Reactions on Unstable Nuclear Targets: Theory and Workflow Developments

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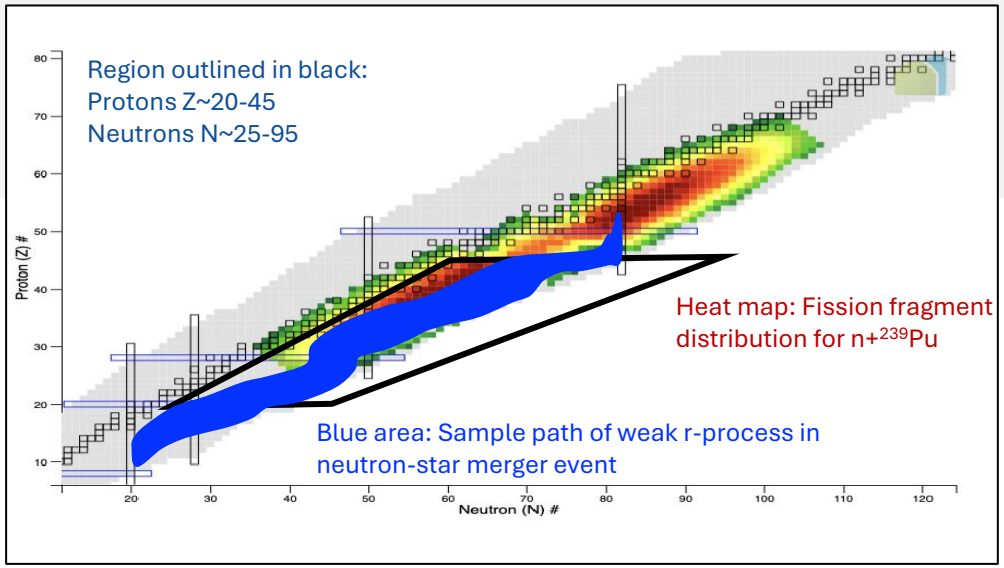
Objectives & Overview

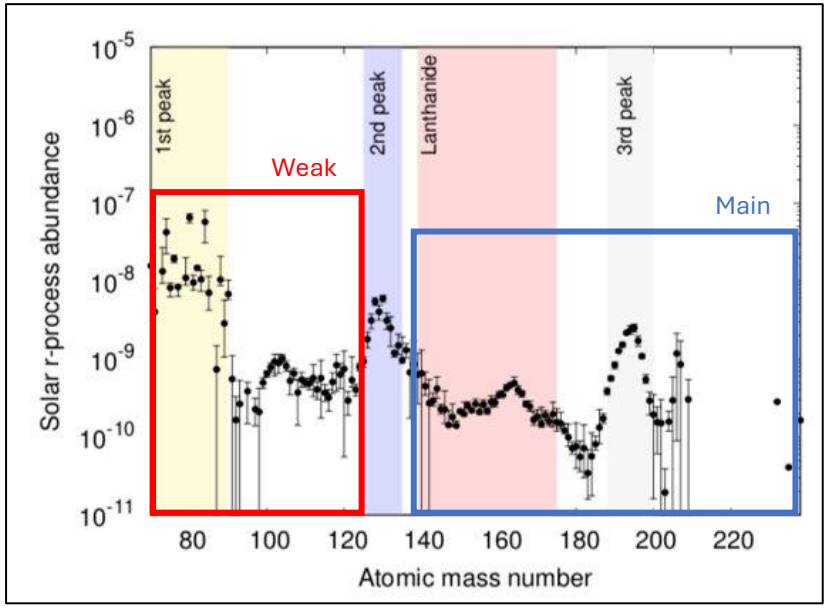
The overarching goal of LDRD 24-ERD-023 is to provide *uncertainty-quantified* predictions for neutron capture rates for species relevant for the weak *r*-process.

I'll focus on the uncertainties derived from the projectile-target interaction(s)—specifically, from the *optical model potential*. I will also flag other sources of uncertainty that will need to be considered to enable robust predictions.

To assess these uncertainties requires software assistance for the organization and execution of *large numbers of reaction calculations*.

(While my focus is on astrophysics here, our techniques/results will be more broadly applicable!)





Two views of the (weak) r-process.

The top shows (roughly) the part of the nuclear chart where the weak r-process is operative; the region bounded in black corresponds to the set of species to be considered in this project, which coincides with light fission fragments. (Figure courtesy of Jutta Escher.)

The figure at left shows solar abundances attributable to the r-process; see Hotokezaka et al. (2018) and references therein. The boxes roughly indicate the species populated by the weak and main r-processes. (Figure taken from Jonathan Cabrera Garcia's presentation at APS April Meeting 2024.)

We calculate reaction cross sections using the Hauser-Feshbach reaction framework

We calculate scattering rates in the context of Hauser-Feshbach (HF) statistical theory with LLNL's in-house code YAHFC ("Yet Another Hauser-Feshbach Code")

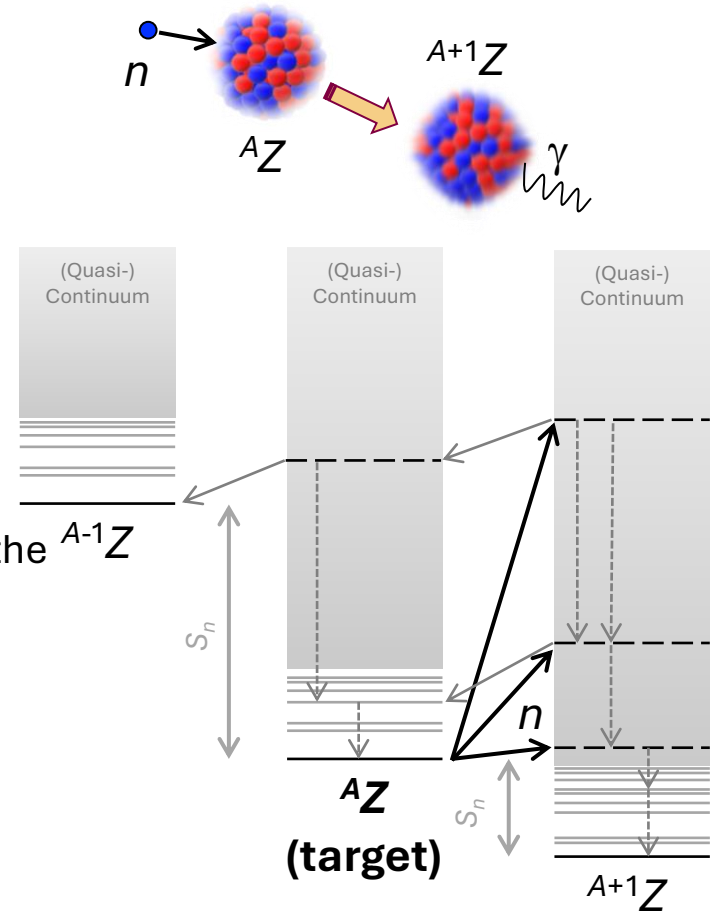
$$\sigma_{(n,\gamma)} = \sum_{J\pi} \sigma_n^{\mathrm{CN}}(E,J,\pi) \times P_\gamma(E,J,\pi)$$

Cross section for formation of a *compound nucleus*

$$\sigma_n^{\mathrm{CN}}(E,J,\pi) = \frac{\pi}{k^2}\frac{2J+1}{2(2J_{\mathrm{tar}}+1)}\sum_{\ell s} T_{n\ell s}^{J\pi}(E)$$

Probability to emit *a photon*

$$P_\gamma(E,J,\pi) = \frac{\sum_{J'\pi'\ell's'}\int dE' T_{\gamma\ell's'}^{J\pi}(E-E')\rho(E',J',\pi')}{\sum_c \sum_{J''\pi''\ell''s''}\int dE'' T_{c\ell''s''}^{J\pi}(E-E'')\rho(E'',J'',\pi'')}$$



The *transmission coefficients* T_c encode the interactions between the compound nucleus, the absorbed/emitted particle *c* and the target/residual nucleus:

$$T_{c\ell s}^{J\pi}(E) = 1 - |S_{cc,\ell s}^{J\pi}|^2$$

Nucleon transmission coefficients are derived from an *optical model potential* (OMP); the gold standard has been Koning-Delaroche (KD) [1]. What are the uncertainties associated with this potential?

