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VELaSSCo

Visual Analysis for Extremely Large-Scale Scientific Computing

D1.1 – End-users requirements and Users panel

Deliverable Information

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1 Introduction

This report includes the user's requirements that VELaSSCo platform should address for the analysis and visualisation of DEM-Discrete particle data and FEM-Continuum data. Moreover, the methodology used with members of the Users panel to obtain these requirements is described.

"**Requirement:** capacity or condition needed by the user to solve a problem or achieve a goal."

1.1 Purpose

The requirements description specified in this document are from the end-user's point of view. From these requirements, tests will be derived which will be used to verify and evaluate the platform.

1.2 Product

The platform to be developed will make possible the analysis and visualisation of huge distributed simulation results which nowadays are impossible to perform.

1.3 Conventions

The requirements have a priority assigned according to the user's specifications:

- **key**: the requirement is key for the usability and good performance and evaluation of the system
- **added-value**: the requirement is considered an extra plus point for the final evaluation of the platform.

1.4 Methodology

The GQM ("Goal, Question, Metric") methodology [Basili et al. 1994] is proposed to be used to achieve the goal of defining a robust description of the end-user requirements for the VELaSSCo platforms for the visual-analysis of big and complex engineering simulation data (see Appendix below). The GQM process will guide the establishment of meaningful metrics to evaluate the quality, assess the progress and support the improvement initiatives over the duration of the project. This document provides the initial draft of the GQM process and the first listing of the user requirements, which has resulted from consulting a limited group of end-users. During the project, the GQM tables will be updated with the feed-back of the users.

2 User Panel

A User Panel with a potential membership of over 100 scientists and industrial R&D engineers including research centres, SMEs and companies form key European industrial sectors such as aerospace, household products, chemical, pharmaceutical and civil engineering has been created. The consortium has already sent an invitation to the potential end-users to join the panel and to encourage their participation and benefits of being part of the User Panel (see Appendix - Flyer). Procter&Gamble, RCPE, IPROCOM Coordinator, Johnson Matthey and the Colorado School of Mines are some of the end-users the consortium has contacted and are willing to facilitate data or work in the test towards achieving the new visualization platform. Some other companies have also shown interest into participate in the User Panel, such as DEM-solutions and John Deere.

This panel will be directly connected to the development of WP1 and WP5, by defining their needs and testing the new developments. The User Panel will:

- Define the end-user requirements (visualization and data analytics) of the system to be developed;
- Provide the scenarios where these requirements should apply;
- Select the examples to be used along the project;
- Define the specific variable to be considered in the evaluation;
- Test the VELaSSCo platform.

The user panel will be organized in four main engagements:

1. The first engagement will define the initial requirements for the users (Deliverable D1.1).
2. The second engagement will analyse the status of the development of the system, and define potential modifications and corrections in the system (Deliverable D1.2, Month 24).
3. Testing of the initial prototype of the system and final corrections/modifications (Deliverable D5.8).
4. Presentation and testing of the final prototype (Deliverable D5.9)

The locations of the meeting will be chosen depending of the specific task and potentially in conjunction with European or International events (conference, workshop, etc.) of related topics.

The first meeting with the User panel members took place during the recent Kick-Off meeting of the ITN T-MAPPP in the University of Edinburgh. The main goal of the session was to obtain the initial user requirements for VELaSSCo platform. A total of 16 DEM/CFD-DEM/FEM users from different Universities, research centres and companies attended to this successful event. The outcomes and the list of the institutions attending to this this session are detailed in the Appendix – User Panel meeting.

3 User requirements

In this section the user's requirements for the analysis and visualisation of DEM-Discrete particle data and FEM-Continuum data are listed. The following requirements are evaluated from the user's point of view as a **key** feature or as an **added-value** feature for the evaluation of the platform.

3.1 DEM – Discrete data User requirements

The VELaSSCo platform should handle three groups of scenario:

- One big model with few time steps.
- One small model with a lot of time steps.
- One model run several times with parameters sensitivity.

