The HCG-16 study

IAA-CSIC

S. Luna, M. Jones, S. Sánchez Expósito, J. Román, J. Garrido, L. Verdes-Montenegro

E-OSSR Onboarding Presentation

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Introduction

- Partner: IAA-CSIC

- Science case: *Evolution of compact groups from intermediate to final stages; A case study of the HI content of HCG 16 (DOI)*

- Heads up: The speaker is a sysadmin helping out astronomers to write a reproducible workflow.

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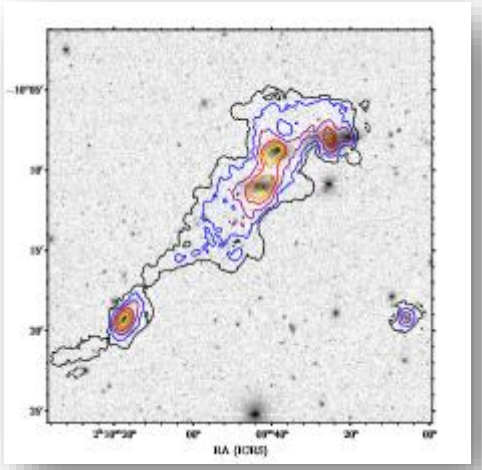
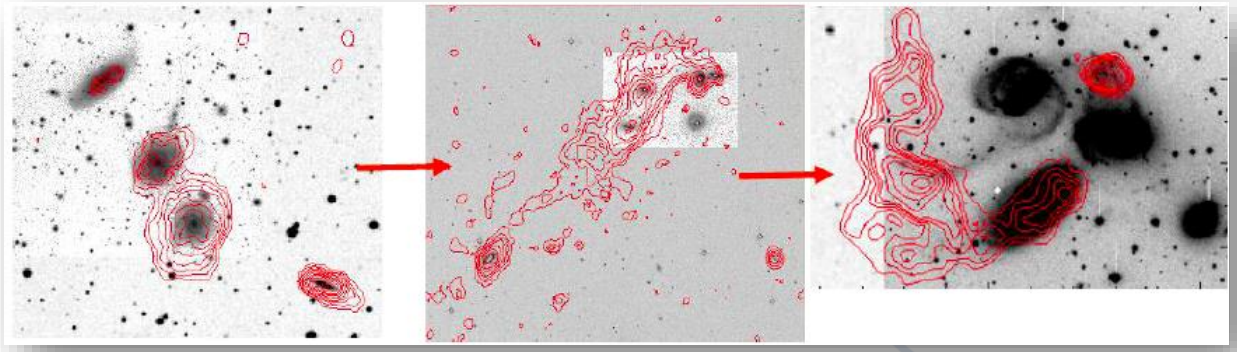
Introduction

- Atomic Gas (HI)
  - HI atoms produce radio emission (1420 MHz)
  - Tracer of galaxy formation and evolution
- Hickson Compact Groups (HCGs):
  - Groups with 4 or more galaxies
  - Nearby galaxies
  - Isolated group
  - There are 100 HCGs, this work focuses on HCG-16



HCG-16
M. Jones et al. 2019



1. HI in galaxies 2. HI in IGM 3. HI out of galaxies

Evolutionary sequence suggested by Verdes-Montenegro et al. 2001

AMIGA

http://amiga.iaa.es

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Introduction

- HI analyses to study galaxy formation and evolution is of interest for the SKA community
  - SKA HI Science Working Group

- No SKA data yet… so:
  - VLA: Very Large Array
  - Radio interferometer
  - 27 dishes, 25m diameter

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Introduction

- Software: pipeline to reproduce the HCG-16 study
- Purpose: enable end-to-end reproducibility, from initial data to plots in the paper. We open up the whole workflow so researchers should be able to:
  - Understand what was done to the data
  - Verify the analysis
  - Reuse data and code
- Use case: From a researcher's point of view, "can I use the ESCAPE ecosystem to share my analysis with a colleague or a referee?"
- Workflow: https://github.com/AMIGA-IAA/hcg-16