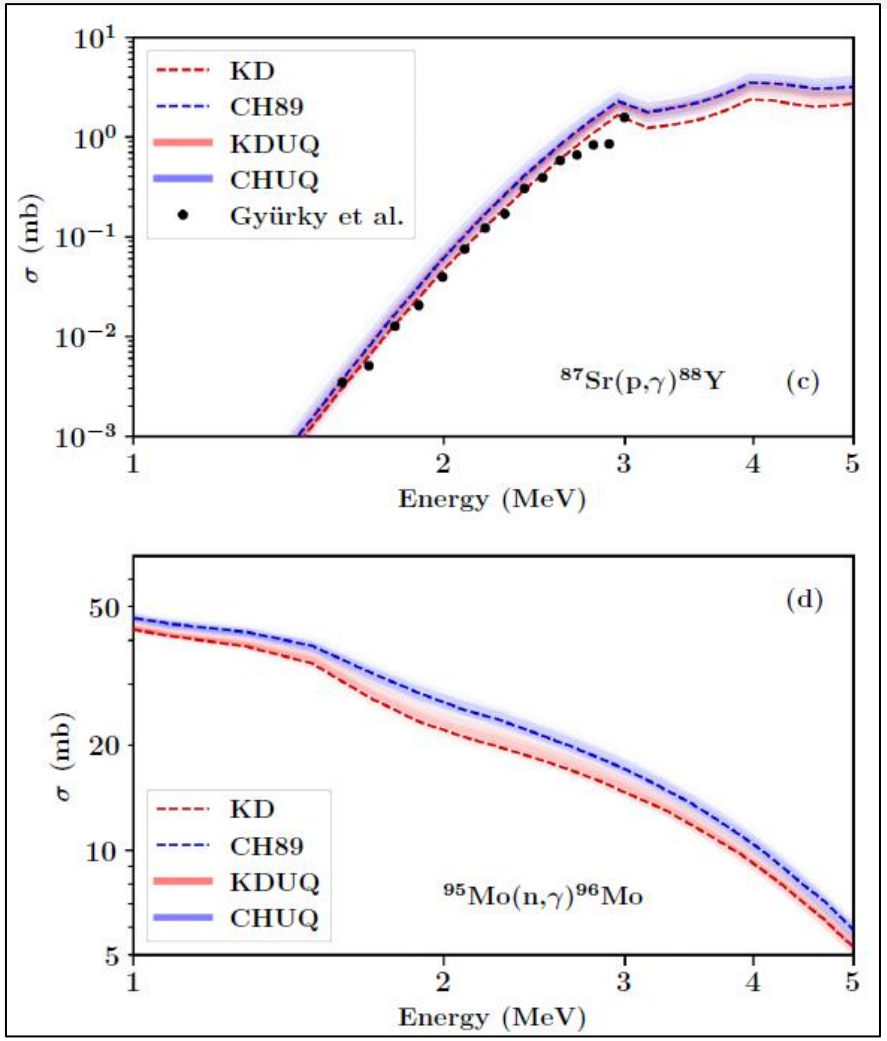
The uncertainties of the nucleon-nucleus interaction are ready for use and propagation

In 2022, Pruitt, Escher & Rahman [2] re-examined and refit both the KD OMPs and, applying more extensive statistical techniques, produced uncertainty-quantified versions of the OMP, called KDUQ. UQ is encoded in the *ensembles of potential parameters*—two flavors of UQ with 416 parameter sets each.

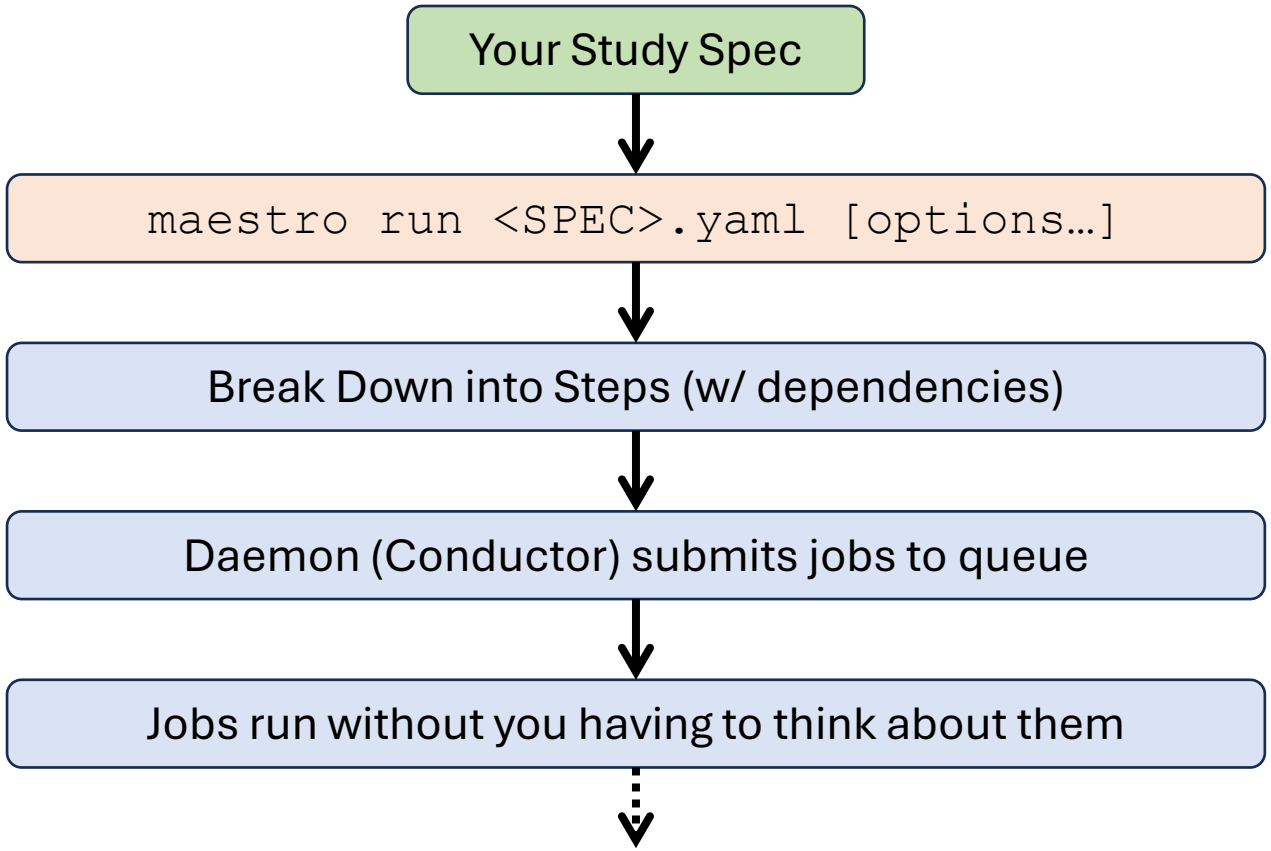
More recently, we have modified the KD potential to use consistent Fermi energies—we call the result "KDEF."

