BioNT - Network for Training

Deliverable 1.3 | Command line and Cluster Computing

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Project partners

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2. BIOBYTE SOLUTIONS GMBH (BIOBYTE)

3. HPC NOW CONSULTING SL (HPCNOW)

4. UNIVERSITETET I OSLO (UO)

5. UNIVERSITAT DE BARCELONA (UB)

6. INFORMATION CENTRE FOR LIFE SCIENCE (ZBMED)

7. SIMULA CONSULTING (SIMULA)

8. ALBERT-LUDWIGS-UNIVERSITAET FREIBURG (ALU-FR)

9. ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL)

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Project overview

The BioNT consortium is dedicated to providing a comprehensive training program and fostering a community for digital skills relevant to the biotechnology industry and biomedical sector. With a curriculum tailored for both beginners and advanced professionals, BioNT aims to equip individuals with the necessary expertise in handling, processing, and visualising biological data, as well as utilising computational biology tools. Leveraging the consortium's strong background in digital literacy training and extensive network of collaborations, BioNT is poised to professionalise life sciences data management, processing, and analysis skills.

Third training workshop report in summary

BioNT delivered its third training workshop in February 2024. This document reports about this workshop regarding its organisation, the applicants and participants, as well as their feedback about it. The report also touches on the different advertising channels used to reach the project's target audience, as well as on the methods developed exclusively for creating and delivering BioNT's training workshops.

Command Line and Cluster Computing

BioNT conducted its third training workshop, an introduction to the command line and cluster computing, from the 6th to the 8th of February 2024. The workshop titled "An Introduction to High Performance Computing" was offered free of charge to the participants and took place fully online.

This introduction to high-performance computing (HPC) outlined key concepts of what an HPC cluster is used for, what needs to be done to access it, and how applications and workflows are run there.

Using online learning materials from The Carpentries and HPC Carpentry (a lesson program in incubation for The Carpentries) proved to be beneficial as they are the result of a community-driven development process and have been improved and validated through extensive workshop evaluation.

Organisation of the workshop

This workshop ran for 3 days, from the 6th to the 8th of February of 2024. The entire event was conducted virtually with no cost to participants. On the first day, a 3-hour session was delivered from 13:00 to 16:00 CET, whereas the second and the third day were delivered from 09:00 to 16:00 CET.

Webpage and registrations

The CECAM event management platform, provided by the EPFL, was used to create a dedicated webpage for the workshop, which included the workshop description, learning objectives, requirements, program (Figure 1), and any further information relevant to potential participants. The webpage is accessible at https://www.cecam.org/workshop-details/-1270.

Tuesday February 6th 2024 - Day 1

- 13:00 to 13:15 – Welcome + Ice-breaker
- 13:15 to 13:20 – Introducing the Shell
- 13:20 to 14:00 – Navigating Files and Directories
- 14:00 to 14:40 – Working With Files and Directories
- 14:40 to 14:55 – Coffee break
- 14:55 to 15:35 – Pipes and Filters
- 15:35 to 16:10 – Shell Scripts
- 16:10 to 16:15 – Summary + Feedback

Wednesday February 7th 2024 - Day 2

- 09:00 to 09:10 – Welcome + Ice-breaker
- 09:10 to 09:30 – Why use a Cluster?
- 09:30 to 10:05 – Connecting to a remote HPC system
- 10:05 to 10:40 – Exploring Remote Resources
- 10:40 to 10:55 – Coffee break
- 10:55 to 12:00 – Scheduler Fundamentals
- 12:00 to 13:00 – Lunch
- 13:00 to 14:00 – Accessing software via Modules
- 14:00 to 14:25 – Transferring files with remote computers
- 14:25 to 14:40 – Coffee break
- 14:40 to 15:55 – Running a parallel job
- 15:55 to 16:00 – Summary + Feedback

Thursday February 8th 2024 - Day 3

- 09:00 to 09:10 – Welcome + summary
- 09:10 to 09:40 – Using HPC resources effectively
- 09:40 to 10:00 – Using shared resources responsibly
- 10:00 to 10:15 – Coffee break
- 10:15 to 11:00 – Running commands with Snakemake
- 11:00 to 11:30 – Running Snakemake on the cluster
- 11:30 to 12:00 – Placeholders
- 12:00 to 13:00 – Lunch
- 13:00 to 13:40 – MPI applications and Snakemake
- 13:40 to 14:00 – Snakemake and the Cluster
- 14:00 to 14:20 – Chaining rules
- 14:20 to 14:35 – Coffee break
- 14:35 to 15:30 – Processing lists of inputs
- 15:30 to 16:00 – Summary + Feedback

Figure 1 - Workshop program as displayed on the [event page](#) at the CECAM platform.

For registration, the CECAM platform was used to manage the applicant's information and communication. In parallel, the EMBL servers were used to collect pre- and post-workshop information through pseudo-anonymised surveys. The survey data was linked to the applicant's data only via a unique identifier, provided in the CECAM registration process, as well as in the EMBL-based survey. This ensured that only the workshop organisers accessed the applicants' personal data while still collecting information relevant to the workshop separately. To register, applicants had to: (i) register on the CECAM platform, (ii) complete and submit the pre-workshop survey, and finally (iii) complete the application on the CECAM platform using the unique identifier provided in the pre-workshop survey.

Applications were reviewed based on answers in the pre-workshop survey (containing no personal information). Applicants working in small and medium enterprises (SMEs) or who identified themselves as job seekers would have been prioritised if needed, but after a thorough assessment of technical and personnel capacity, all 52 applicants were accepted. The communication of the application outcome to all participants, as well as any additional communication, was performed via the CECAM platform.

