ScalaLife

Scalable Software Services for Life Science

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WP2

Web portal: How to improve

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1. What are the main categories that you have clicked on when you first looked on the web?

   a. Competence Center: Applications, HPC Resources, Forum, Activities

   b. News, FAQ, Training

   c. News & Activities. I was looking at News for the forthcoming events, but News referenced to Newsletters from past events. Activities have both future and past activities

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2. Do you find the information on the from page useful, if not what you would prefer to come first?
   a. I think for me the main usage of this website would be for finding information on computational resources and codes, so it would be useful if this information came first.

   b. Front page contains a large description. I'd prefer to see recent and forthcoming activities to complement a briefer description of the project.

   c. No. It is intended for people not familiar with the project. The news is too low down so if you are lucky you see half of the latest news item.

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3. Does the purpose of the web clear from the first sight or did it take you time to figure out why actually this web is needed?

   a. It is pretty clear, but perhaps some “slogans” in larger text on the front page stating your goals and what kinds of services are available would be useful.

   b. No, it wasn't clear to me. The "Competence Center" title is not clear to me, what does it mean? From the topics within, it seems to be related with some application studies. I don't know why I'd be interested on "Who's online" unless I have the chance to contact them directly (this is only applicable for non guests users). Personally, I don't like the main page to be split in 3 columns. At first, I didn't know what to look at and I found the web unnatural to read. The right column seems to contain fast accesses to some parts of the left column, which is a good idea, but it could be implemented differently.

   c. There is some confusion about who it is for. Is it to tell people what ScalaLife is and show what work has been done or is it for researchers who want to run on PRACE but need help with scaling?

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4. What information do you miss on http://www.scalalife.eu/applications ?

   a. I was not missing anything, as you offer a short description of the code and also a link to the code's own webpage

   b. Either more detailed description once single app is clicked on; however, this is problematic as the stuff is constantly further developed and might change. Or just really link to the description on the appropriate websites instead of just the root domain. E.g. http://www.gromacs.org/About_Gromacs for Gromacs rather than www.gromacs.org

   c. Too much text; suggest a case study of a scientific use of the codes with a picture rather than a dry paragraph explaining (or not in the case of DISCRETE) what it does.

5. What kind of video tutorials would you like to see there?

a. I don't feel that video tutorials would be needed if proper README files are attached. However, small & introductory video tutorials would be interesting for graphical applications.

b. For me the live lecture videos are easier to follow

c. I guess video tutorials will only be useful for operations which are not too complex. Also a video for command-line tools is not very useful. So in case of Gromacs, a tutorial for the analysis would be helpful.

d. The GROMACS one is for new users and is from 2007! I like screencasts where you see a screen with e.g. text editor and terminal and so you see the commands being typed as you would while the audio explains what is going on. Ultimately a tutorial of how to tune GROMACS on HPC including PRACE machines would be very useful.

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6. Do you think this web is something your would use on everyday bases to access Gromacs or Dalton for questions etc.?

    a. I definitely think this is a good idea and would use this website when in trouble.

    b. I guess the Gromacs mailing list is more convenient, known and gives a much broader response.

    c. Not everyday, but from time to time. And I'd bookmark it for sure.

    d. Everyday? Nope. If I have problems with GROMACS I look in the manual, ask someone or Google it (which usually ends up in the mailing lists). But it is useful to have a resource telling me how I can run GROMACS optimally on European HPC. I would only need to visit it a few times, however.

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7. What is missing?

    a. If you offer R in the tools, maybe some tutorials, besides the manual, would be nice.

    b. Information for the users of the codes! At the moment there is no reason why they should visit

8. What do you like most on this web?
    a. Access to slides and info regarding the idea behind ScalaLife itself.

    b. For me the best ideas are a place to learn more about available software and also the possibility to get support with using them.

9. Would you use the http://www.scalalife.eu/forum to pose your complains or questions?
    a. Only if there was a critical mass of experts/answers otherwise I'd be probably better off posting to the Gromacs mailing list

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10. Is this http://www.scalalife.eu/HPCresources useful?

a. I was not sure if the idea was to only introduce what resources are available, or are you also able to apply for use of these resources through the webpage?

b. HPC-Resources>Hardware Although the information is useful, it seems a bit poor to me. The web page contains some empty cells. And the cells that contain memory information are non-uniform. What about hard disk size & connection? Life Sciences input tends to use large (if not huge) inputs. HPC-Resources>Resource Allocation Needs fixing size of the table. It looks awful in Google Chrome running at 1024x768.

c. Yes. However, as I am only running simulations on the LRZ, I directly use their website to access the resource allocation etc.

d. Umm, not sure what it is for. Who can use these machines? Can I?

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11. Do you use any of these tools: http://www.scalalife.eu/tools ?

    a. I have used at least Molden
    b. I use Autotools, GNU, IBM and Intel Compilers, GDB, Paraver, gprof, MPI and SVN.
    c. Haven't used yet
    d. GROMACS, R, PyMol, VMD

12. Does the meaning of listing these tools clear for you?

    a. I do not know if I would need this list for anything. Maybe I would want some support also with these tools as a user.

    b. Yes, it is clear and useful, as not every user will have his own analysis package

13. How about the overall design: what grade would you give from 1 to 10?
    a. 9

    b. Design is ok. Layout maybe a bit much, with the left and right side showing a lot of links that's a bit overloaded. Score: 5

    c. I didn't like the 3-column approach. In addition, the links on the right (supposed to be shortcuts) require scrolling down. The section title "Competence center" is not clear to me. There are tables in the webpage that do not fit. I also don't like the color-scheme.

    d. 6

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14. As a Life science researcher did you miss this kind of portal-knowledge base? Is this something you would very much appreciate to have?

    a. I have never thought that I might need something like this but now that I have seen the webpage I think it is agood idea.

    b. It seems interesting but will need continuous tracking&updating as users require and software/hardware evolves. Probably, comparison of accuracy in results and efficiency of the codes using different machines.

    c. Well, I am used to the fact that one always have to search the web and tons of website to get the info one is looking for. I feel that the website is a bit complicated, the structure should be more easy and emphasize should be placed on the most important and needed resources. Maybe one could split this into a more informative part about ScalaLife, and a support/applications/resources website. The password recovery utility never worked for me....

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14. As a Life science researcher did you miss this kind of portal-knowledge base? Is this something you would very much appreciate to have?

    d. This sort of thing only works if it has a critical mass and it is competition with existing ways of finding things out (manuals, mailing lists, asking people in the lab). What is the probability that I will be able to answer my question If I go there? If this is low then chances are I will go somewhere else and never come back except as a last resort.

How do we proceed….