To determine OMP-based uncertainties, we need to pass these parameter ensembles through YAHFC into cross sections/reaction rate ensembles—this gives us O(10^5-10^6) calculations that we need to organize, execute and process. *To do this essentially requires software intervention*.

Fortunately, LLNL has tools that allow us to do precisely this!



Maestro breaks a study down into steps and submits them to the HPC resource manager



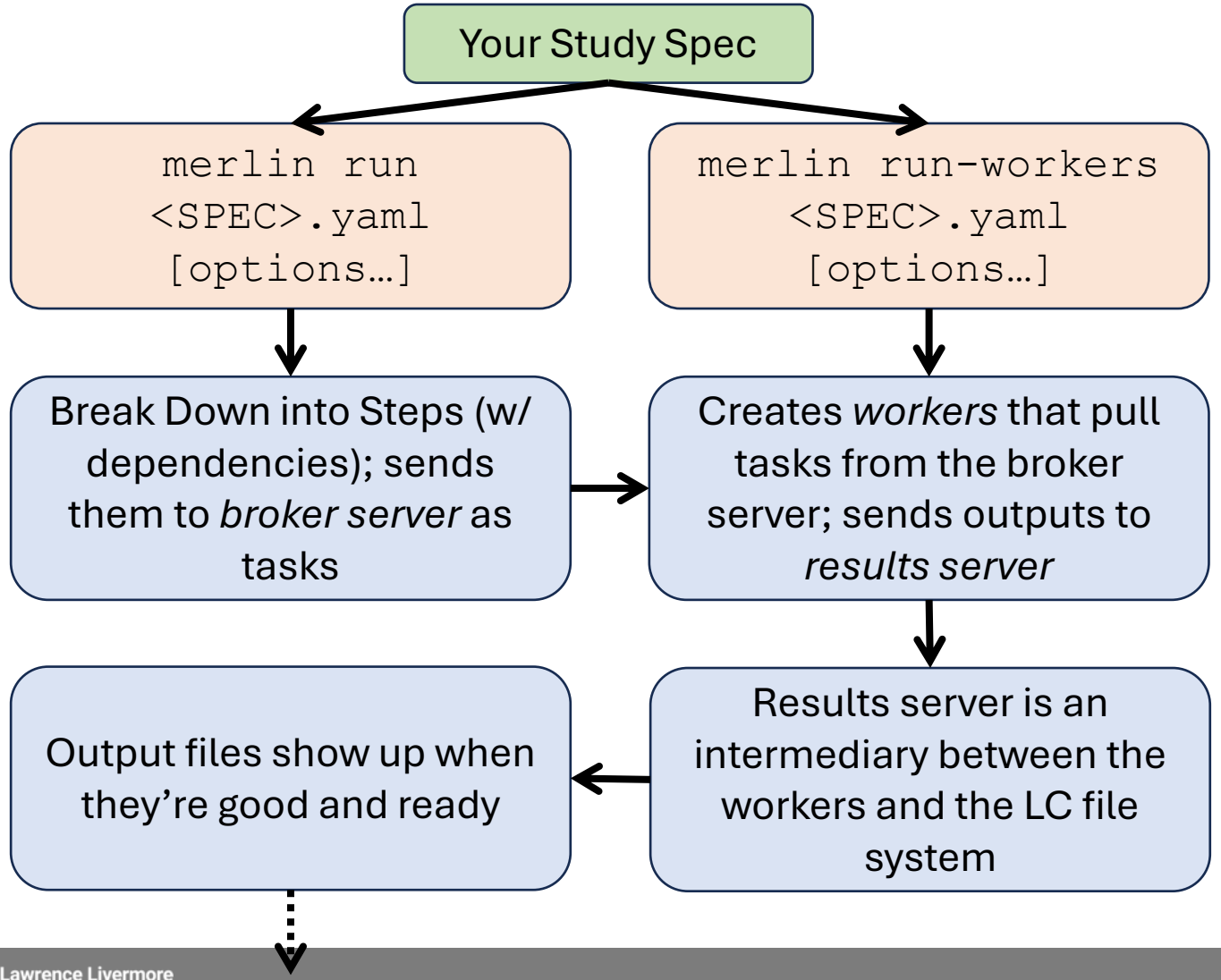
PROS:

- Simple to use—the Conductor lives on the login node and does all the interfacing with the SLURM scheduler
- Simple to monitor/interact with

CONS:

- Jobs submit individually—waiting!
- More difficult to get on-node parallelism.
- No systematic way to restart.
- Every isotope must have its own spec file, and is launched individually

Merlin is based on Maestro, but has more moving pieces; this comes with (dis)advantages



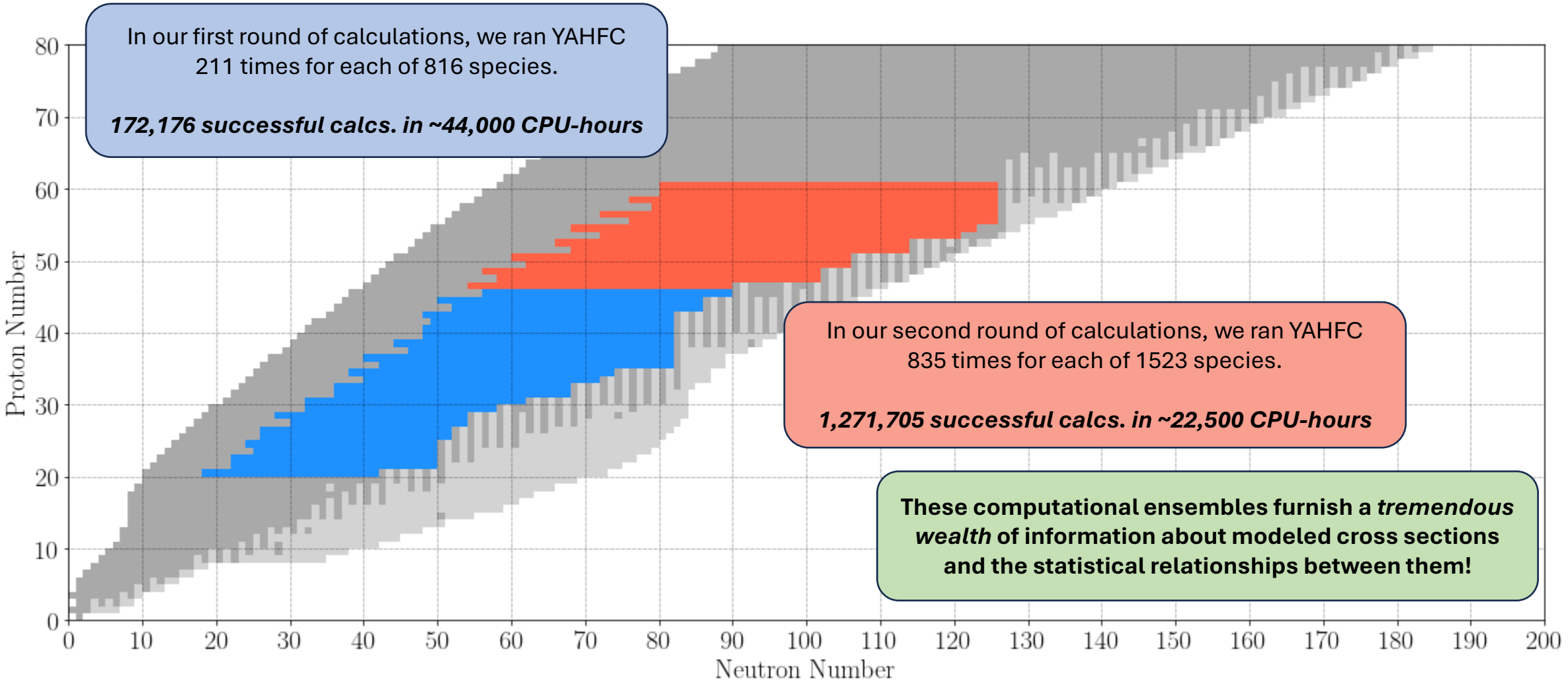
PROS:

- Workers scheduled per core; can run *many* realizations of (serial) YAHFC at a time.
- Studies can create other studies; launch entire isotopic chain at once.
- Restarts are trivial – `merlin restart…`
- Once you have an allocation, you keep going until it ends

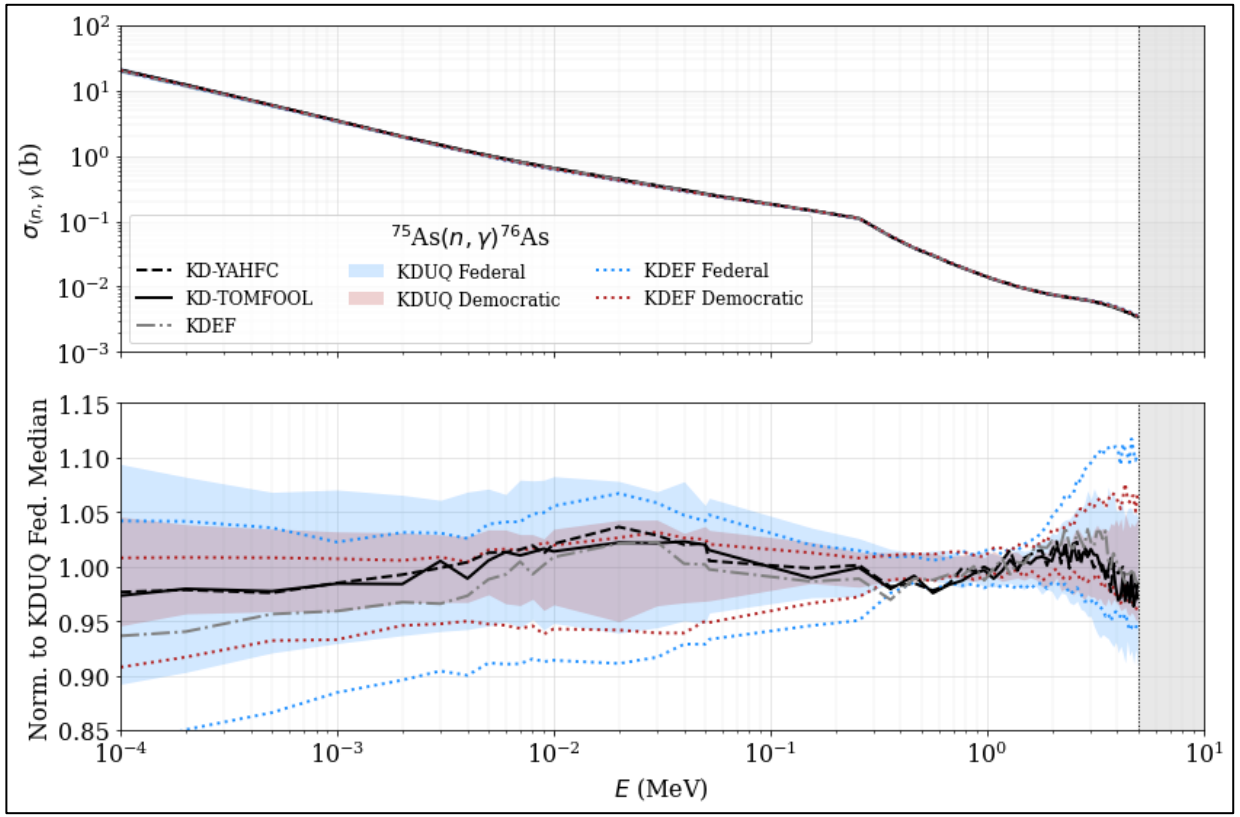
CONS:

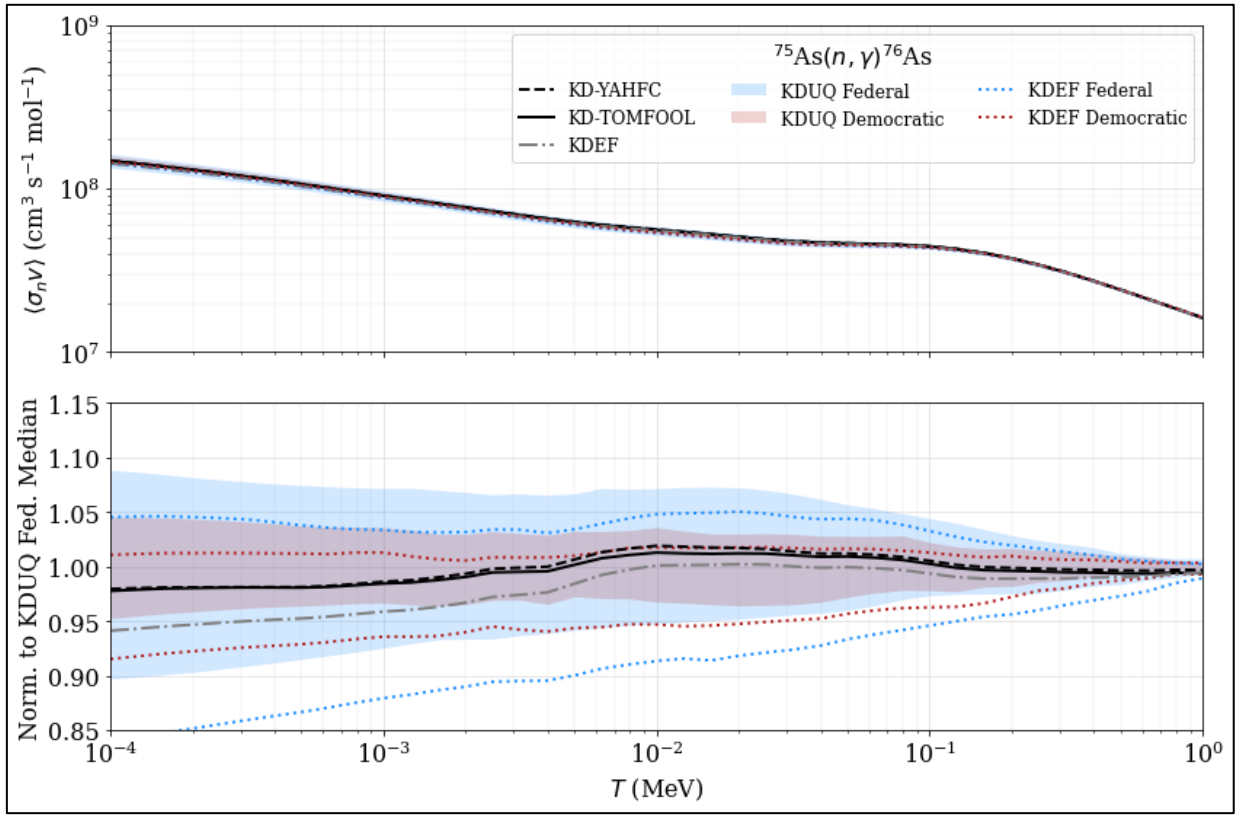
- Reliant on external infrastructure—which can be finnicky.
- More difficult to monitor/interact with.
- Need larger allocations to get started.

