DeiC HPC-Forum

Meeting 4

27/04/21 @ 12.30 – 15.00

Zoom: https://deic.zoom.us/j/63349931083?pwd=Z2dodUVSb0RlN2JUOHBiMGhVTjI0Zz09

Invited members and support that attended the meeting:	**Members, absent (not announced):**
- AU, Christian Storm Pedersen, Director of BiRC (CSP) - AAU, Torben Larsen, Prodekan (TL) - CBS, Carsten Sørensen, Head of Finance Dept. (CS) - CBS, Lars Nondal, Chefkonsulent, Forskerservice (LN) - DTU, Sven Karlsson, Lektor, Computer Science (SK) - DTU, Thomas Bligaard, Professor, Dept. Of Energy (TB) - ITU, Philippe Bonnet, Professor, Computer Science (PB) - KU, Erik Bjørnager Dam, Lektor,Mashine Learning (EBD) - 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., Physics (HJAJ) - DeiC, Eske Christiansen, HPC Chef (EC) - DeiC, Birgitte Vedel Thage, Chefkonsulent (BVT)	- AAU, Christian Nielsen,Head Business Dept.(CN) - SDU, Himanshu Khandelia - DeiC, René Løwe Jacobsen, Specialist (RLJ) **Members, absent (announced):** - AU, Søren Vang, Leading clinical bioinformatician (SV) **Guests:** • None

Minutes from last meeting (meeting 2) was approved on 23/04/21 and can be found here: https://www.deic.dk/Supercomputere/HPC-Forum

Minutes by: ***Birgitte Vedel Thage***

Item	Issue	Comments | Actions
1	**Information** Information items: **A. LUMI Pilot projects. (Eske)** Four pilot projects selected i.e., 2 in LUMI-C and 2 in LUMI-G. It was a selection process on request from the Ministry. Focus will be lessons learned on LUMI and important to share the findings. LUMI-C (Late August): 1. High Performance Computing Quantum Chemistry on LUMI, AU 2. Perfect Antennas for Reconfigurable Intelligent Surfaces (PARIS), AAU LUMI-G 3. BIG-MAP pilot project: Battery Interface Genome – Materials Acceleration Platform, DTU 4. How are stellar systems born, KU The LUMI-LUST people from DeiC will also be involved in the LUMI learning phase. The pilot projects are to TEST the systems, how it works with scaling of code, work needed to get things running, optimal compiling system ect. It was requested that the participants make a report regarding their experiences. It was stated that LUMi is coordinating reporting from the pilot projects as several projects will be running from different countries. What technology that has been used in the pilot projects are meaningful to communicate as well. It was suggested to make Zoom meeting with learnings from the pilot projects and the projects will be addressed at the DeiC conference as well. It was discussed that there are contractular penalties that the vendor needs to pay EuroHPC for delays regarding the LUMI project, however, there are expected some delays.	→ Comments: A: It was highlighted as being of high importance to organize for the community what is learned from the projects and not just to communicate findings on the web page. It was suggested to make learning reports from each of the pilot projects. This was assumed to be coordinated by LUMI.

	B. Project 5 steering committee (p5 styregruppe) (Torben) Brief sharing of information. The DeiC board has decided to form a steering committee to follow the project. Members: Eske (DeiC), Michael Rasmussen (DTU), Hans Henrik Happe (KU), Claudio Pica (SDU), Brian Vinter (AU), Torben Larsen (Chair). **C. PRACE usage (Eske)** Tier-0 PRACE projects with Danish participation (N=36) are now collected, and highlights were presented. If universities have ideas to who can benefit from joining PRACE, Eske can be contacted for assistance. There are people to help. Will also inform the Front Offices about this. The project data was extracted from: https://prace-ri.eu/hpc-access/project-access/project-access-awarded-projects/ **CP:** Useful to have a summary like this. Success rate is high however the process is demanding. There are also resources from UK or US to access. **SK:** Add that there are other interesting initiatives in PRACE e.g. PhD schools and training facilities. There has to be an infrastructure in order to support the researchers in the application process. LUMI steering committee offered possibility for quantum computing. A call presumed to appear end of this year. Does it make sense to look into this? **HJAJ:** DK should join if possible, from the beginning. **SK:** The investment is relatively high and may require 50% co-funding. Not easy to string this together for a Danish collaborative effort. Lessons learned: DTU was part of a proposal last year but had to back out as it was difficult with the co-funding part.	→ Action: B: There was an interest to share the "p5 terms of reference " with the group. **TL** investigate how to share it. → Comments: C: Overview of PRACE projects will be available at www.eurocc.dk during May/June Quantum computing at LUMI: be aware of co-funding part.
2	**Status of National HPC facilities.** Each hosting university gives an update on the status of the national HPC facilities. How is the front office for each university moving along? **Type 1 (CP)** Now up in full capacity at SDU and AU and number of users increasing (170 new users per month). Around 1400 users and 60% from SDU, 40% other universities. Hope for the opportunity to advertise more through the Front Office network. Discussion of financing the storage part together with the HPC facility is important. GPUs are requested from the users. Feedback from users: barriers, improvements – one challenge is a lot of user requests that are pushed to Front Office. When ask for feedback it is positive. Requests for new features e.g., more flexible access to the machines, better way to get access to data platform and possibility to deploy interactive dashboards and run multiple jobs. **EBD:** Users asking for SSH access, some users prefer to use their own terminal. To use there own tools for convenience. **Type 2 (CSP)** AU part of type 2: Genome-DK is used and organization of support to other HPC types is being discussed with local Front Office. CP: comment to type 2. Challenge to be aware of – some architecture of the machines (e.g., Fat nodes/GPU on Computerome2) is not part of DeiC deal. Write an email to Eske about the challenge. HJAJ: Soft limit when reaching the limit instead of wasting the resources. General guidelines – miss a notification of "how big is my allocation". Resource issue (lack of usage data) – provide an overview for HPC forum. The idea is to share the information btw Front Offices. **Type 3 (CP)** Large memory system since March 1st. Not many users. Test projects from SDU – 3 projects. Who does the advertisements in order to attract new users? Are the nodes the best investment? Not many applications in DK that can use it. 4 TB per note maybe to excessive. What is the right profile for type 3? Maybe have a few 2 TB nodes on type 1. Type 1 have a max of 1 TB nodes today. It was encouraged to direct potential users to the different HPC types! **Type 4 (EBD)** No one representing type 4. PB and TS to follow up on the progress. Few	→ Actions: Type2 challenge (**CP**) – send email to EC with details. Hard limit for Comuperome2 –why or why not? (**EC**) Usage data overview (**EC**)

