IAEA 60 Years
Atoms for Peace and Development

Update on Nuclear Data Evaluation Pipeline Prototype

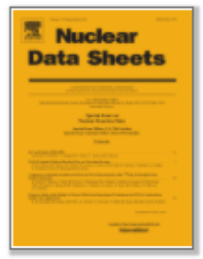
Georg Schnabel
g.schnabel [at] iaea.org

Nuclear Data Section
Division of Physical and Chemical Sciences NAPC
Department for Nuclear Sciences and Applications
IAEA, Vienna

WPEC Subgroup 49
11 May 2021

Publication

Nuclear Data Sheets
Volume 173, March–April 2021, Pages 239-284



Conception and Software Implementation of a Nuclear Data Evaluation Pipeline

G. Schnabel [a, 1] ✉, H. Sjöstrand [b], J. Hansson [b], D. Rochman [c], A. Koning [a], R. Capote [a]

Show more

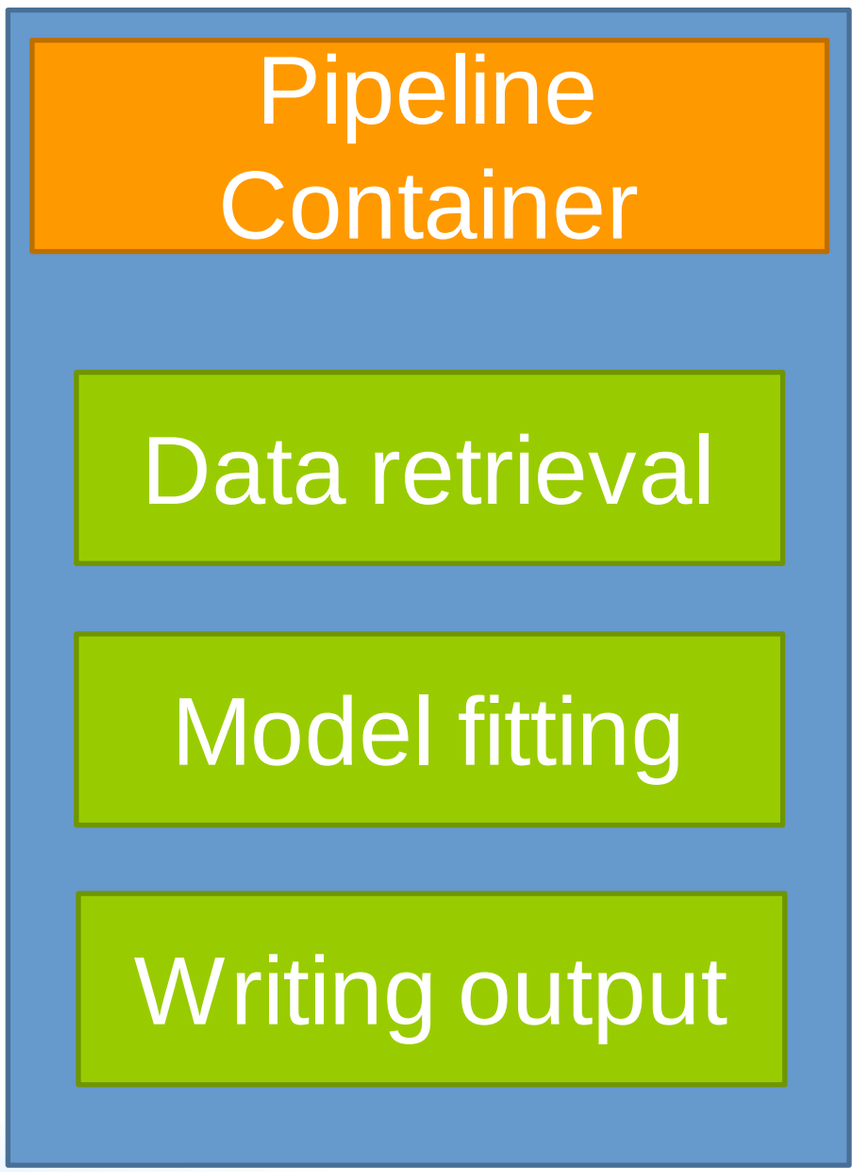
+ Add to Mendeley Share Cite

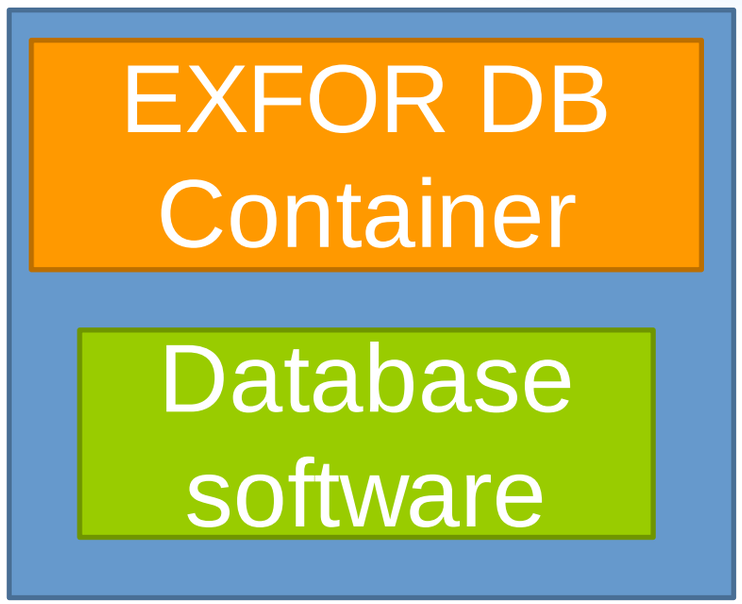
https://doi.org/10.1016/j.nds.2021.04.007

