Community Hydrological Modelling Workflows

Online Training Session with Federal, Provincial, and Territorial Partners

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Acknowledgements

GLOBAL WATER FUTURES

Ouranos

Environment and Climate Change Canada

Environnement et Changement climatique Canada

Alberta Government

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

Yukon

Water Security Agency

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Outline

- Community Hydrological Modelling Recipe
- Digital Infrastructure on Digital Research Alliance of Canada's HPCs
- Introducing Community Workflows & Tools
- Practice Example – Bow River At Banff
- Troubleshooting

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Outline

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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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- Developing relevant workflows on High Performance Computing (HPC) facilities
- Keeping workflows open source and reproducible for the scientific community
- Keeping workflows efficient for real-world applications
- Separate “model-agnostic” and “model-specific” configuration parts

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.

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Digital Infrastructure

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

Science and Policy Decisions

Credit: Dr. Shervan Gharari

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Digital Infrastructure

Remote access accounts

- `rpp-kshook`
- `rrg-mclark`

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Digital Infrastructure

Our recommendation is to access Graham using either of the following methods:

jupyterlab

https://jupyterhub.sharcnet.ca/

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

Terminal

```
$ ssh USERNAME@graham.alliancecan.ca
```

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

MobaXTerm PuTTY MacOS Terminal

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Digital Infrastructure

jupyterhub

https://jupyterhub.sharcnet.ca/

jupyterhub

- Multi-user Server Service for Jupyter Sessions
- User Authentication Capability
- Resource Customization
- Customizable Work Environment

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Digital Infrastructure

Safe to ignore

rpp-kshook

rrg-mclark

Today's session is 3 hours only

How much memory you need? 16000 MB is enough for today

How many cores you need? 4 is more than enough for today

Do we do any Deep Learning? No.

Strong recommendation is to use JupyterLab interface

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Digital Infrastructure

https://jupyterhub.sharcnet.ca/

jupyterhub

DALLE generated image

General tips:

- Understand your setup: Be resourceful! Asking too much computational resource can keep you in the queue forever; public HPCs are shared resources. Asking for too little resources can make your Jupyter session slow and laggy.

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.

DALLE generated image

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Digital Infrastructure

Simple file browser

List of running kernels

GPU list
(is your workflow for Deep Learning?)

Headers of your notebooks
(just like your physical notebooks)

List of HPC modules
(explained later)

Jupyter Extensions
(disabled)

Kernel Status

Debug tools

List of kernels
as Notebooks

List of kernels
as consoles

Useful tools

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Digital Infrastructure

HPCs comes with various "**modules**"

But where are they?

Flexibility

Different users have different requirements

Customization

Users may need specific versions of software or libraries

DALLE generated image

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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Digital Infrastructure

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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Digital Infrastructure

All instructions are available on this presentation's repository:

https://github.com/kasra-keshavarz/community-modelling-workflow-training

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Digital Infrastructure

Exactly similar to what we can do in this tab

All instructions are available on this presentation's repository:

https://github.com/kasra-keshavarz/community-modelling-workflow-training

Loading "Standard Environment"

Loading Gnu C Compiler version 9.3.0

Loading every module we need

Saving all modules as a "collection" called "science modules"

Digital Infrastructure

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

Check out what module collections you have

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

Restore the "`scimods`" (science modules)

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

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Digital Infrastructure

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

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Digital Infrastructure

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

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Digital Infrastructure

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

The idea is to expand horizontally, instead of vertically.

HPC "nodes" are located inside a "rack enclosure"

DALLE generated image

jupyterhub

JupyterHub server lands your JupyterLab session on one these nodes
or, more clearly, "computing" nodes

On Digital Research Alliance HPCs, computing nodes do not have access to an active internet connection unfortunately

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Digital Infrastructure

First, we need to switch to the “login node”