3.1.1 Data handling

- Fast Handling of big data size involving very large number of particles and time steps (key).
- Reduce the storage requirements by optimization of the data files size (key).
- Standard format to import simulation data into the post-processing tool (key).
- Efficient communication between simulation solver and post-processing :
  - Run time & Offline analytics (key).
  - Selective parameters for run time/ offline (key).
  - Self-optimization of simulation parameters (added-value).

3.1.2 Visualisation

- Real time visualisation of results to make decisions on the simulations (key).
- Temporal and Spatial averaging of the results:
  - Adjustment of the interval time for temporal averaging (key).
  - Adjustment of length scale for spatial averaging (key).
  - Tools to decide the relevant temporal and spatial averaging scales for each problem (added-value).

- Visualisation and tracking of complex particle shapes:
  - Easy way to import and define particle shape (key).

- Visualisation of large data sets over many time steps
  - Fast visualisation of results (key).
  - Adaptive resolution for the different zoom scales (key).
- Multi-platform and portable visualisation: from HPC to PC (key).

- Visual comparison of results from different datasets (key).

3.1.3 DEM Analysis

- Analysis of different datasets and easy comparison (key).
- Easy customization of analysis procedures (added-value).
- Statistical analysis of results and easy comparison (added-value).

3.1.4 Usability

- Friendly and intuitive graphical user interface (key).
- Detailed user manual and tutorials.

3.2 FEM – Continuum data User requirements

The VELaSSCo platform should handle two possible scenarios:

- Huge simulation with distributed results and several time steps of an hpc cluster.
- Plenty of simulations distributed on several computers.

3.2.1 Data handling

- Handling of big distributed simulation data (key):
    - from ~30 GB (100 M elements, 40 steps) to 12 TB (1G elements, 1,500 steps),
    - from ~140 GB (8 M elements, 2,300 steps) to 50 TB (240 M elements, 25,000 steps),
    - Between 1 GB and 10 GB of distributed results per time-step.
- Able to track errors in data, control of missing data (key).
- Visualisation and modification of simulation parameters (key).
- Usage of open data formats, optimization of data representation for storage, communication and visualisation.
- Able to export and store animations and results from queries (added-value).

3.2.2 Visualisation

- Ensure usability and interactivity:
    - Efficient communication between simulation solver and post-processing
    - Run time & Offline analytics.

  - Able to interact with the model (or a simplified representation) at interactive rates: zoom, rotate, etc. (key).
  - Able to get full-resolution results (key).
  - Acceptable waiting time of minutes for some queries, if longer, some feed-back should be provided (key).
- Visualisation of results over the results of the queries like:
  - Contour fill of user selected result over skin (key), cut-planes (key) or iso-surfaces (key).
  - Vector visualisation (with some kind of filtering or coarsening) on the volume data (added-value), skin (key), cut-planes (key) or iso-surfaces (key).

3.2.3 FEM Analysis

- Able to perform 0D queries:
  - inquiries about selected nodes, point (requires interpolation) and element (key).
- Able to perform 1D queries:
  - graph of a node or point along the time-steps (key),
  - line-cut and line-graph across the domain and showing the results along this line for a given time-step (key),
  - stream-line or particle tracing (added-value).
- Able to perform 2D queries:
  - boundary/skin extraction of the volume mesh (key),
  - cut planes on the volume domain, and get results interpolated on them (key),
  - iso-surface extraction of a result and interpolation of other results on this iso-surface (key),
  - computation of pressure forces over a structure (normal integral) (added-value).
- Able to perform animated queries, some of the above queries along some or all time-steps of the analysis, for instance:
  - animation of results over iso-surfaces, cut-planes, skin (key),
  - animation of stream-lines, graphs (added-value).
- Able to perform statistic queries:
  - minimum, maximum and average of a result on the whole model for a single time-step (added-value),
  - minimum, maximum and average for each node of the results along some or all time-steps (added-value).

