

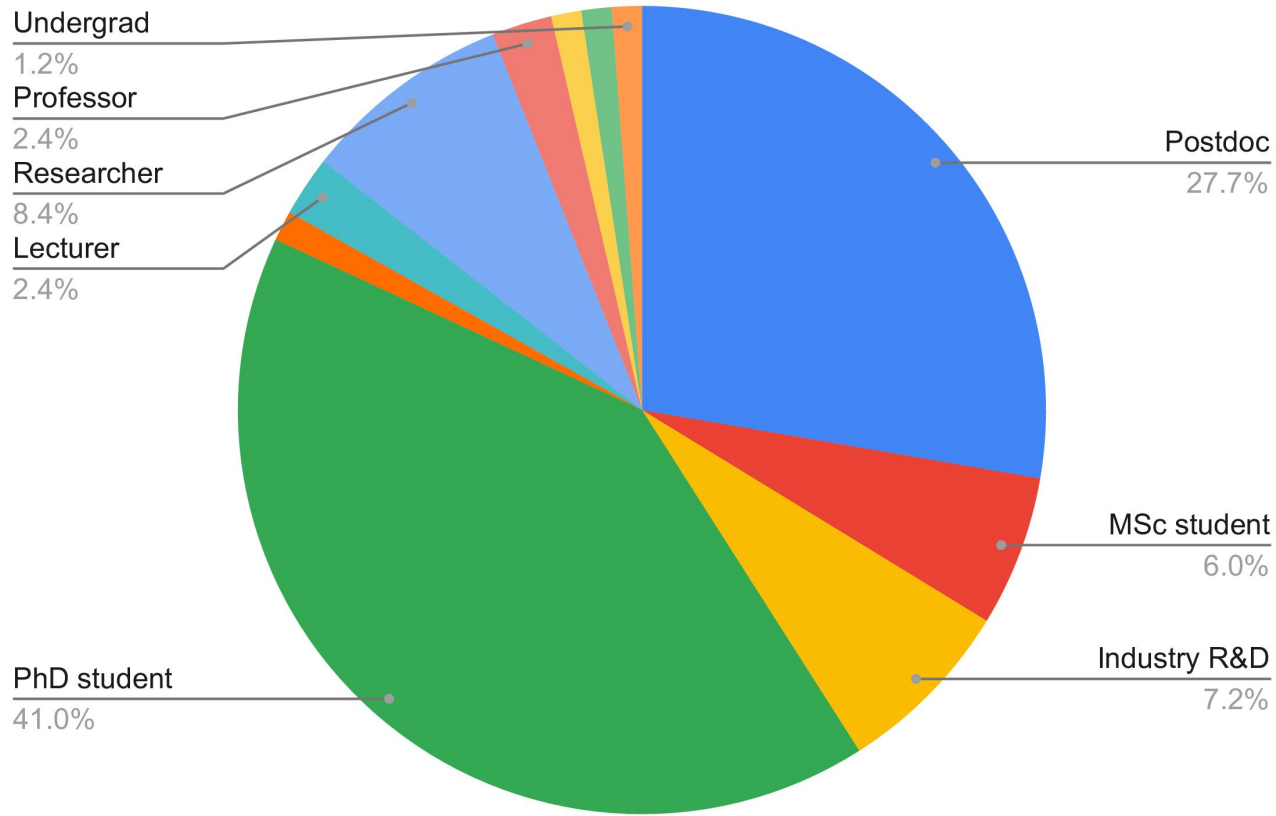


AiiDA Tutorial Overview

Marnik Bercx

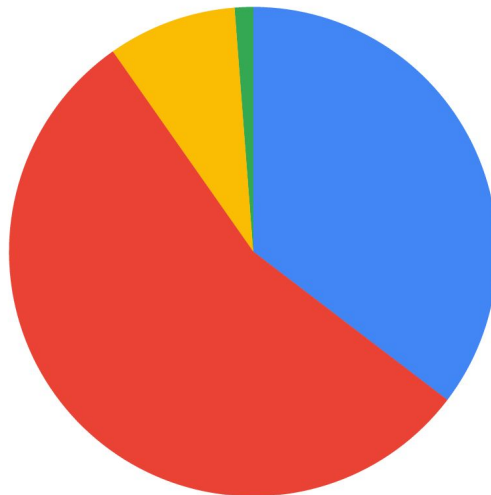
- Participants
- Format and schedule
- Practical information
- Team and sponsors

