry use Menu > View > Render or the Mouse Menu (right button).



Meshing the geometry

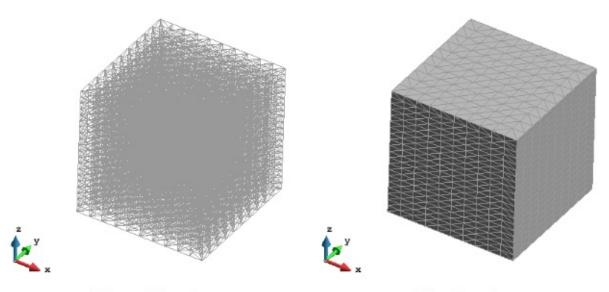
Ones the geometry is created, can be discretized using different unstructured, structured or semi- structured mesh elements. The detail of all the meshing options can be found in <code>Help > Preprocessing > Mesh Menu</code>.

Using the previous example, the instructions to generate a structured mesh of tetrahedral elements with 10 elements in X and Y directions, and 20 elements in Z direction:

- Select structured mesh: Menu > Mesh > Structured > Volume > Assign number of cells.
- With the mouse, click the volume in the screen ().
- Enter the number of cells/elements in for X and Y directions: 10, and Assign clicking over one line following X direction and one line following Y direction. *ESC* to finish.
- Enter the number of cells/elements in for Z direction: 20, and Assign clicking over one line following Z direction. *ESC* to finish.

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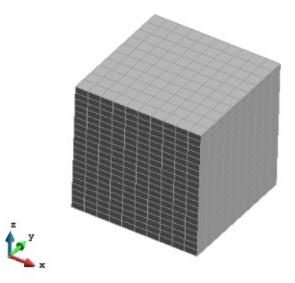
- Generate the mesh by: Menu > Mesh > Generate. As the structured condition for the mesh has been assigned over the geometry, the *Element size* asked in the *Mesh generation* windows will not have effect over our mesh. Click OK.
- Ones the mesh is generated, click *View mesh* to visualize the mesh. Change the render to *Flat* for a better visualization of the mesh.



Nornal Render

Flat Render

• The tetrahedra is the default type of 3D element in GiD. To use Hexahedra (Prism is reserved for semi-structured meshes), change the element type in: Menu > Mesh > Element type > Hexahedra, and click over the volume to assign the type and ESC to finish. Now generate again: Menu > Mesh > Generate.



Note:

- For the processing with P4, structured or semi-structured meshes are recommended.
- The element/cell size do NOT have any influence in the precision of the averaged values, and is just related with the resolution (number of points) of the mesh where the values are projected.
- As the resolution of the averaged values is just related with the amount of points/nodes in the mesh, can be useful the use of quadratic elements in the mesh to minimize the number of elements required maintaining the number of nodes. This is useful to decrease the output file size and for a better visualization. To activate the quadratic elements: Menu > Mesh > Quadratic type > Quadratic.

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Processing options

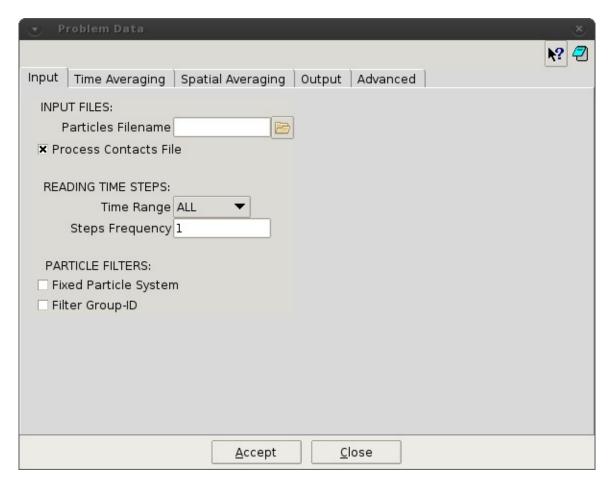
This is the main P4 processing control setting. It is used to define the input files, averaging parameters, and output options.

Frames:

- Input
- Time Averaging
- Spatial Averaging
- Output
- Advanced

Input

This section is used for the definition of the particles files to be processed. The files can be selected and filtered by time ranges, steps frequency and particle groups.



INPUT FILES

- Particles Filename. This options allows the user to chose the input (.p3p/.p4p) file to be processed. In the case of the experimental liggghts dump file, the file extension expected is (.p).
- Process Contact Files. [on/off] This options activates the processing of particle-particle and particle- wall contact files if they are detected. P4 assumes that contact files have the same name that the particle files, with extensions .p3c and .p3w

READING TIME STEPS

- **Time Range.** [ALL / CUSTOM] This option allows the user to chose all time steps in the input files (ALL), or define a custom time range (CUSTOM).
- TimeStart. When CUSTOM Time Range is chosen, define the time to initiate the input file processing.
- TimeEnd. When CUSTOM Time Range is chosen, define the time to finish the input file processing.
- Steps Frequency. Chose the frequency for reading the time steps from the input files.

PARTICLE FILTERS

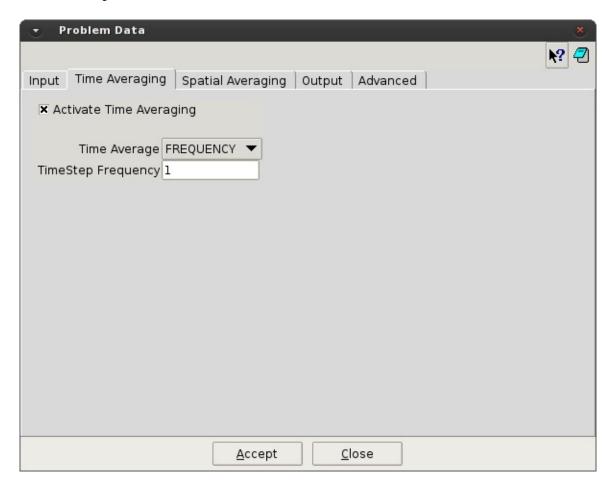
• Fixed Particle System. [on/off] Indicate to P4 that the number of particles and IDs are fixed for the duration of the

simulation being analysed.

- Filter Group-ID. [on/off] This option is used to indicate that a specific group ID of particles will be processed.
- Use Group-ID. When Filter Group-ID activated, indicate the group ID of particles to be processed.