Advertisement

The workshop was advertised via social media, several websites, mailing lists or Slack spaces of networks and communities (ELIXIR, Research Data Alliance (RDA), NFDI4Microbiota, LifeSciTrainer and the Open Life Science (OLS), National Competence Centres for High Performance Computing).

For the advertising of this workshop, a tailored image was generated, which included a QR code to facilitate access to the registration platform.

Figure 2 - Examples of workshop advertisement (left - LinkedIn post, right - advertisement image).

Infrastructure for the workshop

The workshop was delivered in a Zoom webinar format, with participants' visibility disabled to preserve their privacy. Participants were able to see and learn from the trainers but direct interactions (e.g. chat or voice) were not possible within Zoom during the sessions. All direct interaction took place in written form via a collaborative document, where anonymous participation was possible. To serve the collaborative documents, a [HedgeDoc](#) collaborative space was set up by BIOBYTE, and was hosted on their server.

A **Main** collaborative document, set up by the instructors and organisers, was shared with the participants before the workshop. Each section of the workshop had dedicated *Hands-on* boxes to report on the task status, ask questions or raise issues. Helpers engaged and assisted participants by answering the questions and issues directly in this document. This Main document was updated live during the workshop. Separate boxes to answer questions were used to improve participant engagement and as an indirect learning assessment (Figure 3).
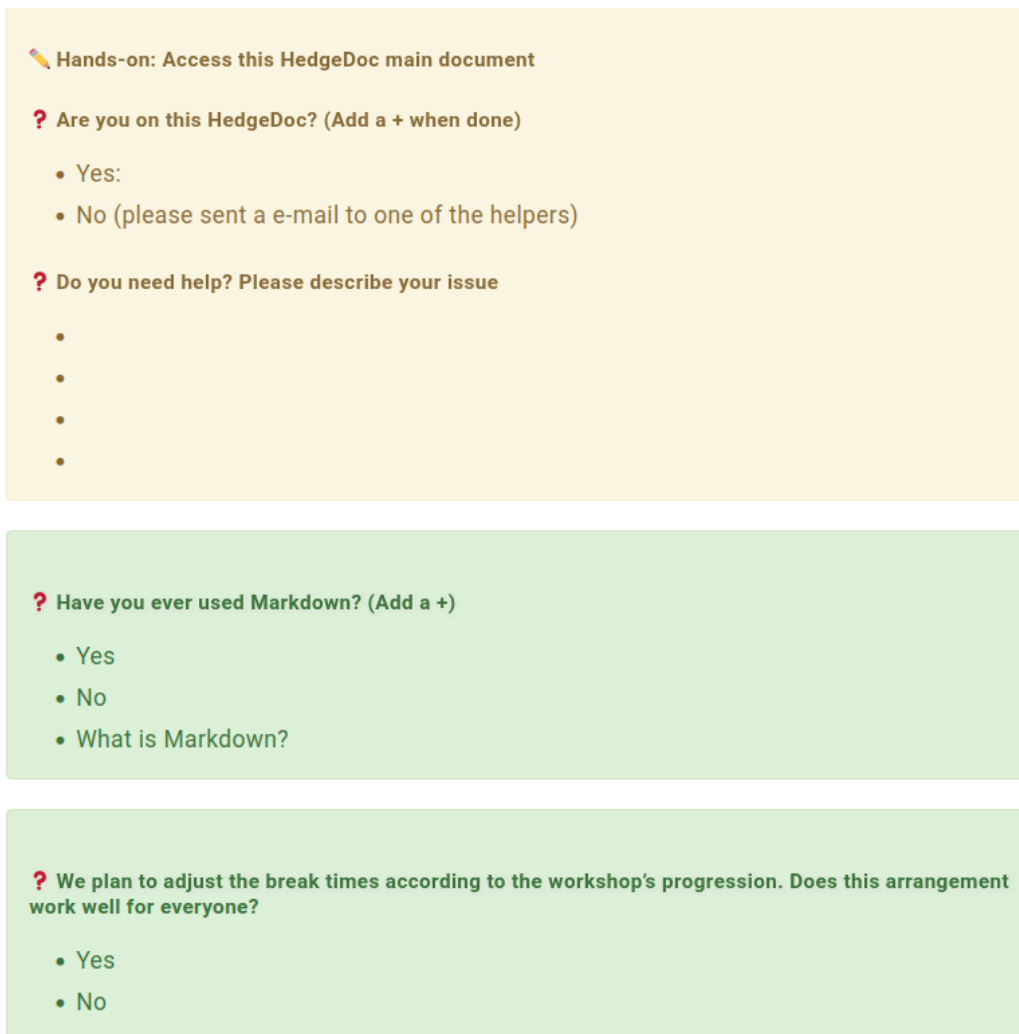
Figure 3 - Example of question and hands-on boxes in the collaborative document.

To help with the organisation, four HedgeDoc documents were used: (i) a **Template** with all instructions and boxes for hands-on, questions, etc; (ii) the **Main** document with the information for the participants during the workshop, filled with boxes related to the section covered by the instructor to help with the navigation and cleaned during each break to avoid an overcrowded document; and (iii) a **History** document collecting all the content from the Main document. This document was shared with participants during the workshop, to grant them access to all prior conversations. In addition, (iv) a document for Helpers & Instructors was created providing the workshop setup, interactions and explaining tasks of the helpers and instructors.

To enhance the structure of the workshops, an improved version of the document for Helpers & Instructors was used: The roles of the Helpers were clearly defined, including step-by-step information for their tasks before, during, and after the workshops.