Participants - Position



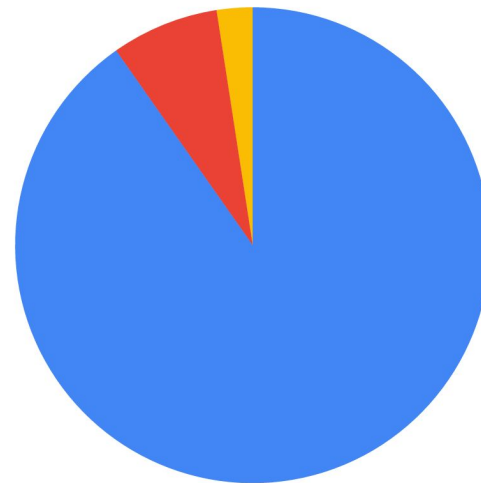
Python Experience

- basic - written a Python script
- medium - familiar with object oriented programming in Python
- advanced - familiar with frameworks like django, sqlalchemy, click, ...
- none - never written a Python program

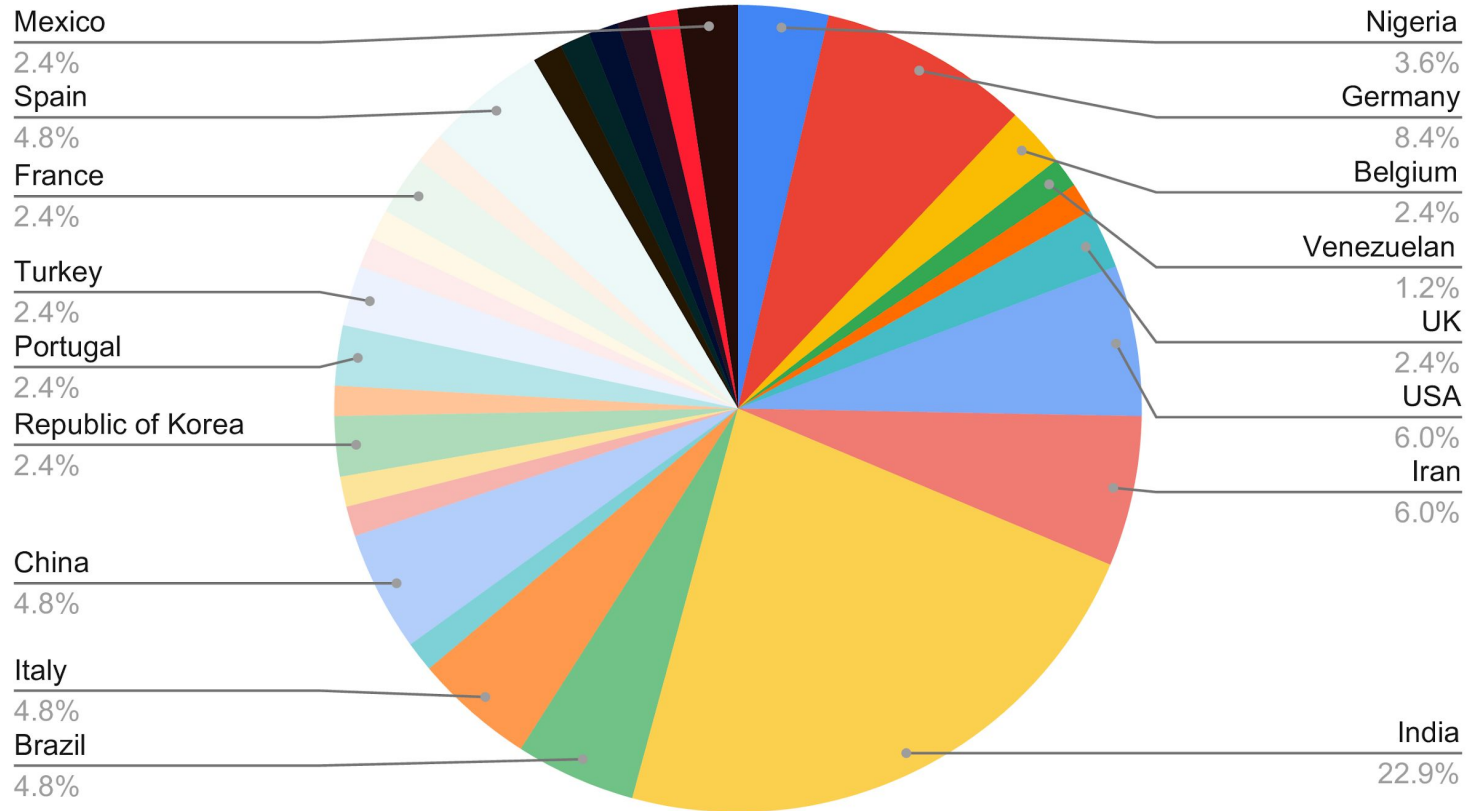


AiiDA Experience

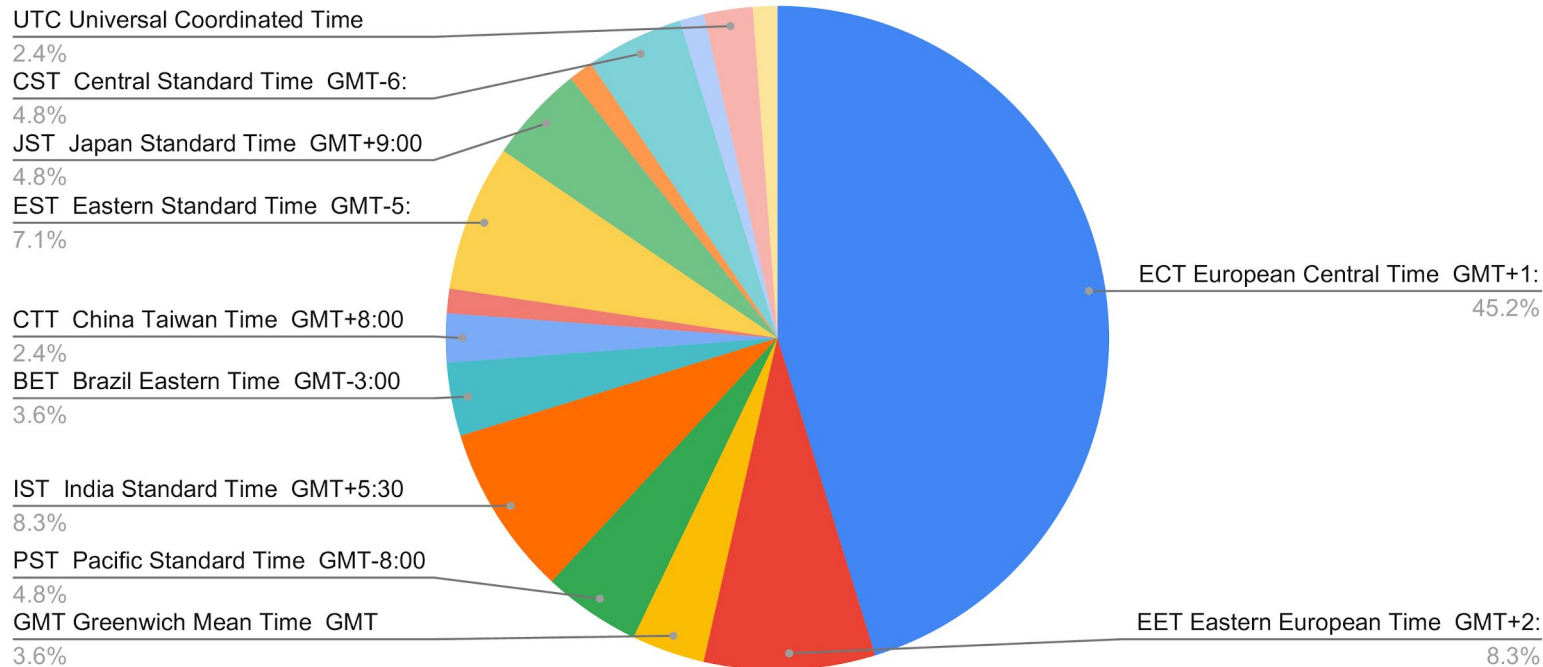
- I am new to AiiDA and have not used the program much
- I have used AiiDA before but mostly restricted to the command line features
- I am an advanced user of AiiDA and have already written workflows with it



