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Title: Enhancing Workflow Manager and Resource Manager to Support Elastic Scientific Workflows in HPC Systems

Abstract:
As scientific workflows grow increasingly complex, integrating AI tasks with traditional high-performance computing (HPC) simulations, dynamic resource management, and elastic execution become essential for optimizing resource utilization in HPC supercomputers. Furthermore, dynamic resource management is necessary for workflows since the computational requirements may not be known when workflows are submitted to HPC systems for execution, and may change over time. Current resource management systems and workflow managers in HPC systems provide limited support for dynamic resource allocation. Static allocations of resources can lead to an overprovisioning of resources, with the risk of underutilization, or an underprovisioning of resources, resulting in workflows terminating prematurely. In this work, we identify some key enhancements needed in HPC software stacks, specifically in Workflow Managers and Resource Managers, in order to support elastic workflows. We develop and evaluate a prototype for dynamic resource management based on the elastic PMIx-enabled Parsl workflow manager and a customized hierarchical scheduler built on top of Slurm. Through experiments and case studies involving some real applications, we demonstrate that dynamic resource management and elastic workflows can improve system and workflow performance by enhancing resource utilization and reducing workflow execution times.