Community Hydrological Modelling Workflows

Online Training Session with Federal, Provincial, Territorial, and International Partners

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February 18th, 2025

Acknowledgements

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GLOBAL WATER FUTURES

Environment and Climate Change Canada

Environnement et Changement climatique Canada

Digital Research Alliance of Canada | **Alliance de recherche numérique** du Canada

Outline

- Community Hydrological Modelling Recipes
- Computational Resources for the Training Session
- Setting up ECCC's National Water Model—MESH
- Introduction and Preview of CONFLUENCE

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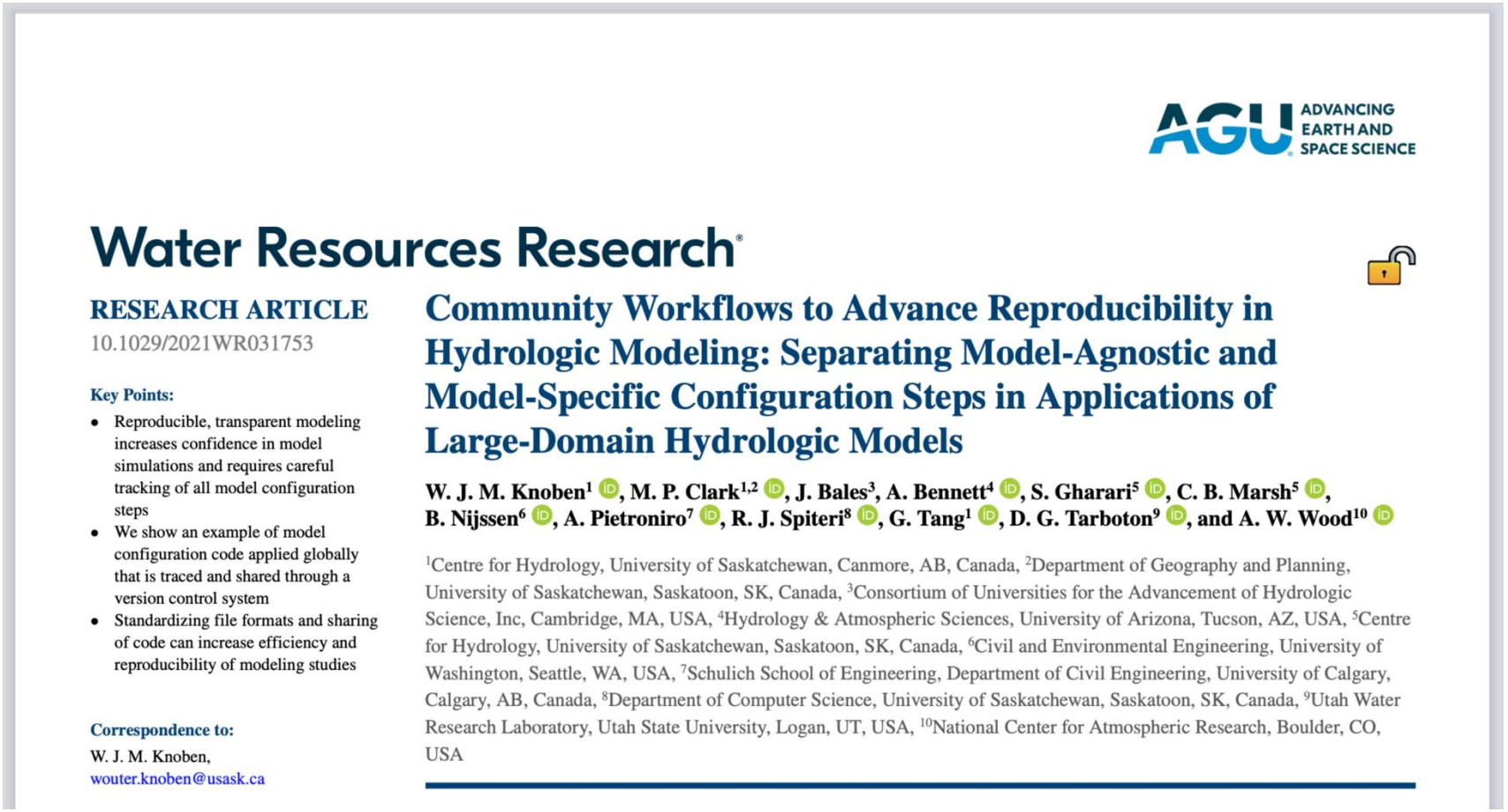
Recipe for Community Hydrological Modelling



AGU ADVANCING EARTH AND SPACE SCIENCE

Water Resources Research

RESEARCH ARTICLE

10.1029/2021WR031753

Key Points:

- Reproducible, transparent modeling increases confidence in model simulations and requires careful tracking of all model configuration steps
- We show an example of model configuration code applied globally that is traced and shared through a version control system
- Standardizing file formats and sharing of code can increase efficiency and reproducibility of modeling studies

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Community Workflows to Advance Reproducibility in Hydrologic Modeling: Separating Model-Agnostic and Model-Specific Configuration Steps in Applications of Large-Domain Hydrologic Models

W. J. M. Knoben[1], M. P. Clark[1,2], J. Bales[3], A. Bennett[4], S. Gharari[5], C. B. Marsh[5], B. Nijssen[6], A. Pietroniro[7], R. J. Spiteri[8], G. Tang[1], D. G. Tarboton[9], and A. W. Wood[10]

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Knoben, W. J. M., Clark, M. P., Bales, J., Bennett, A., Gharari, S., Marsh, C. B., Nijssen, B., Pietroniro, A., Spiteri, R. J., Tang, G., Tarboton D. G. & Wood, A. W. (2022). Community Workflows to Advance Reproducibility in Hydrologic Modeling: Separating Model-Agnostic and Model-Specific Configuration Steps in Applications of Large-Domain Hydrologic Models. *Water Resources Research*, *58*(11), e2021WR031753.

- Community Workflows to Advance Reproducibility in Hydrologic Modeling (CWARHM)
- Developing first generation of community hydrological modelling workflows
- Keeping workflows open source and reproducible
- Keeping workflows efficient for real-world applications
- Separating model-agnostic and model-specific configuration parts

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Recipe for Community Hydrological Modelling

manuscript submitted to *Water Resources Research*

Streamlining hydrological model applications by enhancing extensible model-agnostic and model-specific configuration engines

Kasra Keshavarz[1]*, Alain Pietroniro[1], Darri Eythorsson[1], Mohamed Ismaiel Ahmed[1], Paul Coderre[1], Wouter Knoben[1], Shervan Gharari[1], Martyn Clark[1]

[1]Department of Civil Engineering, Schulich School of Engineering, University of Calgary, Calgary, AB T2N 1N4, Canada

Key Points:

- A generalized model-agnostic framework is proposed to streamline configurations of process-based hydrological models
- The framework advances reproducibility in hydrological modelling by addressing complexities involved in handling dynamic and static datasets
- Prototype applications in a high-performance computing environment demonstrate the effectiveness of the framework in reducing setup time

Submitted to Water Resources Research, under review

- Enhancing and proposing model-agnostic and model-specific engines for HPC environments
- Modularized methodology for the model-agnostic step for various data types and preprocessing needs
- Expanding model-specific workflows for other community modelling systems including ECCC MESH and SMHI HYPE
- Proposing strategies to objectively orchestrate the configuration stage of hydrological models

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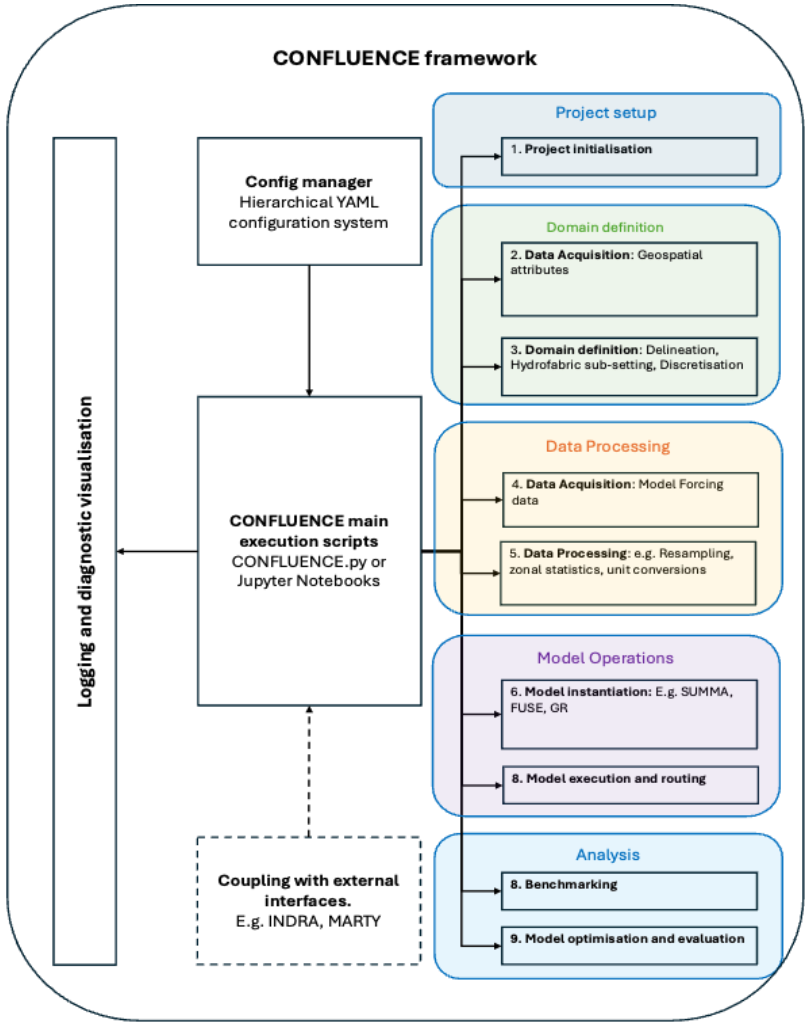
Recipe for Community Hydrological Modelling



CONFLUENCE Workflow (Eythorsson et al., In prep.)

Extended workflow to seamlessly include:

- Domain definition
- Model execution
- Model evaluation and optimization
- Benchmarking
- Visualization and reporting

Design principles:

- Modularized methodology for extendibility and interoperability
- Isolation of model decisions in a central configuration system
- Facilitating machine operability for computational exploration and optimization

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Computational Resources

- Wikipedia (accessed February 13th, 2025)
  "High-performance computing (HPC) is the use of supercomputers and computer clusters to solve advanced computation problems."

- The idea is to expand computational performance horizontally (multiple CPUs), instead of vertically (one massive CPU)

- High Performance Computing (HPC) systems are comprised of various "nodes"

- HPC nodes are located inside rack enclosures

https://top500.org/

Computational Resources

Our recommendation is to connect to HPCs using either of the following methods:

jupyterlab

- Multi-user environment
- Resource efficient
- Collaborative environment
- Reproducibility mechanisms
- Strong community support
- Ease of use

Terminal

```
$ ssh USERNAME@HPC_URL
```

- Maximal flexibility
- Remote Access
- Steep learning curve
- Full control of command sessions
- Strong community support

MobaXTerm PuTTY MacOS Terminal

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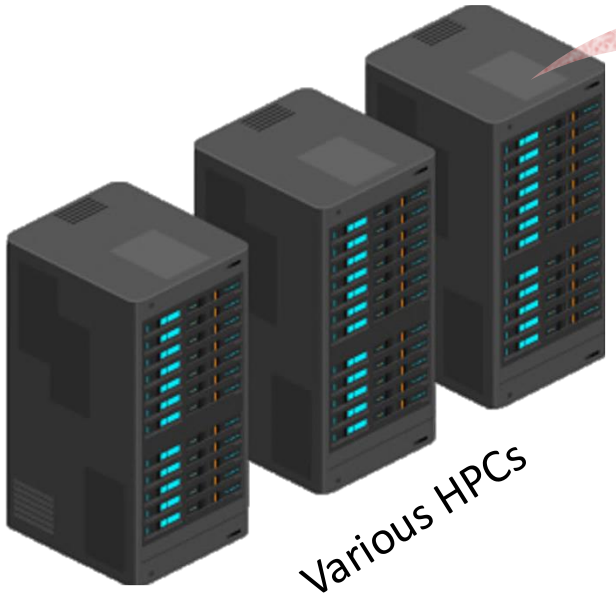
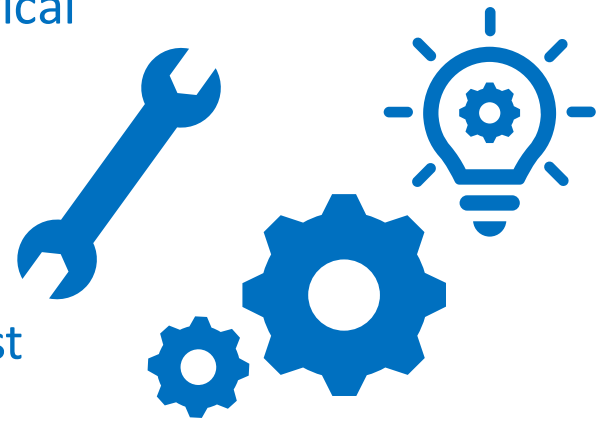
Computational Resources



Various HPCs

Suite of tools to facilitate hydrological modelling and data processing:

- Generalizing approaches applicable to data processing applications
- Using stable tools to assure robust performance on HPC platforms



HPC Tailored

Visualize

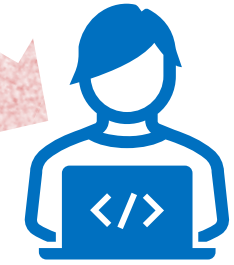
Regrid

Subset

Temporal Disaggregate

Remap

Science and Policy Decisions



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Computational Resources

How can we launch a Jupyter session on HPCs? A few examples…

Anvil at Perdue University

OPEN OnDemand

Digital Research Alliance of Canada | Alliance de recherche numérique du Canada

Fir at Simon Fraser University

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ARC at the University of Calgary

OPEN OnDemand

Computational Resources

Since not everybody has access to an HPC, we need to separate into two groups:

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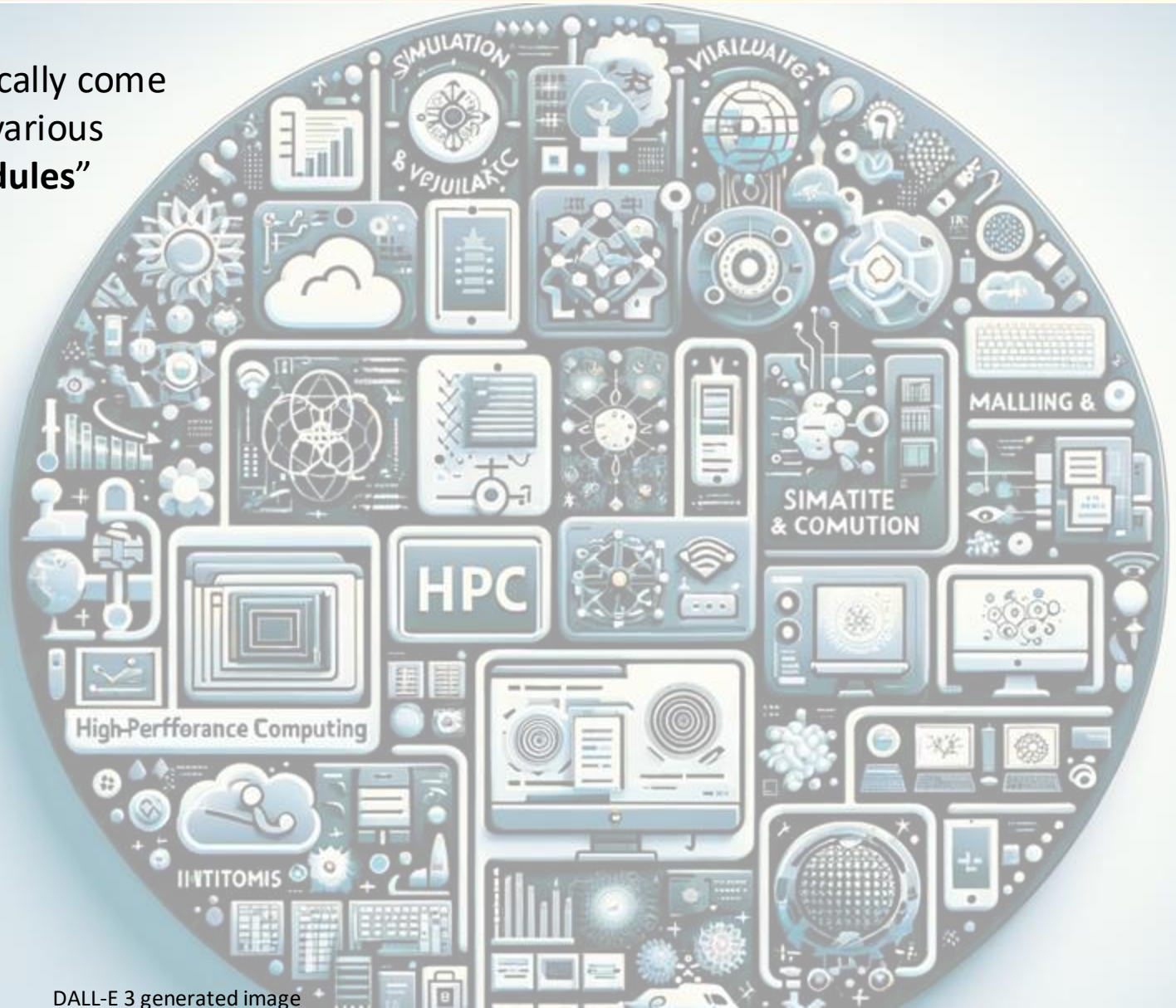
ARC at the University of Calgary

OPEN OnDemand

binder

Computational Resources

HPCs typically come with various "**modules**"



DALL-E 3 generated image

Flexibility

Different users have different requirements

Customization

Users may need specific versions of software or libraries

Optimization

software packages are often optimized for the underlying hardware architecture

Productivity

Having commonly used software readily available, saves users time and effort

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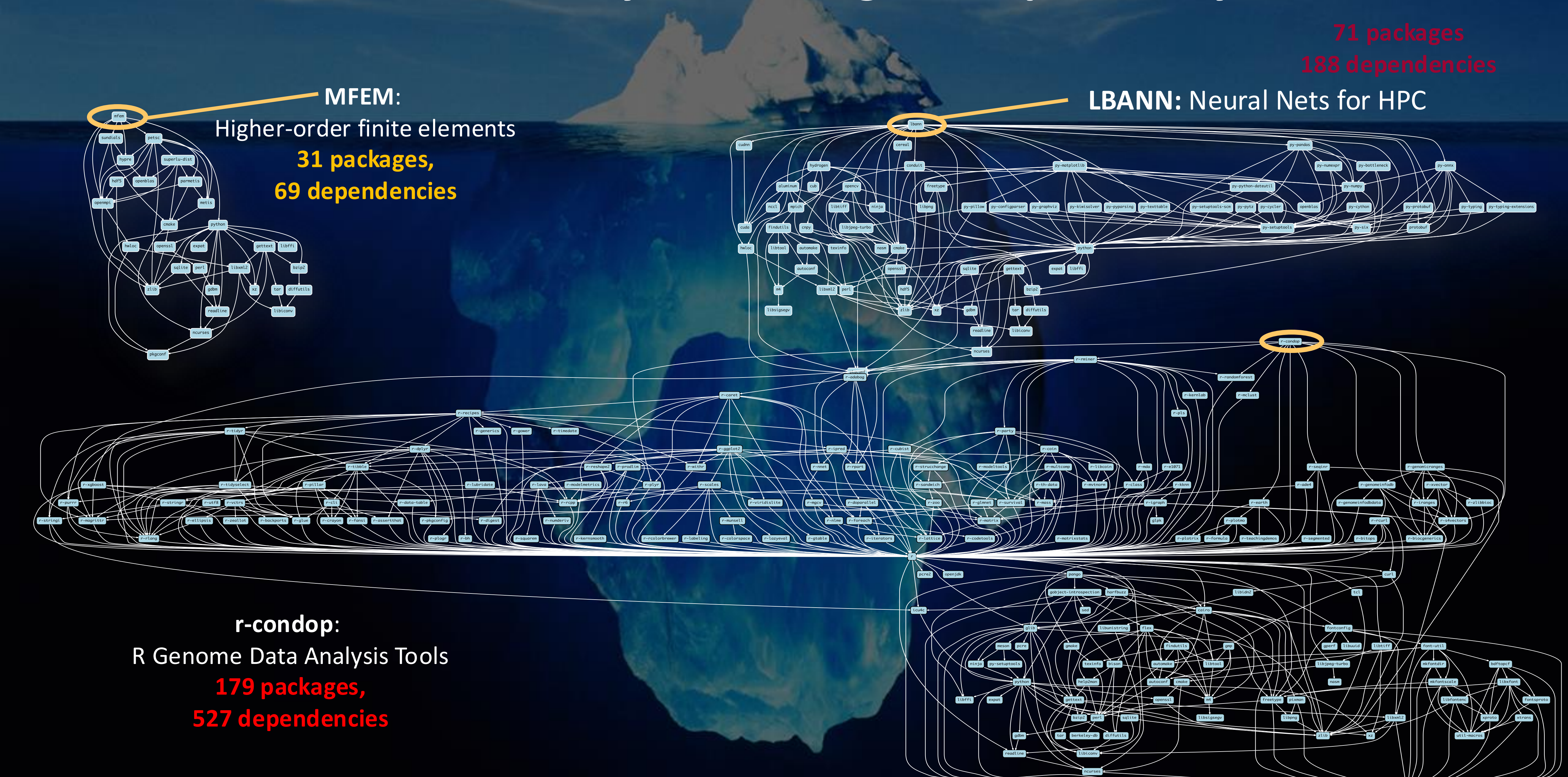
Modern scientific codes rely on icebergs of dependency libraries

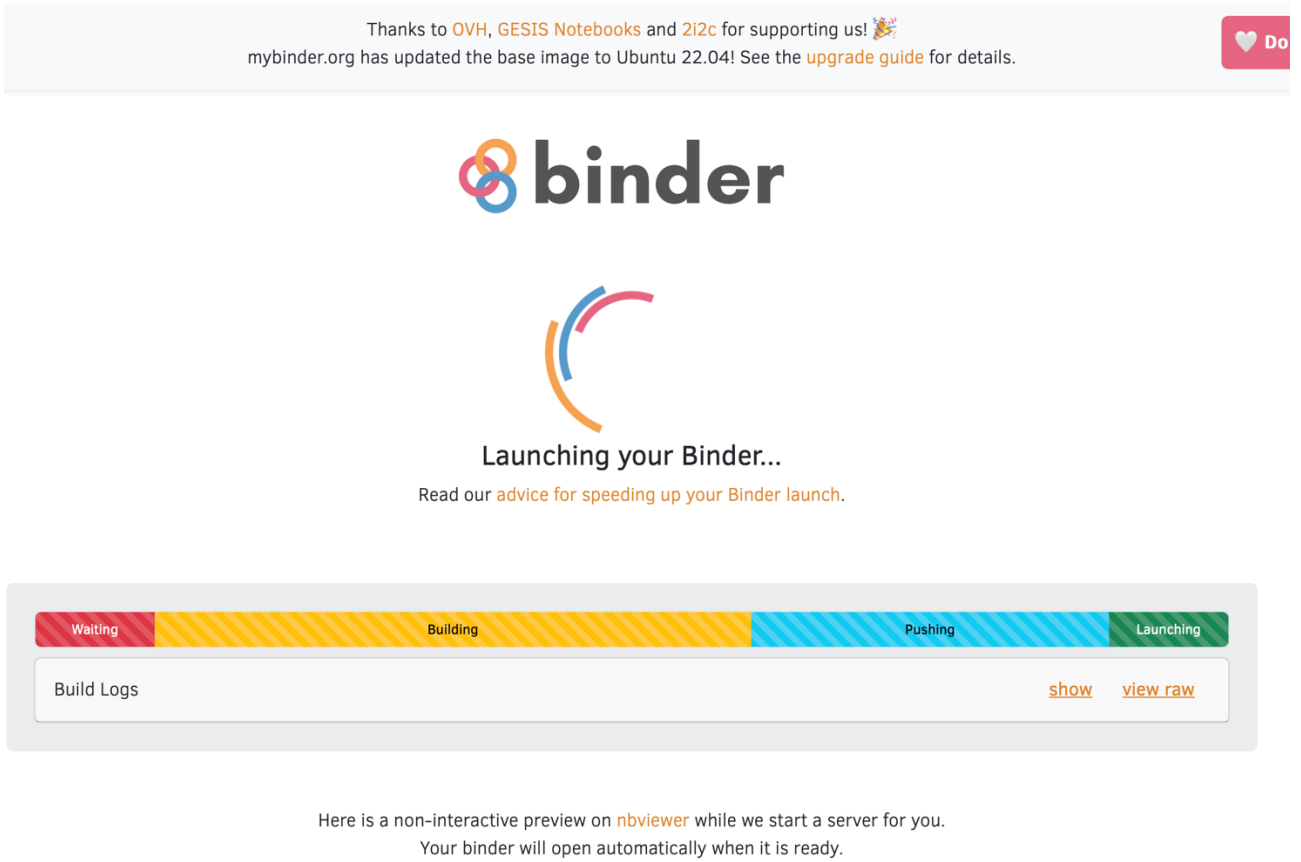


Slide is obtained from Spack's presentation titled: "Spack: Package Management for HPC." ATPESC 2024 Software Track. Todd Gamblin.