The training materials used during this workshop (Table 1) were slides and tutorials partially sourced from The Carpentries. Their volunteer instructors (4287) have run 4000+ workshops in 65 countries since 2012, with 450+ alone in 2022 (data from the annual report). The

material for Days 2 and 3 of the lesson is sourced from HPC Carpentry, which is a lesson program in incubation for adoption by The Carpentries. **This workshop was the first time that the complete official lesson program for HPC Carpentry was delivered**. As a result, it was a valuable opportunity to gather lesson feedback from a diverse audience.

All lesson materials are freely reusable under the Creative Commons - Attribution licence and are stored on The Carpentries website and on the HPC Carpentries website. For Days 1 and 2, mostly existing tutorials and exercises were used. For the HPC workflow lesson of Day 3, the content was created de novo based on other Carpentries-style lessons for the workflow tool used (in particular "Snakemake for Bioinformatics" and "Getting Started with Snakemake"). The customised tutorial was designed to be broadly applicable and reflect on the wide availability and usage of HPC in academic and industrial environments, particularly relevant when considering the growth of AI.

Day	Topic	Tutorial
Day 1	The Unix Shell	1. Introducing the Shell 2. Navigating Files and Directories 3. Working With Files and Directories 4. Pipes and Filters 5. Shell Scripts
Day 2	Introduction to High-Performance Computing	1. Why use a Cluster? 2. Connecting to a remote HPC system 3. Exploring Remote Resources 4. Scheduler Fundamentals 5. Accessing software via Modules 6. Transferring files with remote computers 7. Running a parallel job
Day 3	Introduction to High-Performance Computing HPC Workflow Management with Snakemake	8. Using resources effectively 9. Using shared resources responsibly 1. Running commands with Snakemake 2. Running Snakemake on the cluster 3. Placeholders 4. MPI applications and Snakemake 5. Chaining rules 6. Processing lists of inputs

Table 1 - Program and training material per day.

HPC Cluster

To hold the workshop, access to an HPC resource was required. For this purpose, Magic Castle was used to create a virtual HPC cluster in a public cloud environment. This tool has been used for training purposes for a number of years by the Digital Research Alliance of Canada, and BioNT has delivered a tutorial on how to use the tool at SC23, The International Conference for High Performance Computing, Networking, Storage, and Analysis (together with the main developers). Magic Castle is what will allow HPC Carpentry to be a scalable lesson program within The Carpentries.

In addition, the course has leveraged the software environment provided by the [European Environment for Scientific Software Installations](#) (EESSI, pronounced as "easy"), which is available as an option via Magic Castle.

Certificates

Certificates (Figure 5) were provided to those participants who explicitly requested them and fulfilled these criteria: (i) they joined at least one session on Zoom or notified the organisers that they could not attend, (ii) it was verified that they created an account for the HPC cluster and submitted a number of jobs to the scheduler, and (iii) they completed the post-workshop survey.
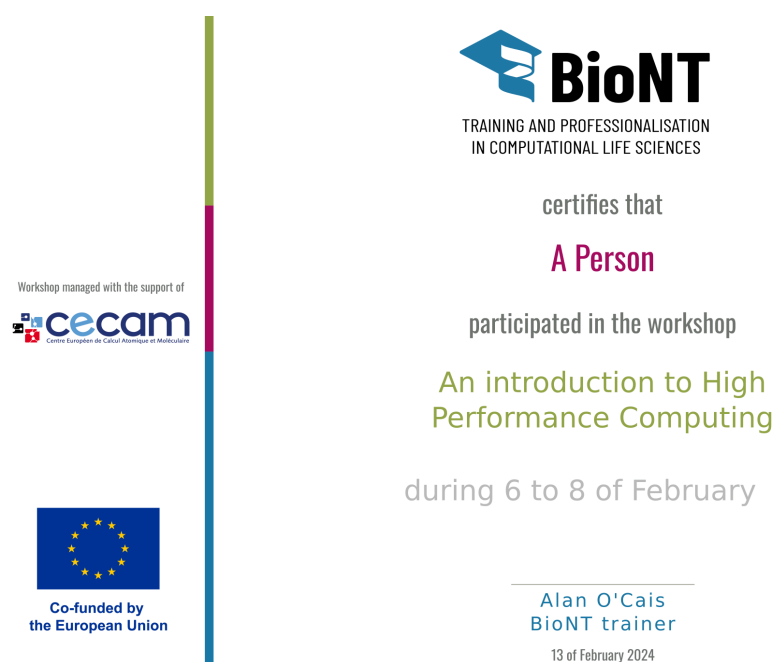
Figure 5 - Template used to generate certificates.

Outcomes of the workshop

Applications and pre-workshop survey

58 applicants completed the pre-workshop survey and 52 submitted their application form via the CECAM platform. From these, 45 participants completed all the registration process and were accepted to the workshop. These 45 survey answers are therefore shown in the following sections. The pre-workshop survey comprised 10 questions covering skills, demographics, and miscellaneous topics. The majority of questions were optional for the successful completion and submission of the survey.

General information

Of 42 applicants, with 69% male and 31% female, were from and were working in 28 different countries (Table 2), and described themselves as 38% White, 43% Asian, 10% Black or African American and 10% Hispanic or Latino(a).