3.2.4 Context

- The system should be able to co-exists with existing HPC resource management systems.
- Different users should be able to use it without interferences and ensuring security and confidentiality.

3.2.5 Usability

- Friendly and intuitive graphical user interface.
- Detailed user manual and tutorials

4 GQM process

This section includes the information obtained from DEM and FEM users in the format of the GQM methodology.

4.1 GQM for DEM user requirements

A meeting took place with a finite number of DEM users from within University of Edinburgh to go through the GQM process and to establish the initial goals, questions and metrics. This information is used to define the user requirements for particle discrete data.

4.1.1 GOALS

Goal	Description	Parent Goal	WP linked to
	DATA HANDLING		
G#1	Handle very large and complex data files	-	WP2
G#2	Simulation & Post-processing communication	-	WP2
G#3	Runtime/Offline Data handling/Analytics	G#2	WP2, WP3
G#4	Self-optimization of simulation parameters	G#2	WP2, WP3
	VISUALISATION		
G#5	Real time/Offline visualisation of large datasets over many time steps	-	WP2, WP3, WP4
G#6	Temporal and Spatial Averaging	-	WP2, WP3, WP4
G#7	Complex particle shape handling	-	WP2, WP3, WP4
G#8	Multi-platform: HPC, workstation, PC	-	WP2, WP4
G#9	Dataset comparison	-	WP3, WP4
	ANALYSIS		
G#10	Dataset analysis	-	WP3
G#11	Statistics of variables	-	WP3

	USUABILITY		
G#12	Ease of use	-	WP1, WP5

4.1.2 QUESTIONS

Question	Description	Associated Goal
Q#1	What is the size of the data files?	G#1
Q#2	How many particles are involved in the simulation?	G#1
Q#3	How many time steps per simulation?	G#1
Q#4	How many results/variable can be handled?	G#1
Q#5	How can data file size be optimized?	G#1
Q#6	How fast can be the communication solver-post-processing?	G#2, G#3
Q#7	How long does the data loading process take?	G#2, G#3
Q#8	How long does the data writing process take?	G#2, G#3
Q#9	How many simulation parameters can be optimized?	G#2, G#3, G#4
Q#10	Are selective parameters during runtime possible?	G#1, G#2, G#3, G#4
Q#11	What is the ratio of visualisation time/ data save interval (sampling frequency)?	G#1, G#5
Q#12	What type of visual outputs?	G#5
Q#13	How much time is necessary to visualise the results?	G#5
Q#14	How to adjust temporal and spatial scales?	G#6
Q#15	How to manage and track irregular shaped particles over time and space?	G#1
Q#16	How to visualise complex irregular shaped particles?	G#7
Q#17	What is the level of graphical detail required for different spatial scales or zoom levels?	G#5, G#6, G#7
Q#18	What are the minimum required hardware specifications (GPU, CPU and RAM) for PC?	G#8

Q#19	How to simultaneously visualise different datasets for comparison? (e.g. parametric study)	G#9
Q#20	How to analyse differences between datasets?	G#9, G#10
Q#21	What Statistics parameters can be obtained?	G#11
Q#22	How long does post-processing set-up take for the user?	G#12

4.1.3 METRICS

Metrics	Description	Associated Question	Value
M#1	Dataset Size	Q#1, Q#5	up to petabyte but the great majority are a lot smaller - approx. 50Gb
M#2	Number of particles	Q#2, Q#5	up to 10^7
M#3	Number of computational time steps	Q#3, Q#5	up to 10^9
M#4	Number of results at particle level	Q#4, Q#5	Min. of 10 variables
M#5	Number of results at bulk/continuum level (Stress calculation)	Q#4, Q#5	Min. of 14 variables
M#6	Number of simulated time steps/Number of post-processed time steps	Q#6	Less than 50
M#7	Processing time per simulated time step (s)	Q#7, Q#8, Q#13	Less than 10 seconds
M#8	Number and type of parameters	Q#7, Q#8	Less than 10 seconds
M#9	Number of parameters to be optimized	Q#9	Minimum of 3
M#10	Ability to discard unwanted information	Q#4, Q#10	NA
M#11	Visualisation frame rate	Q#11	
M#12	Contour fill, contour lines, vectors,	Q#12	NA