Features of the pipeline

- Programmatic data retrieval (EXFOR MongoDB)
- Data-driven uncertainty correction of inconsistent data (MLO)
- Gaussian processes on energy-dependent model parameters (of TALYS)
- Robust Bayesian fitting to obtain MAP estimate, accounting for non-linear model using a prior-aware Levenberg-Marquardt algorithm
- Evaluated covariance matrix obtained by an (incomplete) second-order Taylor approximation at posterior maximum (Laplace approximation)
- Designed to scale: Large number of experimental data (matrix decomposition tricks) and cluster computing
- Production of random files using TEFAL possible; Production of ENDF files with covariance matrix via TASMAN + TEFAL

Implemented Docker containers

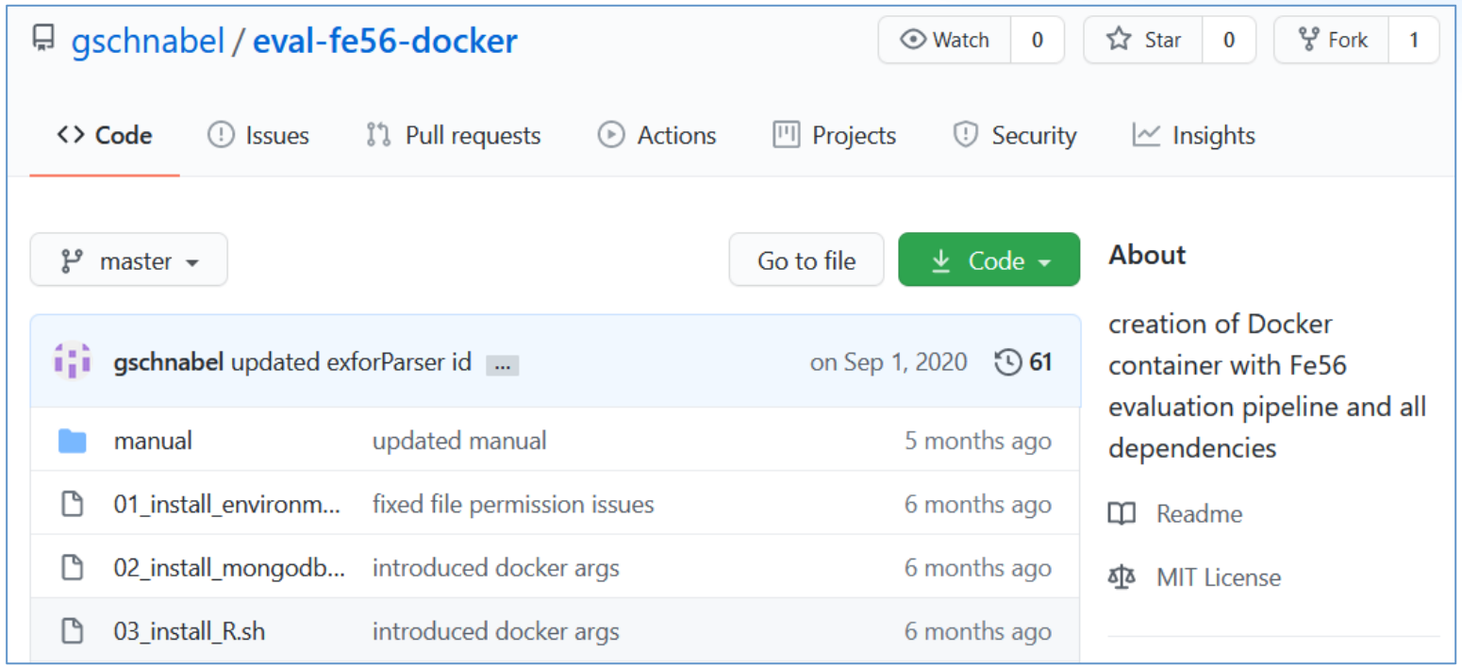




Reproducible evaluation:

```
docker run -it -p 9090:8787 \
-v outdata:/home/username/eval-fe56/outdata  \
-v talysResults:/home/username/talysResults  \
-v /dev/shm:/dev/shm \
-e extUID=<UID> -e extGID=<GID>  \
-e maxNumCPU=32 \
--name eval-fe56-cont eval-fe56-img test_eval
```

GitHub Repos



https://github.com/gschnabel/eval-fe56-docker
(with manual explaining internal structure of container and pipeline)

https://github.com/gschnabel/compEXFOR-docker