OGS Process Simulations and Containerization with Apptainer

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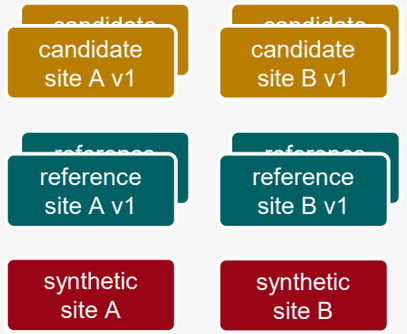
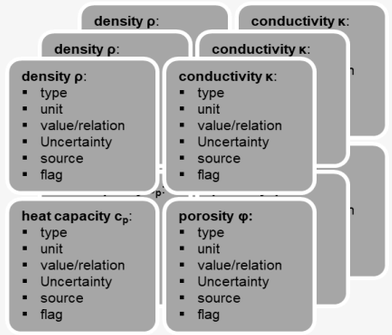
Smart Data Hub – the project's core element

Impact model requires **site specific** information

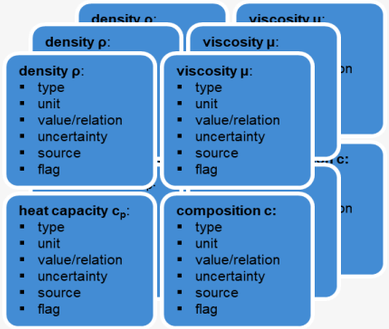
(i) structure & geometry

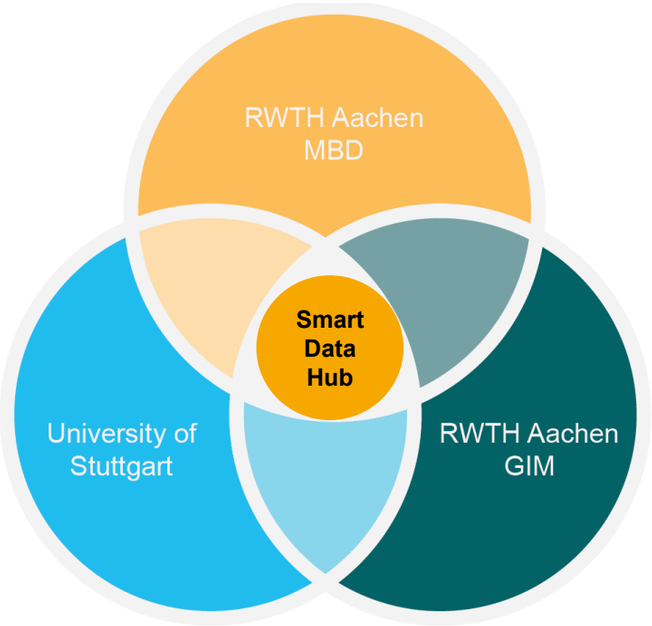


(ii) rock properties



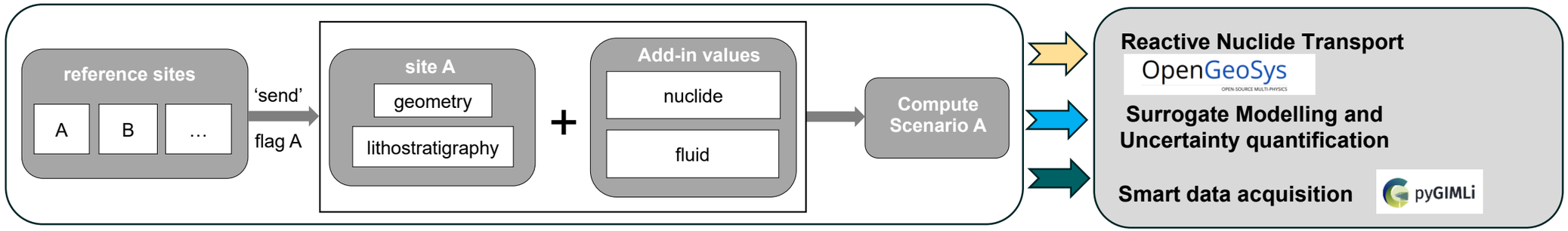
(iii) fluid / nuclide properties



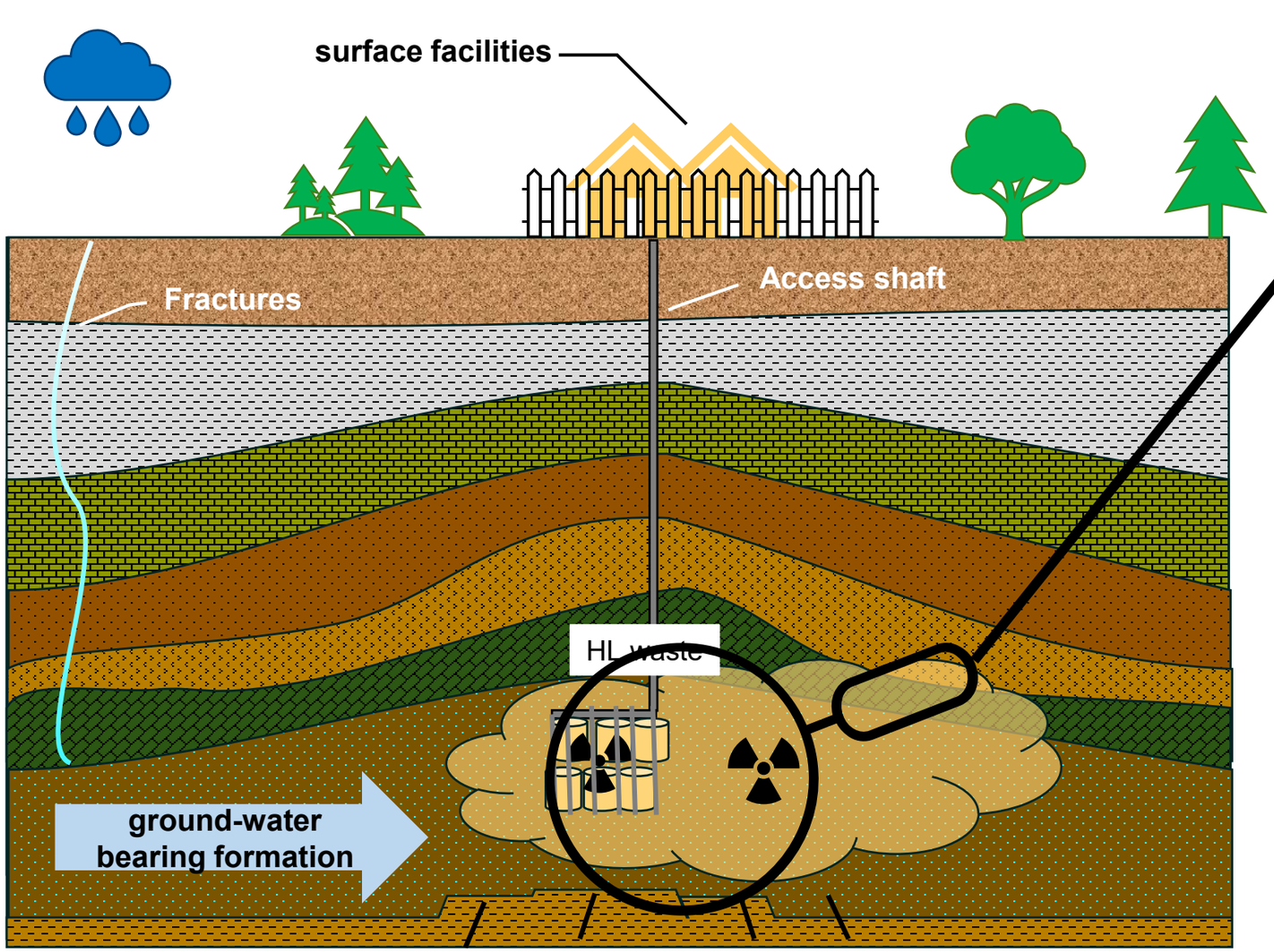