Country	Nationality	Employment
Argentina	1	1
Austria		1
Bangladesh	6	6
Belgium		1
Botswana		1
Brazil	1	
Cameroon	1	
Canada	1	1
Colombia	1	1
Egypt	1	1
France	1	1
Germany	1	5
Greece	2	1
India	8	5
Ireland		3
Israel	1	
Italy	1	2
Lithuania	1	1
Malaysia	2	1
Namibia	1	1
Nigeria	1	1
Poland		1
Portugal	1	
Romania	1	1
Singapore	1	

Slovakia	1	1
Spain	3	2
Sudan	2	2
Sweden	1	1
Turkey	1	
UK	1	
United States of America		3
Vietnam	1	

Table 2 - Workshop applicants' nationality and country of employment from the pre-workshop survey.

Most applicants worked or studied in the fields of Genetic, Genomics or Bioinformatics (data not shown) and were academic employees (Figure 5-B) in the category of graduate students (24%) or research staff (36%) (Figure 5-A).
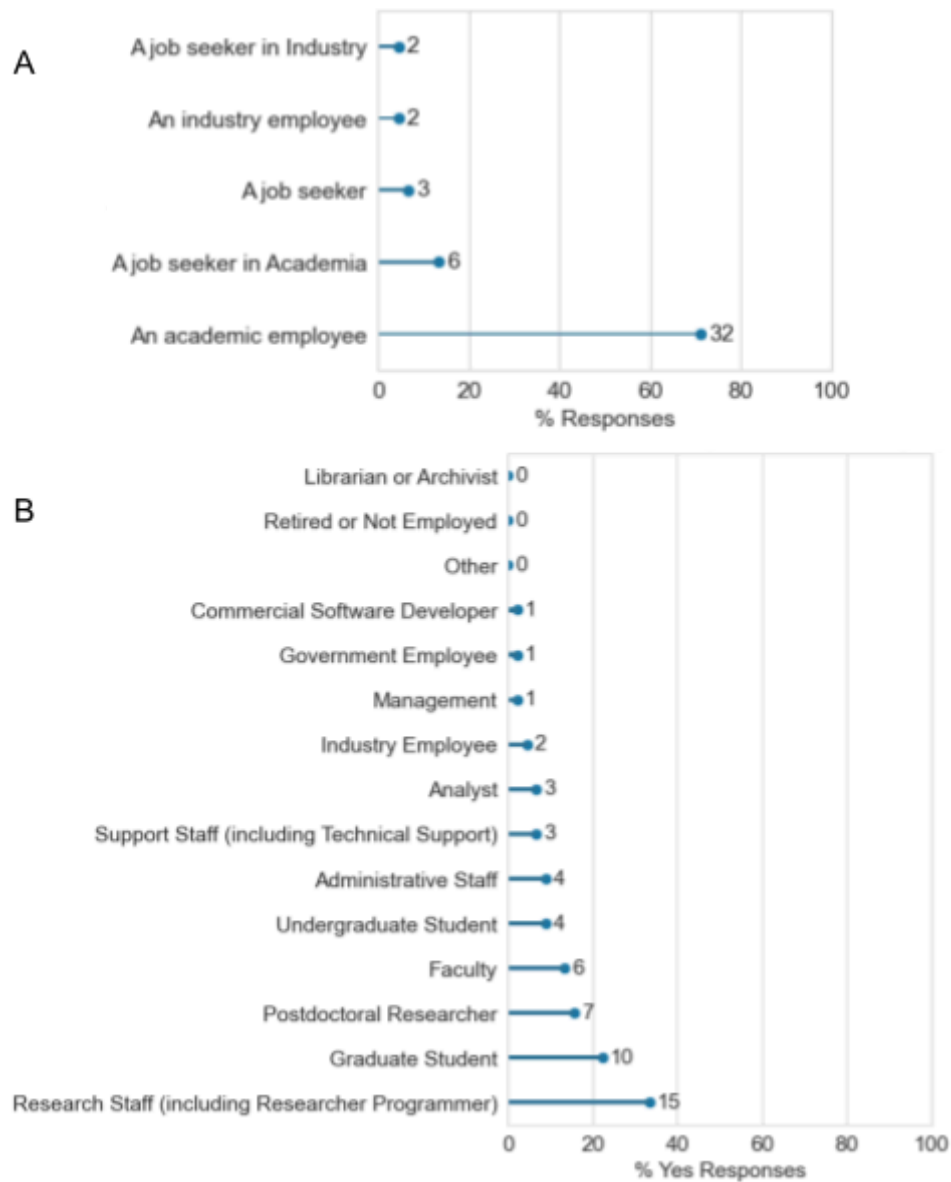
Figure 5 - The current job definition of the applicants (**A**) for n = 45, and the current occupation/career stage (**B**) for n = 42, according to the pre-workshop survey.

Additionally, 2 applicants were industry employees and 11 were job seekers (with 6 in Academia, 2 in Industry and 3 either in academia or in industry). Regarding the connections with SMEs, 4 mentioned to be working in an SME, 9 collaborating with SME(s) and 20 aiming to work in an SME.

