# Management and Deployment of Scientific Applications with SIMULOCEAN Science Gateway

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Abstract

SIMULOCEAN is a web-based scientific application and visualization framework for the management and deployment of software serving the coastal modeling community. The framework helps to collect observational data, schedule modeling codes for execution, manage data transfer, and visualize both observational and numerical results. With all the information collected, SIMULOCEAN can also provide direct validation and verification for models, and generate high quality technical reports. With the help of the Coastal Model Repository (CMR), a coastal researcher can start running state-of-the-art models on the latest cloud-ready computing systems in minutes. The SIMULOCEAN science gateway can take advantage of CMR to quickly deploy coastal models on academic and commercial cloud platforms, in addition to traditional HPC systems.

System Architecture
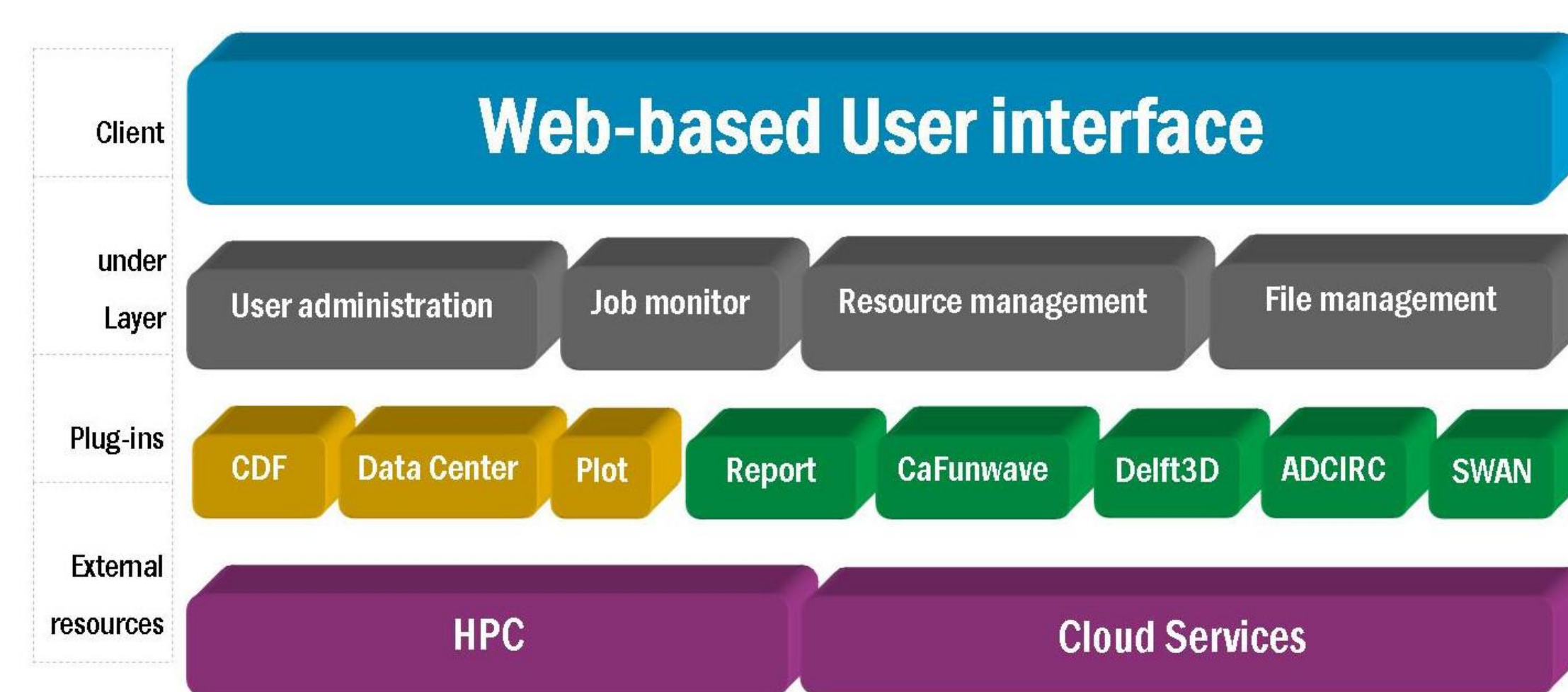
SIMULOCEAN has a multi-layer structure. Each layer in the diagram provides essential functionalities required by the upper layer. Such a multi-layer system separates the programming concerns, thus enables multidisciplinary collaboration and development.