Time Averaging

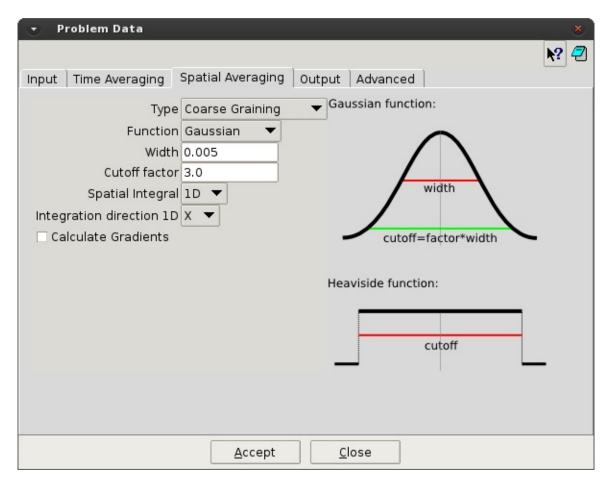
This section allows the activation of the temporal average processing. The average can be chosen for all the results loaded or local time ranges.



- Activate Time Average. [on/off] This option activates the averaging process in the time domain.
- **Time Average.** [ALL / FREQUENCY] Chose if the time average will be performed over all the simulation (ALL) or using a local time average for a number of time steps (FREQUENCY).
- TimeStep Frequency. The number of steps used for the local time average.

Spatial Averaging

this section is used for the definition of the spatial average processing. Allows the user chose between Binning (cell-based averaged values) or Coarse graining (point-based average values), and for the case of Coarse graining, activate the calculation of gradients and spatial integrals.



- **Type.** [Coarse_Graining / Binning] The type of spatial averaging can be chose as Coarse Graining or Binning. (See below for details)
- Function. [Heaviside / Gaussian] When Coarse Graining is chosen, the spatial average function can be chosen between Heaviside and Gaussian functions.
- Width. For Gaussian function, the Width is the standard deviation of the function.
- Cutoff factor. For Gaussian function, the Cutoff factor define the total length of the function, as a factor (>1) of the standard deviation. As the Gaussian function is infinite, the cutoff will define the maximum range of action for the spatial average.
- **Cutoff.** For Heaviside function, the Cutoff defines the range of action of the function to consider the surrounding particles in the spatial average.
- Spatial integral. [NO / 1D / 2D] Allows the user to perform the integral of the spatial average. In 1D integral, all the particles in the integral direction are used to compute the spatial average, resulting in a projection over the plane. In the 2D integral, all the particles in the range of the integral planes are used to perform the spatial average, resulting in a projection over the line. [NEED A BETTER EXPLANATION]

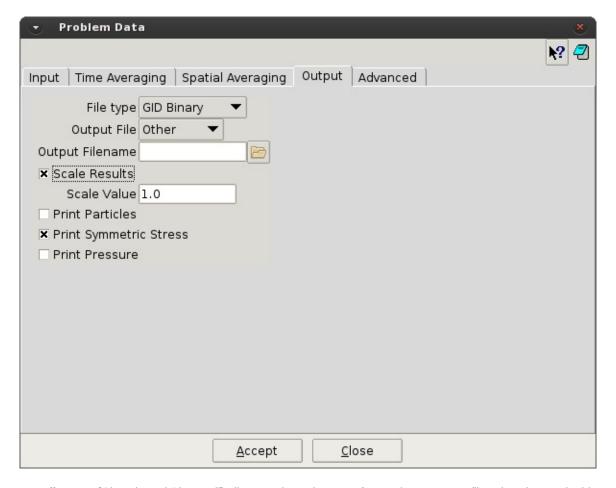
- Integration direction. [X / Y / Z] When Spatial Integral 1D activated, define the integration direction.
- Integration plane. [XY / YZ / XZ] When Spatial Integral 2D activated, define the integration plane.
- Calculate Gradients. [on/off] Activate the calculation of spatial gradients during the averaging process. The gradients will be chosen in results menu for the standard results: Density, Solid fraction, Momentum, and Velocity.

Note:

- For most of the cases, the use of Coarse_Graining averaging procedure with Gaussian function is recommended. Binning averaging and Coarse_Graining with Heaviside function are used just for special cases, because their limitation of capabilities.
- For the Gaussian function, the values of Width and Cutoff_factor are problem dependent, but for quasi-static problems or low speed flows a Width of 2.5-3.0 times the average particle radius can be considered a safe value. For high speed flows and high sampling frequencies, this value can decrease until 0.5 times the average radius. The Cutoff_factor of 3.0 can be considered safe. In case of high speed flows or sampling frequencies, this value can decrease to obtain a better resolution close to the boundaries.

Output

This section is used to define the output generation from P4. Allows activate the particles/contacts visualization files, activate special results or scale the results.



- File Type. [GiD_Binary / GiD_Ascii] Allows to chose the type of output/post-process file written in P4. The binary file reduce the file size, but no problems can be checked in the file. The Ascii file, allows to access and read the results directly in a text editor, but increase the file size.
- Output File. [Default / Other] Allows the user to use the default name for the output file (DEFAULT) or define a
 different one (OTHER).
- Output Filename. When Other Output File is chosen, define the user name for the output/post-process file.
- Scale Results. [on/off] Used to scale the results of P4. This option, combined with the spatial integrals, is useful to calculate the average in a certain direction or plane.
- Scale Value. When Scale Results is activated, define the value used to scale the results.
- **Print Particles.** [on/off] Used to write an extra output file with the particles information. This is required to visualize the particles in the post-processor, but increase the processing time.
- **Print Particles Contact.** When Print Particles is activated, this option is used to add the contact information in the particles output file.
- **Print Symmetric Stress.** [on/off] Normally, the stress calculated in P4 produce a non-symmetric tensor and the 9 components of the tensor should be written. This option is used to force the symmetry in the stress tensor, and just 6

components are required.

