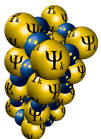




Writing reproducible workflows using AiiDA

May 21st-24th, 2019, Lausanne



swissuniversities

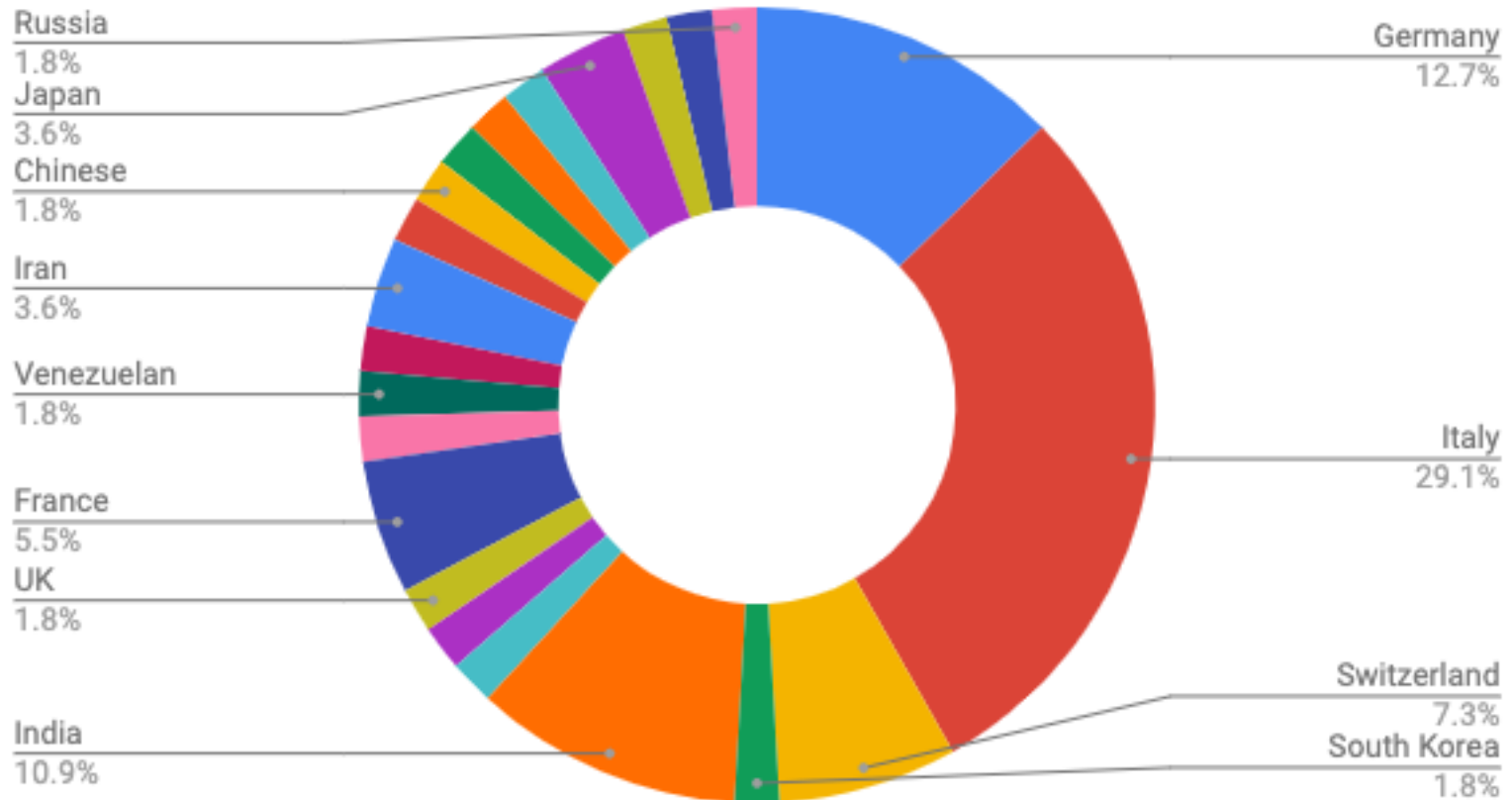


Outline

