Nexus-e

Release 0.0.1

Nexus-e

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CHAPTER

ONE

SETUP

1.1 Get permissions

Before setting up, ask for permission from nexus-e@ethz.ch to access the codes and the input database.

Note: Currently, the codes and databases are only accessible with an ETH account.

1.2 Local setup

Even though the current Nexus-e platform is **not** yet suitable to run locally because of high consumption of resources such as memory, we do recommend to at least get the codes and connect to the database locally in order to view, understand, and edit them easily.

Most the instructions below have been tested both on Windows and on Mac.

1.2.1 1. Get the codes

Make sure you have installed git.

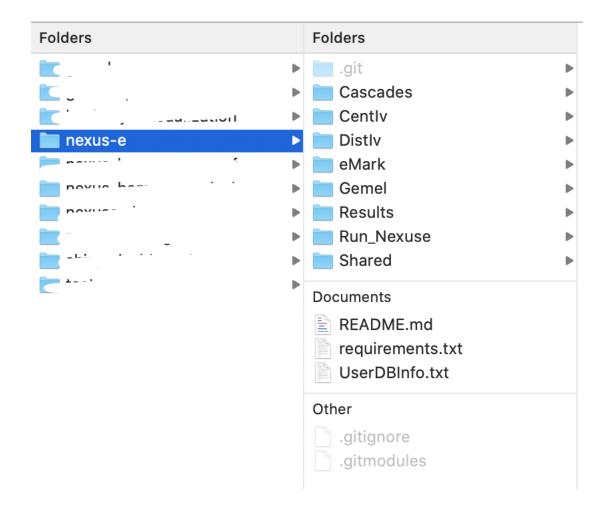
The instructions here use **command lines**. If you have a GUI tool for git, you could use the corresponding operations in the GUI tool instead. An example using a GUI tool "GitKraken" can be found in section Nexus-e repository instructions.

- · Create a folder where you want to put the codes
- cd to that folder
- Clone the overarching repository with this command:

git clone --recursive https://gitlab.ethz.ch/nexus-e/nexus-e-framework.git

You will be asked for your username and password for the repository and its submodules.

In the end, the folder will look like the screenshot below. Note: You might not see the hidden files whose names start with a dot, and the Results folder will be automatically generated when you run Nexus-e.



1.2.2 2. Connect with the input database

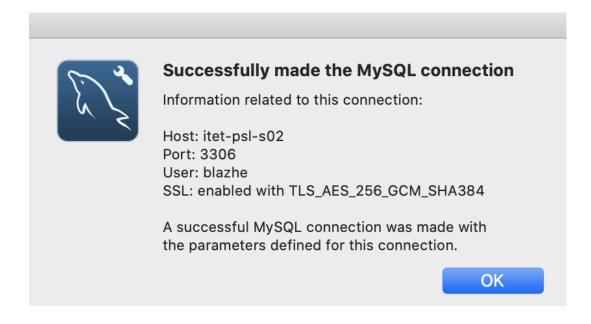
• Find information to connect with the database in UserDBInfo.txt in the repository. The file contains four lines (for confidentiality the username and password is not written here, but can be found in the file):

itet-psl-s02 3306 DATABASE_USERNAME DATABASE_PASSWORD

- View the database
 - Install MySQL (Version 8.0 is recommended) and MySQL Workbench. For Windows, following this instruction. For MacOS, follow this instruction.
 - Connect to ETH VPN
 - Connect to the database with MySQL Workbench

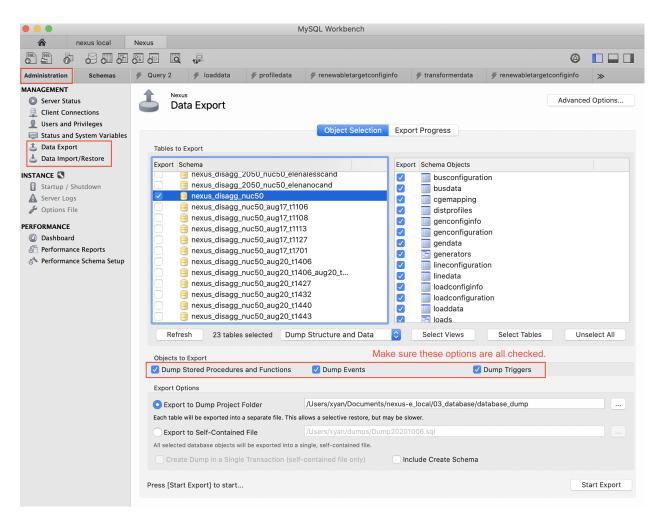
•••		MySQL Workbench	
	MySQL Workbench is t create and browse yc	e to MySQL Wo he official graphical user interface (GUI) tool for MySQL. It bur database schemas, work with database objects and ir ries to work with stored data. You can also migrate schem database vendors to your MySQL database.	t allows you to design, Isert data as well as
	Browse Documentation >	Read the Blog >	Discuss on the Forums >
	MySQL Connections ⊕9		
	Local instance 3306 # root # blazhe # blazhe # blazhe # blazhe	ETH personal database ₤ xyan ☆ mysql1.ethz.ch:3306	
* Add a new MySQL connection			
		Manage Server Connections	
MySQ	L Connections Connection Name: Nexus	Give a name	
Loca	instance 3306	Connection Remote Management	System Profile
Nexu ETH	personal database	Standard (TCP/IP)	S Method to use to connect t
		Parameters SSL Advance	ced
	Hostname: i	itet-psl-s02 Port: 3306	Name or IP address of the serve IP port.
	Username:	YOUR_DATABASE_USERNAME	Name of the user to connect wit
	Password:	Store in Keychain Clear	The user's password. Will be rec not set.
	Default Schema:		The schema to use as default so to select it later.
* Input connection information	ew Delete Duplicate Mo	Move Up Move Down	Test Connection
* input connection information			

* Click the button Test Connection. You will be asked to input your database password. Then you will see a seccess message:



1.2.2.1 2.1. (Optional) Make a local copy of the database

By default, everyone has write permission to the database. Therefore, to be safe, always make a local copy of the database before playing with it - i.e., first "Dump" it to a local folder, then import it to your personal MySQL account. These can be done in this window:



You might encounter the following problems when you run Nexus-e with a local database, follow the link for possible solutions:(1) Error: "Access denied for user 'your_username'@'your_host_address' ..."(2) Error: "The server time zone value 'xxx' is unrecognized ..."(3) Error: "The user specified as a definer ('xxx'@'%') does not exist ..."

1.2.3 3. Prepare software & license

Apart from MySQL introduced above, we also need the following software to run Nexus-e locally. This will be introduced in this section. You could skip this section if you don't plan to run the whole Nexus-e platform locally.

- Matlab
- Python
- Gurobi
- GAMS
- Latex
- ImageMagick

1.2.3.1 Matlab

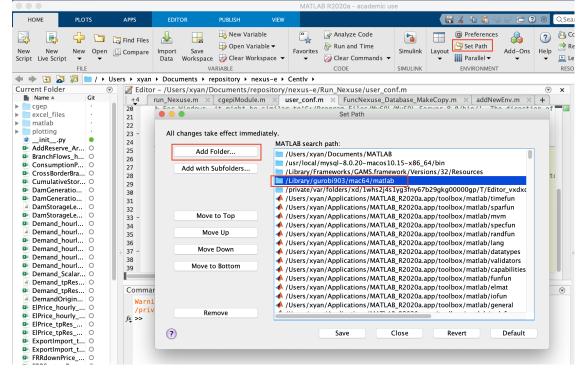
- Download Matlab (R2020a or higher). Available at ETH IT shop.
- During installation, you need to install the "Database Toolbox", the "Financial Toolbox", and the "Communication Toolbox" as well by ticking the box for each toolbox (This option is available if you downloaded Matlab through the ETH IT shop). If this is not an option during installation, you can download it seperately here. If possible install all toolboxes to avoid any inconveniences.
- Set up database connector
 - Download the MySQL connector from here. Unzip the file. Before downloading, select "Platform Independent" from the "Select Operating System" drop-down list.
 - Copy the MySQL connector folder (e.g. mysql-connector-java-8.0.18) into a folder at your preference. We recommend to put it into the **Matlab preferences folder**, which you can find by typing in Matlab Command Window prefdir.
 - Create a javaclasspath.txt file in the Matlab preferences folder.
 - In the javaclasspath.txt file, write the path to the connector .jar file that you just copied. E.g., On a Windows computer the path is similar to C:\Users\user\AppData\Roaming\MathWorks\ MATLAB\R2018a\mysql-connector-java-8.0.18\mysql-connector-java-8.0.18. jar.
 - Reload Matlab
 - Test whether a database connector is set up successfully. Write the following commands in Matlab (substitue YOUR_USERNAME and YOUR_PASSWORD with your credentials for the database). If the second command returns 1, it means success.

