PARSIFAL
V. 1.0
PARticle SImulation For AnaLysis

Developed by

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ABSTRACT

The finite difference and finite element simulation of heterogeneous materials, such as concrete, hinges on our ability to generate an appropriate finite difference grid or mesh for the considered representative volume element (RVE).

PARSIFAL (PARticle SImulator For AnaLysis), http://civil.colorado.edu/~saouma/parsifal , is the program used to generate a heterogeneous material model in RVE. In addition, it can be used to generate a finite difference grid, and also as the input data for the finite element mesh generator program Kumonosu (http://civil.colorado.edu/~saouma/kumonosu) based on T3D (http://power2.fsv.cvut.cz/~dr/t3d.html).

PARSIFAL is a window application, written in C++ and based on the PhD thesis of Dr. Puatatsananon[1], in turn based on an earlier generator developed by Dr. Volker Slowik

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[1] Puatatsananon, W., "*Deterioration of Reinforced and Massive Concrete: A Multi-Physics Approach*", University of Colorado, Boulder, August 2002.

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1. Introduction

PARSIFAL is a flexible, user-friendly environment through which the user can define the RVE in terms of numerous variables. It also includes editing capabilities, which are very useful to perform minor refinements of the RVE definition. Finally, it can generate both a finite difference grid, and a set of boundary definitions for an accompanying finite element mesh generator, Kumonosu[2] (developed by Dr. Hansen).

There are six menu options:

- **File**: Lists options for analysis file controls and exporting the output figure file.
- **Generator**: Provides options for preparing input information for the RVE definition (matrix and inclusions). This menu option also launches and stops the particle generator.
- **Editor**: Gives options for editing the state of the located particle inside the RVE. This menu option also allows the user to set up the display properties of PARSIFAL.
- **Finite Difference**: Presents options for preparing grid definition of finite difference grid generation used in both the chloride diffusion model and in the AAR (should spell out AAR before using the acronym) model.
- **Finite Element**: Gives options for preparing mesh definition for finite element mesh generator.
- **View**: Displays options for controlling the model view.

The procedure of running the particle simulator using PARSIFAL can be summarized in the following sections.

2. Run PARSIFAL

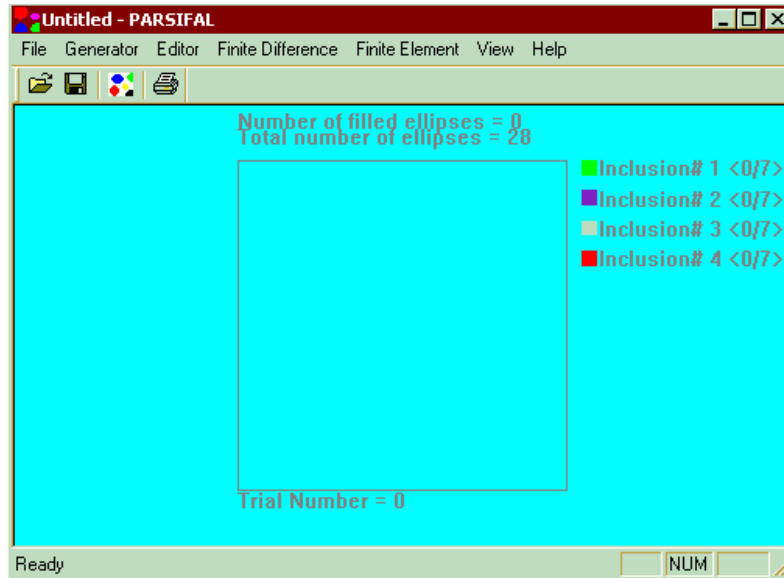Run **Parsifal.exe**. An interface of the program is shown in Figure 1.

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[2] http://civil.colorado.edu/~saouma/kumo

Figure 1: Graphical User Interface of PARSIFAL

3. RVE Definition

There are three user-defined RVE definitions: matrix definition, inclusion definition and crack definition. The steps of defining each are summarized in sections 3.1 – 3.3.