Login nodes do have access to an active internet connection

File Edit View Run Kernel Tabs Settings Help

Filter files by name

/

Name	Last Modified
dask	a month ago
documents	2 days ago
downloads	22 days ago
empty_dir	2 years ago
github-rep...	7 hours ago
hydrologic...	3 months ago
library	13 days ago
nearline	2 months ago
projects	2 months ago
scratch	5 years ago
virtual-envs	5 hours ago
AFFECTED...	2 months ago
AFFECTED...	a month ago
count.sh	15 days ago
requireme...	6 hours ago

kasra545@gra807:~

```
[kasra545@gra807 ~]$ ssh gra-login1
Multifactor authentication is becoming mandatory to connect to this cluste
r.
You can enroll your account into multifactor authentication on this page:
https://ccdb.alliancecan.ca/multi_factor_authentications
by following the instructions available here:
https://docs.alliancecan.ca/wiki/Multifactor_authentication

================================================================================
===

L'authentification multifacteur sera bientôt  obl
ter
à cette grappe. Configurez votre compte  sur
https://ccdb.alliancecan.ca/multi_factor_authentications
et suivez les directives dans
https://docs.alliancecan.ca/wiki/Multifactor_authentication/fr.
Password:
```

Secure SHell (ssh) to a login node of choice

Enter your Digital Research Alliance account password

Simple 1 1 kasra545@gra807:~

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Digital Infrastructure

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

You are logged into a “login node” with an active internet connection

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Digital Infrastructure

File Edit View Run Kernel Tabs Settings Help

Filter files by name

/

Name	Last Modified
dask	a month ago
documents	2 days ago
downloads	22 days ago
empty_dir	2 years ago
github-rep...	7 hours ago
hydrologic...	3 months ago
library	13 days ago
nearline	2 months ago
projects	2 months ago
scratch	5 years ago
virtual-envs	5 hours ago
AFFECTED...	2 months ago
AFFECTED...	a month ago
count.sh	15 days ago
requireme...	7 hours ago

kasra545@gra-login1:~

```
[kasra545@gra-login1 ~]$ mkdir -p ./github-repos
[kasra545@gra-login1 ~]$ git clone https://github.com/kasra-keshavarz/comm
unity-modelling-workflow-training.git ./github-repos/
fatal: destination path './github-repos' already exists and is not an empt
y directory.
[kasra545@gra-login1 ~]$ git clone https://github.com/kasra-keshavarz/comm
unity-modelling-workflow-training.git ./github-repos/community-workflows
Cloning into './github-repos/community-workflows'...
remote: Enumerating objects: 64, done.
remote: Counting objects: 100% (64/64), done.
remote: Compressing objects: 100% (52/52), done.
remote: Total 64 (delta 11), reused 56 (delta 7), pack-reused 0
Receiving objects: 100% (64/64), 521.57 KiB | 4.01 MiB/s, done.
Resolving deltas: 100% (11/11), done.
[kasra545@gra-login1 ~]$
```

Create a “github-repos” directory to organize downloaded repositories

“clone”-ing the repository

Simple 1 1 kasra545@gra-login1:~

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Digital Infrastructure

1	Only for personal use	Home space 50 GB per user
2	Only for data processing	Scratch space 20 TB per user
3	NOT for personal use – only for shared resources	Project space rrp-kshook: 2.5 PB rrg-mclark: 0.2 PB

Digital Infrastructure

Let’s set up our Python virtual environment

DALLE generated image

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Digital Infrastructure

Although the modules are loaded in your JupyterLab session, Terminal is a separate entity, and we must reload the modules there as well:

Filter available modules...

LOADED MODULES

CCconfig
gentoo/2020
imkl/2020.1.217
intel/2020.1.217
ucx/1.8.0
libfabric/1.10.1
openmpi/4.0.3
StdEnv/2020
mii/1.1.2
libffi/3.3
python/3.10.2
ipykernel/2023b
ipython-kernel/3.10

AVAILABLE MODULES (1233)

StdEnv/2016.4
StdEnv/2018.3
StdEnv/2023
abaqus/2021
abinit/9.2.2
abinit/9.6.2
actc/1.1
adf/2019.305
admixture/1.3.0