1.2.3.2 Python

- Download Python. Version 3.8.6 is recomended. Python 3.9 is not compatible with Gurobi 9.0.x yet.
- (Optional) If you (will) use Python for multiple projects, it is recommended to create a virtual environment for Nexus-e (for example, using virtualenv).
- Install the required python packages listed in requirements.txt (e.g., with command pip install -r requirements.txt).

1.2.3.3 Gurobi

- Download Gurobi (9.0 is recomended) and set up a free Gurobi academic license from here.
- Connect Gurobi with Python following this instruction.
- Save Gurobi path for Matlab
 - Find out the path of gurobi_setup.m. (E.g., for mac, it is similar to /Library/gurobi903/ mac64/matlab.)
 - Open Matlab; under the tab "Home", click Set Path; select Add Folder...; browse to the folder containing gurobi_setup.m; click Open.



- A new entry of the selected path will appear on the right side of the Set Path window; click Save.

1.2.3.4 GAMS

- Download GAMS. Version 32.2 is recomended. Our current license doesn't support versions newer than 32.
- Set GAMS License
 - Use the gamslice.txt provided in polybox 02_Model/02_Model_Setup_Instruction.
 - Install the license: here or here or (for MacOS) here.
- Save GAMS path for Matlab
 - Find out your GAMS path. It varies largely depending on your PC's operating system and the version of GAMS. For example, GAMS 32 on Mac has the path: /Library/Frameworks/GAMS. framework/Versions/32/Resources.
 - Similar to how you configured Gurobi for Matlab: Open Matlab; under the tab "Home", click Set Path; select Add Folder...; browse to the GAMS path; click Open.
 - A new entry of the selected path will appear on the right side of the Set Path window; click Save.
- Connect GAMS with Python
 - Follow the instruction here.

1.2.3.5 Latex

• Download Latex.

1.2.3.6 ImageMagick

- Instructions for Windows:
 - Download ImageMagick from here. Install ImageMagick from the .exe file. Tick **all** boxes when asked which packages to be installed (by default only the first three are selected).
 - Download dependable software "Ghostscript" from here. Select Public License Ghostscript. Install the Ghostscript.
 - Optional (if ImageMagick does not work), download and install Visual studio from here.
- Instructions for Mac:
 - Install ImageMagick from here
- Test if ImageMagick works:
 - Open Windows command prompt and browse to folder that contains a pdf file, e.g., testch.pdf
 - Use the following command to convert file: convert testch.pdf testch.jpg

1.2.4 4. Edit conf_local.m

- Make a copy of example_conf_local.m in the folder Run_Nexuse/conf_local. Name the copy as conf_local.m. (Note: You should only work with the local copy, because the original example_conf_local.m will be synchronized to git and it shouldn't be changed.)
- In conf_local.m uncomment and modify the following variables based on your local computer's settings. More instructions can be found in the script conf_local.m itself.
 - PATH_MYSQL
 - PATH_PYTHON
 - PATH_GUROBI_FOR_PYTHON
 - PATH_LATEX
 - PATH_CONVERT
 - PATH_GAMS

Note: You don't necessarily need all software paths here. For example, if you only want to run the postprocess scripts, PATH_GUROBI_FOR_PYTHON is not needed; if you only want to run DBcreation scripts, only DB_INFO_FILE and PATH_MYSQL are needed.

- (Optional) If you want to work with a *local copy of the database*
 - Make a copy of example_UserDBInfo_local.txt in the folder Run_Nexuse/conf_local. Name the copy as UserDBInfo_local.txt. (Note: You should only work with the local copy, because the original example_UserDBInfo_local.txt will be synchronized to git and it shouldn't be changed.)
 - Edit example_UserDBInfo_local.txt based on your local settings:

```
127.0.0.1 (or "localhost")
3306
YOUR_LOCAL_USERNAME (e.g. "root")
YOUR_LOCAL_PASSWORD
```

- Uncomment the variable DB_INFO_FILE in conf_local.m.
- Test conf_local.m: in Matlab, run the script conf_local/conf_test.m.
 - If your conf_local.m is set up correctly, you should see outputs like "xxx works."
 - If you see "xxx FAILED", there will be information in the output showing why xxx failed. However, this is
 not necessarily a problem. Because as mentioned above, you don't always need all software. For example,
 if you only want to run postprocess scripts, PATH_GUROBI_FOR_PYTHON is not needed; if you only
 want to run DBcreation scripts, only DB_INFO_FILE and PATH_MYSQL are needed.

1.2.5 5. Run Nexus-e

- Connect to ETH VPN (in order to connect with the database)
- Open Matlab
- (Optional) Run bench_Nexuse.m. This is required before you run run_Nexuse.m for the first time, or after major changes have been made to eMark and/or CentIv. Running bench_Nexuse.m will create a file /Gemel/results/benchmark_2015.mat which is necessary to run run_Nexuse.m.
- Run the script run_Nexuse.min the Run_Nexuse folder. There are a few parameters that you can customize in the beginning of this run script:
 - You could change the variables scen, scenShortName, tpRes, limDifference, and dbSuffix as instructed in the script
 - If you don't want to run all 4 years, adjust endY for the case you are running. E.g., if endY=staY, it will only run one year.
- Consult the Nexus-e team if you want to run other scripts in the Run_Nexuse folder.

1.3 Software for interacting with Euler from local machine

In our experience, it is usefull to have two tools available for

- transferring files between Euler and your local machine and
- interacting with the command prompt on Euler.

GUIs for file transfer

For transferring files between Euler and your personal computer, a graphical user interface (GUI) is useful. We suggest FileZilla since it is available for "all" platforms. The scicomp wiki also has information on this.

Command prompts for secure shell connections

Unix systems (Linux/Mac) come with shells (command prompts) from which useful interactions with Euler are possible. E.g., type ssh <username>@euler.ethz.ch to make a "secure shell" connection to Euler and issue commands to the Euler command prompt. Windows users are less fortunate and have to install additional software to achieve this functionality. Examples are

- putty.exe and
- MobaXterm.

We can highly recommend MobaXTerm.

Login

• Log-in with ssh on Unix-based operating systems:

```
ssh <ethz-username>@euler.ethz.ch
```

Lacking SSH keys, ssh will ask you for your ETH (LDAP) password and after that your following commands are issued to Euler. See scicomp wiki for instructions for setting up SSH keys if desired.

- File transfers between local and Euler in FileZilla can be made through sftp (secure file transfer protocol). For this, enter sftp://euler.ethz.ch in the 'server' field and your ETH-user name and password in the respective fields, then hit 'connect'.
- Access to Euler: since May 2020, first time access to Euler is only granted upon request. ETH account holders just write an email to cluster-support@id.ethz.ch; If you used the Euler cluster before the 15. May 2020, then you would need to change your LDAP password to get again access to the Euler cluster (wait for 1 day until the change takes effect). (see https://scicomp.ethz.ch/wiki/Getting_started_with_clusters for more info).