Participants - Nationality



Participants - Time Zone



Lausanne (CEST)	Tokyo (JST)	New York (EDT)	San Francisco (PDT)	Tuesday 07 Jul 2020		Wednesday 08 Jul 2020		Thursday 09 Jul 2020		Friday 10 Jul 2020		GROUP A		
9:00	16:00	3:00	0:00	AiiDA tutorial overview (10 min) Introduction to AiiDA (30 min) Setting up an environment (15 min)	1	(Optional) Plugin developer talks			AiiDA & the Materials Cloud (25 min) The AiiDA lab ecosystem (25 min)				Presentations	
9:30	16:30	3:30	0:30										Plugin developer talks	
10:00	17:00	4:00	1:00	Q&A session		Writing workflows in AiiDA (30 min) [1]	6, 12, 14, 15	The AiiDA plugin ecosystem (30 min)	10, 17	OSSCAR (15 mins) AiiDA & OPTIMADE (10 mins)			Hands on Sessions	
10:30	17:30	4:30	1:30	Setting up the machines	2	Q&A session		Q&A session		Q&A session (plugin developers)			Breaks	
11:00	18:00	5:00	2:00											
11:30	18:30	5:30	2:30	AiiDA Basics	2, 3, 4, 11	Working with data and querying your results	7, 8, 15	Advanced workflows	6, 14	Installing and managing AiiDA on your computer/laptop and connecting to your supercomputer/cluster	3, 9		Documentation Reference	
12:00	19:00	6:00	3:00										Introduction:	
12:30	19:30	6:30	3:30	Lunch Break		Lunch Break		Lunch Break		Lunch Break			What is AiiDA	1
13:00	20:00	7:00	4:00										Getting Started	2
13:30	20:30	7:30	4:30										Detailed Installation	3
14:00	21:00	8:00	5:00	Running computations	5, 12, 13	Workflows: Basics	6, 14	Interfacing with external codes and writing plugins	5, 10, 17	Closing remarks and feedback Q&A session and wrap up discussion			Basic tutorial	4
14:30	21:30	8:30	5:30										How-to-guides:	
15:00	22:00	9:00	6:00										How to run external codes	5
15:30	22:30	9:30	6:30										How to run multi-step workflows	6
16:00	23:00	10:00	7:00	AiiDA tutorial overview (10 min) Introduction to AiiDA (30 min) Setting up an environment (15 min)	1	(Optional) Plugin developer talks			AiiDA & the Materials Cloud (25 min) The AiiDA lab ecosystem (25 min)			GROUP B	How to work with data	7
16:30	23:30	10:30	7:30										How to visualize provenance	8
17:00	0:00	11:00	8:00	Q&A session		Writing workflows in AiiDA (30 min)	6, 12, 14, 15	The AiiDA plugin ecosystem (30 min)	10, 17	OSSCAR (15 mins) AiiDA & OPTIMADE (10 mins)			How to manage your installation	9
17:30	0:30	11:30	8:30	Setting up the machines	2	Q&A session		Q&A session		Q&A session (plugin developers)			How to package plugins	10
18:00	1:00	12:00	9:00										Topics:	
18:30	1:30	12:30	9:30	AiiDA Basics	2, 3, 4, 11	Working with data and querying your results	7, 8, 15	Advanced workflows	6, 14	Installing and managing AiiDA on your computer/laptop and connecting to your supercomputer/cluster	3, 9		Command line interface	11
19:00	2:00	13:00	10:00										Processes	12
19:30	2:30	13:30	10:30	Lunch Break		Lunch Break		Lunch Break		Lunch Break			Calculations	13
20:00	3:00	14:00	11:00										Workflows	14
20:30	3:30	14:30	11:30										Provenance	15
21:00	4:00	15:00	12:00	Running computations	5, 12, 13	Workflows: Basics	6, 14	Interfacing with external codes and writing plugins	5, 10, 17	Closing remarks and feedback Q&A session and wrap up discussion			Database	16
21:30	4:30	15:30	12:30										Plugins	17