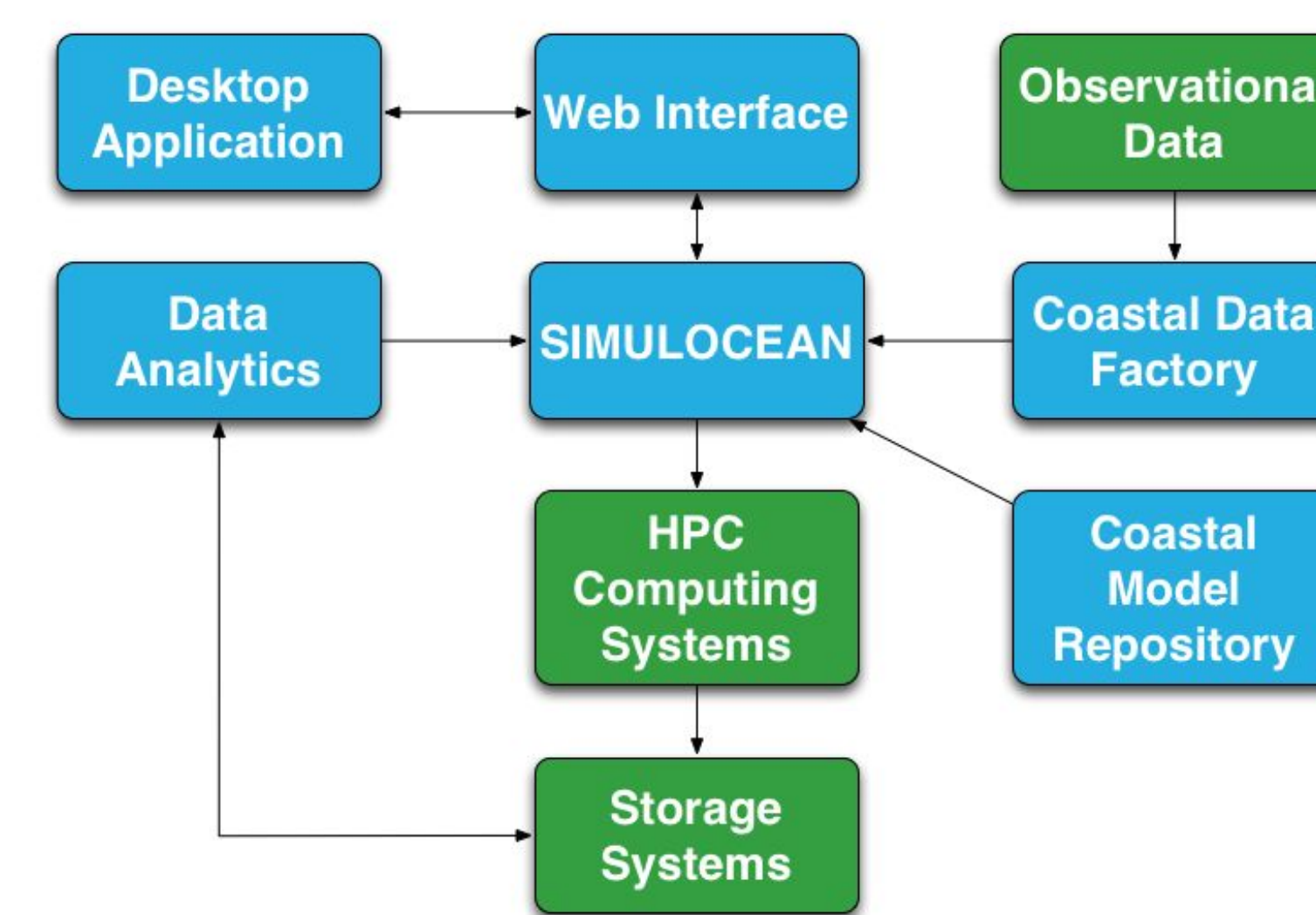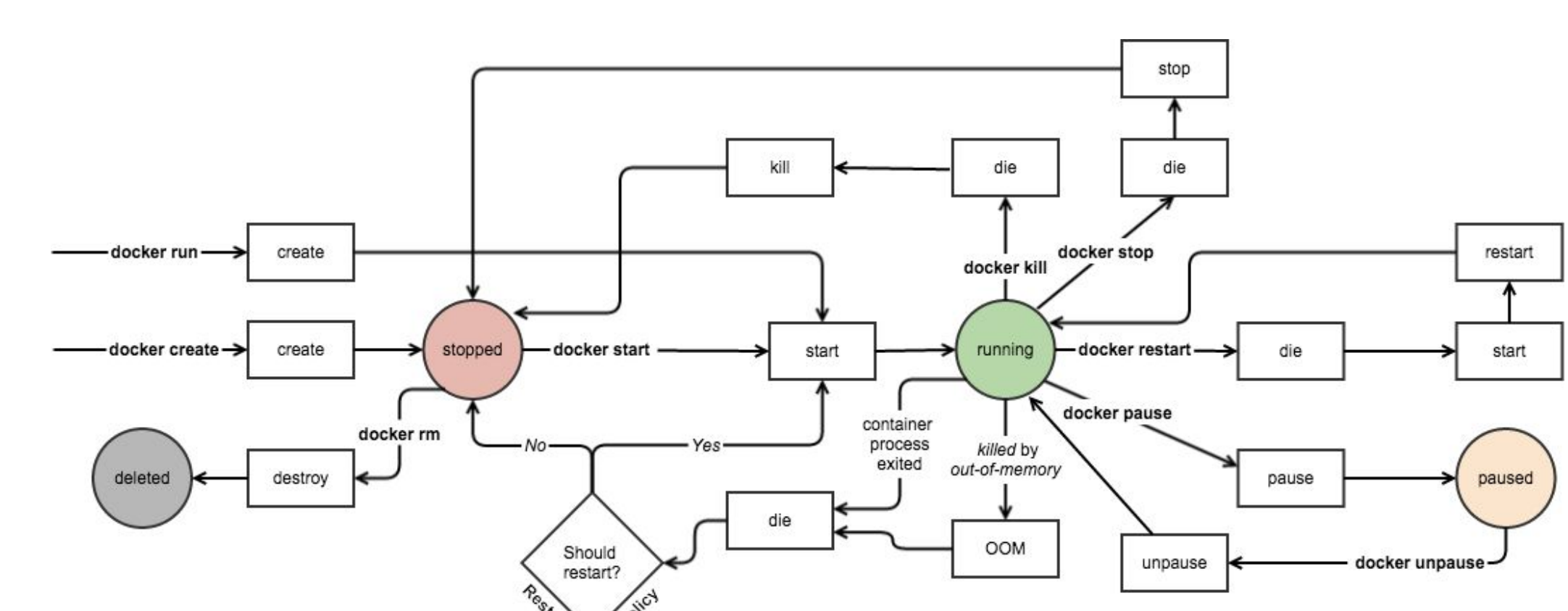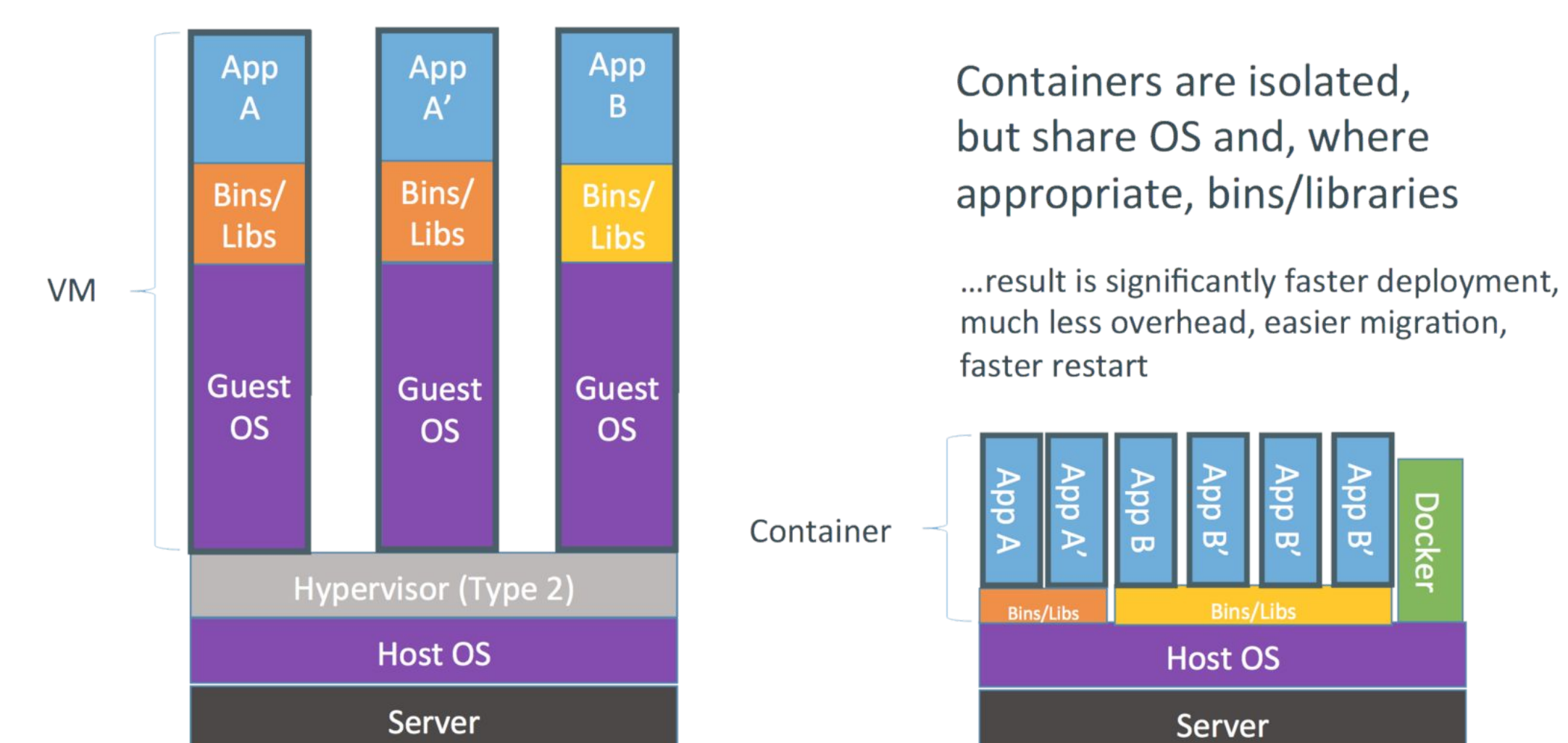