1. Questionnaire results
2. Schedule: the next 4 days
3. Questions?
4. Go!

Participants - Nationalities

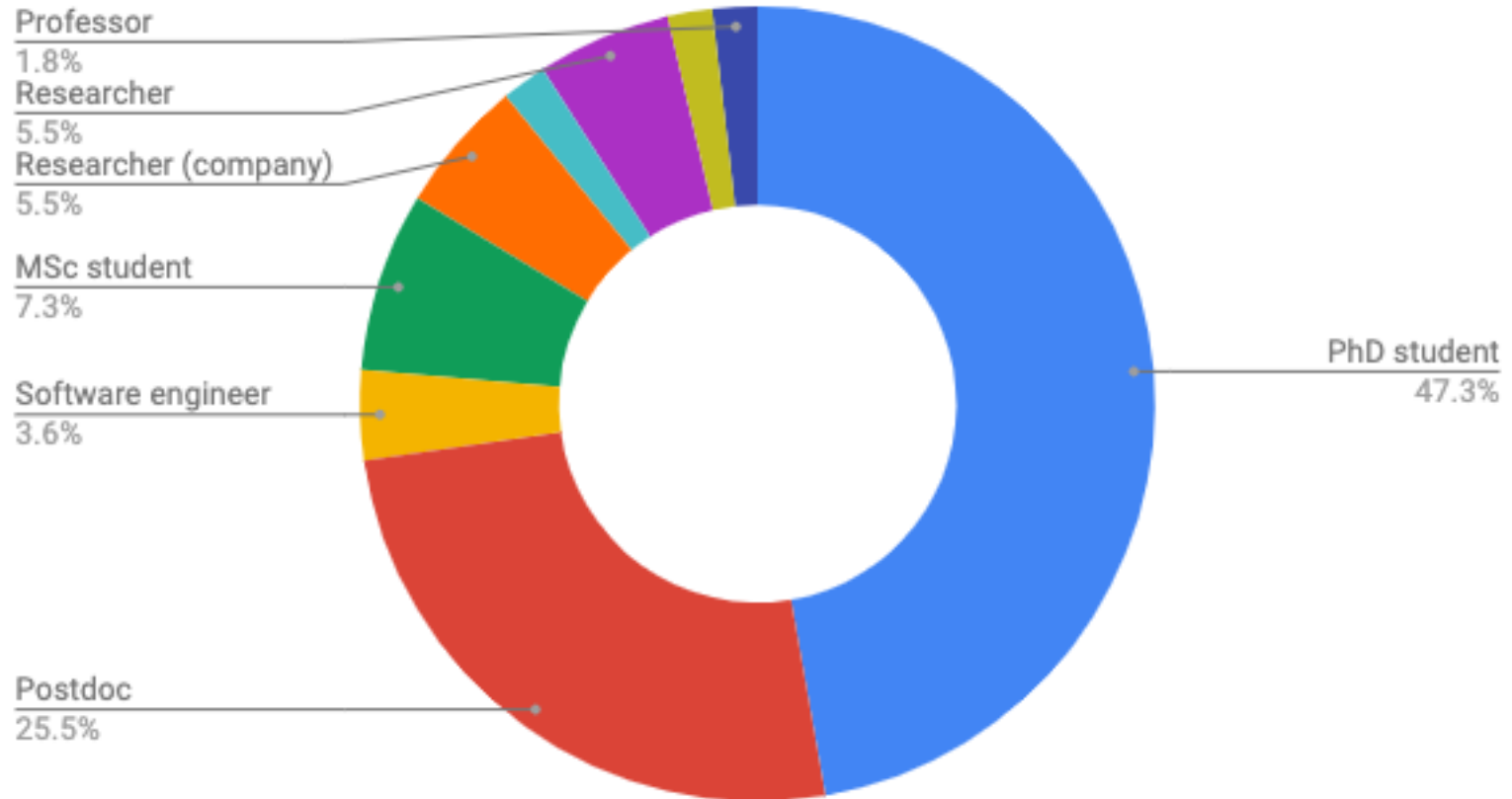
Nationalities



> 20 nationalities represented

