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Containerization and microservices for nuclear data

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Workshop for Applied Nuclear Data Activities
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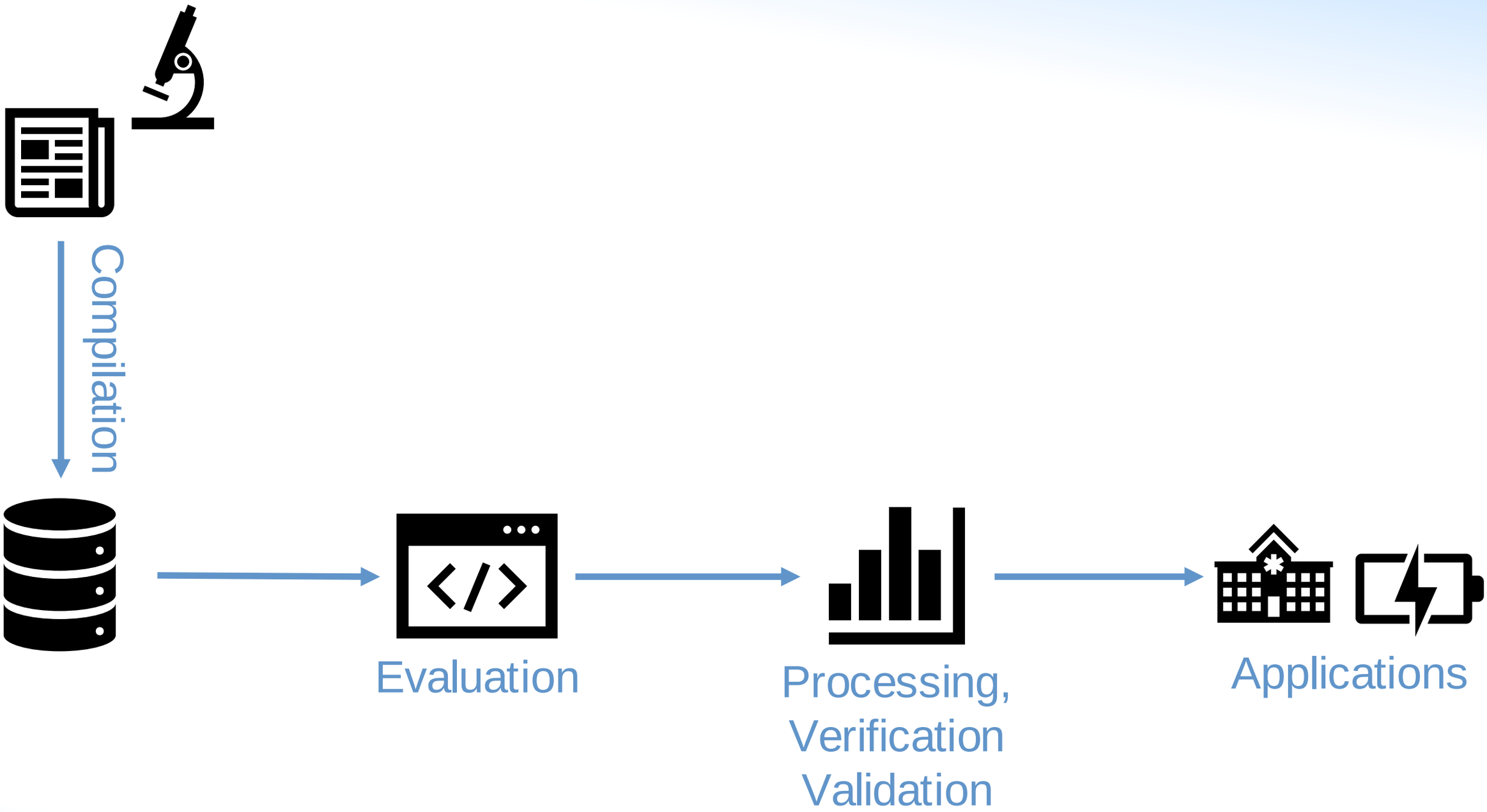
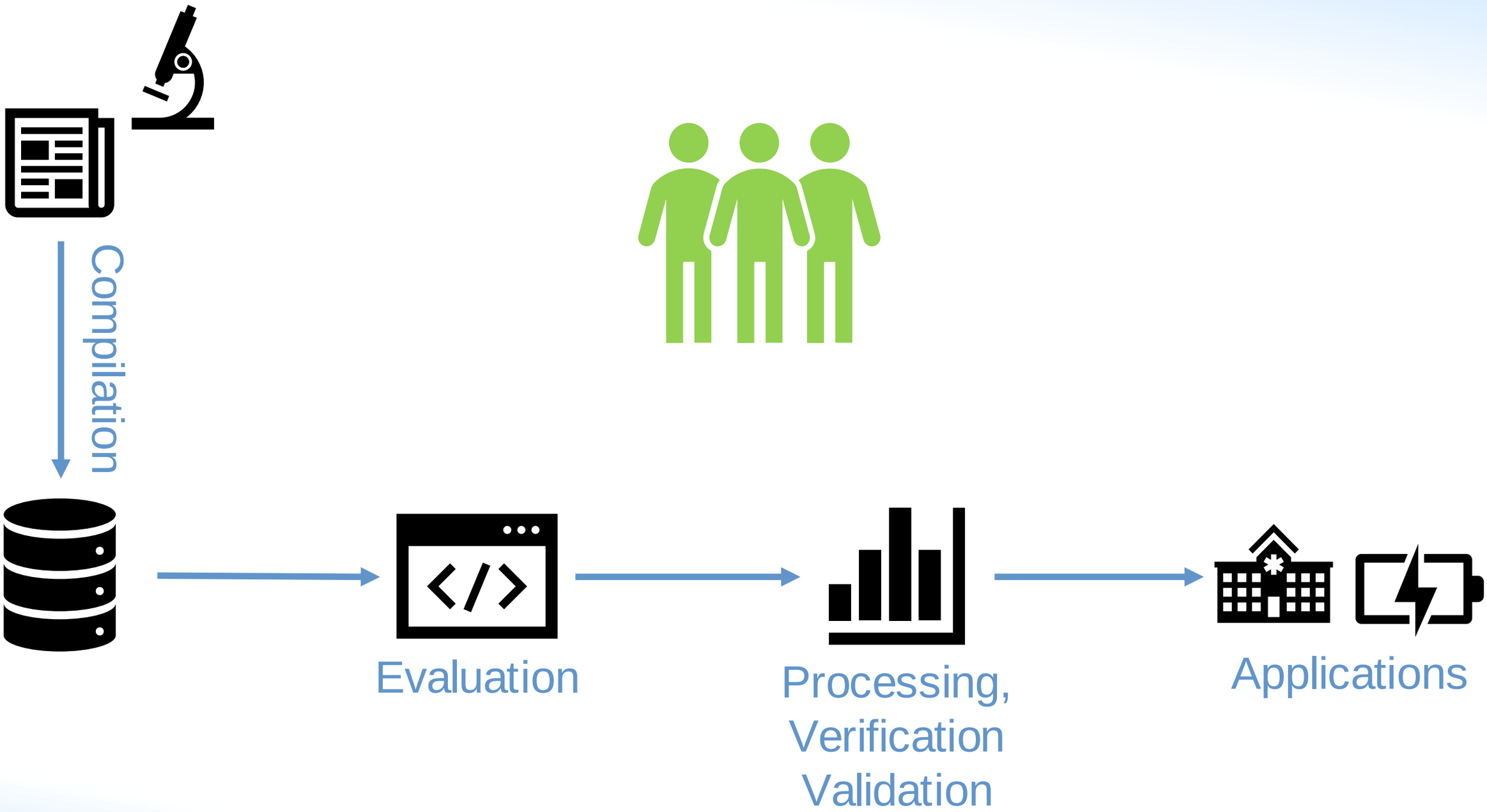
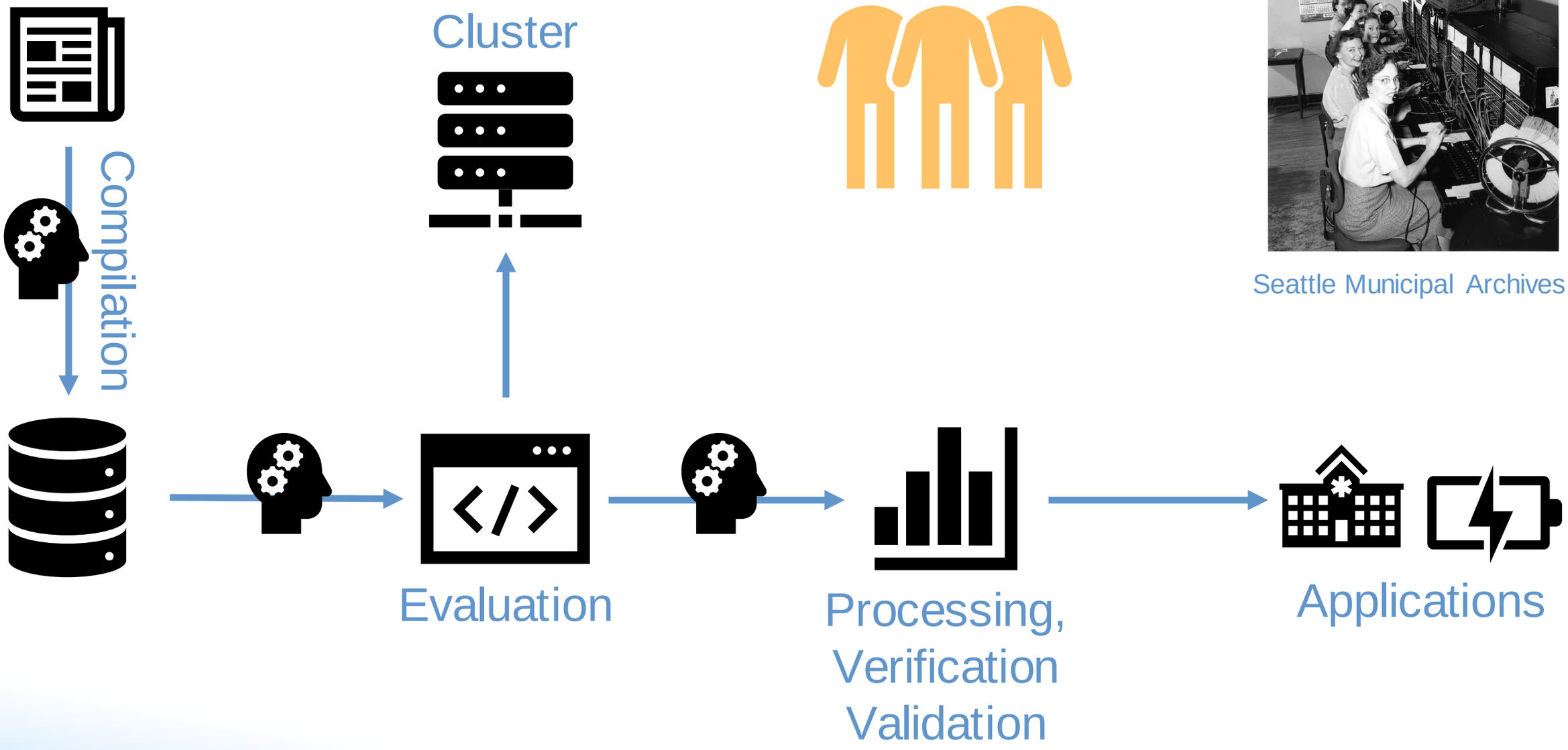
Nuclear data pipeline



