SKAO Open Science School

Building reproducible Scientific Software with Open Source Package Managers and Containerisation tools

Manuel Parra-Royón
Instituto de Astrofísica de Andalucía
IAA-CSIC

Contents of this workshop

- 1. Software reproducibility and distribution: challenges.
- 2. Overview of package managers and containers for scientific software
- 3. Using package managers to install and manage software dependencies
- 4. Working with software containerisation
- 5. Best practices for creating and sharing container images and python environments for scientific software

Resources

- Workshop material: https://github.com/spsrc/SKA-Open-Science-School/

- Software requirements:
  - Python virtual environments
    https://packaging.python.org/en/latest/guides/installing-using-pip-and-virtual-environments/
  - Conda/Miniconda
    https://docs.conda.io/projects/conda/en/latest/user-guide/install/linux.html
  - Docker
    https://docs.docker.com/engine/install/
  - Singularity
    https://docs.sylabs.io/guides/3.0/user-guide/installation.html

Extra material

- SKA Regional Centre Training on Containerisation

  https://gitlab.com/ska-telescope/src/ska-src-training-containers
  https://ska-telescope.gitlab.io/src/ska-src-training-containers/

- Reproducibility course - CSIC

  https://github.com/spsrc/reproducibility-course

- SPSRC Droplets

  https://github.com/spsrc/droplets/tree/master/sessions

Let's get to work!

https://github.com/spsrc/SKA-Open-Science-School/