Dellingr Phase 2: Deliverable 6

Nordic availability of shared resources

Dellingr team *

Thursday 12th March, 2020

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1 Executive Summary

The NeIC Dellingr project is investigating how a lightweight framework for sharing High Performance Computing (HPC) resources [1] can be implemented between participating countries [2]. The Dellingr project has established two temporary trials (pilots) of cross border e-infrastructure resource sharing in order to validate the policies and practicalities. The e-infrastructure resources were opened to eligible researchers [3] from the participating countries who wished to access resources in other participating countries.

This document describes approach and results of the second pilot for sharing resources across borders. In particular, a common lightweight process for the application for resources was agreed by the participating services providers. It was implemented using several tools, in particular Jekyll for displaying available resources to the wider audience, Waldur for self-service request management and accounting, and Atlassian Service Desk aka Jira for implementing the workflow for resource delivery.

Finally, we provide also results of the run of the second pilot, including summary of allocated resources. To make it easier to compare and account for heterogeneous resources, a Billing Unit (BU) was used to convert CPU (100 hours = 1 BU) and GPU (10 hours = 1 BU) consumption to a common value. In total, 6406 Billing Units were consumed with 12000 Billing Units allocated.

The user feedback from the first test of a Nordic resource-sharing framework is included in Appendices A and B and is generally positive.

1.1 Outline of document

The contributed shared resources will be made available to researchers in the Nordics through merit-based competitive mechanisms. These mechanisms, for example a support structure for the open call and an “allocation committee", will balance the capabilities, timelines and loads on the resources. This would be done through an open call from the National Providers.

1.1.1 Intended recipients

The National e-infrastructure Providers and NeIC.

1.1.2 Delivery process

Delivery is an operational process that supports research based usage of resources across national boundaries. The operational process for sharing the resources is based on the process in [1]. This process is facilitated by a modified Waldur [2] framework. An open call to solicit participants to test this framework was issued in June 2019. The first test of a Nordic resource-sharing framework is run and the requests and usage of the projects and the experiences of the participants are reported in this document.

1.1.3 Delivery date

February 2020.

[1] Defined generally as compute, network and storage e-infrastructure.
[2] Currently this includes the Nordic countries and Estonia.
[3] At the moment we do not address commercial users that some countries have agreements to provide/use resources.

2 Purpose of the Document

The purpose of this document is to be the Dellingr project deliverable that describes how Nordic e-infrastructure resources can be made available to be shared across borders.

3 Test of Cross Border Resource Sharing Framework

The Dellingr project has come up with a process to enable resource sharing across national borders and be common enough so that national resource allocation policies could be integrated in a consistent manner. In order to test the resource sharing process, test participants (users) are needed. A framework is provided [4] to provide these test users with an easy way to access e-infrastructure resources. The e-infrastructure resources are provided by the national providers, through the Dellingr project, on a time and amount-limited basis to attract the test users. Below we describe the framework we have used to facilitate the sharing and highlight how user requests have been processed.

3.1 Framework

The main target of the first test of a Nordic resource-sharing framework were researchers that wanted to get access to computational resources.

A diagram of the process that was setup is below along with more detailed explanation. Overall the process was done according to the description in Section 8 of [1].

First of all, we have adjusted the Dellingr project website so it can be used as a landing page [3] for new users willing to get access to resources and used in promotional activities. The website is public and does not require any authentication. The main components of the website included:

- Description of rules of participation in the second pilot: `https://dellingr.neic.no/apply/`.
- Guide for applying for resources via Dellingr self-service: `https://dellingr.neic.no/guide/`.
- Up to date list of computational services available to the users along with some basic technical and performance properties: `https://dellingr.neic.no/offerings/`.

Once the user had decided that some e-infrastructure resources available in the Dellingr offer were interesting, the application process would start.

3.2 Application Process

As the first step of the application process, a user had to authenticate into the Dellingr self-service portal using an identity provider from eduGAIN [4]. Two results were received through the usage of eduGAIN:

- A reliable name and unique ID of the user in the eduGAIN federation;
- The domain of the organization that user belongs to.