Collaborative effort of experts



Technical overhead



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Cluster

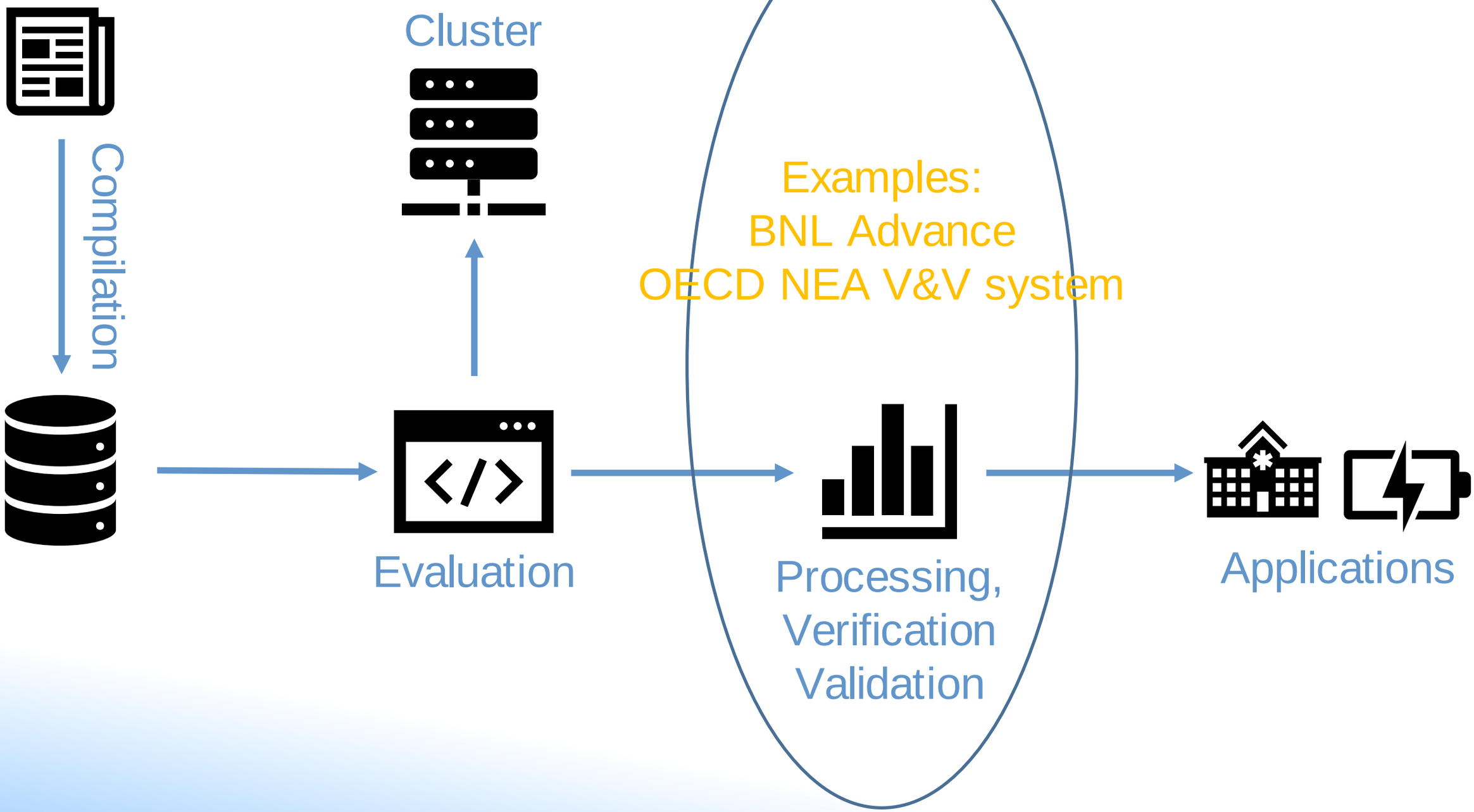
Compilation

Evaluation

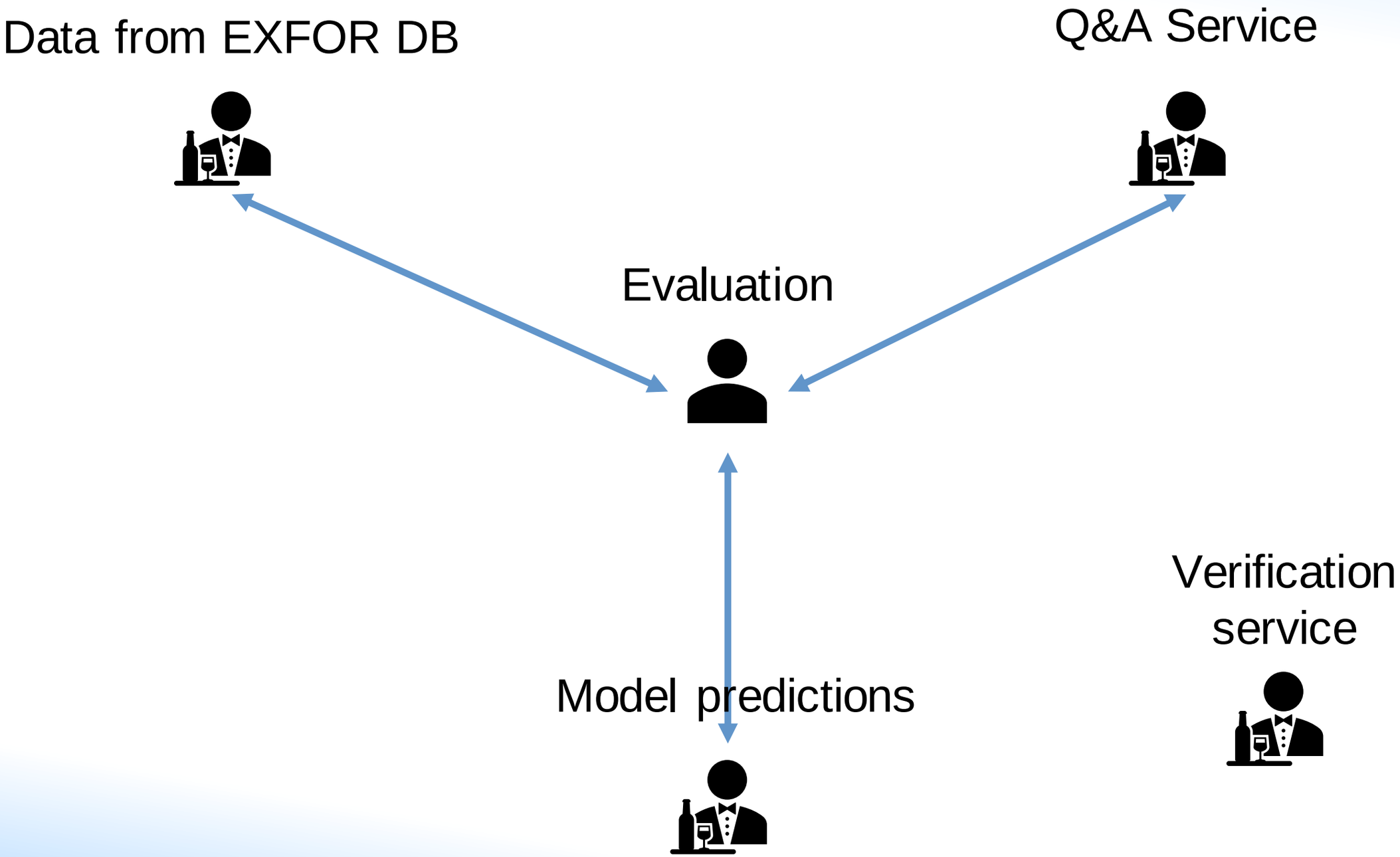
Processing,
Verification
Validation

Applications

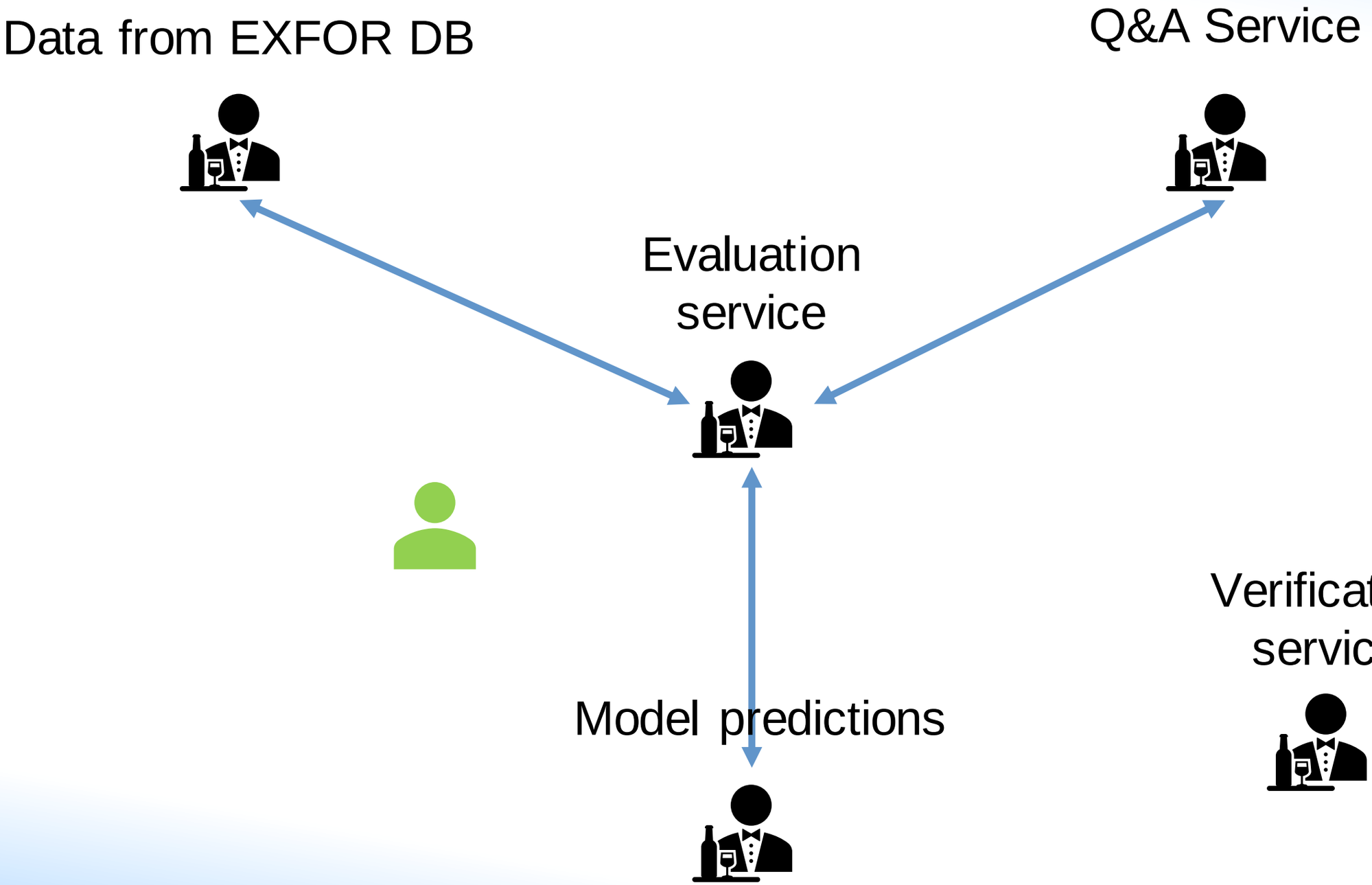
Automation


Compilation
Cluster
Examples:
BNL Advance
OECD NEA V&V system
Evaluation
Processing,
Verification
Validation
Applications

Microservices