kasra545@gra-login1:~

```
[kasra545@gra-login1 ~]$ module restore scimods
Restoring modules from user's scimods
[kasra545@gra-login1 ~]$ module list

Currently Loaded Modules:
  1) CCconfig                    20) cdo/2.2.1                    (geo)
  2) gentoo/2020        (S)      21) libffi/3.3
  3) StdEnv/2020        (S)      22) hdf5/1.10.6                  (io)
  4) cmake/3.27.7       (t)      23) libgeotiff-proj901/1.7.1
  5) sqlite/3.38.5               24) librttopo-proj9/1.1.0
  6) geos/3.10.2        (geo)    25) proj/9.0.1                   (geo)
  7) postgresql/12.4    (t)      26) eccodes/2.25.0               (geo)
  8) udunits/2.2.28     (t)      27) netcdf-fortran/4.5.2         (io)
  9) imkl/2020.1.217    (math)   28) mii/1.1.2
 10) gcccore/.9.3.0     (H)      29) ucx/1.8.0
 11) gcc/9.3.0          (t)      30) python/3.10.2                (t)
 12) jasper/2.0.16      (vis)    31) netcdf/4.7.4                 (io)
 13) libaec/1.0.6               32) cfitsio/4.1.0                (vis)
 14) ipykernel/2023b            33) freexl/1.0.5                 (t)
 15) scipy-stack/2023b  (math)   34) libspatialite-proj901/5.0.1
 16) gdal/3.5.1         (geo)    35) expat/2.4.1                  (t)
 17) libfabric/1.10.1           36) yaxt/0.9.0                   (t)
 18) openmpi/4.0.3      (m)      37) libspatialindex/1.8.5        (phys)
 19) mpi4py/3.1.3       (t)      38) arrow/13.0.0                 (t)

  Where:
   S:      Module is Sticky, requires --force to unload or purge
   m:      MPI implementations / Implémentations MPI
   math:   Mathematical libraries / Bibliothèques mathématiques
   io:     Input/output software / Logiciel d'écriture/lecture
   t:      Tools for development / Outils de développement
   vis:    Visualisation software / Logiciels de visualisation
   geo:    Geography libraries/apps / Logiciels de géographie
   phys:   Physics libraries/apps / Logiciels de physique
   H:                Hidden Module
```

Simple 1 1 kasra545@gra-login1:~

restoring "`scimods`"

Checking what has been loaded

Is it equal to the list on left?

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Digital Infrastructure

Filter available modules...

LOADED MODULES

CCconfig
gentoo/2020
imkl/2020.1.217
intel/2020.1.217
ucx/1.8.0
libfabric/1.10.1
openmpi/4.0.3
StdEnv/2020
mii/1.1.2
libffi/3.3
python/3.10.2
ipykernel/2023b
ipython-kernel/3.10

AVAILABLE MODULES (1233)

StdEnv/2016.4
StdEnv/2018.3
StdEnv/2023
abaqus/2021
abinit/9.2.2
abinit/9.6.2
actc/1.1
adf/2019.305
admixture/1.3.0

kasra545@gra-login1:~

```
 10) gcccore/.9.3.0     (H)      29) ucx/1.8.0
 11) gcc/9.3.0          (t)      30) python/3.10.2                (t)
 12) jasper/2.0.16      (vis)    31) netcdf/4.7.4                 (io)
 13) libaec/1.0.6                32) cfitsio/4.1.0                (vis)
 14) ipykernel/2023b             33) freexl/1.0.5                 (t)
 15) scipy-stack/2023b (math)    34) libspatialite-proj901/5.0.1
 16) gdal/3.5.1         (geo)    35) expat/2.4.1                  (t)
 17) libfabric/1.10.1            36) yaxt/0.9.0                   (t)
 18) openmpi/4.0.3      (m)      37) libspatialindex/1.8.5        (phys)
 19) mpi4py/3.1.3       (t)      38) arrow/13.0.0                 (t)

  Where:
   S:     Module is Sticky, requires --force to unload or purge
   m:     MPI implementations / Implémentations MPI
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   io:    Input/output software / Logiciel d'écriture/lecture
   t:     Tools for development / Outils de développement
   vis:   Visualisation software / Logiciels de visualisation
   geo:   Geography libraries/apps / Logiciels de géographie
   phys:  Physics libraries/apps / Logiciels de physique
   H:                Hidden Module


[kasra545@gra-login1 ~]$ python -m venv --version
usage: venv [-h] [--system-site-packages] [--symlinks | --copies]
            [--clear] [--upgrade] [--without-pip] [--prompt PROMPT]
            [--upgrade-deps]
            ENV_DIR [ENV_DIR ...]
venv: error: the following arguments are required: ENV_DIR
[kasra545@gra-login1 ~]$ python -m virtualenv --version
virtualenv 20.13.0 from /cvmfs/soft.computecanada.ca/easybuild/software/20
20/avx2/Core/python/3.10.2/lib/python3.10/site-packages/virtualenv/__init_
_.py
[kasra545@gra-login1 ~]$
```

Are we all using the same version?

Simple 1 1 kasra545@gra-login1:~

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Digital Infrastructure

Filter available modules...