Unfortunately without the authentication service containing reliable information on the group information about the user (affiliation, role), the only reliable affiliation information that could be obtained came from the domain attribute in the SAML assertion from eduGAIN. This meant that the user had to register their own organization by filling in the form in the self-service portal and that this affiliation information had to be manually confirmed at a later stage.

[4] See `https://share.neic.no`

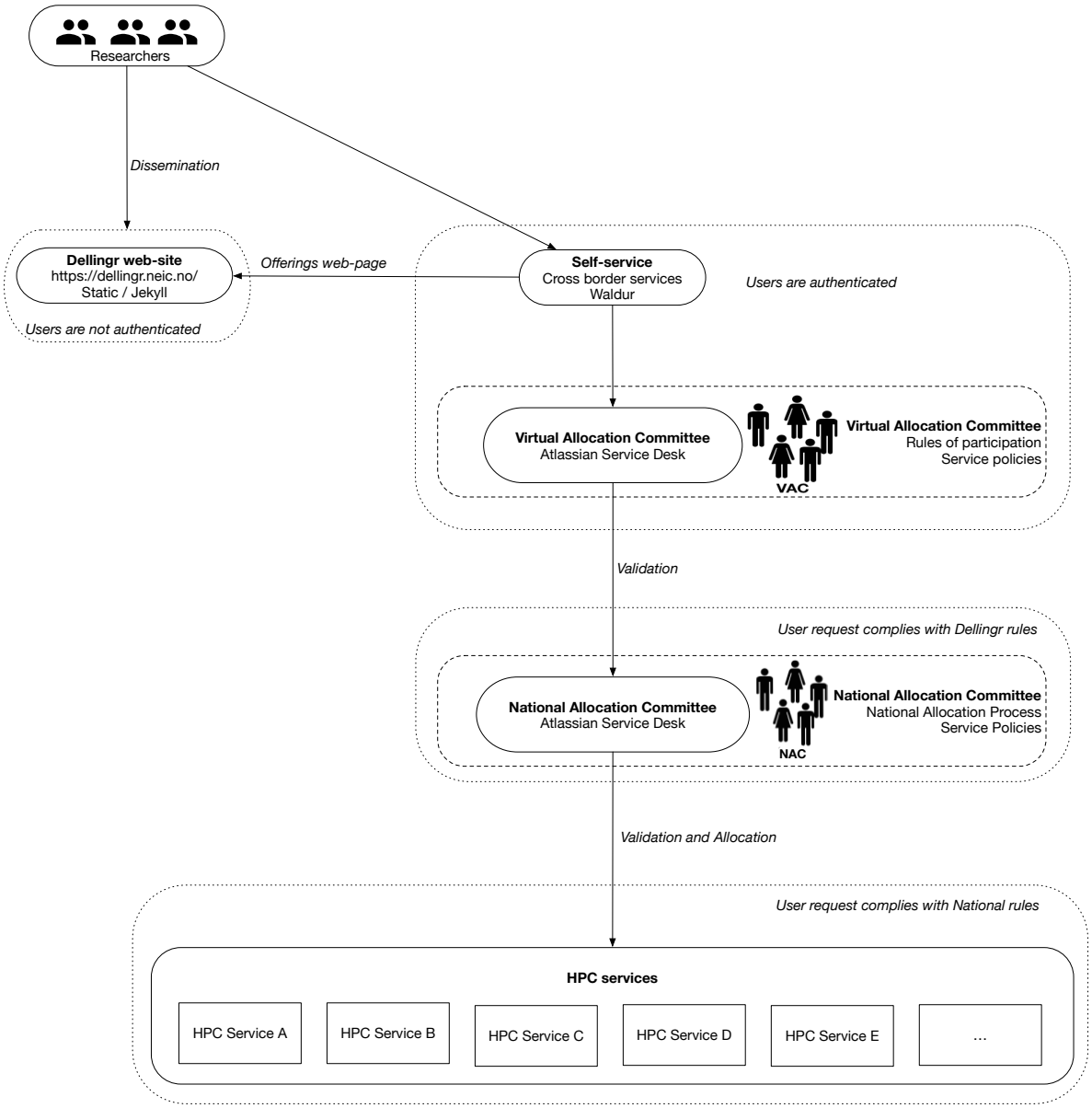


Figure 1: Overview of the second Dellingr pilot setup

Once the user has created their organization, they are able to browse resources available for request at that moment in time. Over the period of the second pilot, some resources can be activated, archived or paused by the resource owners. These actions cause the system information to be updated in the self-service portal and the user can see these changes at once.