1.4 Euler setup

In order to run the full Nexus-e platform efficiently, we use Euler, an ETH cluster for High Performance Computing. To set up the Nexus-e platform on Euler, you first need to access Euler. Instructions on accessing Euler and commands for Euler can be found here.

1.4.1 1. Join the Nexus-e user group

We have a user group for access to Nexus-e specific licenses (e.g. GAMS) and the Euler pre-paid share. The user group is called: **MAVT-esc-nexus-e**, and is set and maintained by D-MAVT IT. To join the user group, ask Blazhe Gjorgiev gblazhe@ethz.ch to send an email to servicedesk@mavt.ethz.ch.

To check whether you are added to the user group, use command line ssh to Euler (type ssh username@euler.ethz.ch), then type groups to show a list of groups that your user account is linked to, which should contain "MAVT-esc-nexus-e".

1.4.2 2. Get the codes

- Create a folder where you want to put the codes
- cd to that folder
- Clone the overarching repository with this command: git clone --recursive https://gitlab. ethz.ch/nexus-e/nexus-e-framework.git You will be asked for your username and password for the repository and its submodules.

the end, the folder will like tThe In look the screenshot below. Note: Results folder will automatically be generated when you run Nexus-e.

[xyan@eu-lo total 60	ogi	n-12 i	nexus-e]\$ ls	s -la				
	11	xyan	xyan-group	4096	Sep	25	09:27	
		-	т0000					
drwxr-x	15	xyan	xyan-group	4096	Sep	24	16:34	Cascades
drwxr-x	7	xyan	xyan-group	8192	0ct	7	11:24	CentIv
drwxr-x	6	xyan	xyan-group	4096	Sep	25	10:30	DistIv
drwxr-x	4	xyan	xyan-group	4096	Sep	24	16:35	eMark
drwxr-x	9	xyan	xyan-group	8192	0ct	7	11:37	Gemel
drwxr-x	9	xyan	xyan-group	4096	Sep	24	16:34	.git
-rw-r	1	xyan	xyan-group	11	Sep	24	16:34	.gitignore
-rw-r	1	xyan	xyan-group	640	Sep	24	16:34	.gitmodules
-rw-r	1	xyan	xyan-group	43	Sep	25	09:26	requirements.txt
drwxr-x	5	xyan	xyan-group	4096	0ct	7	10:05	Results
drwxr-x	2	xyan	xyan-group	4096	0ct	7	11:37	Run_Nexuse
drwxr-x	8	xyan	xyan-group	4096	0ct	7	09:57	Shared
-rw-r	1	xyan	xyan-group	33	Sep	24	16:34	UserDBInfo.txt

1.4.3 3. Prepare dependencies

Unlike setting up Nexue-s locally, we don't need to download any software or license on Euler. Instead, they are all prepared for all users in the user group **MAVT-esc-nexus-e**. You should already be a member of the group if you have followed the *first step*.

But still, we need to explicitely load all the dependencies, including modules (an Euler term for "software") and python packages.

- Load modules
 - Option 1: Manually load modules every time before running Nexus-e

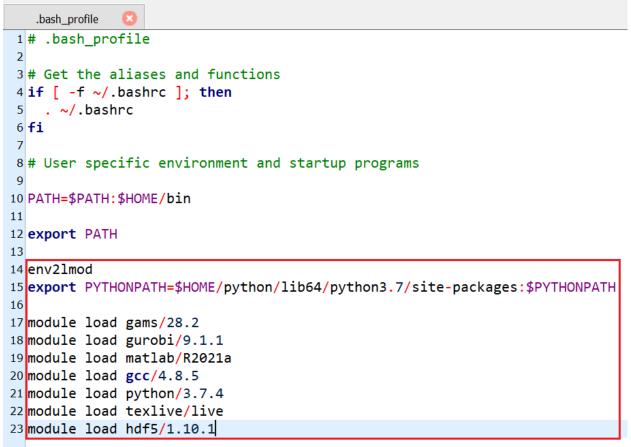
Copy the following commands into Euler:

```
env2lmod
export PYTHONPATH=$HOME/python/lib64/python3.7/site-packages:$PYTHONPATH
module load gams/28.2
module load gurobi/9.1.1
module load matlab/R2020b
module load gcc/4.8.5
module load gcc/4.8.5
module load python/3.7.4
module load texlive/live
module load hdf5/1.10.1
```

env2lmod serves as a switch from the old to the new Euler software stack. Alterntievly one can type in comand set_software_stack.sh new to permently switch to the new software stack.

• Option 2: Edit .bash_profile or .bashhrc so that the modules are automatically loaded upon log in to Euler

Write the same commands at the end of .bash_profile. This is a hidden file in your Euler's home directory. After adding these commands, your .bash_profile should look similar to this:



Test: To test whether the modules have been successfully loaded, type module list in the commaand line. It should then list all loaded modules.

• Install python packages

This you only need to do it once, i.e. you don't need to do it everytime when you run Nexus-e.

In command line under your home directory,

- cd to the folder where you have stored the Nexus-e codes
- type pip install --user -r requirements.txt

You might encounter software compatibility problems when running Nexus-e on Euler, follow the link for possible solutions: Matlab & Python compatibility error: "ImportError: ...pyexpat...: undefined symbol: XML_SetHashSalt"

1.4.4 4. Connect with the input database

- Download the MySQL connector from here. Unzip the file.
- Copy the MySQL connector folder into the hidden .matlab folder (e.g., .matlab/2020a).
 - Tip: To see all folders including the hidden ones, use the command ls -a.
 - If you don't see the .matlab folder, run Matlab once: type in matlab -> you will see Matlab is started in the terminal -> type in exit -> Matlab will stop -> you should then see the .matlab folder.
- Create a **javaclasspath.txt** file in the same folder as above.
- In the javaclasspath.txt file, write the path to the connector .jar file that you just copied. E.g., On Blazhe's Euler account the path is /cluster/home/gblazhe/.matlab/R2018a/mysql-connector-java-8.0.18/mysql-connector-java-8.0.18.jar.
- Logoff and re-login to Euler

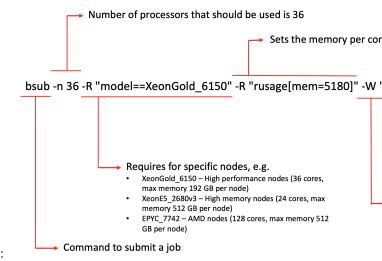
1.4.5 5. Run Nexus-e

- cd to the Run_Nexuse folder
- (Optional) Run bench_Nexuse.m. This is required before you run run_Nexuse.m for the first time, or after major changes have been made to eMark and/or CentIv. Running bench_Nexuse.m will create a file /Gemel/results/benchmark_2015.mat which is necessary to run run_Nexuse.m.
- Customize the run script run_Nexuse.m.
 - You could change the variables scen, scenShortName, tpRes, limDifference, and dbSuffix as instructed in the script. (Recommendation: For quick test, use tpRes = 8 and limDifference = 0.1.)
 - If you don't want to run all 4 years, adjust endY for the case you are running. E.g., if endY=staY, it will only run one year.
- Submit the job (the standard run script is run_Nexuse.m) with a command such as (Note: Don't type .m after the script name.)

```
bsub -n 36 -R "model==XeonGold_6150" -R "rusage[mem=5180]" -W "10:00" matlab -r run_

→Nexuse
```

The parameters in this command can be costomized. Experience with resource usage to run Nexus-e with different time resolution and convergence criteria can be found here. General instructions on bash and Euler commands can be found here.



Here we give a short explanation to the example command above:

After submission, Euler will respond by telling you what the jobID is.

• Consult Nexus-e team if you want to run other scripts in the Run_Nexuse folder.

NOTE: For submissions that require large memory, it is recommended to select EPYC_7742, for submission with smaller memory requirements either select EPYC_7742 or XeonGold_6150.

We have experienced issues with the database connector when computing node is not selected on Euler.

