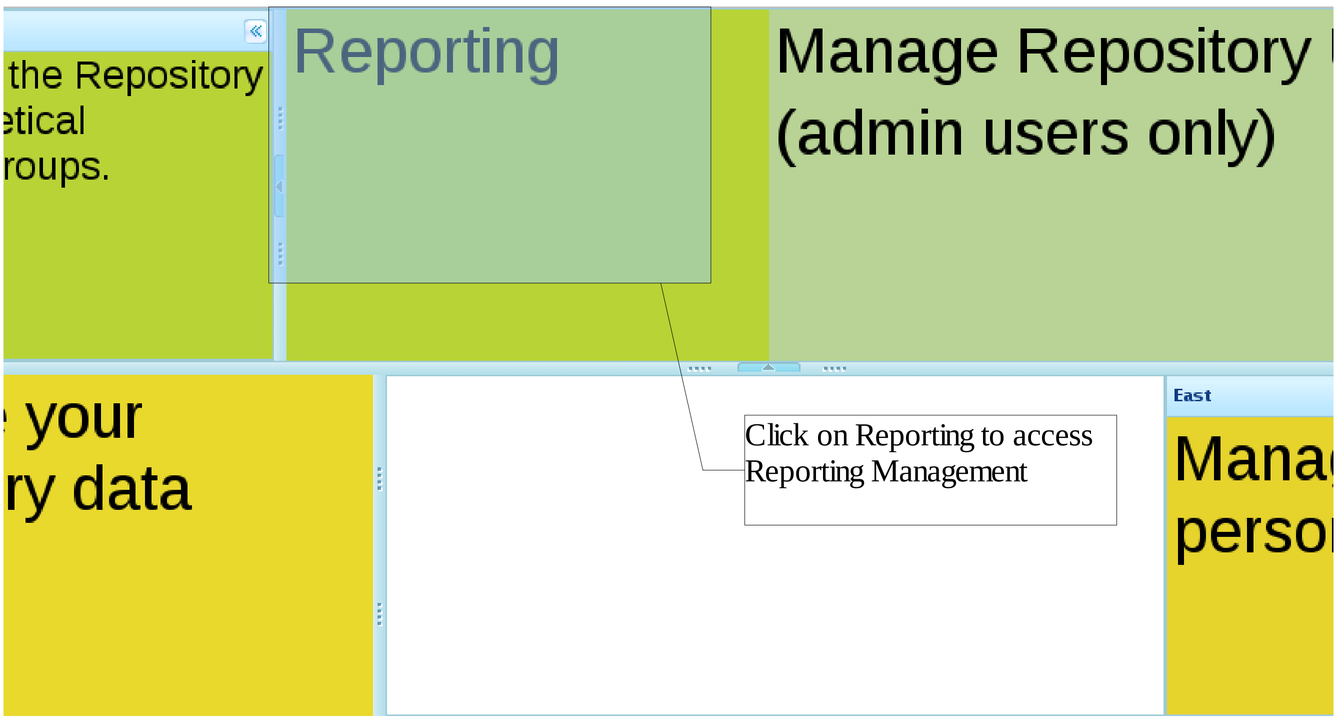
Reporting tutorial

Introduction

This tutorial is about reporting, generating new information in various formats from the stored data in the data base.