	iso-surfaces, stream lines, particles, contact network.		
M#13	Number of time steps	Q#14	Min. 2, Max. All time steps
M#14	Length in particle size	Q#14	Min. 1, Max. up to user
M#15	Format to import particle shape.	Q#15, Q#16	Min. of 2 formats: templates and meshes.
M#16	Pixels/particle size and Pixels/visualizing area	Q#17	Min. 20

Metrics	Description	Associated Question	Value
M#17	RAM memory (Gb)	Q#18	Min 4Gb (benchmark needed).
M#18	CPU specifications (GHz, kB)	Q#18	Min. 2.5 GHz (benchmark needed)
M#19	Number of cores	Q#18	Min 4 (benchmark needed)
M#20	GPU specifications(Gb, MHz)	Q#18	Min. 1Gb per GPU (benchmark needed)
M#21	Number of datasets for visual comparison	Q#19	Min. 2
M#22	Number of datasets to analyse	Q#20	Min. 2
M#23	Number of variables to compare	Q#20	Min. 2
M#24	Statistics parameters: mean, min, max, standard deviation.	Q#21	NA
M#25	Time for setting-up post-processing	Q#22	< 5 minutes

4.2 GQM for FEM user requirements

A meeting took place with some FEM simulation experts from within CIMNE, in order to collect, via questionnaire, their requirements according to the scenarios defined in the DoW and using the two provided CFD simulations (racing car aerodynamics and wave propagation in harbour infrastructure) to get the detailed functionalities and queries which will help to define the tests to validate the platform. This information is used as a starting point for the GQM process, which will help to control the design and implementation of the platform and the validation of the prototypes.

4.2.1 GOALS

Goal	Description	Parent Goal	WP linked to
	DATA HANDLING		
G#1	Able to interact with the remote distributed data from personal computer	-	WP2
G#2	Able to interact with an existing HPC systems	-	WP2
G#3	Confidentiality		WP2
	VISUALISATION		
G#4	Visualisation of FEM simulations and analysis	-	WP2, WP3, WP4
	ANALYSIS		
G#5	Able to analyse FEM simulations	-	WP3

4.2.2 QUESTIONS

Question	Description	Associated Goal
Q#1	Where are the data located?	G#1
Q#2	Which is the layout of the data?	G#1
Q#3	Is the interaction flow the desired one?	G#1
Q#4	What is the time-lag between the user's (first, subsequent) request and the system answer? (May be several questions for the several queries to be performed)	G#1
Q#5	Is this speed improving?	G#1
Q#6	Does the user have a feed-back between request and answer?	G#1
Q#7	Which is the acceptable waiting time to get feed-back between request and answer?	G#1
Q#8	Does the user accept a temporary answer while the exact answer is being computed?	G#1
Q#9	Can the error or missing data be tracked and overcome?	G#1
Q#10	How does the system perform?	G#2
Q#11	How does VELaSSCo platform behave with a production environment?	G#2
Q#12	Can 0D queries be performed?	G#5
Q#13	Can 1D queries be performed?	G#5
Q#14	Can 2D queries be performed?	G#5
Q#15	Can animated queries be performed?	G#5
Q#16	Can static queries be performed?	G#5
Q#17	How long does it take to perform the queries?	G#5
Q#18	Is quick enough for the user?	G#1, 4
Q#19	Does the user need feed-back or temporary results?	G#4

Q#20	Can a contour fill/ vectors be displayed on the queries of any results?	G#4

Question	Description	Associated Goal
Q#21	Is the visualisation interactive or can be made interactive using simplification / decimation?	G#4
Q#22	Can the visualisation or the result of the queries be stored?	G#4
Q#23	Are the data secured?	G#3
Q#24	Is the access secure?	G#3