LOADED MODULES

CCconfig
gentoo/2020
imkl/2020.1.217
intel/2020.1.217
ucx/1.8.0
libfabric/1.10.1
openmpi/4.
StdEnv/202
mii/1.1.2
libffi/3.3

"virtual-envs" directory is in your home directory

Now build a Python Virtual Environment; put it under the "virtual-envs" directory, and call it "scienv" after switching to a "login node"

abaqus/2021
abinit/9.2.2
abinit/9.6.2
actc/1.1
adf/2019.305
admixture/1.3.0

kasra545@gra-login1:~

```
 11) gcc/9.3.0          (t)     30) python/3.10.2                (t)
 12) jasper/2.0.16      (vis)   31) netcdf/4.7.4                 (io)
 13) libaec/1.0.6               32) cfitsio/4.1.0                (vis)
 14) ipykernel/2023b            33) freexl/1.0.5                 (t)
 15) scipy-stack/2023b (math)   34) libspatialite-proj901/5.0.1
 16) gdal/3.5.1         (geo)   35) expat/2.4.1                  (t)
 17) libfabric/1.10.1           36) yaxt/0.9.0                   (t)
 18) openmpi/4.0.3      (m)     37) libspatialindex/1.8.5        (phys)
 19) mpi4py/3.1.3       (t)     38) arrow/13.0.0                 (t)

 Where:
                 Module is Sticky, requires --force to unload or purge
                 MPI implementations / Implémentations MPI
                 Mathematical libraries / Bibliothèques mathématiques
                 Input/output software / Logiciel d'écriture/lecture
   t:            Tools for development / Outils de développement
   vis:          Visualisation software / Logiciels de visualisation
   geo:          Geography libraries/apps / Logiciels de géographie
   phys:         Physics libraries/apps / Logiciels de physique
   H:                      Hidden Module


sra545@gra-login1 ~]$ python -m venv --version
ge: venv [-h] [--system-site-packages] [--symlinks | --copies]
         [--clear] [--upgrade] [--without-pip] [--prompt PROMPT]
         [--upgrade-deps]
         ENV_DIR [ENV_DIR ...]
venv: error: the following arguments are required: ENV_DIR
[kasra545@gra-login1 ~]$ python -m virtualenv --version
virtualenv 20.13.0 from /cvmfs/soft.computecanada.ca/easybuild/software/20
20/avx2/Core/python/3.10.2/lib/python3.10/site-packages/virtualenv/__init_
_.py
[kasra545@gra-login1 ~]$ python -m virtualenv              ./virtual-envs
/scienv
```

Simple 1 1 kasra545@gra-login1:~

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Digital Infrastructure

After creation, let's activate the virtual environment

Install the packages included in the training session's repository

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Digital Infrastructure

Filter available modules...

LOADED MODULES

CCconfig
gentoo/2020
imkl/2020.1.217
intel/2020.1.217
ucx/1.8.0
libfabric/1.10.1
openmpi/4.0.3
StdEnv/2020
mii/1.1.2
libffi/3.3
python/3.10.2
ipykernel/2023b
ipython-kernel/3.10

AVAILABLE MODULES (1233)

StdEnv/2016.4
StdEnv/2018.3
StdEnv/2023

kasra545@gra-login1:~

```
(scienv ) [kasra545@gra-login1 ~]$ python -m ipykernel install --user --na
me "scienv "
Installed kernelspec scienv  in /home/kasra545/.local/share/jupyter/kernel
s/scienv
(scienv ) [kasra545@gra-login1 ~]$
```

"scienv" virtual environment is now accessible through JupyterLab

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Digital Infrastructure

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

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Introducing Community Workflows & Tools

- NCAR-GWF WRF CONUS I
- ECMWF ERA5
- ECCC RDRSv2.1
- NCAR-GWF WRF CONUS II
- CCRN CanRCM4-WFDEI-CaPA
- CCRN WFDEI-GEM-CaPA
- AMES GDDP-CMIP6
- Ouranos ESPO-G6-R2 RDRSv2.1
- Ouranos CRCM5-CMPI6

.
.
.

~1 PB of data
(and growing)

→ Command Line Interface (CLI)

```
./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;
```

Steps:

1. Login to Digital Alliance of Canada (formerly Compute Canada) Graham cluster,
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/kasra-keshavarz/datatool

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DALL-E generate image

Introducing Community Workflows & Tools

- MERIT-Hydro
- Soil Grids V1
- MODIS Land Cover
- Landsat NALCMS
- Depth to bedrock
- Global Soil Dataset (GSDE)

.
.
.