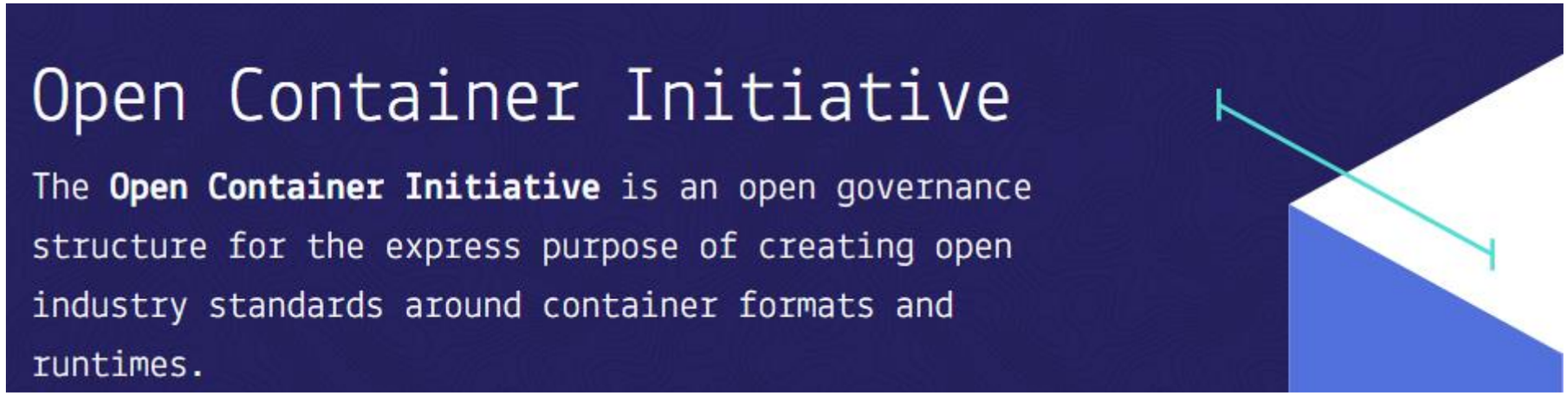
Microservices



Containerization

"A container is a standard unit of software that packages up code and all its dependencies so the application runs quickly and reliably from one computing environment to another. A Docker container image is a lightweight, standalone, executable package of software that includes everything needed to run an application: code, runtime, system tools, system libraries and settings." (quoted from www.docker.com)