4.2.3 METRICS

Metrics	Description	Associated Question	Value
M#1	Number of nodes with data, how are the connected.	Q#1	10^7 … 10^9 nodes on a tetrahedral mesh
M#2	Structured data, redundancy, distributed parts, time steps	Q#2	1 domain, 4 … 1024 sub-domains, 50 … 25,000 time-steps
M#3	Define an interaction flow and rate it by the user.	Q#3	
M#4	Average time	Q#4	Depending on the query, from seconds to minutes
M#5	Percentage over initial timing	Q#5	%
M#6	Feedback for the user	Q#6	questionnaire
M#7	Time between request and any answer	Q#7	seconds

M#8	Similarity between temporary and final answer	Q#8	Visual similarity
M#9	Check traceability of errors	Q#9	Cause and trace an error
M#10	Queries per sec	Q#10	Tens of queries
M#11	Balancing between query engine and HPC's simulations	Q#11	Tools to make possible cohabitation with simulations codes
M#12	Percentage of resources usage	Q#11	CPU / memory / communication / disk usage
M#13	Node/point inquiries	Q#12	Yes / no

Metrics	Description	Associated Question	Value
M#14	Graphs of results of single nodes/points, Line-cut across the domain, Stream lines	Q#13	Yes / No
M#15	Boundary skin extraction, cut planes across the domain, interpolating results on demand, iso-surfaces	Q#14	Yes / No
M#16	Reproduction of queries across the time-steps of an analysis	Q#15	Yes / No
M#17	Min, maximum, average values of results of whole model for a time-step	Q#16	Yes / No
M#18	Min, maximum, average values of results on each node of domain	Q#16	Yes / No
M#19	Average time for queries	Q#17	Between seconds and 1-2 minutes
M#20	Measure time, ask the user	Q#18	questionnaire
M#21	Provide feedback	Q#19	questionnaire

M#22	Check validity of results (may require interpolation of original results to point/cut/iso-surfaces)	Q#20	Yes/no, validation of results
	…		

APPENDIX - GQM Methodology

Generally speaking, the GQM (“Goal, Question, Metric”) methodology [Basili et al. 1994] provides practical guidance for establishing and using meaningful metrics, (which are well defined with the goals of the organizational environment), in order to evaluate the quality, assess progress and support improvement initiatives of a given project.

GQM is a top-down approach to establish a goal-driven measurement system for software development, in that the team starts with organizational goals, defines measurement goals, poses questions to address the goals, and it identifies metrics that provide answers to the questions. Ultimately, the GQM method defines a measurement model based on three logical levels, as depicted in the figure below:

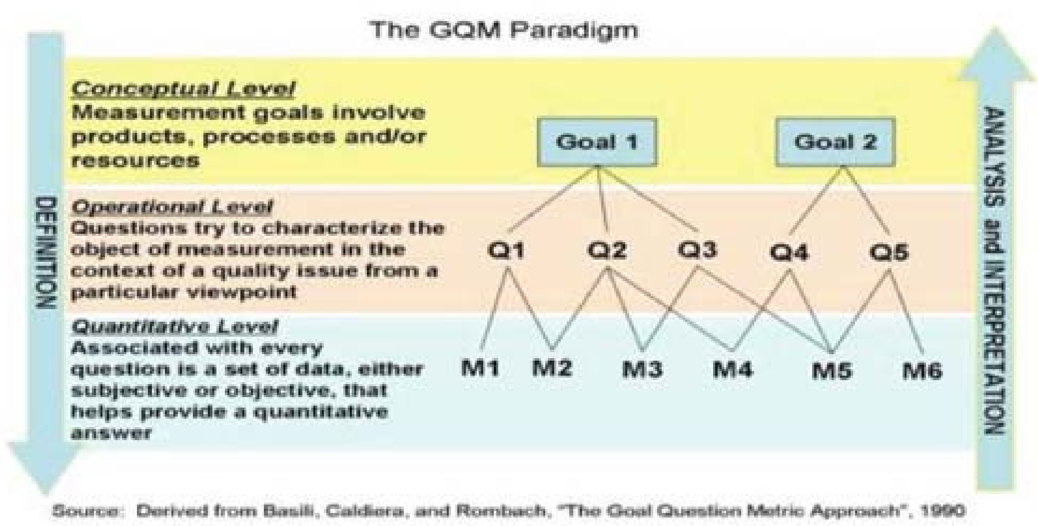


Figure 1. GQM Schema

GQM is described in terms of a six-step process where the first three steps are about using goals to drive the identification of the right metrics to be utilized in the Project and Use cases and the last three steps about gathering the measurement data and making effective use of the measurement results to drive decision making and improvements based on solutions delivered in the UCs.

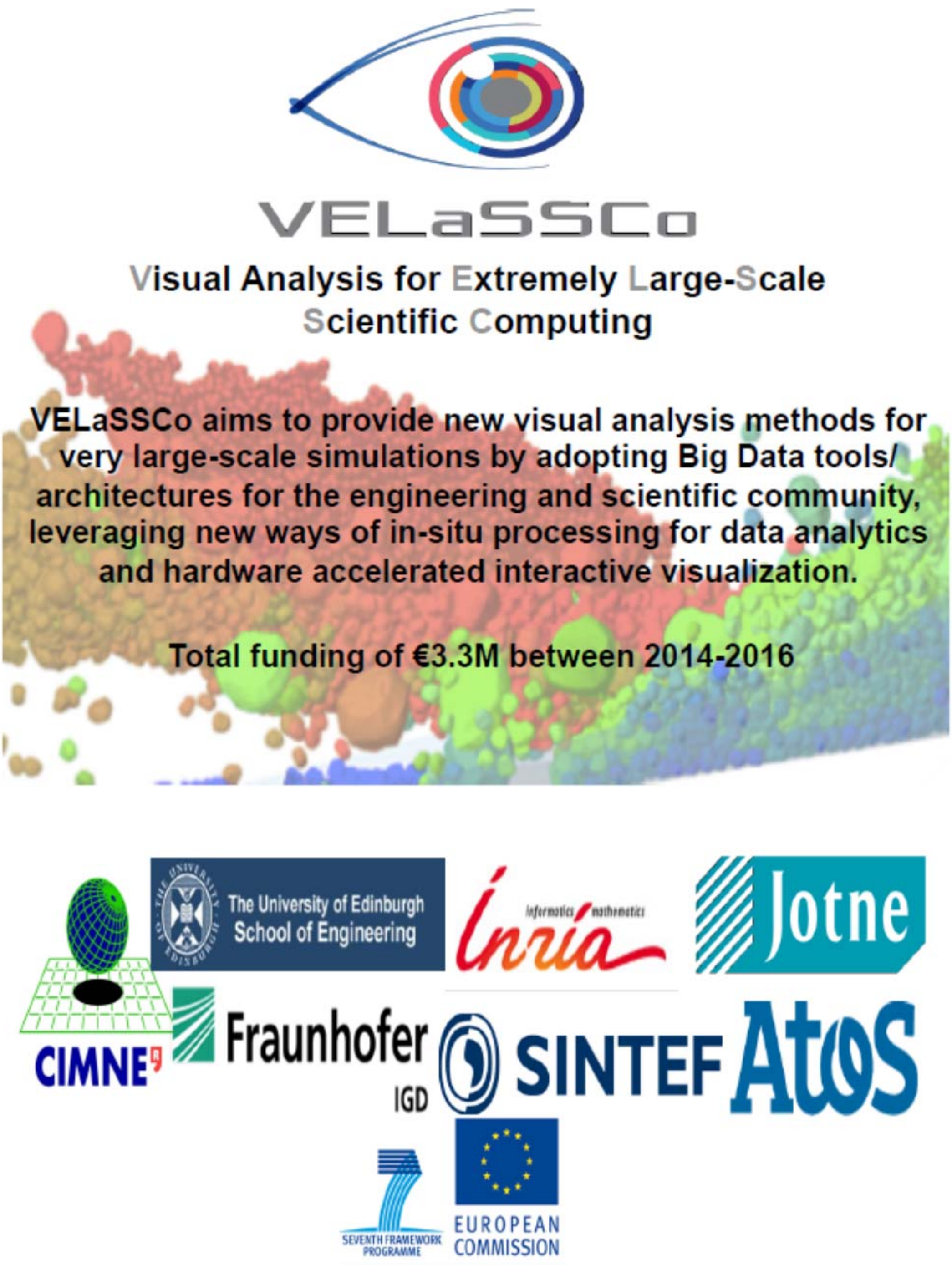
The steps of GQM, adequately contextualized for the VELaSCCo project, are the following:

1. **GOALS** – Develop a set of project goals of paramount importance.
2. **QUESTIONS** – Generate questions that assess goals achievement as completely as possible in a quantifiable way and specify the detailed steps necessary to answer those

questions and track prototypes conformance to the goals, to obtain a significant and objective assessment of the goals.

3. **METRICS** – Specify the measures needed to be collected to answer those questions to track prototype conformance to the goals specified.
4. **TOOL SETUP** – Develop mechanisms for data collection (for example, a spreadsheet gathering comments from the various end-users on the same goal, if applicable).
5. **DATA COLLECTION AND FEEDBACK** – Collect, validate and analyse the data (in quasi-real time) to provide feedback for corrective action.
6. **FINAL ANALYSIS** – Analyse the data in an *a-posteriori* fashion to assess conformance to the goals and to make recommendations for future improvements.

APPENDIX - Flyer



APPENDIX – User Panel meeting

This appendix reports the outcomes from the User Panel discussion with associated T-MAPPP partners that took place last 18th of March 2014 in Edinburgh. The main goal of the session was to obtain the DEM/ CFD-DEM user requirements for VELaSSCo platform. A total of 16 DEM/CFD-DEM users from different Universities, research centers and companies attended to the event. The list of the different institutions participating in the session is the following:

- University of Edinburgh
- University of Twente.
- Univérsite de Technologie de Compiègne.
- CIMNE.
- Research Centre Pharmaceutical Engineering.
- Nestlé.
- Procter&Gamble.
- Johnson Matthey.
- DCS Computing.
- DEM Solutions.

Dynamics of the discussion

First, a brief overview of VELaSSCo project was presented to the participants. Moreover, an engagement speech in order to stress the potential benefits from VELaSSCo project to the User Panel members was given. After the presentation, the following scenario and question were posed for the brainstorming:

Scenario: You can get the "perfect" pre/postprocessing platform for large DEM/DEM-CFD simulation data:

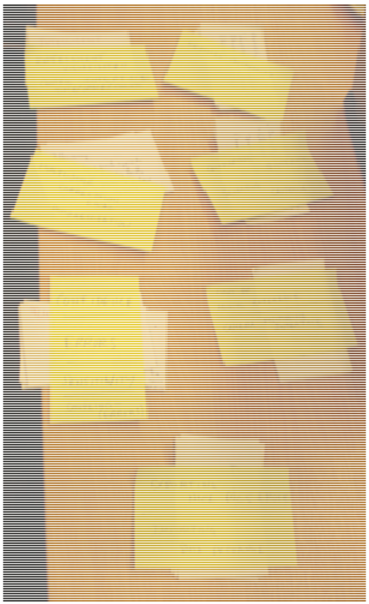
- Many time steps (> 10^9?).
- Large number of particles (> 10^7?).
- Multiple runs of the same model with different parameters.

Question: Which are the key features that you expect from that "perfect" software in terms of Data handling, visualisation, analysis, usability, ...