→ Command Line Interface (CLI) →

- Subsetting Geo-spatial data in GeoTIFF format
- Implementing Zonal Statistics for ESRI Shapefiles efficiently
- Calculating Slope & Aspect [in progress]
- HRUs discretization in any spatial scale [in progress]

Steps:

1. Login to Digital Alliance of Canada (formerly Compute Canada) Graham cluster,
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/kasra-keshavarz/gistool

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Introducing Community Workflows & Tools

```
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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Outline

- Community Hydrological Modelling Recipe
- Digital Infrastructure on Digital Research Alliance of Canada's HPCs
- Introducing Community Workflows & Tools
- Practice Example – Bow River At Banff
- Troubleshooting

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Practice Example – Bow River at Banff

Bow River at Banff

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

All instructions are available on this presentation's repository:

https://github.com/kasra-keshavarz/community-modelling-workflow-training

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Practice Example – Bow River at Banff

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

DALLE generated image

Practice Example – Bow River at Banff

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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Practice Example – Bow River at Banff

Bow River at Banff

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

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

Good read: http://switchfromshapefile.org

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.

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Practice Example – Bow River at Banff

How does `HydrAnT` help us?

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

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?

Practice Example – Bow River at Banff

Navigate using JupyterLab file browser

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Practice Example – Bow River at Banff

File Edit View Run Kernel Tabs Settings Help

Filter files by name

/ ... / community-workflows / 1-geofabric /

Name	Last Modified
bow-at-banff-geofa...	14 hours ago
pre-process-geospa...	14 hours ago
README.md	14 hours ago

README.md | Launcher | pre-process-geospa

Markdown | scienv

Basic preparations

In this Notebook, the geospatial fabric for the "Bow River at Banff" gauge is extracted from the `MERIT-Basins` dataset.

If you are using Graham HPC, and have access to Clark's Research Group allocation (`rrg-mclark`), you may find `MERIT-Basins` layers under the following path: `/project/rrg-mclark/data/geospatial-data/MERIT-Basins/`

Let's get started with our workflow and import necessary Python libraries:

[1]:

```
import geopandas as gpd # version 0.14.3
import pandas as pd # version 2.1.1
import numpy as np # version 1.24.4
import matplotlib.pyplot as plt # version 3.5.1

from shapely.geometry import Point # version 2.0.

import hydrant.topology.geom as gm # version 0.1.

import subprocess # built-in Python 3.10.2
import os # built-in Python 3.10.2
import glob # built-in Python 3.10.2
```

Simple 0 2 scienv | Idle Mode: Command Ln 1, Col 1 pre-process-geospatial-fabric.ipynb

Double click to launch the Notebook

Use “Shift + Enter” to execute Notebook cells

Notebook cells

Tip: review keyboard shortcuts!

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Practice Example – Bow River at Banff

Switching to the relevant Jupyter Notebook webpage

jupyterlab

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Practice Example – Bow River at Banff

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

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Practice Example – Bow River at Banff

Second step is to run the model-agnostic processes

DALLE generated image

Practice Example – Bow River at Banff

- 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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Practice Example – Bow River at Banff

Agnostic workflow execution using its "Orchestrator"

File Edit View Run Kernel Tabs Settings Help

Filter files by name

/ ··· / community-workflows / 2-agnostic /

Name	Last Modified
assets	17 minutes ago
easymore-job.slurm	19 hours ago
model-agnostic.json	
model-agnostic.sh	
README.md	

Open
Open With
Open in New Browser Tab
Rename F2
Delete
Cut ⌘ X
Copy ⌘ C
Paste ⌘ V
Duplicate ⌘ D
Download
Copy Download Link
Copy Path
Copy Shareable Link
New File
New Notebook
New Folder
Shift+Right Click for Browser Menu

JSON
Editor
Vega5
Vega-Lite4
VDOM

Launcher

github-repos/community-workflows/2-agnostic

Notebook

scienv
scienv2
scienv
scienv2

Other

Text File
Markdown File
Python File

Editing "agnostic" configuration step

Simple 0 0 Launcher

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Practice Example – Bow River at Banff

File Edit View Run Kernel Tabs Settings Help

Filter files by name

/ ··· / community-workflows / 2-agnostic /

Name	Last Modified
assets	an hour ago
easymore-job.slurm	19 hours ago
model-agnostic.json	19 hours ago
model-agnostic.sh	19 hours ago
README.md	19 hours ago

model-agnostic.json | kasra545@gra-login1:~/gith