Workflow management tools have enabled calculations for >1500 nuclear species



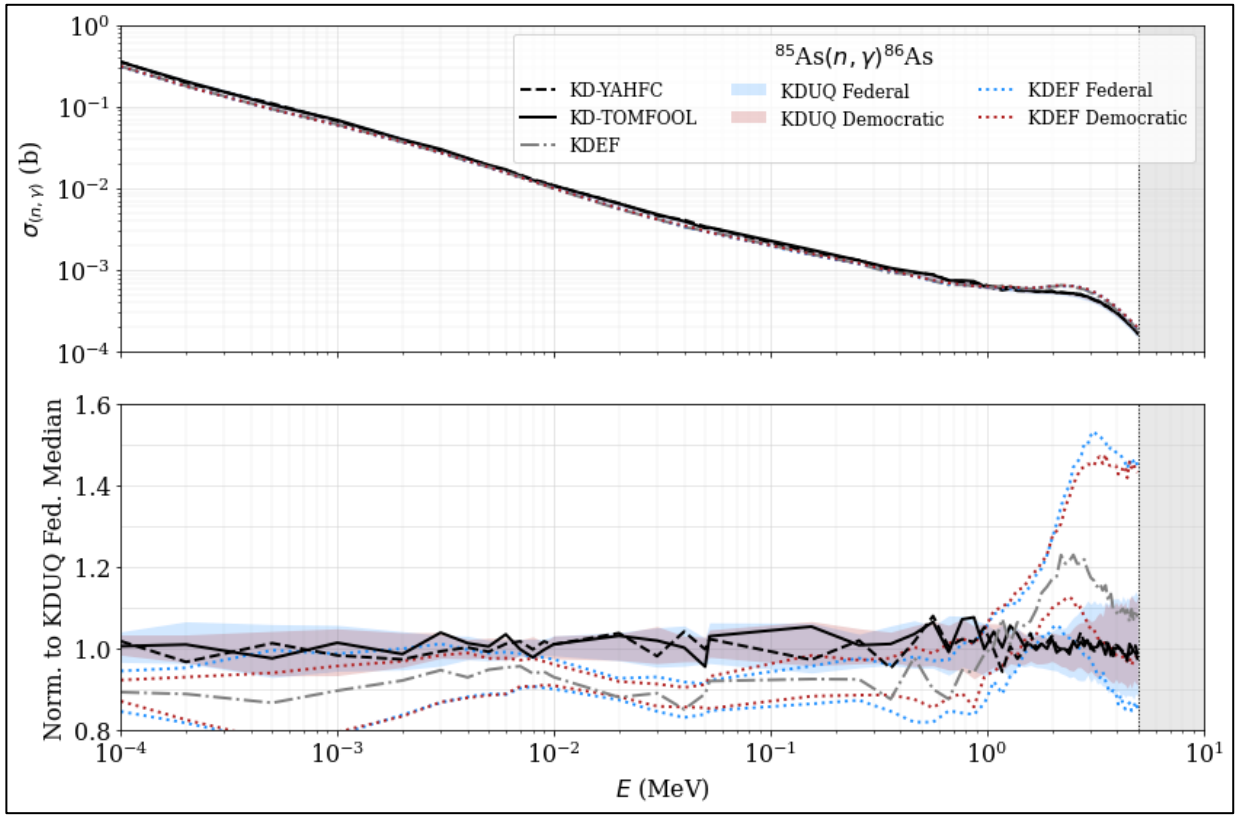
OMP-based uncertainties are at the few-percent level

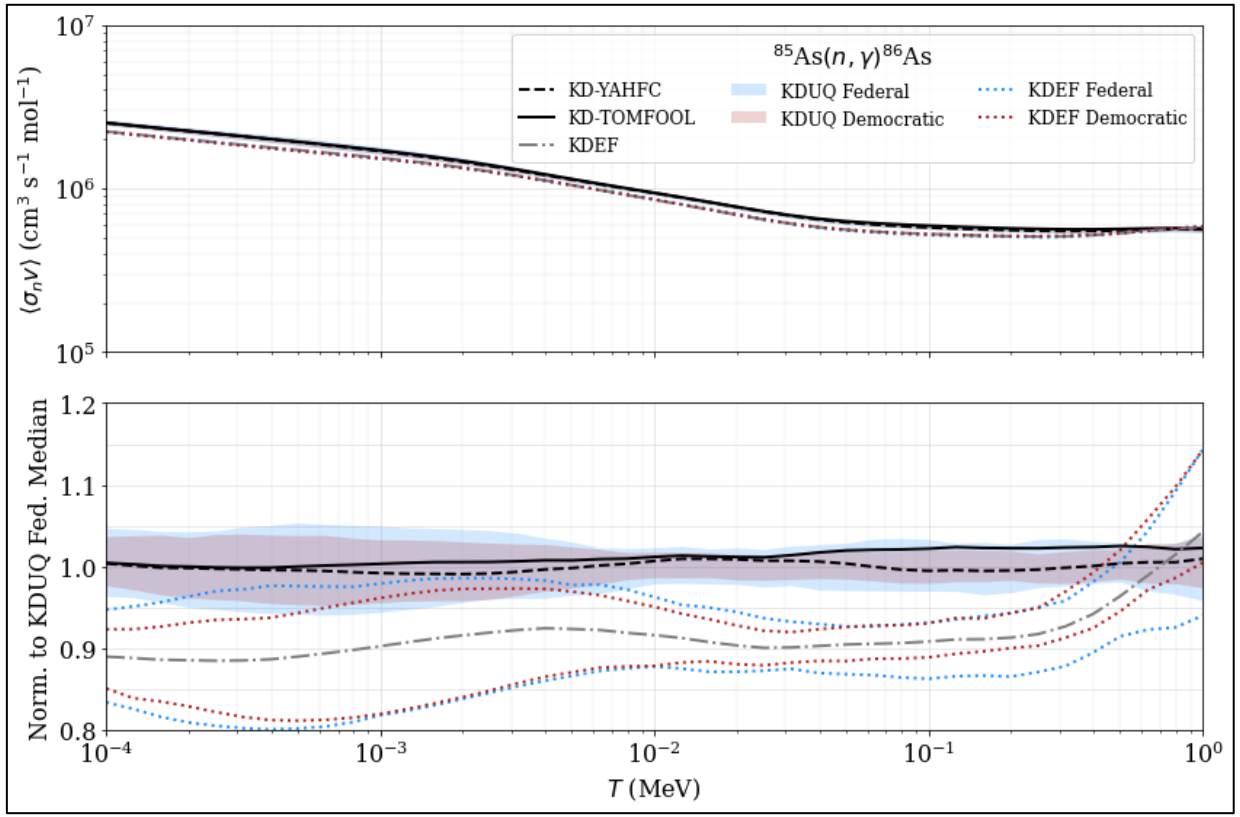




We expect that the OMP is the least significant source of (parametric) uncertainty that we will include.

