JFE-DEMSPH User Manual

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1 Introduction

There are two standard types of simulations that can be run using the JFE-DEMSPH . The block break (dam break) and the steel converter simulation. The first simulation is useful to see if the modelled fluid physically behaves properly. This paper walks the user through a tutorial for both types of simulations. The tutorials will outline the steps in each simulation, from the parameter initialization to the final visualization in Paraview.

2 Requirements

2.1 Compiling

The program can be compiled using the makefile that is located in the same directory as the source files. The makefile will compile and link the following using g++ .

1. Parameters.h
2. Main.cpp
3. Solver.cpp
4. KernelFunctions.cpp
5. utility.cpp
6. Boundaries.cpp
7. Initialization.cpp
8. OutputFunctions.cpp
9. UserInterface.cpp

To create an executable, open a terminal and cd into the directory where the source files and the makefile is located. Type in the command make, and an executable named JFE_DEMSPH will be created. To execute the program type the command ./JFE_DEMSPH into the terminal.

2.2 Ouput Directories

Before running the program ensure that the following ouput directories exist in the same location as the JFE_DEMSPH executable. If the following files are not present, the program will report an error message and the output files will not be be printed.

1. data
   (a) data/vtk
      i. data/vtk/air
      ii. data/vtk/water
      iii. data/vtk/boundary
   (b) data/csv
      i. data/csv/air
      ii. data/csv/water
      iii. data/csv/boundary
   (c) data/run

2.3 Codeblocks (optional)

This program was written using the open source IDE Codeblocks. Any text editor or IDE can be used to edit the code however, Codeblocks is recommended. Included in the main directory is the codeblocks project file SPHDEM. cbp . Codeblocks can be downloaded for free from their website www.codeblocks.org .

2.4 Paraview

The output files can be visualized with the open source software Paraview. Paraview handles both the CSV files (which contain the particle positions and grid indexes), and the native Paraview VTK format files (which can contain any scalar data such as density, position, velocity, acceleration etc.) . Paraview can be also be easily downloaded directly from the Paraview website. Post processing in Paraview will be further discussed later on in the tutorial.

3 The Classic Dam Break

The dambreak simulation initializes a large block of particles in the domain, and then releases it so that the motion of the fluid can be observed within the boundaries. The following tutorial will outline how to simulate molten steel released within the steel converter.

1. Run the program.

- cd into the directory and use the make command to create an executable if one is not already present. Use the ./ command to run the JFE_DEMSPH executable.

2. Setting the Parameters

   - A + ENTER. Set a run name.
   - B + ENTER. Input any appropriate notes.
   - C + ENTER. Change the boundary viscocity to 28 or lower to help simulate the splashing effects of the block.
   - D + ENTER. Set the particle block settings. By default the particle block should set to 0 (off), set it to 1 (on). Set the length, width and height of the block all equal to 20. Change the location of the particle block to (0.4,0.0,0.4). NOTE the spacing of the block refers to the spacing in between the block particles. The spacing is entirely dependant on the properties of the fluid. With different fluid properties there is a different spacing required. The ideal spacing will be just far enough so that particles will not compress or expand. Basically the spacing should be set to ensure that the pressure on each particle is close to zero.
   - E + ENTER. Turn the oxygen lance off by setting it to 0.
   - f + ENTER. Set the number of timesteps to 6000.
   - I + ENTER. Adjust the print settings. Activate printing for Water CSV, Boundary CSV and Water VTK by setting them all equal to 1. Set all other CSV, and VTK options to 0. Set the print frequency to 30.
   - Begin the simulation by typing 1 and ENTER twice. If the output directories (ex. data/csv/water) are not in the same location as the JFE_DEMSPH executable then an error message will occur to prompt the user to create the appropriate directories. If all output directories are properly established then the program will count every tenth step and input it to the terminal .

4 The Steel Converter

The steel converter simulation is more complicated than the dam break simulation. Adjustments and modifications to the settings must be made cautiously as even minor changes can result in numerical explosions.

1. Run the program.

   - cd into the directory and use the make command to create an executable if one is not already present. Use the ./ command to run the JFE_DEMSPH executable.

2. Setting the Parameters

   - A + ENTER. Set a run name.
   - B + ENTER. Input any appropriate notes.
   - D + ENTER. Turn the particle block off by setting it to 0.
   - E + ENTER. Turn the oxygen lance on by setting it to 1. Change the lance position to (0.5,0.8, 0.5)
   - f + ENTER. Set the number of timesteps to 6000.
   - I + ENTER. Adjust the print settings. Activate printing for , Boundary CSV and Air CSV and Water VTK by setting them all equal to 1. Set all other CSV, and VTK options to 0. Set the print frequency to 30.
   - G + ENTER. Fill the converter with molten steel by using Read in Positions. Choose Water Data Type. Type Fill4 as the name of the data file to read in positions from. 174,575 steel particles should be initialized.
   - Begin the simulation by typing 1 and ENTER twice. If the output directories (ex. data/csv/water) are not in the same location as the JFE_DEMSPH executable then an error message will occur to prompt the user to create the appropriate directories. If all output directories are properly established then the program will count every tenth step to the terminal screen.