- Pre-recorded talks, published on youtube
 - Some are required for the hands-on sessions: be sure to watch these before each hands-on!
 - Plugin developer talks can be watched at any time, Q&A session on Friday.

- Hands-on sessions
 - Scheduled Zoom meetings.
 - First hands-on of each day starts with a Q&A session.
 - Introduction to the topic of hands on.
 - Work at your own pace in groups of 5-6.
 - Questions answered either in the group or in one of the Zoom “breakout” rooms.

Presentations: watch before hands-on sessions of that day!

Tuesday 07 Jul 2020	Wednesday 08 Jul 2020	Thursday 09 Jul 2020	Friday 10 Jul 2020
AiiDA tutorial overview (10 min) Introduction to AiiDA (30 min) Setting up an environment (15 min)	(Optional) Plugin developer talks		AiiDA & the Materials Cloud (25 min) The AiiDA lab ecosystem (25 min)
Q&A session	Writing workflows in AiiDA (30 min) [1]	The AiiDA plugin ecosystem (30 min)	OSSCAR (15 mins) AiiDA & OPTIMADE (10 mins)
Setting up the machines	Q&A session	Q&A session	Q&A session (plugin developers)
AiiDA Basics	Working with data and querying your results	Advanced workflows	Installing and managing AiiDA on your computer/laptop and connecting to your supercomputer/cluster
Lunch Break	Lunch Break	Lunch Break	Lunch Break
Running computations	Workflows: Basics	Interfacing with external codes and writing plugins	Closing remarks and feedback Q&A session and wrap up discussion

Group

A

B

- 8:00 15:00 GMT

- 8:30 15:30 GMT

Hands on sessions:

Be sure to double check starting times for your group and time zone!

- 11:30 18:30 GMT

- Amazon Web Services virtual machines:
 - Login instructions in email by Monday July 6th 18:00 GMT
 - Quantum Mobile can also be installed on your computer, but AWS is recommended
- Zoom rooms:
 - Links: One for group A and group B
 - Password protected
 - Details will also be provided in email
- Link to tutorial material:
https://aiida-tutorials.readthedocs.io/en/latest/pages/2020_Intro_Week/index.html

Organising committee:

- Chris Sewell
- Marnik Bercx
- Giovanni Pizzi

Plugin developers:

- Daniele Ongari
- Atsushi Togo
- Bonan Zhu
- Miki Bonnachi
- Emanuele Bosoni
- Philipp Rüßmann
- Dominik Gresh
- Dou Du

Tutors:

- Chris Sewell
- Marnik Bercx
- Giovanni Pizzi
- Sebastiaan Huber
- Leopold Talirz
- Aliaksandr Yakutovich
- Casper Andersen
- Francisco Ramirez

Support:

- Marco Borelli
- Simon Adorf
- Cornelia Bujenita



MARVEL



NATIONAL CENTRE OF COMPETENCE IN RESEARCH



swissuniversities



Platform for Advanced Scientific Computing

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Contributors for the 40+ plugins: Quantum ESPRESSO, Wannier90, CP2K, FLEUR, YAMBO, SIESTA, VASP, CASTEP, CRYSTAL, ...

Contributors to aiida-core and former AiiDA team members —

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