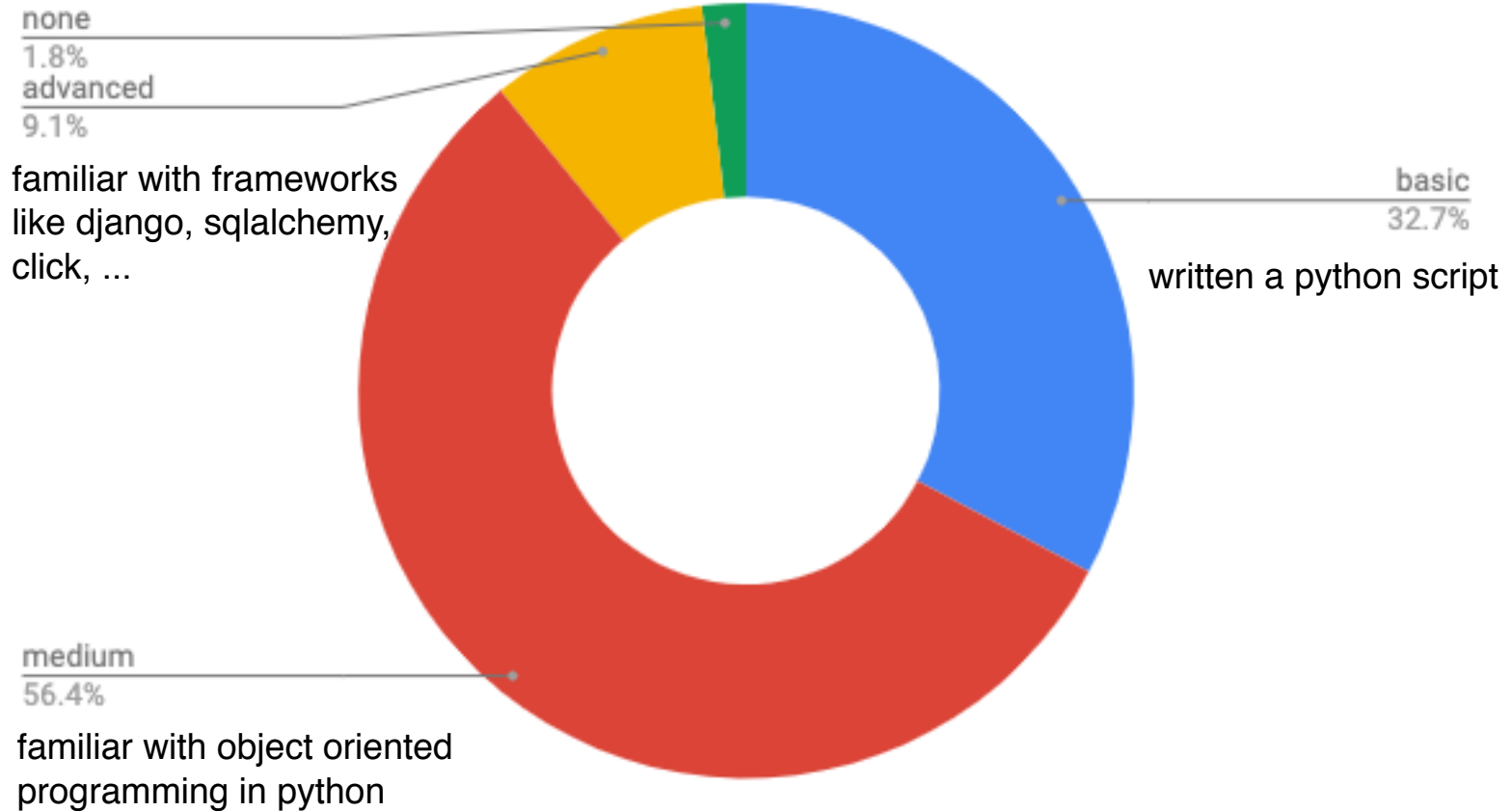
Participants - Current position

Current position



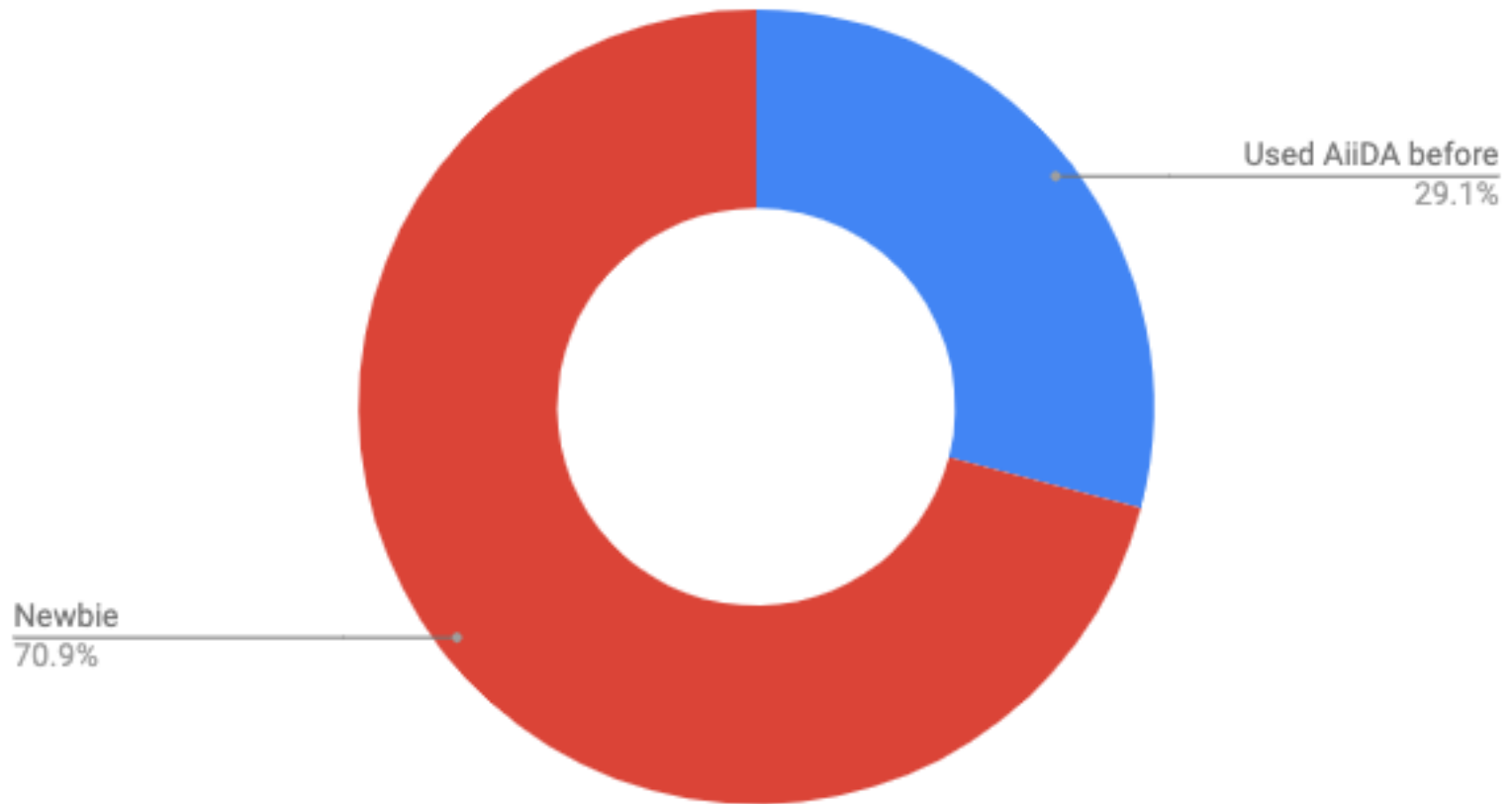
Participants - python proficiency

Level of python proficiency



Participants - AiiDA proficiency