	issues with overall design (accelerators, storage etc.). All decisions not taken with respect to architecture and feedback important. Mixed or one or the other…… **SK:** Essential for type 4 to be open for technical users.	EBD will require info from KU moving forward.
3	**Initial planning of HPC installations for 2021 to 2025?** All universities are in the process of collecting needs for HPC resources for 2021-2023. This is done to provide budget for the different HPC types. This do not answer the question, do we provide the correct types of HPC for researchers? This discussion is used for the DeiC board meeting in may. To discuss: A. Do we have to correct types of facilities going forward? B. Should the mix in Type 2 be different? **LN:** Balance btw the HPC types. CBS interest is 75% in type 1 and 25% in type 2. **SK:** Ongoing discussion at DTU. On EU level, data and data spaces are discussed. Challenges in how to store data and interconnect data spaces. We need to make sure installations can benefit from the data spaces developed. Workflows discussed excessively in EU with respect to how to connect different facilities and scale code across facilities, data access etc. **EBD:** Balance btw the different machines and resources available – difficult to get an overview of hardware in the Type1-4 facilities. What is open to DeiC and what is not? What is the current distribution? Not easy to find e.g. on DeiC webpage. Distribution of resources – usage of different types and CPU/GPU requirements based on a baseline from what is used now (else we are guessing). PhD students and early researchers doing machine learning – many CPUs available, Computerome 30.000 CPUs and 40x4 GPUs – users would like GPUs is the impression. **HJAJ:** Agree with SK and EDB – better website information needed! A little early to state what is needed as no good statistics yet. Important for new users not to expect long waiting time for use of HPC facilities. GPUs: small projects on Type1 and going for LUMI. Need for more GPUs in the Danish landscape is the impression. **CP:** Resources available lead by Front Office. DeiC e.g., not access to fat or slim nodes on Computerome2. DeiC board decision – we have LUMI for GPU nodes. However, we need to try GPUs – do we need another type in DK with GPUs? **CSP:** Genome-DK: CPU part only available on Computerome2. However, there are GPUs available but apparently not part of the agreement. Only few external projects but not requesting GPUs. **TS:** CPU/GPUs. Type 1 – 1 GPU + 16 CPUs is the package. **PB:** Four types of systems is working however we need to have more time for evaluation – be patient and not change too much at this time point. **TL:** Stability issue extremely important, however it should not prevent us from finetuning if subjects are identified. Experience on GPUs – always need for more (AI, ML is a success) and hungry in terms of computational resources. Need for platform that is easily accessible before moving to LUMI. The issue about remembering storage is important to implement. Not an investment for this the next year – and can cause challenges. Important: stability, stick to the plan until we have sufficient data to justify changes to the plan. Not even seen type 4 in action yet. More GPUs and remember to include storage as part of the investment plan. **Comment CP:** Stability important for the ecosystem – cost for services – the higher complexity the higher cost. Uncertainty / money investment a factor in the overall price. Buy in advance and you get a good price compared to if you buy late in the process. **EC:** type 2 more geared for bioinformatics (not originally stated in the description). **HJAJ:** Broaden the focus. State it is too early to state the needs until 2023 and therefore our recommendations are limited. More usage information in November. **CSP:** Computerome2 and Genome-Dk born for bioinformatics but users come from all faculties social science, natural sciences, health etc. Not only	→ Comments: **EC:** On April 14th a request was send to the Universities to plan future needs. In May, there is DeiC board meeting where it will be discussed. Feel free to come with input. Important conclusion: HPC resources will be wasted if storage is not considered in the investment. Come up with a draft that calls for comments and a consensus agreement on the content. **TL** summarize: 1. Consensus on we do not have enough user statistics in order to evaluate at this point. Therefore, no big changes recommended. 2. Agreement on making a statement that highlights that the storage investment must follow HPC investment 3. Acknowledge that there is not a sufficient number of GPUs available within the current DeiC agreement. More GPUs more than welcome. The discussions from today will be directed to the DeiC board – **TL** will attend the meeting in May and will present the ideas.