Any questions so far?

Computational Resources

binder



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Computational Resources

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ARC at the University of Calgary

OPEN OnDemand

Welcome to ARC OnDemand

Pinned Apps A featured subset of all available apps

Interactive Apps

Desktop (Container)
System Installed App

Jupyter Notebook
System Installed App

Jupyter Notebook (Container)
System Installed App

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Computational Resources

jupyter

DALL-E 3 generated image

General tips:

- Understand your setup: Be resourceful—Asking too much computational resource can keep you in the queue forever
- Choose the Right Kernel: Be mindful—Jupyter provides you with all sort of programming environments; make sure to choose the right (customized) programming kernel for your work.
- Monitor Performance and Document: Be diligent—As you work more with the environment, you get to know the requirements of your computations. Keep track of your workflow's performance and document your work.

DALL-E 3 generated image

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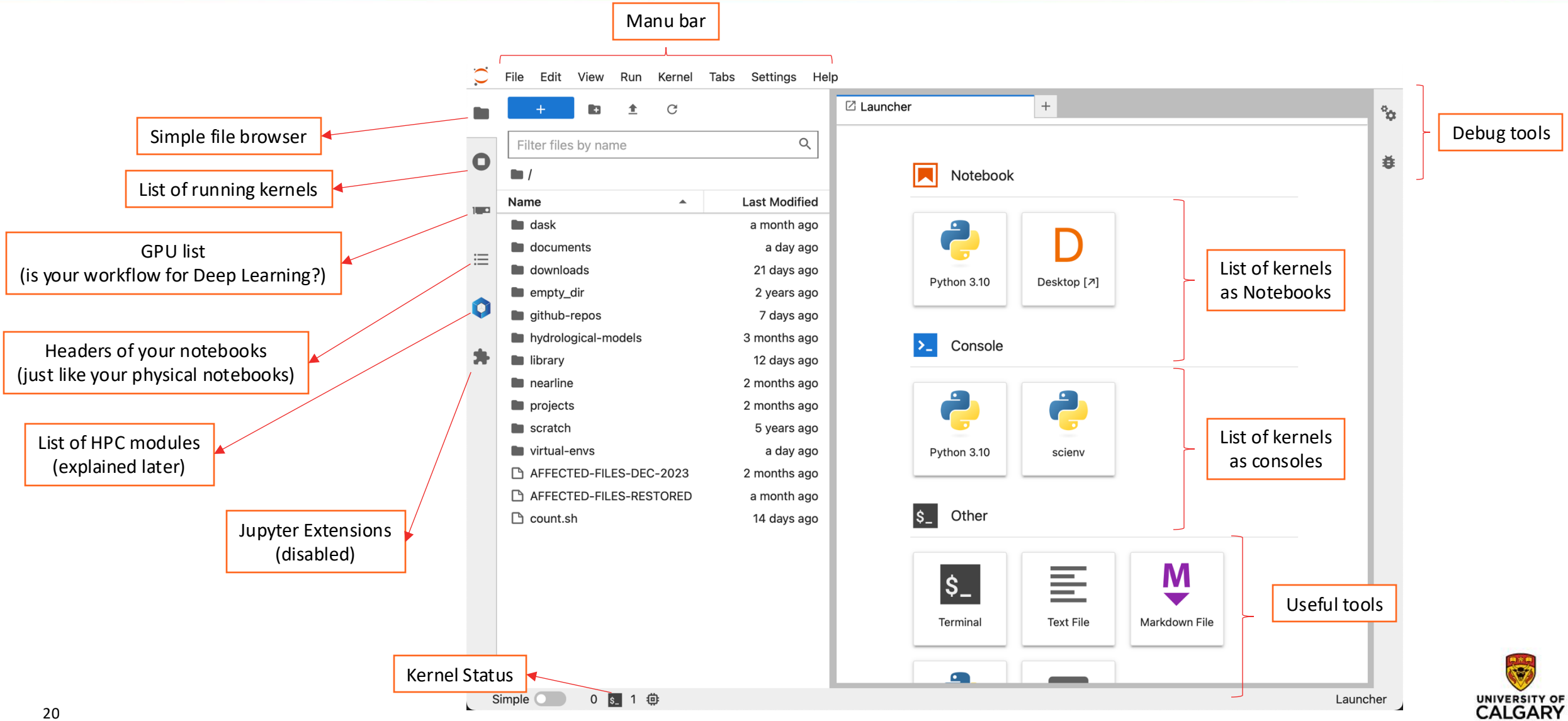
Computational Resources



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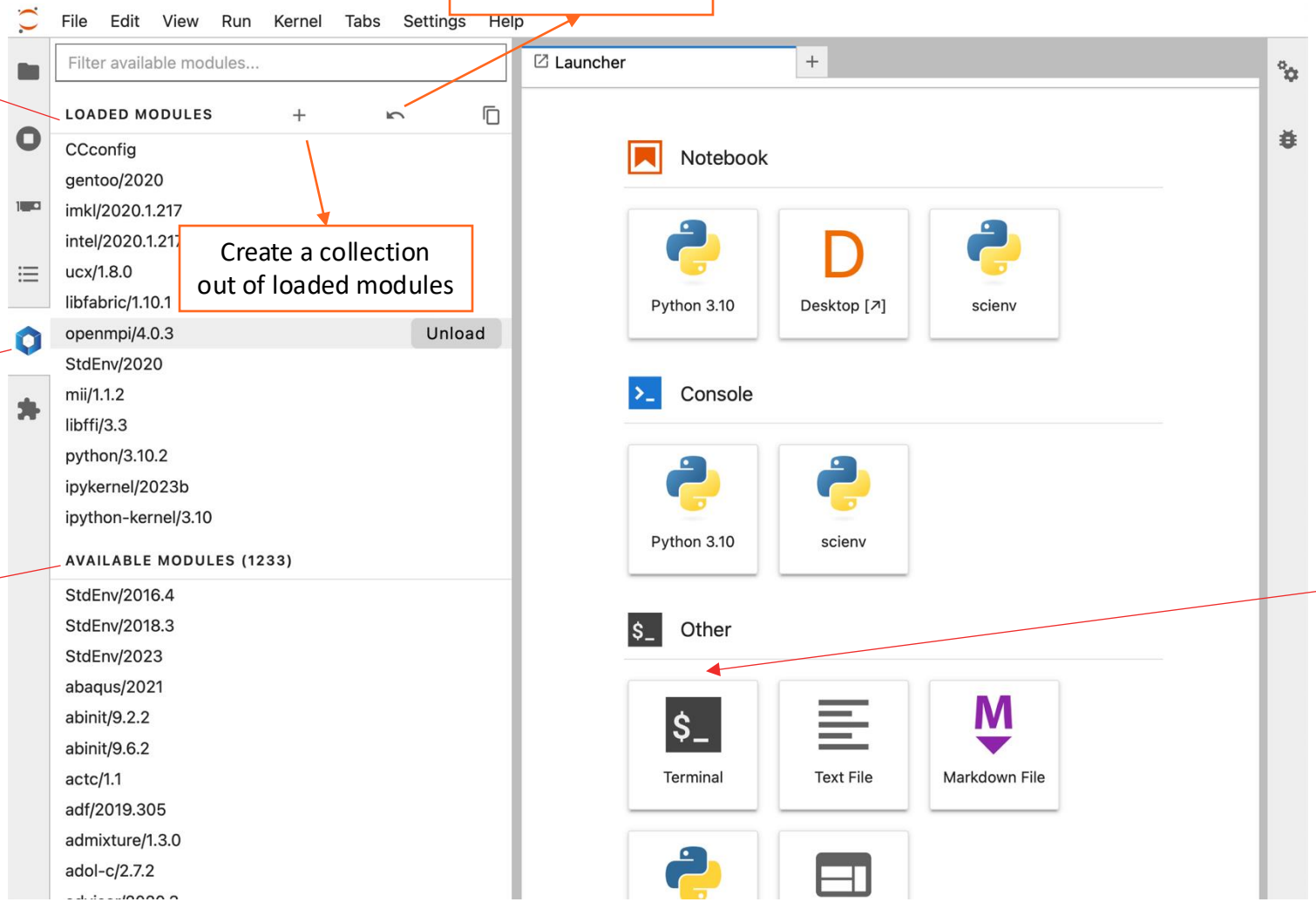
Computational Resources

Restore a previously saved collection

Loaded modules



Create a collection out of loaded modules

List of HPC modules (LMOD Extention)

Unloaded modules

A saved list of modules is called a “collection”

Using JupyterLab interface
For creating collections could be time consuming.

We will use the Terminal to build a collection later.

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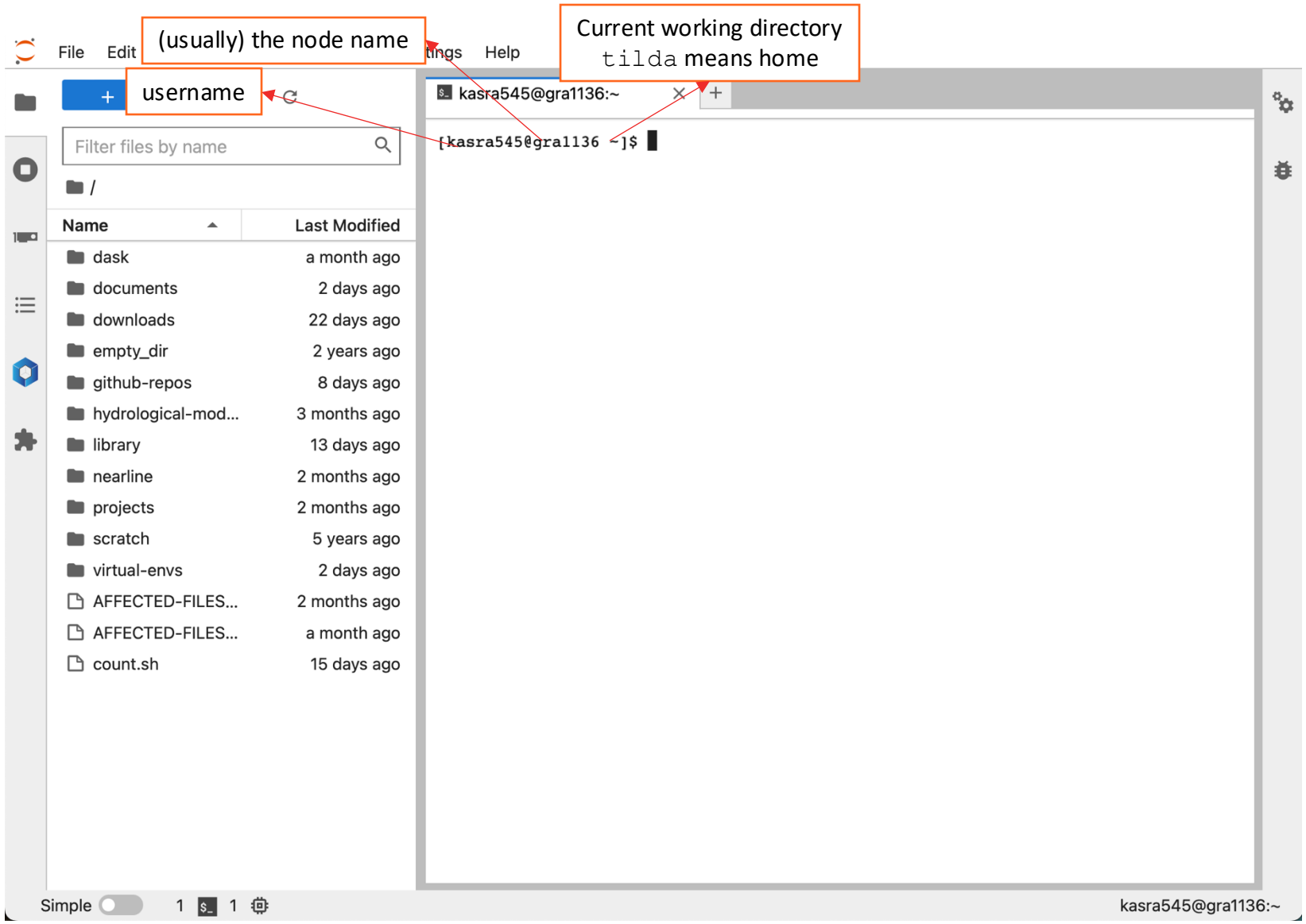
Computational Resources

All instructions are available on this presentation's repository:

https://github.com/CH-Earth/community-modelling-workflow-training



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Computational Resources

Exactly similar to what we can do in this tab

All instructions are available on this presentation's repository:

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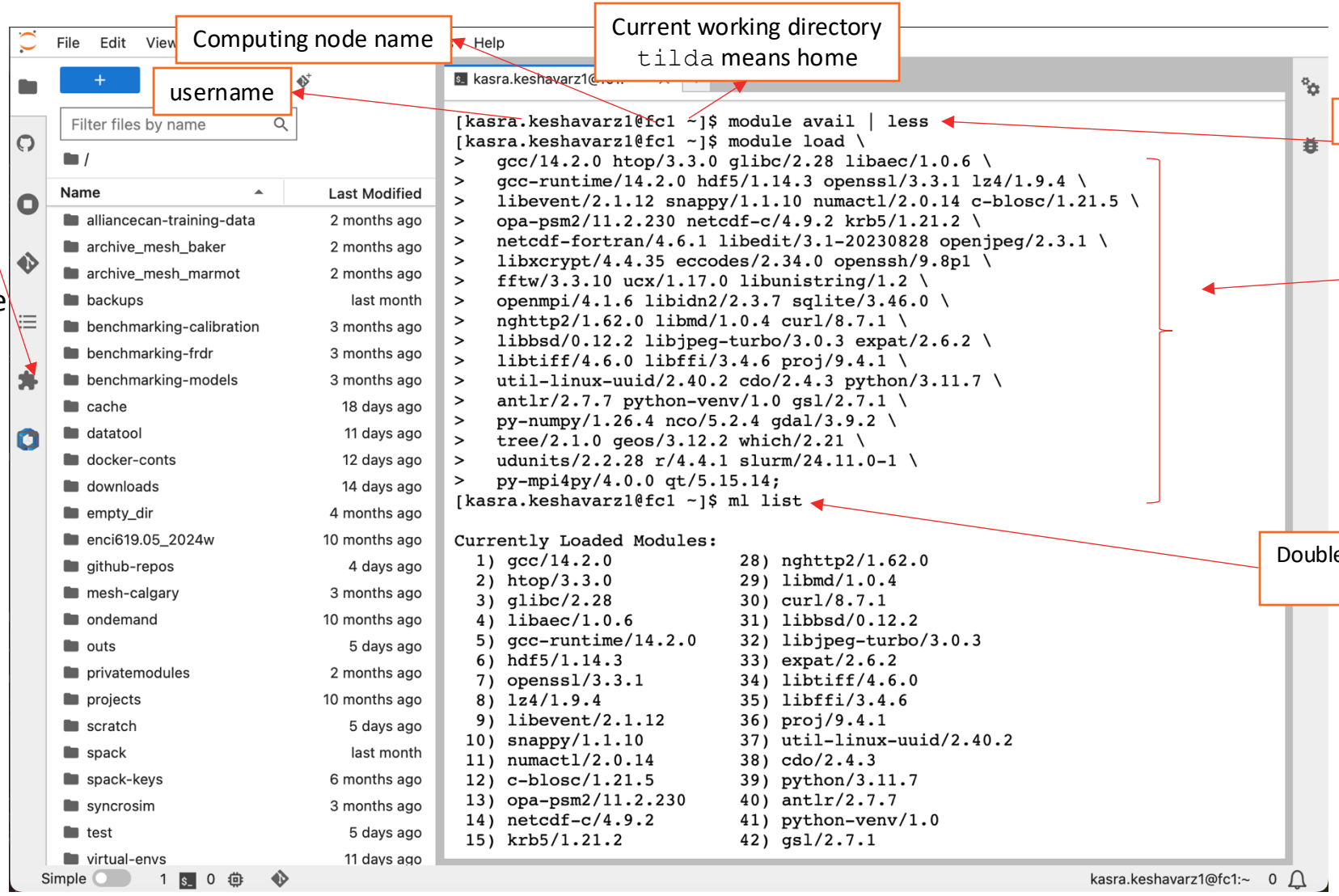

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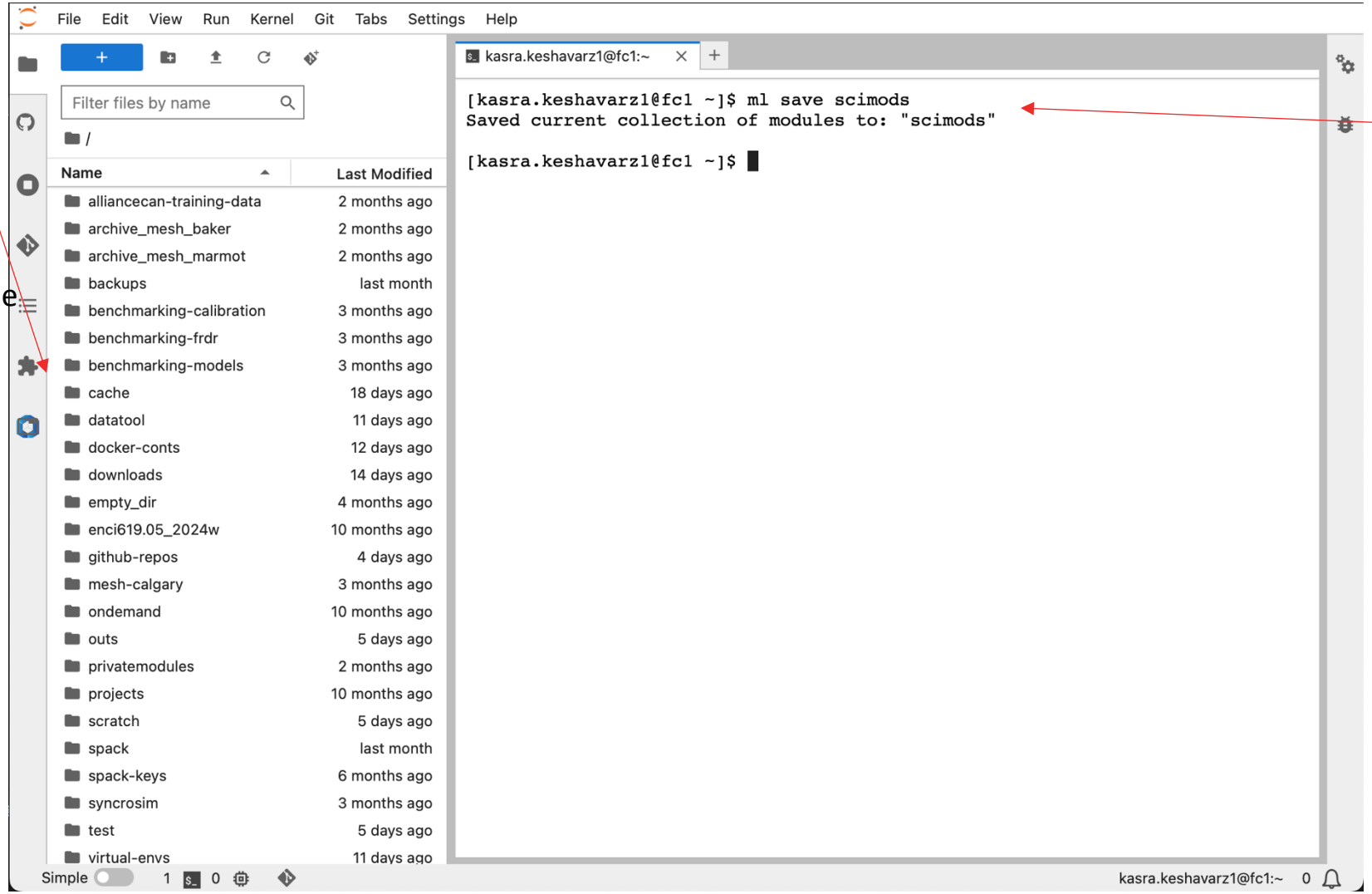

Saving the modules as a “collection”

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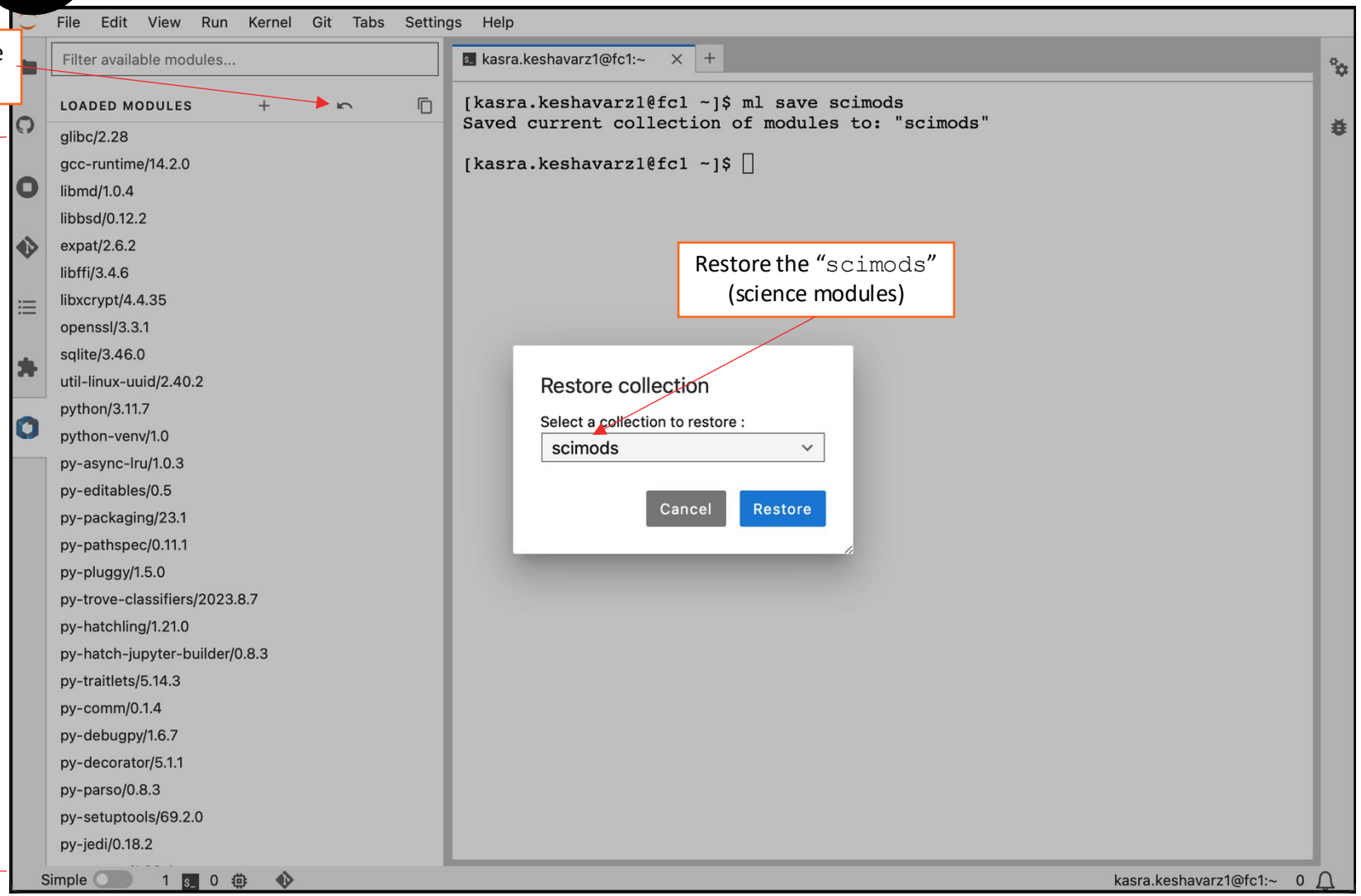
Computational Resources

Refresh the JupyterLab session webpage, and see if you can find the collection you just saved:

Check out what module collections you have



Restore the "scimods" (science modules)

Wait for a few seconds so Jupyter loads all modules saved in "scimods" collection

This is only a one-time process.
You can always access all the collections you saved from Jupyter's module extension tab

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Any questions so far?

