VELaSSCo

Visual Analysis for Extremely Large-Scale Scientific Computing

Evaluation Event

USE CASE 2: Discrete Element Simulation (DEM)

Simulation Tool & Discrete2Continuum (D2C): iFX

Table of Contents

1 iFX Installation Guide

1.1 Download and installation of iFX

- Download current package from:
  https://cloud.igd.fraunhofer.de/owncloud/public.php?service=files&t=2917f738764546efd7adb29e8b1061c6
- Unzip downloaded package.
- Directory structure should look like this :

app	11/14/2016 6:07 PM	File folder	
Discrete To Continuum_StepByStep.pptx	11/2/2016 3:47 PM	Microsoft PowerP…	2,957 KB
iFX-Velassco.bat	2/3/2016 3:43 AM	Windows Batch File	1 KB
Start_VELaSSCo_Eddie.bat	1/29/2016 4:37 PM	Shortcut	2 KB
Tutorial-iFX-Velassco.docx	2/3/2016 5:20 AM	Microsoft Word D…	2,941 KB
VELaSSCo-iFX-VisualizationClient-Manua…	2/3/2016 10:37 PM	Microsoft PowerP…	2,321 KB
VisualizeParticles.pptx	11/2/2016 4:14 PM	Microsoft PowerP…	1,242 KB
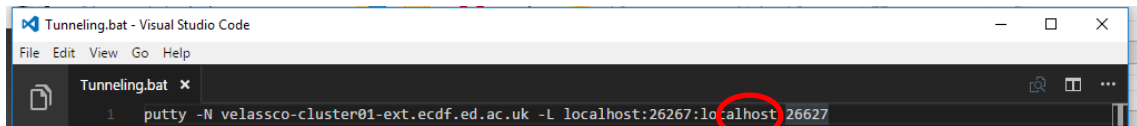
1.2 Connect to EDDIE Cluster

- The usernames created for the Evaluation Event to connect to the VPN network are **velgst2** to **velgst50** (the first 9 have only 7 characters).
- Each one has an initial/registration EASE password set to **"VELaSSCo"**. This will have to be changed through the EASE webpage (https://www.ease.ed.ac.uk/).
- Setup VPN connection to EDDIE cluster following the instructions provided in the URL: http://www.ed.ac.uk/information-services/computing/desktop-personal/vpn/vpn-service-using
- Once connected to VPN, to login in into VELaSCCo platform, following provided information will be required:

- o Multi-user connection:
  - Username: velassco (default)
  - Password: --- (default)
  - VELaSSCo host: velassco-cluster01-ext.ecdf.ed.ac.uk
  - Port: **provided individually by mail. Please check the invitation mail.**

- o Tunnel through:
  - Tunnel host: velassco-cluster01-ext.ecdf.ed.ac.uk
  - Local Port: same value that Port.
  - Username: **provided individually by mail. Please check the invitation mail.**
  - Password: **provided individually by mail. Please check the invitation mail.**
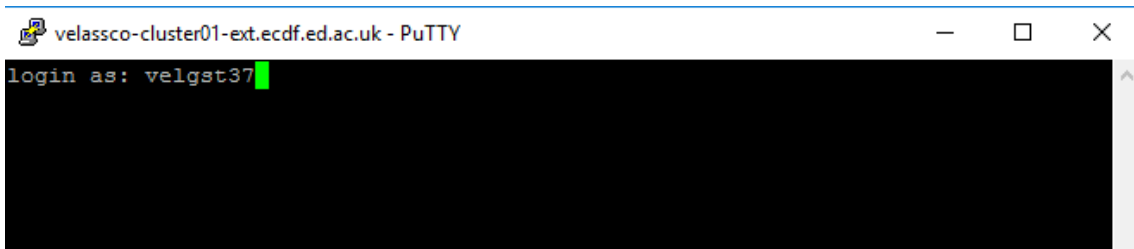
Next, the tunnel should be set up and started:

- Open the *tunneling.bat* file in iFX VELaSSCo Client's folder, and set the proper port for VELaSSCo platform:

- Execute *tunneling.bat*. It will request for the credentials to connect to the VELaSSCo platform. Use the provided user name and password to establish the port tunneling.

2   User instructions and brief tasks description

Thank you for your participation in this study. You will carry out the tasks on your own in the presence of a facilitator. The facilitator will be giving hints, asking questions, observing your responses to the exercises and supporting you during the whole process. The study will comprise a series of tasks, to be completed one at a time; i.e. once the facilitator, who would be observing your interactions, agrees that you have concluded one task, you will be presented another one.

The study is about the use of VELaSCCo Platform by means of GiD or IFX visualizations clients to operate with a FEM or DEM simulation previously calculated and injected into the Platform. You will be asked to carry out tasks that involve simple simulations actions on the client side.

During the session you have the following tools at your disposal:

- **VELaSSCo Open Platform**
- **iFX Client V.8.4** (Visualization Tool)
- Text editor and viewer (e.g. Notepad, Word,…)
- Web browser

Your work may be monitored and at the end you will be asked to fill in a simple questionnaire. This will help us understand how people use VELaSCCo Platform and Visualization Clients, how efficient and effective is the VELaSCCo Platform, etc.

