DeiC HPC-Forum

Meeting 2022-1 10/2/2022 @ 10.30 - 12.00

Zoom: https://deic.zoom.us/j/2909030409

Invited members and support that attended the meeting:

- AU, Søren Vang, Leading clinical bioinformatician (SV)
- AAU, Kåre Lehmann Nielsen, Professor Chemistry and Bioscience (KLN)
- CBS, Lars Nondal, Chefkonsulent, Forskerservice (LN)
- DTU, Sven Karlsson, Associate Professor, Parallel Computer Architecture (SK)
- DTU, Thomas Bligaard, Professor, Dept. Of Energy (TB)
- ITU, Martin Aumüller, Associate Professor, Computer Science (MA)
- KU, Piotr Jaroslaw Chmura, Research programmer (PJC)
- RUC, Thomas Schrøder, Professor IMFUFA (TS)
- SDU, Claudio Pica, Head of eScience Centre (CP)
- SDU, Hans Jørgen Aagaard Jensen, Prof., Chemistry (HJAJ) DeiC, Eske Christiansen, HPC Chef (EC)
- DeiC, Birgitte Vedel Thage, Chefkonsulent (BVT)

Members, absent (not announced):

None

Members, absent (announced):

- AU, Christian Storm Pedersen, Director of BiRC (CSP)
- CBS, Carsten Sørensen, Head of Finance Dept.
- (CS) -- KU, Erik Bjørnager Dam, Lektor, Mashine Learning
- AAÚ, Lars Sørensen, Head of Digitalisation (LS)

Guests:

- AU, Birte Christensen-Dalsgaard, chairperson DMRF

(BCD)

Minutes from last meeting in team's folder and web: https://www.deic.dk/sites/default/files/documents/PDF/HPC%20Forum%20referat%2024092021.pdf

Minutes by: Birgitte Vedel Thage.

Item	Issue	Comments Actions
1	Agenda and approval of minutes from last meeting (5 min) Presentation round	→ Agenda accepted. An extra topic was announced from SK under AOB.
	Approval: A. Minutes from meeting last meeting in 2021 was approved by email.	
2	HPC forum 2022 (Hans Jørgen) (10 min) According to our "HPC forum kommissorium" we provide input for DeiC board decisions. After initial discussions today on topic 5, it is expected that each member go back to their stakeholders as university representatives and provide input for the three questions from the board.	→ See additional comments under 5)
3	Information (10 min) Information items: A. LUMI-C Pilots (Eske) Four Danish pilot projects consumed approx. 33 million CPU core hours in total. Users are happy with the LUMI-C set-up and LUMI LUST. Some problems identified with disk IO, permissions, compiler, and software stack. Feedback is obtained from experienced users on LUMI in their recent survey, and it is noted that it may not reflect issues that midlevel experienced users may encounter. Initial problems with the PUHURI access but now users can be created fast. A question was raised regarding information sharing and availability of material for users to engage quickly on LUMI based on pilot project experiences. Work is ongoing creating guides and recommendations, and the intention is to communicate the LUMI pilot project user experiences. LUMI-G part is delayed, and as there is not access to information about the hardware yet, guides for this will be outlined later. B. LUMI time plan overall (Eske) Huge delay of LUMI-G. Pilots in March or April. Also delays on the object store (S3 interface). Learnings from LUMI-C is that it takes time to move code from LUMI-C to use the LUMI-G part. Can expect considerable rewriting of the code. There were discussions about utilization of GPU nodes. At this point the experience is that a huge speed-up of performance will require a full	A: Activities ongoing regarding communication of pilot project experiences (DeiC) B: No action points C: LUMI-C sandbox access deadline 25th February D: NeiC open call deadline is March 1st

evaluation of code architecture. However, it depends on how computing intensive the coding is. It was requested if one with 10% effort could get 50% pay-off instead of 100% utilization of the GPUs. The experience at this point is that if one tries to optimize code, e.g., 20%, one still does not get benefit of the GPU part.