Computational Resources

Python Programming Language

- Community Hydrological Modelling Workflows: much of our workflows are offered in Python package formats
- Python is Powerful: Python always can offer you a useful workflow
- Reproducible Environments: Python's Virtual Environments enables this requirement
- Supported on HPCs and Commercial Cloud regardless of your Operating System: it can be used everywhere
- Graham is no exception: Python is fully supported on Graham

Computational Resources

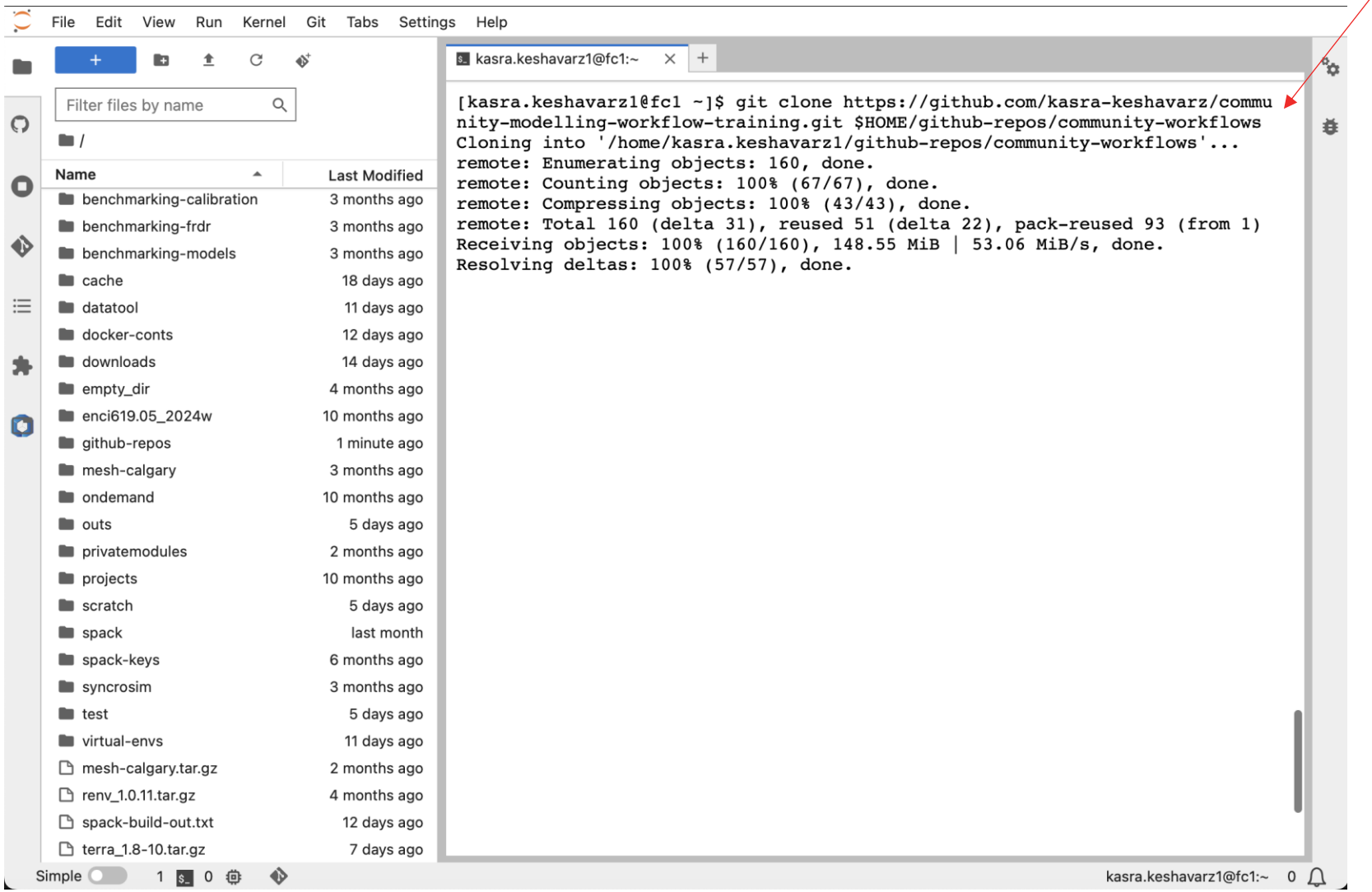
Before setting up the Python Environment, we need to download the training session's GitHub repository

Please note that Binder users, need to run the following command on MyBinder Session due to a bug reported in JupyterLab:

bash --norc --noprofile

See the following webpages for ongoing discussions:
https://github.com/jupyterhub/mybinder.org-deploy/issues/3210#event-16270107011
&
https://github.com/jupyterhub/repo2docker/issues/1405

Computational Resources



"clone"-ing the repository

We use this terminal session now to download the relevant GitHub repository

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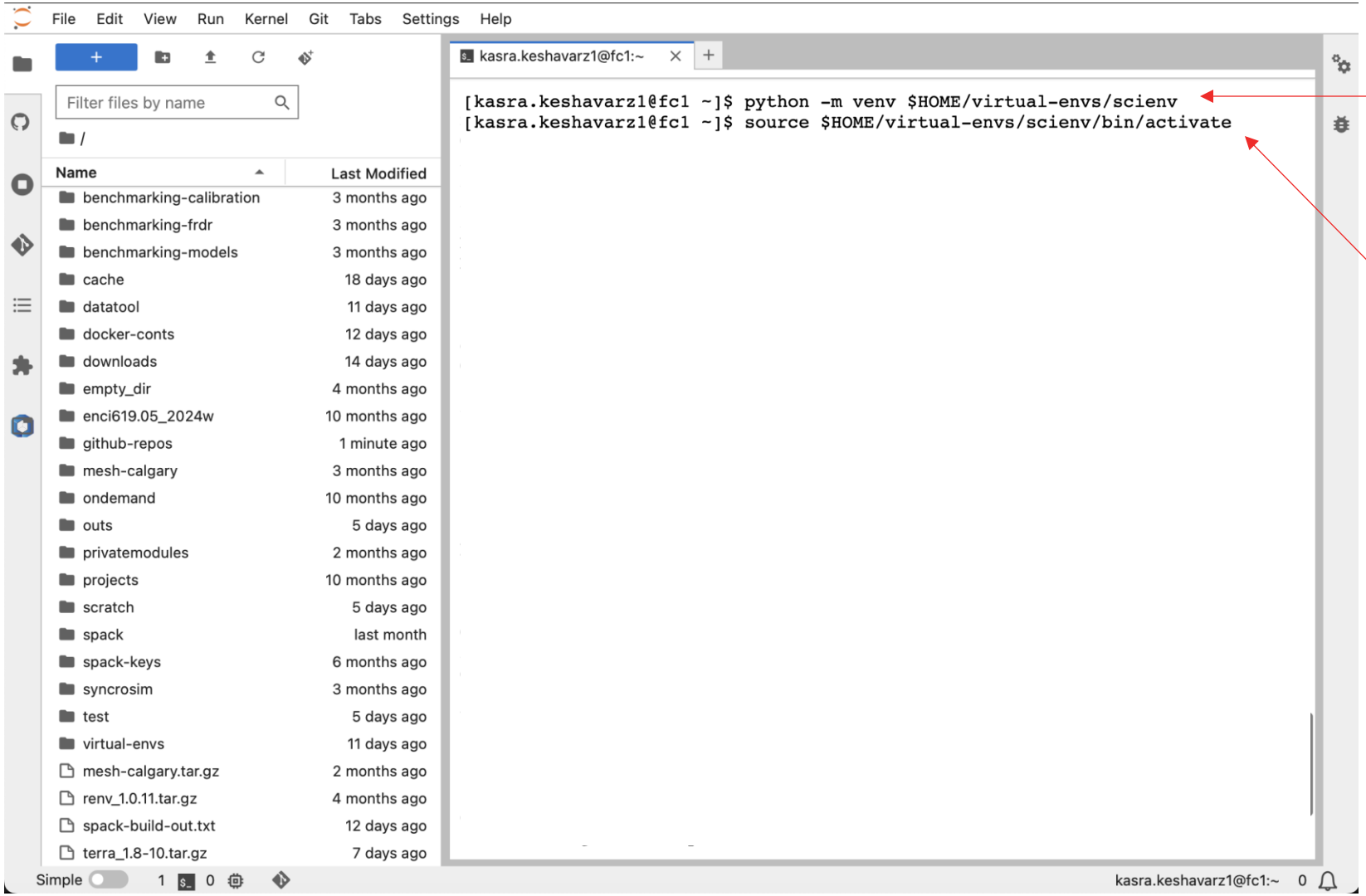
Computational Resources



Creating an empty Virtual Environment

Activating the empty Virtual Environment

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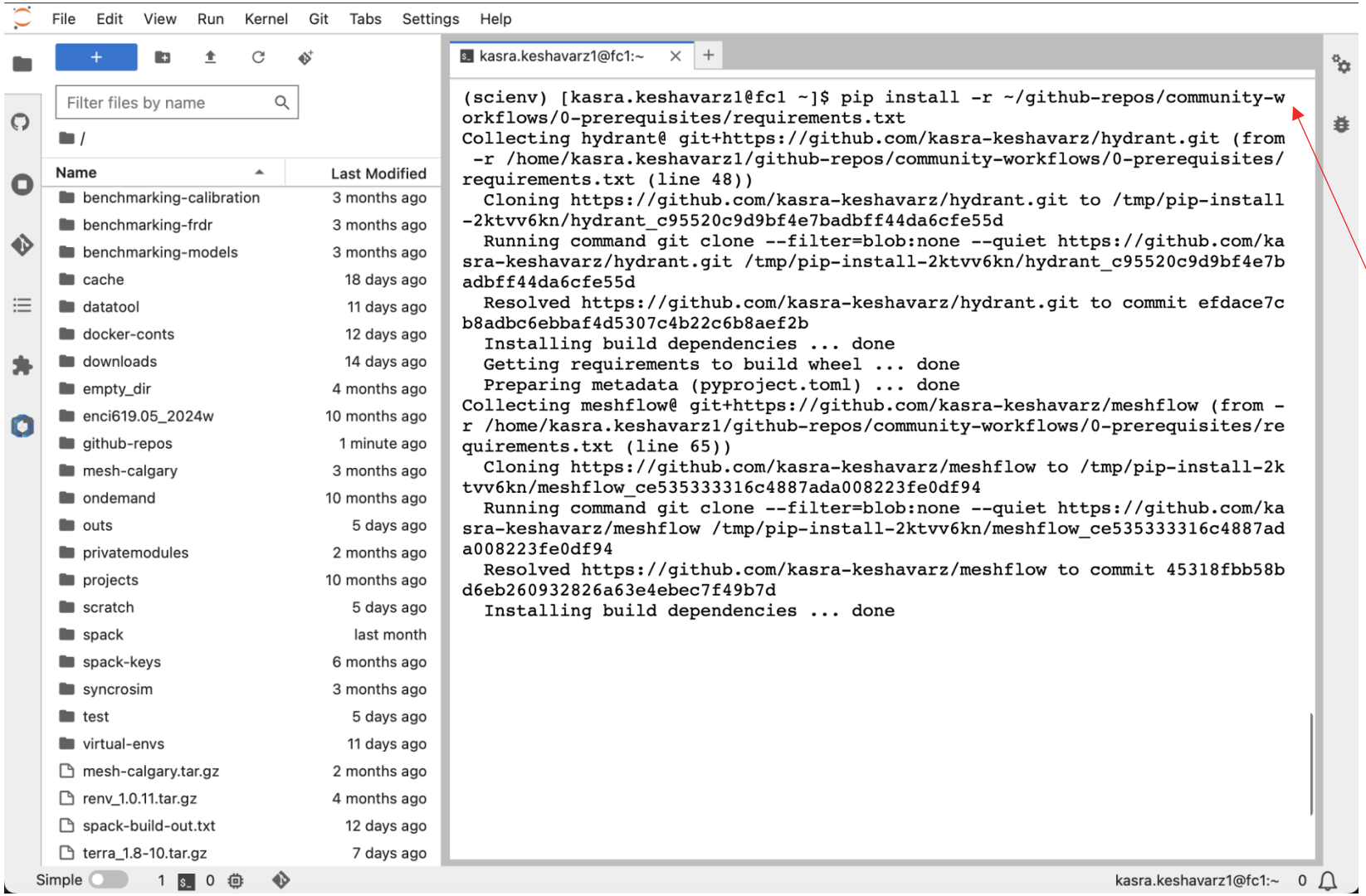
Computational Resources



Installing necessary Python Packages

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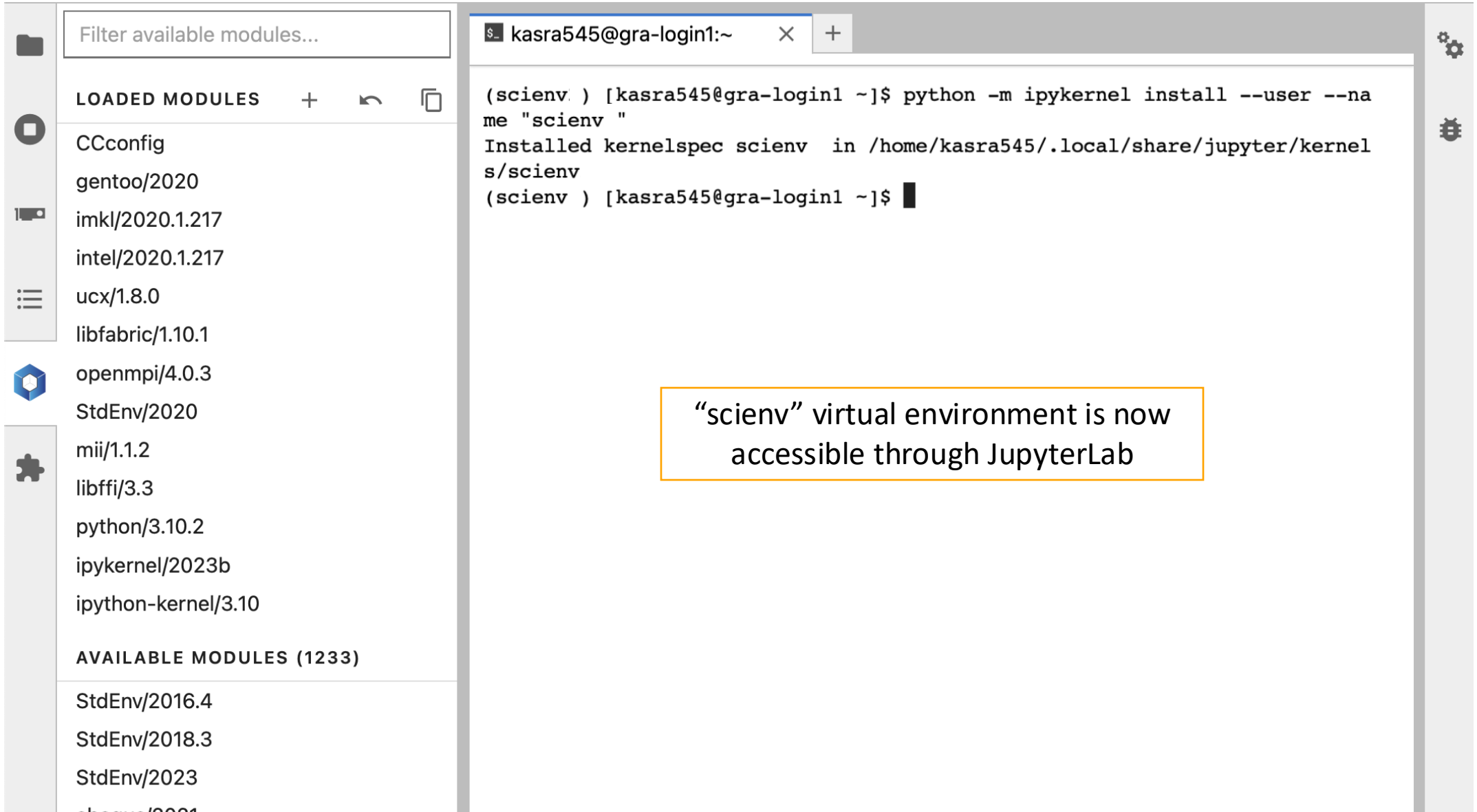
Computational Resources



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Computational Resources

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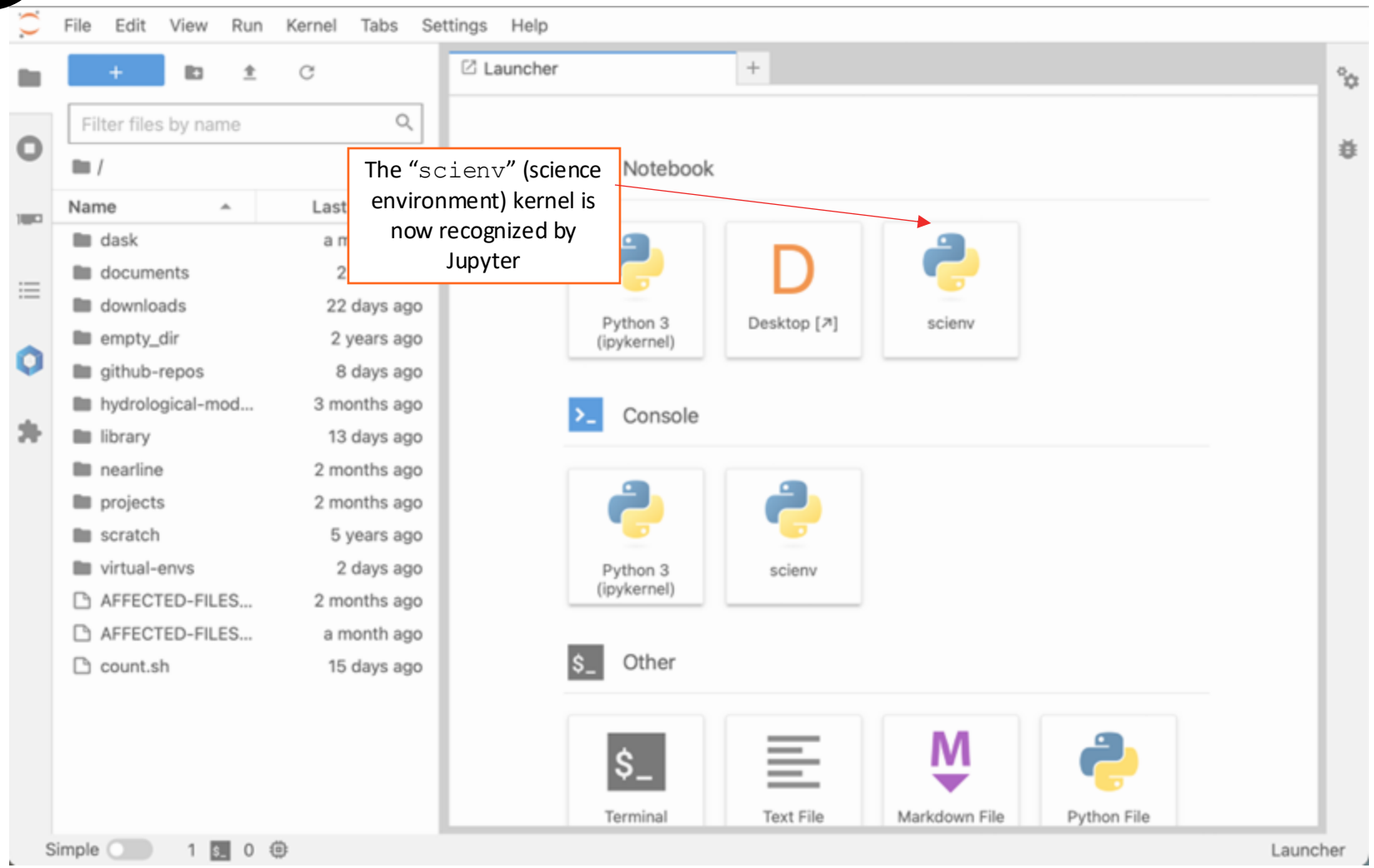

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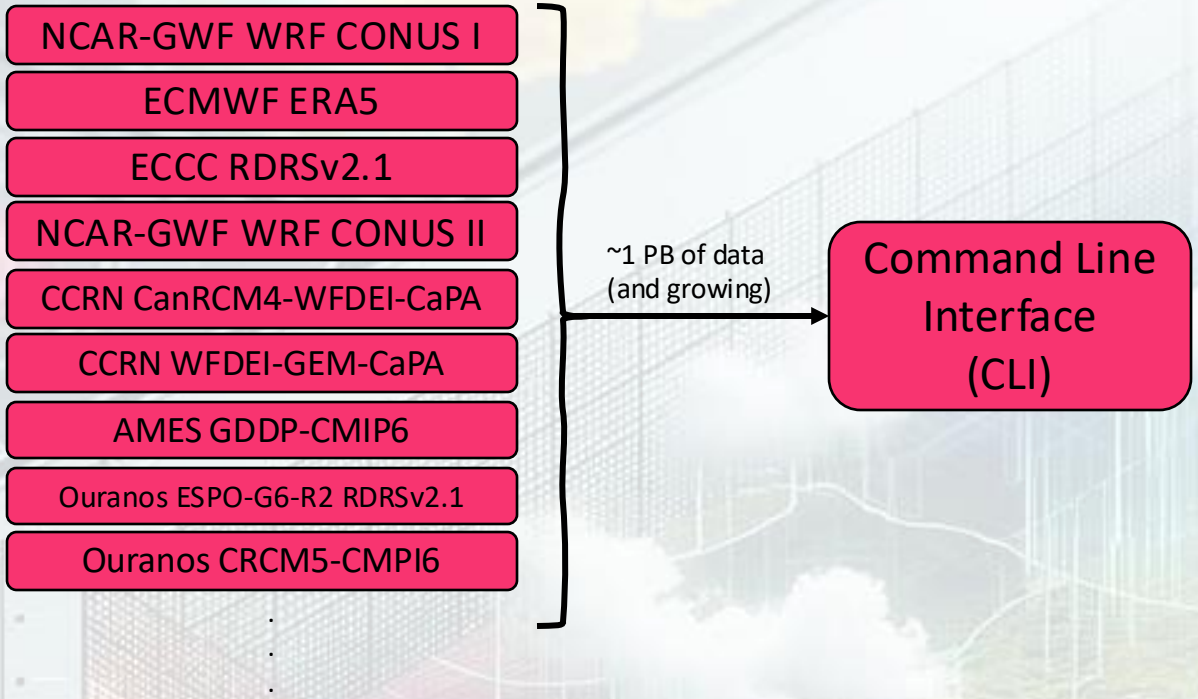
Setting up ECCC's National Water Model—MESH




```
./extract-dataset.sh  --dataset=CONUS1 \
  --dataset-dir="/project/rpp-kshook/Model_Output/WRF/CONUS/CTRL" \
  --output-dir="$HOME/scratch/conus_i_output/" \
  --start-date="2000-10-01 00:00:00" \
  --end-date="2013-09-30 23:00:00" \
  --lat-lims=49,54  \
  --lon-lims=-120,-98 \
  --variable="T2,PREC_ACC_NC,Q2,ACSWDNB,ACLWDNB,U10,V10,PSFC" \
  --prefix="conus_i" \
  --email="youremail@company.ca" \
  -j;
```

datatool

Steps:

1. Login to cluster of choice,
2. Make sure you have access to the designated project space and allocation,
3. Clone the remote GitHub repository,
4. Subset any spatial and temporal extents of interest for any of the available datasets with only **one line of code**.

https://github.com/CH-Earth/datatool.git

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DALL-E generate image

Setting up ECCC's National Water Model—MESH

datatool
(HPC-agnostic)

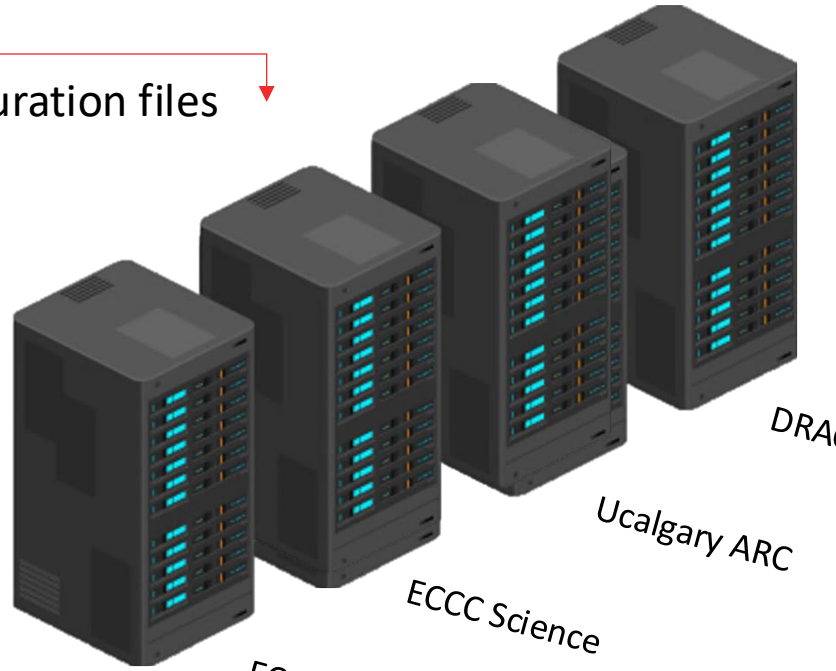
Hardware dependent job settings

HPC-specific settings

Scheduler dependent settings

JSON files

JSON configuration files



DRAC Graham

Ucalgary ARC

ECCC Science

ECCC Collab

… any other HPC

slurm workload manager

Altair | PBS Works™

IBM Spectrum LSF

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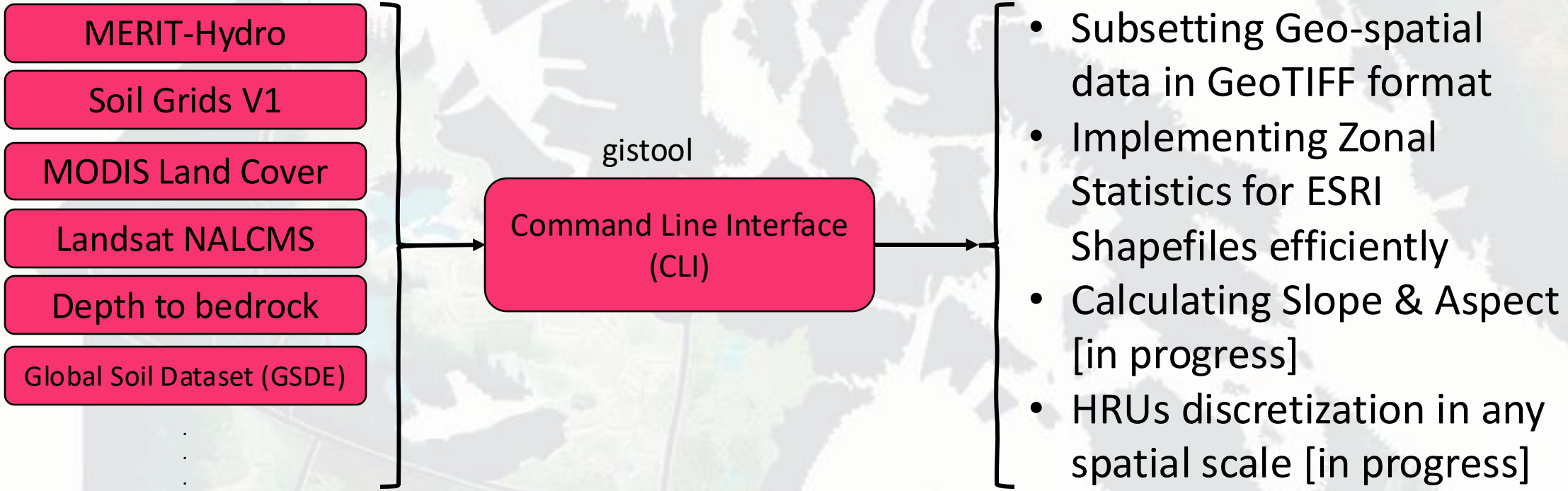
https://datatool.readthedocs.io/

Setting up ECCC's National Water Model—MESH



Steps:

1. Login to your cluster of choice,
2. Make sure you have access to the designated project space and allocation,
3. Clone the repository,
4. Subset and/or implement zonal statistics for any spatial and temporal extents of interest for any of the included datasets with only **one line of code**.

https://github.com/CH-Earth/gistool.git

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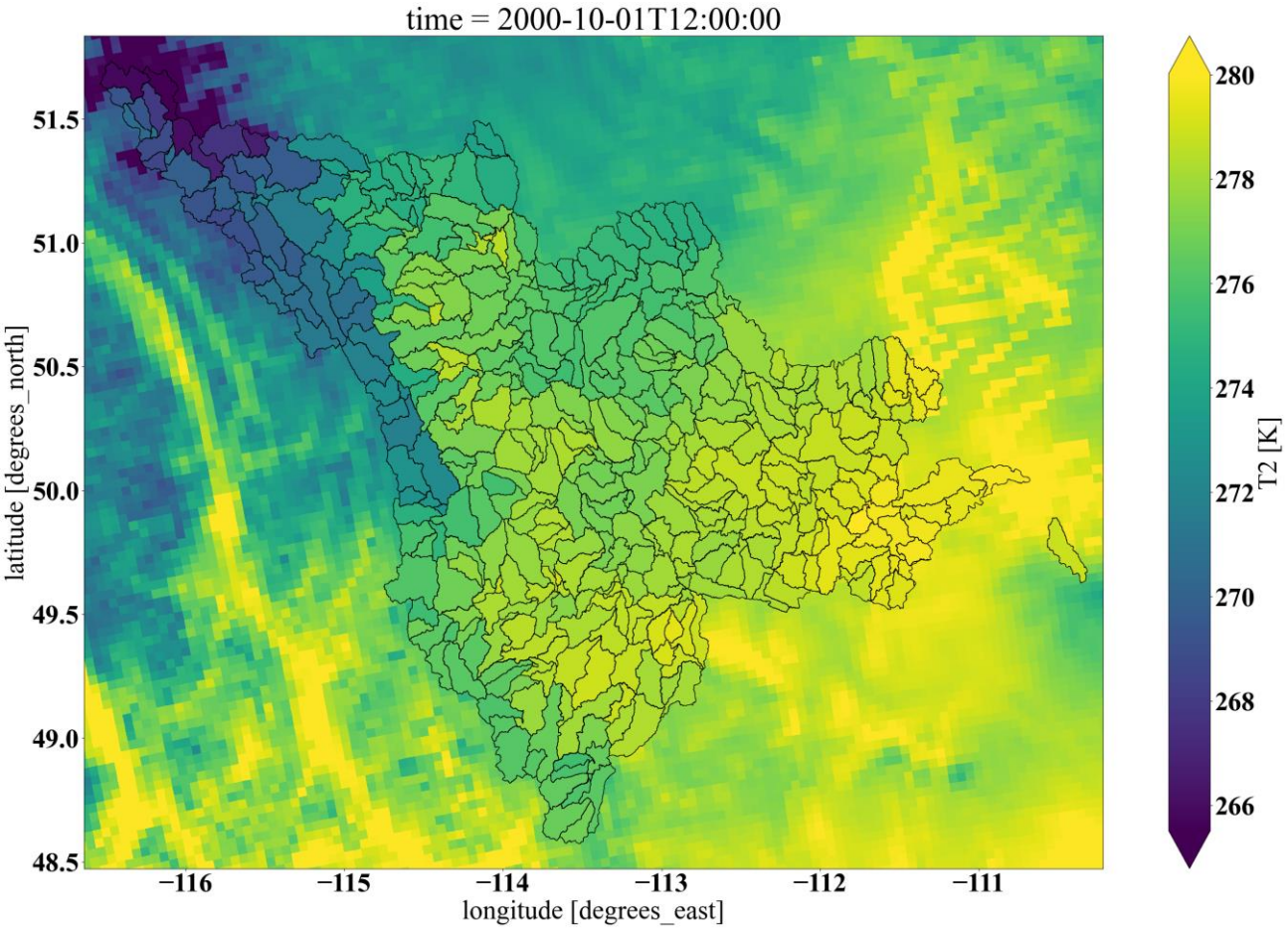
Setting up ECCC's National Water Model—MESH




```
kasras-mbp:easymore ShervanGharari$ easymore
Usage: easymore [OPTIONS] COMMAND [ARGS]...

  EASYMORE is a collection of functions that allows extraction of the
  data from a NetCDF file for a given shapefile such as a basin,
  catchment, points or lines. It can map gridded data or model output to
  any given shapefile and provide area average for a target variable.

Options:
  --version  Show the version and exit.
  --help     Show this message and exit.

Commands:
  cli   Run Easymore using CLI
  conf  Run Easymore using a JSON configuration file

  For bug reports, questions, and discussions open an issue at
  https://github.com/ShervanGharari/EASYMORE.git
```

Command Line Interface (CLI)
and
Python Library

https://github.com/ShervanGharari/EASYMORE.git

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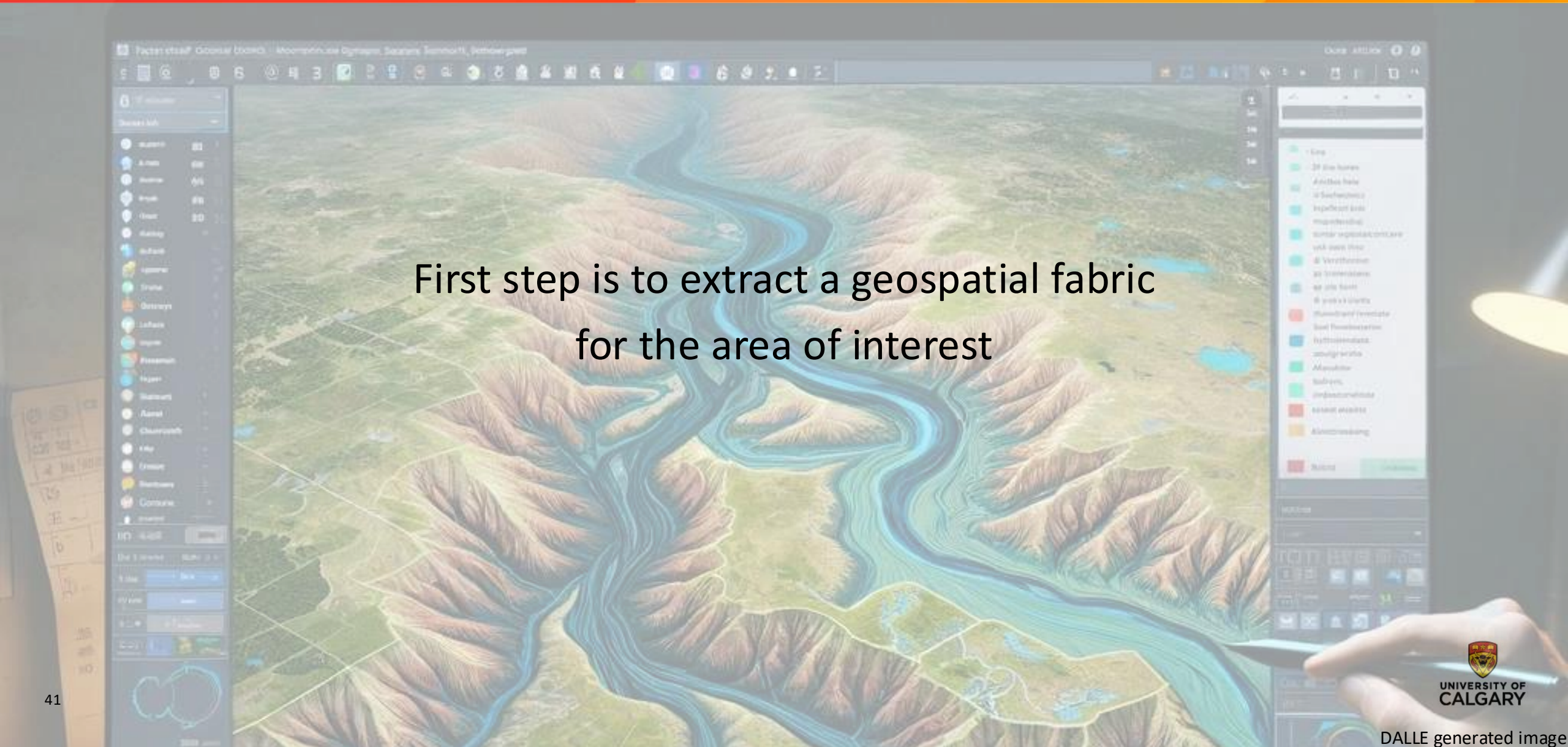
Any questions so far?

Setting up ECCC's National Water Model—MESH

Configuring ECCC's MESH with the following datasets for the Bow River at Calgary:

Meteorological Forcing Dataset	Landcover Dataset	Geospatial Fabric Dataset	Study Area
Regional Deterministic Reforecast System version 2.1 (RDRSv2.1)	North American Land Change Monitoring System 2020 (NALCMS 2020)	MERIT-Basins	Bow River at Calgary

Setting up ECCC's National Water Model—MESH



First step is to extract a geospatial fabric for the area of interest

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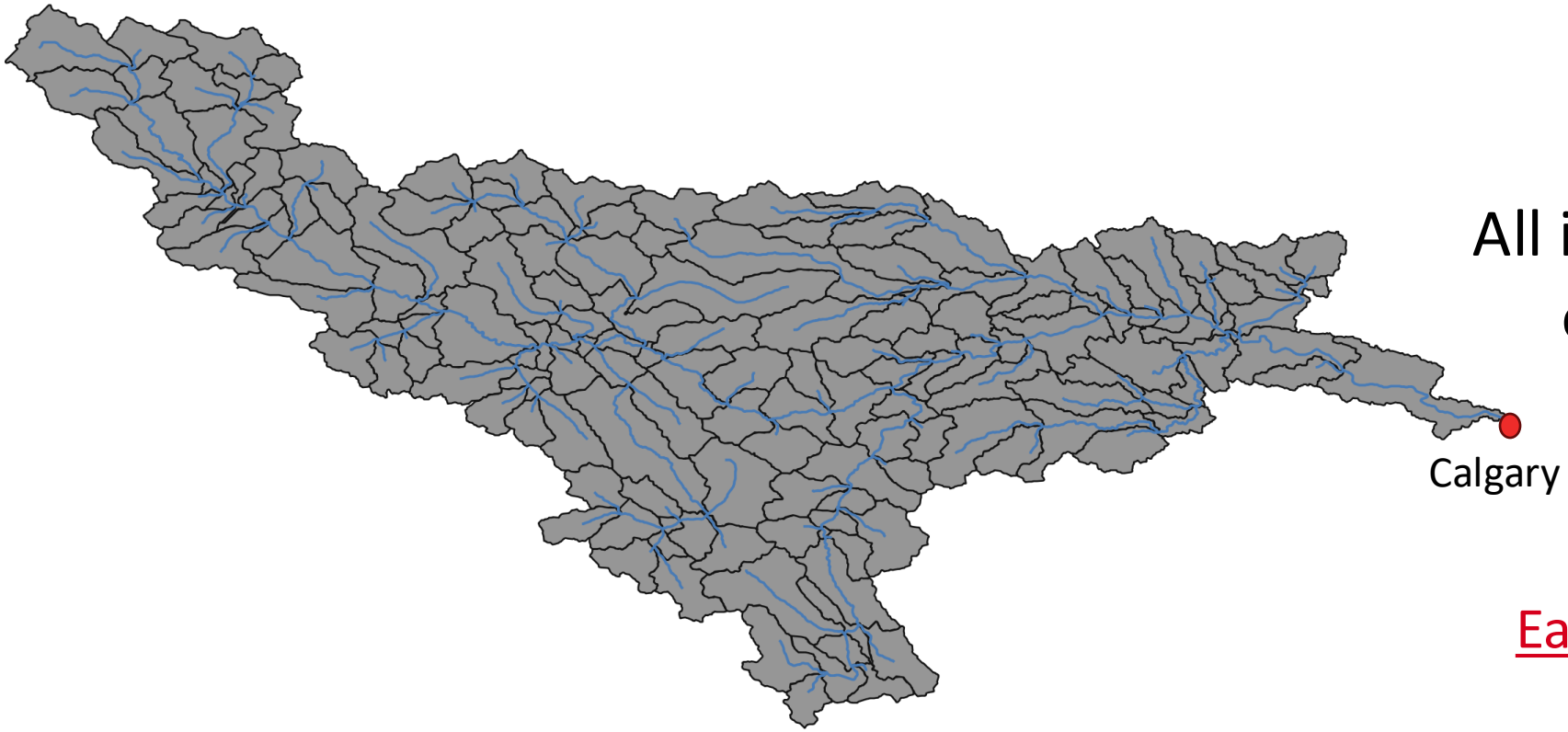
Setting up ECCC's National Water Model—MESH



All instructions are available on this presentation's repository:

https://github.com/CH-Earth/community-modelling-workflow-training

Bow River at Calgary

Sub-basins and river network extracted from `MERIT-Basins` using `Hydrant v0.1.0-dev0`

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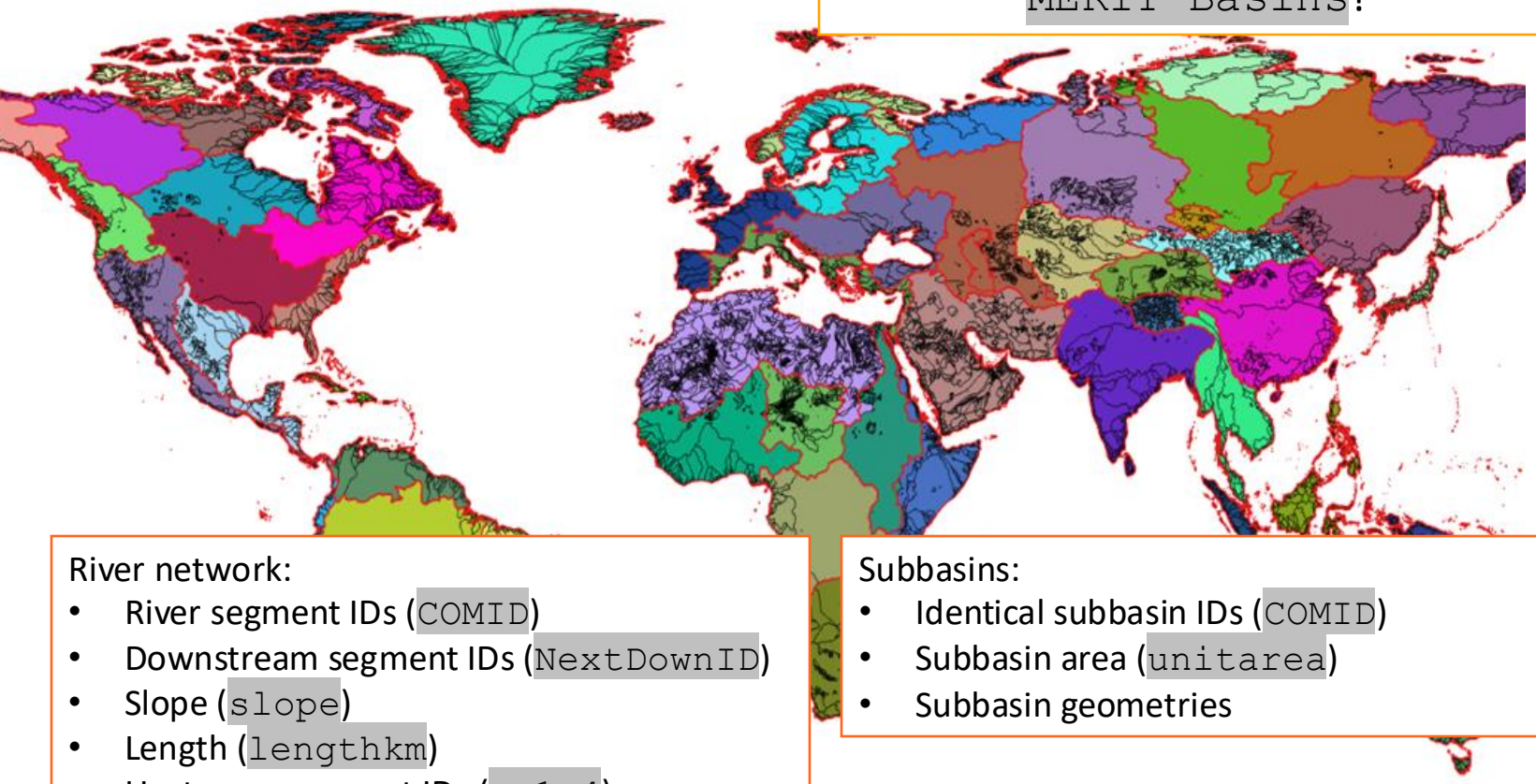
Setting up ECCC's National Water Model—MESH

What information is provided through `MERIT-Basins`?



