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Containerization of numerical ocean model for computational reproducibility and portability in the cloud computing

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Many numerical ocean models have been used to understand and predict ocean dynamics. For global and high-resolution ocean modeling, many information technology (IT) resources are required. The cloud-computing technologies has enabled oceanographers to easily use numerical ocean models that require high-performance computing (HPC) and message-passing interface (MPI) software. Although it is easier today to use computing resources than it was in the past, computational reproducibility and portability in diverse IT environments remain crucial issues. This study proposes numerical ocean model execution or runtime architecture for computational reproducibility, portability, and agility based on container-based virtualization and orchestration technologies. We implement a containerized regional ocean-modeling system (ROMS), an MPI-based numerical ocean model in various public or private cloud environments (e.g., personal computers and multiple-node servers). The pre-requisite time and many efforts for model setup is greatly reduced using container-based HPC architecture. Additionally, we can deploy and test model runtime or execution environments into multiple environments using automation processes based on cloud native methods.

Containerization of ROMS is tested for its support of the portability of numerical modeling in major public-cloud environments and private cloud environments. When leveraging an abstraction layer of infrastructure such as container environments, we can run the ocean model more easily while obtaining computational reproducibility using a shareable deployment code. This advancement can be used to guide the containerization of various numerical models and to run them in parallel in public and private cloud-computing environments.