AiiDA proficiency



Who has used AiiDA before?

The next 4 days

Tuesday

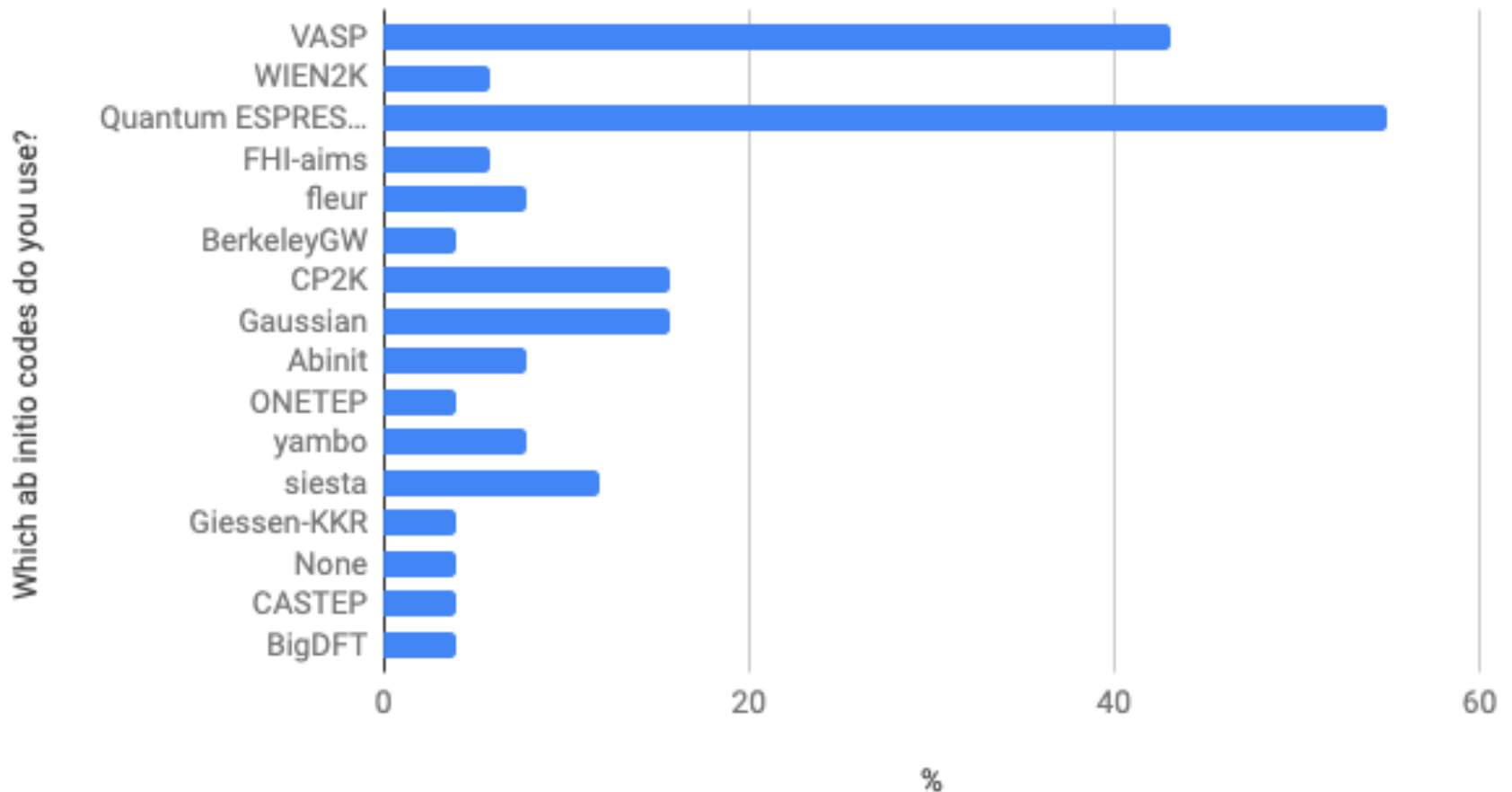
Introduction to aiida-core 1.0
(hands-on tutorial, using **virtual machine**)

