iBridges and Snakemake

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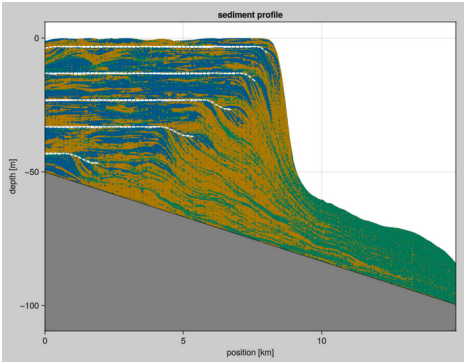
June 18, 2025

Mind the Gap

- Geoscience project with group of Emilia Jarochowska
- With my colleague Christine Staiger
- Simulation of sediment curves



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“How do we...?”

- Manage multiple programming languages (R, Julia)?
- Manage all the computation steps
- Store data on YoDa/iRODS system?
- Keep track of our data?
- Deal with metadata?
- Parallelization?
- Onboard people (students)?

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What is Snakemake?

- Workflow framework based on Python
  - 14 citations/week, 1.2M downloads
- Command line based
- Similar to make: Snakefile
  - input file
  - output file
  - shell commands
- Abstracted access to compute (SLURM, multicore, etc.)
- Abstracted access to storage (local, S3, iRODS)

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Snakemake demonstration

iBridges storage plugin

- Already existing iRODS plugin based on PRC.
- `> pip install snakemake-storage-plugin-irods`
- Why use iBridges?
  - Integrate with ibridges CLI/GUI
  - Simplify the plugin and its maintenance
- New features:
  - Add support for wildcards (`irods://zone/user/{sample}.csv`)
  - Add support for metadata (`irods://zone/user/data.csv.metadata.json`)
- `https://github.com/qubixes/snakemake-storage-plugin-irods/tree/switch-to-ibridges`
- Proposal to merge in the future

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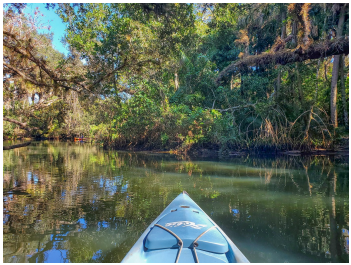
Snakemake iRODS demonstration

Conclusion

- Created iBridges plugins for
  - Galaxy
  - Snakemake
- Galaxy and Snakemake can make researchers' workflows easier
  - Reproducibility
  - Parallelization
  - Data ← YoDa/iRODS
- Now, researchers do not need to understand iCommands/PRC/iBridges



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