Applicants found information about the workshop through various channels, as illustrated in Figure 6, with the majority learning about it via social media or receiving direct recommendations from friends or colleagues. Additionally, 8 applicants reported becoming aware of the workshop in a newsletter or on a university website.
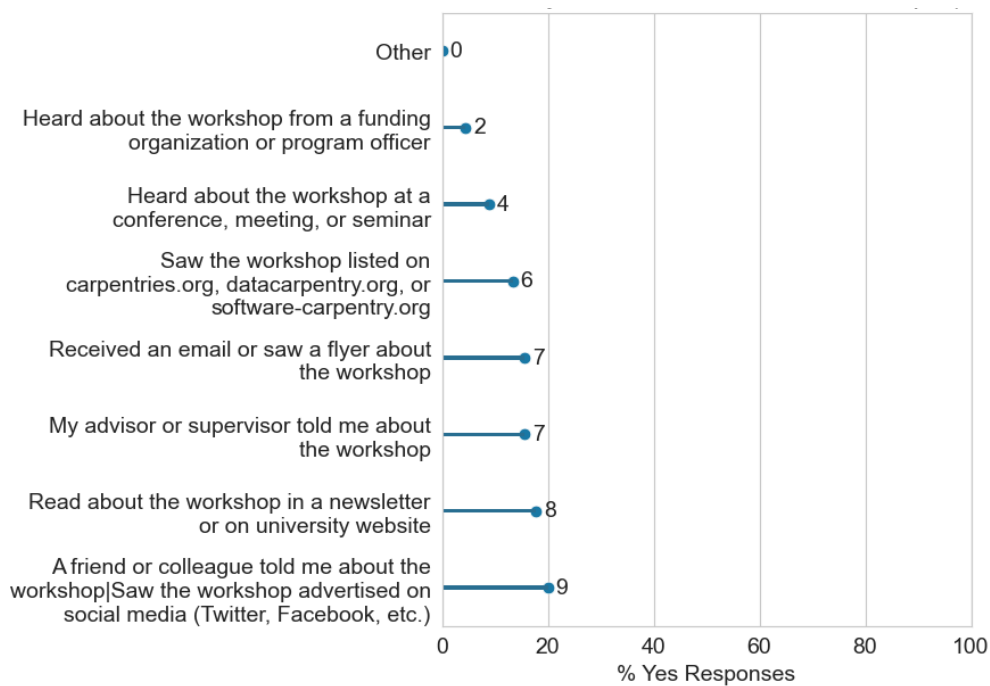
Figure 6 - Answers to the question: "How did you find out about this workshop?" (n = 39).

Of the 45 participants, 43 provided information about the operating system they planned to use for the workshop: 51% planned to use Windows for the workshop, 26% macOS and 23% Linux.

Background information

When asked about how often they use different programming languages (such as R, Python, C++, etc.), 36% answered "Daily", 25% answered "Weekly", and 18% answered "Monthly" (Figure 7).
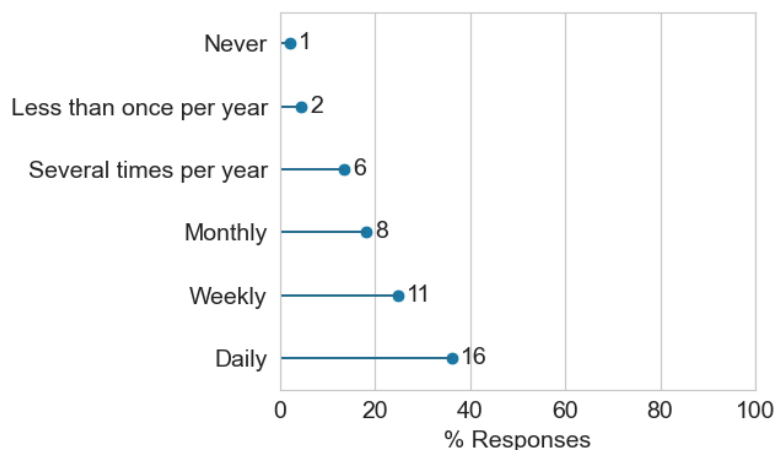
Figure 7 - Answers to the question: "How often do you currently use programming languages: R, Python, C++. etc?" (n = 44).

Most applicants (93%) agreed with the importance of having access to the original, raw data to be able to repeat an analysis (data not shown). The majority agreed that using a programming language can make their analyses easier to reproduce (Figure 8-A), and 35% of applicants were not satisfied with their current data management and analysis workflow (Figure 8-B).

Figure 8 - Answers to the questions: A; "Using a programming language (like R or Python) can make my analysis easier to reproduce" (n = 43). B; "Please rate your level of satisfaction with your current data management and analysis workflow (i.e. how you collect, organise, store and analyse your data)" (n = 42).
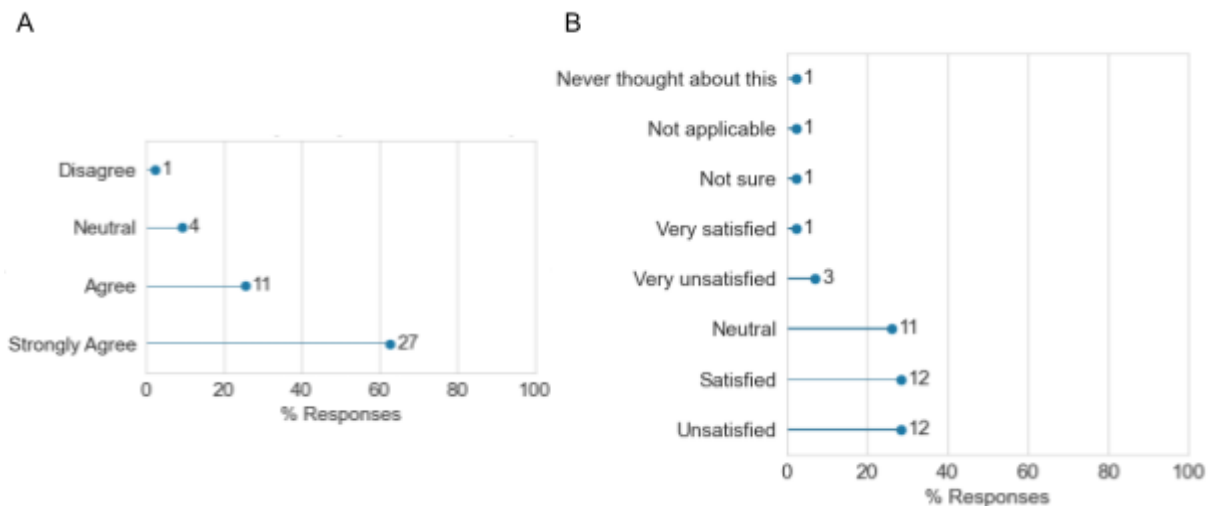
Expectations

Most participants were keen on acquiring new skills, with some specifically interested in learning those applicable to current or future occupations. Notably, 11 participants expressed their intention to leverage the acquired skills either to secure a promotion within their current job or to pursue new employment opportunities (Figure 9).