5 Postprocessing

1. Loading Data Into the Pipeline Browser

   - Open Paraview
   - Enable the Point Sprites Plugin. Go to the tools panel (alt+t) at the top of the screen and select Manage Plugins. A window will open and two screens will appear, to the right Local Plugins and to the left Remote Plugins. Under Local Plugins select PointSprite_Plugin. If in the property panel it reads "Not Loaded" then click "Load Selected" and close the window. The Point Sprites plugin allows the user to view coordinates as sprites which can describe scalar values through a colour gradient. The plugin may have to be reloaded every time that Paraview is run.
   - Open the data files. Click on file-¿open (ctrl+o) and navigate to the directory of the vtk or csv data that you wish to view. If visualizing a dam break simulation select the vtk/water files and also the csv/boundary files. If visualizing a steel converter select; the vtk/water files, the vtk/air files and the csv/boundary files. You will notice that the simulations will be grouped by run name (ex;

w_RunName_..vtk). If you click on the little plus sign to the left the group can be expanded to be able to see each data file at each timestep. Collapse and double click on the entire group (e.g. + w_Tutorial_..vtk and not w_Tutorial_3.vtk).

- To the left in the Pipeline Browser the data files will show up. For the VTK files simply click apply. For CSV files uncheck the Have Headers box and then click apply.
- For VTK files once you have clicked apply you will be able to view the data. There are a few ways to view the data. First view the data in 3D. If Paraview is in spreadsheet view, exit spreadsheet view by clicking the small x to the right in Layout1. Select 3D view and click on the centre of the screen. In the Pipeline browser next to the data, there will be a small eye icon. Make sure this eye is selected. Once selected move to the Representaion tab , above the 3D Layout and select Point Sprite. To the left of the Representation tab choose a scalar field to visualize. Choose velocity. Initially very small sprites will be visualized, the size of the sprites can be adjusted by clicking the gear icon below the Pipeline Browser. Under the Display (UnstructuredGridRepresentation) Tab enter a Point Size. Try 15. Other Representation options are ; outline, points, surface, surface with edges volume and wireframe. Not all these representations will be useful or even visualize anything.
- For CSV files a few more steps need to be taken to view the data in 3D. Once you have clicked apply go to Filters (alt+F) then Alphabetical and choose Table to Points. Set the X Column to Field 0, the Y Column to Field 1 and the Z Column to Field 2. Click Apply. Now in 3D view the data should be viewable when using the points represention or the point sprite representation. The CSV files however cannot view the scalar values so set the scalar tab to Solid Colour.
- To visualize the step data sequentially click on the play button near the top right of the screen. The number to the right of the play button shows which timestep is currently being visualized. To visualize a specific time step, simply input the number of that time step.
- Visualizing using the Delauney 3D filter. The point sprite plugin is very useful for visualizing the fluid body as a set of discrete spheres, however if we want the fluid to appear continuous the Delauney 3D filter would be more appropriate. Select the VTK data in the pipeline browser and then click on the Filters tab (or type alt+F). Go into Alphabetical and select Delauney 3D . Change the Alpha setting to about 0.0258 and then click apply. Once the eye icon is selected the data can now be viewed in the 3D Layout.

2. Recording an Animation

- Before recording an animation make sure all data files to be animated appear in the 3D view. Sometimes only the fluid steel is needed to be viewed at other times we would also like to view the boundaries. More than one 3D layout can be viewed at a time, which is useful for visualizing different particles or angles of a simulation.
- Under the file tab, select Save Animation. Any Data that is inside the Pipeline Browser that has the eye icon selected will appear in the animation. Set the Frame Rate (fps) to 29 . Click Save Animation and select a directory to save the .avi file to .

6 Notes on Modifications

The settings outlined in these parameter initialization tutorials are just examples of systems that worked relatively well(free from numerical inconsistancies and oddities). The particle properties can be tweaked to change the types of fluid simulated altogether. The interaction between the two fluid types are controlled by the DEM type forces. As such by altering the Herztian coefficent, the damping coefficient and the tangential friction the system will be greatly altered. Finding parameters that effectively model the real phenomena is tricky and will require trial and error. To combat numerical instabilities the main parameters that may need to be tweeked are ; the viscocity, the DEM damping coefficient, the lance velocities and the size of the timestep.

7 How to Fill the Converter

To fill the converter, a large block of fluid must be initialized in the converter. Make sure that the print water csv option is on. Make the X and the Z component both 120 (if 120 does not work try other large dimensions, sometimes if there are too many particles the programs will return 0 and an error.), and the Y dimension the desired height. This is much larger than the converter, however since particles are deleted right away this it is ok. The fluid will enventually settle. Keep the last csv file and move it into the main folder where the source files are located. To initialize these particle positions for future simulation simply use the Read in Positions function at the main menu and type in the name of the csv file. Some fill files that have already been made are; MillPhil, Fill4, LowPhil, SteelFill. NOTE: not all these fills will work depending on the fluid type. The particles in these fill files settled based on the densities and other properties of that simulation. If the fill file's particle's settings and the current particle's settings are different the particles may explode during the next simulation.

8 Adding Modules to the Code

To add in additional features to the existing code the Paramaters.h, Output.cpp and the Solver.cpp files need to be modified. Lets look at adding thermo transfer

as an example.

- Add all new necessary particle properties (temperature etc) to the Particle structure in the Parameters.h file.
- Add necessary variables and constants to the Param struct also in the Parameters.h file. Add these variables into the private section, and access and modify them by using getter and setter functions (all Param variable are used in this way).
- In the Solver.cpp file, create another SPH neighbour search loop for each particle type (probably updateDensity function). If particles fall within the smoothing range then execute the appropriate physics. Follow the model of the previous SPH neighbour search loops.
- In the Output.cpp file additional information will need to be printed to the VTK files. Review the format guidelines for VTK files before attempting to modify the code.