A Software Architecture for

Heterogeneous Engineering Workflow Interoperability & Model Provenance

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As the computational workflow landscape becomes increasingly diversified, flexible, and distributed, problems with engineering simulation validation and portable repeatability of results emerge. The lack of interoperability due to variability in the software tooling at nearly every layer of the software computing stack further impedes addressing these challenges, compounding systemic complexity executing engineering workflows such as parametric-sweep ensembles and the orchestration of assorted applications applied in concert. Examples of interoperability barriers include workflow representation, execution and tracking, FAIR data and tool management including provenancial reference to the runtimes which created or used them, and security barriers at organizational perimeters. Abandoning abstraction for access to best-of-breed capability and/or comprehensive functionality, single-vendor or explicitly constrained solutions impose limitations to the fully realized and liberal application of modern MBSE tooling.

Based on our industrial experience, we propose a software architecture consisting of three workflow types – in-situ, intra-enterprise or site, and inter-site. Interoperable and digitally threaded workflows can span all three types. For a site to interoperate in a workflow – be it a local user site, or a corporate, government, or cloud-managed computing facility – the site must provide four architectural pillars including security, runtime, data and resource management. Any commercial, open source, or custom solution which adheres to, or can be made to bend to a published open interface can interoperate in a distributed heterogeneous workflow. This implementation-agnostic view differentiates our approach.

We present the software architecture and provide demonstrated examples of its use across heterogeneous systems for industrial purposes including in-situ simulation steerage, design of experiment-driven workflows with ML training from physics-based simulations, as well as supporting and preparatory software readiness workflows. We will illustrate the general approach of incorporating unique and pre-existing tooling and computing systems into the framework and show how data provenance and model traceability can be maintained throughout the execution process.

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