Unified metadata handling for reproducible simulation workflows

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Summary

- Metadata management framework for simulation workflows to assist with:
  - Reproducibility of simulation experiments
  - Efficient organization, exploration and visualization of simulation data
- Address all components of simulation research and corresponding metadata types
- Cope with modularity and flexibility demands of rapidly progressing science[1]
- Applicable to diverse simulation based research fields, example use cases from:
  - Computational Neuroscience
  - Earth and Environmental Science

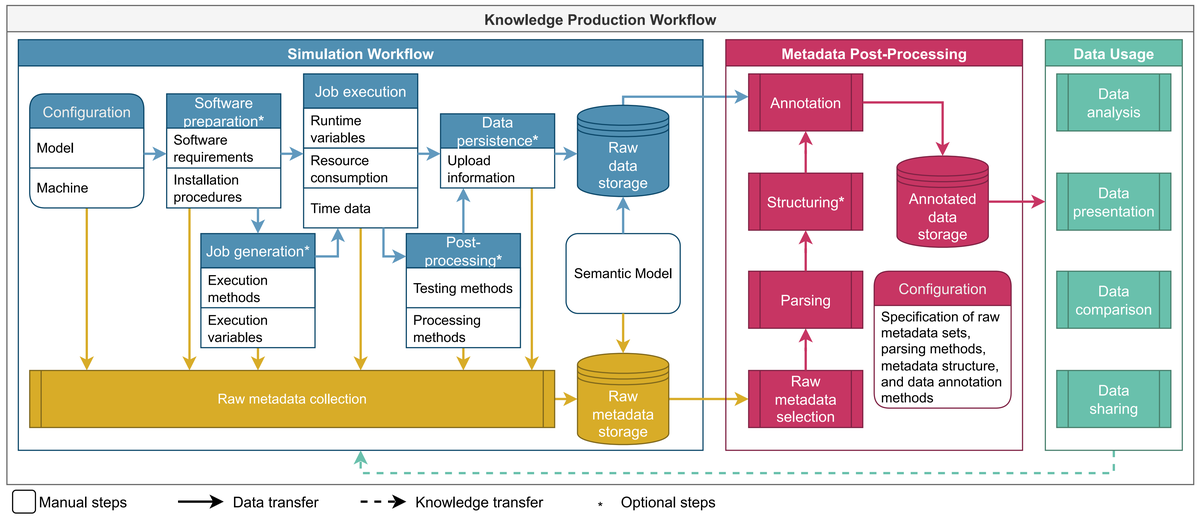
User stories

Story 1 (Model reproducibility):
Scientist X cannot reproduce simulation results of scientist Y due to lack of information on software dependencies and inconsistencies between the article and the code published by Y. Even personal communication with Y does not resolve these inconsistencies[2].

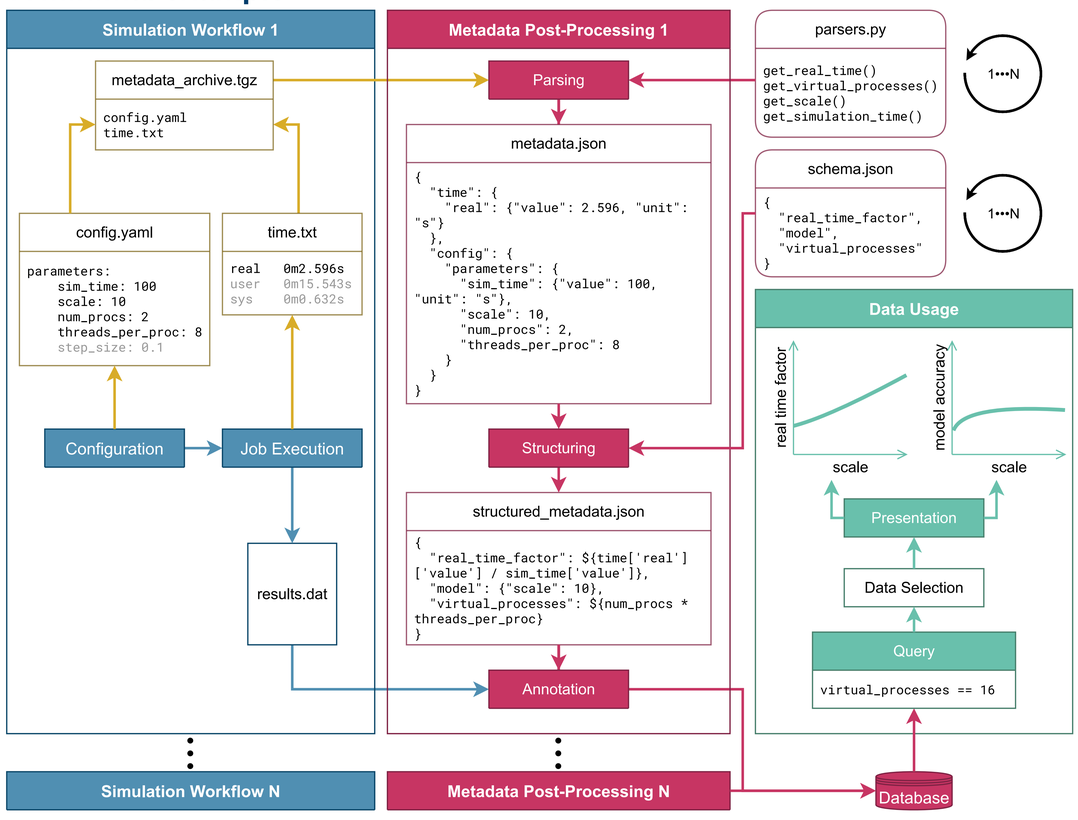
Story 2 (Hardware reproducibility):
Scientist X cannot reproduce their previous simulation performance results even though they are using the same model implementation, software stack, and hardware. Only after personal communication with the IT department, X finds out that the system was actually running at higher clock speed.

Story 3 (Data exploration):
A team of developers is regularly running validation experiments with different configurations and models to continuously monitor software performance. After years of development the group has accumulated large amounts of validation data for each software version with no means of efficient exploration.

Concept of metadata management framework



A minimal example



References:
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- Pauli et al. (2018) Reproducing Polychronization: A Guide to Maximizing the Reproducibility of Spiking Network Models. Front. Neuroinform. 12:46

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