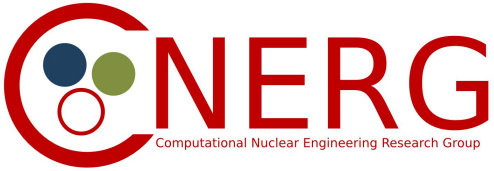
Empowering Fuel Cycle simulation with HTC Condor

B. Mouginot

HTC Condor Week - 05/2019

DEPARTMENT OF
Engineering Physics
UNIVERSITY OF WISCONSIN–MADISON

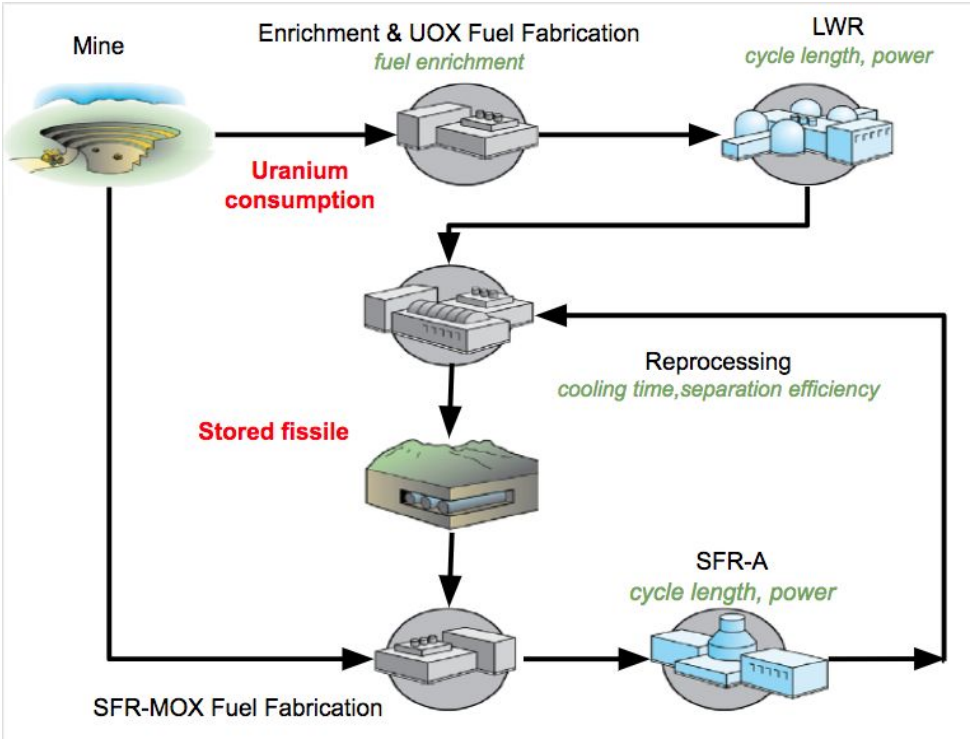


Nuclear Fuel Cycle Simulation - **What ?**

Simulation of the life of the nuclear fuel:

- From the mine to the ultimate waste
- Following all **fuel transformations**:
  - Fuel fabrication
  - Transmutation
  - Decay
  - Separation
  - …

- Scales:
  - Number of unit/facility:
    $10 - 10^3$ (country size)
  - Time scale
    10 days - 10^2 years