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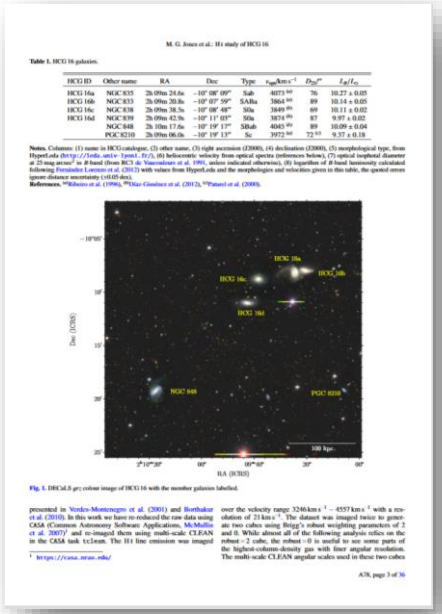
Introduction

- Most figures in the paper can be fully reproduced with a Jupyter notebook [provided in GitHub]



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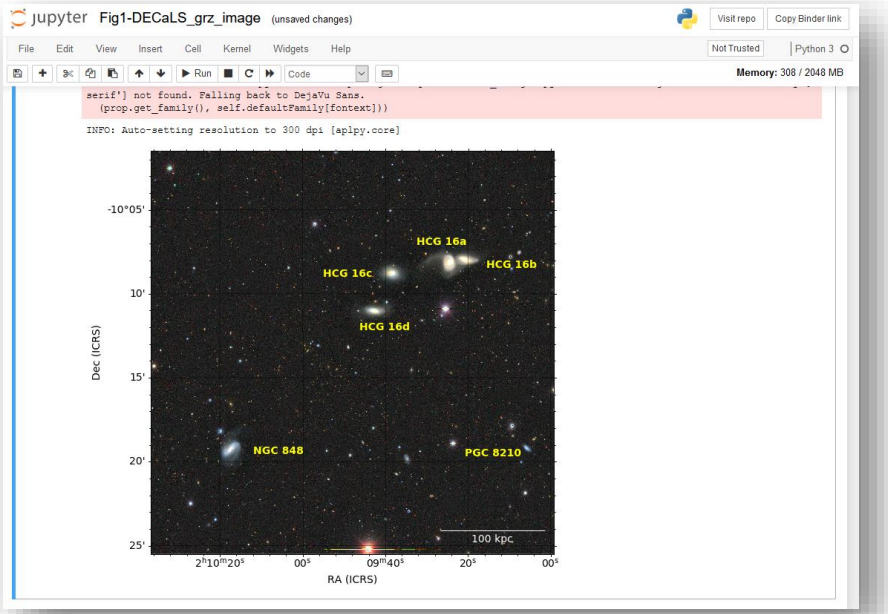

Interactive notebook on [mybinder]

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Introduction

- Workflow:
  - First download and install runtime dependencies
    - Note: the exception is docker, which is expected to be already available on the target computer
    - Runtime dependencies are provided in a conda environment
  - Download source code for the analysis and input data.
    - Code from GitHub
    - Data from EUDAT's B2SHARE service
  - Run the pipeline
    1. Flagging and calibration with CASA (docker container)
    2. Imaging with CASA (docker container)
    3. Masking with SoFiA (docker container)
    4. Plotting with Jupyter Notebooks (conda environment)

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Software/Service Development

- Software Development Lifecycle Strategies
  - GitHub: git brach/pull request/merge
  - Pin dependencies. Use conda first, docker as last resort.
- Development:
  - Coding style: write understandable code for your future self
  - Versioning: released version 1.0.0 for publication, then point releases for solving issues (e.g. docker's change of ToS)
  - Maintenance: only when necessary to preserve functionality
  - Documentation: comprehensive README file provided
  - Software quality standards: no formal approach
- Testing and efficiency optimization strategies
  - None