https://www.docker.com

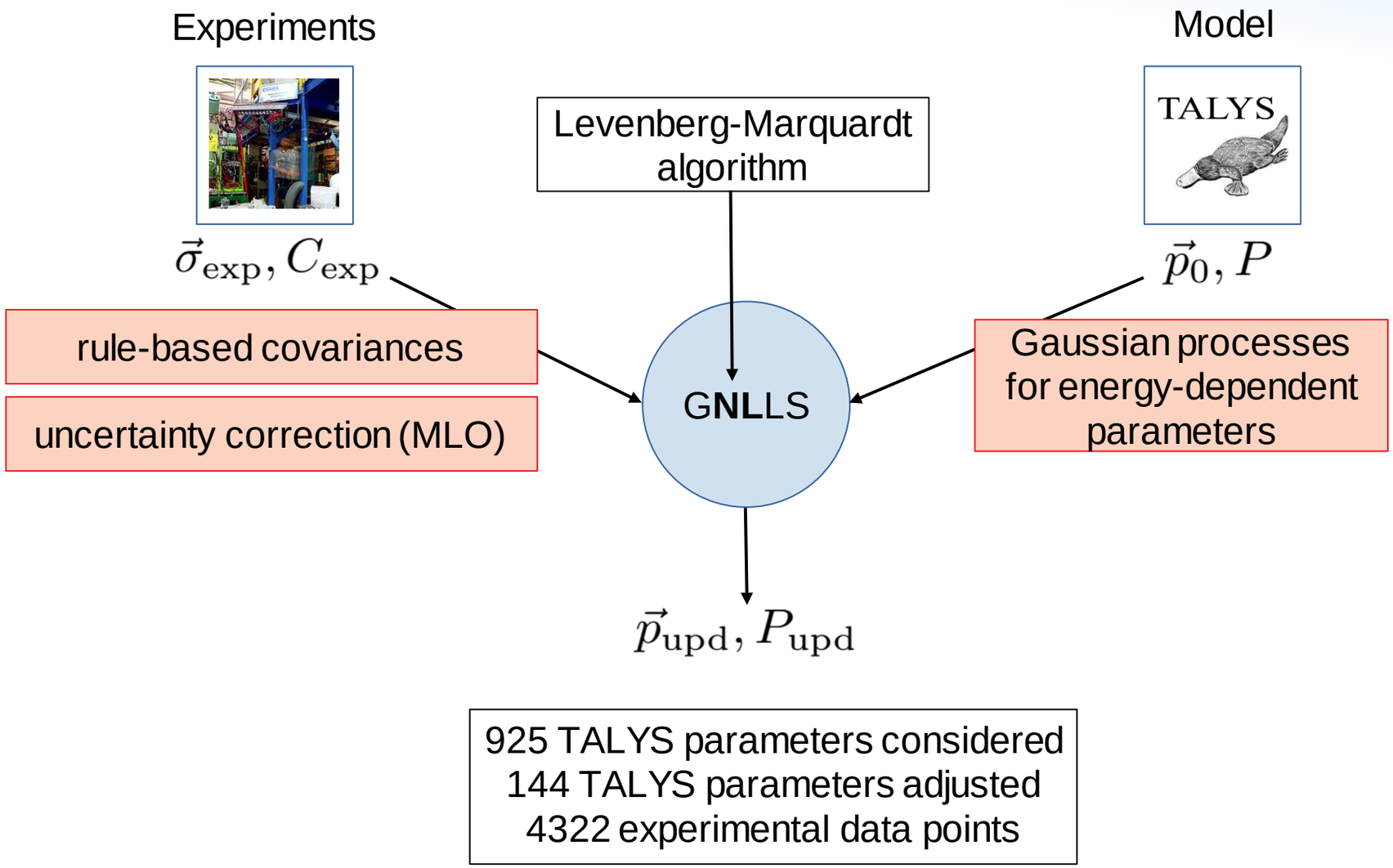


Sylabs.io
SINGULARITY
SIMPLE, FAST, SECURE

docker

podman

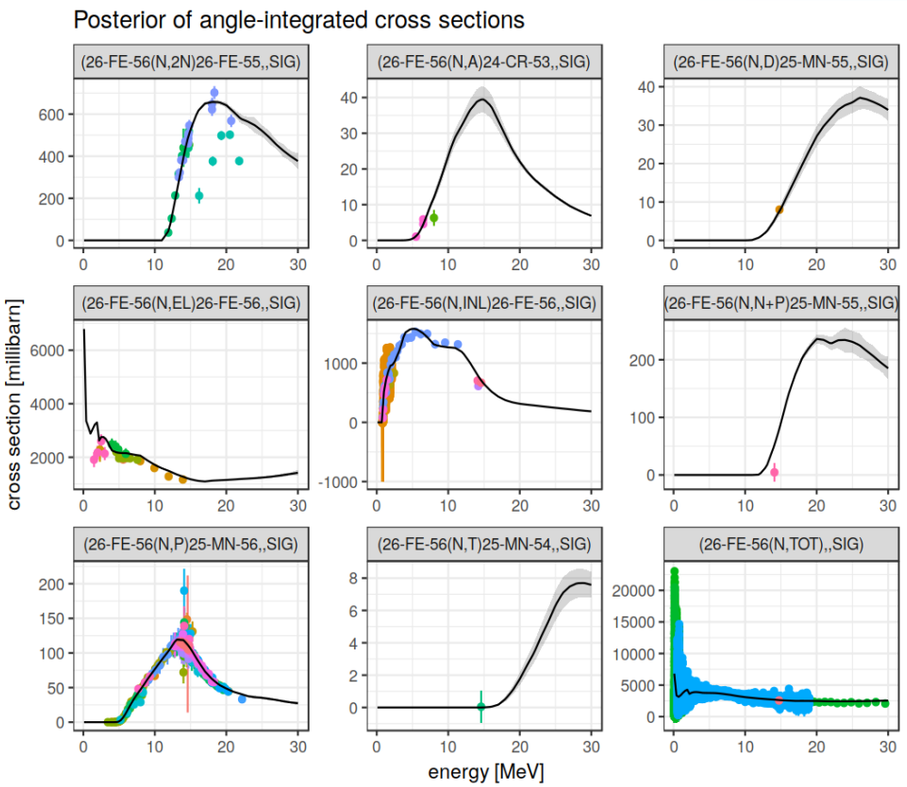
Evaluation with advanced statistical processing