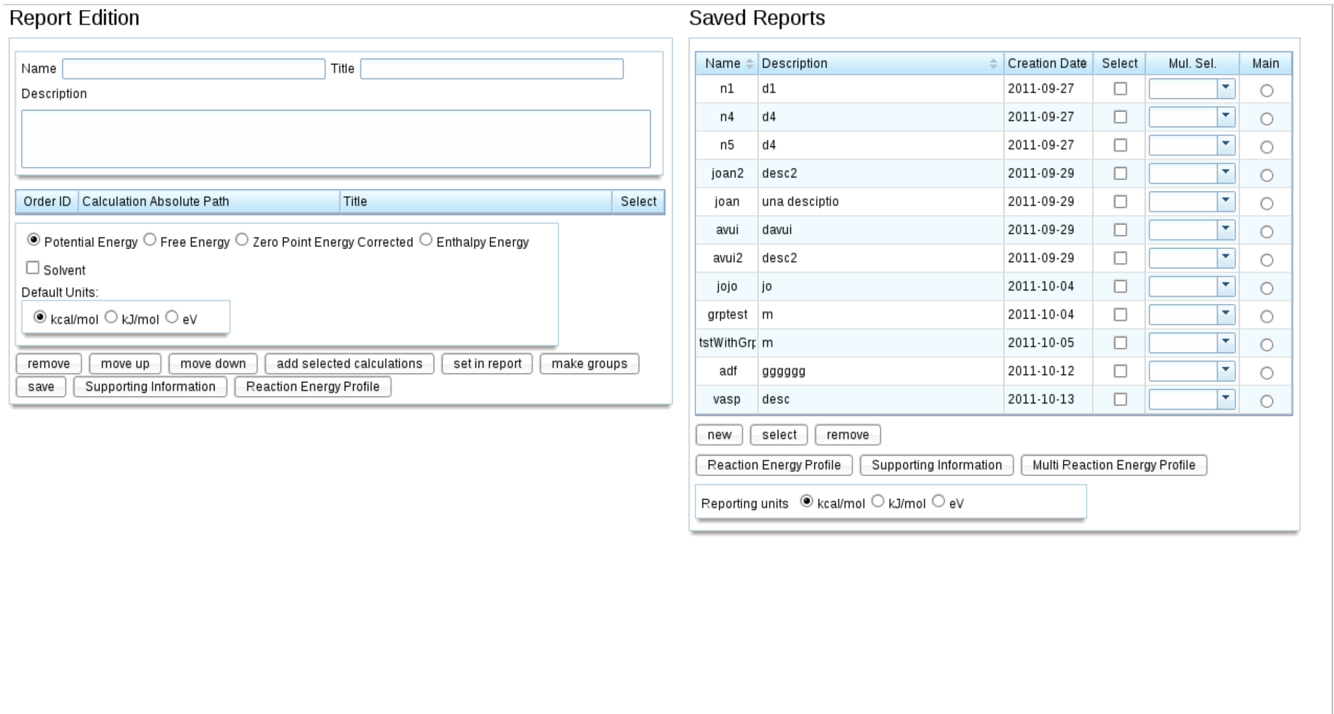
For the moment, there is only on reporting tool: Reaction Energy Profile Generation of the Potential Energy for VASP, ADF and Gaussian. Solvation Energy for the moment is not available, for this kind of reporting generation.

General Reporting Management Introduction



When “reporting” is pressed in the main page of the repository a new browser window is opened.

... and it has the following appearance:



On the right you have a list of your own reports definition. This list is not shareable, it's only visible to you. For the moment most of the functionalities are not programmed. As I mentioned earlier, the only functionality programmed until now is the Reaction Energy Profile Generation for the potential energy.

On the left you can see the detail of the report definition. You have a name for the report, that identify the report, a title, used for future report generations [supporting information], and a description field used for documentation of your own reports [what the report do or pretends to do, and so on].