CHAPTER

EULER INSTRUCTIONS

2.1 Useful bash commands

Euler's command line interface (shell) is called "bash". The scicomp wiki gives a good overview over a list of bash commands. We just give a short list of useful applications of these commands:

- Ctrl-p and Ctrl-n give previous and next commands in the command history.
- Ctrl-r <expression> searches for <expression> in the command history.
- Use cd for changing directories. E.g., cd nexus-e/Run_Nexuse to go to the directory where the main matlab script run_Nexuse.m lives.

Note: avoid white space in directory or file names like the plague.

- Use 1s for listing the contents of the current directory
- Use rm <filename> for deleting file with name filename
- Use rm -r <foldername> for recursively deleting the contents of folder
- Use pwd for printing the current working directory
- grep <expression> <filename> prints all lines of file(s) filename in which expression appears. Use option -i for case-insensitive search.
- <command1> | <command2> employs a "**pipe**" (|) to redirect output of command1 as input to command2. E.g., ls | grep <filename> sends the listing of the current directory contents to grep, which looks for lines in which filename appears. If this command does not return anything, filename does not exist in the current directory.
- Wildcards: bash accepts several wildcards for file name or string completion. E.g.,
 - \star stands for a sequence of characters of arbitrary length
 - ? stands for one character
 - ls lsf.o14*, e.g., will list all files with names starting with *lsf.o14*.
- Use scp for making secure (remote) copies of files and folders. E.g. enter

scp ./run_Nexuse.m <username>@euler.ethz.ch:/cluster/home/<username>/
nexus-e/Run_Nexuse/run_Nexuse.m

To transfer a local copy of run_Nexuse.m to ~/nexus-e/Run_Nexuse/run_Nexuse.m on Euler. Issue this command on your local machine!

This command may come in handy for scripting certain things but is unnecessary if you are happy to make all file transfers using FileZilla.

2.2 Euler specific commands

2.2.1 Account information

To access information about your account on Euler

- lquota checks the amount of data and files you have on the cluster
- busers -w shows resource usage
- my_share_info returns your user group

2.2.2 Modules

Diverse commands exist for organizing and checking the modules that Euler has loaded in your environment. Generally, running Nexus-e should work fine if the modules listed under Setup are loaded. Here's a list anyway (see scicomp wiki for more explanation around the commands).

- module load new loads all new modules
- module list shows currently loaded modules
- module avail shows all available modules
- module help <module_name> brief description
- module show <module_name> what the module would do
- module load <module_name> load a module
- which icc check the compiler
- module unload <module_name> unload module

2.2.3 Batch system: How to run Nexus-e

On Euler, users are asked to run large jobs using Euler's batch system. Scicomp gives an extensive description of this system. Here we summarize what is useful for running Nexus-e on Euler.

Generally, commands like

```
bsub -n 36 -R "model==EPYC_7742" -R "rusage[mem=5180]" -W "10:00" matlab -r run_Nexuse_platform
```

will be used to run Nexus-e from folder nexus-e/Run_Nexuse_platform on Euler.

- -W "10:00" gives Euler 10 hours to run the process
- -R "rusage [mem=5180]" tells Euler to allocate 5180 MB of RAM per core (default is 1GB)
- -R "model==EPYC_7742" tells Euler to use the EPYC_7742 nodes Available nodes:
 - XeonE5_2680v3 High memory nodes (24 cores, max memory 512 GB per node) Recomended!
 - XeonGold_6150 High performance nodes (36 cores, max memory 192 GB per node)
 - EPYC_7742 AMD nodes (128 cores, max memory 512 GB per node) Note that requiring for specific nodes may imply longer queuing times.
- -n 36 tells Euler to use 36 processors
- matlab -r run_Nexuse tells Euler to run the script run_Nexuse using matlab

Other useful options are the following.

• Add -nojvm to matlab command to prevent Java from being used.

```
bsub [...] matlab -nojvm -r run_Nexuse
```

• Add -nodisplay to matlab command to explicitly tell matlab that no graphical interface is available.

```
bsub [...] matlab -nodisplay -r run_Nexuse
```

- Set the output filename using -o <output_filename>. Default is lsf.o<JobID>.
- Add -B and/or -N to be notified via email when your job begins and/or ends (reference). Also, you need to have a file . forward in your home directory containing your email address.

```
bsub -B -N [...] matlab -r run_Nexuse
```

• For parallel computation using OpenMP, the number of processor cores available needs to be specified using the environmental variable OMP_NUM_THREADS. Set this with the command

export OMP_NUM_THREADS=<number_of_cores>

before issuing your bsub ... command. Consider writing this to .bash_profile if you don't want to repeat this each session.

• To use job arrays for parallel calculation, use option -J "arrayname[1-10]" ./program [arguments]

If some jobs fail, it's possible to rerun only those:

brequeue -e <JOBID>

2.2.4 Batch system: How to check the status of your jobs

- bjobs lists jobs
- bjobs -p lists only pending jobs
- bjobs -1 lists jobs with more details
- bkill <JOBID> kills job with JOBID
- bpeek <JOBID> checks the output of a particular running job
- bbjobs <JOBID> checks resources used
- bjobs -1 -aff is another method for checking the resources used

2.3 Recommendations for running Nexus-e

2.3.1 Experience with resource usage

(1) [For final run] 2-day time resolution with convergence criterium 0.1 percent

For this, set tpRes = 2; and limDifference = 0.001 in run_Nexuse.m. The following command works fine.

```
bsub -n 36 -R "model==XeonGold_6150" -R "rusage[mem=5180]" -W "350:00" matlab -r run_Nexuse
```

(2) [For quick test] 8-day time resolution with convergence criterium 10 percent

For this, set tpRes = 8; and limDifference = 0.1 in run_Nexuse.m. The following command works fine.

bsub -n 36 -R "rusage[mem=2180]" -W "15:00" matlab -r run_Nexuse

(3) 8-day time resolution with convergence criterium 2 percent

For this, set tpRes = 8; iand limDifference = 0.02 in run_Nexuse.m. The following command works fine.

bsub -n 36 -R "rusage[mem=2180]" -W "30:00" matlab -r run_Nexuse

(4) 8-day time resolution with convergence criterium 0.1 percent

For this, set tpRes = 8; and limDifference = 0.001 in run_Nexuse.m. The following command works fine. (This is still being tested as of October 22 2020).

bsub -n 36 -R "rusage[mem=2180]" -W "60:00" matlab -r run_Nexuse

(5) [For benchmark] Run the benchmark script bench_Nexuse.m

As instructed in the setup procedure, you sometimes need to run the script bench_Nexuse.m to (re-)calibrate GemEl. This script runs rather quickly because it doesn't run the entire energy-economic loop and has a low time resolution. The following command works fine.

bsub -n 36 -W "2:00" matlab -r bench_Nexuse

2.3.2 Finding your way around output on Euler

After you issue a batch job through bsub, Euler will respond by telling you what the jobID is. After completion, the 'standard output' of running Nexus-e will be written to lsf.jobID and can inspected there using the text *editor of your choice*.

While the job is running, however, standard output can be accessed by means of the command

bpeek

which in turn writes to standard output of your console. To more conveniently browse this, several options exist:

• write the output of bpeek to a file:

bpeek>yourfilename.txt

and then look at it in the text editor of your choice.

• use a pipe ('l') to find lines including certain 'patterns' with grep:

bpeek | grep <pattern>

for example,

bpeek | grep 'maximum difference'

will print all lines that contain information about Gemel's convergence criterion in given iterations.

• use a pipe ('l') to display the output of bpeek using the 'less' command:

bpeek | less

This will bring up an interface that lets the user browse through the output of bpeek without using the mouse. Some basic functions of the interface:

- press "Space" to go down one page,
- press "q" to quit the "less" interface,
- press "/" to enter a pattern to search for.
 - * Pressing "n" (n for next) after having searched for a pattern jumps to the next instance of the pattern;
 - * pressing "N" jumps to the previous.

- A relative to "/" (forward search) is "?" (backward search).
- "G" goes to the end of bpeek's output, "g" to the beginning.