2.1 Fluidized Bed Model Description

Fluidized bed processes are very common in pharmaceutical and chemical industries. The Fluidized Bed model selected has the following settings:

- ~ 12,000 particles per time-step
- ~ 3,000 contacts (p2p and p2w) per time-step.
- 48,000 time-steps.
- Particle results: mass, volume, velocity vector
- Contact results: Force vector.
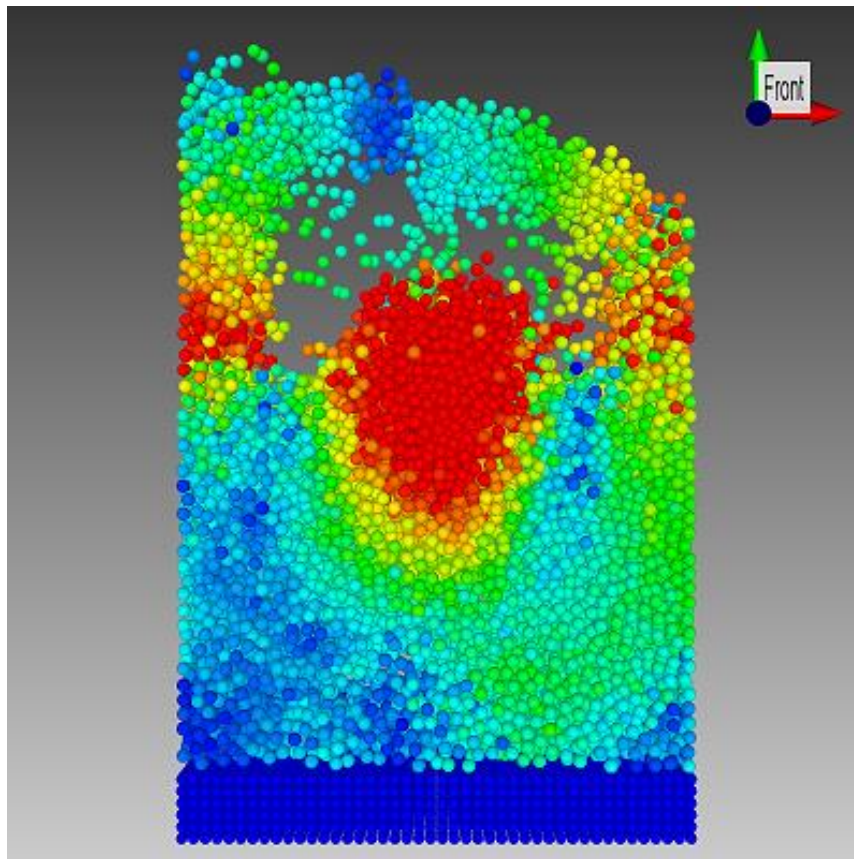
2.2   Rail Embankment Model Description

Simulations with a high frequency output that cover long time durations are difficult to deal with on a desktop machine due to the large quantity of data generated. The rail embankment model selected has the following settings:

- 207,440 particles per time-step

- ~ 560,000 contacts (p2p and p2w) per time-step.

- 9,102 time-steps – 100Hz output.

- Particle results: mass, volume, velocity vector, angular velocity vector

- Contact results: Force vector.
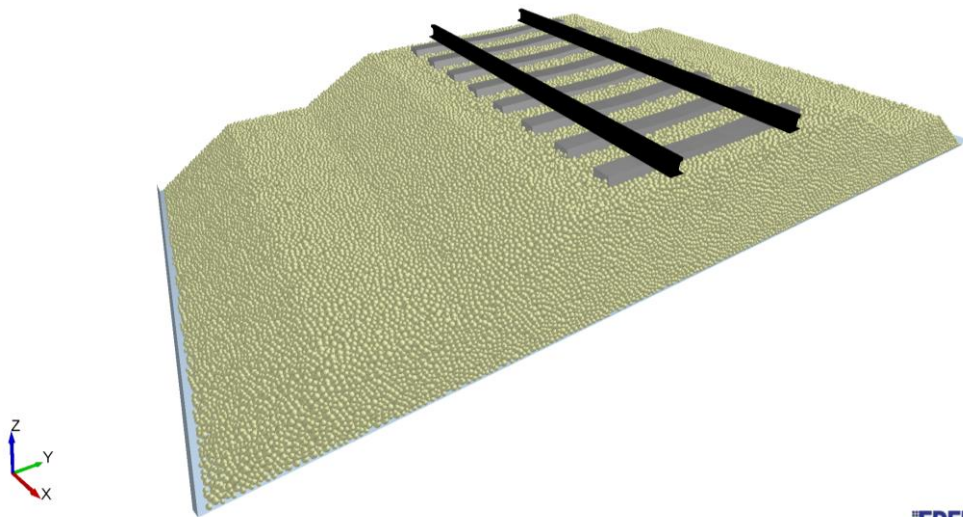
This results in a total data file size of approximately 540 GB generated by the DEM solver.
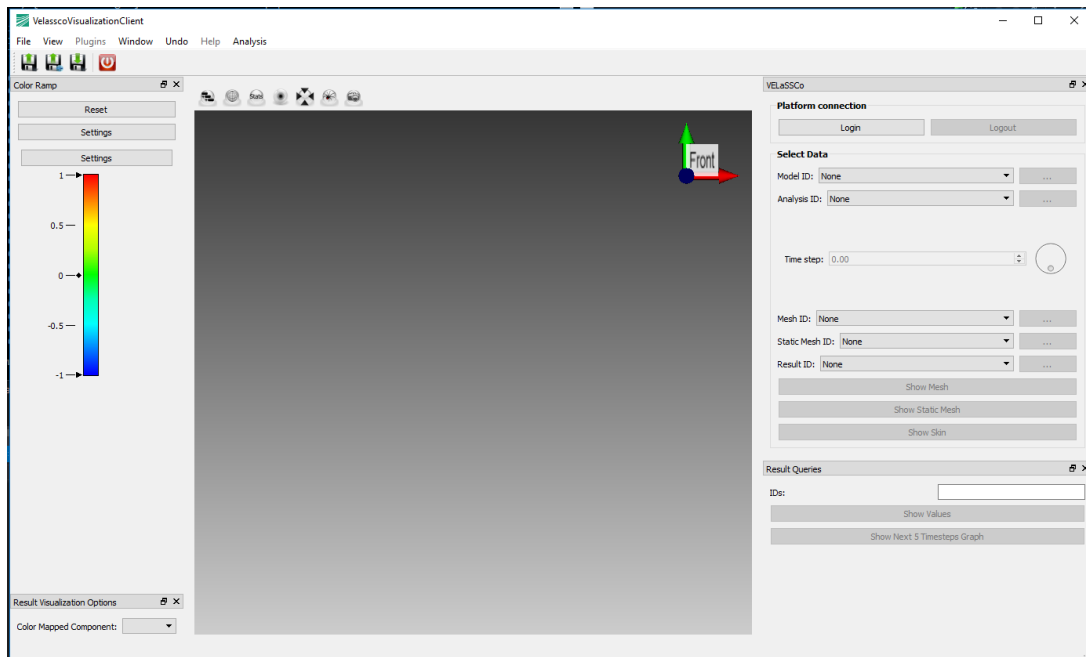
2.3 Task 1: Use Case DEM.M1-01 & M1-02