• Print Pressure. [on/off] This option is used to write the hydrostatic pressure of the contact stress tensor, defined as

$$p = \frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$$

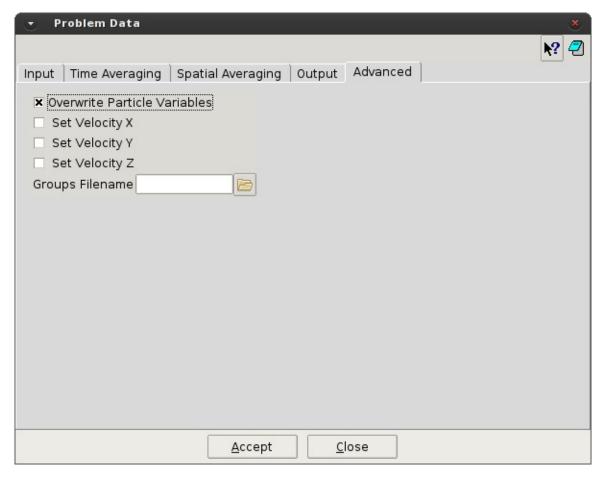
NOTE:

The most common use of the Scale Results option are:

- The change of units in the model.
- The calculation of the average value in a certain direction/plane. This is performed in combination with the 1D/2D integrals.

Advanced

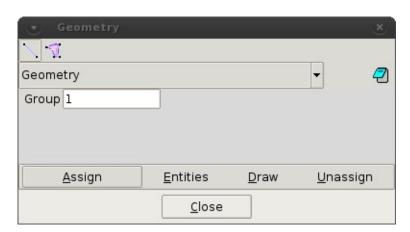
This section give access to advanced features of P4, like overwrite particle variables or groups.



- Overwrite Particle Variables. [on/off] Allows the user to overwrite certain variables from the particle files. At the moment, just the velocity can be overwritten.
- **Set Velocity_[X,Y,Z].** [on/off] When Overwrite Particle Variables is activated, allows the user to chose the component of the velocity vector to be overwritten.
- **Velocity_[X,Y,Z].** When Overwrite Particle Variables is activated, the value of the velocity used to overwrite this velocity component.
- Groups Filename. Define a file used to overwrite the particles group-ID in the particles file.

Assign geometry/surface condition

This command allows the user to select elements/surfaces that are physical walls, for the calculation of pressure and drag force.

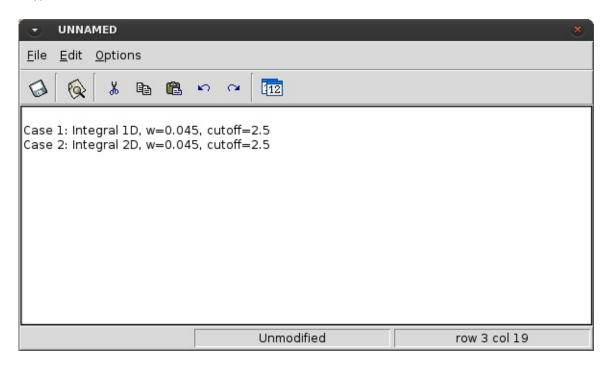


The condition can be assigned over lines () or surfaces ().

• Group. This option allows to assign the line/surface to a different group for the post-process.

Notes

This option allows the user to add notes related with the model. It is useful when working with large models where much information is defined or when working with a set of models where just one parameter (i.e. the material density or the time step) differs from each other.



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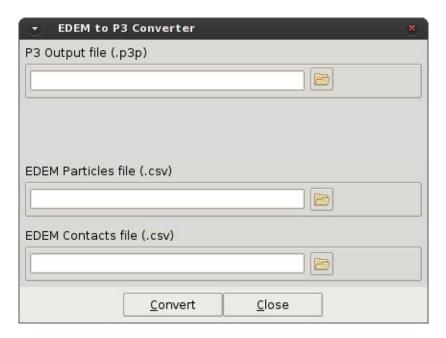
Toolbox

This option give access to the user to different tools defined for the pre-process. Currently just the converter from EDEM exported files to P4 file format are available.

Convert: EDEM to P3Convert: EDEM to P4

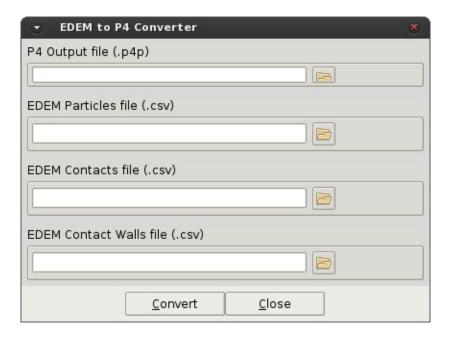
The main difference between each option is related with the use of non-spherical particles in the simulation. The previous version of the file format (P3 format) assume spherical particles in the DEM simulation, while the new version (P4 format) allows the use of non-spherical particles, providing extra information in the contact files, through the use of a API mechanism in EDEM. For more details, please see Appendix A for the converters, and Appendix D for the explanation of the different file formats in P4.

EDEM converter for spherical particles:



EDEM converter for non-spherical particles:

Toolbox 26



Toolbox 27

Processing control

The process control is defined by 3 main commands to execute (), show info () and cancel () the execution of P4.

- Start Process. Initiate the processing of the simulation results. Check the setting and launch the process.
- View Run Info. Shows a window with the evolution of the process, as in Figure below.

```
output info for 'current'
 reading pap/pac/paw rires... crmescep: 4.2403
reading p4p/p4c/p4w files... timestep: 4.2484
reading p4p/p4c/p4w files... timestep: 4.2485
Output file printed.
reading p4p/p4c/p4w files... timestep: 4.2486
reading p4p/p4c/p4w files... timestep: 4.2487
reading p4p/p4c/p4w files... timestep: 4.2488
reading p4p/p4c/p4w files... timestep: 4.2489
reading p4p/p4c/p4w files... timestep: 4.249 ok.
Output file printed.
reading p4p/p4c/p4w files... timestep: 4.2491
reading p4p/p4c/p4w files... timestep: 4.2492
reading p4p/p4c/p4w files... timestep: 4.2493
reading p4p/p4c/p4w files... timestep: 4.2494
reading p4p/p4c/p4w files... timestep: 4.2495
Output file printed.
reading p4p/p4c/p4w files... timestep: 4.2496
reading p4p/p4c/p4w files... timestep: 4.2497
reading p4p/p4c/p4w files... timestep: 4.2498
reading p4p/p4c/p4w files... timestep: 4.2499
reading p4p/p4c/p4w files... timestep: 4.25 ok.
Output file printed.
reading p4p/p4c/p4w files... finished
Finish!
1
                                  Close
```

Cancel Process. Stop the execution. All the processed result until stop the process can be visualized in the post-process.

Processing control 28

After post-processing: Analysis

When the user start the GiD post-processor, GiD will display a new toolbar at the left of your GiD main screen, as shown in the Figure.