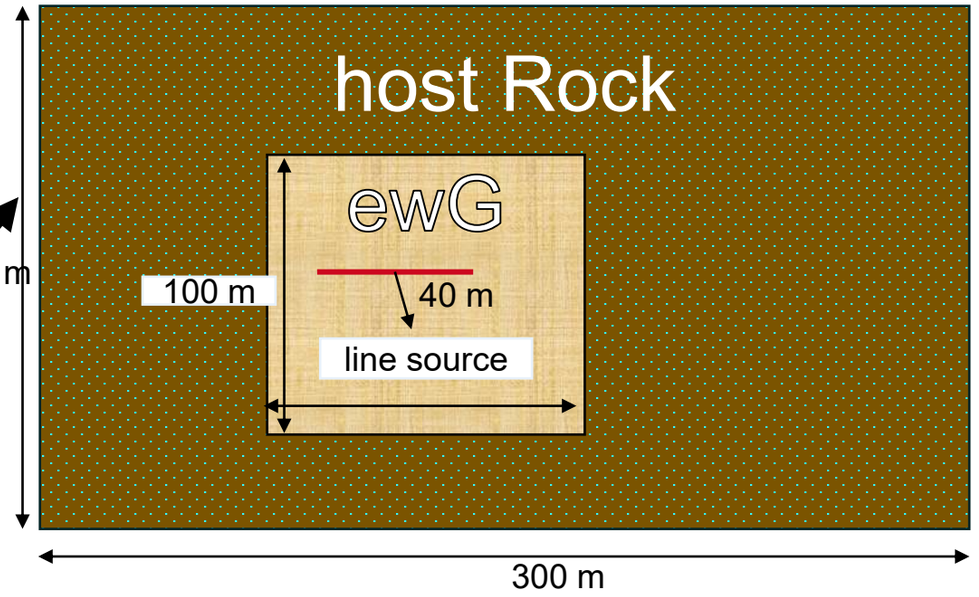
Smart Data Hub:

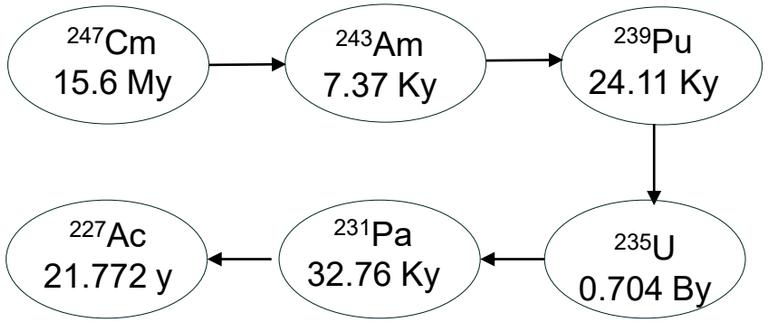
‘flagging’ strategy: form a reference-based compute scenario:



2D leakage scenario





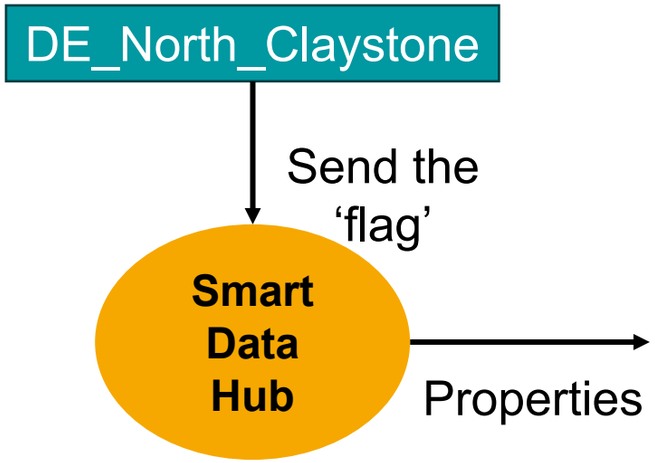


Parameters

Ordinance on Safety Requirements for the Final Disposal of High-Level Radioactive Waste (EndlSiAnfV)
Leakage §4 (5):

- < 10^{-4} # total nuclides over 1 million years
- < 10^{-9} # total nuclides/a

	ewG	host rock
diffusion coefficient (m^2/s)	1e-12	1e-12
porosity	0.0675	0.13
hydraulic conductivity(m/s)	1e-9	1e-7
density(kg/m^3)	2490	2470
…	…	…




```
bulk_density:
  type: scalar
  value: 2450
  dev_pdf: uniform
  dev_value: [2400, 2530]
  unit_str: kg/m^3
  unit: [ 1 -3 0 0 0 0 0 ]
  source: bossart2017mont
```

```
Cm-247:
  effective_diffusion_coefficient:
    type: scalar
    value: 5.e-11
    dev_pdf: uniform
    dev_value: [ 1.e-11, 1.e-10 ]
    unit_str: m^2/s
    unit: [ 0 2 -1 0 0 0 0 ]
    source: nagra2002ntb0206
  sorption_coefficient:
    type: scalar
    value: 17
    dev_pdf: non-symmetric #  the
    dev_value: 8.2
```