Wednesday

Workflows in aiida-core 1.0
(hands-on tutorial, using **virtual machine**)

Participants - ab initio codes

Which ab initio codes do you use?



The next 4 days

Tuesday

Introduction to aiida-core 1.0
(hands-on tutorial, using **virtual machine**)

Wednesday

Workflows in aiida-core 1.0
(hands-on tutorial, using **virtual machine**)

Thursday

Workshop - Your projects

Group A: Write a workflow using existing plugins

Group B: Write a plugin for your code

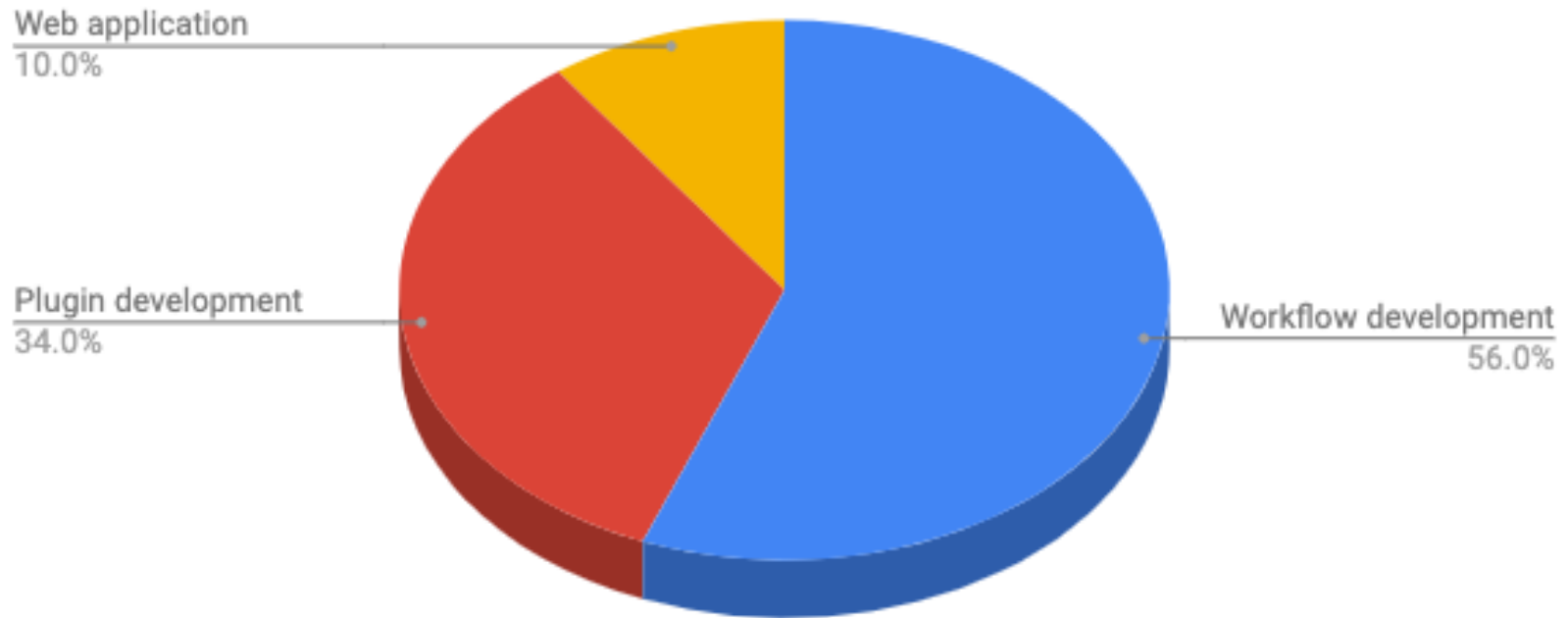
Group C: Wrap a workflow in a web application