- 25 km^2 drainage area threshold for channels
- Corrected/refined basin/region definitions
- Below 25 km^2 non-channelized areas along the coast or some endorheic areas (incomplete catchments or hillslopes) excluded
- ~2.94 million river reaches (unit catchments)

River network:
- River segment IDs (`COMID`)
- Downstream segment IDs (`NextDownID`)
- Slope (`slope`)
- Length (`lengthkm`)
- Upstream segment IDs (`up1-4`)
- Upstream drainage area (`uparea`)
- River geometries

Subbasins:
- Identical subbasin IDs (`COMID`)
- Subbasin area (`unitarea`)
- Subbasin geometries

Non-contributing areas:
- Non-contributing area IDs (`FID`)
- Non-contributing area geometries

`MERIT-Basins` webpage: https://www.reachhydro.org/home/params/merit-basins

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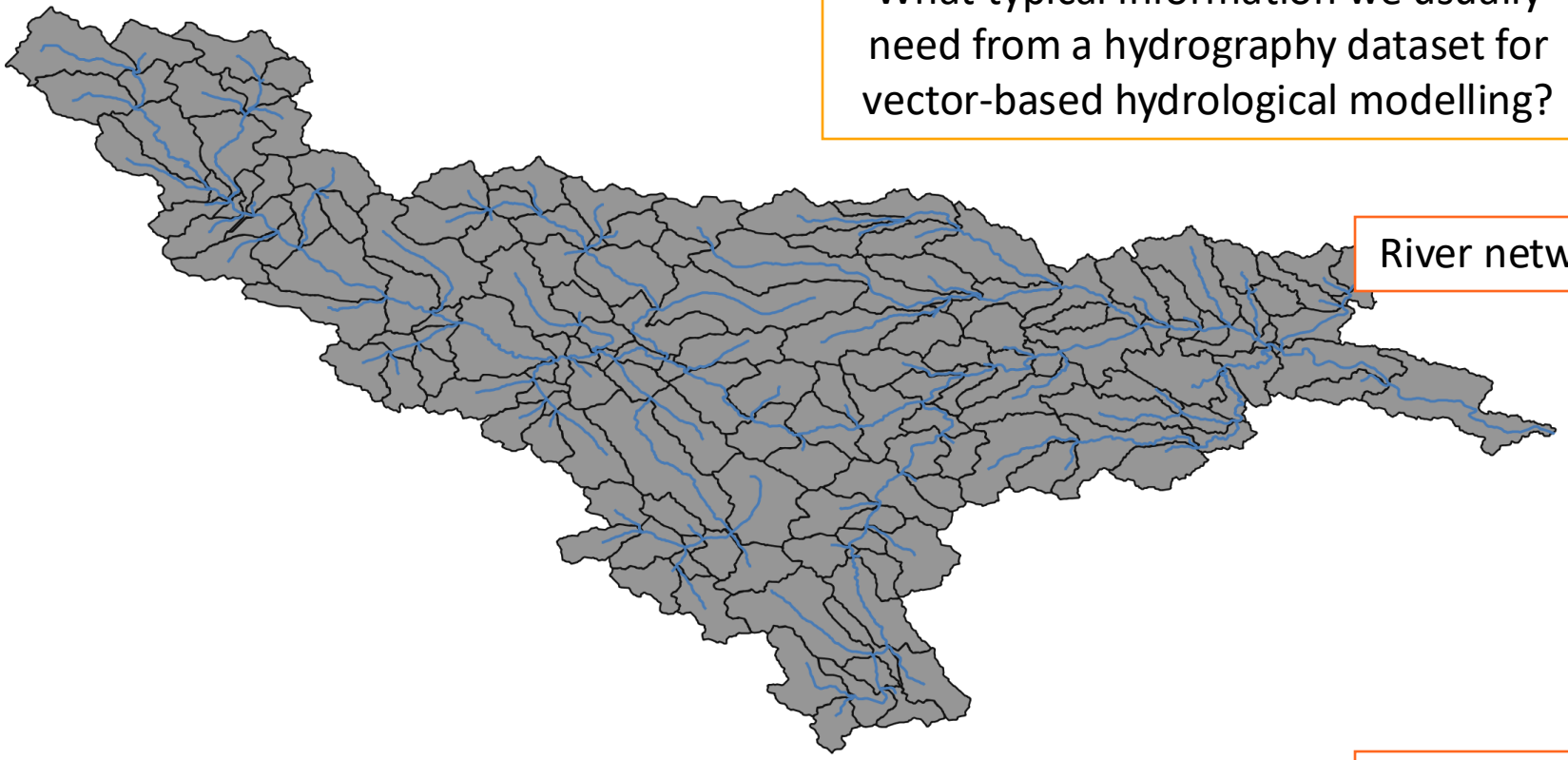
Setting up ECCC's National Water Model—MESH

What typical information we usually need from a hydrography dataset for vector-based hydrological modelling?



Bow River at Calgary

Sub-basins and river network extracted from `MERIT-Basins` using `Hydrant v0.1.0-dev0`

River network:

- River segment ID values
- Immediate downstream segment ID values
- Length

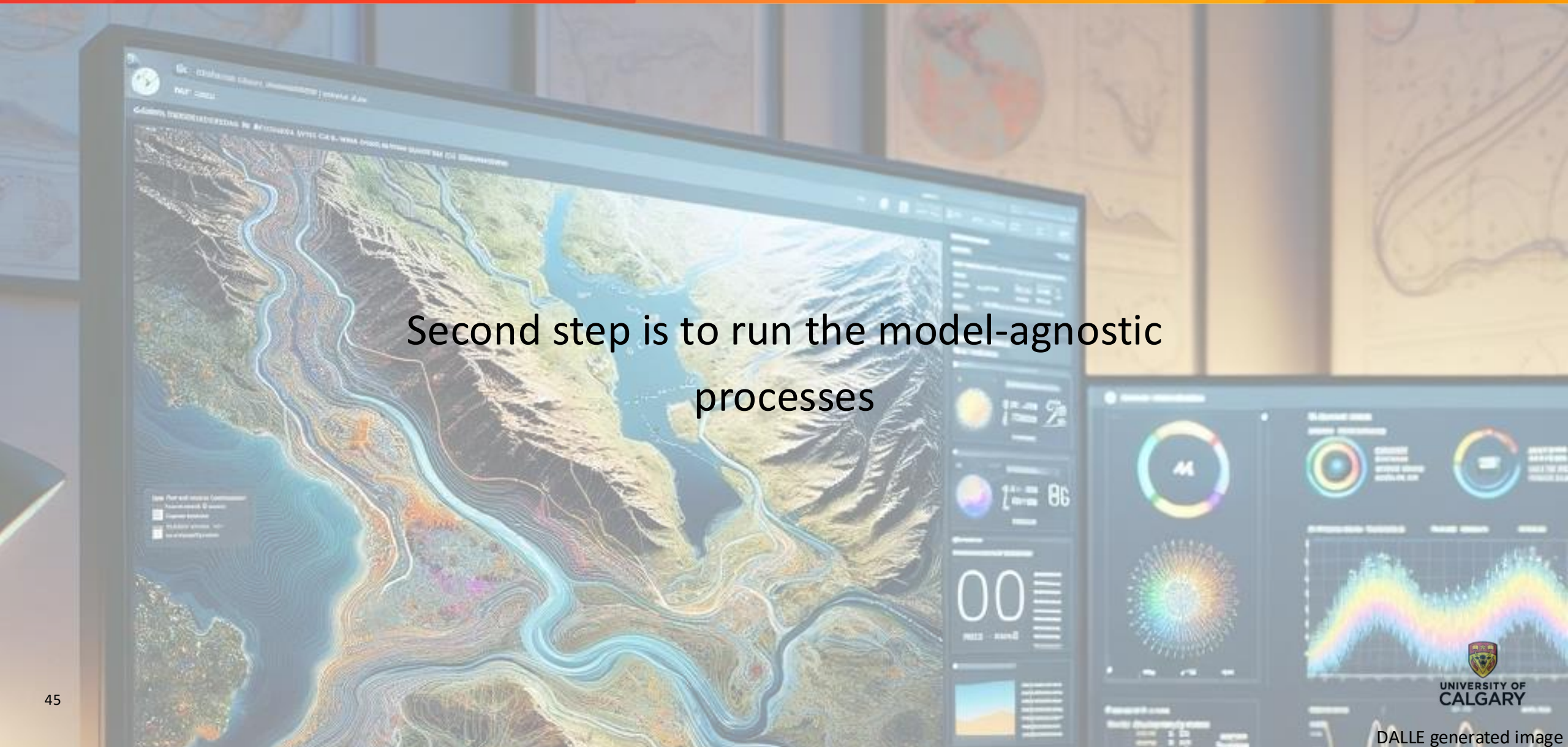
Depending on your routing scheme you may need:

- Slope [optional]
- Width [optional]
- etc.

Subbasins:

- Subbasin ID values
- Correspondence Mapping Table between Subbasin and River Segment IDs (could be identical value)
- Subbasin Area [optional]
- etc.

Setting up ECCC's National Water Model—MESH



Second step is to run the model-agnostic processes

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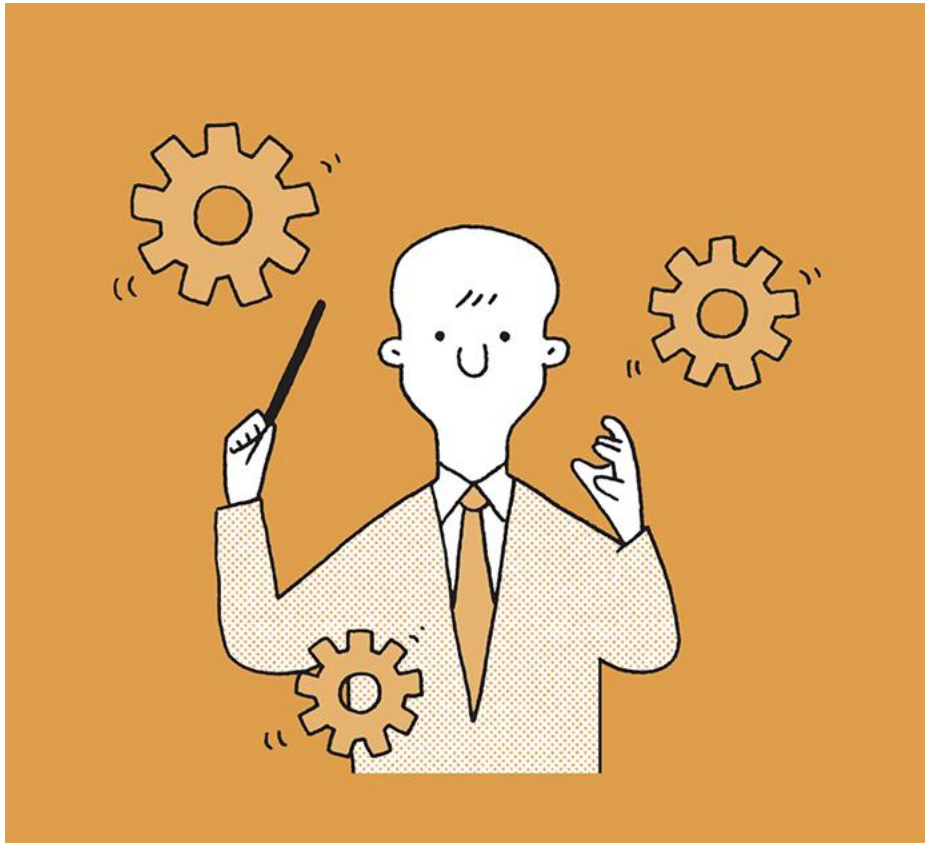

- Through a tool called "agnostic orchestrator" all the relevant data needed for this setup is processed by the Graham HPC
- We have previously downloaded all the relevant tools for the "agnostic" step
- We use the "agnostic orchestrator" configuration file instruct the file processing hierarchy

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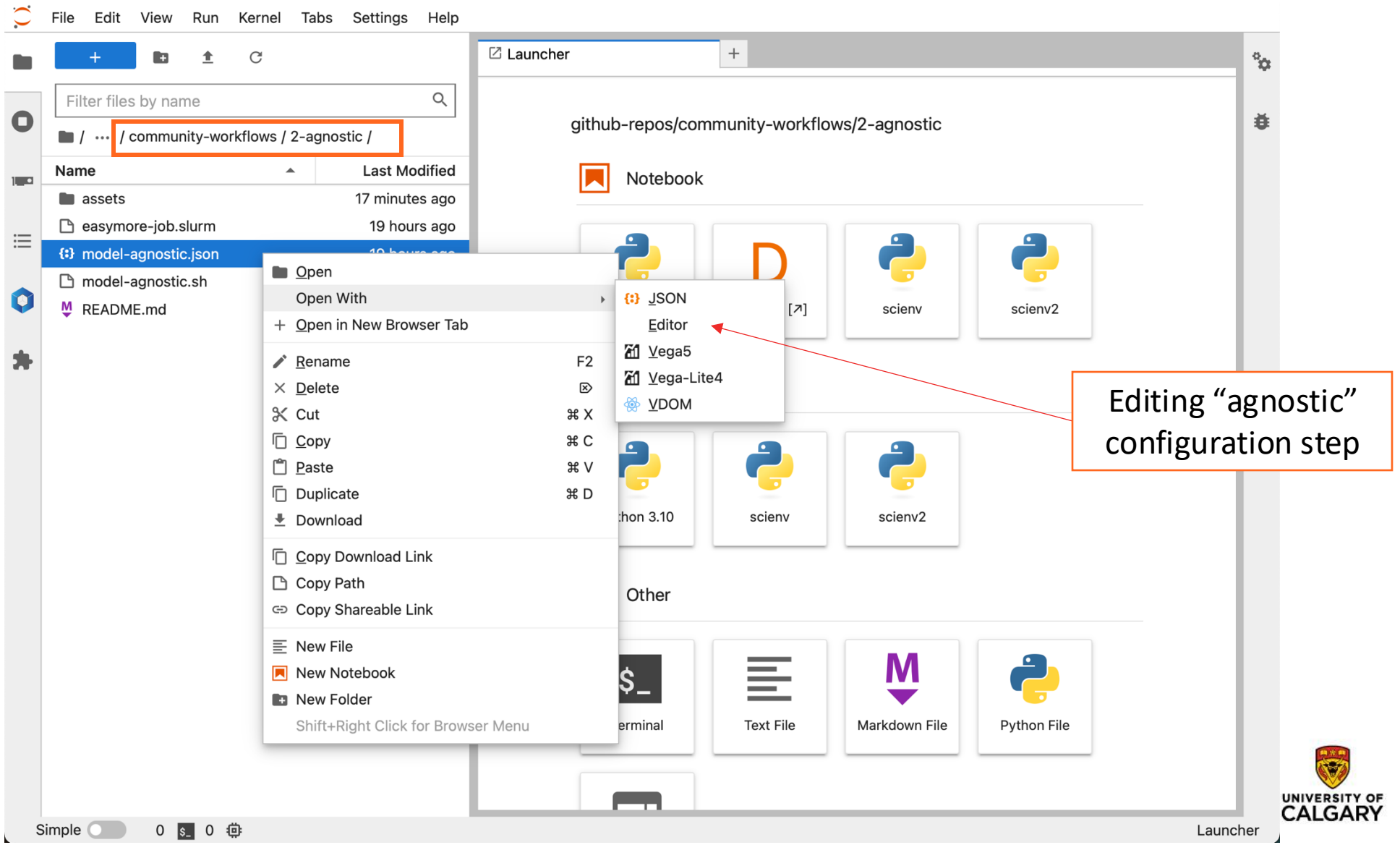
Agnostic workflow execution using its "Orchestrator"



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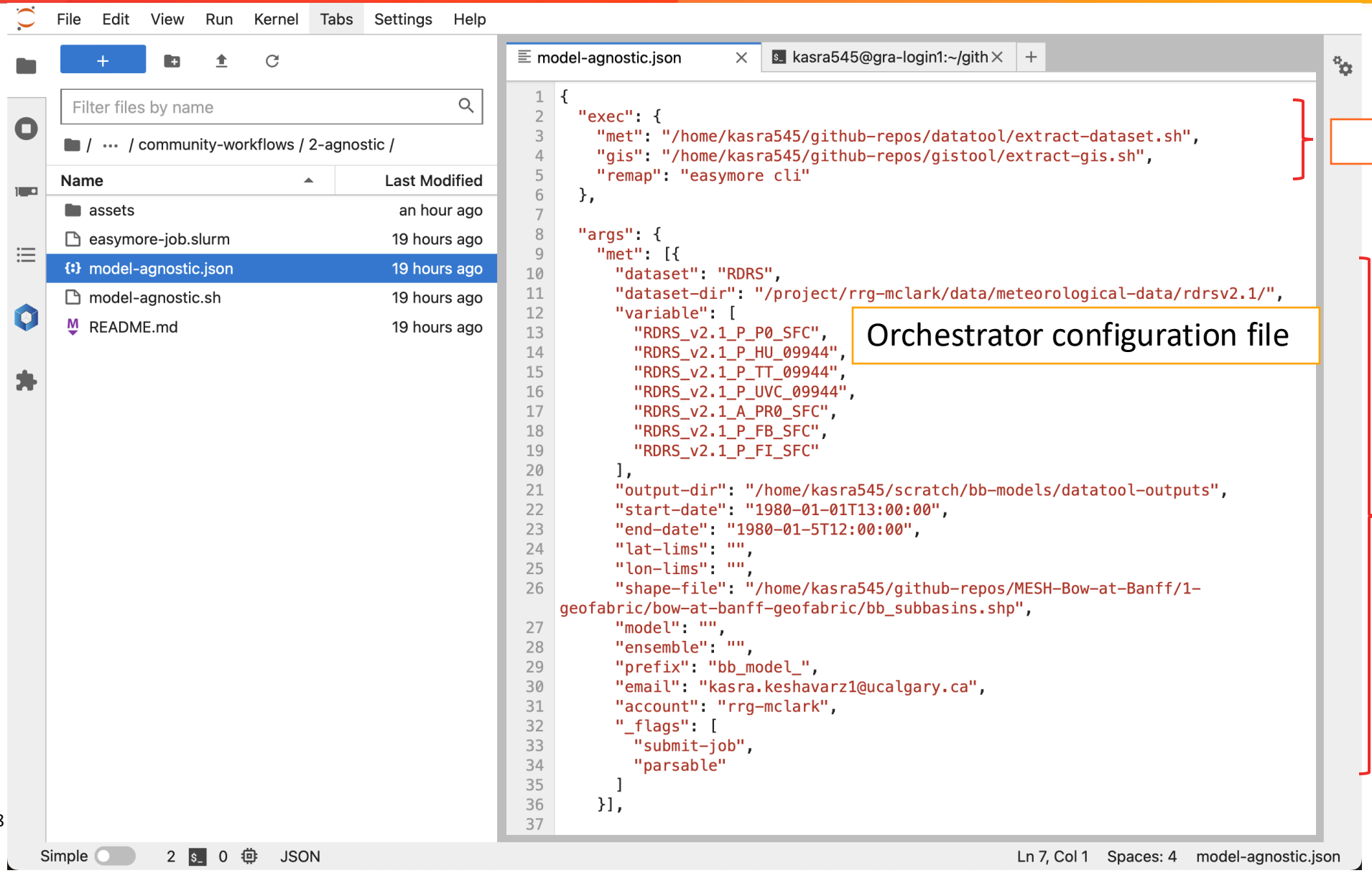

Orchestrator configuration file

Executable paths

Executable arguments and options

(empty options are ignored)

This is the only file for the "agnostic" step

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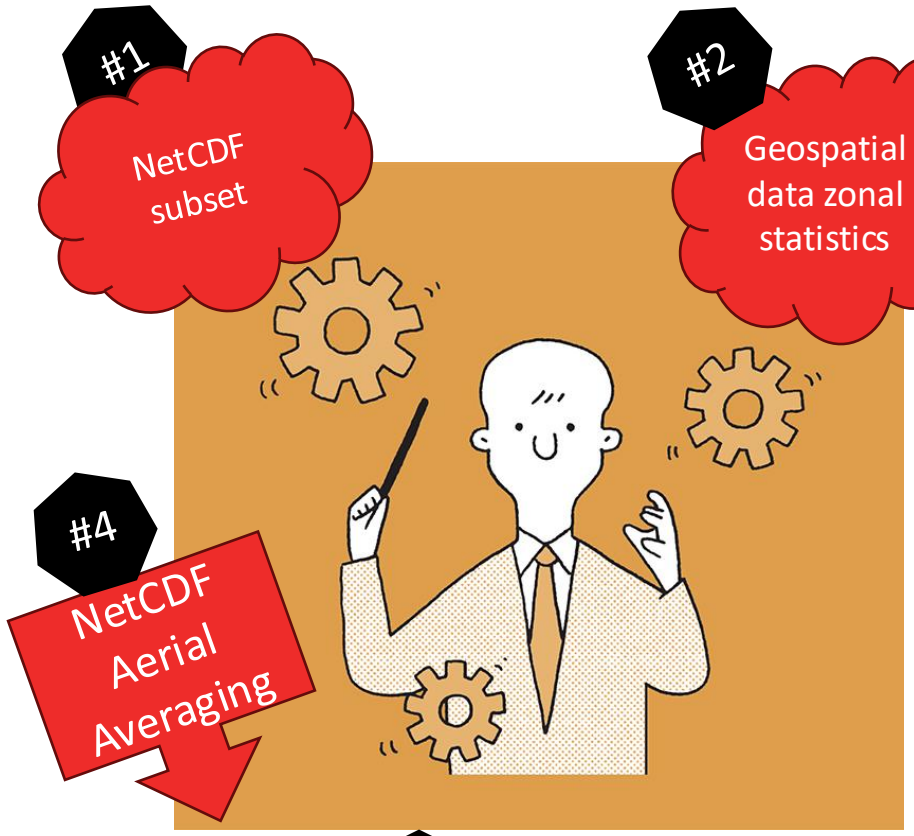
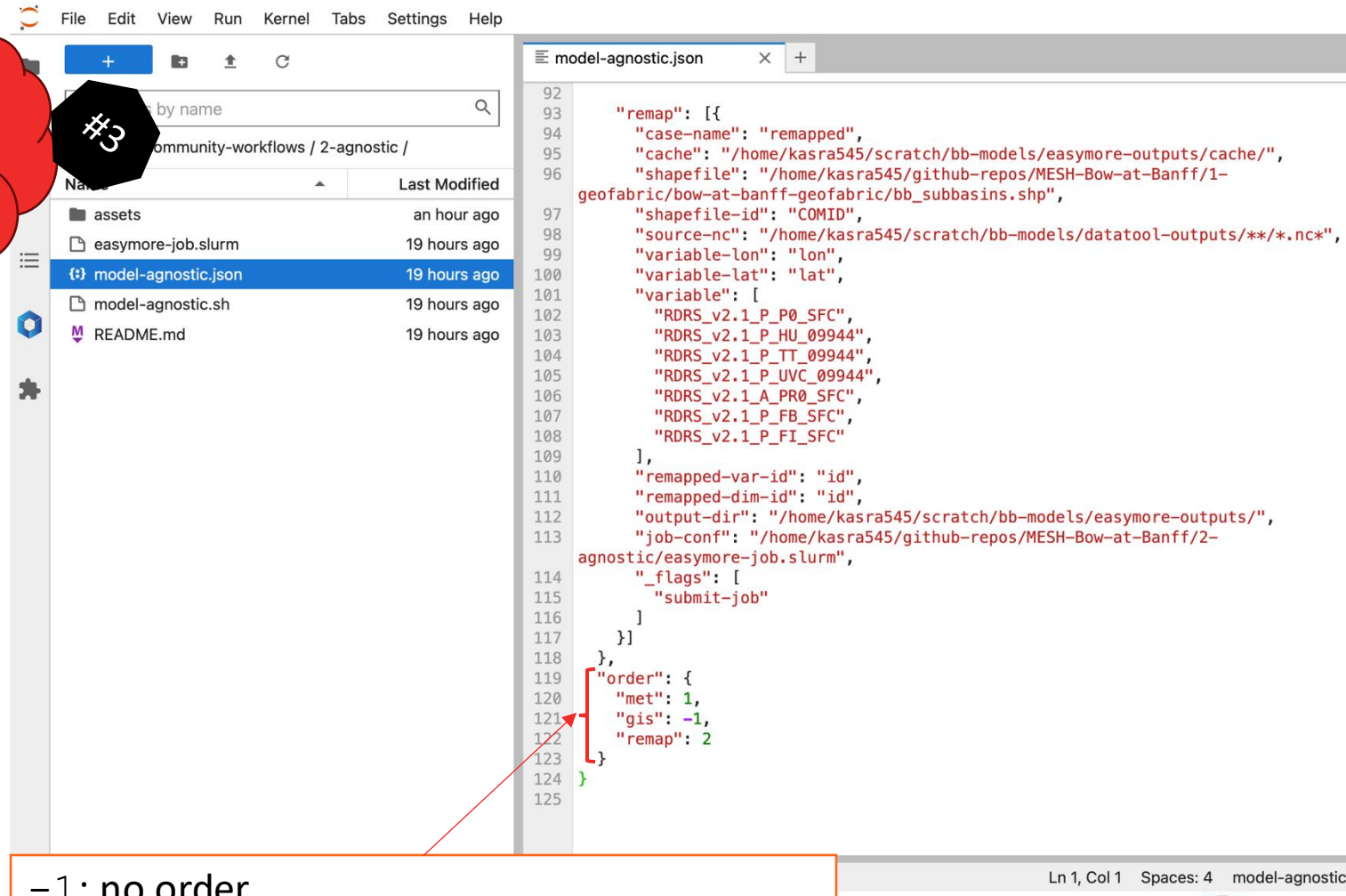
Setting up ECCC's National Water Model—MESH