2.3.2.1 Finding stuff in lsf.o<JobID> files

• grep -i <expression> lsf* searches for <expression> in all files starting with lsf. E.g.,

```
grep -inH nexus_disagg_nuc50_oct20 lsf*
```

searches for copies of database nexuse_disagg_nuc50 mentioned in lsf* files that where made on October 20. This may be helpful for identifying the copies of the database that can safely be removed ("dropped") from the PSL server.

2.4 Viewing output

The output of Matlab is directed to files lsf.o<JobID>. To inspect this output, open it in your editor of choice.

- Several editors are available on Euler, e.g.,
 - emacs
 - vim
 - nano

nano may be a good choice if you don't know emacs or vim (if you do know emacs or vim, you will have strong opinions on which one to use). Nano gives some on-screen instructions on basic key combinations. (E.g., ^G means *type g while holding Ctrl pressed*).

• For better user experience, copy files to your local computer for viewing with a GUI editor (e.g., using FileZilla).

CHAPTER

REPOSITORY INSTRUCTIONS

For a full instruction to work with git repository, please see here.

This document is only used to demonstrate git operations for certain nexus-e-related questions and use cases:

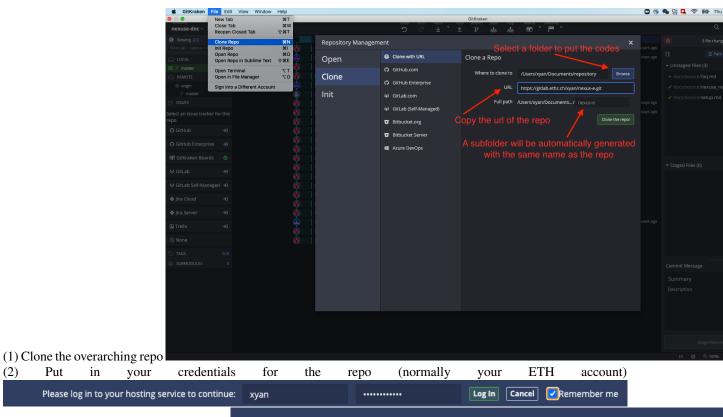
- How do I get the repository?
 - Short answer: you "git clone" it from https://gitlab.ethz.ch/nexus-e/nexus-e-framework.git to a local folder.
- What is the structure of the repository?
 - Short answer: it is an overarching repository called "nexus-e" containing sub-repositories ("submodules" is the official term in git).
- I want to make changes in my own module. What should I do first?
 - Short answer: be aware of where you are in other modules. If needed, pull changes from other submodules.
- *I have made some changes in my own module and tested them in a small scale. How do I test them with the full Nexus-e platform?*
 - Short answer: depending on the scale of your change if small, you might want to copy the changed file(s) to Euler; if large, you might want to push the changes first then pull it on Euler.
- I have fully tested my changes in my own module. What should I do now?
 - Short answer: push what you have tested (maybe not only your own module) into the overarching repo.

We recommend to use a git GUI (e.g. GitKraken, Git Extensions, SourceTree, and many more) to work with git locally. However, Euler doesn't have a GUI, therefore you have to use command line there. In this documentation, we demonstrate with the GUI "GitKraken". You can get a pro account for free as a researcher. The screenshots are taken from MacOS. There should be equivalent operations on other operating systems.

Why GitKraken:

- It is stable in all operating systems (Linux, Mac, Windows)
- It provides a good overview for the status of submodules, which is the key structure of our Nexus-e repo.
- It has an embeded & very handy merging conflict resolution tool.
- It is mature and well-documented.

3.1 How do I get the repository?



Would you like to initialize submodules for nexus-e-demo?

(3) Initialize the submodules (select "Yes")

Afterwards, you will see submodules getting initialized one one (In the screenshot beby low there are 7 submodules. Since January 2021, it is reduced to 5 submodules.):

(2)

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3.2 What is the structure of the repository?

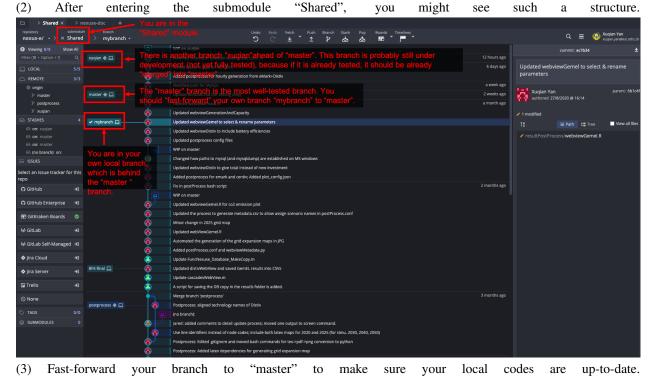
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To help with understanding, we show both interfactes in GitKraken (left) and in the repository (right).

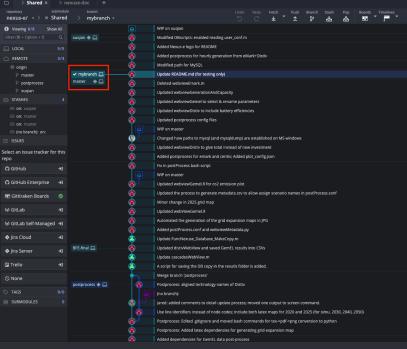
3.3 I want to make changes in my own module. What should I do first?

For example, you want to make changes in the "Shared" module. Note: Since January 2021, "Shared" is not a submodule anymore but a folder directly under the Nexus-e repository, but the procedures demonstrated here can be applied to any submodules.(1) Open the submodule "Shared".

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(4) Now your own branch is at the same level as "master".

(5) Sometimes you might need to update other modules as well.E.g., if your change in the "Shared" module depends on the newest changes in the "CentIv" module which is in the "target_branch" branch (doesn't have to be the "master" branch), you will need to go through a similar procedure:

- Enter "CentIv" submodule.
- Fast-forward your own branch to the "target_branch".

(6) In the end, you could enter all submodules one by one to make sure that you are at the right place in all of them.

3.4 I have made some changes in my own module and tested them in a small scale. How do I test them with the full Nexus-e platform?

To test the full platform, you will need to move your codes with your changes to Euler and run Nexus-e on Euler.

There are two ways to get codes to Euler: (1) copy from your local and (2) use git. Here we list the pros, cons, and use cases of both ways. You could decide which way to use.

- Comparison
 - Copy from local
 - * Pro: (1) This can be done with a GUI tool. (2) You don't need to push to the repository first.
 - * Con: (1) Copying the whole Nexus-e folder takes time (a few minutes). (2) If you only copy selected files where you have made changes, you might by accident forget some.
 - * When to use: (1) when you need to test small changes that you don't want to push to the repository yet, and (2) when you can't push to git, e.g., when you made changes in a repo where you don't have permission to push.
 - Git
 - * Pro: (1) Using git gaurantees that what you run on Euler is exactly the same as in the repository. (2) It is fast because only updated files will be reloaded by git and some files (e.g. results) are ignored by git.
 - * Con: (1) You need to run git commands in a terminal (no GUI). (2) You need to push your codes to the repository first and then pull it to Euler
 - * When to use: (1) When you want to test what is already in the repository, and (2) when you have made lots of changes to the codes and you might forget some files when you copy them to Euler manually.
- · Copy from local
 - Use a graphical tool to transfer files between Euler and your local computer.
 - Copy your whole Nexus-e folder (you don't have to copy the "Results" folder) to Euler.
 - Alternatively, you could also only copy individual files where you made changes, but you risk forgetting some files or forgetting to update some modules on Euler.
- Use gitIn this section, we assume that you already have Nexus-e codes on Euler, so you only need to update the codes where you have made changes. If this is not the case, follow the section Euler setup.
 - First, make sure to have a clean start be aligned with the most updated commit in the overarching repository.
 - (1) On Euler, go to the folder where you put the Nexus-e codes. e.g., cd nexus-e(2) Update the codes
 - * Delete your local changes (e.g., your edits in "run_Nexuse.m")git reset --hard
 - * Pull changes from the overarching repositorygit pull
 - * Update the submodules git submodule update
 - * (Optional) Check the commit numbers of each submodulegit submodule foreach "git rev-parse HEAD"
 - Then, go to the individual submodules where you want to pull changes that are not in the overarching repository. For example, you want to test your changes in the "Shared" submodule which is pushed to a branch named as "postprocess".