We initially hoped to be able to automate the whole process of delivery at least for some services, however the amount of issues connected with that was eventually beyond the scope of Dellingr resources and it was decided to use a service desk system, Jira [5], for processing requests instead. Please note that despite this technical limitation, the process is exactly the same for both the manual and automated way.

The user had to also fill in the project information, which has been attached to all requests for resources under that project. When requesting a resource, users had to:

- Provide estimated requirements of resources in terms of CPU and GPU hours;
- Provide the science domain (following the standard from [6]) for which the resources were planned to be used;
- Provide nationalities of the users that were expected to get access to the resource.
- Agree to the terms of services of the chosen service.

Once the user submitted the information, a request to **Virtual Allocation Committee** (**VAC**) was been created. Upon receiving notification about new requests, the VAC validated input data to see if it complies with the Rules of participation of Dellingr– and if so, forwarded the requests to the representative of the service, aka **National Allocation Committee** (**NAC**).

The NACs took as input the request for am e-infrastructure allocation that had the minimal commonly agreed information (see above) as well as validation of VAC that request conforms to the Dellingr policy. The NAC representative then could decide if the request also matches with the policies at the requested resource and either grant or deny the application. The amount of e-infrastructure BUs requested by the user could be approved unchanged or be modified by the NAC representative resulting in the **allocated BUs**.

To make sure that process works smoothly, a separate role — service manager — was in place to follow up on created tickets and assure that requests are processed in time.

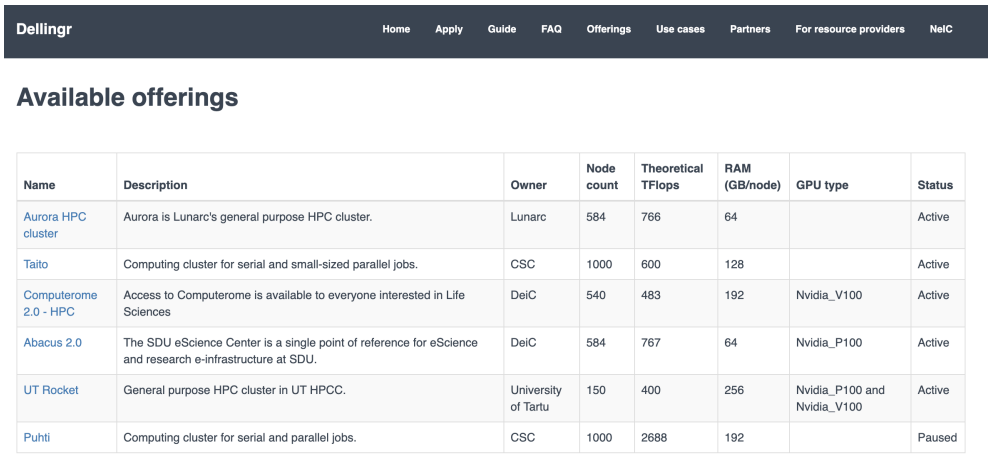
3.3 Resources

One of the most often asked question was 'What resources do you have'? To make sure that the answer is visible to the widest audience, we have collected various technical information about the services and exposed parts of it on the public website. Exposure was semi-automated, taking the JSON from the self-service (automatic) copying it to the Dellingr website (manual) and publishing it as static website in Jekyll (automatic). This has allowed to significantly reduce getting authenticated requests from users (which lead to request processing flow), who would not benefit from the provided offerings.

Over time some service offerings have been taken of the list due to different reasons, an example of state of affairs in the middle of February is shown below. Site properties were selected based on the main questions asked. One of the most requested resources was GPU access, however only one offering was providing that, which has hindered high number of requests from arriving.