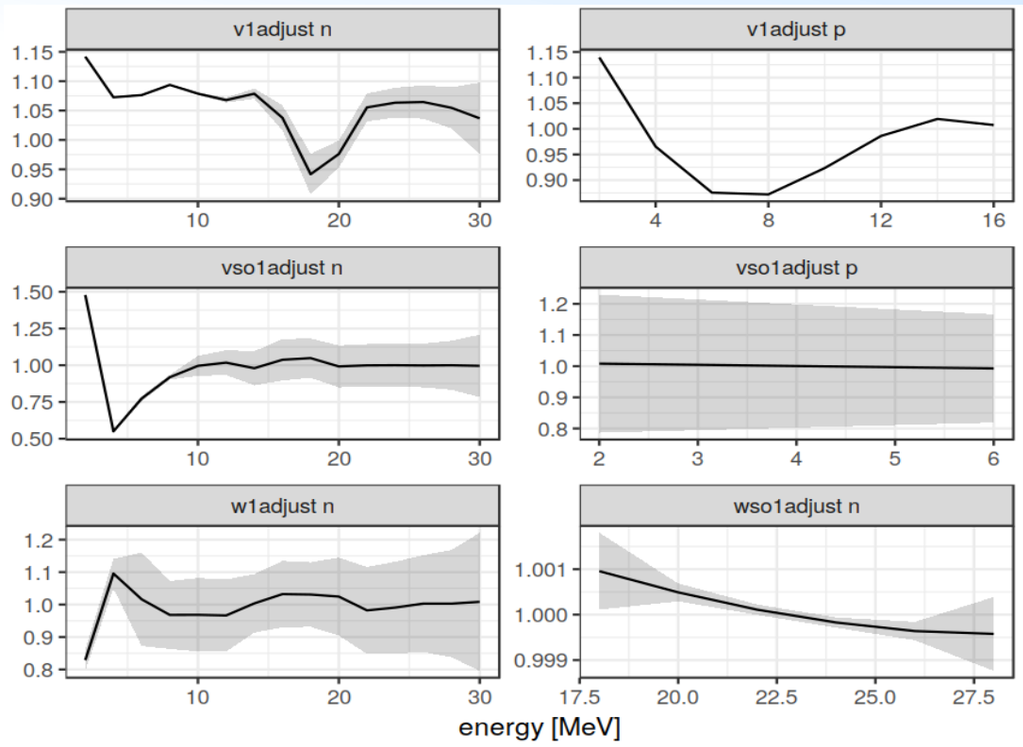


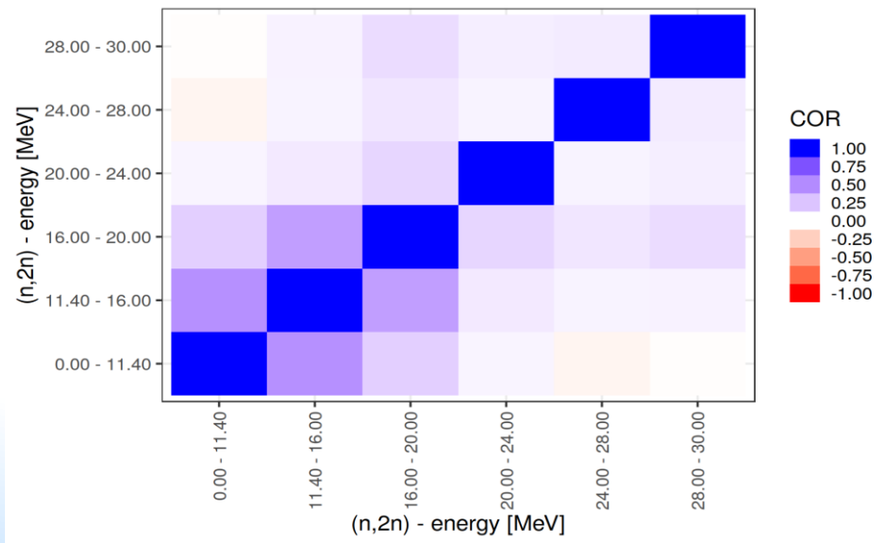
In this work: parallel computing on ~80 CPU cores sufficient; statistical inference could benefit from use of GPU in the future (but not the bottleneck at present)

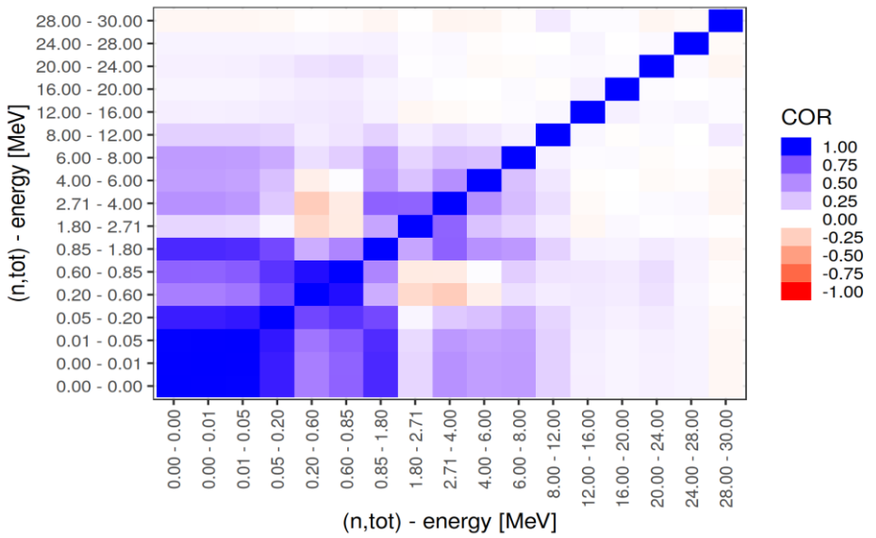
[2009.00521] Conception and software implementation of a nuclear data evaluation pipeline (arxiv.org)

Results


Posterior of angle-integrated cross sections
(26-FE-56(N,2N)26-FE-55,,SIG)
(26-FE-56(N,A)24-CR-53,,SIG)
(26-FE-56(N,D)25-MN-55,,SIG)
(26-FE-56(N,EL)26-FE-56,,SIG)
(26-FE-56(N,INL)26-FE-56,,SIG)
(26-FE-56(N,N+P)25-MN-55,,SIG)
(26-FE-56(N,P)25-MN-56,,SIG)
(26-FE-56(N,T)25-MN-54,,SIG)
(26-FE-56(N,TOT),,SIG)
cross section [millibarn]
energy [MeV]


v1adjust n
v1adjust p
vso1adjust n
vso1adjust p
w1adjust n
wso1adjust n
energy [MeV]


(n,2n) - energy [MeV]
(n,2n) - energy [MeV]
COR


(n,tot) - energy [MeV]
(n,tot) - energy [MeV]
COR

Evaluation as pipeline

Step	Description
1	Retrieval of relevant experimental data
2	Generation of predictions based on a reference calculation
3	Rule-based correction of experimental uncertainties
4	Correction of systematic experimental uncertainties using MLO
5	Evaluation of the Jacobian associated with the reference calculation
6	Setup of Gaussian processes for energy-dependent model parameters
7	Optimization of TALYS parameters using the LM algorithm
8	Calculation of a MVN approximation of the posterior pdf
9	Generation of representative random files