3.1 Matrix Definition

Click on the **Generator** menu, and then **Matrix Definition**. The **Matrix Definition** dialog box is then loaded as shown in Figure 2. The user can define the dimension of the RVE, and can set up the **Random Number Generator's Seeds** of xy-coordinates and an angle with respect to the x-axis. Each particle can be defined to be either automatic or defined numbers.
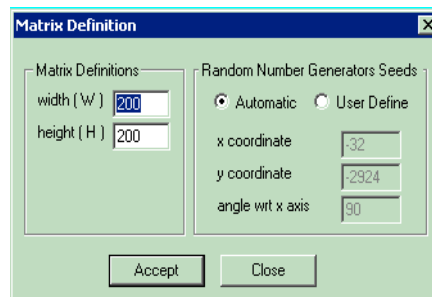

Figure 2: Matrix Definition Dialog

3.2 Inclusion Definition

Click on the **Generator** menu, and then **Inclusion Definition**. The **Inclusion Definition** dialog box is loaded as shown in Figure 3. The user can define the number of each group of particle either by percentage of matrix area of by number of inclusions. The user can

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define five different groups of particles. By checking the **ID** box, the selected ID group will be activated to be included in the generation process. The information required in each group is;

◆ **Geometry** (ellipse)
◆ **Model**: This selection can either be voided or included. By checking **Void**, the particle of the selected ID group will be considered as void, otherwise they are inclusions.
  ○ Type of particle: The type of particle can be ellipse, ellipse with one crack or ellipse with two cracks.
  ○ Interface: This option is used in the generation of mesh definition of the finite element model. If checked, the particles will have interface elements around them.
◆ **Crack Inclusion**: If the type of particle is ellipse with one crack or ellipse with two cracks, the user needs to provide the following information to define the crack of those particles:
  • **Crack Inclusion**: This option is available only in the case of the ellipse with two cracks model. If checked, there will be a crack connecting both radiating cracks through the particle.
  • **Angle**: The user can define the random crack angle, which will use the random number generator to generate the crack angle during the filling particle process. Otherwise, the user can define the exact number of the crack angle so that the same crack angle will be used throughout the filling process for that particular particle group.
  • **Length**: Length of crack.
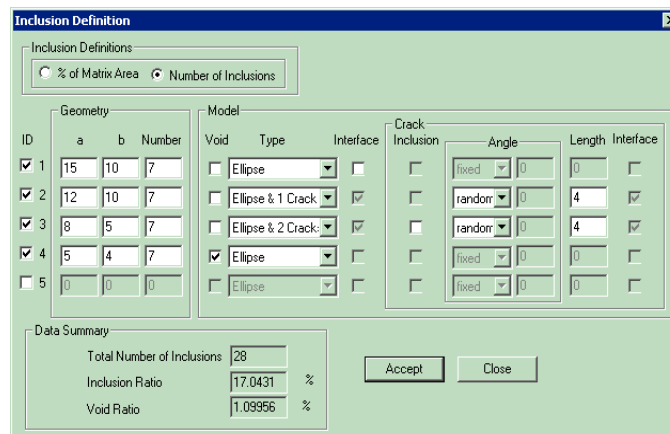 • **Interface**: This option is for the generation of the finite element mesh definition only.

Figure 3: Inclusion Definition Dialog

3.3 Crack Definition

Click on the **Generator** menu, and then **Crack Definition**. The **Crack Definition** dialog box is loaded as shown in Figure 4. The crack in the generation process of the RVE will be represented as an ellipse. The bounded size of the crack represents the length of the minor axis of the ellipse. By checking on the **ID** box, the selected ID group will be activated to be included in the generation process. The information required in each group is;

- ◆ **Number**: The number of cracks in that group ID.
- ◆ **Length**: Length of crack.
- ◆ **Angle**: The user can define the random crack angle, which will use the random number generator to generate the crack angle during the filling particle process. Alternately, the user can define the exact number of the crack angle so that the same crack angle will be used throughout the filling process for that particular particle group.
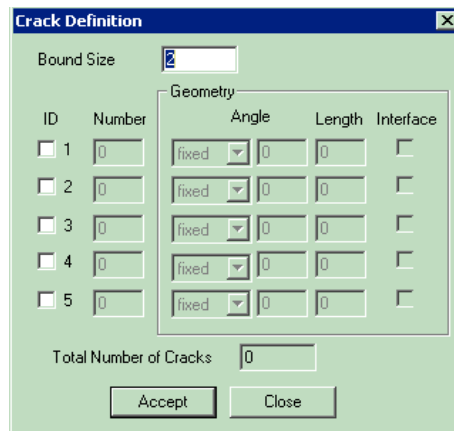- ◆ **Interface**: This option is for the generation of the finite element mesh definition only.