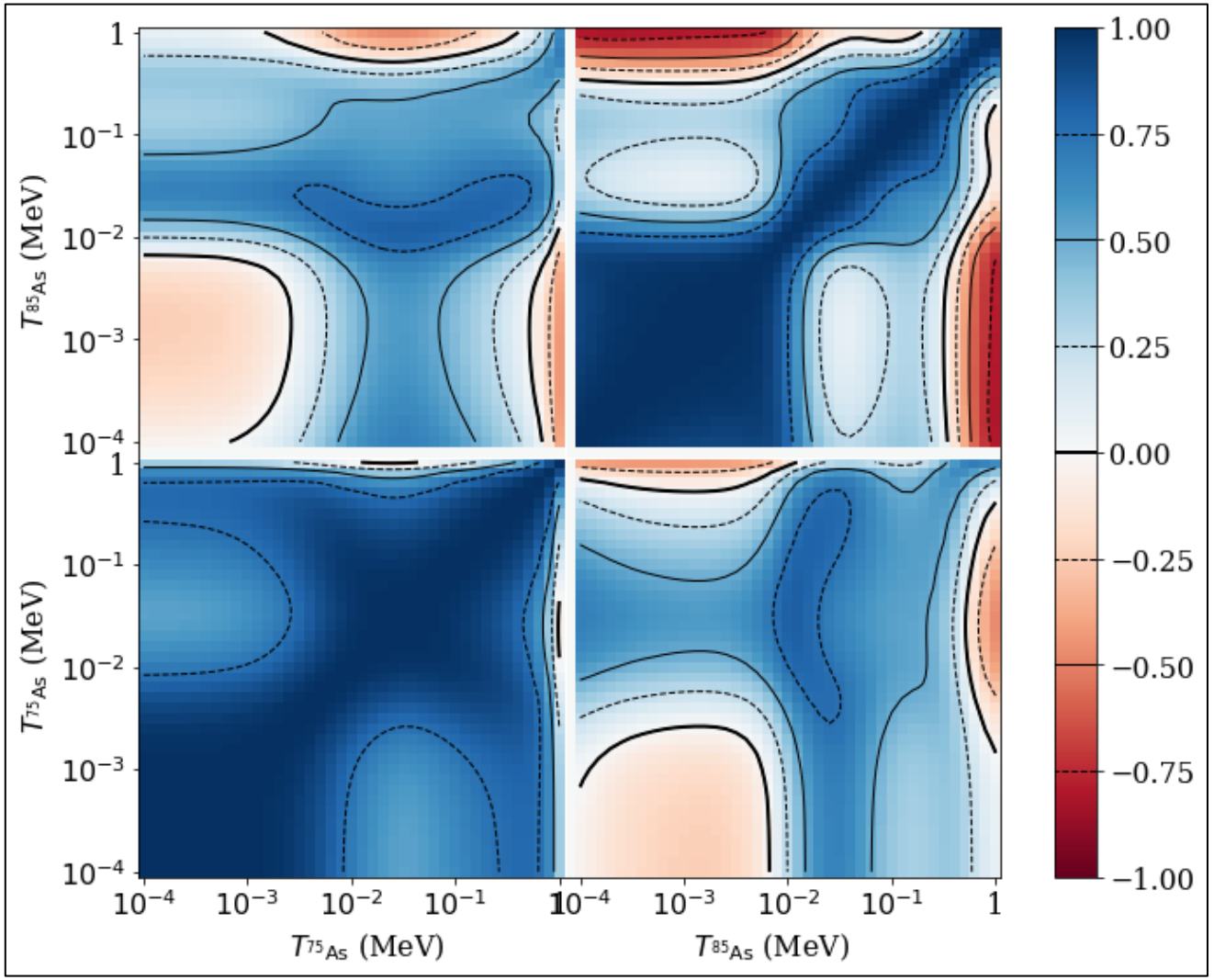
Off stability, changing the Fermi energy prescription engenders O(10%) changes to cross sections





Changing the model form induces a bias that is larger than the parametric uncertainties!

The use of a common OMP engenders strong correlations across energies—and across species



Strong correlations in model predictions have interesting implications for UQ: *Not including these predictions can lead to incorrect assessments of uncertainties in applications!*

The astrophysicists on this project have propagated our reaction rates into nucleo-synthesis calculations; it remains to be seen what impact this has on astrophysical abundances. (*Expect results soon!*)

It's worth noting that cross-species correlations are *not included in nuclear data libraries*. The relevance of these correlations is likely application dependent, but it's not clear *a priori* that they won't affect outcomes—what does this mean for an activation library?

There are other sources of (parametric & epistemic) uncertainty to be considered

Depending on the energy, this may not be the correct physical picture. The compound nucleus is formed *by assumption*; the reaction may instead proceed, e.g., by *capture on an isolated, low-energy resonance*.

We've discussed KD(UQ), but if the potential misses essential physics, *then no amount of UQ is going to help you capture that*. More sophisticated approaches to the OMP are being developed.

$$\sigma_{(n,\gamma)} = \sum_{J\pi} \sigma_n^{\mathrm{CN}}(E,J,\pi) \times P_\gamma(E,J,\pi)$$

$$\sigma_n^{\mathrm{CN}}(E,J,\pi) = \frac{\pi}{k^2} \frac{2J+1}{2(2J_{\mathrm{tar}}+1)} \sum_{\ell s} T_{n\ell s}^{J\pi}(E)$$

The T_γ are connected to the *γ strength function*, which is also a *modeled and uncertainty-laden object;* UQ treatment of this is in the works.

$$P_\gamma(E,J,\pi) = \frac{\sum_{J'\pi'\ell's'} \int dE'\, T_{\gamma\ell's'}^{J\pi}(E-E')\rho(E',J',\pi')}{\sum_c \sum_{J''\pi''\ell''s''} \int dE''\, T_{c\ell''s''}^{J\pi}(E-E'')\rho(E'',J'',\pi'')}$$

The denominator connects all possible final states; uncertainties in the modeling of one type of reaction affect the probabilities of all of them.

The *nuclear level density* is tremendously important – YAHFC implements some models for this that rely on *external input*. For unstable species, there are no data to inform these; one needs theory input, which is also in development.