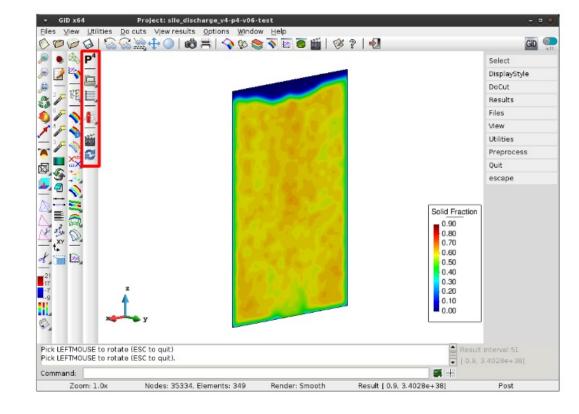
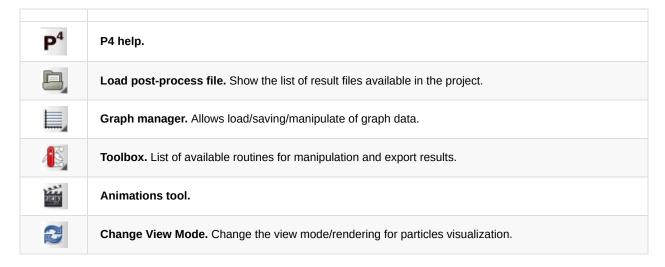


Figure. Example of P4 Toolbar for post-processing results.

The description of the different commands in the post-process toolbar is shown below:



Contents:

- Load post-process file
- Graph manager
- Toolbox for analytrics
- Animations tool

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- Change view mode
- Visualizing particles
- Visualizing averaged results

After post-processing 30

Load post-process file

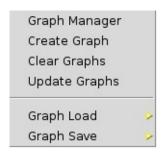
This command shows the list of result files available in the project.

The option [Others...] open the Post-process Read windows to load results in a different folder.

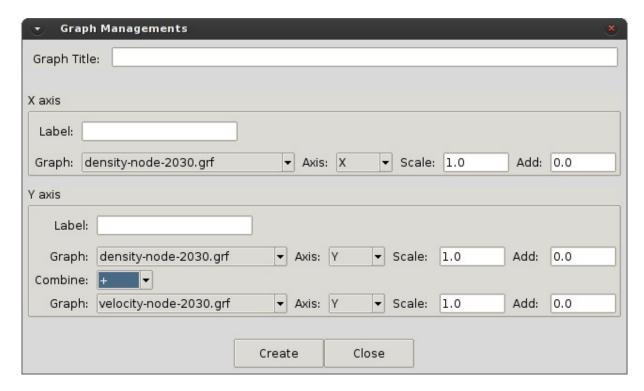
Load post-process file 31

Graph manager

This command displays a sub-menu to create/edit/save graphs.



- **Graph Manager.** Open the Graphs Manager of GiD. (See GiD help on Graphs manipulation: Menu > Windows > View graphs)
- **Create Graph.** Open the Graphs Creation window. This command is used to create a new graph as a combination of existing graphs.

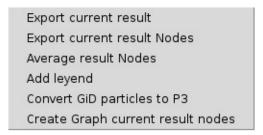


- Clear Graphs. This option clean the graphs buffer in GiD.
- **Update Graphs.** Update the list of graphs in the menu.
- Graph Load. Display the list of graphs available in the project to be loaded.
- Graph Save. Display the list of graphs in the graph buffer (plotted in the graph window) and save the selected graph.

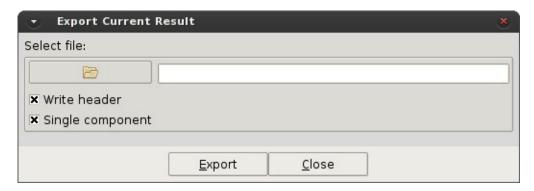
Graph manager 32

Toolbox for analytics

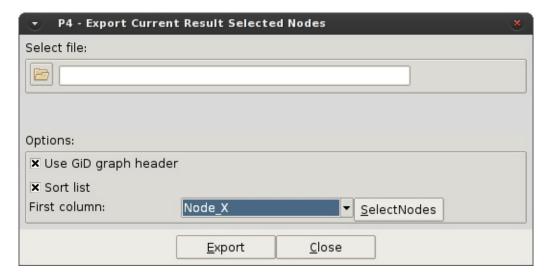
This option display the list of available tools to export/manipulate results defined for the post-process.



• Export current result. This option export in a plain text the coordinates and the selected result for each node in the mesh.

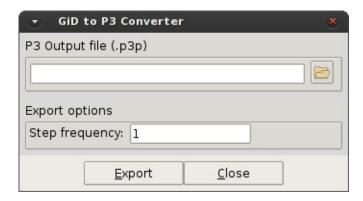


• Export current result nodes. This option exports in a plain text a chosen coordinate/ID and the selected result for a group of nodes in the mesh.

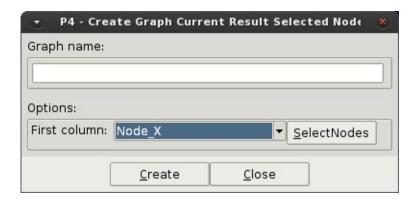


- Average result nodes. The option calculates the average value for the selected result in a user defined group of nodes. The results shown are: Number of nodes for the average, the average value, and the standard deviation of the value.
- Add legend. Display the Comment windows to visualize a legend with the present result. (To see the detailed list of options available in GiD help: Help > General Aspects > Utilities Menu > Tools > Comments > Postprocessing)
- Convert GiD particles to P4. The option write a P4 file with the particle information using the P3/P4 format. This is useful to process old simulations available in GiD post-process format.

Toolbox for analytrics 33



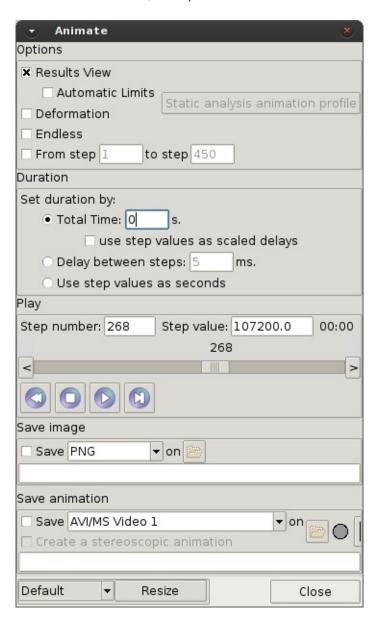
• Create Graph current result nodes. The option generate a graph with a defined group of nodes for the current result, over a chosen coordinate/node-ID. Similar to [Export current result nodes], but sending the information to the graph buffer without write a file.