Figure 4: Crack Definition Dialog

4. Run Generator

After the user is finished preparing all input information of the REV definition, particles can be generated. To generate particles into the REV, click on **Generator**, and then **Run Generator** as shown in Figure 5. The filling process using the random number generator and collision detection algorithm then begin. The process runs until one particle cannot be filled into the available space inside the matrix within the limitation of the trial number, or until the user clicks on **Generator** and then **Stop Generator**. The result after completion of the generation process is shown in Figure 6.
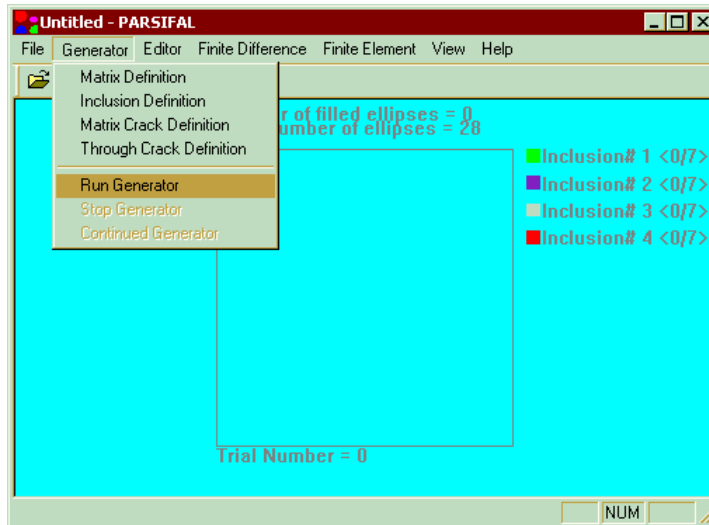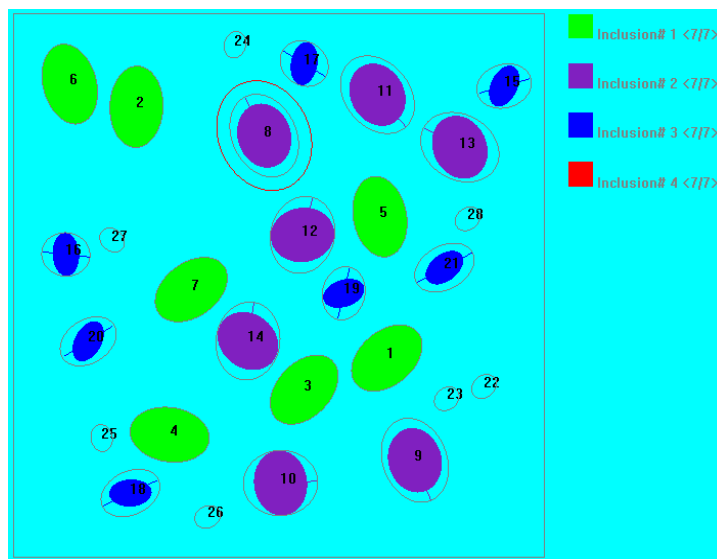
Figure 5: Run Generator Menu

Figure 6: REV after finishing the generation process

5. <u>Editor Mode</u>

After the generation process is completed, the user can move and also can rotate the located particle in the editor mode. To do so, click on the **Editor** menu and then select **Move Ellipse**. The **Moving Ellipse** dialog box is then loaded. The user can then input the ellipse or particle number to be edited. To activate the selected particle, the user must press the **Edit** button. The particle location and orientation can then be changed using slider bars as shown in Figure 7.
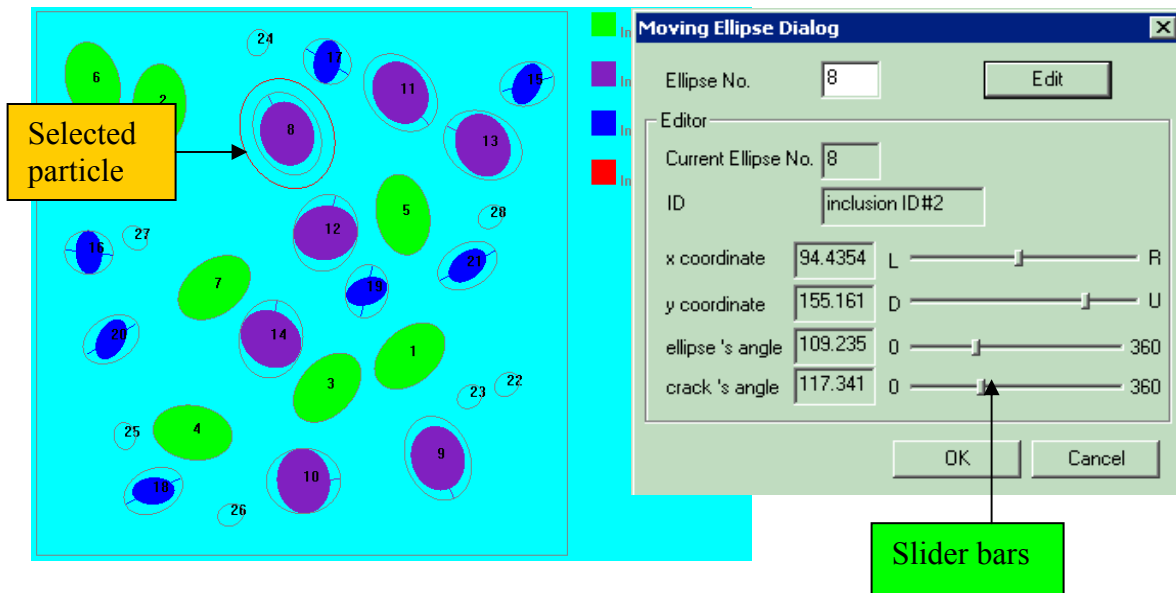
Figure 7: Editor Mode

