![PAUL SCHERRER INSTITUT PSI]

WIR SCHAFFEN WISSEN – HEUTE FÜR MORGEN

AiiDA Team :: MSD :: Paul Scherrer Institute

Result of Questionnaire 2024

June 2024

PAUL SCHERRER INSTITUT
PSI

AiiDA Questionnaire 2024

- **Estimated Total Time to Complete:** Less than **5** minutes
- **Sections:** 3 or 4 short sections (based on initial answer)

khsrali@gmail.com Switch account

Not shared

Draft saved

* Indicates required question

Are you currently using AiiDA for your research? *

○ Yes, frequently (e.g. every week)
○ Yes, occasionally (e.g. few projects per year)
○ No, but I used it a long time ago
○ No, I never used it for my research

We are planning to **highlight** a number of top research papers that have utilized AiiDA in a new dedicated section on the AiiDA website. If you're interested in featuring your work, please share details here or get in touch with us.

Your answer

Have you been part of any projects supporting AiiDA, either currently or in the past?

☐ NCCR MARVEL
☐ MaX CoE
☐ H2020 MarketPlace
☐ H2020 Intersect
☐ NFFA
☐ BIG-MAP
☐ Other:

Next   Clear form

AiiDA Tutorials

Your answer: I use AiiDA

Have you participated in any AiiDA tutorials? (Whether in person or online)

○ Yes
○ No

If the answer is "yes," can you recall the year you took part?

Your answer

If the answer is "no," how did you learn to use AiiDA?

☐ My research group knew how to use it, I learned from them
☐ AiiDA documentation and online resources
☐ Other:

For how long have you been utilizing AiiDA in your research work?

○ less than 1 year
○ 1-2 years
○ 2-5 years
○ more than 5 years

Would you like to participate in our next tutorial? It's aimed for beginners and will go over the newest features of AiiDA.
If so, please enter your email address below, we will keep you posted!

Your answer

Back   Next   Clear form

Enhancing User Experience

When you were **first** exploring and learning AiiDA, what aspect did you find most difficult to grasp?

Please be specific, for instance, "was hard to query data using nodes" or "I couldn't fetch the calculation folder" or "difficult to set up workflows"

Your answer

What is the most challenging aspect of using AiiDA **today**?

Please be very specific, as we are planning to work on these points. For instance, "I would have preferred if 'verdi computer delete ' also allowed for the deletion of all its associated nodes..."

Your answer

Which AiiDA plugins have you utilized so far?

For example, aiida-quantumespresso, aiida-vasp, ... [see the full list]

Your answer

Anything else that we can improve?

Your answer

Back   Next   Clear form

Collect contact-info if agreed.

The end.

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☐ NFFA

☐ BIG-MAP

☐ Other:

Next   Clear form

Your answer: I don't use AiiDA

Have you participated in any AiiDA tutorials? (Whether in person or online) *

○ Yes

○ No

Would you like to participate in our next tutorial? It's aimed for beginners and will go over the newest features of AiiDA.
If so, please enter your email address below, we will keep you posted!

Your answer

Back   Next   Clear form

Your answer: I don't use AiiDA, and I have not participated in any AiiDA tutorials.

What is AiiDA?
AiiDA is an open-source Python infrastructure to help researchers with automating, managing, persisting, sharing and reproducing the complex workflows associated with modern computational science and all associated data. Follow this link to learn more.

If you **ever** were exploring and learning AiiDA, what aspect did you find most difficult to grasp?

Please be specific, for instance, "was hard to query data using nodes" or "I couldn't fetch the calculation folder" or "difficult to set up workflows "

Your answer

What other AiiDA learning methods have you tried?

☐ My research group knew how to use it, I learned from them

☐ AiiDA documentation and online resources

☐ Other:

Back   Next   Clear form

Your answer: I don't use AiiDA, but I have participated in an AiiDA tutorial

Can you recall the year you took part in an AiiDA tutorial?

Your answer

Why did you stop using AiiDA?

☐ I needed a feature that AiiDA doesn't have

☐ I use other workflow managers

☐ I was stuck at the learning process

☐ I changed my research field

☐ Other:

Please be more specific about the your answer above. This would assist us in understanding how to get better (e.g., I expected this particular code behavior from AiiDA, because...).

Your answer

When you were **first** exploring and learning AiiDA, what aspect did you find most difficult to grasp?

Please be specific, for instance, "was hard to query data using nodes" or "I couldn't fetch the calculation folder" or "difficult to set up workflows "

Your answer

Back   Next   Clear form

Collect contact-info if agreed.

The end.

- The questionnaire* was sent to:
  - Discourse
  - MARVEL mailing list (with an additional reminder)
  - Emails of past participants in AiiDA tutorials **

- It was roughly available for about one month May to June.

- We've collected 38*** responses, of which only 17 (~46%) responses recorded from MARVEL.

- Considering sampling group and reachability of users, presumably we have **more external users** than those associated with MARVEL, although they may not have been immediate to publish their work.[++]

* Most of questions were not obligatory to answer, to avoid compulsive responses.

** Note: many of these emails never delivered, because many of these users students/postdocs who were not affiliated anymore with their previous institution, still some retrieved manually.

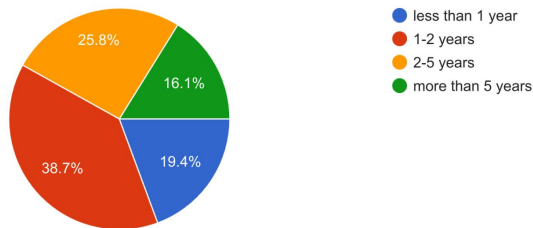*** Only one person from PSI (we didn't fill ourselves)

++ We explicitly asked if you want to highlight your publication in our website, and only got a few responses. Meaning many of our external users, haven't reached to publication point, yet.