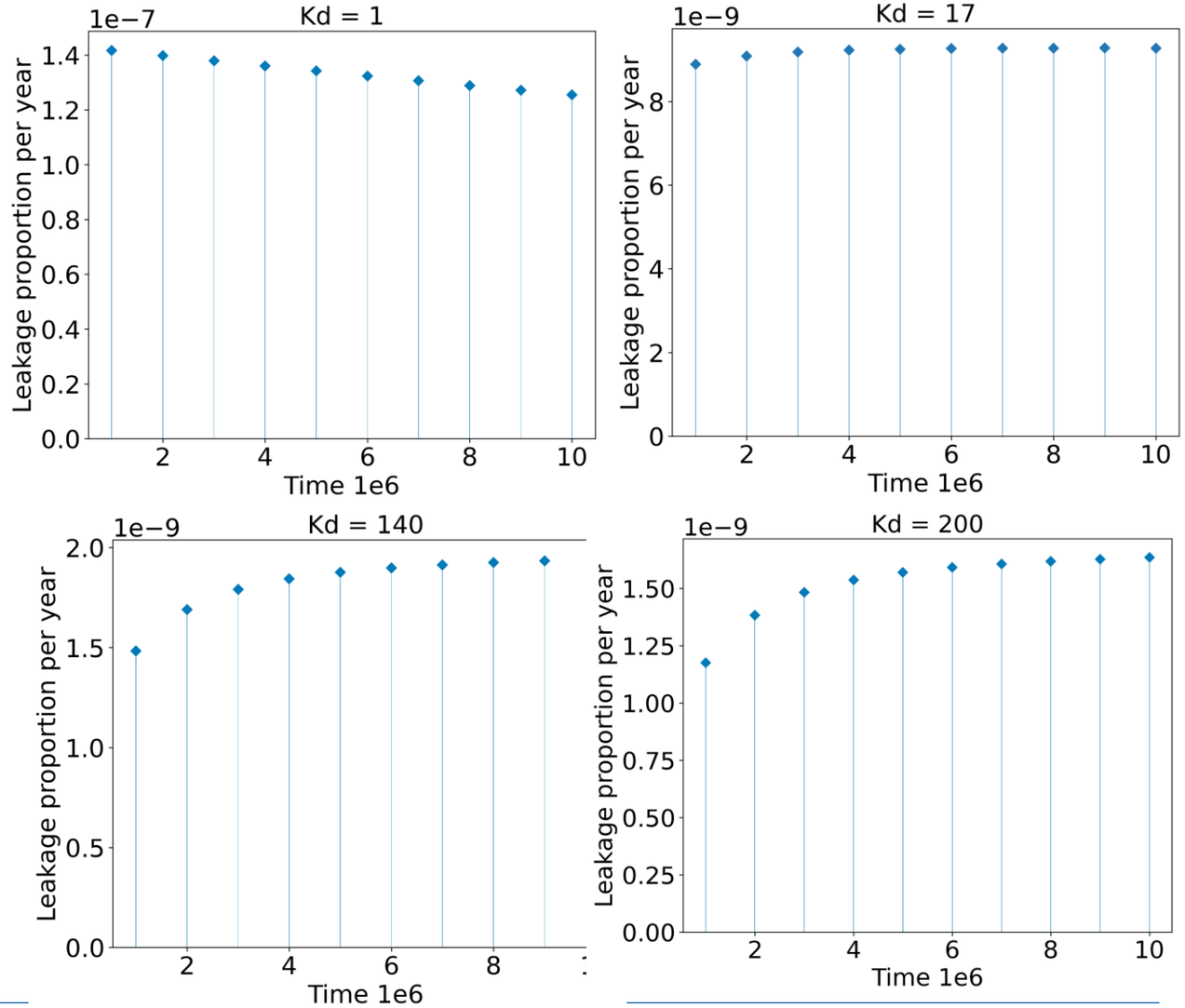
	sorption coefficient (m^3/kg)
Pessimistic value	1
Reference value	17
Optimistic values	140, 200