2.3.1 Motivation

Connect to the VELaSSCo platform and visualise the particle assembly in the visualisation client. Get a result on a particle; concretely get the velocity value specifying a concrete particle id and time-step.

2.3.2 Specification

- Execute the iFX velassco client:

- Connect to VELaSCCo Server using iFX:

  o **Credentials**:
    - Tunnel one of the local ports to the query manager port of VELaSSCo platform that you have received by email.
    - Now that the port tunneling is established, click on the login button in the visualization client:
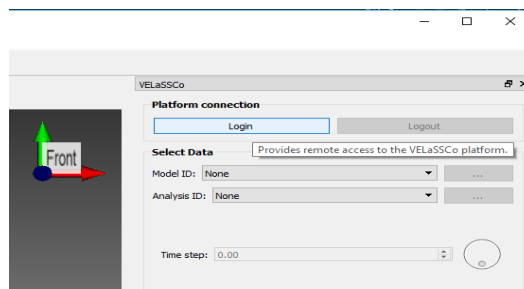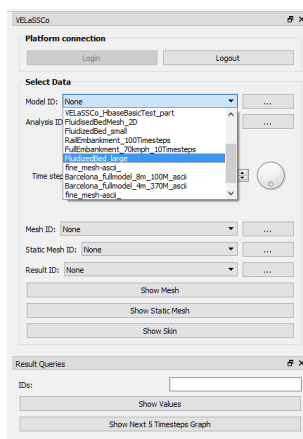
- Press login again in the opened dialog to establish connection between visualization client and VELaSSCo platform:
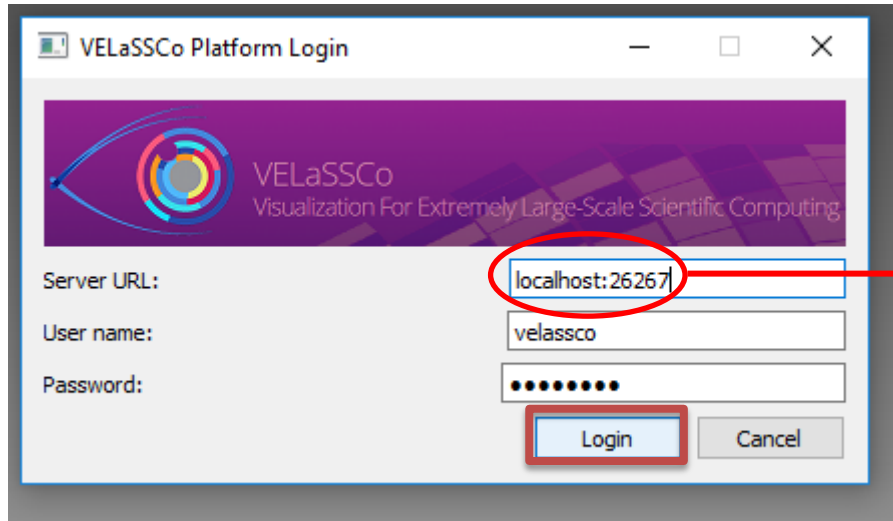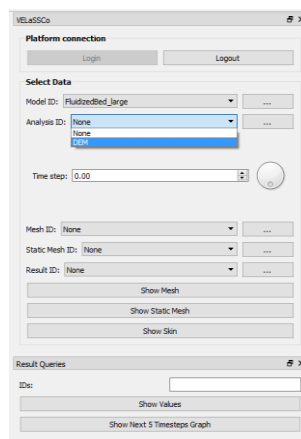

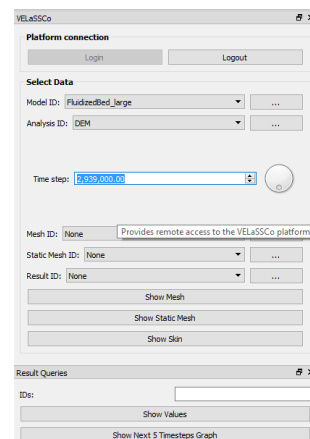Local port tunneled to the VELaSSCo platform's port.