Toolbox for analytrics 34

Animations tool

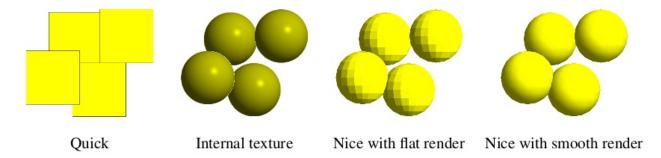
This window lets you create an animation of the current Results View, where the limits can be fixed along the animation with Automatic Limits, and/or an animation of the Deformation of the meshes. To the right of the Step: label, the step value is shown. On the slide bar, the step number is shown.



Animations tool 35

Change View Mode

Change the view mode/rendering for particles visualization. GiD have the ability to use different rendering techniques for the particle visualization. This option automatically change between: Internal Texture, Nice and Quick. For further details, please check the GiD help: Help > Postprocessing > Options Menu > Geometry > Sphere options.



NOTE:

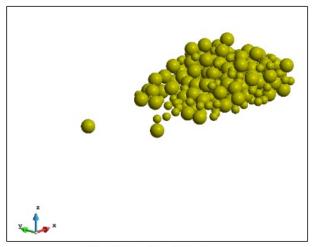
- The recommended view mode for large models is Internal Texture. The Nice view mode should be reserved for small models or special cases due to the high computational cost involved in the rendering.
- When Nice view mode is activated, the render mode can be changed in: Menu > View > Render, or with the Mouse Menu (right button) and Render.

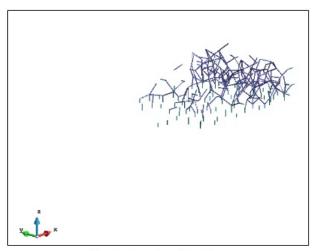
Change view mode 36

Visualizing particles

After activate *Print Particles* in the OUTPUT options of P4 and run the P4 processing, the user can load the particles in the *Load post-process file* section of the toolbar (with GiD in post-process mode). The files containing the particles, and optionally the contacts, have the extension particles after the user defined name.

By default, the Internal-texture visualization mode is activated and both, particles and contacts, are plotted in the screen. The control for activate/deactivate, transparencies and style for the different groups of particles or contacts, the Display Style windows of GiD can be used []. The particles file just contain the information of particles and contacts, and no information of geometry is stored.

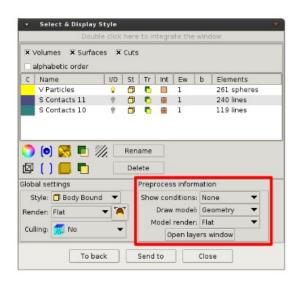


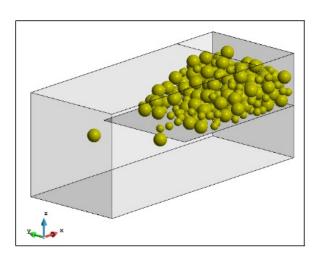


Particle visualization

Contacts visualization

If the geometry or mesh is required in the visualization of the particles, the option *Draw model* in Display Style can be used. This requires to have loaded the geometry/mesh in the pre-processor and transparency/deactivation for the geometry are available through the *Open layer window*.



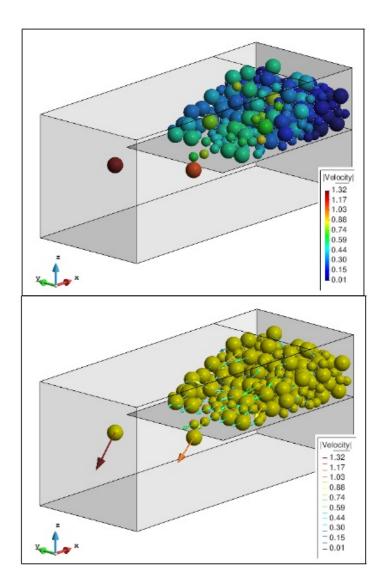


To visualize the particle results, the toolbar *View Results Menu* can be used (Menu > View results), or through the *Results Window* [].

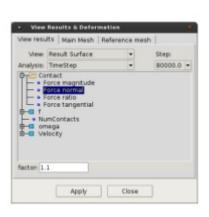
Visualizing particles 37

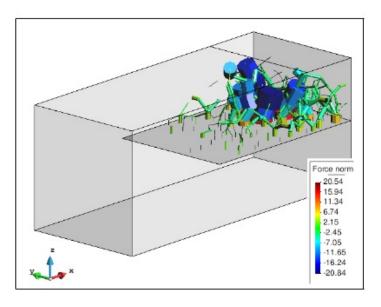






The visualization of the Force Chain with the particle contacts can be performed using the result option *Result Surface*. Please be sure that the contacts are activated for visualization and the particles are deactivated or with transparency.





For more details about the visualization options and capabilities, please check the GiD help in: Help > Postprocessing > View Results Menu.

Visualizing particles 38

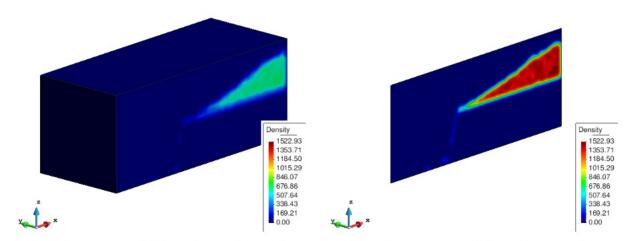
Visualizing averaged results

After the model is processed and the P4 output files are generated, the standard visualization capabilities of GiD can be used, together with a set of special tools and commands specific of P4 for the analysis of the results.

The output file can load the particles in the Load post-process file section of the toolbar (with GiD in post-process mode).

Ones the file is loaded, the different meshes used in the process will appear in the Display Style window. To visualize the averaged results, the toolbar *View Results Menu* can be used (Menu > View results), or through the Results Window [].

Based in the same previous example of particle visualization, the figure below depicted the density projected over a 3D volumetric mesh (Tetrahedra) and a fine 3D surface mesh (triangles) as a slice (XZ) in the middle of the domain.



