Comments raised related to the CMMST-VRC Proposal Document

Sergio Maffioletti

Generally speaking the document seems too much focused on the technologies available rather than an idea how to organize the existing VOs and create value for the researchers.

Maybe a sort of 1 page executive summary will help us condensing all the ideas into a coherent structure

The document should probably state more clearly:

. What is the overall objective (like "create a self-sustained CMMST community that organize itself with access to a large plethora of tools and services to improve collaborative research")

. How it is proposed to achieve the objective ( where are the money coming from ? why one would contribute with own resources ? )

. Who is the target (researchers, research groups, IT providers, communities,... )

 . what would be the value for them

 . Why would they be interested in using the services provided by the proposed VRC

. I would suggest to simplify the "4.3 The adoption of a credit system in the CMMST VRC" it raises too many questions that are, imho, not relevant for the scope of the document;

if we want to make the case that different level of involvement of the end-users will be mapped to different roles and, eventually, different contribution models, we could simply state that the new users will be offered a 'fremium' access to the services and then they could either be end-users (will be charged for their usage on a 'pay-per-use' model of some sort) or will become members of the VRC and contribute to the service portfolio.

Task for the VRC will be to come with a marketplace and a business model to balance the different level of contribution/usage.

. Provide resources: To me this point is unclear, I thought the resources were coming from EGI. Is it foreseen the VRC will have its own resources not taken from the EGI pool ? what is the rational behind this ?

. "2.2 M2-M5 outcomes" I'm not sure I follow here, are we talking about a scenario where the VRC collects money from the different partners and buys resources for them ? or a sort of joint purchase to be placed/operated centrally ? how this is even legally possible (cross institution purchases)

. "4.4.6 Sustainability" This part needs to be expanded and clarified. I must have missed the discussions on the sustainability...

Jelena Tamuliene

An ide of the CMMST:

To  bring together research teams in computational chemistry area into a virtual research community at a worldwide level, focusing on the application of  quantum mechanics in physical models and experiments of chemical systems. The VRC covers the following scientific interest:
• To predict the molecular structure of molecules by the use quantum chemical methods.
• Storing and searching for data on chemical entities.
• Identifying correlation between chemical structures and properties.
• Creation of the computational approaches to help in the efficient synthesis of compounds as well as to design molecules that interact in specific ways with other molecules.

Target group: recearches or researches group of the computational chemistry domain, IT provider and creator ( more detailed clasification)

The value for target group:  large IT resources ( it is written in the document); data basis of the researches, program and tools; share of knowledge and results; share of self-created (unique) program for research; rapid communication; independed-testing of  new approches and program packages.