```
{
  "exec": {
    "met": "/home/kasra545/github-repos/datatool/extract-dataset.sh",
    "gis": "/home/kasra545/github-repos/gistool/extract-gis.sh",
    "remap": "easymore cli"
  },

  "args": {
    "met": [{
      "dataset": "RDRS",
      "dataset-dir": "/project/rrg-mclark/data/meteorological-data/rdrsv2.1/",
      "variable": [
        "RDRS_v2.1_P_P0_SFC",
        "RDRS_v2.1_P_HU_09944",
        "RDRS_v2.1_P_TT_09944",
        "RDRS_v2.1_P_UVC_09944",
        "RDRS_v2.1_A_PR0_SFC",
        "RDRS_v2.1_P_FB_SFC",
        "RDRS_v2.1_P_FI_SFC"
      ],
      "output-dir": "/home/kasra545/scratch/bb-models/datatool-outputs",
      "start-date": "1980-01-01T13:00:00",
      "end-date": "1980-01-5T12:00:00",
      "lat-lims": "",
      "lon-lims": "",
      "shape-file": "/home/kasra545/github-repos/MESH-Bow-at-Banff/1-geofabric/bow-at-banff-geofabric/bb_subbasins.shp",
      "model": "",
      "ensemble": "",
      "prefix": "bb_model_",
      "email": "kasra.keshavarz1@ucalgary.ca",
      "account": "rrg-mclark",
      "_flags": [
        "submit-job",
        "parsable"
      ]
    }],
```

Simple 2 0 JSON Ln 7, Col 1 Spaces: 4 model-agnostic.json

Executable paths

Orchestrator configuration file

Executable arguments and options

(empty options are not provided to the script)

This is the only file for the “agnostic” step

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Practice Example – Bow River at Banff

: Order of process

Automated and ordered job submission to HPC

`-1`: no order

`ordered integers`: order of processes

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Practice Example – Bow River at Banff

Switching to the JupyterLab webpage
for a quick overview

jupyterlab

Execute the “agnostic orchestrator” in the Terminal using:

```
$ ./model-agnostic.sh model-agnostic.json
```


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Practice Example – Bow River at Banff

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

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DALLE generated image

Practice Example – Bow River at Banff

Filter files by name

/ ··· / community-workflows / 3-specific /

Name	Last Modified
setting_files	20 hours ago
meshflow_bb.ipynb	seconds ago
README.md	20 hours ago

The specific part is written into a Jupyter Notebook

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

meshflow_bb.ipynb

Markdown

scienv

Build MESH Model Setup for the Bow River at Banff

We use the `MESHFlow` Python package to build a `MESH` model setup for the Bow River at Banff.

It's also better to keep the geospatial fabric files next to the "agnostic" step's outputs:

[ ]:
```
!cp -r ../1-geofabric/bow-at-banff-geofabric/ /home/kasra545/scratch/
```

Let's start by importing the necessary libraries:

[ ]:
```
# import necessary libraries
import meshflow # version v0.1.0-dev1

import os # python 3.10.2
```

Now, let's provide necessary information to set up the `MESH` model:

[ ]:
```
# main work path - modify
work_path = '/home/kasra545/scratch/bb-models/'

# using meshflow==v0.1.0-dev1
# modify each segment to match your settings
config = {
    'riv': os.path.join(work_path, 'geofabric', 'bb_rivers.shp'),
    'cat': os.path.join(work_path, 'geofabric', 'bb_subbasins.shp'),
    'landcover': os.path.join(work_path, 'gistool-outputs', 'bb_mode
    'forcing_files': os.path.join(work_path, 'easymore-outputs'),
    'forcing_vars': [ # does the variable list match those of the "
```

`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

Simple 0 1 scienv | Idle Mode: Command Ln 1, Col 1 meshflow_bb.ipynb

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Practice Example – Bow River at Banff

Filter files by name

/ ··· / community-workflows / 3-specific /

Name	Last Modified
setting_files	20 hours ago
meshflow_bb.ipynb	20 hours ago
README.md	20 hours ago

Launcher | meshflow_bb.ipynb

Markdown | scienv

[2]:

```python
# main work path - modify
work_path = '/home/kasra545/scratch/bb-models/'