Conclusions and Outlook

- We have constructed computational pipelines to turn nuclear physics inputs into astrophysical reaction rates *with robust (albeit incomplete) uncertainty quantification*.
- These pipelines provide gobs of information about the model-induced correlations between these rates.
  - Most work neglects these correlations—what are the impacts on astrophysical observables? On other applications?
- We are identifying shortcomings within this framework and developing additional ingredients to fill out these UQ pipelines.
  - Nuclear level densities and gamma-strength functions are explicitly within the purview of the project.
  - *Low-energy resonances* lead to order-of-magnitude differences relative to HF; working to treat these statistically.
  - *(Semi-)Direct processes* may be relevant for neutron-rich species; YAHFC may include *pre-equilibrium* contributions, but we have disabled these for this work.

The Team:

LLNL: JMB, Jutta Escher, Oliver Gorton (PD), Erika Holmbeck, Kostas Kravvaris, Gregory Potel (fmr.), Cole Pruitt, Andre Sieverding

NC State: Atul Kedia (PD), Gail McLaughlin

Notre Dame: Jonathan Cabrera Garcia (GS), Rebecca Surman

Thank you for your attention!

References

1. A. J. Koning & J. P. Delaroche, “Local and global nucleon optical models from 1 keV to 200 MeV,” Nucl. Phys. A 713 (2003) 231
2. C. D. Pruitt, J. E. Escher & R. Rahman, “Uncertainty-quantified phenomenological optical potentials for single-nucleon scattering,” Phys. Rev. C 107 (2023) 1, 014692, arXiv:2211.07741 [nucl-th]

Some other work worth perusing (not intended to be comprehensive and in no particular order):

- T. Rauscher & F.-K. Thielemann, “Astrophysical reaction rates from statistical model calculations,” ADNDT 75 (2000) 1
- C. J. Horowitz et al., “*r*-Process Nucleosynthesis: Connecting Rare-Isotope Beam Facilities with the Cosmos,” J. Phys. G 46 (2019) 8, 083001
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- A. Gade et al., “White Paper On Nuclear Structure Reactions and Astrophysics,” https://www.osti.gov/biblio/1999724
- A. J. Koning et al., “TENDL: Complete Nuclear Data Library for Innovative Nuclear Science and Technology,” Nucl. Data Sheets 155 (2019) 1-55
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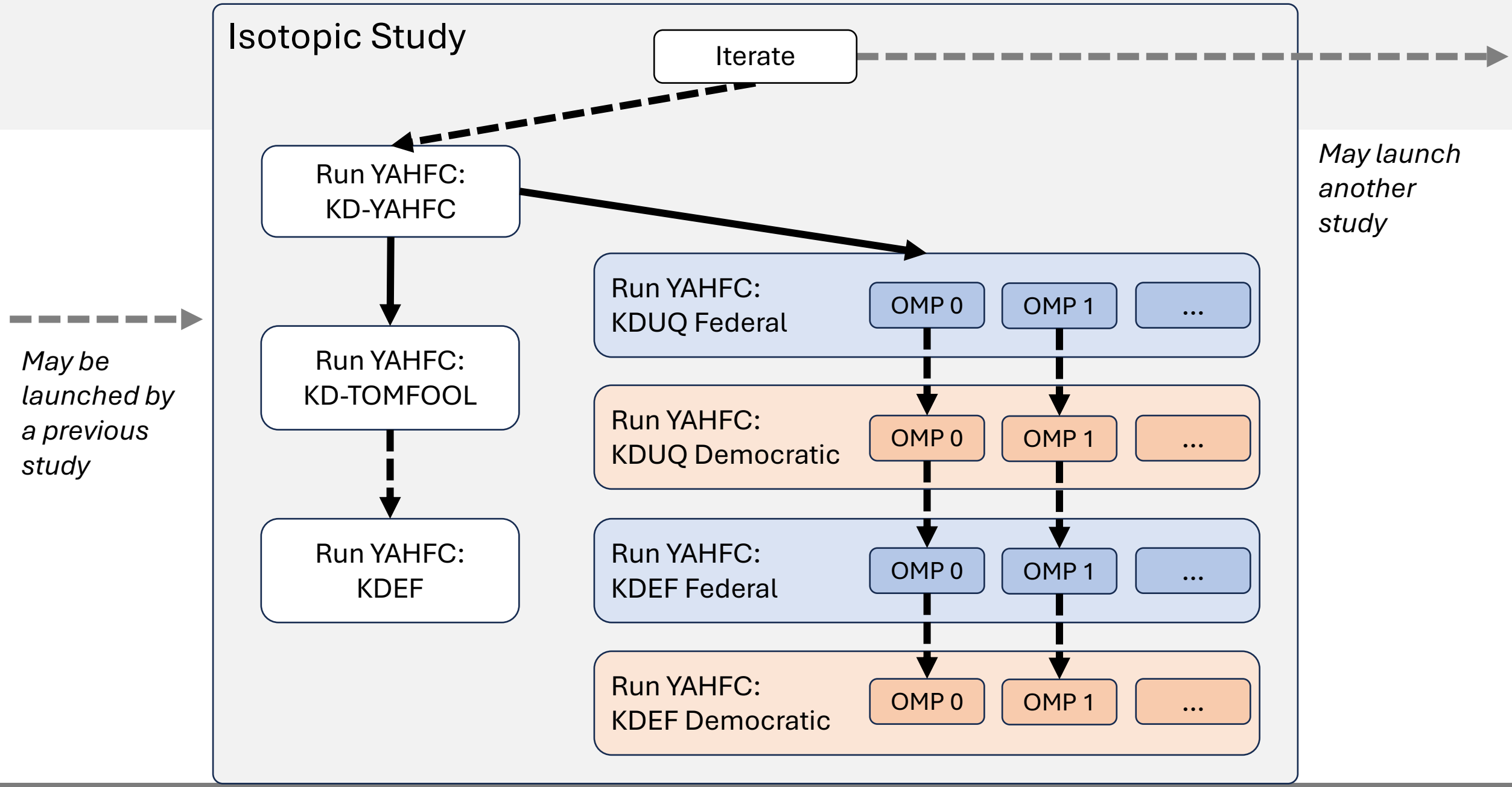
- T. Kawano, P. Talou & H. A. Weidenmüller, “Random-matrix approach to the statistical compound nuclear reaction at low energies using the Monte Carlo technique,” Phys. Rev. C 92 (2015) 044617
- D. Rochman et al., “From average parameters to statistical resolved resonances,” Ann. Nucl. En. 51 (2013) 60-68
- D. Rochman et al., “Radiative neutron capture: Hauser-Feshbach vs. statistical resonances,” Phys. Lett. B 764 (2017) 109-113
- D. Rochman, A. J. Koning and J.-Ch. Sublet, “A Statistical Analysis of Evaluated Neutron Resonances with TARES for JEFF-3.3, JENDL-4.0, ENDF/B-VIII.0 and TENDL-2019,” Nucl. Data Sheets 163, (2020) 163-190
- N. Furutachi, F. Minato, and O. Iwamoto, “Statistical properties of thermal neutron capture cross sections calculated with randomly generated resonance parameters,” Phys. Rev. C 100 (2019) 014610
- G. E. Mitchell & J. F. Shriner Jr., “Missing Level Corrections using Neutron Spacings,” IAEA Report INDC(NDS)-0561 (2009)
- https://maestrowf.readthedocs.io/en/latest/
- https://merlin.readthedocs.io/en/latest/