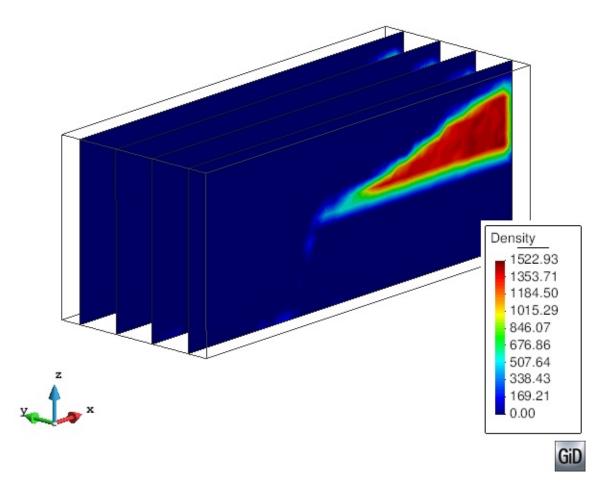
Density contour fill in volumetric mesh

Density contour fill in surface mesh

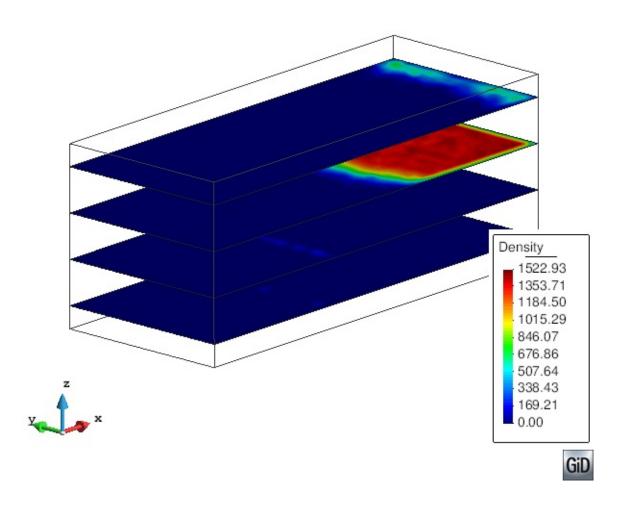
The interior of the volumetric mesh can be visualized through cut planes defined over different directions:

- Menu > Do cuts > Cut plane > Succession.
- Define the cutting axis by two points. Enter first point: (0.0 -0.2 0.0), and second point: (0.0 0.2 0.0).
- Enter the number of cut surfaces along the defined line: 4. Each cut surface will appear as a different layer in *Display Style* window, and can be visualized deactivating the volume mesh ().

Visualizing averaged results 39



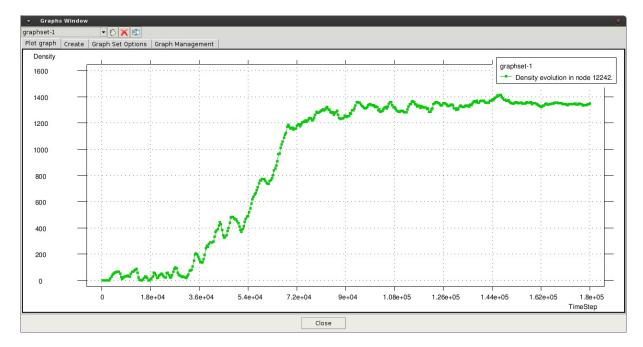
- Activating again the volumetric mesh and deactivating the cuts, it is possible generate new cuts in a different direction
- Selecting a new set of successions in direction Z. First point: (0.0 0.0 -0.2), second point: (0.0 0.0 0.2), and 4 cut surfaces.



Graphs

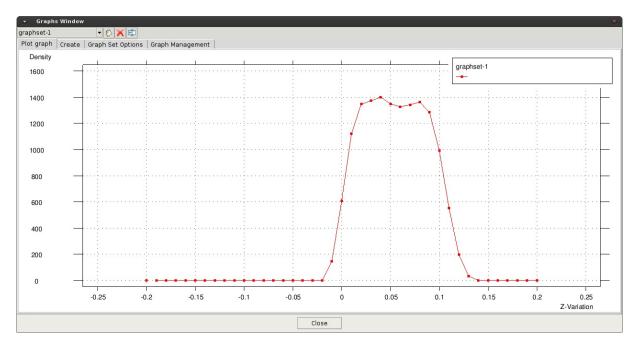
To analyze the results in the mesh, graphs can be generated for the temporal evolution of a variable in a defined point or the spatial distribution of a certain variable. The generation of a graph with the temporal evolution of a variable in a predefined point can be performed by:

- Menu > View results > Graphs > Point evolution > Variable (density) .
- Enter the coordinates of the point: (0.3 0.0 0.05). More points can be entered or ESC to finish.



In a similar way, the spatial distribution of a variable in a defined direction can be plotted:

- Set the spatial direction in X axis: Menu > View results > Graphs > Line graph > Set X axis > Z variation.
- Set the variable to plot: Menu > View results > Graphs > Line graph > Variable (density).
- Enter the initial point of the plot: (0.3 0.0 -0.2), and the second point: (0.3 0.0 0.2). More points can be entered or ESC to finish



The graphs can be modified using the options in the Graph window, or can be used a more specialized software (like MS Excel or Matlab), exporting the graphs as 2 columns ascii files: Menu > File > Export > Graph and select the graph to export, or export all the graphs in the screen.

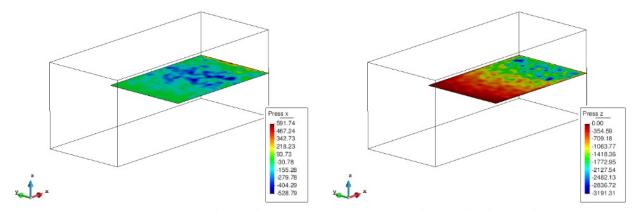
NOTE:

• Explain something about the Integral 1D or 2D visualization...

Pressure/drag force in surfaces

When the user define physical surfaces (geometries), the pressure and drag forces over those surfaces will be calculated during the precessing.

For the previous example, if the condition is applied for the surface in the middle of the domain (the conveyor), the drag forces and pressure will appear in the results menu. In the figure below, the resultant drag force in X and Z directions are depicted.