- Open a simulation model
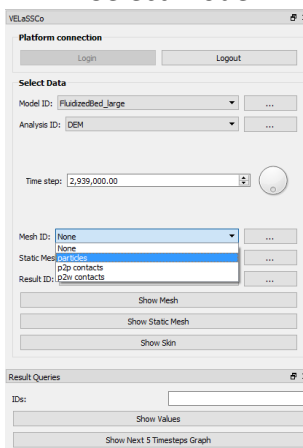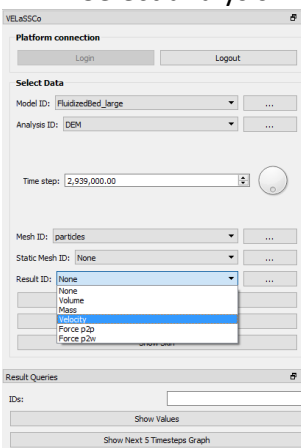 - Select **Fluidized Bed Large** model (FluidizedBed_large)

1. Select model

2. Select analysis

3. Set time step

4. Select Mesh

5. Select Result
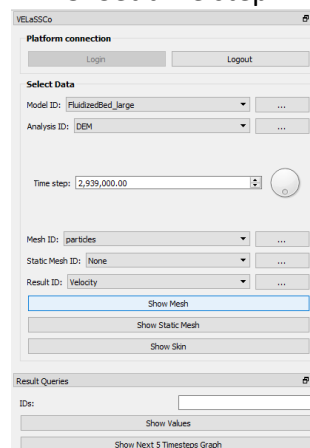
6. Query for particles

- Reset the viewport
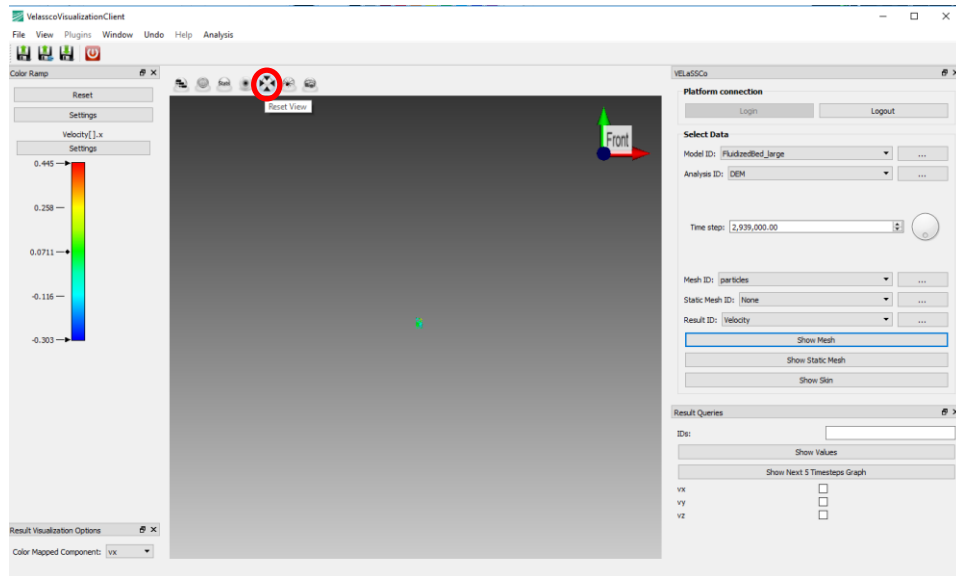
- Visualize a contour fill of a particle result.

    o Visualize the velocity-Y in the skin of the particles in selected time step
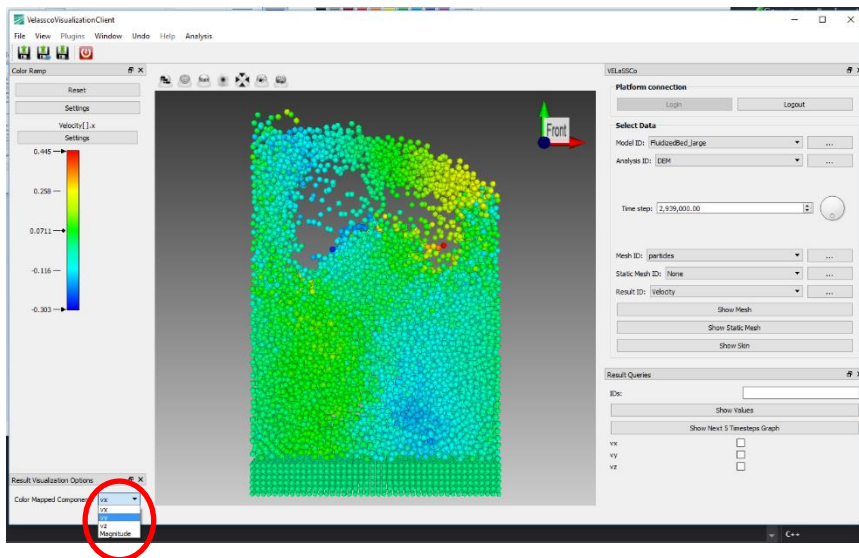
    o Rotate the model