4 Results

In this first test of a Nordic resource-sharing framework the resources were allocated in a different manner than the first pilot. In this case the users requested specific resources not in their country through the portal. In the first pilot,



Dellingr Home Apply Guide FAQ Offerings Use cases Partners For resource providers NeIC

Available offerings

Name	Description	Owner	Node count	Theoretical TFlops	RAM (GB/node)	GPU type	Status
Aurora HPC cluster	Aurora is Lunarc's general purpose HPC cluster.	Lunarc	584	766	64		Active
Taito	Computing cluster for serial and small-sized parallel jobs.	CSC	1000	600	128		Active
Computerome 2.0 - HPC	Access to Computerome is available to everyone interested in Life Sciences	DeiC	540	483	192	Nvidia_V100	Active
Abacus 2.0	The SDU eScience Center is a single point of reference for eScience and research e-infrastructure at SDU.	DeiC	584	767	64	Nvidia_P100	Active
UT Rocket	General purpose HPC cluster in UT HPCC.	University of Tartu	150	400	256	Nvidia_P100 and Nvidia_V100	Active
Puhti	Computing cluster for serial and parallel jobs.	CSC	1000	2688	192		Paused

Figure 2: Example of service offerings shown to users and accessible via the Dellingr self-service portal.

the users requested an amount of computing time and were assigned to a resource manually by the Dellingr project. Also, the self-service portal expressed the e-infrastructure resources in a common format “Billing Units" (BU) [5].

The Dellingr first test of a Nordic resource-sharing framework was launched in June 2019 and the last applications were received in December 2019. These figures summarize the extent of the Pilot [6]:

- 13 applications were received;
- 11 projects were accepted;
- 12000 BU were granted to the accepted projects;
- 6406 BU were consumed by the projects.

Only two applications were rejected. Two of the eleven applications accepted were handled through channels other than the self-service portal. One was a Danish continuation of resource usage from the first Dellingr pilot and was handled through the Swedish SUPR [7] portal. The other was am Icelandic continuation of resource usage from the first Dellingr pilot and was handled through the CSC Service Desk [8].

Table 1 shows the orders for resources received from users. As can be seen in Table 1 the amount of BUs allocated varies. The amount of BUs consumed by each project also varies from very little (zero) to multiples of the original allocation. One project, with a BU consumption of "n/a" was not correctly assigned an allocation due to a misunderstanding in the project setup stages.

Table 2 shows the resource allocations between client and hosting countries. As the number of accepted projects was 11 and the number of entries in Table 2 is 8, it can be seen that most countries managed to generate 1 request. The exception to this was Iceland that generated 6 projects and, to a lesser extent, Denmark that generated 3 projects. It can be seen in Table 2 that two countries (Finland and Sweden) hosted the majority of the projects and BUs and one country (Iceland) generated the majority of the projects but not the majority of the BUs allocated.

[5] In general for all Dellingr resources, 1 CPU core has been set to cost 0.01 BU per hour and one GPU core cost is 0.1 BU per hour.
[6] As of Thursday 12th March, 2020

Project Title	**From**	**To**	**Allocated BU**	**Used BU**
Exploring mechanisms of roughness creation at the nanoscale using a systematic set of large time and length scale Molecular Dynamics simulations	DK	EST	500	2085
Acetonitrile parametrization	DK	FI	500	482.94
Local structural correlations in Sn doped BCZT ferroelectric relaxors	DK	SE	3000	1569
GETM high-resolution modelling for the Baltic Sea	EST	SE	500	594
Simulation of ions in solutions using QM/MM method	IS	FI	1000	3.58
Simulating Electronic and Nuclear Dynamics in Dye-Sensitized Solar Cells	IS	FI	500	6.99
Benchmark comparison of pure, hybrid, double-hybrid DFT functionals against the highly accurate wavefunction methods for reliability for quantum dynamics simulations	IS	FI	500	3.85
Configuration space sampling of solvated hexaaquairon(II) and hexaaquairon(III)	IS	FI	500	51.30
Polarizable Embedding of Ions in Solution	IS	FI	500	0
Fluid reactions mechanism on mineral surface in planet interior	IS	SE	2000	n/a
Atomistic insight into difference and similarities of copper sulfide and oxide corrosion films	SE	FI	2500	1609.42
Total			12000	6406

Table 1: The accepted projects in the first test of a Nordic resource-sharing framework. (DK=Denmark, EE=Estonia, FI=Finland, IS=Iceland, NO=Norway, SE=Sweden).