Contour fill of drag force in X direction

Contour fill of drag force Z direction

Integrals

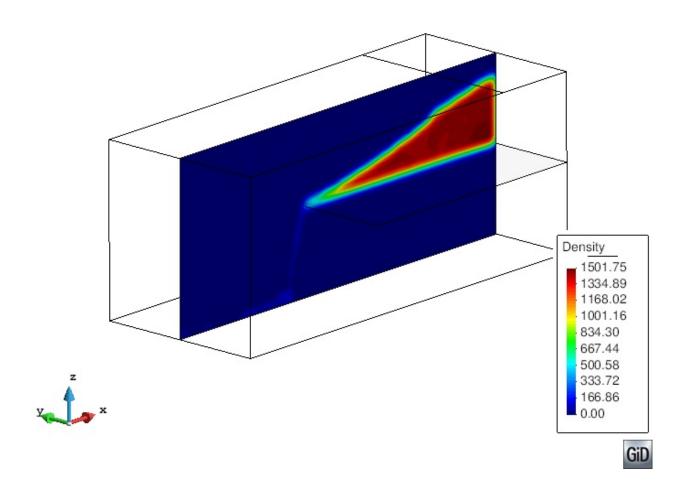
The calculation of the integrals in a direction (1D) or a plane (2D) can be specially useful in certain situations, like the calculation of mass or volumetric flow rate. Other case in which the integral can be used is the calculation of the average values in a certain direction when the results should be uniformly distributed. For this, the averaged results can be projected over a surface, decreasing the amount of information required.

With the previous example, the average density over the Y direction is calculated following as:

- Activate the integral in Axis-Y. In the *P4 Options:* Spatial_Integral = 1D, and Integral_direction = Y.
- \bullet In Output options: Scale Results = yes and Scale Value = 1/L (L is the length in Y direction).
- Generate a geometry (surface) over the plane XZ, considering the dimensions of the domain (the position of the surface in the Y direction is not relevant and any value can be used).

The results of the simulation now can be defined as $\langle \rho \rangle_y$, as presented in the figure

Visualizing averaged results 43



Visualizing averaged results

Using P4 with EDEM

While EDEM has a post-processing tool included in the Analyst, it's abilities are limited. Visualisations and movies can be made easily, but the information displayed is limited to particle properties such as velocity and angular velocity. Force chain networks are also easily visualised with the option to apply colour-maps to the network also.

The graphing tool is limited to plotting a single value at a time. Checking multiple pieces of data requires external post-processing.

In order to calculate stress, strains and other values for an assembly we use the P4 toolbox.

Data Export

EDEM currently does not support exporting directly to the P4 file format so data needs to be exported from EDEM using a normal .csv file with a specific set of queries to provide the necessary data. Details on setting up query configurations can be found in the EDEM manual.

For spherical particles only the P3 file for particles (.p3p) and for all contacts (.p3c) are required. These queries are detailed in A.1. In the case of non-spherical, clustered particles, the ID of the two contacting particles is also required for the output. In this case data files of the P4 type are exported. These are detailed in A.2 for particles (.p4p), particle-particle contacts (.p4c) and for all particle-geometry contacts (.p4w).

In order to provide the ID for particles in contact, an additional API contact model has been written to determine and store the necessary contact data. The **Track_ID API contact model** (available as either a windows .dll file or linux .so file) must be loaded for both particle-particle interactions and particle-wall interactions to generate P4 file types.

NOTE: While it is possible to us the P4 Toolbox for spherical particles using the P3 export configuration, that is the simulation is run without the Track_ID API to reduce the simulation run-time, doing this may lead to errors. Due to the limitations in the export formatting in EDEM, consistent and/or sufficient level of significant figures in the coordinates may lead to the rejection of a certain number of contacts when the exported EDEM file is being converted. The P4 converter will automatically increase the tolerance to accept all particle-particle and particle-wall contact and display a warning message detaining how many ambiguous contacts were found.

The P4 toolbox has the minimum requirement listed in the A.1 and A.2 but also supports additional queries. An example of such additional queries is highlighted in A.1 and A.2 where the queries marked with an * represent additional queries of interest for particle data If the X, Y and Z components are provided, the magnitude will also be calculated and averaged. If all three components are not found the items will treated as individual scalars.

Table 1. P3 Export Queries

P3P File	P3C File
Q01:Total Number of Particles:	Q01:Total Number of Contacts:
Q02:Particle ID:	Q02:Contact Vector 1 X:
Q03:Particle Volume:	Q03:Contact Vector 1 Y:
Q04:Particle Mass:	Q04:Contact Vector 1 Z:
Q05:Particle Position X:	Q05:Contact Vector 2 X:
Q06:Particle Position Y:	Q06:Contact Vector 2 Y:
Q07:Particle Position Z:	Q07:Contact Vector 2 Z:

Using P4 with EDEM 45

Q08:Particle Velocity X:	Q08:Contact Position X:
Q09:Particle Velocity Y:	Q09:Contact Position Y:
Q10:Particle Velocity Z:	Q10:Contact Position Z:
*Q11:Particle Angular Velocity X:	Q11:Contact Normal Force X:
*Q12:Particle Angular Velocity Y:	Q12:Contact Normal Force Y:
*Q13:Particle Angular Velocity Z:	Q13:Contact Normal Force Z:
	Q14:Contact Tangential Force X:
	Q15:Contact Tangential Force Y:
	Q16:Contact Tangential Force Z:

Table 2. P4 Export Queries

P4P File	P4C File	P4W File
Q01:Total Number of Particles:	Q01:Total Number of Contacts:	Q01:Total Number of Contacts:
Q02:Particle ID:	Q02:Contact IDfirst:	Q02:Contact IDfirst:
Q03:Particle Volume:	Q03:Contact IDsecond:	Q03:Contact Position X:
Q04:Particle Mass:	Q04:Contact Position X:	Q04:Contact Position Y:
Q05:Particle Position X:	Q05:Contact Position Y:	Q05:Contact Position Z:
Q06:Particle Position Y:	Q06:Contact Position Z:	Q06:Contact Normal Force X:
Q07:Particle Position Z:	Q07:Contact Normal Force X:	Q07:Contact Normal Force Y:
Q08:Particle Velocity X:	Q08:Contact Normal Force Y:	Q08:Contact Normal Force Z:
Q09:Particle Velocity Y:	Q09:Contact Normal Force Z:	Q09:Contact Tangential Force X:
Q10:Particle Velocity Z:	Q10:Contact Tangential Force X:	Q10:Contact Tangential Force Y:
*Q11:Particle Angular Velocity X:	Q11:Contact Tangential Force Y:	Q11:Contact Tangential Force Z:
*Q12:Particle Angular Velocity Y:	Q12:Contact Tangential Force Z:	
*Q13:Particle Angular Velocity Z:		