It was discussed how to organize the support to LUMI via the Danish Front Offices. It was considered important to explain the set-up and how to coordinate with LUMI LUST back office. It was also pointed out that there is an international angle to consider using Lumi architecture – important to share knowledge on CRAY systems with other parties.

It was also addressed how to get "most value for money" from the LUMI support team from DeiC.

C. LUMI-C sandbox call (Eske)

Researchers at Danish universities can apply for CPU resources at LUMI-C. It includes UFM resources, and only resources for the first 6 months of the year. The LUMI-G part is not part of the call, as it will be available medio 2022. The national resources will be in play second part of this year including LUMI-G. **Deadline for LUMI-C access application is 25**th of February 2022.

https://www.deic.dk/news/2022-2-3/lumi-c-sandbox-application

D. NeiC calli (Eske)

Consortia consisting of e-infrastructure providers, developers, researchers and related communities around the Nordic region can propose collaboration projects within e-infrastructure (digital infrastructure) of joint Nordic interest. Model: 50/50. Total budget 21.3 mill NOK. **Deadline is March 1**st https://neic.no/news/2022/01/12/invitation-for-development-projects/

4 EuroHPC 2022 work programmeⁱⁱ (Eske). (5 min)

A short presentation on some of the possibilities in the EuroHPC JU work programme for 2022 including calls for

- EuroHPC Centres of Excellence
- EuroCC v2 taskforce is working
- Call for Exa-, pre-exa and peta-scale and quantum computing
- DK could take part in a consortia as LUMI
- High level support teams across EuroHPC facilities
- Often software stack technologies and algorithms
- EuroHPC summit week 22-24 March

It was encouraged to include Math, Physics and Chemistry departments to engage and send out information to the computer science departments as well. It was considered to be important to use the pre-established communication channels that already are available at the universities in order to be effective.

It was highlighted that there still is a need for better flow of information through Front Offices.

It was emphasized that EuroHPC JU projects has co-financing – it may be a challenge to engage in the calls as you need to bring in finance.

5 Do we have the right HPC offerings for research in DK 2023-2026. (Hans Jørgen) (30 min)

From the DeiC board:

At their meeting on November 26, 2021, DeiC's Board of Directors invited the HPC Forum to reflect on the long-term development of the national HPC area:

- 1) Which path should the HPC landscape go? (the composition, including national international)
- 2) What opportunities does the HPC Forum see for development?
- 3) Are users satisfied with the current composition of the landscape? is something missing?

Overall, the desire is to get an input on what the board should focus on in the coming years.

The Chairman of the HPC Forum is invited to present the thoughts of the HPC Forum on this at the Board meeting on 18 March 2022.

The objective for HPC forum was to outline how to proceed on this task.

→ No action points

Prepare clear position from each university for next meeting and send to EC.
Before 4th of March.

Ask DeiC board for more time (HJAJ). Do the best we can before deadline but the topic is so important that more time is needed to describe the assigned task from the board more thoroughly.

See more details in mail from HJAJ to HPC forum 16022022.

Presentation of current plan (Eske)

Some questions to consider:

- Type 1 DeiC interactive HPC
- Type 2 DeiC Throughput HPC
 Type 3 DeiC Large Memory HPC
- Type 4 Reopen Type 4 call DeiC Accelerated HPC
- Type 5 LUMI Capability HPC
- Move some of the investment to EuroHPC consortiums
- More capability beside LUMI
- Ftc.

It was decided:

Prepare clear position from each university for next meeting.