Back-up Slides


Isotopic Study
Iterate
Run YAHFC:
KD-YAHFC
Run YAHFC:
KD-TOMFOOL
Run YAHFC:
KDEF
Run YAHFC:
KDUQ Federal
OMP 0
OMP 1
...
Run YAHFC:
KDUQ Democratic
OMP 0
OMP 1
...
Run YAHFC:
KDEF Federal
OMP 0
OMP 1
...
Run YAHFC:
KDEF Democratic
OMP 0
OMP 1
...
May launch another study
May be launched by a previous study

How does a Maestro/Merlin spec file look?

```yaml
# Use:
# merlin run Merlin_Cr_Study.yaml --pgen scripts/pgen4.py --var PGenFile=scripts/pgen4.py
# sbatch run_workers.slurm.sh
#
# J. Berryman, 01/2025

description:
   name: $(TARGET_CR) Merlin
   description: Calculating cross sections for low-Z species, out to the neutron drip line

batch:
   type: slurm
   host: ruby
   bank: ncap
   queue: pbatch
   shell: /bin/zsh

env:
   variables:
      OUTPUT_PATH: /usr/workspace/jberryma/MERLIN/LDRD/lowZ/studies
      SCRIPTS: /usr/workspace/jberryma/MERLIN/LDRD/lowZ/scripts
      ITER: 48
      MAX_ITER: 74
      TARGET_CR: Cr48            # The target for this study
      REVERSED_TARGET_CR: 48Cr   # The target name, but A before symbol
      P_TARGET_CR: V48           # Need proton TCs; find species that gives same compound nucleus for proton reaction
   dependencies:
      paths:
         - name: TemplateInput
           path: $(SCRIPTS)/yahfc_input_template.com
         - name: CustomEnergyGrid
           path: $(SCRIPTS)/custom_yahfc_grid
         - name: TCscript
           path: $(SCRIPTS)/createTransCoeffFile.py
         - name: MassFile
           path: $(SCRIPTS)/mass-frdm2012-yahfc.dat
         - name: NewTargetScript
           path: $(SCRIPTS)/getNextTarget.py
         - name: PGenFile
           path: $(SCRIPTS)/pgen.py
```

Resource coordination; Merlin ignores this part

Study variables; Merlin allows you define these at the command line

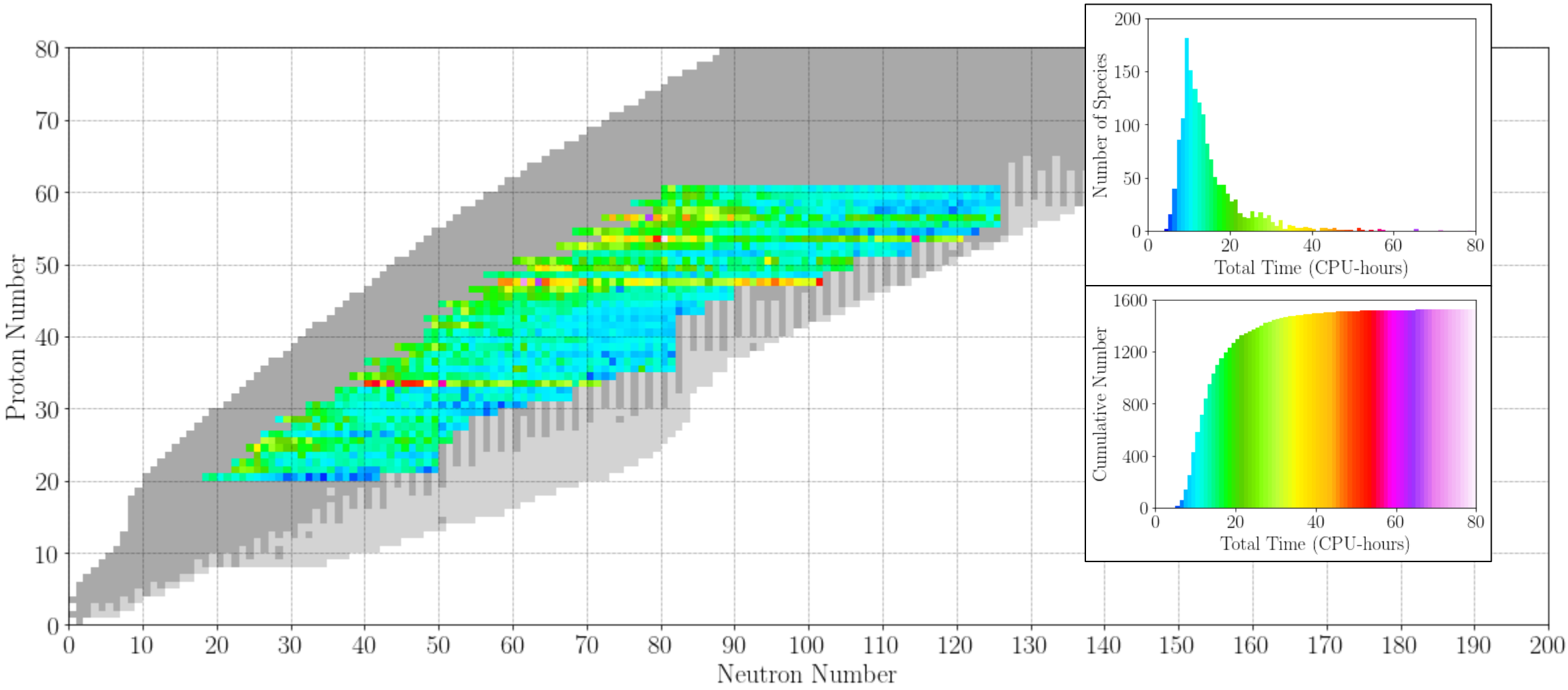
```yaml
study:
   - name: Iterate
     description: Generate the next isotope in our study
     run:
        cmd: |
           # Check to see if we should stop iterating
           if [ $(ITER) -ge $(MAX_ITER) ] ; then
              echo "done"
           else
              # Up the iteration count by one
              next_iter=$(ITER)
              ((next_iter=next_iter+1))
              echo "Starting iteration " $next_iter

              # Move back to the SPECROOT so that the output of our next run isn't nested in the current run
              cd $(SPECROOT)

              # Use command line substitution to pass in the next iteration value
              python $(NewTargetScript) $(SPECROOT)/Merlin_Cr_Study.yaml Cr $next_iter -pgen $(PGenFile)
           fi
        task_queue: iterate
        max_retries: 1

   - name: KD-YAHFC
     description: Running YAHFC with YAHFC's version of the Koning-Delaroche OMP
     run:
        cmd: |
           ln -sf $(MassFile) .
           cp $(TemplateInput) ./$(TARGET_CR)-Model.com
           sed -i 's/TARGETNAME/$(TARGET_CR)/g' $(TARGET_CR)-Model.com
           ln -sf $(CustomEnergyGrid) .
           ./$(TARGET_CR)-Model.com
           tar -czf $(REVERSED_TARGET_CR).tar.gz $(REVERSED_TARGET_CR)
           rm -r Fresco-*
           rm -r $(REVERSED_TARGET_CR)
        depends: [Iterate]
        task_queue: kd
```

Step definition—“cmd” represents what Maestro puts in the .slurm.sh file.

Merlin can use a study to launch another study!

Maestro maps out dependencies between steps; “task_queue” only relevant for Merlin

Timing Information



Timing Information