Results

Ordinance on Safety Requirements for the Final Disposal of High-Level Radioactive Waste (EndlSiAnfV)
Leakage §4 (5):

- < 10^{-4} # total nuclides over 1 million years
- < 10^{-9} # total nuclides/a

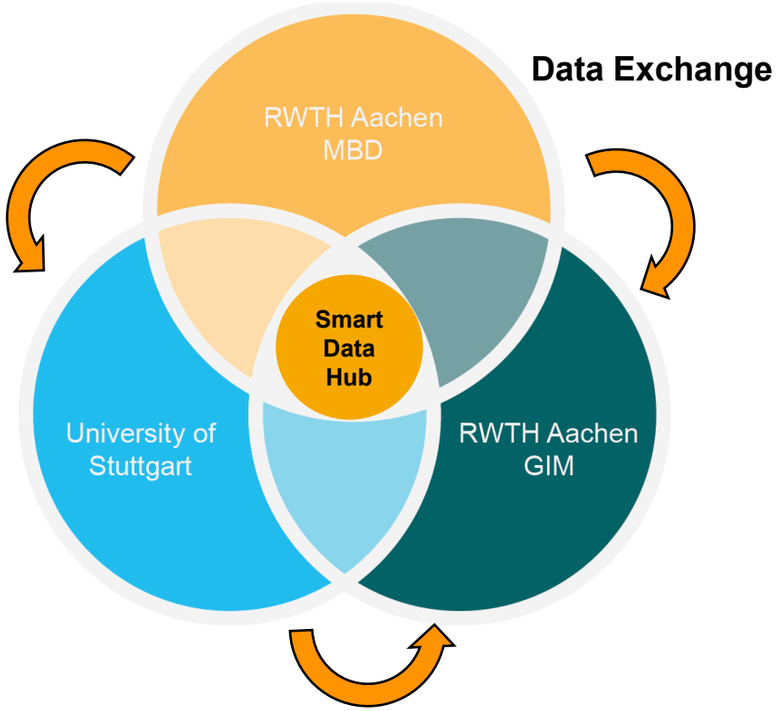
	Relative leakage over 1 million years
Kd=1	0.125509
Kd=17	0.009275
Kd=140	0.001941
Kd=200	0.000918