    o Now, the color mapping can be modified by dragging the color mapping min, max, or center. The color mapping can also changed by double right clicking on it.
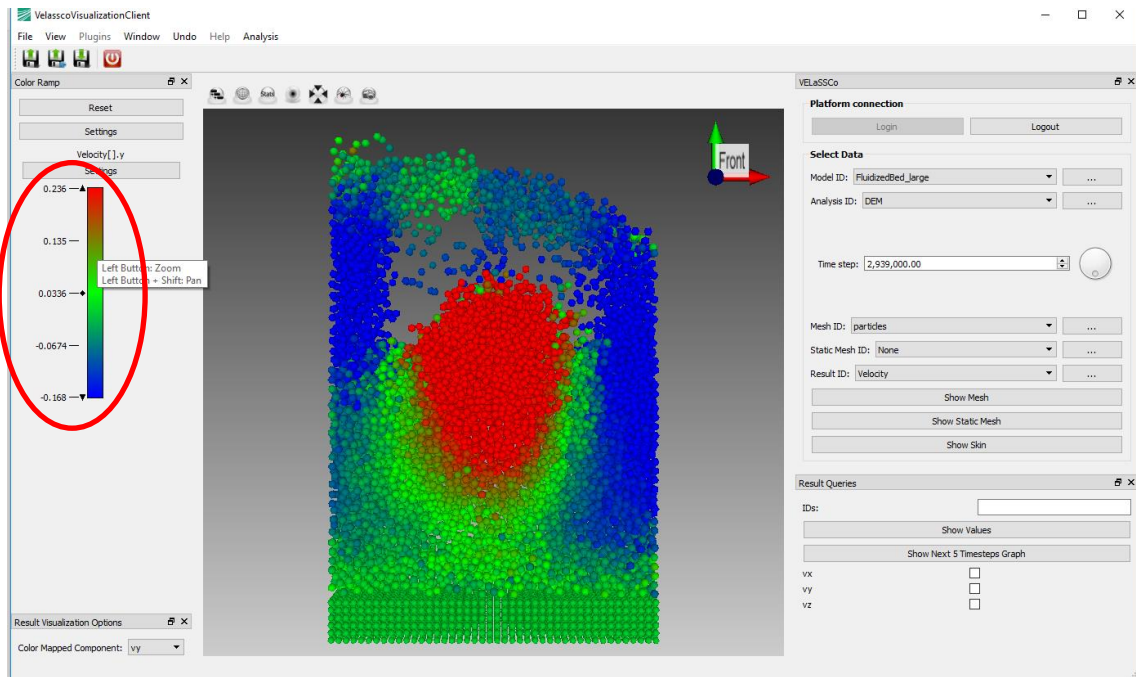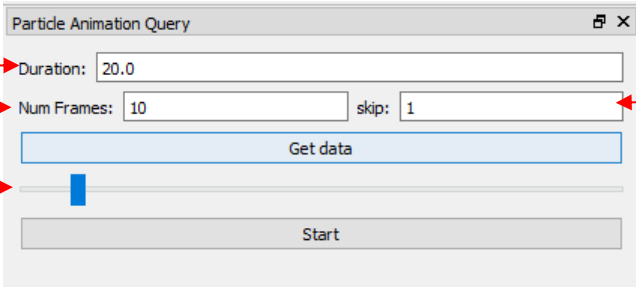
- Visualizing multiple timesteps of particles as animation

    o Open **Particle Animation** dialog
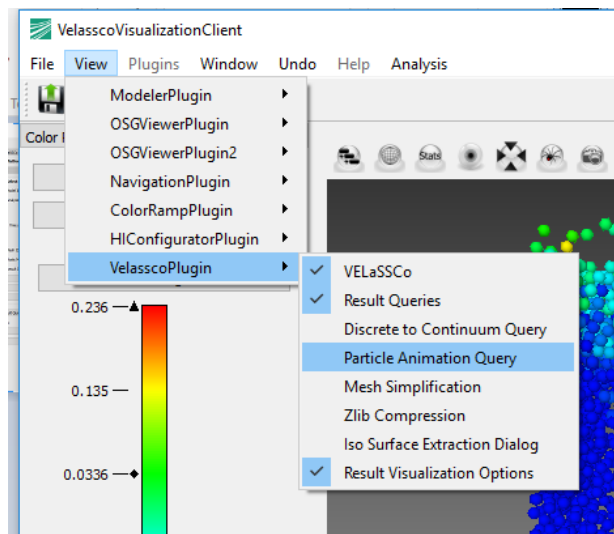
    o Switch to the Particle Animation tab
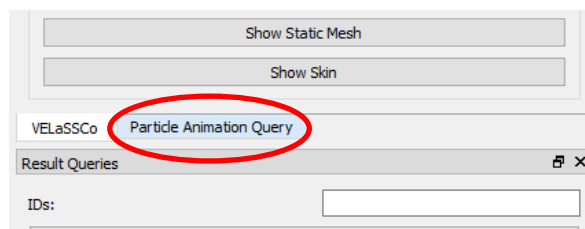
o   Set the parameters as follows:

Duration of animation in seconds

Number of frames to be queried

Number of frames to skip in between

Animation time slider

Particle Animation Query

Duration: 20.0

Num Frames: 10   skip: 1

Get data

Start

o   Press **Get Data**.

o   Press **Play** to see the animaton.