Host/Guest	Denmark	Estonia	Finland	Iceland	Norway*	Sweden	Total	
							BU	#
Denmark	x						0	0
Estonia	500	x					500	1
Finland	500		x	3000		2500	6000	7
Iceland				x			0	0
Norway*					x		0	0
Sweden	3000	500		2000		x	5500	3
Total BU (#)	4000 (3)	500 (1)		5000 (6)		2500 (1)	12000	11

Table 2: The number of BUs allocated and hosted per country. The horizontal (vertical) view gives the number of BUs hosted (allocated) per country. ∗ Norway has observer status only.

PN: In Table 1, are all numbers in the fourth column the allocated resources (and not requested)?
PN: In Table 2, are all numbers the allocated resources (and not requested)?
PN: In Table 1, should Estonia be EST (as in the table) or EE (as in the caption)?
PN: I will update FI usage figures in Table 1 on 13th March.
PN: Remember to finally update Total allocated (BUalloc) and Total used (BUcons) in main.tex.

5 Conclusions

Overall, we see that the process implemented during the second pilot of the Dellingr project is:

- Not very intrusive for the service providers;
- Scalable in the number of participating users and organizations, both consumers and service providers;
- Provided additional benefits beyond the initial scope, e.g. creating a small up-to-date public catalogue of HPC services in the Nordic region without extra effort.

perhaps add an item like: Sensitive to miscommunications, i.e. the process needs a high level of automation so that project continuations and requests are not missed in the reporting and/or creation process. But still not so automatic that the review process is removed.

User feedback was requested from the participants during the first test of a Nordic resource-sharing framework. There was a first set of questions sent out on 2019/10/02 to participants as it was noted that users had logged in an registered but very little activity on projects had been seen. These questions attempted to find out of there were fundamental problems in the way that users viewed the self-service portal. These questions and the responses are given in Appendix A.

Looking at these responses from the self-service portal users and also feedback from the Dellingr project steering group, some changes were made to the portal. In part, these changes were made in an attempt to reassure users to feel that a monetary transaction was taking or about to take place. This included: removing references to “shopping carts"; explaining BUs are only used for common accounting purposes; explanatory text on the landing page that NeIC sponsors the costs for these e-infrastructure resources; resolving the difference between an organization and a

user; simplifying the creation of an organization by using the user eduGAIN affiliation as default. These changes, once communicated to the users, resulted in an uptake of project creation.

A second set of questions was later (2020/01/21) sent to users who requested and received an allocation of BUs in the pilot. These questions and responses are given in Appendix B. Of the 11 projects accepted, we received answers from 6 of the users. The respondents are split evenly between those that had participated in the first pilot and those who had not. The users generally found it easy to access the "foreign" e-infrastructure resources, probably due to the refined procedures to accept users developed by the NACs of the national e-infrastructure providers. In general, these users did not have application or licencing support issues. This might be because users are requesting through a self-service portal to run on non-local resources and are therefore more likely to have open-source software. Of the users that have not used their allocated resources [7], all indicated that they intend to do so. None of the respondent users replied that this type of resource sharing/access is not useful. A response from more than one user indicated that this is useful for early stage researchers and method development. The user feedback, provided in the Appendix below, has been generally favourable, which is both motivating and hints that such service could be sustained beyond the Dellingr lifetime.

As part of the "contract" between Dellingr, NeIC and the pilot participants is that any work resulting from the e-infrastructure resources accessed should have an attribution attached: "This work was made possible (in part) by usage of computing resources at (institution) through the NeIC Dellingr resource sharing pilot." The publications from the 1st Dellingr pilot can be seen at [9]. Due to the length of time for the process from data analysis to publication, it is not expected to receive notice of publications attributed to this second pilot before the official end of the Dellingr project.