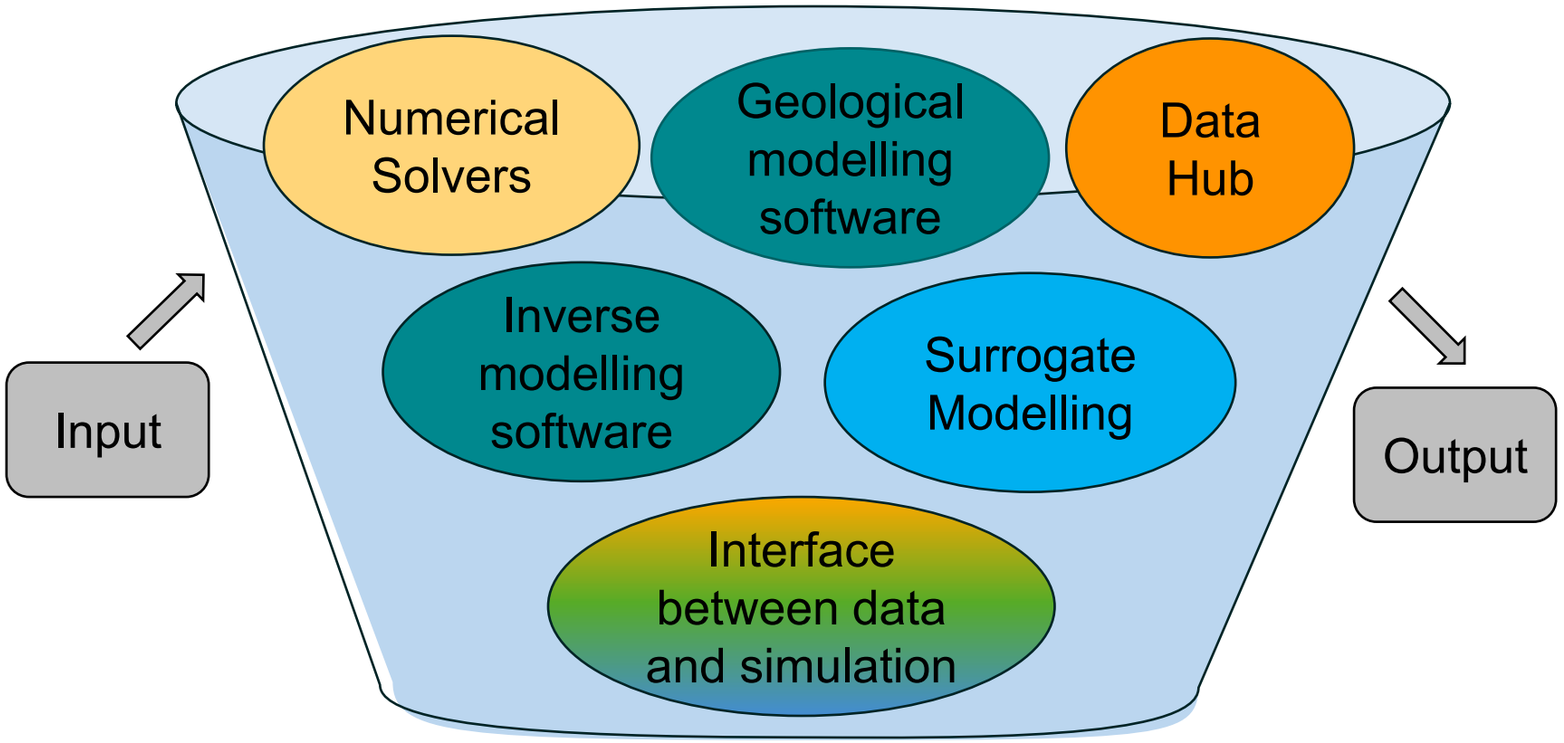
Part 2: Apptainer technology

Challenges: Reusability

- Complex workflow



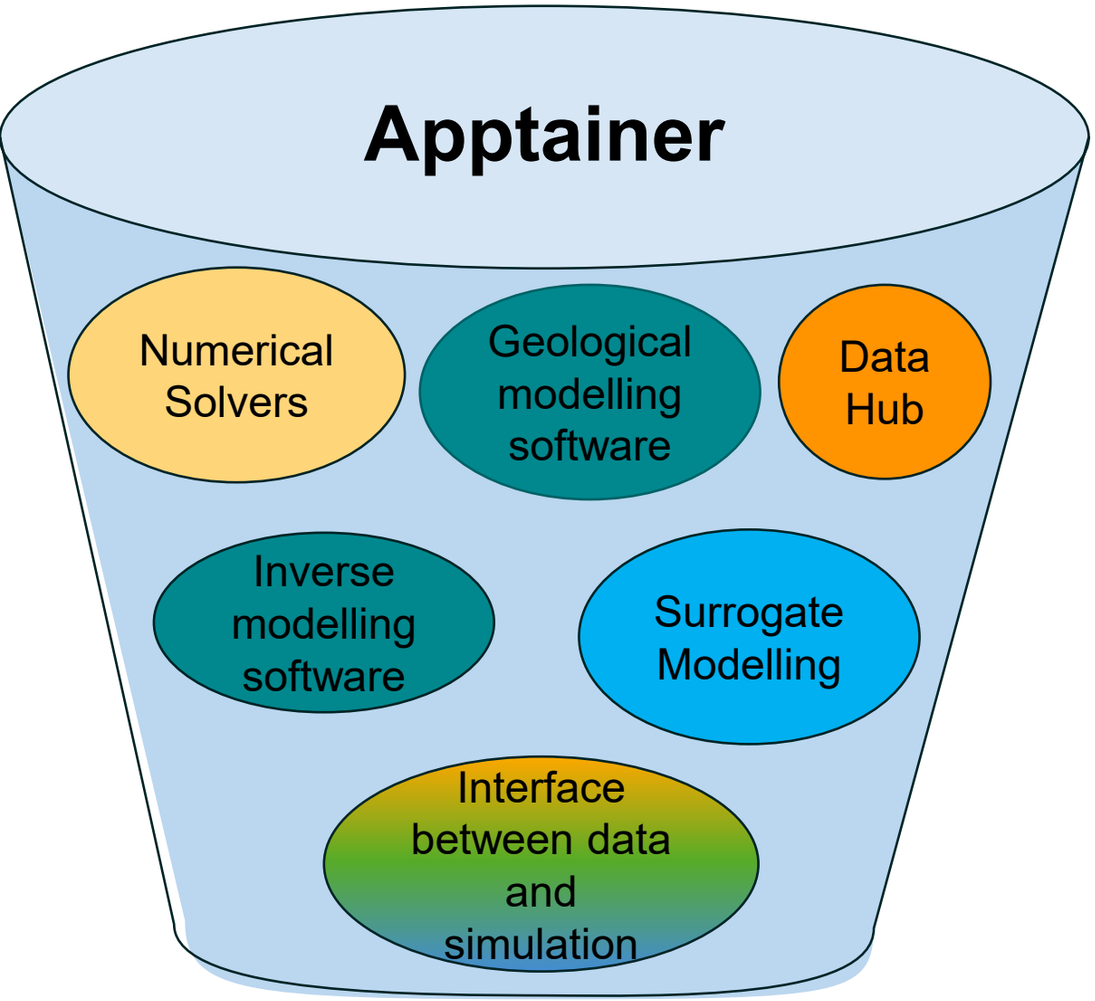
- Heterogenous software



- TTFX (Time To First ~)
