

# AiiDA Hackathon: developing code plugins and robust scientific workflows

@Cineca, Casalecchio di Reno (BO) 17 Feb - 21 Feb 2020

## AGENDA

|    | Monday | Tuesday                                                                                                        | Wednesday                                                                        | Thursday                                                                                | Friday          |                    |             |
|----|--------|----------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|-----------------|--------------------|-------------|
| 9  |        | Calculation and Workchain design (Sebastian Huber)                                                             | Containerization of codes and integration in AiiDA (Luigi Genovese)              | Plugin design, maintenance and distribution (Leopold Talirz)                            | Work Session    | 9                  |             |
| 10 |        | Workchain ideas best practices (Aliaksandr Yakutovich)                                                         | <b>Follow-up Discussion:</b> Containerization of codes and integration in AiiDA. | <b>Follow-up Discussion:</b> Standard guidelines for plugin package design/maintenance. |                 | 10                 |             |
| 11 |        | Coffee Break                                                                                                   | Coffee Break                                                                     | Coffee Break                                                                            |                 | Coffee Break       | 11          |
| 12 |        | <b>Follow-up Discussion:</b> Turn-key solution common interfaces: SCF, Relax and Band structure.               | Unit & Integration tests (Giovanni Pizzi et al.)                                 | Work Session                                                                            | General Wrap up | 12                 |             |
| 13 |        | Lunch Break                                                                                                    | Lunch Break                                                                      |                                                                                         |                 | Lunch Break        | Lunch Break |
| 14 |        | Work Session                                                                                                   | Work Session                                                                     | Work Session                                                                            |                 | 14                 |             |
| 15 |        | Introduction & Week Overview<br>Overview of AiiDA 1.0 (Sebastian Huber)                                        | Coffee Break                                                                     | Coffee Break                                                                            |                 | Coffee Break       | 15          |
| 16 |        | Coffee Break                                                                                                   | Work Session                                                                     | Work Session                                                                            |                 | Work Session       | 16          |
| 17 |        | <b>Preparations:</b> Setting up computers, develop environment, inventory of extra topics for discussion, etc. | Wrap up Discussion                                                               | Wrap up Discussion                                                                      |                 | Wrap up Discussion | 17          |
| 18 |        |                                                                                                                |                                                                                  |                                                                                         |                 |                    | 18          |
| 19 |        |                                                                                                                |                                                                                  |                                                                                         |                 |                    | 19          |

|                 |
|-----------------|
| Presentations   |
| Discussions     |
| Breaks          |
| Work (8 x 1.5h) |

SOCIAL DINNER (Cantina Bentivoglio, BO)