Note: Don't logout, because the following use case is also using this model.

2.4 Task 2: Use case DEM.M1-03

2.4.1 Motivation

Get the evolution of a result on a particle over time; for instance, get the velocity y-component value for all simulation time-steps of specific particle id.

2.4.2 Specification

- Get the evolution of a result on a particle over time.
    - Get the particle number 2724's evolution of velocity y-component value for next five time steps:
        - Enter the particle IDs, select **vy**, and press **Show Next 50 time steps**.
        - The results should look like the following figure:
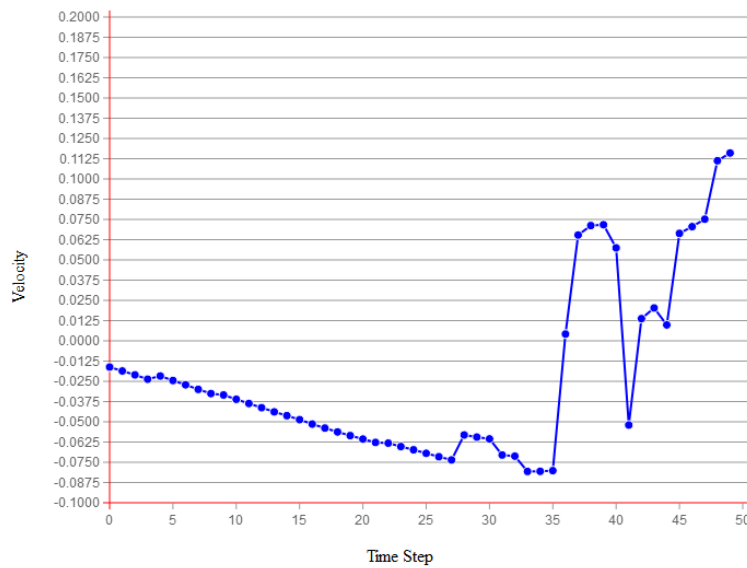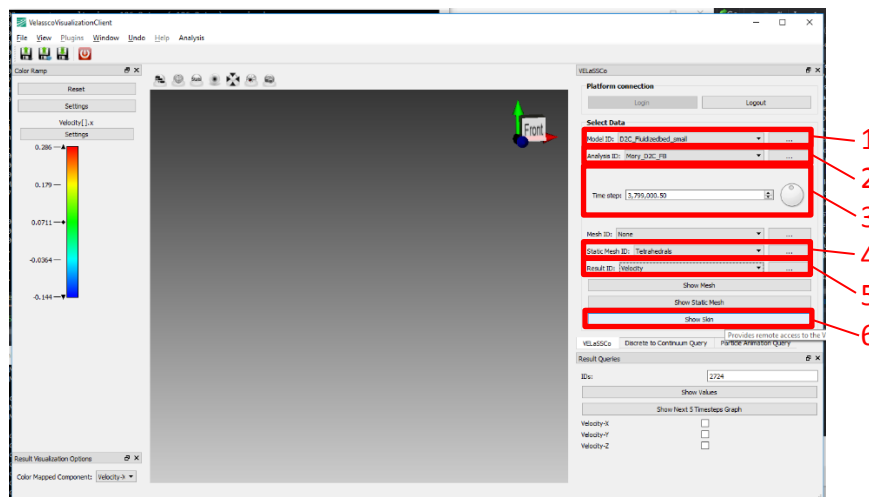

- vy (Node 2724)

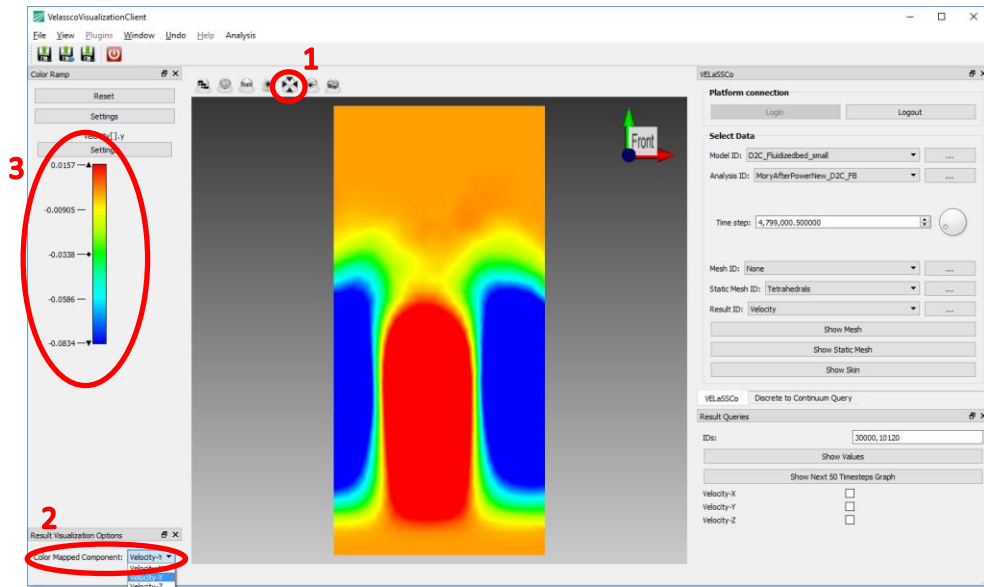## 2.5   Task 4: Use case DEM.M1-05 and DEM.M1-07

2.5.1   Motivation

Compute Discrete to Continuum (d2c) values of the model, get the result in a specific node of the d2c Mesh, and visualize the contour fill of a discrete2continuum result.