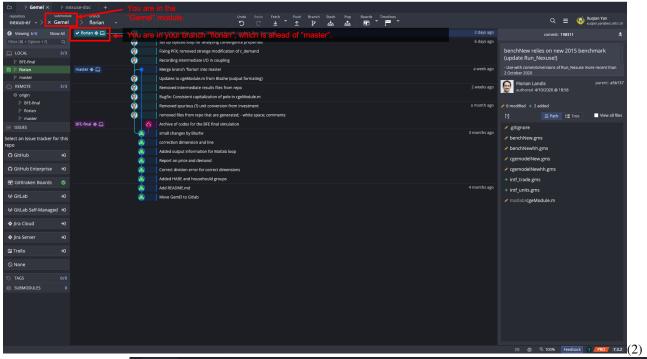
(1) Go to the folder where you want to pull the changes, e.g., cd Shared(2) Check which branch you are at right now withgit branchE.g., in the screenshot below, it is at the "xuqian" branch (seen from the "*" sign) and there is **no "postprocess" branch yet**. (Note: This is the most complicated case. For example, if you already have the "postprocess" branch and you are already at the "postprocess" branch, you could skip the following steps and only run git pull. See more information on switching branch with git checkout and updating the current branch with

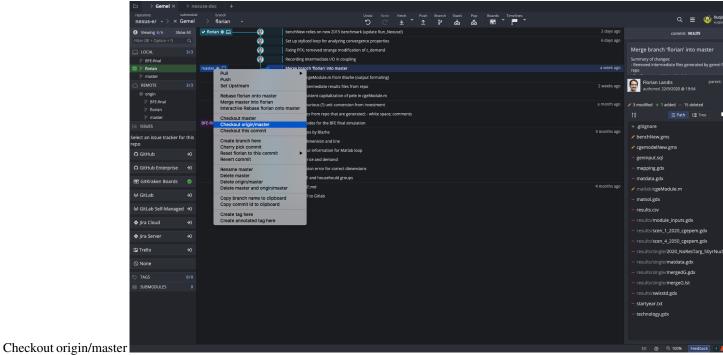
```
[xyan@eu-login-19 Shared]$ git branch
          master
git pull.) * xuqian
                                                      (3) Fetch the origingit
fetch origin(4) Pull changes in the "postprocess" remote branch withgit pull origin
postprocessYou will see the following message asking for your credentials for the "Shared" repo.
[xyan@eu-login-19 Shared]$ git pull origin postprocess
Username for 'https://gitlab.ethz.ch': xyan
Password for 'https://xyan@gitlab.ethz.ch':
From https://gitlab.ethz.ch/jaredg/nexus_shared
 * branch
                          postprocess -> FETCH_HEAD
Already up-to-date.
                                                                      (5)
Create and check out local branch "postprocess" withgit checkout -b postprocess origin/
            [xyan@eu-login-19 Shared]$ git checkout -b postprocess origin/postprocess
            Branch postprocess set up to track remote branch postprocess from origin.
postprocess Switched to a new branch 'postprocess'
Check your branch again with git branch to make sure that you are at the "postprocess" branch.
 [xyan@eu-login-19 Shared]$ git branch
   master
 * postprocess
   xuqian
```

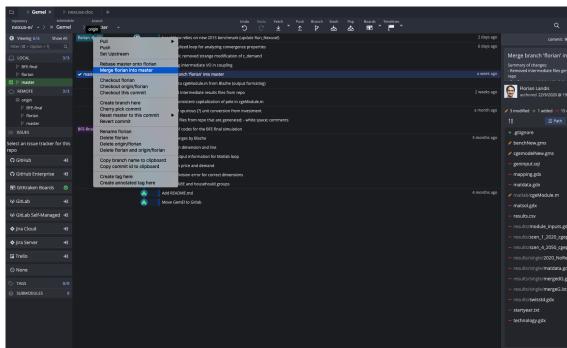
- Sometimes you need to do the branch switching (as instructed in the step above) for other submodules as well. From *here*, you should already know which branch you are at in each submodule.

3.5 I have fully tested my changes in my own module. What should I do now?

For example, you have made changes on the branch "florian" in the submodule "Gemel". The changes have been tested together with the updated module "Run_Nexuse". Now you are confident about the codes and you want other researchers also use your updates.Note: Since January 2021, "Run_Nexuse" is not a submodule anymore but a folder directly under the Nexus-e repository, but the procedures demonstrated here can be applied to any submodules.(1) Enter the "Gemel" submodule.



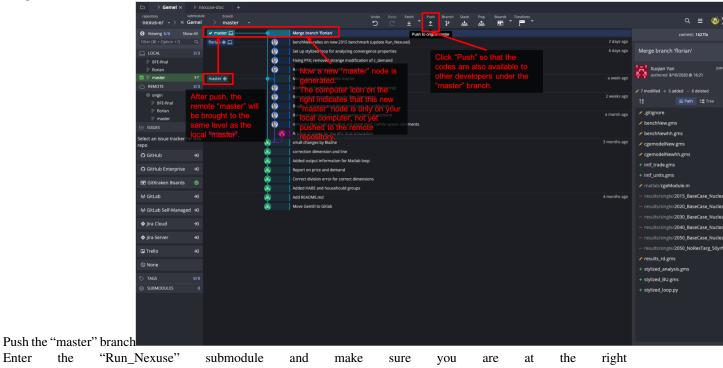




Merge "florian" into "master"

Enter

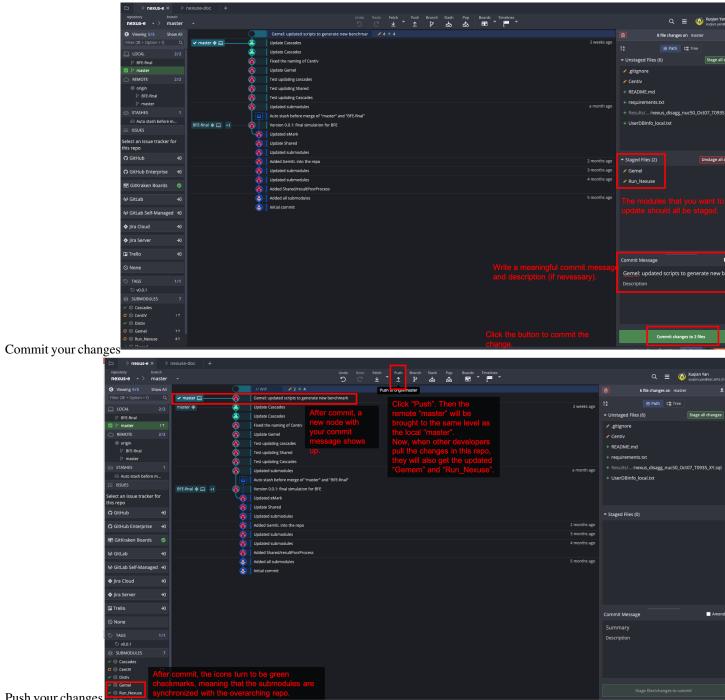
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💠 Jira Cloud 🗧	→)		Update run_Nexuse.m and run_Nexuse_1s.m		
♦ Jira Server ÷	→)		Update run_Nexuse.m and run_Nexuse_1s.m		
			Improved the displaying of informations regarding the execurtion of each loop and module.		
🛛 Trello 🗧			Update run_Nexuse.m	4 months ago	
⊗ None			Update run_Nexuse.m		
			Update run_Cascades_eMark.m, run_Nexuse.m, and 2 more files		
🕆 TAGS 🛛 0			Updated for the convergence check in the first loop.	5 months ago	
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			Update run_Nexuse.m		
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			Update run_Nexuse.m		
			Update run_Cascades_eMark.m, run_Nexuse.m, and run_Nexuse_1s.m		
			Updated to build the web-plot tables for the Cascades results.	6 months ago	
4			Update run_Nexuse.m and run_Nexuse_1s.m		
t			Merge branch 'master' of https://gitlab.ethz.ch/gblazhe/run-nexus-e.git		



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Push your changes

MODIFY INPUT DATA

Input data for Nexus-e are organized in two ways: (1) Collected in one common MySQL database and (2) Stored separately in each module. When modifying input data, you first need to figure out where the data is stored, and then take the corresponding approach to modify.