Figure 9 - Answers to the question: "Why are you participating in this workshop?" (n = 45).

Participation

All 45 applicants who submitted their complete application were chosen to take part in the workshop. Of these 45 applicants, a total of 32 participants attended the workshop live, although not all of them stayed for the entire duration (Table 3). All 45 received the self-learning materials for them to consult at any time.

Day	Participants	Instructors	Helpers
1	33	1	4
2	27	1	4
3	26	1	4

Table 3 - Number of participants, instructors and helpers per day. The number of participants was obtained from the participant login information captured by Zoom.

After the workshop, 15 participants requested a certificate. The certificate was provided to those participants who attended the Zoom live session at least once, completed the post-workshop survey and carried out a substantial portion of the exercises on the provided HPC resource.

Daily feedback

At the end of each day, participants were asked for feedback on the following three points:

- Please share one thing that was good about today
- Please share one thing that could be improved about today
- Do you have any other comments?

The daily feedback is summarised in the following Table 4.

Day	Good about today	To improve	Any other comments?
1	Covered all the basics needed to refresh old knowledge, Love the use of hedge doc Velocity was good I like this live tool for the training Learned from basic Learned all the basic commands of linux, and pace is also good for the beginner Thank you for the initiative of teaching HPC :)	Please make the "standard" gallery, so screen sharing can be bigger. Confirm comfortability with the entry level items, to allow for skipping of some topics, in order to - aid with time Use the same directory	Are we going to learn how to perform batch jobs? And changing the memory limits due to the command to be executed? Good explanations, speed was at the beginning too fast, but time for the exercises was good enough Are we going to

	well explanation This platform is pretty good in interactive session Renato is really didactic Recordings will be made available later. You will be able to review	structure, for all to explain some bash concepts. A little bit faster in the beginning i like the live tools training somebody is constantly highlighting the text in the HedgeDoc, it would be nice to not do that :) The last 10 minutes was really fast, I couldn't follow a little bit fast for me in certain sections Was a little rush at the end, but overall is good provide the lecture material	have at some point, applications for python in real life problems ? Will there be a video available of today's and the rest of the days explanations for the participants	
2	Very helpful, especially on the data transferring and parallel jobs Covered what felt like a lot of information in good pace Very nice practice Good intro to HPC Very precise and interesting Good pace & Interesting Knowledge	Starting part of day was little bit fast, but then the speed was alright Please set the gallery into "standard", not the "speaker", so the "screen sharing" becomes larger more time to see the commands on screen Maybe the creation of account could be done earlier, as it was a little messy in the morning Kindly see if you are able to display a bar (like yesterday) which shows the commands entered break should be longer (~15') Need the changes made in code during the explanation More breaks/more often	Thanks so much Alan Thank you Thanks Thank you very much Thanks Alan! LFB Thank	

| 3 | More advanced concepts of HPC were introduced which was good

Well explained and at a good pace | I would have liked the topic of this day to be allotted more time. | |

**Table 4** - Daily feedback collected in the HedgeDoc document.

Postworkshop survey

At the end of the workshop, participants were asked to complete the post-workshop survey consisting of 20 questions, 19 of them optional. In total, 19 participants completed this survey.

Regarding the workshop environment and the possibility of interacting with the trainer and helpers, the answers were overall positive. (Figure 11 A-B). A significant number of participants perceived the instructors as enthusiastic about the workshop and knowledgeable about the material being taught (Figure 11 C-D). Except for two participants, all others could get clear answers to their questions from the instructors (Figure 11-E). 74% of the participants expressed confidence in their ability to immediately apply what they learned at the workshop (Figure 11-F). Only one participant marked the answer "Strongly disagree" to all the questions shown in Figure 11. As this participant indicated to be very likely to recommend the workshop, it is plausible that a misinterpretation of the questions occurred from their end.

When asked about accessibility requirements, 7 participants replied "Yes", but none included further explanations about their requirements, therefore no actions were taken.