2.5.2   Specification

- Compute d2c of the model
  - Open Discrete to Continuum Dialogue (Similar to Particle Animation dialog).
  - Set the dialog parameters as follows:
    - Static mesh = D2C_FluidizedBed_small
    - D2C analysis name = user initials + "_D2C_FB"
    - Time-step options = INTERVAL
    - List of time-steps = 2799000,6799001
    - Coarse-graining method = Gaussian
    - Coarse-graining options:
      - Width = 0.0024
      - Cut-off factor = 3
    - Process contacts = True
    - Do temporal averaging = True

      - Temporal Averaging options = ALL

      - DeltaT = 30000
  - Now, the calculated mesh is stored in the database.
- Visualize a contour fill of a result

  - User: Visualize the contour fill of **velocity-Y** in the skin of the volume mesh of the computed d2c (model "D2C_Mesh" and analysis name "user initials + "_d2c_FB"") for **time step 4799000.5**

- o Reset the view and set the color mapped component to **Velocity-Y**
- o Play with color map, to get the result shown in the figure.

- Get the result in a specific node of the d2c mesh
  - o User: Open D2C_Mesh model
  - o User: *Get the **Bulk density** value for:*
    - *Analysis = user initials + "_d2c_FB"*
    - *Time-step # **4799000.5***
    - *Result = **Density***
    - *Node number **300, 1000***

2.6 Task 4: Use case DEM.M2-01 and DEM.M2-02

2.6.1 Motivation

Compute temporally averaged Discrete to Continuum (d2c) values of the model, get the result in a specific node of the d2c Mesh and visualize the contour fill of a discrete2continuum result.
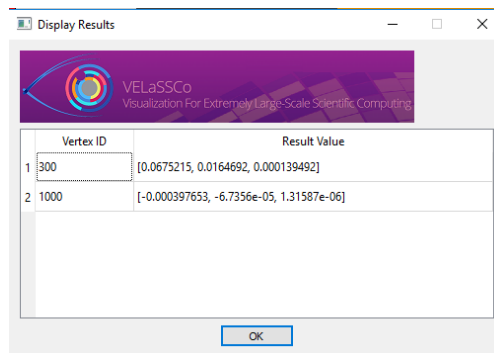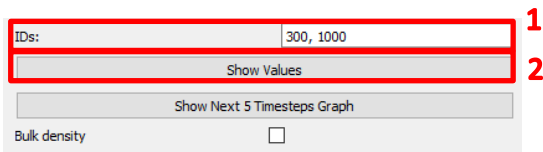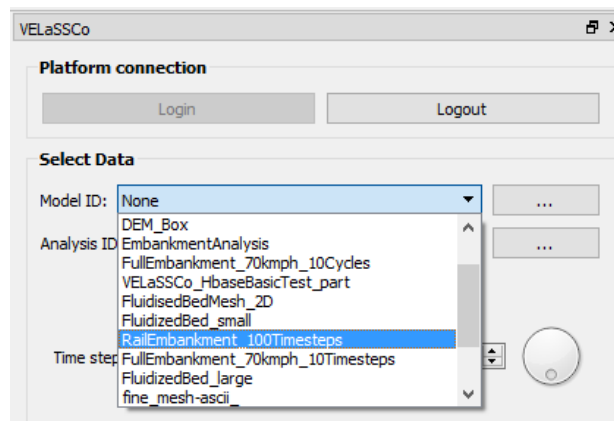
2.6.2 Specification

- Select **Rail Embankment** model (RailEmbankment_100TimeSteps)