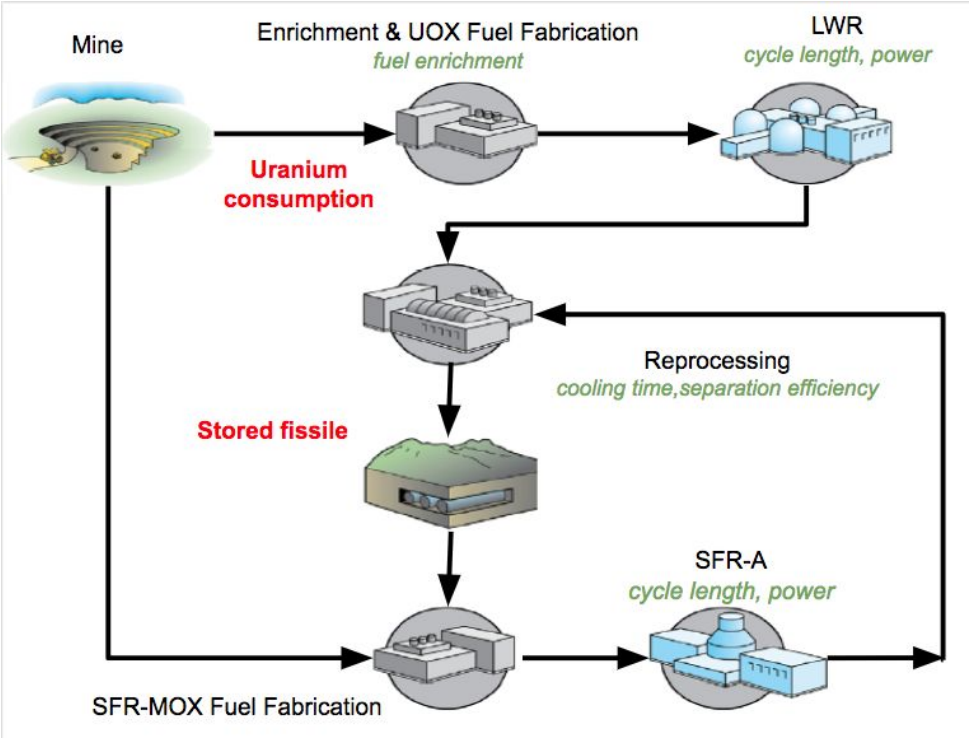


Nuclear Fuel Cycle Simulation - **Why ?**

Simulation of the life of the nuclear fuel:

- Assessing possible future:
  - Cost
  - Waste production
  - Proliferation risk
  - Deployment optimisation
  - Phase-out

- Retrieve past production:
  - Benchmark
  - Non-proliferation:
    - Verification
    - Nuclear archeology



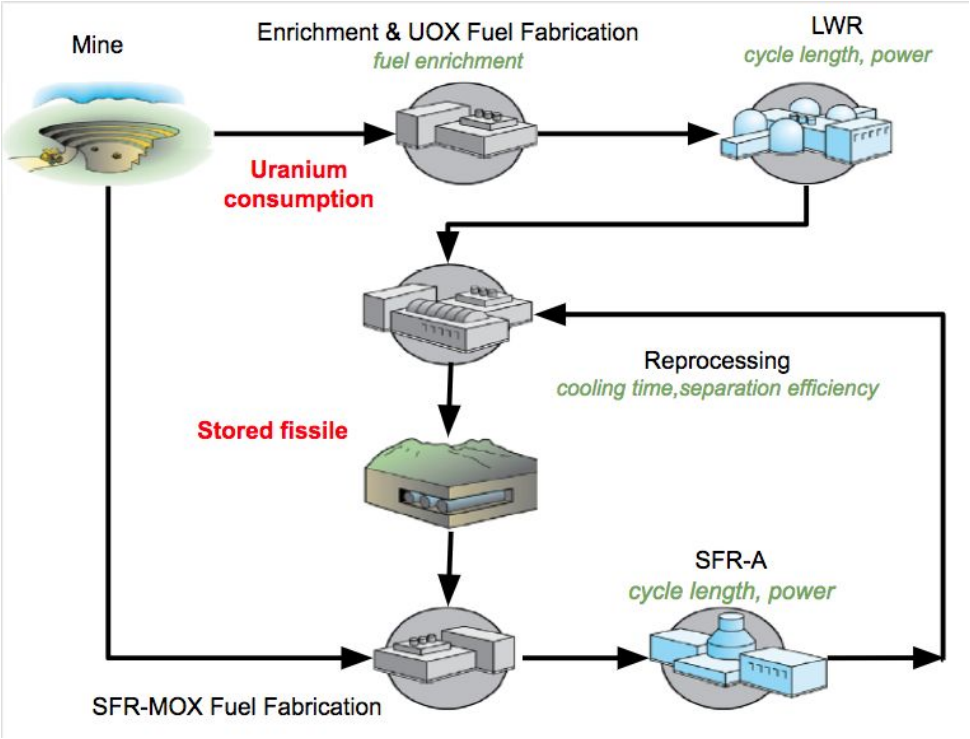
Nuclear Fuel Cycle Simulation - **How ?**