Participants mostly viewed the interaction with the HedgeDoc document and the questions answered on the fly by the helpers as positive and helpful for their learning experience. Not only the assistance of the helpers but also the support from the instructors in addressing individual issues and the repetition of exercises were positively received. The possibility to access the overall discussion within the shared document, during and after the workshop, seemed to have improved the participant's learning experience, as indicated by their feedback.
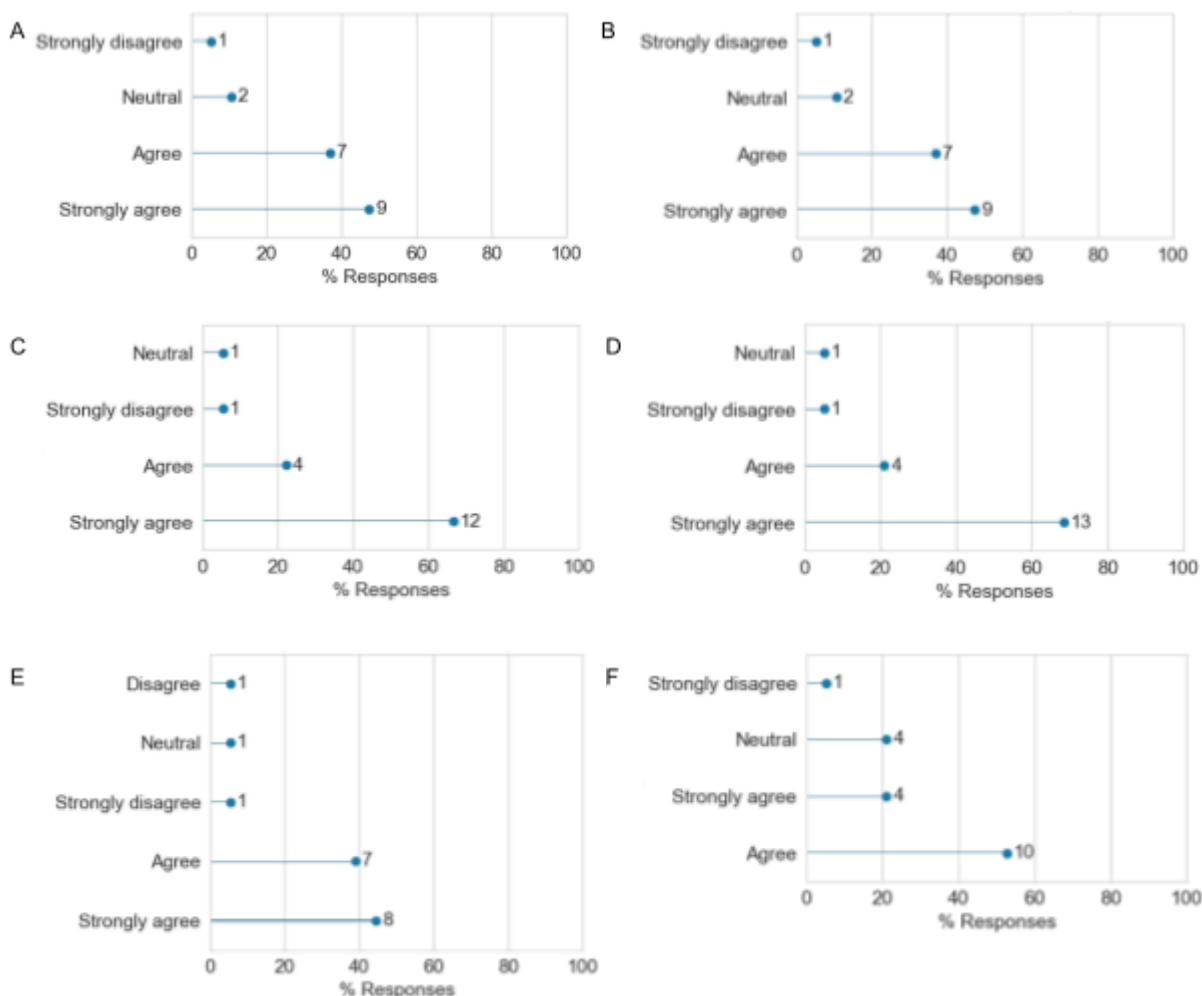
Figure 11 - Rating of participant's agreement with the following statements: **A** - I felt comfortable learning in this workshop environment; **B** - I felt comfortable interacting with the instructors; **C** - The instructors were enthusiastic about the workshop; **D** - The instructors were knowledgeable about the material being taught; **E** - I was able to get clear answers to my questions from the instructors; **F** - I can immediately apply what I learned at this workshop (n = 19).

Participants were also asked about strengths and ways to improve the workshop. All answers are reported in the following Table 5.

| Major strengths of this workshop	Ways the workshop could be improved
Wide breadth of topics but also enough depth and enough time given to each to feel as though I have a good grasp on what was covered. HedgeDoc is a great way of interacting and asking questions. Good instructors.	Some more frequent recaps after each 30-45 minutes or so would be useful if having lost track slightly. For example, waiting for an answer to be answered in the HedgeDoc whilst the instructor continues. First half day was a lot more basic than the other days.
Well organised with step by step tutorial for	I have no suggestion

beginners	
It partially went too far and was difficult to follow. The snakemake part was very good, but could be much longer as it is not straightforward to understand but can be very helpful.	More of snakemake
I really liked following this workshop with HedgeDoc tool. It's an efficient way for conducting such workshops	Some of the stuff like making of the cluster account and maybe the very basics of HPC can be done on the first day, so there is more time for HPC fundamentals and some advanced stuff for the next two days.
Thank you for the training. Simple hands-on but I think after doing all the hands-on I quite understand the basic fundamentals to use HPC. I will highly recommend to my colleagues and undergraduate students to join and learn this. It is just that I have lost the snakemake session as I need to leave to take my child from the school.	Not so far until now.
Very good explanations, the possibility to work in parallel with the instructor	Documentation to follow the workshop

Prerequisites. I think it is necessary to make separate workshops. For example shell basics. Mixing it with this workshop is not good.

Save the workshop with screen (to have after the workshop a complete history for the commands, and for the editions

Need work with more real examples. |
| In this workshop I gained familiarity with parallel computing techniques. Although I had a rudimentary understanding of the concept, the practical exercises involving connecting to a cluster and executing commands concurrently truly enhanced my comprehension. As a daily Linux user, connecting to a real cluster significantly deepened my understanding of the concepts involved. Another strength of the workshop was the presence of responsive support staff who quickly addressed any issues that arose.