: Order of process

Automated and ordered job submission to HPC



`-1`: no order
`ordered integers`: order of processes

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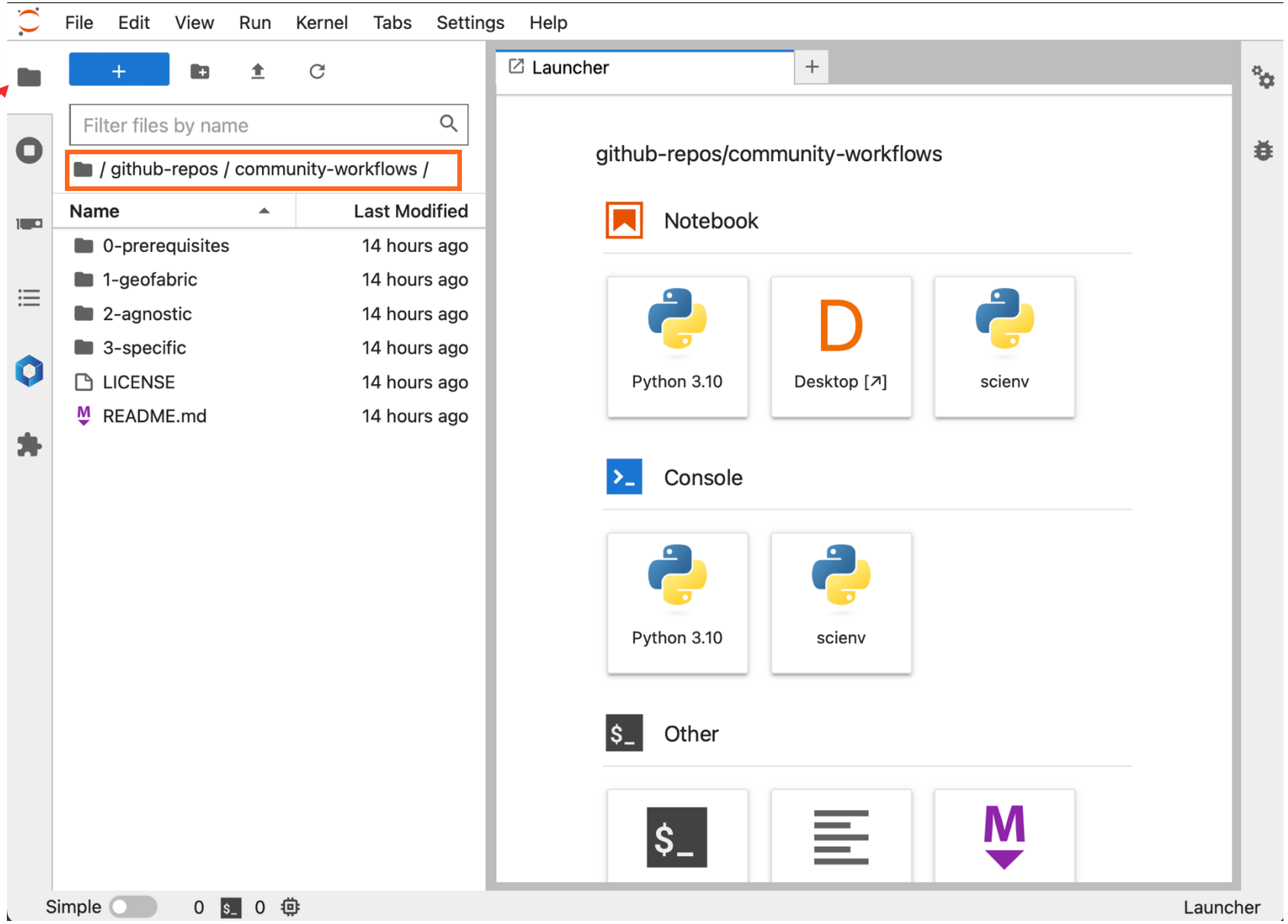
Any questions so far?

Setting up ECCC's National Water Model—MESH

Navigate using JupyterLab file browser



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Setting up ECCC's National Water Model—MESH

Third and final step is to run the model-specific processes

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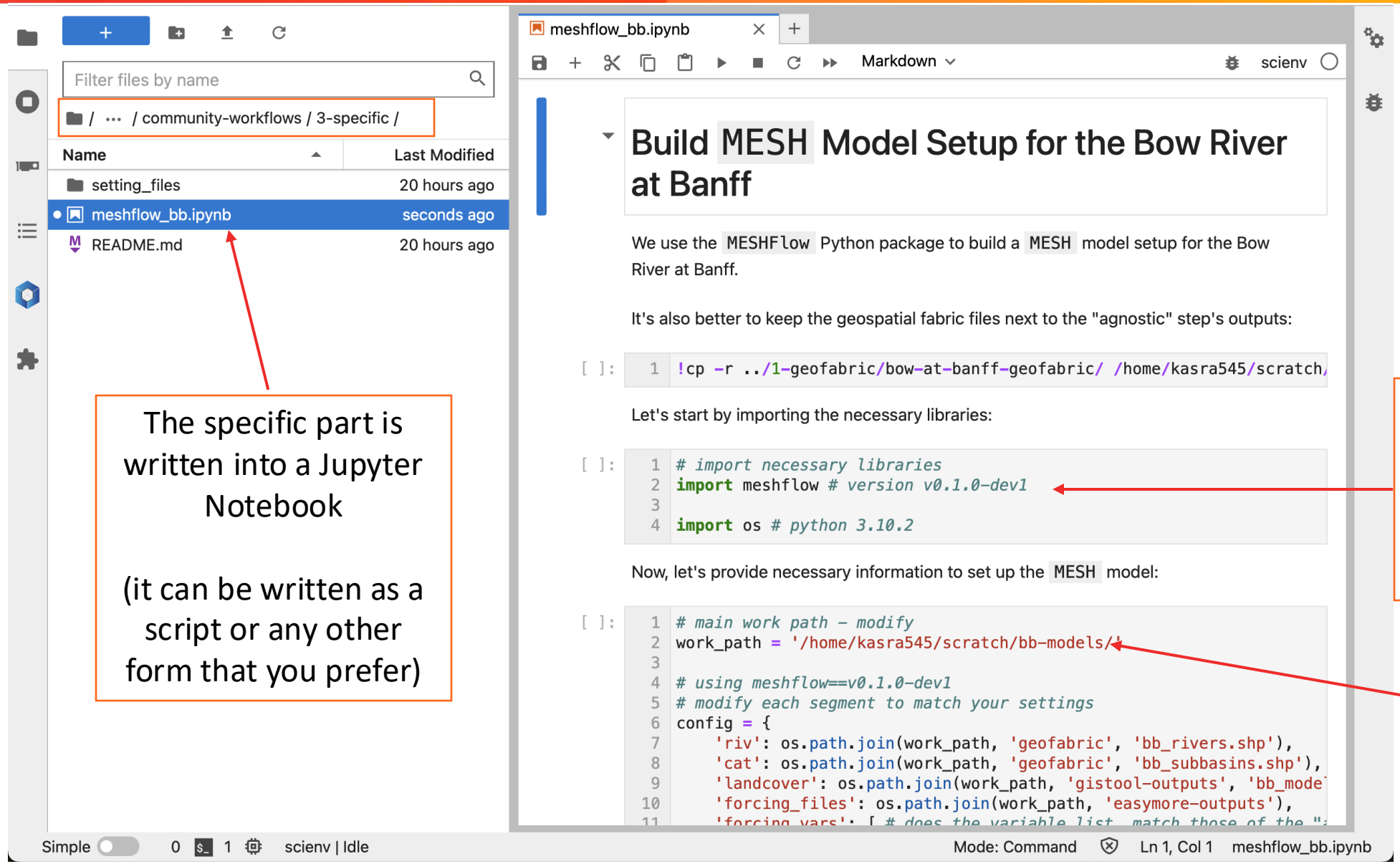
Setting up ECCC's National Water Model—MESH



The specific part is written into a Jupyter Notebook

(it can be written as a script or any other form that you prefer)

`Meshflow` is the package to build a MESH model out of all the data we processed so far

The root address of where the data is stored

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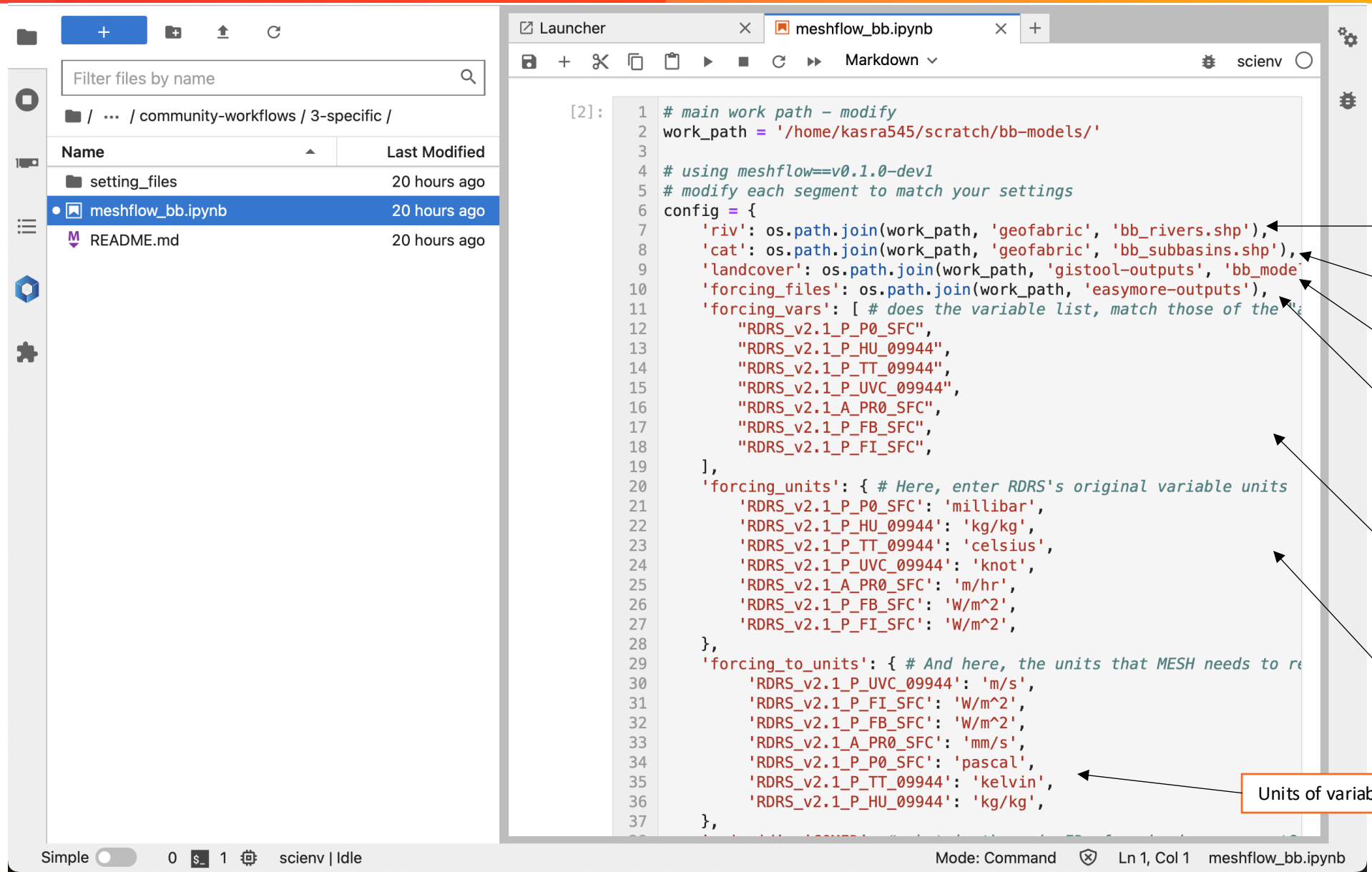
Setting up ECCC's National Water Model—MESH



River network geometry file

Subbasin geometry file

Landcover fractions file(s)

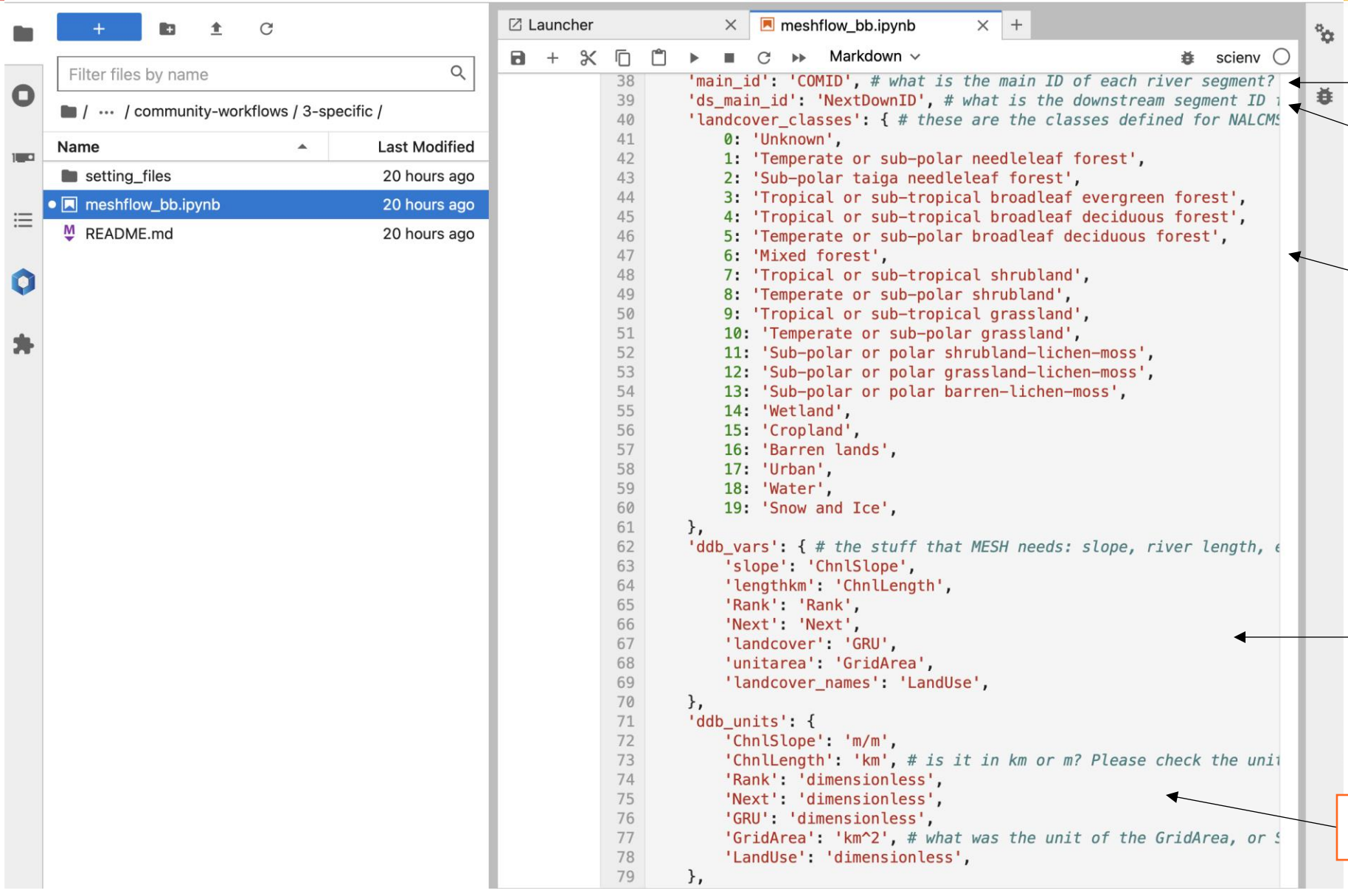
Prepared forcing file(s)

List of variables to be used

Variables' default units in the NetCDF files

Units of variables that MESH requires

Setting up ECCC's National Water Model—MESH



River Segment/Subbasin ID

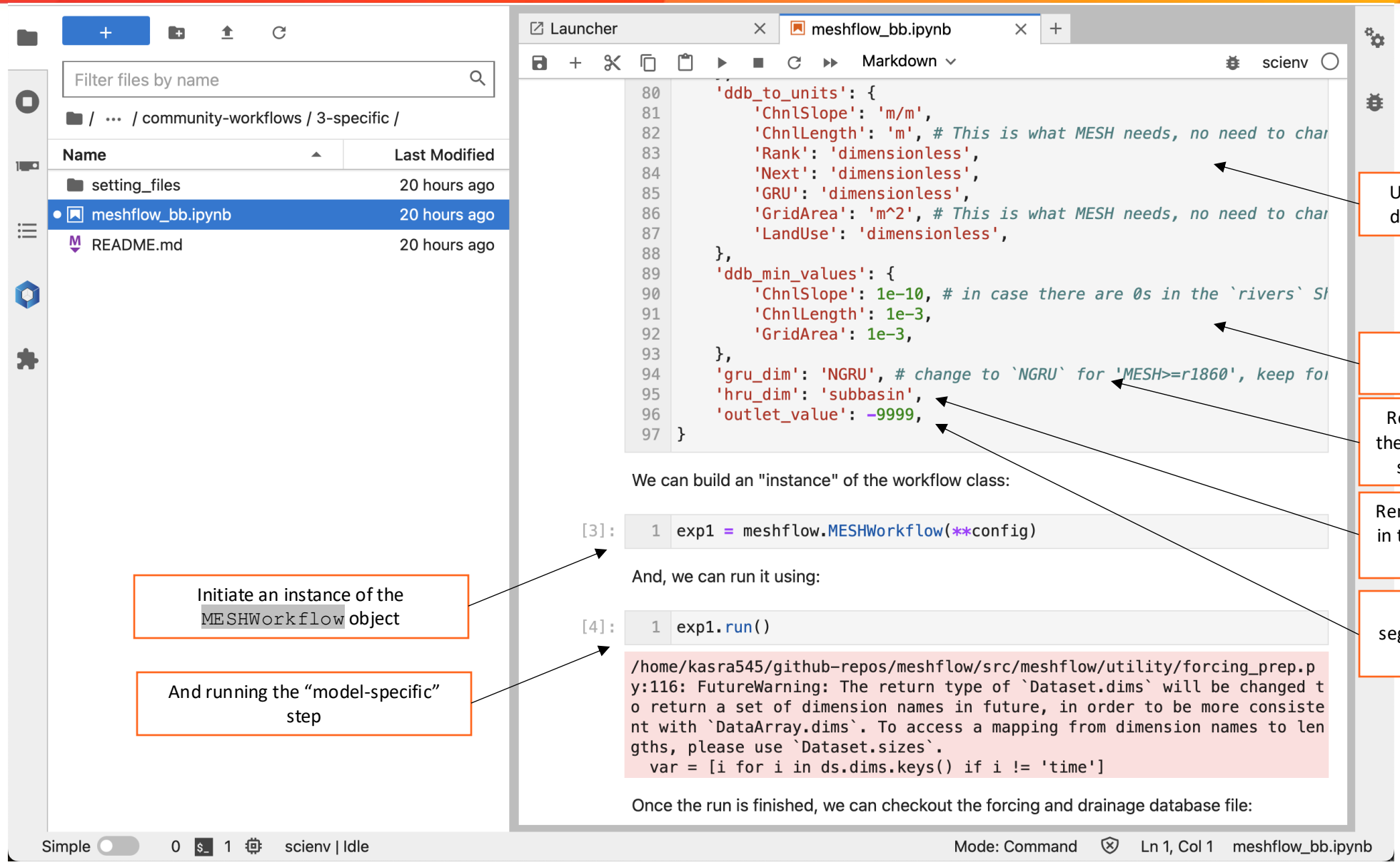
Downstream river segment/subbasin ID

Landcover classes of the landcover dataset used

All the variables to be used in the "drainage database" MESH file

Units of variables to be included in the "drainage database" MESH file

Setting up ECCC's National Water Model—MESH



Units of variables in the "drainage database" file that MESH requires

Minimum values of "drainage database" MESH file

Renaming GRU dimension name in the MESH "drainage database" file to satisfy diverse versions of MESH

Renaming sub-basin dimension name in the MESH "drainage database" file if needed

The value of the outlet river segments created using "`Hydrant`" (`Hydrant` default is `-9999`)

Initiate an instance of the `MESHWorkflow` object

And running the "model-specific" step

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Any questions so far?

Setting up ECCC's National Water Model—MESH

Switching to the relevant Jupyter Notebook webpage

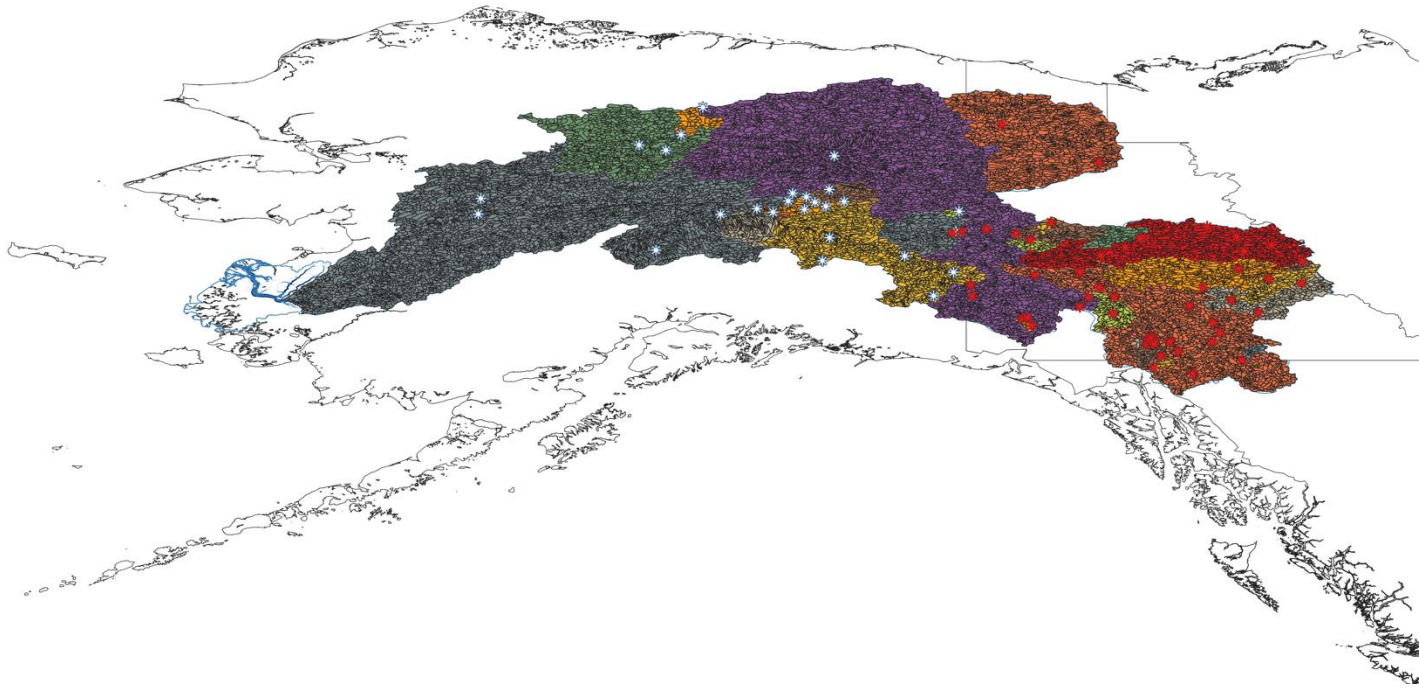
Outline

- Community Hydrological Modelling Recipes
- Computational Resources for the Training Session
- Setting up ECCC's National Water Model—MESH
- Introduction and Preview of CONFLUENCE

Brief background: Yukon River basin study

Research Question:

How can we optimally represent hydrological processes across diverse landscapes in modern process-based hydrological models?



Observations:

- 53 Stream gauges
- 86 Snow observation stations
- 35 sub-basins with in-situ snow observations

Model: SUMMA

- Flexible framework for model comparison
- 40 processes with multiple representation options
  - Space of possible combinations > 10^7
- 126 parameters to optimize for each combination

External decisions:

- Domain representation
- Forcing data
- Attribute data
- Etc.