Simulation of the life of the nuclear fuel:

- NFC Simulators:
  - ORION[1], DYMOND[2], VISION[3],
  - CLASS[4], COSI[5], CYCLUS[6]

- CYCLUS: the (real) Agent based simulator

- Each facility:
  - individual decision making algorithm
  - Interacts through the Dynamical Resource exchange
  - could be as detailed as possible



First use of HTC

Neural network (NN) Prediction :

- 1 fuel/reactor type
- Neutron multiplication factor evolution
- ~700 Macroscopic reaction cross sections

Neural network (NN) training :

- trained on 1.10^3 to 10.10^3 nuclear fuel evolutions
- Each evolution requires:
  - ~10 CPU.h
  - 180 Mo raw data produced
  - 1.9 Mo of useful data
- Up to:
  - ~100 000 CPU.h per model
  - ~1.8 To of raw data
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Solution:

- tar.gz raw datas (from 180 to 50 Mo)
- Increased disk quotat
- batch of 5000 jobs

- Directly upload raw data on Box

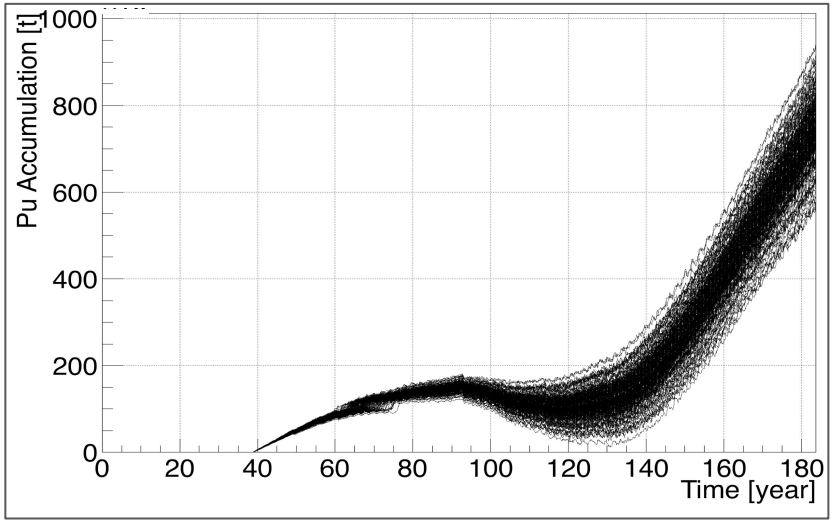
```
> cp $home/.netrc ~/

> curl -1 -v --disable-epsv --ftp-skip-pasv-ip
--ftp-ssl --upload-file ${1}_raw.tar.gz  -netrc
ftp://ftp.box.com/.../${1}_raw.tar.gz

 > rm -rf ~/.netrc


.netrc:
"machine ftp.box.com login YYYYY password XXXXXXX"
```

Stochastic Uncertainty Propagation

Stochastic uncertainty propagation:

- 1/10 of the US nuclear fleet over 180 years
- Main uncertainty propagation: 400 simulations
- Parameters normally distributed

- Output metrics uncertainty: std deviation
- Individual contribution One At the Time:
  200 simulations each



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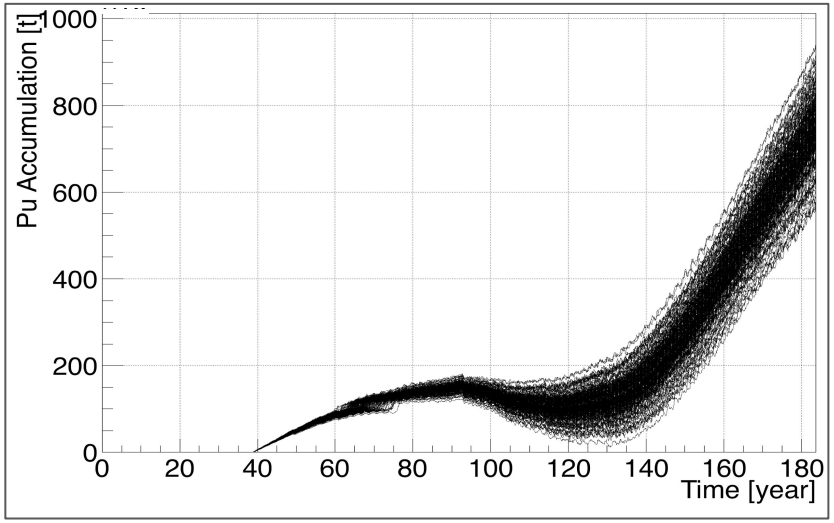