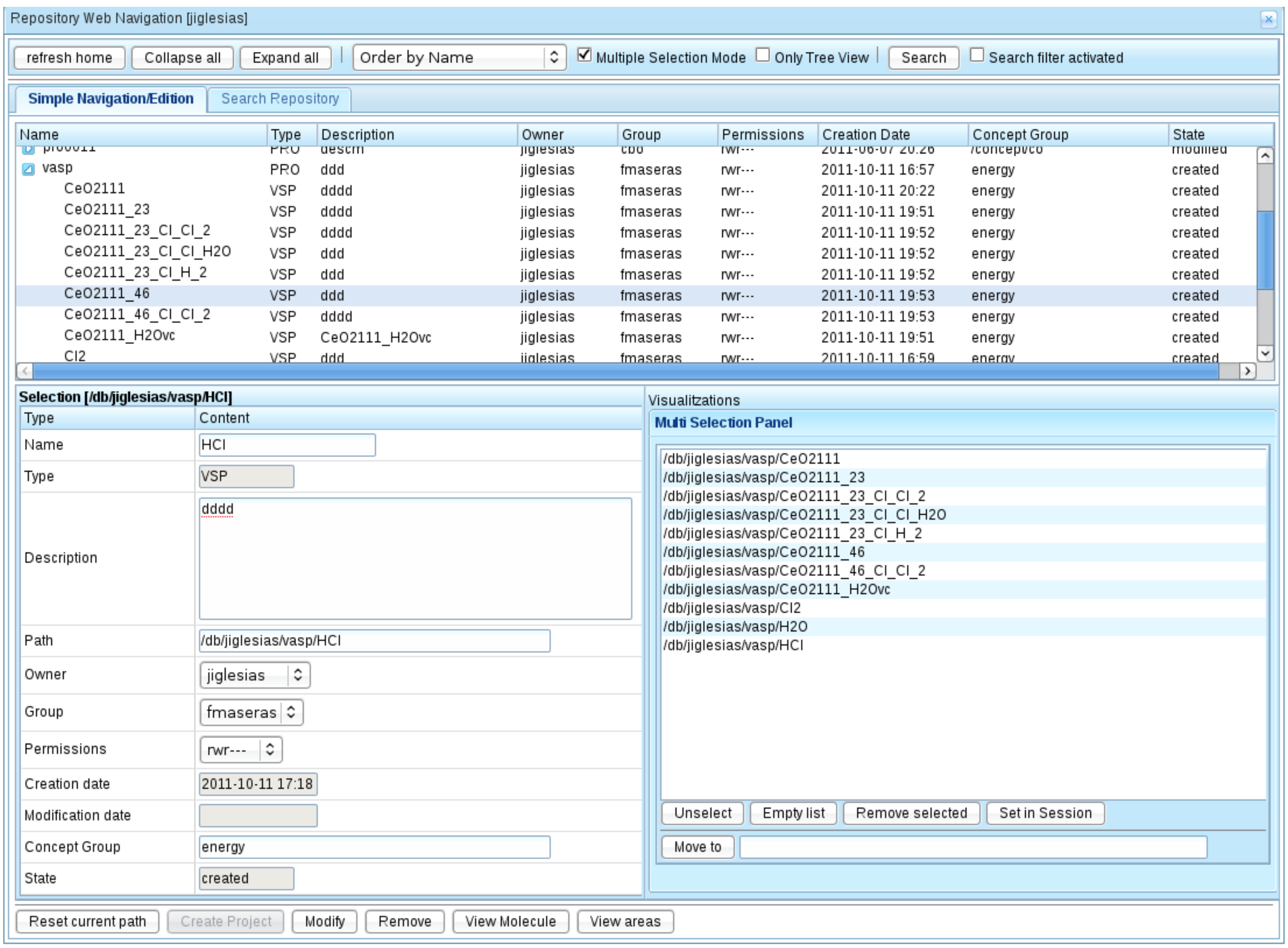
On the right, you can manage the reports, that means you can create, select and delete a report. Multiple selection of reports, for the moment has no effect or doesn't have any functionality associated. You can only select one report at a time. Of course, you can order the reports by clicking on the title of each column. The report definition is paginated, that means you can access the list of reports definitions by clicking on “next page” symbol.

Lets go into a sample of report generation, step by step and screen by screen:

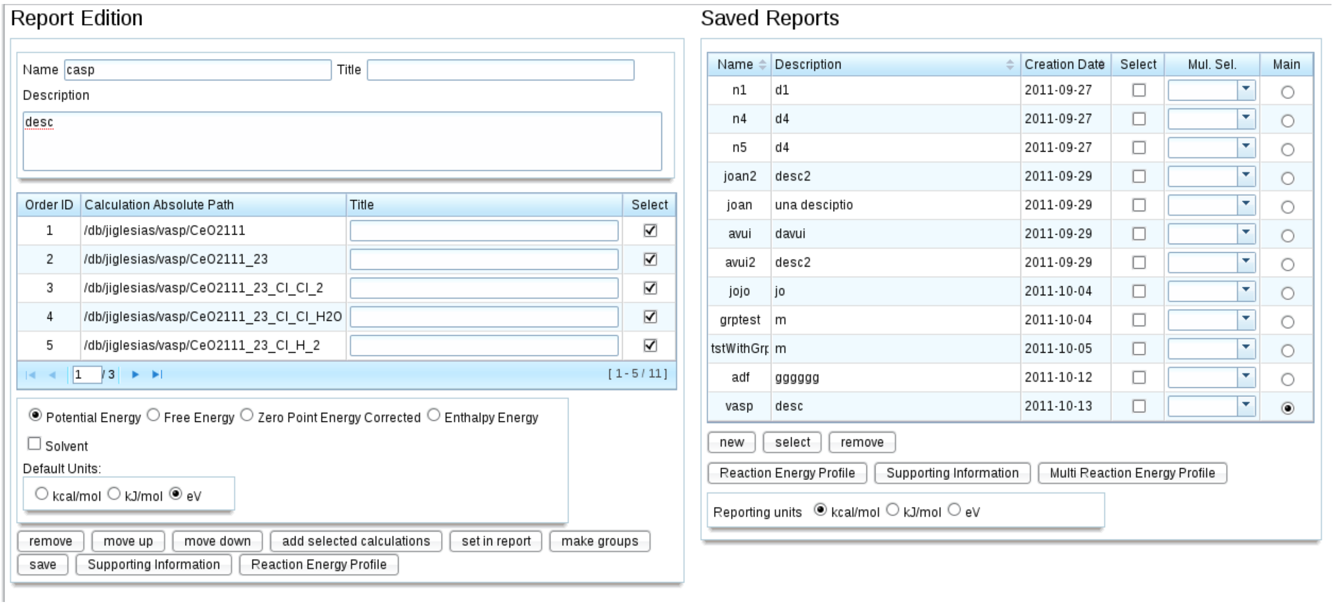
First of all press new on the right panel and a clean panel will appear on the left. Fill the main fields: name, description, and so on...

Now we will associated a group of calculation to the report, for doing the Reaction Energy Profile. For this selection go the the main page, and click on “Manage your repository Data”.

In our example we will define a VASP report. In that case, I have single project, called vasp, and into it I have a group of VASP calculations. Press the flag of Multiple Selection Mode on the top of the screen and a new panel will appear on the right bottom corner and click on each calculation you want to be processed for doing your Reaction energy profile. After the selection is made, press the button “Set in session”. This button makes available the selection for the other browser window, that allows you to manage the reports. You have a sample on the following screen-shot:



After the selection is made, go to the reporting window. Press the button “add selected calculations” and the selected calculations will appear in black color. Those selected calculations are not really “into” the report, they are only in selection mode, and they are accessible for all the defined reports to be added, if you want. In our example we want all the calculations to be added to the report definition. Select all the calculations and press “set in report”. After that the selected calculation will change their color from intense black to soft black. Take a look to the screen shot:



At this moment, has no effect if you press any other energy, or solvation. It only operates using the potential energy. For the coherence of the database, please select Potential Energy.

You can choose the units, that is fully functional. In our case it's pressed eV.

Because the reports has in mind the calculation order in this screen you can reorder the calculations, selecting them and moving up and down, using “move up”, and “move down” buttons.

Position 1, means calculation 1 potential energy [abbreviated c1], position 2 means calculation 2 potential energy [abbreviated c2], and so on. The “c” stands for calculation, in that case is a reference to the potential energy of each calculation.