Friday

(on your hardware, if you prefer)

Participants - Working groups

What would you like to focus on in the second half of the workshop?



Decide until Open Mic session Thursday

Tutorial Schedule

	Tue, 21 May	Wed, 22 May	Thu, 23 May	Fri, 24 May
09:00 - 09:30	Registration	Highlight talk M. Govoni (R)	AiiDA Q&A	
09:30 - 10:00	AiiDA intro (R)		Highlight talk F. Mohammed (R)	Highlight talk G. Petretto (R)
10:00 - 10:30		1. Getting set up	Highlight talk S. Cottenier	AiiDA lab (R)
10:30 - 11:00				
11:00 - 11:30	Coffee break	Group photo & Coffee break	Coffee break	Coffee break
11:30 - 12:00	2. verdi CLI	Workflows intro (R)	AiiDA plugins (R)	Feedback forms
12:00 - 12:30		6. Workflows	Open Mic round + split into groups	Group work
12:30 - 13:00	3. verdi shell			
13:00 - 14:30	Lunch	Lunch	Lunch	Closing remarks
14:30 - 15:00	4. Managing calculations	6. Workflows	Intros to topics of group work	
15:00 - 15:30			Group work & setting up AiiDA on your laptop	
15:30 - 16:00				
16:00 - 16:30				
16:30 - 17:00	Coffee break	Coffee break	Coffee break	
17:00 - 17:30	QueryBuilder intro	7. Band structure	Group work	
17:30 - 18:00	5. QueryBuilder + Appendices			
18:00 - 18:30		Error handling & real-life WorkChains (R)		
18:30 - 19:00	Problems during hands-on			
...				
Evening		Standing dinner, poster session	Social dinner, 7:30pm	

Tutorial Schedule

	Tue, 21 May	Wed, 22 May	Thu, 23 May	Fri, 24 May
09:00 - 09:30	Registration	Highlight talk M. Govoni (R)	AiiDA Q&A	
09:30 - 10:00	AiiDA intro (R)			talk to (R)
10:00 - 10:30				
10:30 - 11:00	1. Getting set up			Cloud
11:00 - 11:30	Coffee break			break
11:30 - 12:00	2. verdi CLI	Workflows intro (R)	AiiDA plugins (R)	Feedback forms
12:00 - 12:30		6. Workflows	Open Mic round + split into groups	Group work
12:30 - 13:00	3. verdi shell			
13:00 - 14:30	Lunch	Lunch	Lunch	Closing remarks
14:30 - 15:00			Intros to topics of group work	
15:00 - 15:30	4. Managing calculations	6. Workflows	Group work & setting up AiiDA on your laptop	
15:30 - 16:00				
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17:30 - 18:00	5. QueryBuilder + Appendices		Group work	
18:00 - 18:30		Error handling & real-life WorkChains (R)		
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...				
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**Split up 50/50: COVIZ2
(MED 2 1124)**

Tutorial Schedule

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10:00 - 10:30			AiiDA lab (R)	Materials Cloud
10:30 - 11:00	1. Getting set up			
11:00 - 11:30	Coffee break	Group photo & Coffee break	Coffee break	Coffee break
11:30 - 12:00	2. verdi CLI	Workflows intro (R)	AiiDA plugins (R)	Feedback forms
12:00 - 12:30	3. verdi shell	6. Workflows	Open Mic round + split into groups	Group work
12:30 - 13:00				
13:00 - 14:30	Lunch	Lunch	Lunch	Closing remarks
14:30 - 15:00	4. Managing calculations	6. Workflows	Intros to topics of group work	
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16:00 - 16:30				
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11:00 - 11:30	Coffee break	Group photo & Coffee break	Coffee break	Coffee break
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12:30 - 13:00				
13:00 - 14:30	Lunch	Lunch	Lunch	Closing remarks
14:30 - 15:00	4. Materials calculation		Intros to topics work	
15:00 - 15:30			work	
15:30 - 16:00			work + AiiDA laptop	
16:00 - 16:30				
16:30 - 17:00	Coffee break	Coffee break	Coffee break	
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see map in booklet
+ EPFL Campus app