The brainstorming and the discussion were structured as following:

1) Individual ideas: each person wrote down his/her.
2) Discussion in groups: individual ideas were discussed and summarized.
3) Presentation of the main ideas: each group presented their main ideas.

Lively discussions of the individual ideas in different groups



Clustering and presentation of the main ideas

Group ideas and clustering

DATA HANDLING

- Exporting nice pictures and movies.
- Importing data/ data exchange.
- Data compression.
- Change time scale for averaging.
- Determination of important time and length scale automatically.

- Ability to filter what to keep and discard.
- Complex particles.

DATA ANALYSIS

- Confidence/ Errors/ Sensitivity.
- Comparison of multiple dynamic runs.
- `”On the fly” averaging.
- Easy calculator of fluxes.
- Define filters
- Fast conversion from micro to macro.
- Automatic outputs “on the fly”.
- Comparison of experiment/ numerical data.

VISULISATION

- Control simulation through visualisation.
- Camera positioning interface.
- Moving reference.
- Dynamic manipulation of 3D objects in real time.
- Define filters.
- Localized visualisation.
- Complex particles visualisation.
- Visualisation for large scale particles.
- Intelligent visualisation.
- Control interface for time/space/color.

USUABILITY

- Reduced complexity
- Verbal control.
- HPC friendly.

Individual ideas

- Intuitive methods to visualise results respect to high number (> 3 independent varibales).
- 3D tensor fields.
- Efficiency multiscale approach allowing for changing locally timesteps in DEM (eg. Shear zones vs static regions).
- Need techniques to visualise confidence in predictions (error bars or distributions).

- Intelligent representation of log vs lin scale.
- Identify particle only in specific areas.
- Collisional information for large number of particles .
- Handling incomplete data.
- Scripting for videos, camera positioning.
- Able to move coordinate system.
- Data visualisation for large (high number of particles) simulations.
- Data compression.
- “Downscale” to smaller file sizes at any moment.
- Choose temporal/spatial file variables.
- Multi-scale visualisation.
- Multi-particle >> 10^6.
- Parameter sensitivity analysis.
- Complexity reduction for movie/visualisation.
- Scale dependent resolution.
- Detection and comparative tools.
- Identify data the fulfil criteria – or not.
- Fast coarse-graining of large data-sets.
- Export to SVG, copy to clipboard.
- Different representation of images for screen and paper.
- Tools to compare results from multiple run.
- Open formats allowing for an easy data exchange.
- Homogenized discrete data (space+time).
- Spatial averaging of 3D DEM dynamic data “on the fly”.
- Temporal averaging of 3D DEM dynamic data “on the fly”.
- Deriving BC conditions for multiscale analysis.
- Possibility of visualising results for a sector of the whole domain.
- Dynamic manipulation of graphical object in real time while simulation is running.
- Touch screen manipulation of graphical objects in real time to generate geometries as well as better visualisation solution.
- Flux averaging on easily selected surfaces.
- Define filters to select particles or fluid behavior and switch between them rapidly.
- Select zones to generate video animations of selected features.
- Verbal control.
- Control simulation through visualisation.
- Interactive time-averaging.
- “Automatic” determination of “important time and length scales.
- Fast and userfriendly temporal and spatial averaging for some parameters.
- To allow work on multiprocessor workstation and not only big HPC computer.
- To be able to integrate some bulk quantitates on changing temporal and spatial scales.
- To do parameter sensitivity analysis.
- Automated output (real time) of key factors.

- Fast conversion of microscale data to macroscale and visualisation.
- Filtering and saving of "important" results (eg. Discarding slowly varying results across most timesteps).
- Can this be made HPC friendly (Shared memory)?
- On the fly coarse-graining.
- Good visualisation of non-spherical particles.
- Postprocessing of DEM (CFD-DEM) simulations: temporal + spatial averaging.
- Ability to cross reference experiments vs DEM (or DEM-CFD) simulations 3D and calculate objective function.
- Fast movie generation.