[7] As of Thursday 12th March, 2020

References

[1] Dellingr DO5: Resource exchange implementation and agreement.
https://wiki.neic.no/wiki/Dellingr#DO5_Resource_exchange_implementation_and_agreement

[2] Waldur cloud brokerage.
https://waldur.com/

[3] Dellingr public project page.
https://dellingr.neic.no/

[4] eduGAIN - enabling worldwide access.
https://www.edugain.org/

[5] Atlassian Jira.
https://www.atlassian.com/software/jira

[6] OECD Science Domains.
https://en.m.wikipedia.org/wiki/Fields_of_Science_and_Technology

[7] SUPR - SNIC User and Project Repository.
https://supr.snic.se/

[8] CSC Service Desk.
https://research.csc.fi/support-and-training

[9] Publications from Dellingr 1st Pilot.
https://wiki.neic.no/wiki/Dellingr_Publications_1st_Pilot

Appendix A First Questions to and Responses from Framework users

Responses 1

* Did you experience any technical issues with the page?

Yes there was some login issue, but it got resolved

* Is the procedure to apply for computing resources too complex?

A bit yeah. It was unclear to me what I was getting and how I would get it

* Does the design of the page (BUs, shopping cart etc) imply a direct
cost to you?

Yes it does. I still dont know what a BU is or how I would get billed.

* Were the computing resources available of no interest to you?

They might be. If it was super easy to just logon and start using it. I
think I got my resource request rejected for my test application.

Responses 2

It is true that I logged in. I am also interested in applying for time. That's why I logged in, to check what is required.

I was looking for information regarding if I as a postdoc can apply myself, or if it I should go through my PI. I could not find an answer to this, maybe you know?

Primarily, I believe the problem so far has been a lack if time from my side. We
(the research group), will most probably apply for resources soon.

Responses 3

Yes, I logged in to the portal, mostly to see the specs of clusters and get knowledge of the service and possibilities.

* Did you experience any technical issues with the page?

no

* Is the procedure to apply for computing resources too complex?

don’t know, since I did not apply / open the application. Probably not.

* Does the design of the page (BUs, shopping cart etc) imply a direct cost to you?

I don’t think so.

* Were the computing resources available of no interest to you?

They were interesting, and I’m mostly interested in GPU clusters. I did google the other clusters a bit to find out more information, so maybe the pages could benefit from more information about specs.

I’m already using CSC cluster (Espoo) so I did not see a reason for applying the "same resource’’ twice, if I was to be allocated to CSC.

Responses 4

Thanks for the follow up and nice to hear from you! I am obviously not the target user, but I did not know how to use the website. What would be an organization?
As someone who just followed a link I was completely lost as to what to do. Some introductory words about the site, intended audience, etc would help.

Responses 5

I didn’t use the requested resources due to delays that affected my project "Simulating Electronic and Nuclear Dynamics in Dye-Sensitized Solar Cells".

Is it possible to extend the time frame for using the requested resources on the supercomputer Taito?

Appendix B Responses from Framework users

The responses from the participants of the first test of a Nordic resource-sharing framework are given below. The identities of the participants are intentionally removed.

Responses 1

```
- If you are a user of both the first and second Dellingr pilots... How
     does the experience compare between the two pilots?

I wasn't.

- How easy was it to get the account on the "foreign" shared resources?

To be perfectly honest, I found the infrastructure around getting accounts and project management
etc slightly byzantine. But it probably wasn't helped by the fact that I kinda got stuck with two
accounts for some reason related to my dual employment at two different universities, both using
the wayf login. What I'm saying is, it was 50%-75% my own fault :)

- Did you need application support? If so, did it work well?

No.

- Did you have licensing issues? Were they solved?

No issues

- If your project did not use all the allocated resources, why was this
     the case?

I think I used almost all of them, if not all.

- Other comments on the application framework and/or process?


None i can think of currently. Thanks for letting me be  part of the pilot!
```

Responses 2

```
- If you are a user of both the first and second Dellingr pilots... How does the experience
compare
between the two pilots?

I have been using resources from CSC/Finland in both pilots. The experiences have been rather
similar, in both cases positive throughout. Their are two large differences between the rounds
are:
```

i) the new application system for the latest round, which was a bit tricky to understand at first but the platform seems to have good future potential;
ii) the new computer cluster at csc (puhti), which works very well.