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14:30 - 15:00	4. QueryBuilder + Appendices	7. Band structure	Intros to topics	
15:00 - 15:30				
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in COVIZ2, broadcast to MED 2 1512

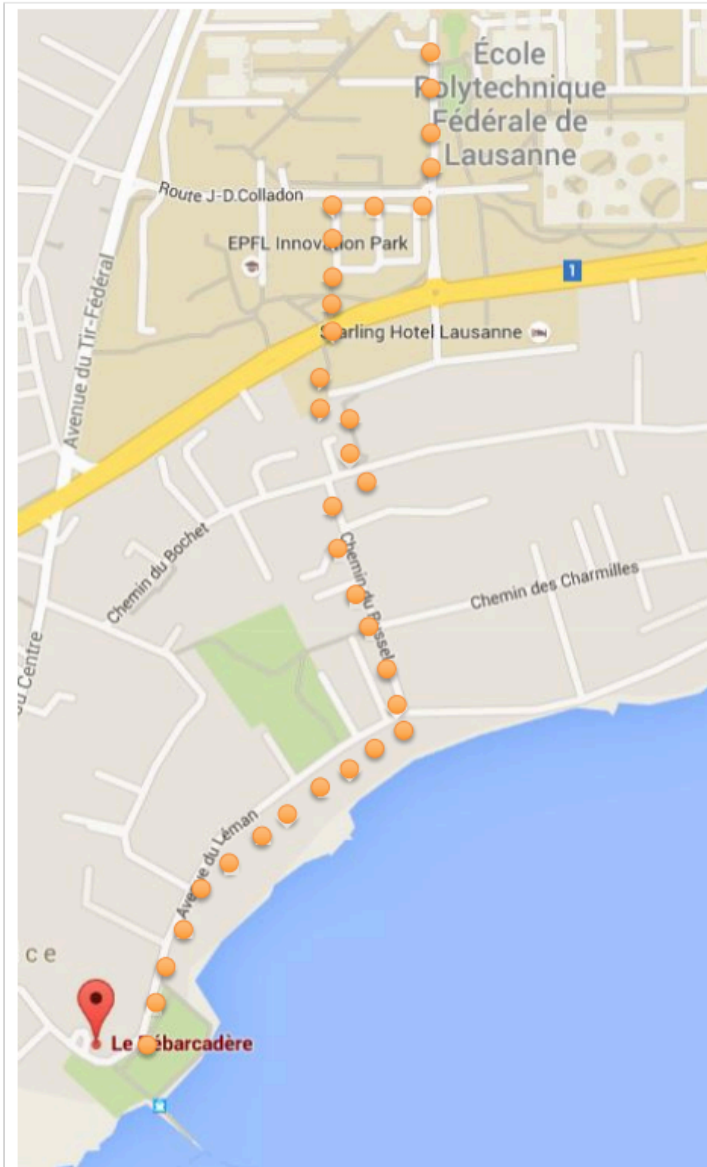
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11:00 - 11:30	Coffee break	Group photo & Coffee break	Coffee break	Coffee break
11:30 - 12:00	2. verdi CLI	Work	downstairs, MED 0 1418	
12:00 - 12:30				
12:30 - 13:00	3. verdi shell	6.		
13:00 - 14:30	Lunch	Lunch	Lunch	Closing remarks
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15:30 - 16:00				
16:00 - 16:30				
16:30 - 17:00	Coffee break	Coffee break	Coffee break	
17:00 - 17:30	downstairs in the hall put posters tomorrow or this evening			
17:30 - 18:00				
18:00 - 18:30				
18:30 - 19:00				
...				
Evening		Standing dinner, poster session	Social dinner, 7:30pm	

Tutorial Schedule



22 May	Thu, 23 May	Fri, 24 May
light talk ovoni (R)	AiiDA Q&A	
light talk tottenier	Highlight talk F. Mohammed (R)	Highlight talk G. Petretto (R)
photo & ee break	AiiDA lab (R)	Materials Cloud
ws intro (R)	Coffee break	Coffee break
workflows	AiiDA plugins (R)	Feedback forms
	Open Mic round + split into groups	Group work
lunch	Lunch	Closing remarks
workflows	Intros to topics of group work	
	Group work & setting up AiiDA	
ee l		
d s		
ha		
real		
Chains (R)		
ng dinner, r session	Social dinner, 7:30pm	

Le Débarcadère
15 minutes walk
Free food & drinks!