- Initial discussion HPC Forum meeting 10. February 2022
- 2. The HPC Forum members discuss the HPC needs for the next three years with the HPC stakeholders at their home universities. The HPC Forum members e-mail a short document describing the outcome of this to Eske; deadline Friday 4th March 2022
- 3. Final discussion based on the inputs from point 2 at next HPC Forum meeting 10, March 2022
- 4 HPC Forum chairman presents the outcome on the DeiC board meeting 18. March 2022

Some discussion points raised regarding HPC needs:

With respect to type 4, it was suggested to look at the next step beyond GPUs - may be a strategic problem if there is not a possibility for experimenting with new technologies. An idea could be to mirror some of the EuroHPC activities and partner up with others. A number of specialized accelerators are emerging and could be good to build up small set-ups to explore some of the possibilities teaming up with others. It was also discussed if it should be considered to focus on less national HPC types due to limited money.

Some comments on the process for defining HPC needs: Does this process in HPC forum reflect the needs of the researchers? Ideally, one would list a number of HPC options and measure what is used. For the future, maybe a workshop-based approach could be used trying to predict HPC needs. It was stated by HPC forum that it could be worth to discuss a broad and inclusive approach for estimating the needs in order to design a process on this task on the long run. Too little timeframe for doing this in a careful way. Ask for more time. We need a better way to do this in the future.

National AAI I samarbejde med DMRF (Hans Jørgen) (15 min) DMRF have created a set of working groups to look at AAAI. To ensure a coherent national research e-infrastructure, members of HPC forum should join the work to ensure that the result will be from both HPC forum and DMRF and bring the requirement from HPC into the work on a early stage. Guest: Birte Christensen-Dalsgaard, chairperson DMRF

Important to discuss commonalities between DM and HPC activities. DMRF has mapped the research data cycle (planning, data generation, analysis, publishing). They are currently working on "the glue" to make the services from each area possible to work together. FAIRification is on the agenda as well. May include a substantial work on legal framework, joint infrastructures as well as demonstrators.

CP is head of a technical working group that is working on the technical aspects of "national architecture & AAI" for DeiC national services. This is a joint effort between the DeiC Data Management and HPC fora. Outcome of the work from the group will be forwarded to the DeiC board. HPC forum members were encourage to contact CP if they wanted to be involved.

A question was raised regarding what type of data DMRF are looking at. The answer was that it could indeed be sensitive data looking at the metadata attached to the sensitive data. However, main focus is sharing of non-sensitive and non-IPR data.

The complexity around actors around data is huge. The intention is to build a technical solution for that. The people involved in the work are technology oriented and with experience from the library and university

CP to inform HPC forum of the DMRF activities on a regular basis and send out an email to the HPC forum to invite to participate in the work. Email from CP has been sent to HPC forum 16022022.

Deadline for joining "national architecture & AAI" group is February 25th 2022.

	world as well. Role of DeiC is to bring in the technology structure. Other part is support role from the different universities working with researchers. It is a top down process where the challenge is to show the benefit of using DM for the researcher. Try to make a bottom-up approach with different tools as e.g. seed money to engage groups to test the solutions and give feedback. Storage will be free.	
	A feedback from HPC forum was to look for groups with emerging data needs that may be more responsive and eager to engage rather than people that already generate data. It was asked to consider if there may be a core scaffold of most important areas/ target points to address.	
	It was encouraged to share vision reports between DMRF and HPC forum.	
	Nomenclature: AAI: Authentication – Authorization - Infrastructure AAAI: Accounting + AAI	
7	Next meeting (Hans Jørgen) (5 min) Select the next meeting date. Suggested date: 10 March 2022	→ Doodle with suggested time sloths has been sent out
8	Around the Table (10 min) What happens at the universities related to HPC? This is both for research and teaching but also for usage and resource allocation etc. Skipped this time due to time constraints	→ No action points
9	AOB. SK Presenting a research project. Danish National AI Innovation Arena (Sven Karlsson (DTU), Torben LArsen (AAU), Anders Pall Skött (KU)). No collaboration with DeiC on the infrastructure part in this project.	→ No action points

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i https://neic.no/news/2021/01/14/open-call/

ii https://eurohpc-ju.europa.eu/sites/default/files/2022-01/Decision%2028_2021_%20Work%20Plan%202022fix.pdf