  ⟹ **TTFR** (Time To First Reuse)

~days/weeks

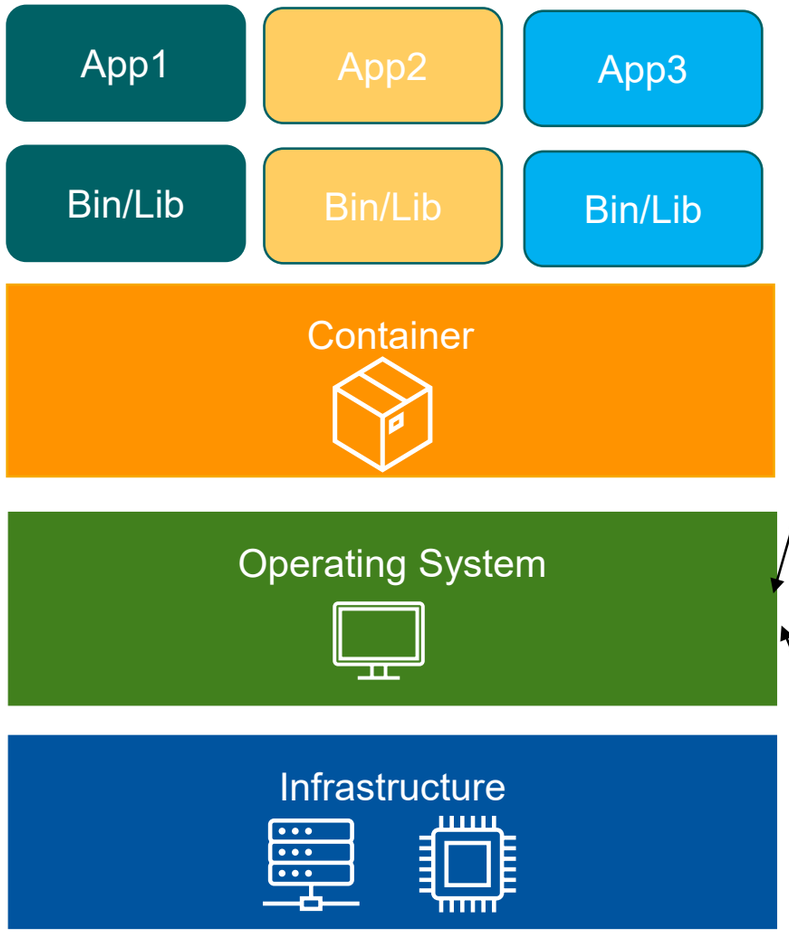
Solution: Apptainer



- **Apptainer** is an open-source **container** platform,
- A container for apps,
- Run complex applications on HPC clusters,

