Optimizing Simulation-based Scientific Workflows
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Workflow in the context of simulation is a term used to capture the entire process of using application codes and computers in pursuit of scientific discovery and mission goals. Before a simulation is ever run on a high-performance computer, the software must be built for optimal execution on the target platforms, and an expert or team of experts must model the system by setting up the problem inputs. During a simulation run (which in some cases can span weeks or months) the user must manage large data sets, monitor progress, monitor system health, and adjust course as necessary. After a simulation is run, that same expert or team must aggregate the results, decide what’s worthy of attention, and perform a deeper analysis in order to turn the raw data into actionable information. It is this conception-to-conclusion series of steps that we refer to as the workflow management and making users of simulation tools efficient and productive along that path can be just as important as speeding up the core simulation on resources like those available in the NNSA laboratories.

Managing scientific workflow is an increasing area of interest within the NNSA and broader HPC community and is highly complementary to the goals of exascale computing, uncertainty quantification, machine learning, reproducibility, and productivity - all of which work together to allow the user to gain deeper insight into their problem as efficiently and productively as possible. In fact, workflow should be considered the unifying element between simulation and those areas outlined above - with workflow management tools acting as the harness that pulls it all together to provide the user with a positive and productive experience.

Not all simulation-based problem-solving environments need to focus on workflow management, but in large multidisciplinary centers such as those that exist in our PSAAP centers, the additional effort can have wide-ranging benefits. These include providing the center with a unifying focal point for execution, cross-disciplinary training, bringing experimental and simulation results together, passing knowledge by capturing and automating best practices, and allowing users to bypass the complications often found in complex simulation environments to focus on their problem development and solution, to just name a few.

Containers are an emerging technology that are embraced in the broader IT world and cloud computing as a means for software deployment that allows one many of the benefits of OS virtualization without the execution overhead. Think of a container as an advanced executable which also contains other user-selected elements of the environment that it relies on (e.g. libraries and runtimes), but still uses the host OS directly. This allows a user or developer to work in an ideal (and validated) environment for developing or running the simulation. This can in turn be assembled for parameter studies, large-scale runs, in situ post-processing or any combination to build a useful complex workflow. Portability is enhanced by decoupling the application dependencies from the underlying system, and by passing the control of the environment back to the application development teams to determine. This in turn insulates the team from potentially disruptive system upgrades and improves provenance by allowing simulations to be rerun months or even years after their original result with less fear of change in results incurred by updated compilers or system libraries. The use of containers in HPC starting to take root, with projects such as LANL’s Bee and CharlieCloud focusing on HPC-specific workflows that can span multiple systems and even the cloud.
Uncertainty Quantification remains a key component of predictive science by allowing large ensembles of runs to vary uncertainties either incurred by statistical uncertainties due to natural stochastic behavior (aleatoric) or by limited knowledge of the inputs and boundary conditions to the simulation (epistemic). With typical UQ ensembles reaching into the 1000’s of coordinated runs, it is increasingly unthinkable to run them without the aid of a workflow management system (such as SNL’s Dakota).

In-situ visualization is another emerging element of workflow management aimed at increasing the availability of actionable information (visual data) to the user without the interim steps of writing files out to disk and using a separate visualization tool and HPC partition and job for analysis. Originally conceived as a necessity for reducing the I/O bottleneck in simulations that are dealing with extremely large data sets, in-situ visualization has the potential to change the way users interact with a running simulation by providing continuous streaming output. As the information flow turns into a 2-way exchange through languages like Python and Lua interacting with the simulation via the users - the ability to steer the simulation without a halt and restart becomes easier to implement. However, computational steering provides its own potential pitfalls, and should be considered only as part of a larger workflow system that can record and replay and track provenance of realtime changes necessary for reproducibility.

Computational notebooks first emerged in tools such as Mathematica and Matlab as workflow management systems aimed at capturing interactive runs, documentation, and output all in a single often browser-based interface. Initially popularized in scientific computing through IPython, notebooks are merging as an extremely powerful tool for capturing and standardizing workflow, transferring knowledge, and presenting results in a unified system. IPython has grown up into Jupyter Notebook (and its multi-tenant complement JupyterHub) popular in the open-source world, and has advanced features supporting a number of languages (e.g. Python, C++) and analysis systems (e.g. Spark). The Apache Zeppelin project is another notebook gaining in popularity, with a tight integration with Spark aimed at data-intensive workflows.

Workflow management is gaining in popularity and remains an area ripe for additional research and development – particularly in the context of simulation-based HPC. A recent NNSA-hosted workshop held a breakout session on the topic, and raised the question of “what research questions are paramount in workflows”? The ideas included:

1. Reducing reliance on file I/O (esp. on slow spinning disk) as an intermediary form for coupling applications into a workflow
2. Scheduling complex workflows across diverse machines (including cloud resources)
3. Using system monitoring data, machine learning, and other data for purpose of optimizing system performance or energy
4. End-to-end security and encryption of workflow management tools
5. Use of key-value stores for bulk data (e.g. instead of HDF5) to better leverage fast queries available in systems such as Spark

These examples show that workflow is a very broad area that can encompass a large number of subdisciplines. Indeed, there is no one “right” workflow or workflow management system – even within a single PSAAP center or NNSA simulation campaign. As more general-purpose workflow tools penetrate the HPC world, we envision the ability for teams to quickly pull together pieces from a toolkit of workflow components to rapidly build custom workflows using standard APIs and new features of exascale systems (e.g. NVRAM, resource managers, containers, accelerators, etc). The NNSA labs all have efforts underway at different levels of maturity, and
look forward to working with the PSAAP community to advance this technology. By considering workflow management as key productivity enabler, PSAAP centers can focus on adopting, adapting, or even inventing the tools that will best encompass their workflow.

In summary, the goal is to persuade potential PSAAP centers to consider workflow management tools and their continued development as a key cross-cutting feature that can enable HPC simulation, large-scale data management, machine learning, uncertainty quantification, coupled applications, developer productivity – all the major areas we in the NNSA hope to see innovations occur within the PSAAP centers.