6. Finite Difference Grid Generator

To generate finite difference grids for this REV, the user must first define the finite difference grid definition. The grid is defined by clicking on the **Finite Difference** menu and then on **Grid Definition**. The **Grid Definition** dialog box is then loaded as shown in Figure 8.
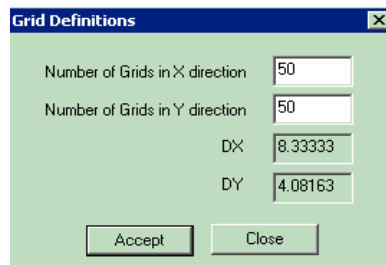

Figure 8: Grid Definition Dialog

In the **Grid Definition** dialog box, the user can define the number of grids in both x and y directions. After the user has clicked on the **Accept** button, the **Finite Difference** menu must be opened and the **Generate FD Grids** selection must be made. Then the user must select the type of analysis for which this REV will be used. The **For Chloride** model will generate a finite difference grid for the chloride diffusion model which will then be used by the CDAP program. In addition, the **For AAR Model** will result in the generation of finite difference grids for the **Alkali-Aggregate Reaction Model** simulated in SIMSAR. The result of the grid generation for chloride diffusion model is illustrated in Figure 9.
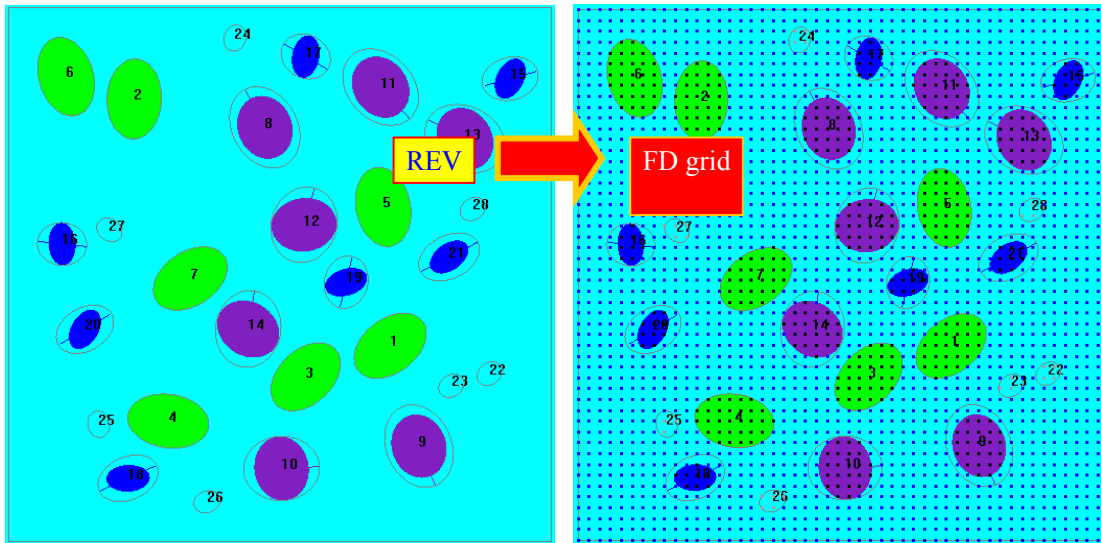
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Figure 9: Example of the result of grid generation for chloride diffusion model

To export the grid definition data to a file, click on the **Finite Difference** menu and then **Export Data**. The user will be asked to provide the file name. The grid definition data file will have a "**.clg**" extension for the chloride diffusion model, and "**.arg**" extension for the alkali-aggregate reaction model.