singularity

Apptainer Vs Regular Containers



Apptainer

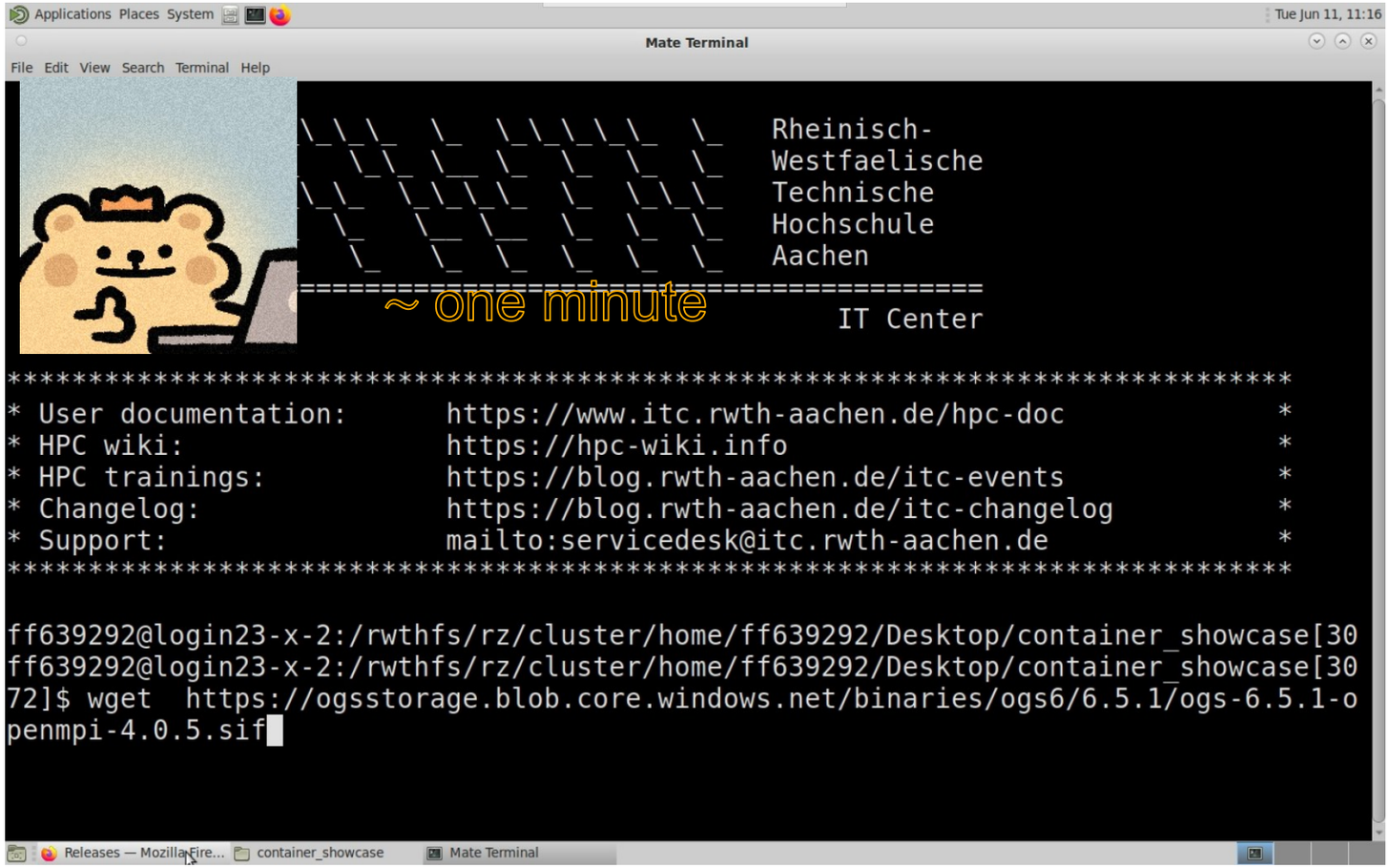
Regular container

- container system for high-performance computing,
- A simple, effective security model,
- allow containers to be executed as if they were native programs or scripts on a host system.

- microservices

Time To First Reuse (TTFR)

- a single file SIF container



- Create a SIF file:
  - ➢ pull from docker;
  - ➢ from definition File (apptainer.org)

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Thank you for your attention