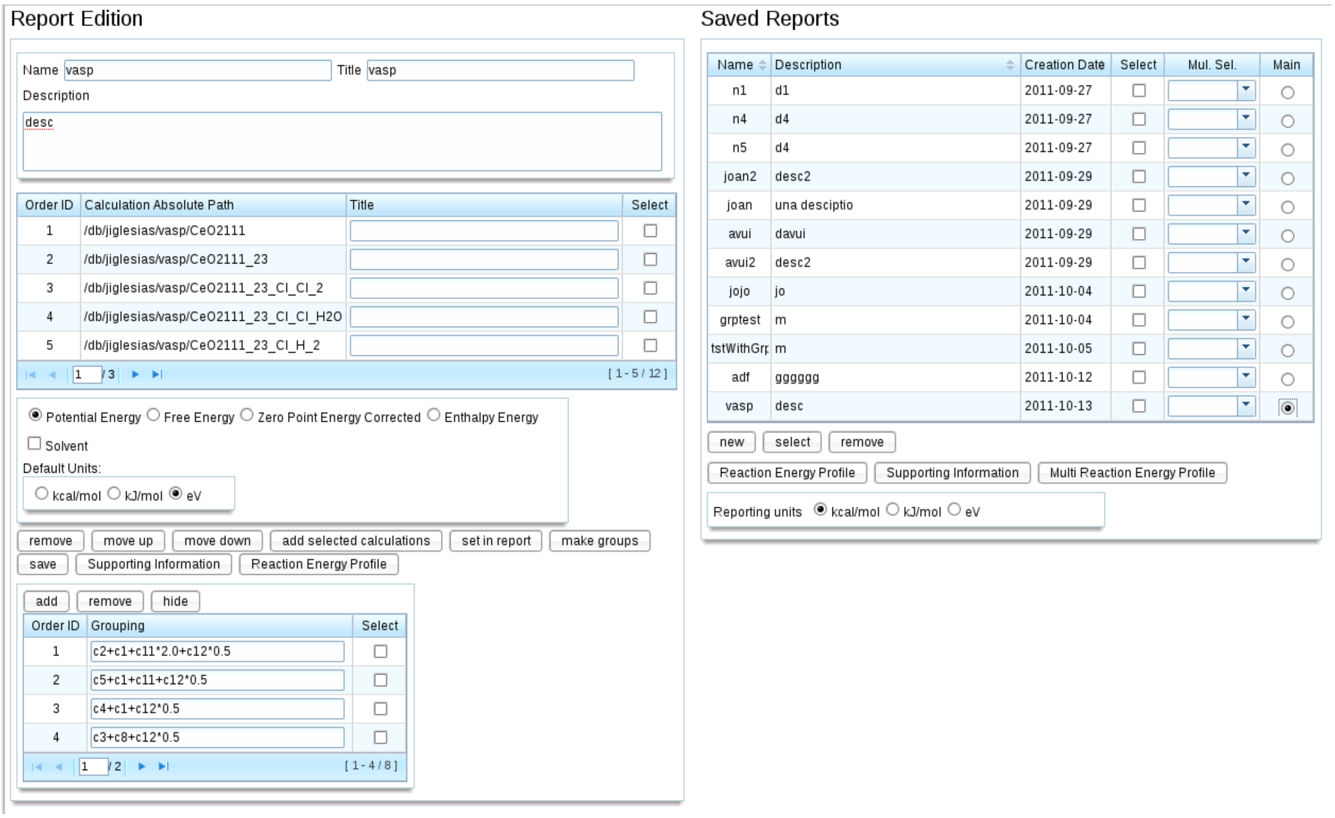
For the Reaction Energy Profile definition you must create “groups”, each group corresponds to an “step” in the reaction. The first group corresponds to the “Reactants”, the intermediate groups are each transition state. The last group, of course, are the products. In our sample we will define 8 reaction steps. Press add to create a reaction step boxes, fill each box with the calculation you want to be processed for this step.

You can define the following kind of formulas:

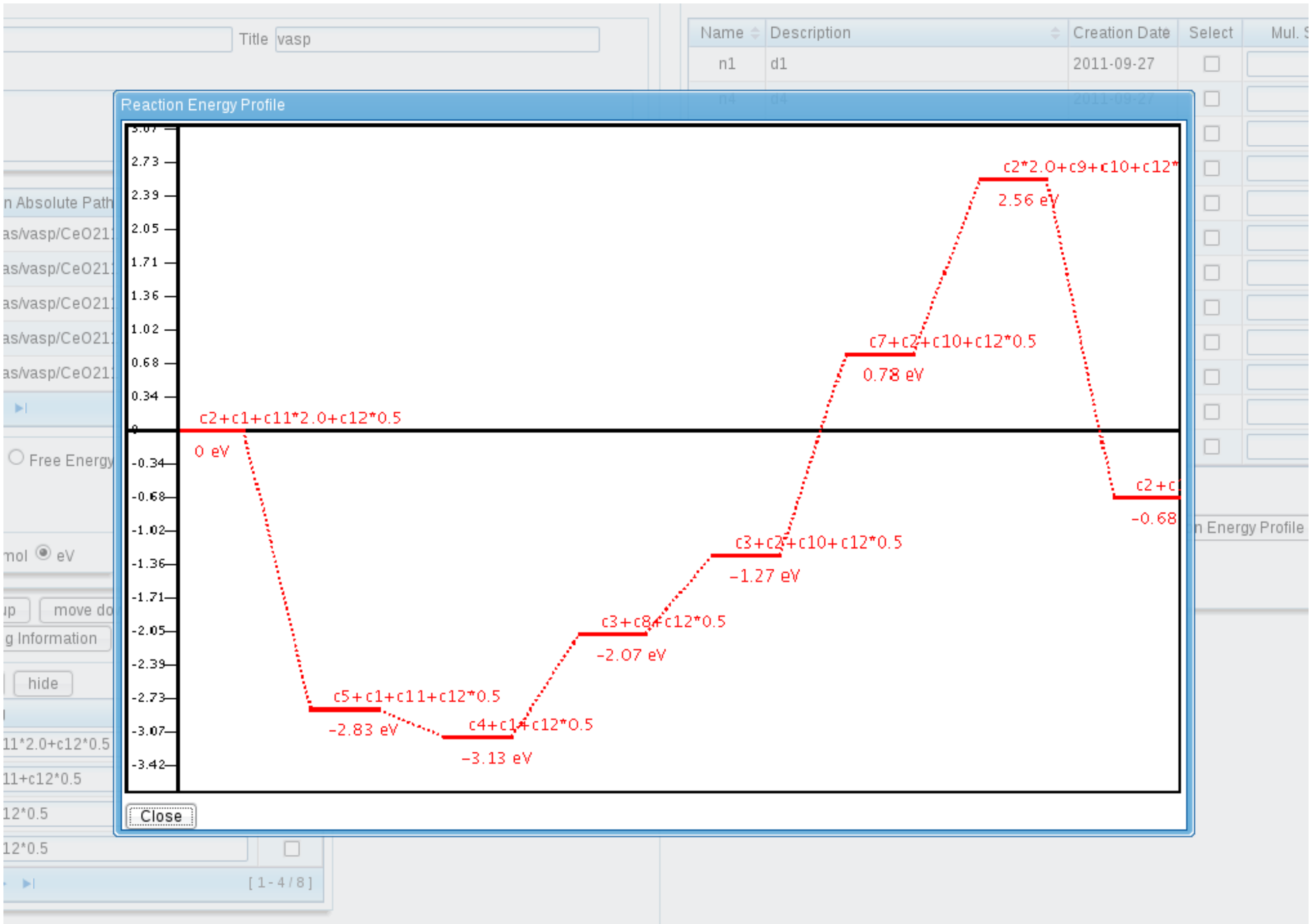
1. Single calculation potential energy reference. Example: **c1**
2. Addition and subtraction of potential energies. Example c1+c2-c3
3. Multiplication for a constant of each potential energy. Must be a decimal one ALWAYS. That means a number a dot and another number. Multiplicands cannot be negative Example: c1+c2***0.5**+c3***1.0**

4. And finally you can define a positive multiplicand for the whole formula. Like the other multiplicands, those must be decimal also: digit, a dot and a digit. If this multiplicand is specified, parenthesis are needed. Examples: **(**c1+c2*22.2**)*2.0** or this one : **(**c2**)*0.5**

Here you have another screen shot of the groups definitions:



At this moment, you have two options: or save the report or not to save. If “save” is pressed, it will appear in the Reporting list. At this moment, event it's not save, you can press the button “reaction energy profile”, and an image will be generated with the data specified in the report. Here you have another screen shot:



Already defined Reports can be selected and modified using save, or generated again.