Tutorial Team

Organising Committee

- Leopold Talirz
- Sebastiaan Huber
- Andrea Ferretti
- Espen Flage-Larsen
- Alberto Garcia

Support

- Admin: Cornelia Buenjita
- Video: Marco Borelli
- Materials: Snehal Kumbhar, Elsa Passaro

Tutors

- Giovanni Pizzi
- Sebastiaan Huber
- Leopold Talirz
- Aliaksandr Yakutovich
- Casper Andersen
- Oscar Arbeláez
- Daniele Tomerini

Tutorial Team

Organising Committee

- Leopold Talirz
- Sebastiaan Huber
- Andrea Ferretti
- Egon Elger
- A...

contact person for
accommodation reimbursements
cornelia.bujenita@epfl.ch

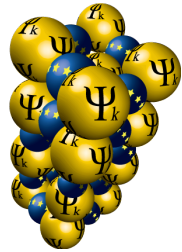
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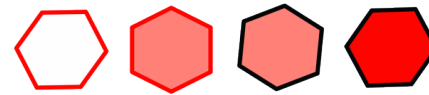
Tutors

- Giovanni Pizzi
- Sebastiaan Huber
- Leopold Talirz
- Aleksandr Yakutovich
- Sasper Andersen
- Oscar Arbeláez
- Daniele Tomerini

Sponsors



MARVEL



NATIONAL CENTRE OF COMPETENCE IN RESEARCH



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EPFL

Questions?



Go!

1. Check your email for **SSH key** to log into your virtual machine
2. Split 50/50: COVIZ2
3. Head to **aiida.net**

Go!

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Automated Interactive Infrastructure and Database for Computational Science

AiiDA is a flexible and scalable informatics' infrastructure to manage, preserve, and disseminate the simulations, data, and workflows of modern-day computational science. Able to store the full provenance of each object, and based on a tailored database built for efficient data mining of heterogeneous results, AiiDA gives the user the ability to interact seamlessly with any number of remote HPC resources and codes, thanks to its flexible plugin interface and workflow engine for the automation of complex sequences of simulations.

Journal ref: G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari, and B. Kozinsky, AiiDA: automated interactive infrastructure and database for computational science, *Comp. Mat. Sci.* 111, 218-230 (2016)

Open access link: [arXiv:1504.01116](https://arxiv.org/abs/1504.01116)

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TUTORIAL MATERIALS

aiida-core 1.0.0b3 (2019, EPFL, Switzerland)

aiida-core 0.12.2 (2019, University of Amsterdam, Netherlands)

aiida-core 1.0.0a1 (2018, Cineca, Italy)

aiida-core 0.11.4 (2018, EPFL, Switzerland)

aiida-core 0.9.0 (2017, EPFL, Switzerland)

aiida-core 0.7.1 (2017, ICTP, Italy)

aiida-core 0.6.0 (2016, EPFL, Switzerland)

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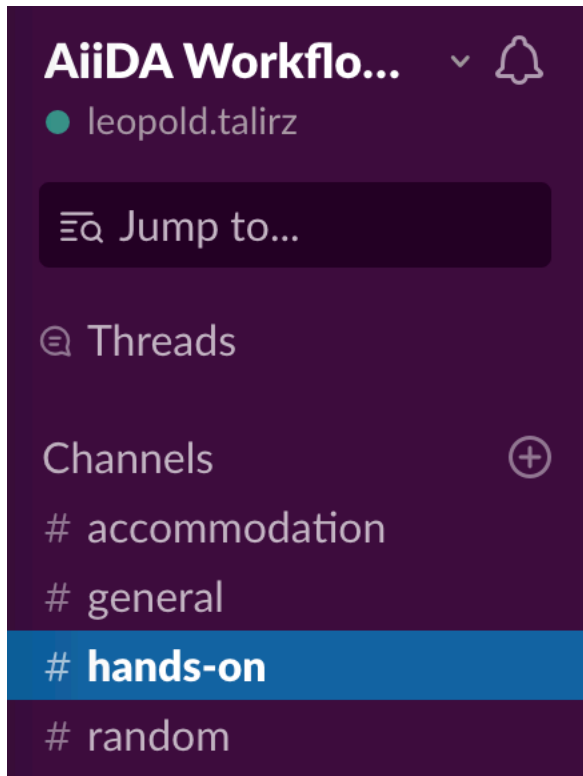
Get a GitHub account!
report issues, fix typos, ...
we love pull requests :-)

Tutorial materials

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aiida-tutorials.readthedocs.io

Final remarks



- Lectures marked with (R) are recorded
Oscar is taking pictures
- Let us know if you don't want to be filmed/photographed
- We'll be using the
#hands-on channel in slack
bit.ly/aiida-workflows2019-slack