Usage

- More than 80% of responsive users are currently using AiiDA for research.

- Among those who were participating in AiiDA tutorial, there is an **increasing** number of those got hooked on, and using it since the last three tutorials.

- About 60% of responsive users have been utilizing AiiDA for only less than two years. Which means their results might not have been ready to publish, yet.
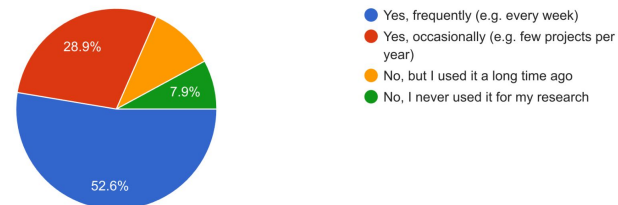
Are you currently using AiiDA for your research?
38 responses

- Yes, frequently (e.g. every week)
- Yes, occasionally (e.g. few projects per year)
- No, but I used it a long time ago
- No, I never used it for my research

28.9%
7.9%
52.6%

For how long have you been utilizing AiiDA in your research work?
31 responses

- less than 1 year
- 1-2 years
- 2-5 years
- more than 5 years

25.8%
16.1%
38.7%
19.4%

Can you recall the year you took part in an AiiDA tutorial?

- Total responsive
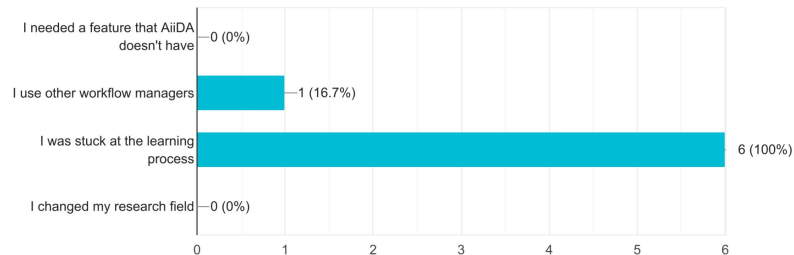- Actively using
- Not actively using

Year
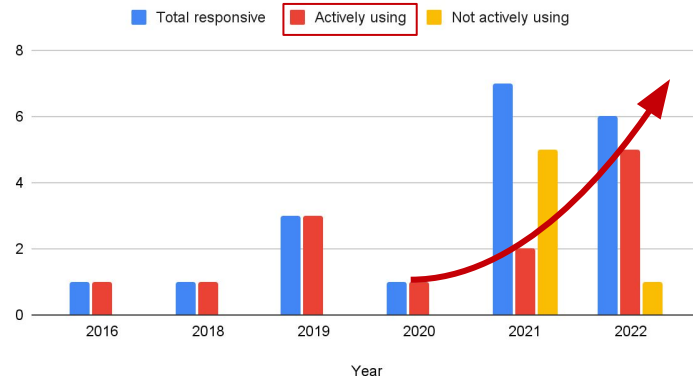
Learning Curve: users who dropped out

- Those who participated in AiiDA tutorials, but never used it afterwards mainly said:
  "I was stuck in learning process"

Why did you stop using AiiDA?
6 responses

I needed a feature that AiiDA doesn't have	0 (0%)
I use other workflow managers	1 (16.7%)
I was stuck at the learning process	6 (100%)
I changed my research field	0 (0%)

(bar chart, x-axis 0 to 6)

- We asked *"Please be more specific about the your answer above."*
  Some were referring to not having enough computer resources, or have being totally new in this field of research. **Apparently lack of a clear research idea, also played a rule.**

- We asked again "what aspect of AiiDA did you find most difficult to grasp", and many pointed to **difficulty of setting up workflows**.

Learning Curve: users who stayed put

Among those active users, 58% have never participated in an AiiDA tutorials. We asked how did you learn, they equally weighted the **knowledge of their research group** and **online documentations**.

We asked three main question: what they found difficult to understand in AiiDA in the past and now, and what can we improve.

* Among answers we came across a self learner from <u>Colorado said:</u> **"The documentation is pretty fantastic and I think researchers can pretty easily self-teach. [...]"**
* A person from <u>Germany</u> said: **"**[It's difficult] **To know when to apply which concept (calcfunctions, -jobs, workflow chains, ...) to my specific use case. But the docs are great, I have to simply read it again and let all those concepts sink in to my brain."**
* A person <u>Canada</u> who is using AiiDA for less than a year, didn't know how: **"Fixing and resubmitting jobs that did not exit successfully"**
* Somebody from <u>Netherlands</u> found it challenging: "**If I want to do something that's not inherently supported by either AiiDA core or one of the plugins, but I would like to do it from within AiiDA to preserve provenance."**

Some others found it difficult:
    - "to get use to database structure rather than folder based"
    - "lack of "unsafe" no-provenance mode for quick-and-dirty use cases"
    - the simple add & multiply example in tutorial useless, and not practical in real use case.
    - "querying data is not straight forward and difficult"
    - "to set up a first workflow"
    - ...

What's next? Action plan summary

The following tracks that we are already implementing seem to be in the right direction:

- WorkGraph [final stages of development]→ providing easier logic than workflow
- **aiida-shell*** [developed] → able to run custom scripts
- verdi presto [developed] → quick setup
- verdi dump [developed] → downloading data as local folder

In addition, based on the feedback, we plan to start the following actions:
- verdi git/mirror [in discussion] → folder based behaviour

* Increasing number of users: the most frequently mentioned plugin is **aiida-quantumespresso** with 15 mentions, followed by **aiida-vasp** with 5 mentions, and **aiida-shell** and **aiida-pseudo** each with 4 mentions, in the responses.