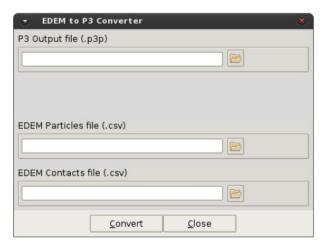
File Conversion

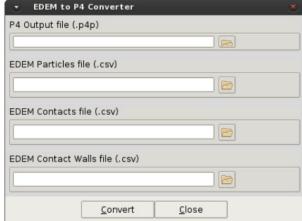
In order to carry out post-processing with the P4 Toolbox, the data exported from EDEM needs to be converted into the file format used by the P4 Toolbox. The P4 toolbox comes with an inbuilt converter which converts the .csv files exported from EDEM to the required P3 or P4 files for use in the toolbox. The converter can be selected as shown in 3.1. Upon selection, the option to convert to either P3 or P4 files is displayed in the *P4 toolbox* submenu as:

Converter: EDEM to P3 Converter: EDEM to P4

Selecting either option displays an input box such as those presented in A where the EDEM input files and P3/P4 output files are specified. Once the files have been correctly selected, the conversion process is started by pressing the convert button. Pressing the convert button will open the info window (A), which provides details of the conversion for each timestep as the files are being processed.

Using P4 with EDEM 46





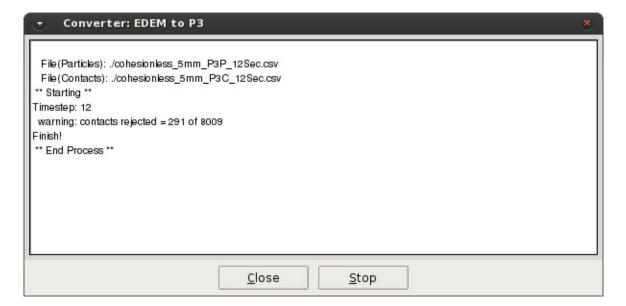
EDEM to P3 file converter

EDEM to P4 file converter

Once the files have been converted to the P3/P4 file format, the data can then be used with the P4 Toolbox for advanced post-processing of the data. Calculation and post-processing of the data can only take place if a mesh of nodes has been created within GiD. This will be discussed in the following section.

NOTE:

During the file conversion process, it is possible that some contacts will be rejected such as shown in the file conversion Info window. However, only contacts that occur between virtual-virtual particles and virtual particles-geometry will be rejected. Virtual particles are generated in the case where periodic boundaries are employed in the simulation and this is the only time contacts should be rejected.



EDEM to P3/P4 file converter info window

Using P4 with EDEM 47

Using P4 with LIGGGHTS

As a experimental feature, P4 can read alternatively liggghts dump files for the processing, considering few restrictions in the structure of the files.

The dump files generated by liggghts for the particles variables can have different variables and no order is required, nevertheless to be processed in P4 a minimum number of variables and the order should remains constant. The same restriction affect to the particle-particle and particle-wall contact dump files.

In the particles file, the file name must have the extension ".p". The variables in the command must follow this rules:

- id: column one
- type: column two
- x,y,z: columns three to five
- vx,vy,vz: columns nine to eleven
- · radius: column eighteen

The rest of columns will be considered as user defined variables, and will be processed on that way. An example of the liggghts dump command for the particles file is:

```
dump Pfile all custom 400 dumpfile.p id type x y z ix iy iz vx vy vz fx fy fz \
  omegax omegay omegaz radius
```

The particle-particle contacts file must have the same name of the particles file, with the extension ".c". On this file, just the IDs of particles in contact and forces will be read:

- id: IDs of particles in contact. Columns seven to nine
- fx,fy,fz: Contact forces. Columns two ten to twelve

The rest of the columns will not be considered.

In the case of the particle-wall contact files, the file name must have the same name of the particles file, with the extension ".w". The rules for the files is similar to the particle-particle contact files, plus the contact point position:

- cx,cy,cz: Contact point position. Columns one to three
- id: IDs of particles in contact. Columns seven to nine
- fx,fy,fz: Contact forces. Columns two ten to twelve

An example of the liggghts dump command for both contact files is:

```
compute cp all pair/gran/local
compute cw all wall/gran/local
dump Cfile all local 400 dumpfile.c c_cp[1] c_cp[2] c_cp[3] c_cp[4] c_cp[5] \
    c_cp[6] c_cp[7] c_cp[8] c_cp[9] c_cp[10] c_cp[11] c_cp[12]
dump Wfile all local 400 dumpfile.w c_cw[1] c_cw[2] c_cw[3] c_cw[4] c_cw[5] \
    c_cw[6] c_cw[7] c_cw[8] c_cw[9] c_cw[10] c_cw[11] c_cw[12]
```

Using P4 with Liggghts 48

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The Particle Pre- and Post-Processor uses GiD as a front-end. Consequently, the GiD end-user licence agreement applies to users of the Particle Pre- and Post-Processor.

The following table lists third-party licences used in libraries that are supplied alongside the Particle Pre- and Post-Processor.

Component	Description	Licence
Assimp	Open Asset Import Library	Assimp Licence
Boost	Boost C++ Libraries	Boost Software License - Version 1.0
GiD Post	For writing postprocess results for GiD	GiD Post licence
Tcl	Tool Command Language	Tcl licence
zlib	Compression Library	Boost Software License - Version 1.0

Licensing 49

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Licences Used in The Particle Pre- and Post-Processor

The Particle Pre- and Post-Processor uses GiD as a front-end. Consequently, the GiD end-user licence agreement applies to users of the Particle Pre- and Post-Processor.

The following table lists third-party licences used in libraries that are supplied alongside the Particle Pre- and Post-Processor.

Component	Description	Licence
Assimp	Open Asset Import Library	Assimp Licence
Boost	Boost C++ Libraries	Boost Software License - Version 1.0
GiD Post	For writing postprocess results for GiD	GiD Post licence
Tcl	Tool Command Language	Tcl licence
zlib	Compression Library	Boost Software License - Version 1.0

3rd party licences 53