Input → Run → Output

FE Simulation

Mesh
- Nodes
- Elements

Model
- Interpolation
- Integration
- PDE
- Boundary Cond.

NonLinearSolver
SparseLinearSolver

Soft. Hard. stack

- Software/Script Version
- compilation options
- dependencies Versions
- OS
- Hardware Spec

FE Output

Mesh
- Nodes
- Elements

Fields
- Nodal
- Elemental

Accuracy
- Convergence
- Error measure

Post-Process/graphics

Package

- Versions, metadata (yaml, json, …)
- Results in standard format
- Limit number of files
- Spack/Python lock files
- CMakeCache.txt / build config and log file
- Docker file
- Run logs, execution times, cpu-hours
- How to strictly attach to output results ?