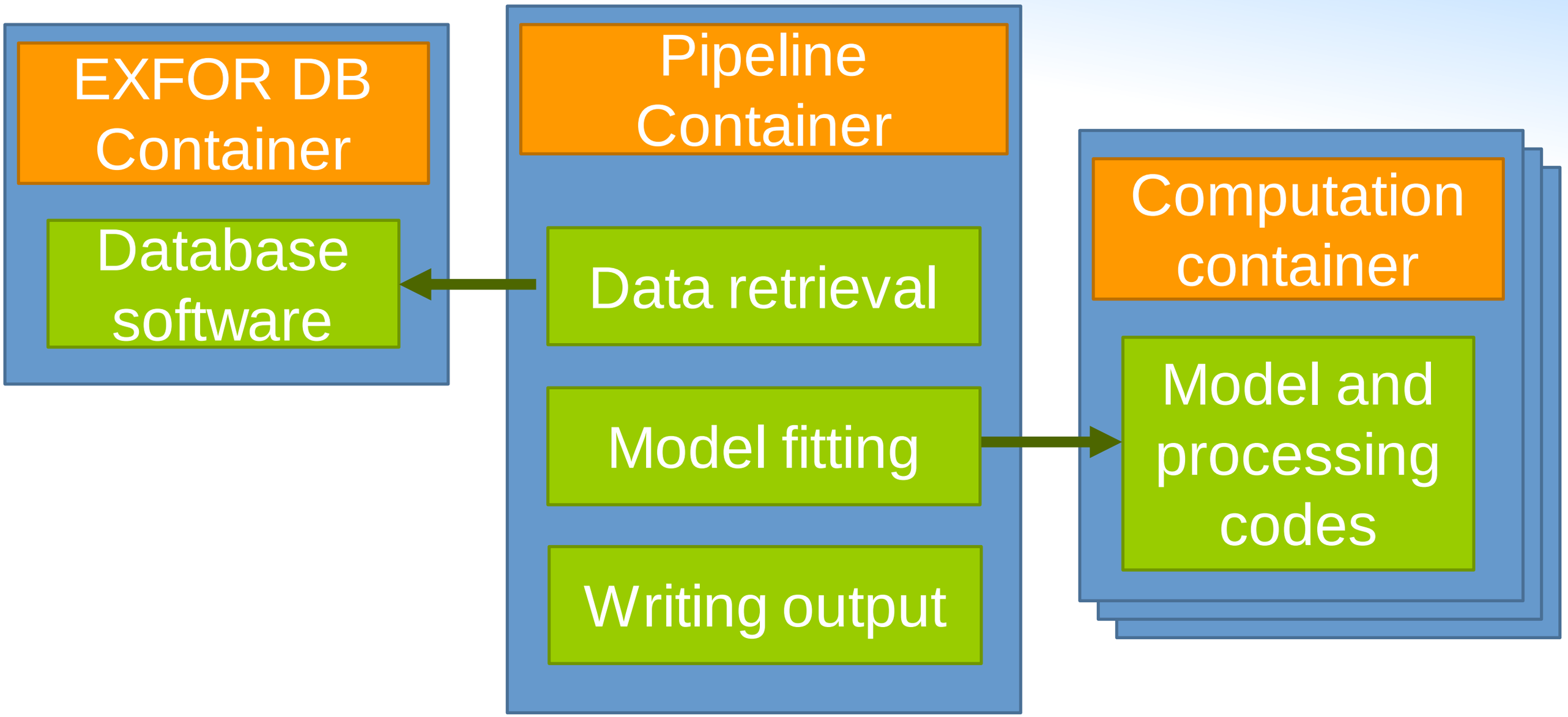
Evaluation as pipeline

Database interaction

Step	Description
1	Retrieval of relevant experimental data
2	Generation of predictions based on a reference calculation
3	Rule-based correction of experimental uncertainties
4	Correction of systematic experimental uncertainties using MLO
5	Evaluation of the Jacobian associated with the reference calculation
6	Setup of Gaussian processes for energy-dependent model parameters
7	Optimization of TALYS parameters using the LM algorithm
8	Calculation of a MVN approximation of the posterior pdf
9	Generation of representative random files

Model calculation on computer cluster

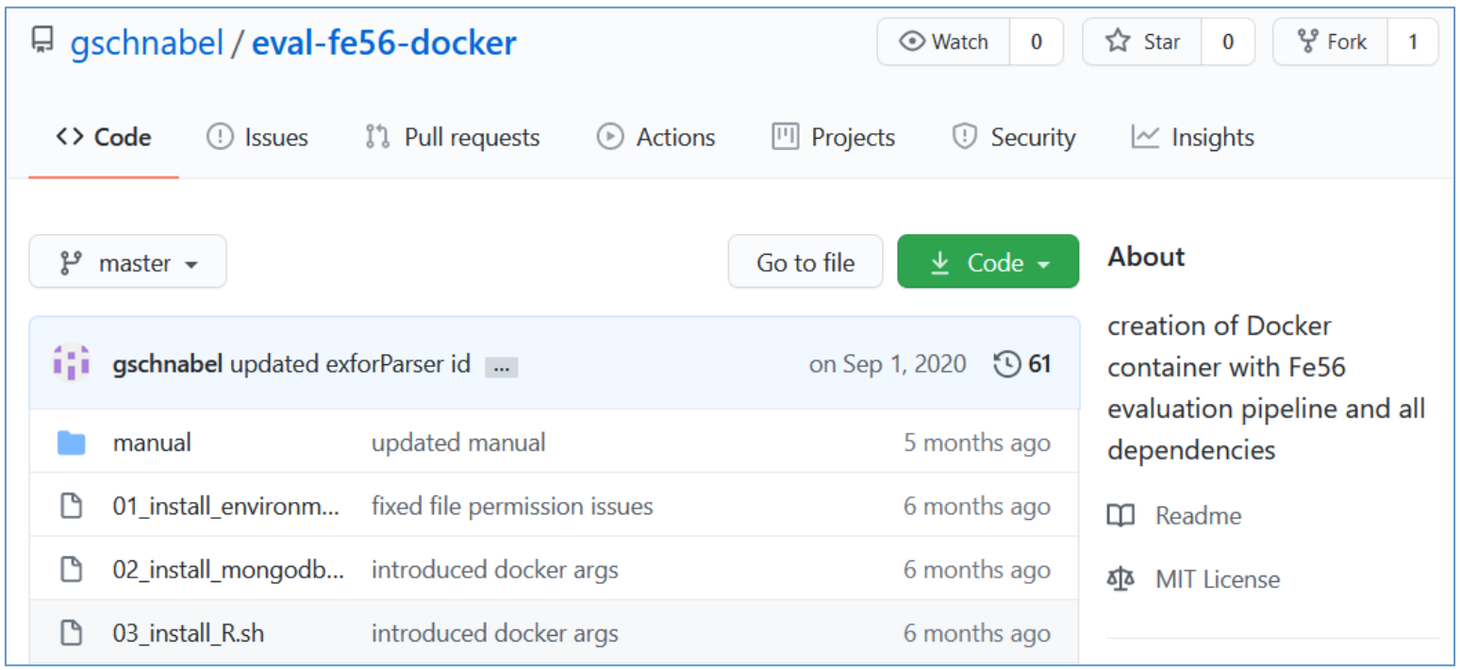
Implemented Containers (Prototypes)