- Compute d2c of the model by opening Discrete2Cointinuum query dialog and entering the following parameters:
    - *Static mesh = NewEmbankmentTest_0_1m_77K*
    - *D2C analysis name = user initials + "_D2C_RAIL"*
    - *Time-step options = INTERVAL*
    - *List of time-steps = 0.2, 1*
    - *Coarse-graining method = Gaussian*
    - *Coarse-graining options:*
        - *Width = 0.09*
        - *Cut-off factor = 3*
    - *Process contacts = True*
    - *Do temporal averaging = True*
    - *Temporal averaging options = ALL*
    - *DeltaT = 30000*
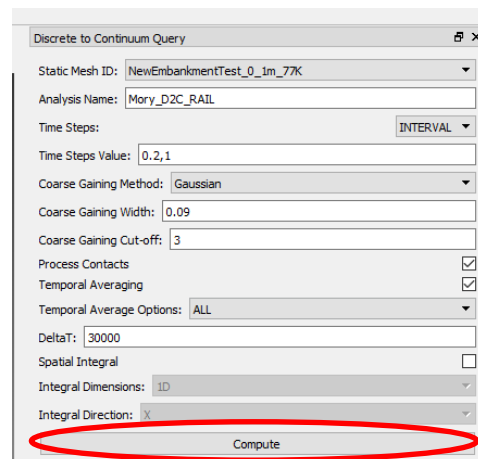
- Visualize a contour fill of a result
    - User: *Visualize the contour fill of **Bulk Density** in the volume mesh of the computed d2c (model "D2C_Mesh" and analysis name "user initials + "_d2c_FB"") for **temporarily averaged time step 0.595.***
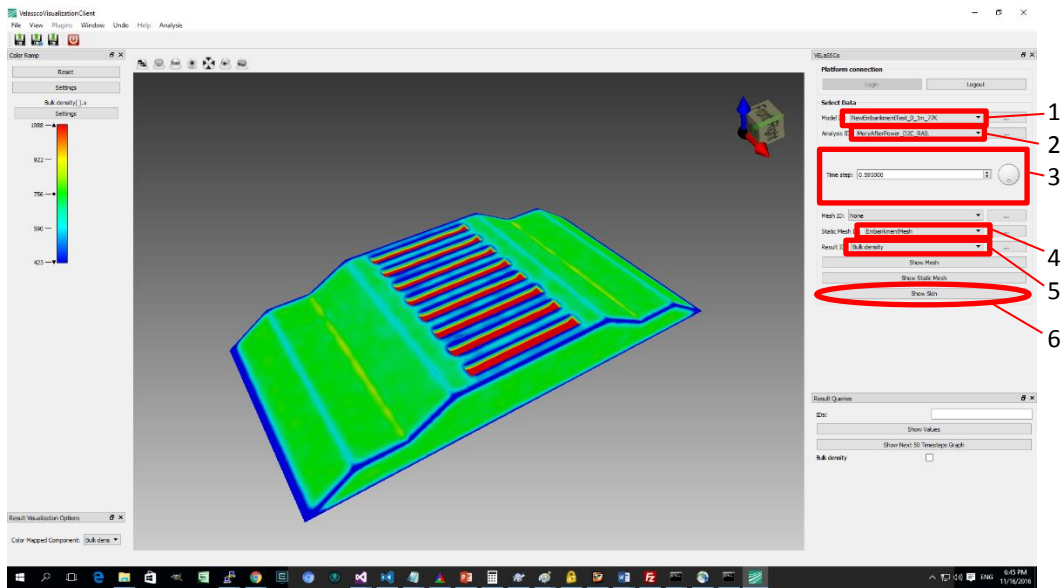
- Get the result in a specific node of the d2c mesh
  - User: Open D2C_Mesh model (*NewEmbankmentTest_0_1m_77K*)
  - User: *Get the* **Contact stress** *value for:*
    - *Analysis = user initials + "_d2c_RAIL"*
    - *Time-step # 0.595*
    - *Result = **Contact stress***
    - *Node number **30000, 10120***
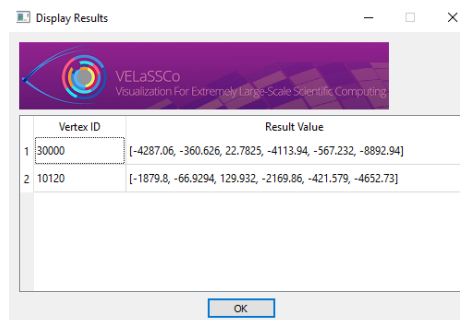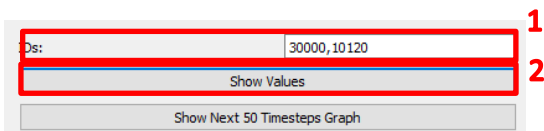
3   Questionnaire for participants

Measuring the quality of a service can be a very difficult exercise. Unlike product where there are specific specifications such as length, depth, width, weight, colour etc. a service can have numerous intangible or qualitative specifications. In addition there is there expectation of the customer with regards the service, which can vary considerably based on a range of factors such as prior experience, personal needs and what other people may have told them.

The questionnaire below is in three sections. On the one hand the first section asks you to rank all software tools for pre and post processing of numerical simulations in science and engineering according to your expectations i.e. what you expect all these tools to provide. On the other hand the second section asks you to rank the iFX's VELaSSCo visualization client according to your experiences and perceptions. The third section asks you about the overall satisfaction of iFX's VELaSSCo visualization client.

Expectations deals with your opinions of software tools for pre and post processing of numerical simulations. What we are interested in here is a number that best shows you expectations about software tools for pre and post processing of numerical simulations offering services.

Perceptions relate to your feelings about the iFX's VELaSSCo visualization client. Please show the extent to which you believe this tool has the feature described in the statement. Here, we are interested in a number from 1 to 7 that shows your perceptions about the iFX's VELaSSCo visualization client.

You should rank each statement following a seven-point Likert-style scale from 1=very unimportant to 7=very important

The questionnaire is available in the following URL to be filled:

https://docs.google.com/forms/d/e/1FAIpQLScEQWrvk07eriIBNCb2xhjpeizZyYTtyQWEHbNE3SgbX6WgwA/viewform#responses

In summary, our purpose is to get your valuable feedback about your experience with the VELASSCO Platform and its usability against expectations.

We would also appreciate your impressions on practical issues and any other comment or criticisms that you may find interesting.

Please send your completed questionnaires telematics using the URL indicated above.

Thanks for your time.

The VELASSCO project.