# using meshflow==v0.1.0-dev1
# modify each segment to match your settings
config = {
    'riv': os.path.join(work_path, 'geofabric', 'bb_rivers.shp'),
    'cat': os.path.join(work_path, 'geofabric', 'bb_subbasins.shp'),
    'landcover': os.path.join(work_path, 'gistool-outputs', 'bb_mode
    'forcing_files': os.path.join(work_path, 'easymore-outputs'),
    'forcing_vars': [ # does the variable list, match those of the "a
        "RDRS_v2.1_P_P0_SFC",
        "RDRS_v2.1_P_HU_09944",
        "RDRS_v2.1_P_TT_09944",
        "RDRS_v2.1_P_UVC_09944",
        "RDRS_v2.1_A_PR0_SFC",
        "RDRS_v2.1_P_FB_SFC",
        "RDRS_v2.1_P_FI_SFC",
    ],
    'forcing_units': { # Here, enter RDRS's original variable units
        'RDRS_v2.1_P_P0_SFC': 'millibar',
        'RDRS_v2.1_P_HU_09944': 'kg/kg',
        'RDRS_v2.1_P_TT_09944': 'celsius',
        'RDRS_v2.1_P_UVC_09944': 'knot',
        'RDRS_v2.1_A_PR0_SFC': 'm/hr',
        'RDRS_v2.1_P_FB_SFC': 'W/m^2',
        'RDRS_v2.1_P_FI_SFC': 'W/m^2',
    },
    'forcing_to_units': { # And here, the units that MESH needs to re
        'RDRS_v2.1_P_UVC_09944': 'm/s',
        'RDRS_v2.1_P_FI_SFC': 'W/m^2',
        'RDRS_v2.1_P_FB_SFC': 'W/m^2',
        'RDRS_v2.1_A_PR0_SFC': 'mm/s',
        'RDRS_v2.1_P_P0_SFC': 'pascal',
        'RDRS_v2.1_P_TT_09944': 'kelvin',
        'RDRS_v2.1_P_HU_09944': 'kg/kg',
    },
```

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

Simple 0 1 scienv | Idle Mode: Command Ln 1, Col 1 meshflow_bb.ipynb

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Practice Example – Bow River at Banff

Filter files by name

/ ··· / community-workflows / 3-specific /

Name	Last Modified
setting_files	20 hours ago
meshflow_bb.ipynb	20 hours ago
README.md	20 hours ago

Launcher | meshflow_bb.ipynb

Markdown | scienv

```
38      'main_id': 'COMID', # what is the main ID of each river segment?
39      'ds_main_id': 'NextDownID', # what is the downstream segment ID i
40      'landcover_classes': { # these are the classes defined for NALCMS
41          0: 'Unknown',
42          1: 'Temperate or sub-polar needleleaf forest',
43          2: 'Sub-polar taiga needleleaf forest',
44          3: 'Tropical or sub-tropical broadleaf evergreen forest',
45          4: 'Tropical or sub-tropical broadleaf deciduous forest',
46          5: 'Temperate or sub-polar broadleaf deciduous forest',
47          6: 'Mixed forest',
48          7: 'Tropical or sub-tropical shrubland',
49          8: 'Temperate or sub-polar shrubland',
50          9: 'Tropical or sub-tropical grassland',
51          10: 'Temperate or sub-polar grassland',
52          11: 'Sub-polar or polar shrubland-lichen-moss',
53          12: 'Sub-polar or polar grassland-lichen-moss',
54          13: 'Sub-polar or polar barren-lichen-moss',
55          14: 'Wetland',
56          15: 'Cropland',
57          16: 'Barren lands',
58          17: 'Urban',
59          18: 'Water',
60          19: 'Snow and Ice',
61      },
62      'ddb_vars': { # the stuff that MESH needs: slope, river length, e
63          'slope': 'ChnlSlope',
64          'lengthkm': 'ChnlLength',
65          'Rank': 'Rank',
66          'Next': 'Next',
67          'landcover': 'GRU',
68          'unitarea': 'GridArea',
69          'landcover_names': 'LandUse',
70      },
71      'ddb_units': {
72          'ChnlSlope': 'm/m',
73          'ChnlLength': 'km', # is it in km or m? Please check the unit
74          'Rank': 'dimensionless',
75          'Next': 'dimensionless',
76          'GRU': 'dimensionless',
77          'GridArea': 'km^2', # what was the unit of the GridArea, or S
78          'LandUse': 'dimensionless',
79      },
```

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

Practice Example – Bow River at Banff

Filter files by name

/ ··· / community-workflows / 3-specific /

Name	Last Modified
setting_files	20 hours ago
meshflow_bb.ipynb	20 hours ago
README.md	20 hours ago

Launcher | meshflow_bb.ipynb

Markdown | scienv

