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Good practices for handling metadata in simulation workflows

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Computer simulations are an essential pillar of knowledge generation in science.
Understanding, reproducing, and exploring the results of simulations relies on tracking and organizing metadata describing numerical experiments.
However, the models used to understand real-world systems, and the computational machinery required to simulate them, are typically complex, and produce large amounts of heterogeneous metadata.
Here, we present general practices for acquiring and handling metadata that are agnostic to software and hardware, and highly flexible for the user.
These consist of two steps: 1) recording and storing raw metadata, and 2) selecting and structuring metadata.
As a proof of concept, we developed a Python tool to help with the second step, and use it to apply our practices to distinct high-performance computing use cases from hydrology and neuroscience.
Our practices and the tool support sustainable numerical workflows, facilitating reproducibility and data reuse in generic simulation-based research.

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References

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