Current limitations:
- Pipeline container specialized to Fe56,
- Communication with computation container coupled to R programming language

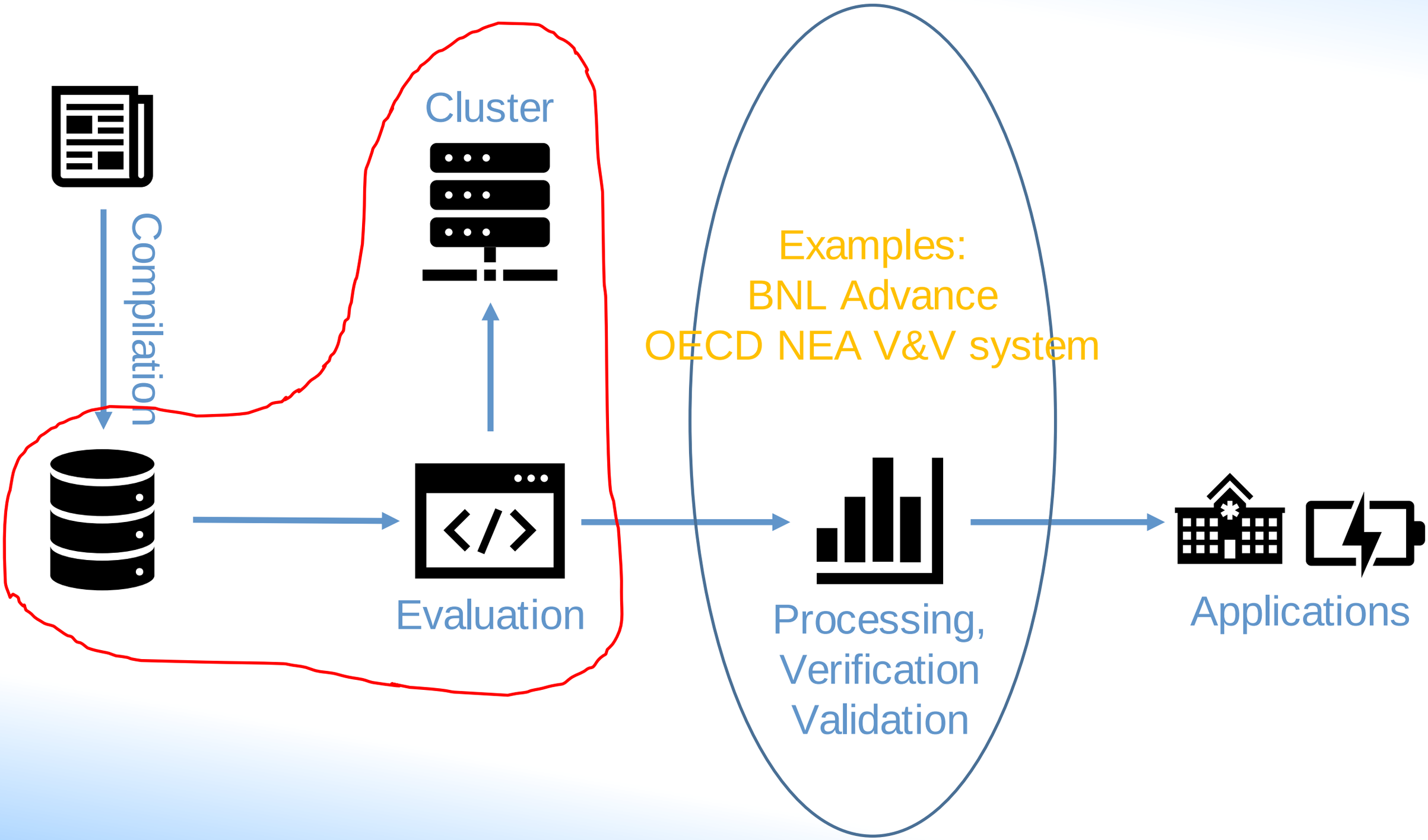
Advantages

- Composability
- Transparency
- Extensibility
- Reusability
- Transferability
- Reproducibility
- Collaboration




```
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
```

Nuclear data pipeline



Conclusion

- Nuclear data pipeline requires diverse expertise and depends on a variety of codes
- Microservices for nuclear data enable human experts to write evaluation scripts concisely codifying what data should be used and what should be done with it
- Microservices as containers allow their easy shipping and reuse
- Prototypes of a nuclear database container and evaluation container available online

Outlook & Challenges

- Interaction with containers should be language agnostic, e.g., use widely employed data structures and protocols
- Microservices & data should be discoverable and usable, i.e., the conception that something is stored somewhere on a specific architecture becomes more and more irrelevant
- (Simple) Programmatic access to databases, model codes, statistical microservices and compute power will be an accelerator for AI/ML as enabling technology

Thank you for your attention!

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Dimitri Rochman, Arjan Koning,
Roberto Capote

UPPSALA UNIVERSITET

PAUL SCHERRER INSTITUT PSI

IAEA

Links & References

- Pipeline paper
  https://arxiv.org/abs/2009.00521
- Pipeline code
  https://github.com/gschnabel/eval-fe56
- EXFOR CouchDB database
  https://github.com/IAEA-NDS/exfor-couchdb-docker

Related work

- NEA NDS V&V System

  https://nds1.gitlab.io/nds/files/jeffdocs/jefdoc-2020.pdf

  https://nds1.gitlab.io/nds/files/jeffdocs/jefdoc-2012.pdf
- BNL ADVANCE (V&V System)
- https://www.sciencedirect.com/science/article/pii/S0090375214001264