4.1 Where the input data are stored

Input data for Nexus-e are organized in the following two ways.

4.1.1 (1) Stored in one common MySQL database

By gathering input data in one common database, (1) it alignes the data used by different modules, (2) it easies the procedure to tune the parameters, and (3) the data become more transparent and have a clearer structure. Data that are collected in the database include - data that are used by multiple modules (e.g., grid parameters) - data that vary across scenarios (e.g., macroeconomic assumptions)

The structure of our current database can be found here.

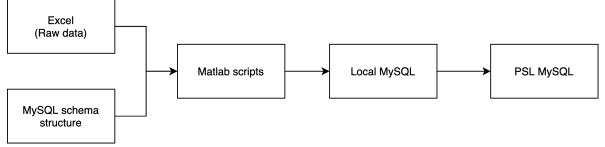
4.1.2 (2) Stored separately in each module

Storing data separately saves the effort to transfer the data into/out of the database. This is especially beneficial for complex data formats, because MySQL is only suitable for table-like data formats and other small & simple data formats that can be transformed into a BLOB. Data that are stored separately include - data that are only used for one module - data that do not need to be changed frequently - data with a complex format

4.2 How to modify

- If the data is stored within a certain module, contact the module owner (i.e., the administrator of the module's repository).
- If the data is stored in the input database, tutorial videos on how the database is created and how one can modify the input data can be found in Polybox 00_Administration/05_Internal

Meetings/2021/2021.05.03_MySQL-Tutorial. Here we briefly describe the workflow:



- The ending point: The input database of Nexus-e is served by a MySQL server from the Power Systems Laboratory (PSL) at ETH Zurich. This is the PSL MySQL block shown on the right side of the diagram above, i.e., the ending point of the workflow.
- The starting point: The left side of the diagram shows the starting point of the workflow. It contains (1) one Excel file of the raw data and (2) a MySQL schema structure (i.e., an empty schema without data but with the strucutre). the Excel is shared through Git and is available in \scenario_data\source_excel, while the schema structure can be found in the folder Shared/DBcreation/schema_structure.
 - * What to do: (1) get the Excel file (either find it on Git (as instructed above) or ask the Nexus-e team (nexus-e@ethz.ch) for it) and (2) upload the schema structure to your local MySQL server (instructions on how to work with the local MySQL).
- The intermediate steps: The raw data in the Excel is organized and populated into the MySQL schema structure in your local MySQL. This is conducted with the Matlab script Shared/DBcreation/addNexusExcel2dataBase.... This script calls other Matlab functions. Basically (but not always) each function takes care of one sheet in the Excel or one table in the schema. After running the script and making sure that the schema in your local MySQL is correctly populated, you can move the populated database to the PSL MySQL server.
 - * What to do: (1) At the beginning of the addNexusExcel2dataBase... script (look for the sign ###>---<###) edit the inputs as instructed in the script, (2) in Run_Nexuse/ conf_local provide the credentials to your local MySQL in UserDBInfo_local.txt, (3) edit the DB_INFO_FILE and PATH_MYSQL variables in conf_local.m (instructions), (4) run the script addNexusExcel2dataBase..., (5) when ready, export your local database and import it to the PSL MySQL (instructions on how to import/export a database).
- In summary, if you want to modify the data stored in the database:
 - * To **change** a data that is already in the input database, you only need to change the data in the Excel file and run the Matlab script with the existing schema structure. (You could theoretically also directly change the MySQL database, but to keep the workflow consistent, we recommend to always start from the Excel file.)
 - * To **add new** data to the input database, you will also need to adjust the schema structure and the Matlab script.

CONNECT NEW MODULE

- Before connecting a new module to the Nexus-e platform, the answer of following questions is needed:
 - 1. Is it going to be a substitute/replacement for an existing module?
 - 2. Is it an additional module that will be part of the existing or new convergence loops?
- In case question one is true, the existing interfaces can be used, including the convergence criteria that already exists. Furthermore, these interfaces may be extended if new points of connections are identified. This process requires consultation with the involved modelers.
- In case question two is true, clear interfaces has to be defined, i.e., the data exchange between the new module and the existing modules. Also, if the new module is part of any of the existing loops, the convergence criterion may need to be revised. Otherwise, new loop and convergence criteria need to be defined. These processes require consultation with the involved modelers.
- Each model within Nexus-e is connected to the platform using a wrapper, i.e., Matlab class. As an example use the existing wrappers, i.e., emModule.m (\eMark\electricity_markets\marketsModule) or CascadesModule.m (\Cascades\03_Run_models&methods). The class contains of properties and methods.
- In properties, assign your property attributes, e.g., wkspace (workspace information).
- In methods, we suggest that you set three types of functions:
 - Object constructor, which creates the module object. There you can have, e.g., additional paths to your subfolders, reed your input parameters, assign data structures (e.g., input parameters) to the module object, etc.
 - Run method, which executes the module. This function, besides the module object, as an inputs can use data from other modules with which interfaces are established.
 - Interface functions, which gather the data which will be stored and later send to other modules. You can
 have multiple interface functions. The number of these functions depends on the number of modules and
 type of information your module is sending data to. It is not necessary that the data exchange between two
 modules is going in two directions.
- Note that the aforementioned instructions are general directions, and therefore, the class is subject to customization based on the needs and preferences of the modelers.

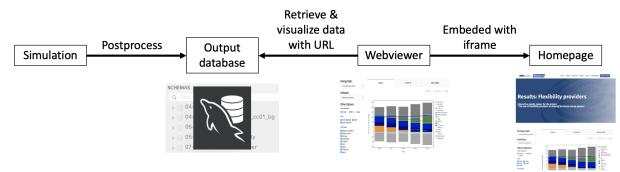
RESULTS VISUALIZATION

The simulation results from Nexus-e can be interactively viewed through a visualization tool (also called the "webviewer"), developed with Python Dash.

- Repository for the tool: https://gitlab.ethz.ch/nexus-e/nexus-homepage-dash.git
- A frontend example: https://nexus-e.org/results-flexibility-providers/

This documentation only introduces the general workflow of developing the visualization tool. Detailed instructions can be found in the README.md files in the associated repositories.

The visualization of achieved in workflow shown the simulation results is the in the figure. The key processes will be explained in the sub-sections



below.

6.1 Postprocess

After a simulation finishes, selected results are **postprocessed** and uploaded to the output database. This postprocess procedure is carried out in the following two ways. The two ways are designed for different purposes and both are needed.

- 1. Embedded in the run_Nexuse.m script
 - **Purpose**: Automatically process the results when finishing a simulation, so that the reseacher could promtly see the results of this simulation from the webviewer.
 - How it work: After the simulation finishes, run_Nexuse.m calls the MATLAB script Shared/ resultPostProcess/postProcess.m. This scripts calls other MATLAB/Python scripts to postprocess the results.
- 2. Stand-alone
 - Purpose: Batch-process multiple simulations, fine-tune/modify/test/debug the post-process scripts.