	for bioinformatics. **HJAJ:** Type 2 is less than we need – suggests putting the money in type 1. **TB:** Niflheim – Computerome2 (5 times more expensive). Large amount of people doing simulations in materials/chemical reactions – A problem this is not represented in the National HPC architecture. **CP:** Main issue is prize! Node hours make a difference. Should not expect to build something like LUMI. Stay faithful to the GPUs we have (type 1 and LUMI). **SK:** GPUs paves the way for users to use LUMI. Users also have specific acceleration needs. Storage and access to data important – data transfer back and forth btw locations is a challenge at relevant data volumes.	
4	**EuroHPC Access policy** The first version of the EuroHPC access policy has now been approved. This first version is in effect until the end of 2021. A process is planned to be initiated to review this version so that we have an updated second version that will be used from 2022. We wish to start collecting changes from Danish users now. A formal process will be announced but so fare feel free to start collecting comment and questions. Link: https://eurohpc-ju.europa.eu/sites/default/files/2021-03/Decision%2006.2021%20-%20Access%20policy.pdf To discuss: A. Initial comment and suggestions of the first version of the access policy are discussed. Only allow for one-year projects (E.g. on PRACE 2- and 3- years projects). **CP:** good policy and also standard in PRACE (can apply for multi-year allocation) and extension also possible. **SK:** Non-research comment: It is not clear how industrial actors can engage. How to handle collaborative projects where IP is generated? How does this relate to the focus on open R&D? Not clear in the current draft! Can you engage with EuroHPC in projects that generate IP?? Welcome to send comments to EC. Latest in 2-week time. Send mail to all HPC members (the way the feedback is wanted). Make a formal letter on behalf on DeiC to the Ministry. All should have a chance to see the letter for approval before it is handed over to the Ministry. Send out an overview of the process to all HPC members. Only EuroHPC access to scientists for H2020 program. SK: There are established Danish working groups for H2020 calls – may also be important to engage them. (representative is e.g., SK).	→ Actions: As agreed, an email has been forwarded to all HPC forum members by EC on 29/04/2021: • 12.05.2021 – Deadline for comments • 13.05.2021 – Circulation of draft material to HPC forum members. • 15.06.2021 – Submit material to UFM and INFRAG
5	**LUMI task force** To provide better synchronization of the LUMI knowledge a small LUMI task force was created with people that have been doing to different LUMI tasks. The task force consists of Claudia Pica, Torben Larsen, Brian Vinter, Eske Christiansen, and Sven Karlsson. CP is appointed as first chairman. Many topics and lack of information. Main goal is to open up the process and try to organize requests from the LUMI organization. Roles: From LUMI – TL is a representative Advisor- Brian Vinter Operational manager - CP European overview – SK Other that has an interest in joining the task force is welcome. There will be short deadlines and important to work on short notice. Make shared folder for transparency of the work accessible for HPC forum. First task: nominate persons for 6 special interest groups in LUMI. To discuss: **A. Special Interest groups.** Security (closed) – special conditions only nominate one person. Draft of groups, expectations will be circulated. If agree on persons, then no need for approval via DeiC board. Include DM forum. Consider if you want to join the task forces. Come up with nominations. CP circulate the SIG document. Spread information about LUMI.	→ Comments: A: **CP** circulate relevant material **All** – find nominees to the interest groups

	B. Competences building for LUMI. Increase involvement of interest for engaging in LUMI.	B: Focus on share experiences for LUMI
6	**Around the Table** What happens on the universities related to HPC. This is both for research but also for usage and resource allocation etc. **SK:** Ongoing process with respect to governance at DTU. Research wise DTU engage in projects with partners cross Europe. In some cases heading the effort. Proposal for master program. **TL:** AAU investment for 2021 DeiC resources. **PB:** DeiC science forum versus HPC forum – any news? Nominating people is initiated and there seems to be lack of clarity about the process. **SK:** DTU same question – how does it relate to the HPC forum. The intent is to look at long term perspectives – role and work distribution needs to be clarified. **CP:** It is part of the new DeiC organization – two different functions – both technical and scientific persons in the science forum. **EC:** Note the mail for resosurces demand in 2022 sent to university CIOs	→ Actions: DeiC science forum versus HPC forum. **EC** will check with Gitte and revert to HPC forum members.
7	**AOB.**	

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