A Software Architecture for

Heterogeneous Engineering Workflow Interoperability & Model Provenance

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[DRAFT] Abstract for NAFEMS World Congress ‘23[[2]](#footnote-2)

The wide and broadening computing and workflow landscape and its increasingly distributed nature results in widely acknowledged problems with engineering simulation validation and portable repeatability of results. These are not unidimensional problems but impeding progress on these and other important aspects of total quality is the lack of interoperability caused by variability in the software tooling at nearly every layer of the software computing stack. Since most engineering use cases are not satisfied by the execution of a single application, but at minimum by the execution of that application repeatedly, or more likely, in concert with other orchestrated applications in a workflow, the complexity is compounded. 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. Short of single-vendor or pre-down selected solutions which are also myriad, often non-comprehensive, and at a level of software abstraction strikingly similar, this high bar imposes limits 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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2. An expansion of our paper presented at Oak Ridge’s SMC22. See pre-print here: <https://ge.box.com/s/veuq1rgxnh1x0n5a71aemqjqq9tji4vq> [↑](#footnote-ref-2)