Brief background:

Research Que

How can we optimally represent
processes across diverse landscape
hydrological m

Observations:

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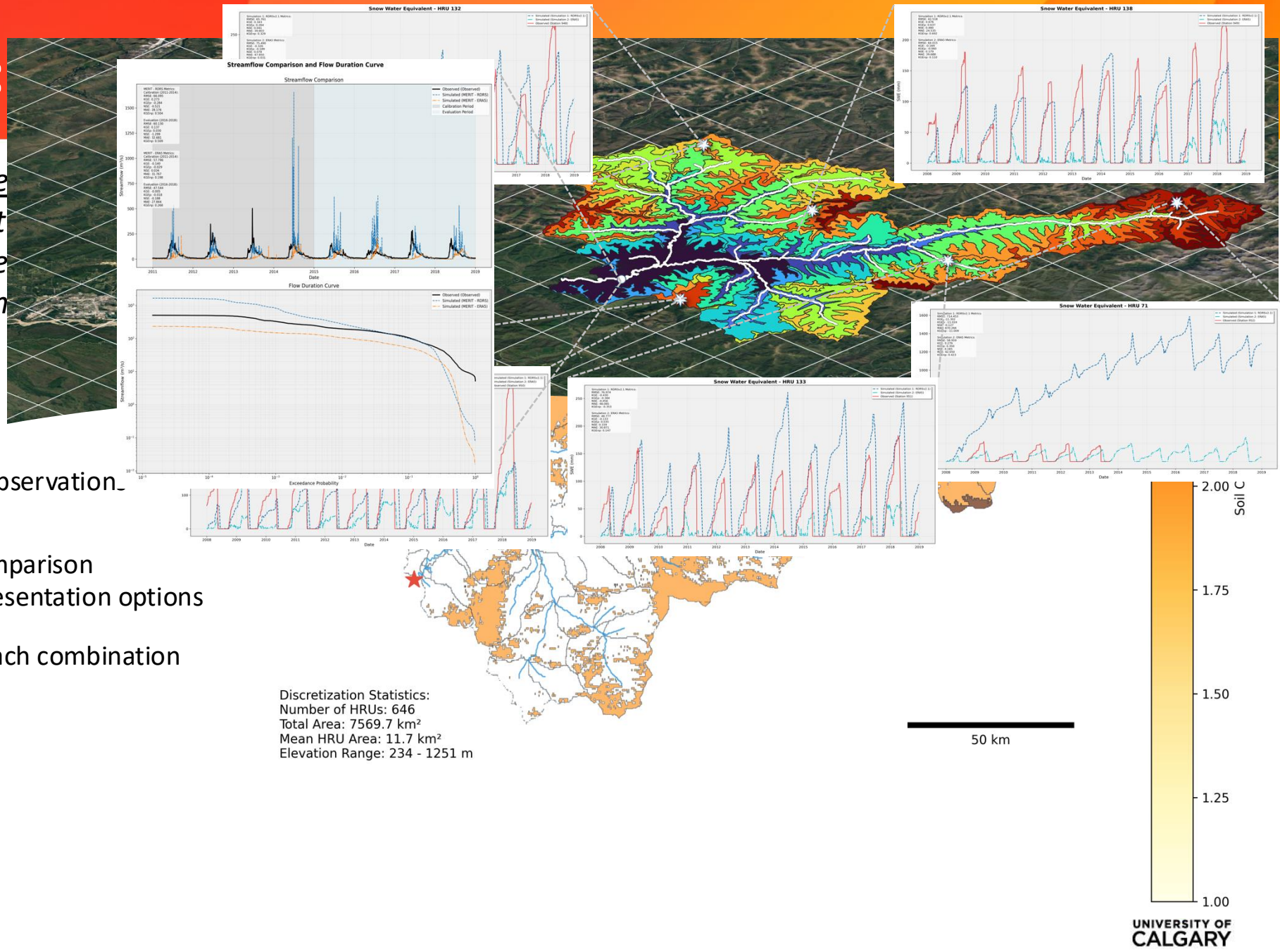
Model: SUMMA

- Flexible framework for model comparison
- ~40 processes with multiple representation options
  - Space of possible combinations > 10^7
- 126 parameters to calibrate for each combination

External decisions:

- Domain representation
- Forcing data
- Attribute data
- Etc.



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CONFLUENCE: Community Optimization Nexus For Large-domain Understanding of Environmental Networks and Computational Exploration

Problem:

The inherent complexity of modern process based hydrological models poses substantial challenges to researchers and operators, particularly due to the high dimensionality of the modelling decision space

Solution:

Automation of routine task through seamless integration of existing workflows with clear separation of technical implementation and scientific decision making.

Implementation:

- Single configuration file (YAML)
- Central workflow orchestration script
- Central workflow logging
- Modular design
- Extendable code base

CONFLUENCE

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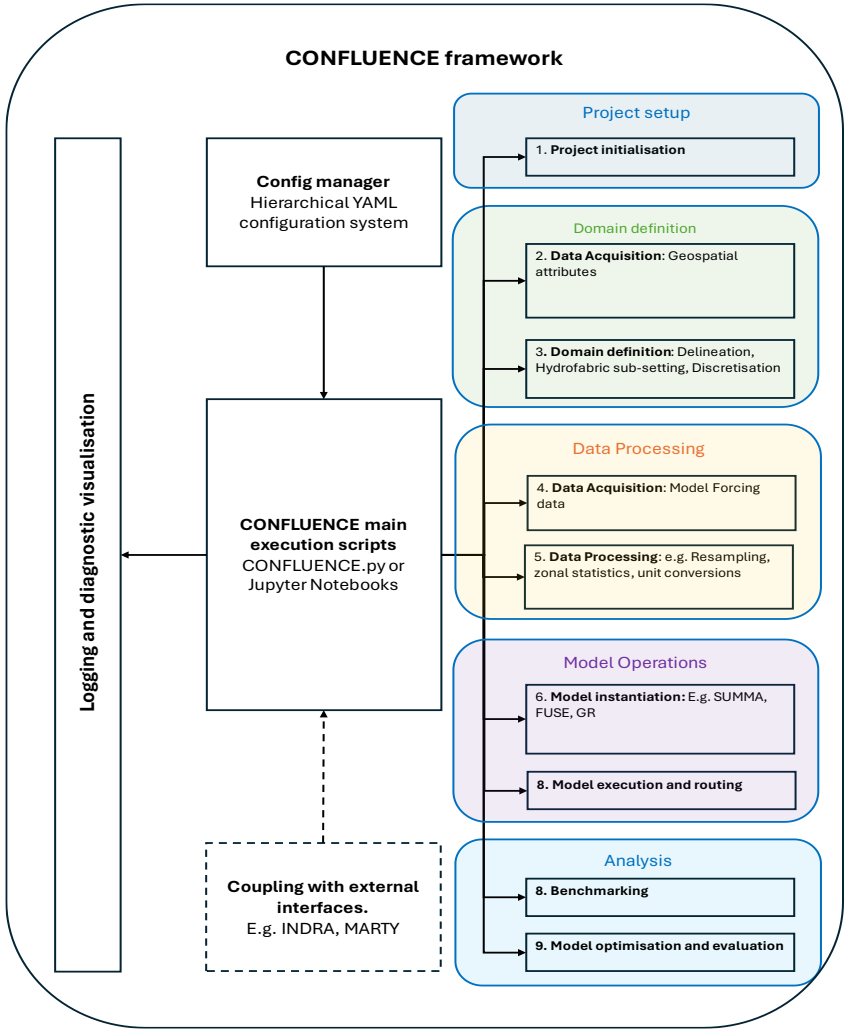

CONFLUENCE Workflow (Eythorsson et al., In prep.)

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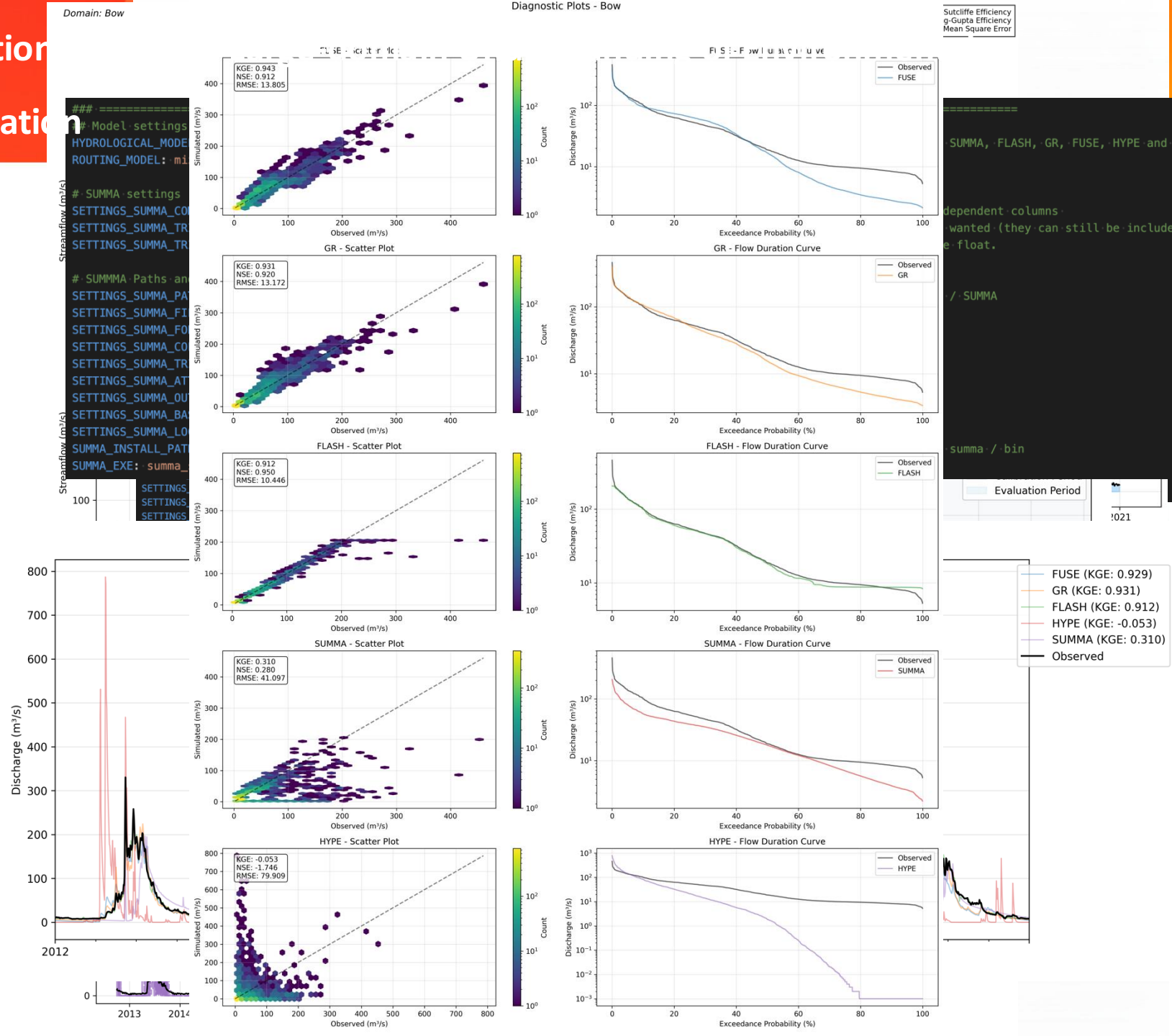
CONFLUENCE: Community Optimization Networks and Computational Exploration

- Configuration examples
  - Delineation
  - Discretization
  - Benchmarking
  - Model initiation
  - Model comparison



INDRA: Intelligent Network for Dynamic River Analysis

New problem:

Computational resource restrictions prohibit exhaustive search of the modelling decision space using current optimization algorithms

Solution:

Reduce dimensionality of decision space by selection of a domain expertise informed subset. Leverage novel developments in LLM contextual understanding and multi-agentic AI for decision support and automation of non-essential technical implementation through configuration generation.

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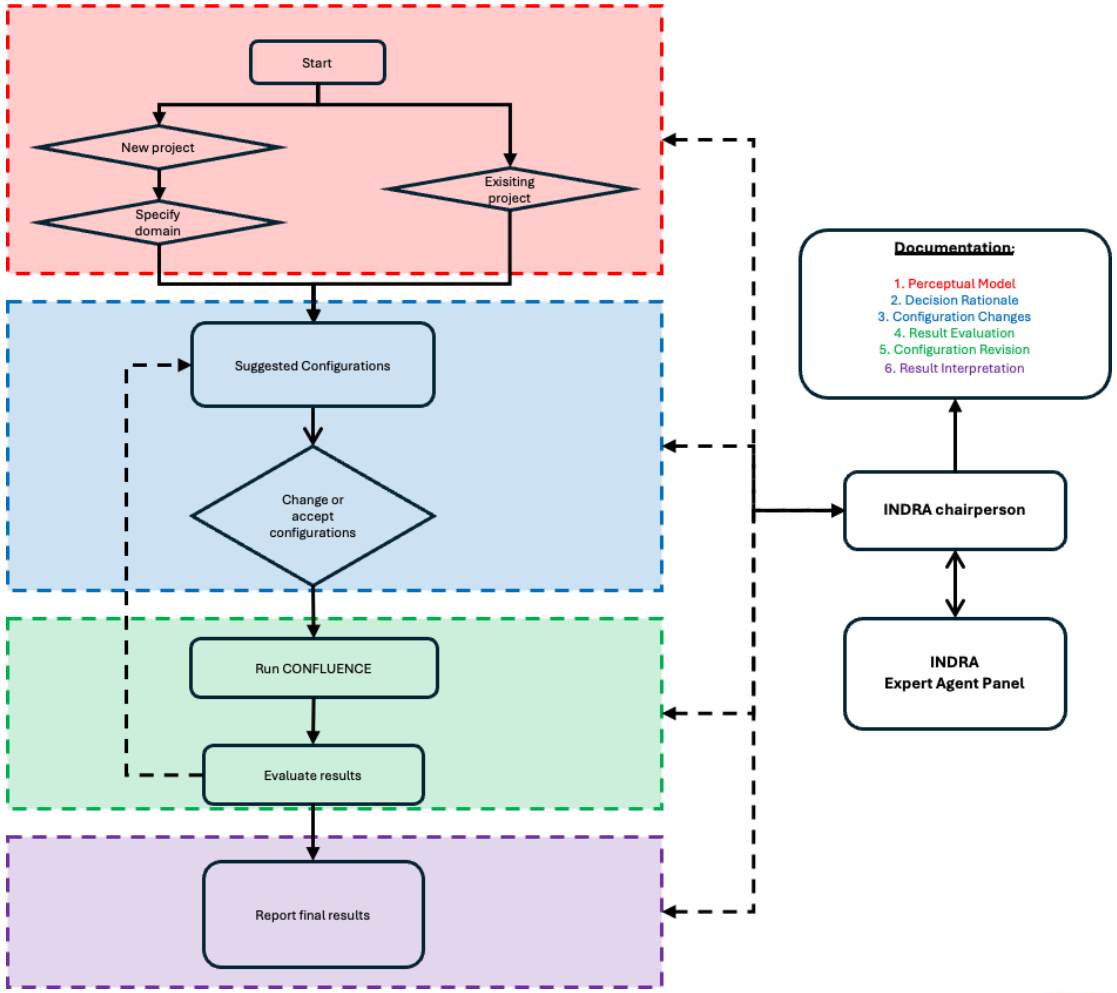
INDRA: Intelligent Network for Dynamic River Analysis

Implementation:

- CONFLUENCE coupling with a multi agent framework orchestrated by central LLM Moderator
- Moderator interacts with human operator and analyses natural language input to provide actionable decision support
- Moderator can create a panel of project appropriate AI subject matter experts to deliberate on each decision
- Moderator summarizes panel discussions and generates a CONFLUENCE config file with the suggested settings for the operator to consider.
- If approved moderator executes CONFLUENCE.
- After completed simulation Moderator generates a panel to analyze the results and suggest refinements
- Repeat until results are acceptable



INDRA (**I**ntelligent **N**etwork for **D**ynamic **R**iver **A**nalysis, (Eythorsson & Clark, 2025))

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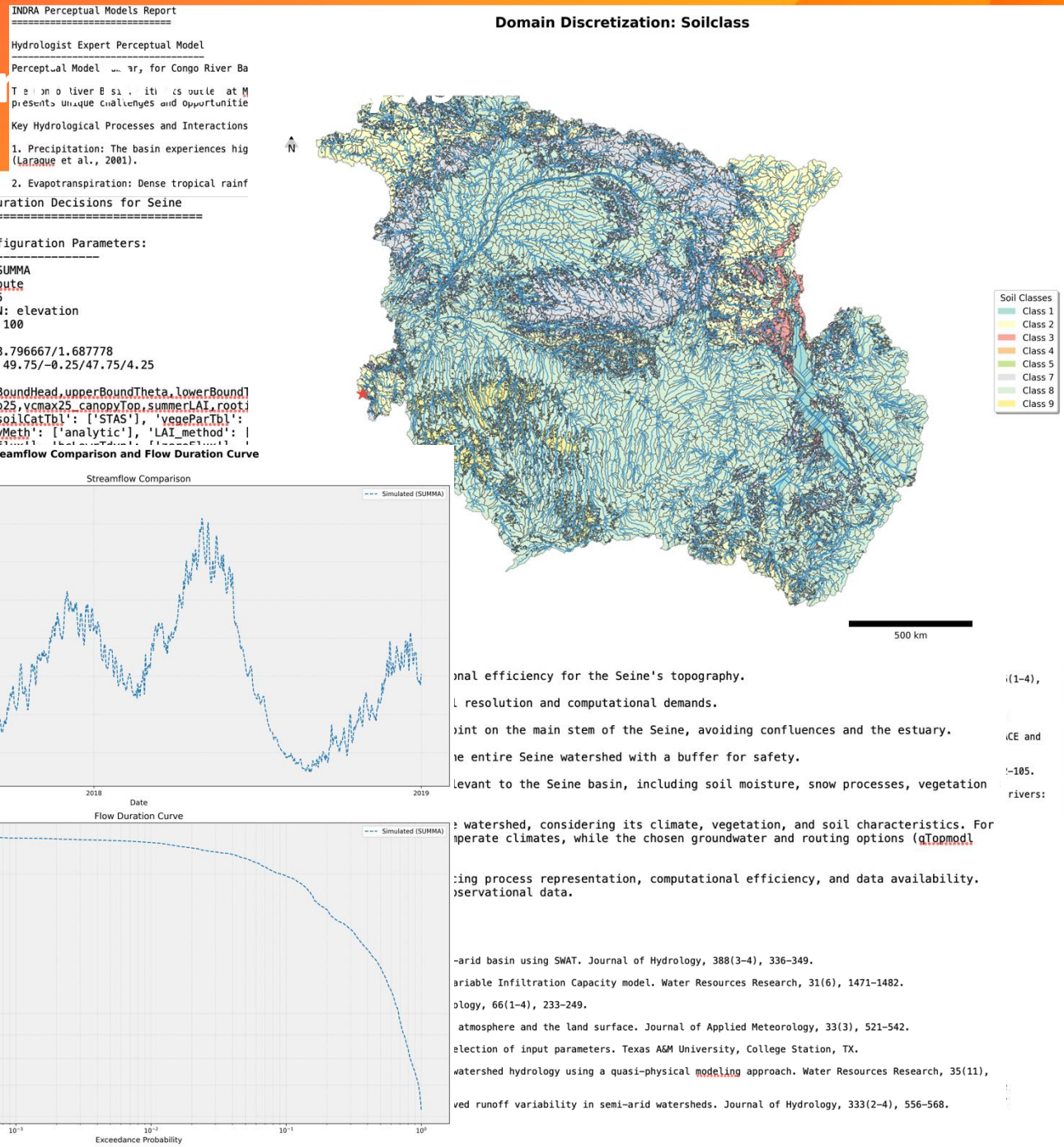
INDRA: Intelligent Network for Dynam

- Perceptual model generation
  - Not all LLMs created equal
  - Fast moving technology
- Configuration rationale
  - Collaborative conversation summary
- Prompt parsing, e.g.:
  - *python INDRA.py --purpose “Please create a SUMMA model for the Congo River”*



DELTA: Deliberately Expert Liquid Topography Assistant

Next problem:

Human and economic resource restrictions bottlenecks scientific exploration and documentation.

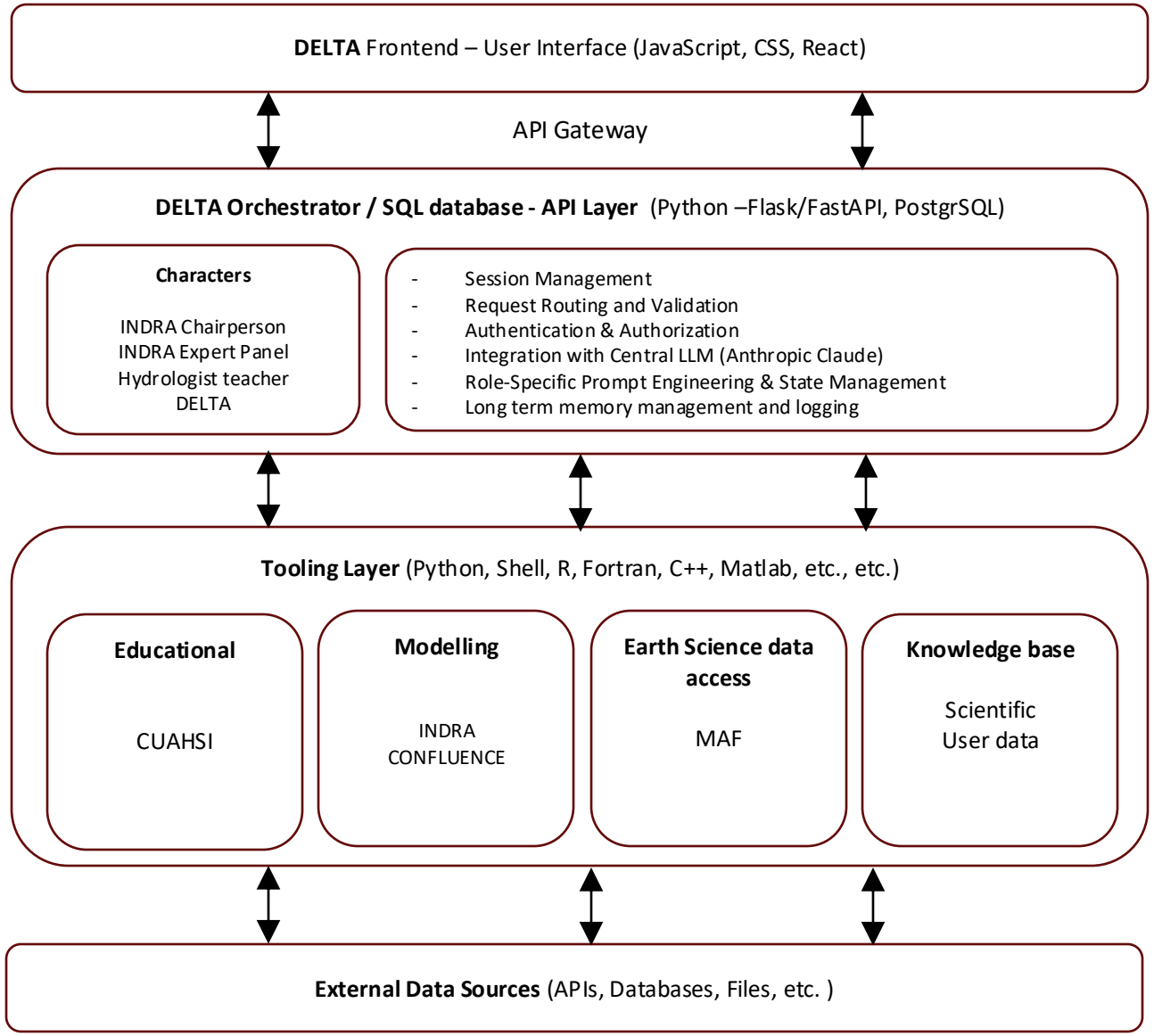
Solution:

Individual and domain tailored AI research assistance. With appropriate access to research tools such as MAF/INDRA/CONFLUENCE along with data and computational resources to use them. Freely available and easily accessible online in all languages.