- How easy was it to get the account on the "foreign" shared resources?
It was easy the first round, and this time I already had an account making it very smooth.

- Did you need application support? If so, did it work well?
Not this round. Last round we had minor issues that the support could solve quickly

- Did you have licensing issues? Were they solved?
Not this round. Last round we needed to confirm our VASP license, which took a few days.
This is however very common for this program.

- If your project did not use all the allocated resources, why was this the case?
We have not yet had time to use all, but we will.

- Other comments on the application framework and/or process?
Not at this point, other than that is has been working well and that I consider this a very useful and good initiative

Responses 3

- If you are a user of both the first and second Dellingr pilots... How does the experience compare between the two pilots?

I did not participate to the first Dellingr pilot.

- How easy was it to get the account on the "foreign" shared resources?

The process for setting up an account to use the CSC resources was easy.

- Did you need application support? If so, did it work well?

I did not.

- Did you have licensing issues? Were they solved?

I did not have any licensing issues.

- If your project did not use all the allocated resources, why was this the case?

I did not use all of the allocated resources because the development and implementation part of my project took longer than what initially expected.

- Other comments on the application framework and/or process?

My Dellingr project on CSC terminates on 29.01.2020. Would it be possible to extend the end of the project so I can continue using the allocated resources? Or should this be handled by CSC?

Responses 4

"If you are a user of both the first and second Dellingr pilots... How does the experience compare between the two pilots?"

-> I cannot answer this question because I am a user of the second Dellingr pilot project.

"How easy was it to get the account on the "foreign" shared resources?"

-> It was easy as I got the computational budget within 48 hours. The application form was also straightforward and did not require many details.

- Did you need application support? If so, did it work well?

-> I filled in the online form myself. The manual for completing the application is clear.

- Did you have licensing issues? Were they solved?

-> No, I do not.

- If your project did not use all the allocated resources, why was this the case?

-> This case did not apply to me as I just got the resources a month ago.

- Other comments on the application framework and/or process?

-> Please continue the project as it is really helpful for early-stage researcher.

Responses 5

- If you are a user of both the first and second Dellingr pilots... How does the experience compare between the two pilots?

We had positive experience with both pilots. It took us some time in the first pilot to setup things, but afterward everything was very smooth. For the second pilot, it didn't work initially because of some misunderstanding (it was not clear on the other side if we got the approval for the second pilot), but it is working now!

- How easy was it to get the account on the "foreign" shared resources?

Since it was the first time from our university (Aarhus University), it took us some time to create an account and to make it work. But we did not had any problem afterward.

- Did you need application support? If so, did it work well?

Not that much as we only used LAMMPS software which is straightforward to install.

- Did you have licensing issues? Were they solved?

No as we only used open-source software

- If your project did not use all the allocated resources, why was this the case?

I believe we used even more than allocated resources

- Other comments on the application framework and/or process?

It would be nice to hear about future perspectives of the project and how one can access these resources. As I mentioned before, it really helped us a lot.

Responses 6

- If you are a user of both the first and second Dellingr pilots. How does the experience compare between the two pilots?

The dashboard introduced during pilot phase two was a great boon. Applying for, and monitoring resources, was more streamlined.
Pilot phase one was however quite easy to apply for and use.

- Did you need application support? If so, did it work well?

Yes, there was some support needed during pilot phase one,
which was resolved quickly.

- Did you have licensing issues? Were they solved?

No licensing issues. All software used was GNU GPL.

- If your project did not use all the allocated resources, why was this the case?

We still have access to and are using resources from pilot phase two.
Resources from pilot phase one were used fully.

- Other comments on the application framework and/or process?

Keep up the good work. Having an option of applying for computational resources through a shared network like this is invaluable for method development.

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