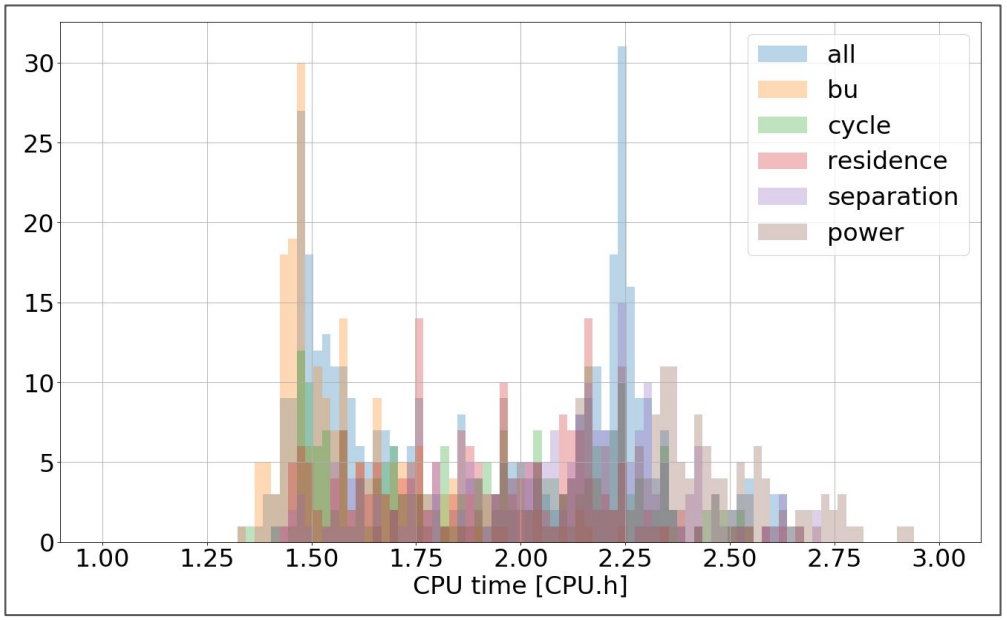

Computational needs:

- Per jobs:
  - ~ 2.2CPU.h
  - 20 Go memory
  - 22 Mo of generated
- 1400 jobs
- Total of ~2700 CPU.h
- x 2 (bug fixing, errors, crashes, data loss, …)

Issues: setup

Worker setup:

- Build a tar.gz package:
  - simulation software
  - Dependencies
  - Need to update the tar.gz frequently

    once/twice a year

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Typical dependency list:

- c/cpp compiler
- python
- CMake
- Boost
- libxml2
- libxml++
- sqlite3
- HDF5
- Coin-Cbc
- py_Jinja2
- py_NumPy
- py_Pandas
- py_Cython
- ROOT + pyROOT
- *CLASS*
- *cyCLASS*
- *cycamore*
- ...

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- Script:
  - No direct intervention:
    hard to debug and fix problem
  - Need to wait for the job to come back

- Interactive:
  - Wait to get an interactive worker
  - Connection issues:
    - connection/wifi loss
    - Not done when need to move
      (meeting, back home, …)

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Solutions:

- install scripts
- tmux/screen (from desktop computer) to keep connection alive

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Solutions:

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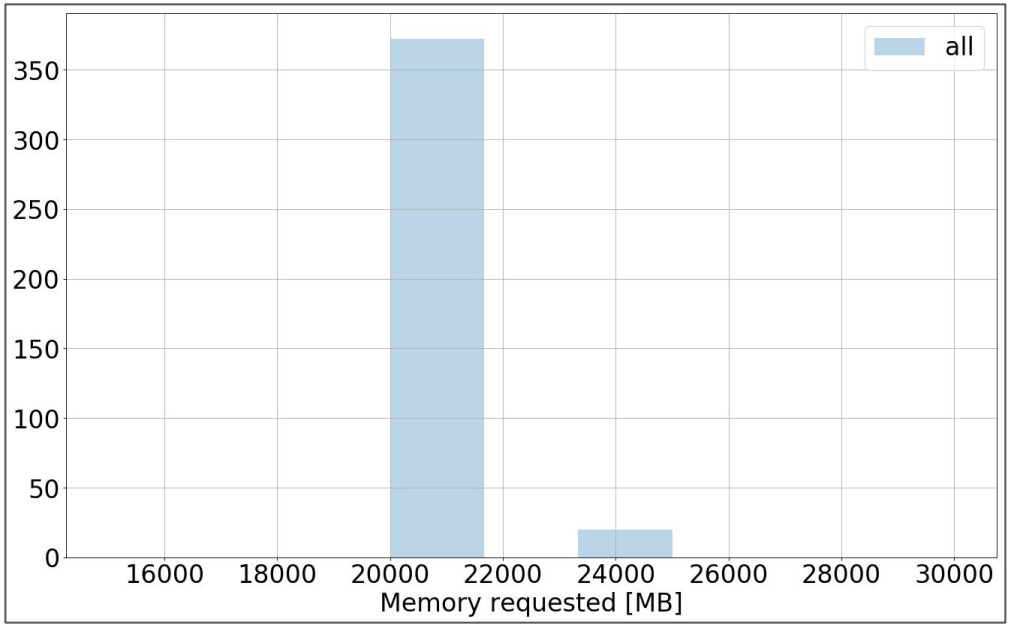
Future workflow:

- Docker:
  - pro:
    - Complete control of the environment
    - Easy to test and install softwares
  - Cons:
    - Image size
    - Speed ?

Issues: exceeding memory allocation

5-10% of the job on hold:

- Some jobs used too much memory



- Solution: restart them requesting more memory (x1.2) up to 4 times

```
cvt.sub:
# Conditionnal memory request
request_memory = ifthenelse(MemoryUsage =?= undefined, 20000, (MemoryUsage * 1.2))

# Periodidic release
periodic_release = (JobStatus == 5)
                        && ((CurrentTime - EnteredCurrentStatus) > 180)
                        && (JobRunCount < 4)
                        && (HoldReasonCode =?= 34)
```

Workflow Improvement

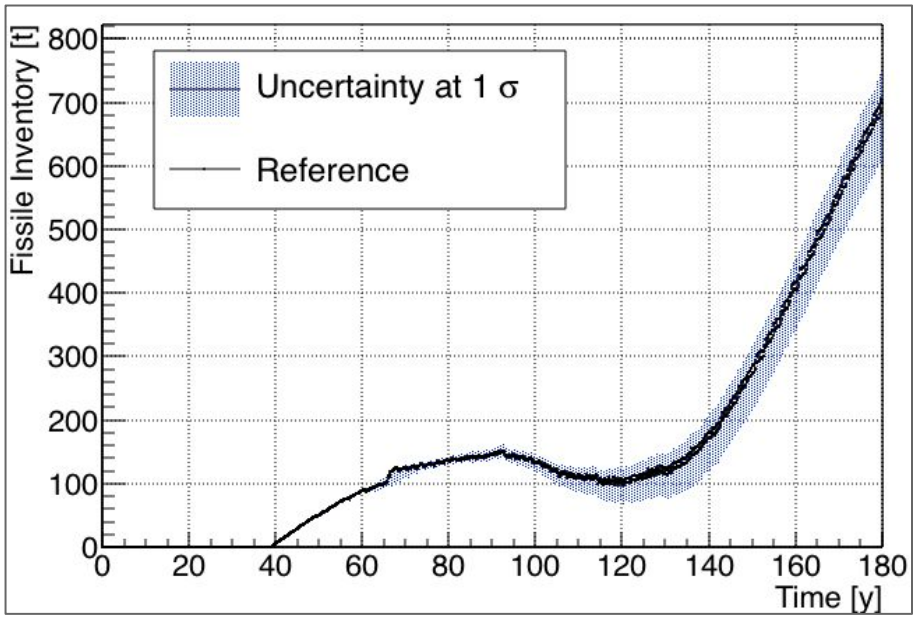
Post-processing:

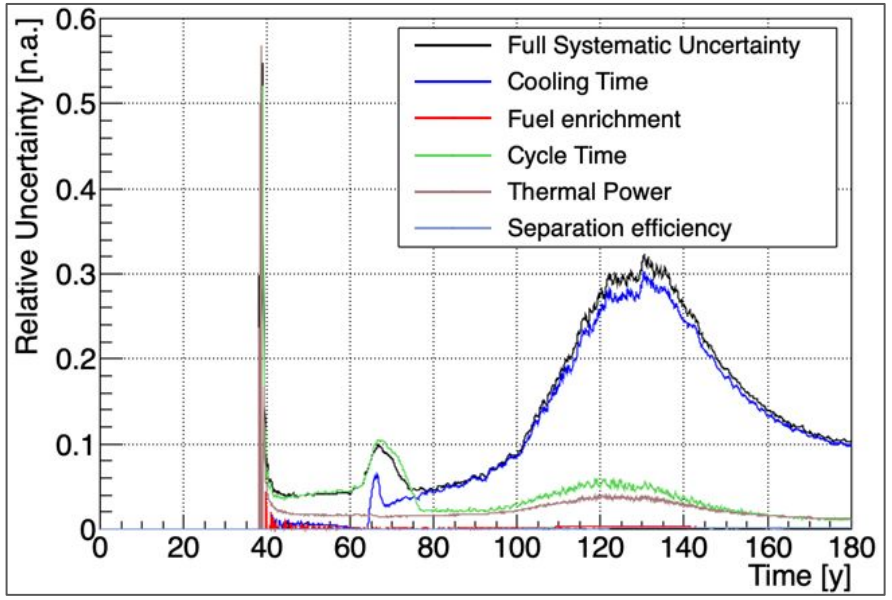
- Combining different simulations
- Computing the uncertainty
- ~2h per set / ~12h total
- Was run locally :(

Use flow manager (*makeflow* / *dagman* / *?*):

- combine simulation
- compute the main interesting metrics
- Produce plots

Final Results





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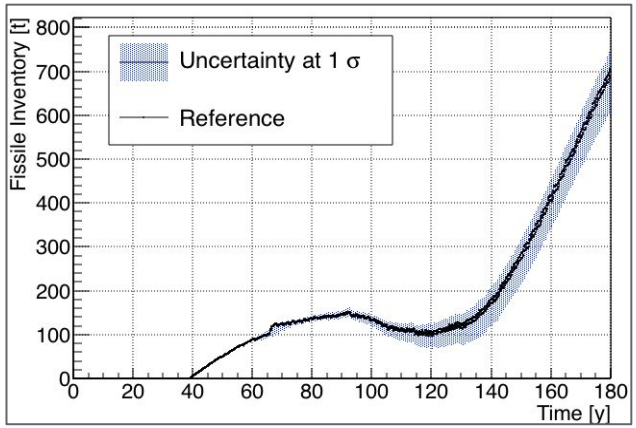
CONSORTIUM FOR VERIFICATION TECHNOLOGY

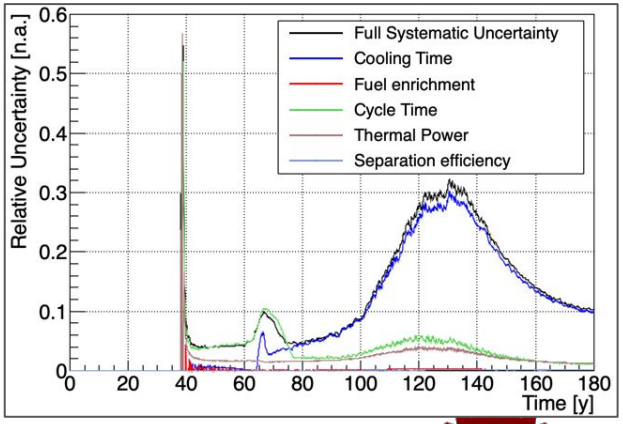
CNERG
Computational Nuclear Engineering Research Group

Thank you !

Questions/Comments ?

Thanks to the Research Computing Facilitators for all the help and advices.





CENTER FOR HIGH THROUGHPUT COMPUTING

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