FabSim3 for Automation and Tool Integrations in VECMAtk

**High-Performance Computing (HPC)**
- High-performance computing has unlocked a new dimension in scientific research and simulation-based decision making.
- With this ever-growing forefront of computational power, we can simulate increasingly complex systems of interest.
- Exascale computing systems can perform >1 exaFLOPS, or a quintillion calculations per second.
- We currently sit on the brink of the exascale.

**Multiscale Modelling and Simulation**
- Systems of interest can be examined at a wide range of physical and temporal scales using high performance computing.
- Multiscale modelling and simulation combines different scales in order to make new discoveries and inform critical decisions.
- It is widely applied in fields ranging from the physical sciences, engineering, and the life science domain.
- VECMA project deals with the following domains: Climate Modelling, Migration Prediction, Material Science, Fusion Energy and Biomedicine.

**VVUQ**
- VVUQ - Validation, Verification, and Uncertainty Quantification.
- Verification - Determines if the computational model fits the mathematical description.
- Validation - Determine if the model accurately represents the real-world application.
- Uncertainty Quantification - Determine how variations in the numerical and physical parameters affect simulation outcomes.

VECMAtk: An open-source toolkit for multiscale VVUQ based on generic multiscale VV and UG patterns (software solutions to recurring problems).

**FabSim3 Architecture**
- By abstracting the low-level required activities, FabSim3 features a flexible plugin system that allows users to have a customizable version of their own application, in a modular and lightweight manner, to be employed for automating simulation runs and performing tasks such as search, store, transfer, visualize, or any other analysis on the inputs/outputs data. This helps developers to curate complex and dynamic ensemble workflows in an easier way, and also make their simulations more robust and reproducible.
- FabSim3 plugin API philosophy follows these three main goals:
  a) Stability:
     i. should not require any changes in the application core development, i.e., it should be only used as a wrapper functionality around the application.
     ii. the installation and usage should be applicable across devices and users.
  b) Ease of Development:
     i. should be easy enough to develop and support.
     ii. should have a sufficient level of simplicity and generality for an average user.
  c) Performance:
     i. should provides a range of functionalities for common use cases.

**FabSim3 Plugins**
- FabSim3 is designed to support automation of large scale simulation workflow from data preparation step to results analysis in such a way as to reduce the burden on application developers. The tool is generic and is oriented towards developers from different research disciplines and with at least basic programming experience. To enable users to rapidly prototype and evolve their domain-specific workflows, FabSim3 supports the development of application-specific plugins. Once developed, these plugins can then be shared with the wider community, eliminating the need to duplicate machine configurations, workflow definitions or deployment instructions.

**Future Work**
- Improving the total job submission;
- Supporting more VV and UG patterns;
- Close integration of FabSim3 with QCG-PJ, EasyVVUQ, and MUSCLE3.

**VECMAtk**
- FabSim3 Architecture
- FabSim3 Plugins
- FabSim3 Performance and Scalability

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