DELTA: Deliberately Expert Liquid Topography Assistant

Implementation:

- Online frontend
  - User Interface
  - Collaborative exploration
  - Result exports
- Backend orchestration
  - Frontend API
  - LLM / AI / TTS service APIs
  - Misc. communication with tools
- Toolbox (extendable)
  - Modeling workflows (CONFLUENCE / INDRA)
  - Data analysis (MAF)
  - Knowledge database (SQL)
  - Educational content
- External data sources
- Protype framework online



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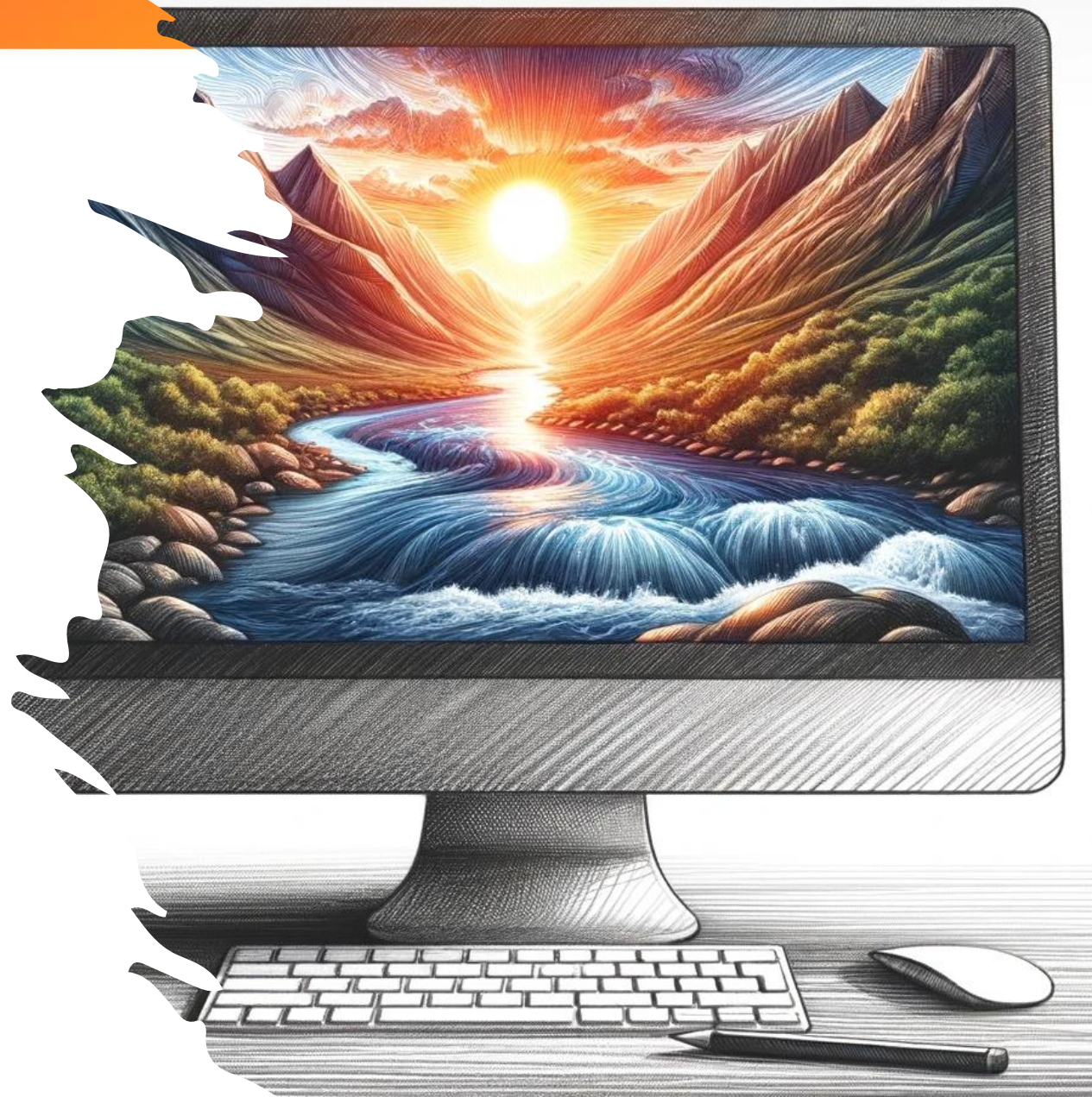
Future Directions

- Continue fusion of community assets
  - Design wrappers for individual assets
  - Optimize central architecture
- Develop AI enhancement, e.g.:
  - Validation protocols
  - Evaluation philosophy
  - Retrieval Augmented Generation (RAG)
  - Prompt engineering
- Develop interfaces
  - Develop integration philosophy
  - Estimate resource requirements



Thank you for attending

https://ucalgary.ca/civil

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Backup slides

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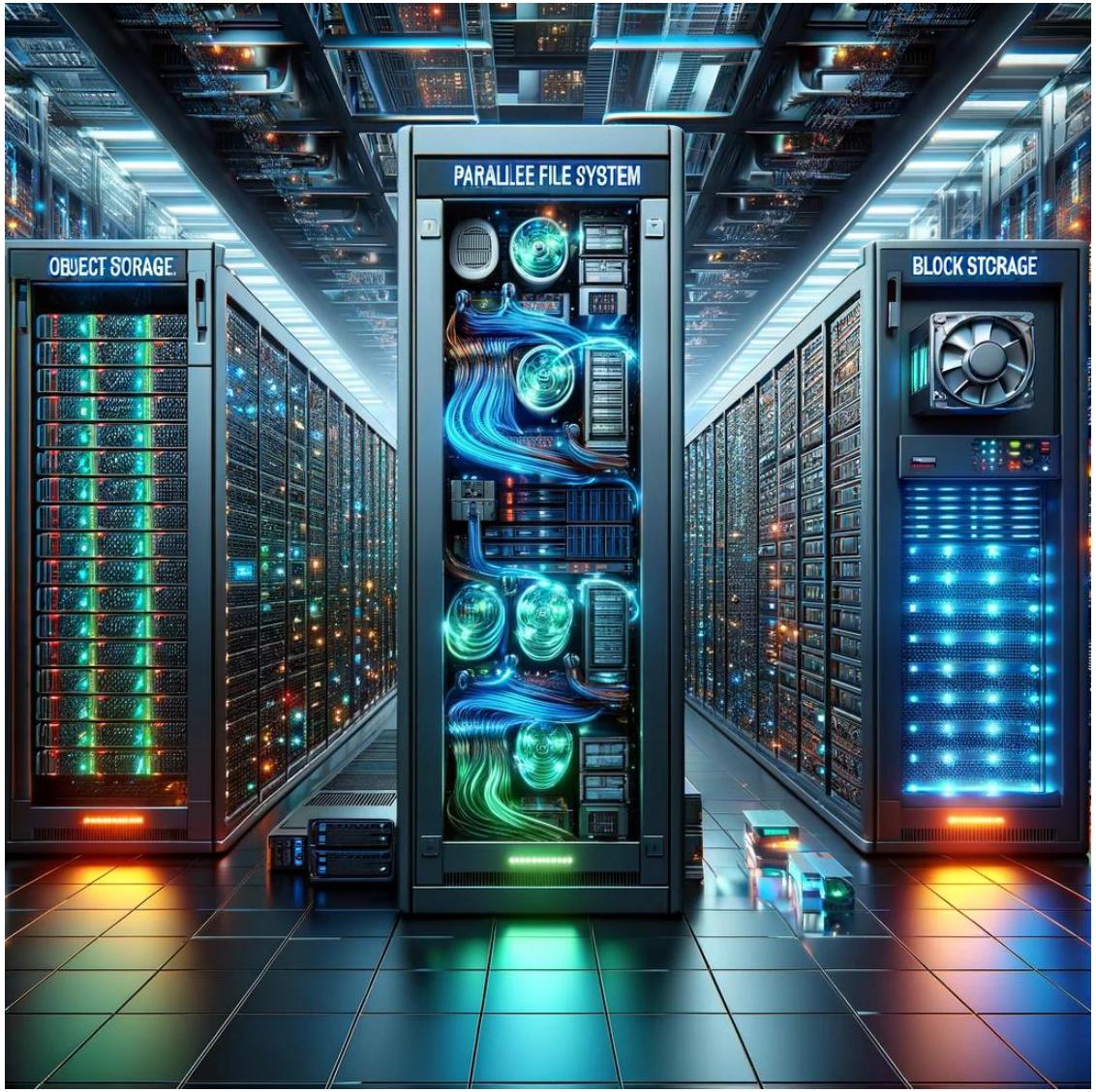
Computational Resources

1	Only for personal use	Home space 500 GB per user on ARC
2	Only for data processing	Scratch space 15 TB per experiment
3	NOT for personal use – only for shared resources	Project space comphyd_lab: 0.2 PB



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Any questions so far?

Computational Resources

Let’s set up our Python virtual environment

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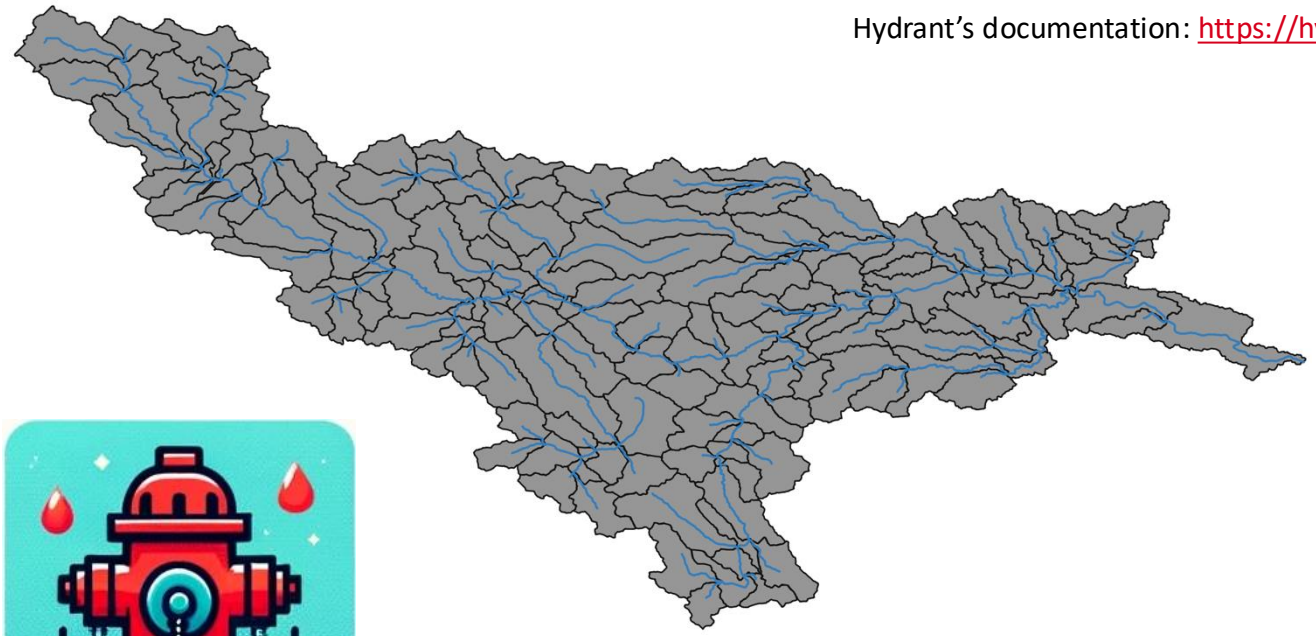
Setting up ECCC's National Water Model—MESH

How does `HydrAnT` help us?

Hydrant's documentation: https://hydrantpy.readthedocs.org

NetworkX
Network Analysis in Python



HYDRANT

Bow River at Banff

Sub-basins and river network extracted from `MERIT-Basins` using `Hydrant v0.1.0-dev0`

- Extracting subsets of hydrography datasets given a point or a boundary area,
- Hydrant is data-agnostic; if the input hydrography is valid and standard, you can use `Hydrant`,
- Common sanity checks for datasets:
  - Is water going upstream?
  - Is there a cycle of river segments?
  - etc.
- Aggregation methods to dissolve elements of hydrography datasets
- Knowledge extraction:
  - What is the longest branch of river segments?
  - What are the upstream segment of a certain point in the river network?
  - What are the downstream segments of a river segment?
  - What are the Strahler order of river segment?

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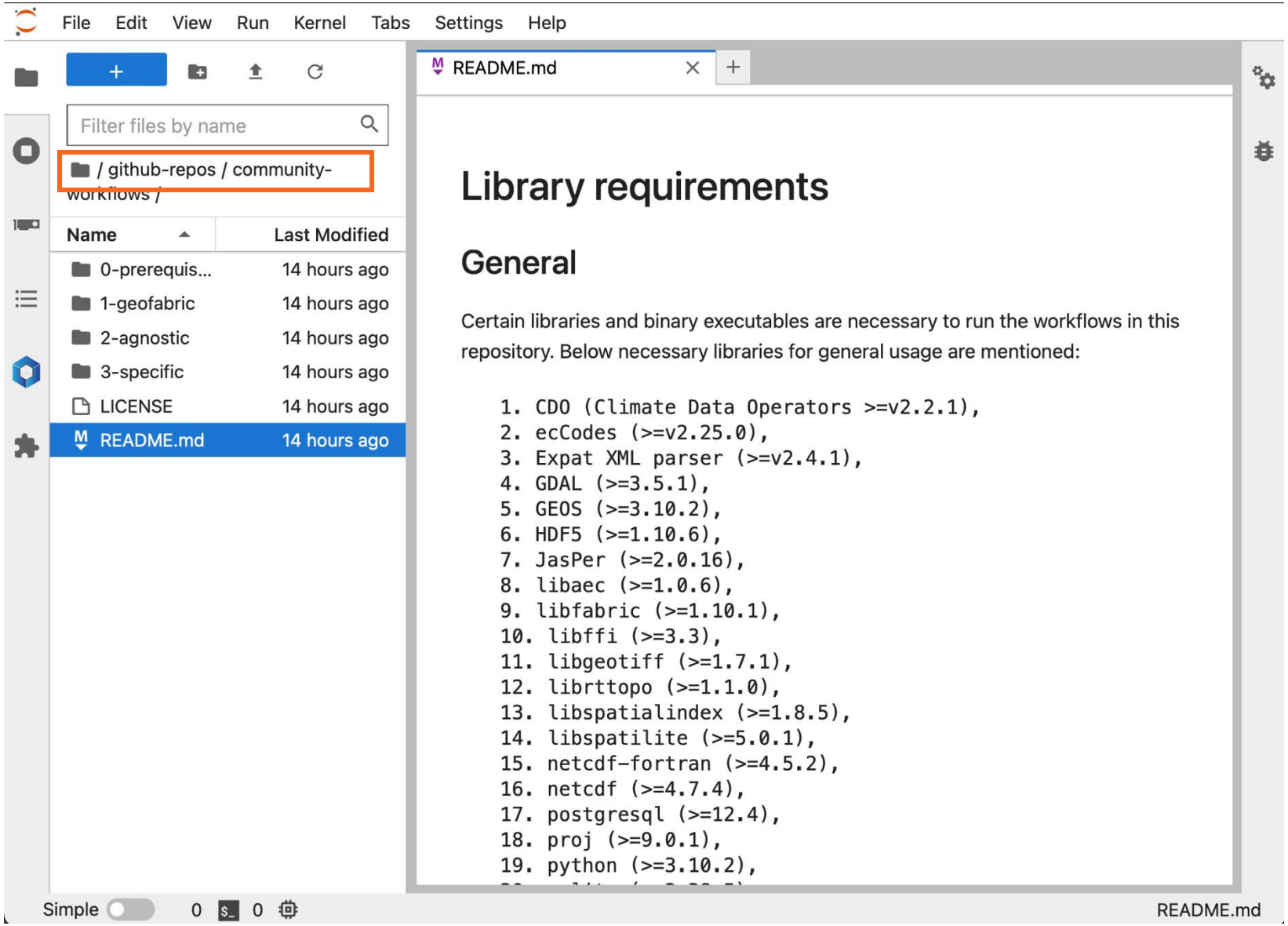
Practice Example – Bow River at Banff

Navigate using JupyterLab file browser



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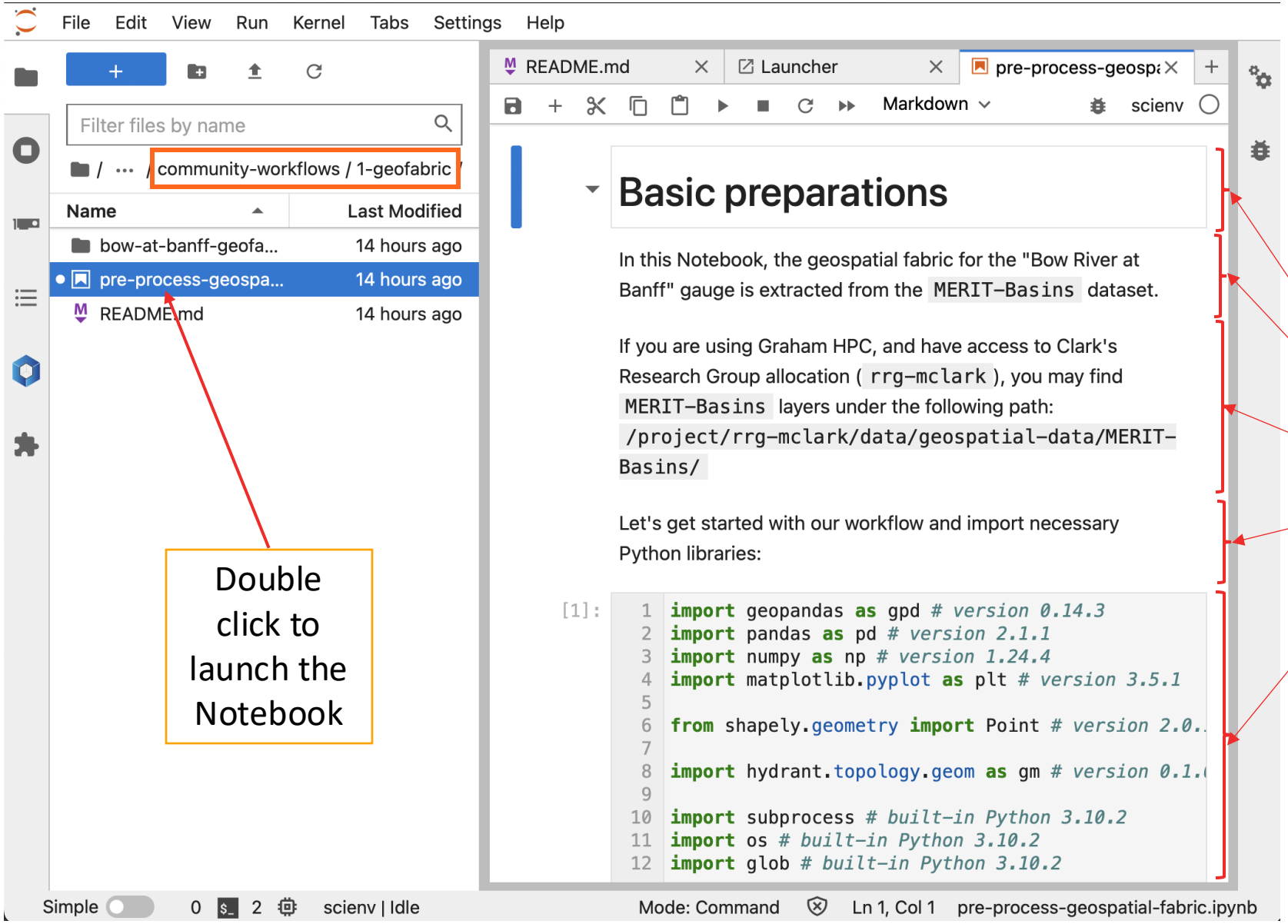
Setting up ECCC's National Water Model—MESH



Double click to launch the Notebook

Use "Shift + Enter" to execute Notebook cells

Notebook cells

Tip: review keyboard shortcuts!

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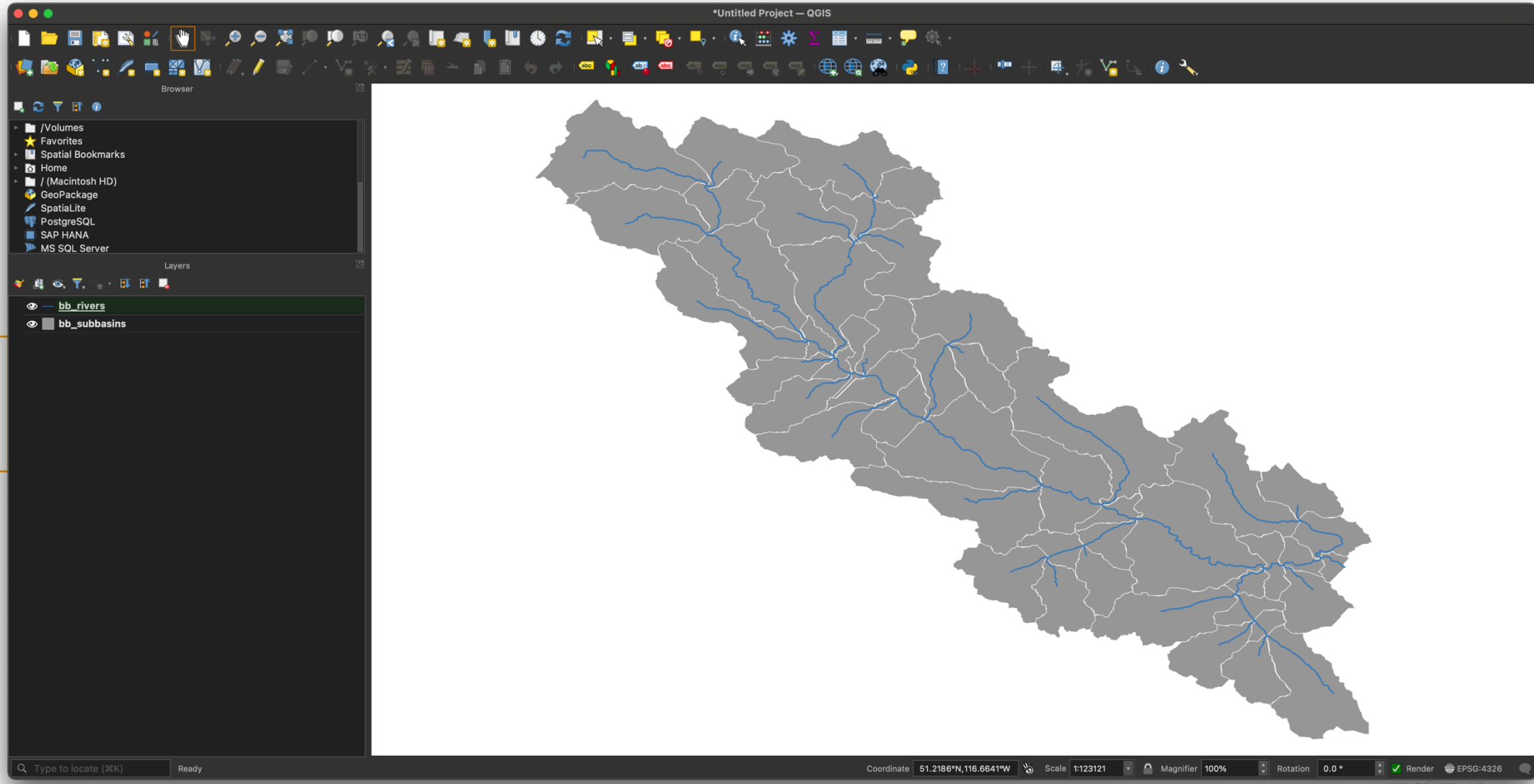
Setting up ECCC's National Water Model—MESH

You can view the extracted geospatial fabric in a typical GIS program, such as *QGIS*



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Future Directions