• How it works: Run the MATLAB script postProcess_batch.m locally. This script loops through multiple simulations and runs only the required post-process scripts (e.g., we don't have to run the complete post-process for quick debugging). Which simulations to loop through and which post-processes to run can be configured at the "To be edited" section in the script. Details can be found in the comments in the script.

Note: To properly run the postProcess_batch.mscript, you need to set up the paths for the required software (e.g., Python, GAMS). To do this, follow the instructions in Run_Nexuse/user_example_conf.m and the online documentation.

6.2 Output database

In the output database (host: itet-psl-s02, port: 3307), each simulation's results is stored in one **schema** named with the simulation **submission date** and the **scenario name** (e.g., the scenShortName variable in run_Nexuse.m), which looks like "01-dec-2020_baseline".

The output database can be viewed with MySQL Workbench in the same way as introduced here.

6.3 Retrieve & visualize data with a URL

After the postprocessed data has been uploaded to the output database, the data can be retrieved and visualized by **provideing a URL through the webviewer**. Three types of URL are accepted.

- 1. https://nexus-e.org/results/JOB-SUBMISSION-DATE_SCENARIO_NAME, e.g., https://nexuse.org/results/01-dec-2020_baseline. This will retrieve and visualize only the data from the **exact** MySQL schema named as "JOB-SUBMISSION-DATE_SCENARIO_NAME".
- 2. https://nexus-e.org/results/JOB-SUBMISSION-DATE, e.g. https://nexus-e.org/results/01-dec-2020. This will retrieve and visualize the data from all the MySQL schemas whose name start with "JOB-SUBMISSION-DATE". In other words, results from all simulations submitted on the same day will be shown on the website.
- 3. https://nexus-e.org/results/MANUALLY_DEFINED_URL, e.g. https://nexus-e.org/results/project. This will retrieve and visualize the results from all simulations associated with the MANUALLY_DEFINED_URL. This is particularly useful if we run multiple scenarios for one project. The mapping of URL and simulations is specified in the constants.py in the repository for the webviewer.

Note: Synchronizing data between the web server and the database

Not all changes in the output database will be automatically sychronized to the webviewer. The reason lies in how the data is downloaded from the database to the web server: based on the given URL, the webviewer checks the output database and decides which simulation(s) will be shown, i.e., which schema(s) should be downloaded to the web server; the webviewer then checks (by comparing the existing folder names and the schema name) whether the needed schema has already been downloaded; if the viewer finds a folder with the same name as the needed schema, it won't re-download the schema.

Therefore, to show a changed data in the output database (e.g., after changing the postprocess script, added new data), you need to **first delete the corresponding data folder on the web server** so that the webviewer will re-download the data from the database.

6.4 Embed the webviewer into the homepage

The webviewer itself is plainly a Python Dash application without much Nexus-e branding. To change this, it is embedded into the homepage with iframe - a html element to display a nested webpage within another webpage. By doing so, we can easily have the same header, footer and menubar for the visualization tool as in other Nexus-e webpages.

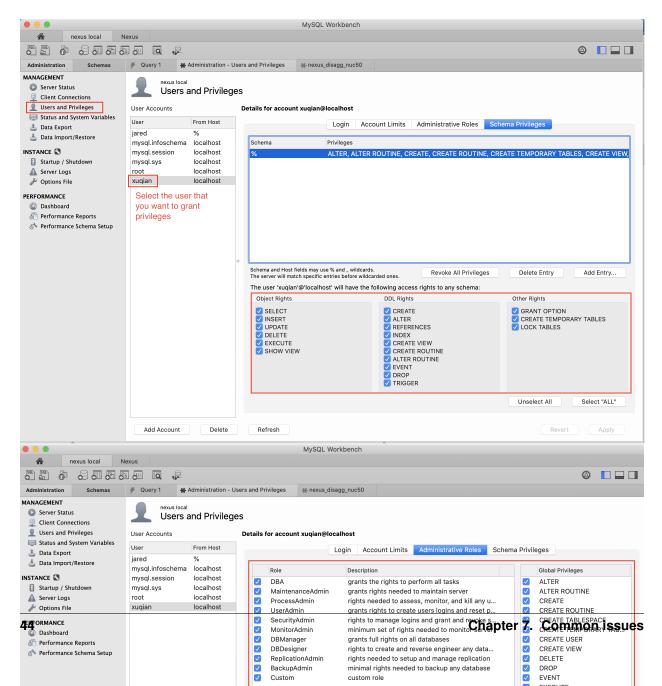
The embedding can only be done by the administrators of the homepage. If you are an administrator, you could login to the homepage and check the backend of this page to learn how it is done.

SEVEN

COMMON ISSUES

7.1 Database

7.1.1 Grant full privileges to a user in MySQL Workbench



7.1.2 Access denied to access database

- In Matlab, print out the variables connInfo.user, connInfo.pw, and connInfo.host to make sure that they are exactly what you provided in the your UserDBInfo file.
- Make sure you database user account has full permission to the database

7.1.3 Database server timezone issue

There are two ways to solve this issue: (1) using command line, but this only takes effect for the duration of the current service uptime, i.e., when the MySQL services restarts, you need to type in these commands again; (2) editing the MySQL configuration file, but the configuration file is platform-dependent, e.g., MacOS doesn't even have a default configuration file.

Here we introduce the 1st approach using command line. For the 2nd approace of editing the MySQL configuration file, see here.

- Open command prompt and login to mysql using the command:mysql -u root -p
- Enter your MySQl password for the root user, this should start mysql and you should see the prompt mysql>
- Type the following two command to reset the MySQL time zone:SET @@global.time_zone = 'Europe/Paris'; SET @@session.time_zone = 'Europe/Paris';
 - If you get the error "Unknown or incorrect time zone: 'XXX'", use the command (ref):mysql_tzinfo_to_sql /usr/share/zoneinfo | mysql -u root mysql -pThen rerun the SET @@... commands.
- You can check that these were properly set using the command:SELECT @@global.time_zone, @@session.time_zone;
- After confirming these are now correct you can exit mysql using the command:exit

7.1.4 Database definer missing

Add a dummy user (same name as the missing definer - you can see it from the error message) to the database and *grant all previleges*.

7.2 Software compatibility

7.2.1 Matlab & python

On Euler, sometimes you get a similar error ImportError: ...pyexpat...: undefined symbol: XML_SetHashSalt. This might be because of conflice between Matlab's and Python's libexpat.so.1 library. If you encounter this, it is better to consult IT. Or, you could try different combinations of Matlab and python by yourself.Here is an example to compare the versions of the libexpat.so.1 library of Python 3.7.1 and Matlab R2020a:

• Input command ldd /cluster/apps/python/3.7.1/x86_64/lib64/python3.7/ lib-dynload/pyexpat.cpython-37m-x86_64-linux-gnu.so. It gives libexpat.so.1 => /lib64/libexpat.so.1 (0x00002b00348bd000). This means the Python 3.7.1's library pyexpat.cpython-37m-x86_64-linux-gnu.so is linked against the operating system's libexpat.so.1 library and not the one from Matlab (/cluster/apps/matlab/R2020a/bin/ glnxa64/libexpat.so.1). • The screenshot below shows that the operating system's library links to the version 1.6.0; while Matlab R2020a's library links to the version 1.6.9. Experiences show that when if Matlab has a newer version than Python (namely, newer than the operating system), it should

[xyan@eu-login-47 ~]\$ ls -l /cluster/apps/matlab/R2020a/bin/glnxa64/libexpat.so.* lrwxrwxrwx 1 apps ID-HPC-APPS 17 Aug 24 14:14 /cluster/apps/matlab/R2020a/bin/glnxa64/libexpat.so.1 -> l -r-xr-xr-x 1 apps ID-HPC-APPS 188640 Apr 1 2020 /cluster/apps/matlab/R2020a/bin/glnxa64/libexpat.so.1.6.9 20a/bin/glnxa64/libexpat.so.1 -> libexpat.so.1.6.9 [xyan@eu-login-47 ~]\$ ls -l /lib64/libexpat.so.1 -> libexpat.so.1.6.0