Ultimately, the best aspect of this workshop was the practical exposure to | Increase Hands-on Practice

 Diverse Examples |

high-performance computing concepts, which was invaluable for my learning experience.	
Able to communicate with instructor easily	Slow the speed
Broadly addressed the main themes and difficulties encountered in HPC; listed the most used and most necessary commands	Instructors could make typed codes available for longer on the screen, to give students time to understand what they are doing and be able to visualise and reproduce them at the same time. Furthermore, the lack of help when we are learning prevents us from following the content. When we encounter a failure on our laptops or typed codes wrongly, we end up missing part of the instructor's explanation and, as a result, we are unable to follow the next steps. An example: regarding downloading the amdahl data. The commands failed for me (probably because I copied some code wrong at the moment) and I was unable to perform this task even the next day, following the link provided. And, as a result, I was unable to perform any job that referred to amdahl.
Very compact but insightful introduction	
Well structured lessons Good instructors Supportive	Some last minutes are often faster than beginning.
The workshop exhibited a commendable structure, providing all necessary software in advance—an appreciated gesture. It comprehensively covered essential features, seamlessly introducing new processes that facilitated the organic integration of various topics. The instructors were adept at addressing queries, generously sharing insights, and the live demonstration of command line operations proved immensely beneficial. The incorporation of HedgeDoc significantly enhanced interaction, fostering collaborative problem-solving with the participation of multiple individuals. This collaborative approach added depth to the learning experience by leveraging collective expertise to overcome challenges. The opportunity to use my personal computer contributed significantly to my comfort level throughout the course.	I encountered challenges with one of the topics, specifically in determining the p-value, as the Bash output consistently presented an error. Despite my efforts to repeat the steps, the issue persisted. To enhance the learning experience, it would be beneficial to incorporate a post-session Q&A opportunity. This would provide a dedicated time for troubleshooting, allowing participants to address issues without falling behind in the course. Furthermore, introducing a pre-workshop video that explains the principles or provides a brief demonstration of the upcoming topic could be immensely helpful. This preparatory content would give participants a foundational understanding before the workshop, reducing the risk of getting lost during troubleshooting. Additionally, incorporating a related assignment mirroring the workshop content would offer an invaluable opportunity to solidify comprehension. This approach ensures that even if one falls

Looking ahead, I am confident that revisiting this course in a few months would not only bolster my proficiency but also deepen my knowledge of bioinformatic methods and command line usage. Overall, the course laid a solid foundation for continued growth and skill development in this field.	behind, they can independently verify their understanding of the new and novel concepts introduced in the course.

Table 5 - Strengths and possible improvements for this workshop, as suggested by participants in the post-workshop survey.

The feedback on the post-workshop survey was positive and participants were likely to recommend this workshop to a friend or colleague (Figure 12).
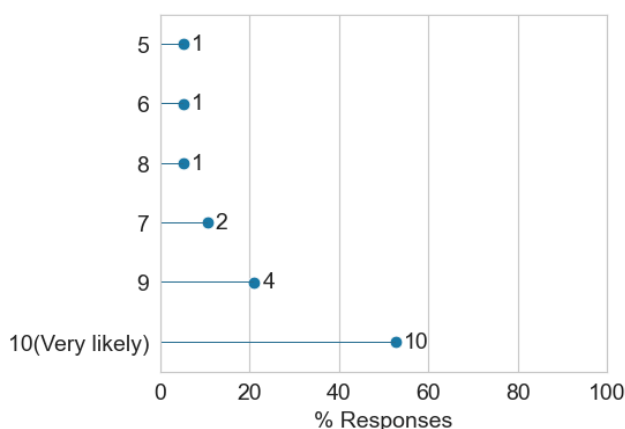
Figure 12 - Answers to the question: How likely would participants recommend this workshop to a friend or colleague? (n = 19). The answers from "0 - Very unlikely" to 4 are not shown as no responses were given in this range.

Conclusion

The third BioNT workshop, "An Introduction to High Performance Computing", was successfully held on February 6th - 8th of 2024, online and cost-free for participants.

The setup for the third workshop benefited from the experience gathered during the first two BioNT workshops. In particular, the general approach to interaction with the participants was appreciated. However, the setup for the third workshop posed some additional challenges:

- Account creation and getting SSH access to the HPC resource was not well suited to the webinar environment as people tended to have non-content related issues. This would have been better suited to a drop-in session before the main webinar session.
- Attendees were very keen to see the history of commands run by the instructor. This can be done in the shell itself for bash, but when moving between a local and remote environment other tools are necessary. On the second day, no such tool was used but for the 3rd day, Shellshare was used and this seemed to be appreciated.

- Some content was sensitive to syntax, and typos may be hard to catch, this meant it was important to periodically provide working versions of the files the instructor was working on. This helps avoid a situation where participants get lost while bug-hunting.

Successful participation in the training required: (a) the installation (or availability) of certain packages before the course, and (b) the use of a dual-screen setup was recommended.

One significant issue for the course in general is that self-paced learning is not entirely possible. The course requires the availability of an HPC resource on which to carry out the content, something that is unlikely to be the case for many self-paced learners.

The consortium will take the improvements and the individual challenges of the third workshop into consideration to further enhance the training provided by BioNT, especially regarding the upcoming fourth workshop scheduled for March 2024. Overall, the BioNT consortium concludes that the workshop successfully achieved its goals.