```
    'ddb_to_units': {
        'ChnlSlope': 'm/m',
        'ChnlLength': 'm', # This is what MESH needs, no need to char
        'Rank': 'dimensionless',
        'Next': 'dimensionless',
        'GRU': 'dimensionless',
        'GridArea': 'm^2', # This is what MESH needs, no need to char
        'LandUse': 'dimensionless',
    },
    'ddb_min_values': {
        'ChnlSlope': 1e-10, # in case there are 0s in the `rivers` Sh
        'ChnlLength': 1e-3,
        'GridArea': 1e-3,
    },
    'gru_dim': 'NGRU', # change to `NGRU` for 'MESH>=r1860', keep for
    'hru_dim': 'subbasin',
    'outlet_value': -9999,
}
```

We can build an "instance" of the workflow class:

[3]:
```
exp1 = meshflow.MESHWorkflow(**config)
```

And, we can run it using:

[4]:
```
exp1.run()
```

```
/home/kasra545/github-repos/meshflow/src/meshflow/utility/forcing_prep.p
y:116: FutureWarning: The return type of `Dataset.dims` will be changed t
o return a set of dimension names in future, in order to be more consiste
nt with `DataArray.dims`. To access a mapping from dimension names to len
gths, please use `Dataset.sizes`.
  var = [i for i in ds.dims.keys() if i != 'time']
```

Once the run is finished, we can checkout the forcing and drainage database file:

Simple | 0 | 1 | scienv | Idle | Mode: Command | Ln 1, Col 1 | meshflow_bb.ipynb

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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Practice Example – Bow River at Banff

Switching to the JupyterLab webpage

for a quick overview

jupyterlab

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Outline

- Community Hydrological Modelling Recipe
- Digital Infrastructure on Digital Research Alliance of Canada's HPCs
- Setting Up Your Account on HPCs
- Introducing Community Workflows & Tools
- Practice Example – Bow River At Banff
- Troubleshooting

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Troubleshooting

Whenever you face an issue, follow the steps below:

- "Agnostic" log files are located in the following directories:

```
$HOME/.datatool
$HOME/.gistool
/path/to/EASYMORE/s/temp/directory
/path/to/agnostic/orchestrator/s/directory
```

Look for files with the following extensions:

```
.out, .err, .log
```

Try to understand what has gone wrong. In 80% of the time, there is a minor human error involved.

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Troubleshooting

Continuing…

- Make sure Graham storages are responsive, very often than not, the `home`, `scratch`, or `project` spaces experience technical difficulties
- Make sure you have enough space on any storage you are working; the `quota` command can show you how much storage you are using
- If the `project` space gets full, communicate this with your PI; users do mistakenly fill up the shared storage without much justification,
- Try troubleshooting technical issues using ChatGPT or any online ChatBot you have access to

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Troubleshooting

- Try troubleshooting by Google-ing and searching Stackoverflow
- Avoid using chat mechanisms to exchange critical information; everything needs to be documented properly; undocumented work equals to null
- If nothing worked out, open an “Issue” on the relevant GitHub repository(-ies) providing an MCVE
- Feel free to contribute to any repository you are interested in. Whenever you `commit`, follow the `commit` guidelines recommended by the creator of `Git`
- Fix `MESH` bugs

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Troubleshooting

Linus Torvalds – creator of Linux and Git

```
Header line: explain the commit in one line (use the imperative)

Body of commit message is a few lines of text, explaining things
in more detail, possibly giving some background about the issue
being fixed, etc.

The body of the commit message can be several paragraphs, and
please do proper word-wrap and keep columns shorter than about
74 characters or so. That way "git log" will show things
nicely even when it's indented.

Make sure you explain your solution and why you're doing what you're
doing, as opposed to describing what you're doing. Reviewers and your
future self can read the patch, but might not understand why a
particular solution was implemented.

Reported-by: whoever-reported-it
Signed-off-by: Your Name <youremail@yourhost.com>
```

Same philosophy applies to GitHub Issues

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Thank you for attending

https://ucalgary.ca/civil

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