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Software/Service Development

- Information on how to run the software
  - Step-by-step guide on the repository's README file
- software licenses
  - MIT license
- General guidelines that are followed
  - Document as much as possible to help others reuse it
  - Automate every possible step
  - Streamline deployment to enhance portability between systems

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Software/Service Requirements

- Operating System, compilation environment
  - It has been tested on Ubuntu 18.04
  - In theory you just need bash and docker pre-installed
  - Everything else installs automatically with conda
- Hardware requirements
  - Minimum of 10GB disk space on the working directory
  - Recommended minimum of 2 CPU cores, 2GB RAM
- Containerisation and portability requirements
  - Password-less “sudo docker” is a pre-requisite
- Workflow / interface requirements to other software/services
  - Internet access: docker hub, conda packages, input data

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OSSR Integration

- What is available?
  - Code, data, scientific publication
  - https://github.com/AMIGA-IAA/hcg-16
- What will be onboarded (source code, container, test workflow incl. data)?
  - Code, data
- Are there open points and requirements?
  - From the OSSR integration point of view, we don't know

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OSSR Integration

- What is the ”user story” of a EOSC user taking on the software/service?
  - From the data side (what data can be analysed and how)
    - All the data and the code are publicly available, so as long as the installation works, the analysis workflow should be fully reproducible.
  - From the OSSR side (how to find data and easy use demos, tutorials, documentation, …)
    - Our aim is to provide a self-explanatory README, with steps to reproduce the workflow, and links to everything: code, data and scientific publication.

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Time for a short demo (~10 min)

- Show how the software is used and what is the outcome
  - Let's go to the README (showcase mybinder link)
- What should and can a EOSC user do with the software?
  - Understand what was done to the data
  - Verify the analysis
  - Reuse data and code

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Open Points and Discussion Time

- Which of your questions have not been covered so far?
- What do you want to discuss?
  - Our main goal here is to check whether end-to-end reproducibility is feasible, and how much is the effort
    - What are the blockers?
      - Overhead associated when trying to achieve reproducibility
      - The original data could not be downloaded automatically so we had to re-host it on the EUDAT's B2SHARE service
      - SlicerAstro: interactive tool whose commands could not be scripted in the pipeline
      - IDL: proprietary software hinders Open Science. Hopefully for this specific case we are looking into the alternative, open source GDL

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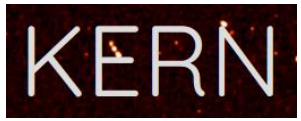
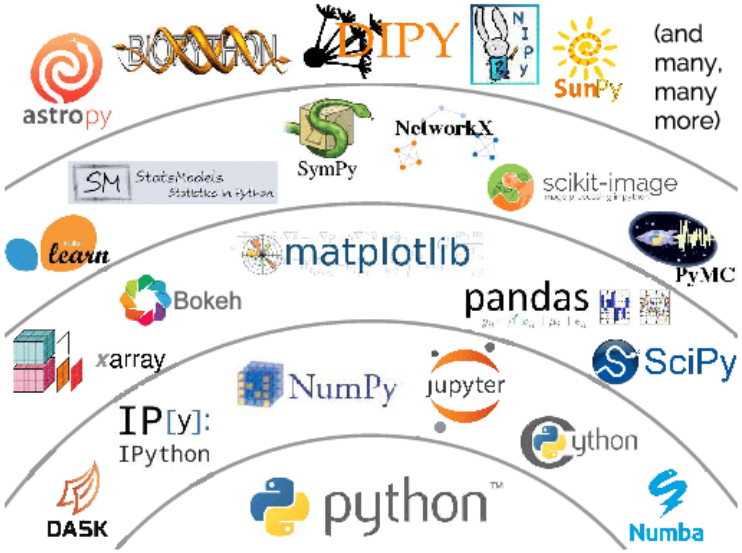
Open Points and Discussion Time

- This work would have not been possible without:





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