7. Finite Element Mesh Definition Generator

To generate a finite element mesh definition for this REV, the user must first define a finite element mesh definition by clicking on the **Finite Element** menu and then on **Mesh Definitions**. The **Mesh Definition** dialog box is then loaded is shown in Figure 10.
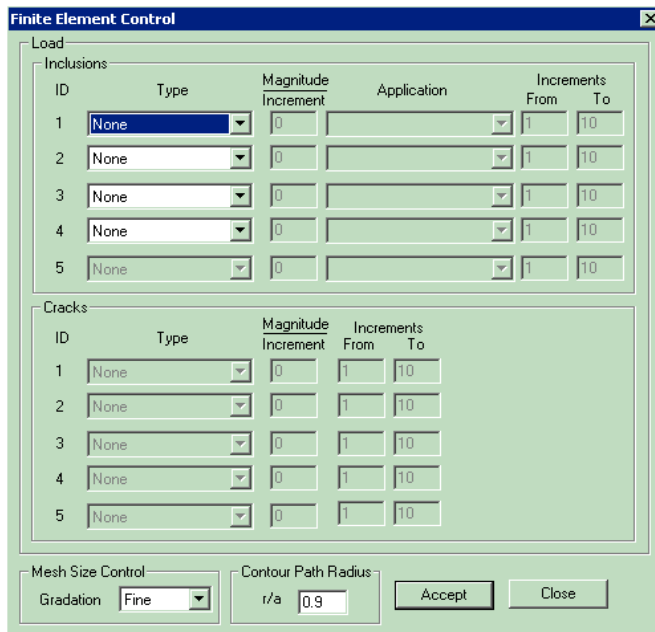

Figure 10: Mesh Definition Dialog

In this dialog, the user can define traction or displacement, their magnitudes, and the number of increments, on each particle ID. The user can also define mesh size control and contour path radius.

After finishing the preparation of all mesh definitions, click the **Accept** button to close the dialog box. To export the mesh definition data to a file, click on the **Finite Element** menu and then **Export Data**. The user will be asked to enter a file name in which to save the data, and then must press **Enter** to finalize the save. The mesh definition will be saved into the file with extensions of ".**bd**" and ".**ctrl**." An example of the mesh generated by Kumonosu (should this be capitalized) is shown in Figure 11.
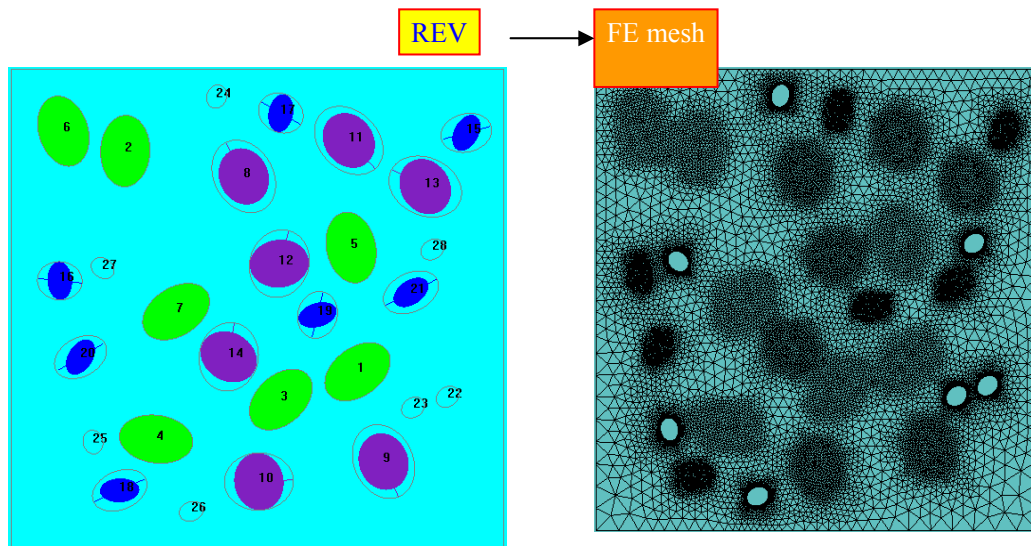

Figure 11: An example of the mesh generated by Kumonosu