SIMULOCEAN includes multiple components (as shown above in blue boxes) that are coupled together to provide user interfaces to prepare model input and run models on high performance computing systems.
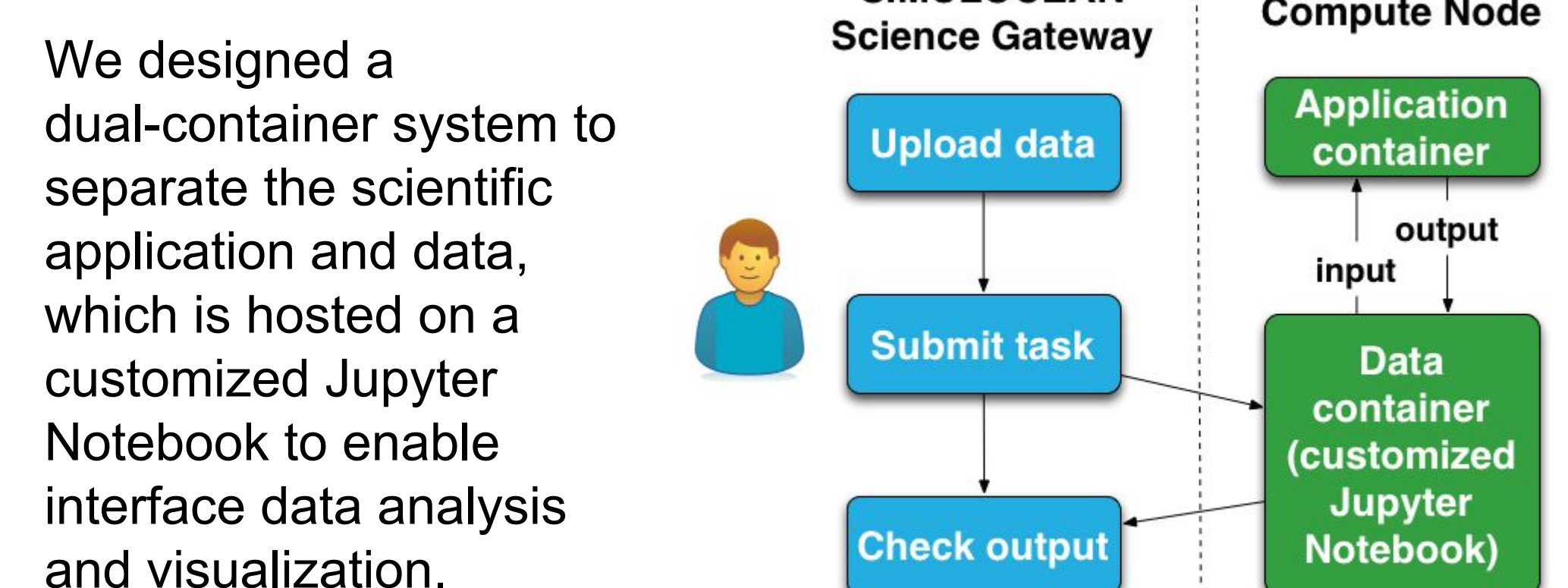
Resilient Container Cluster
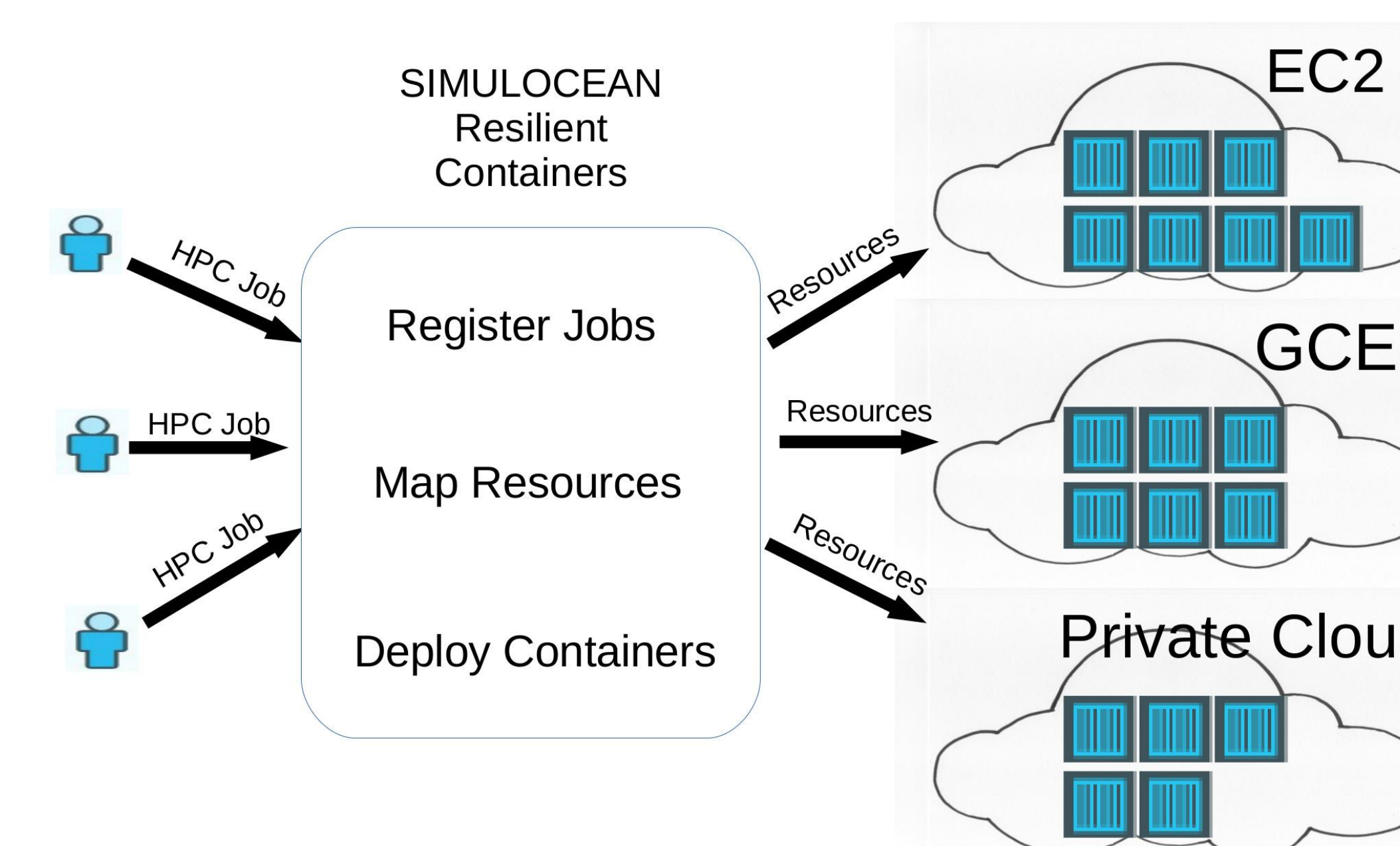
SIMULOCEAN has a built-in resource manager which, on a given cloud computing platform, creates and maintains a resilient container cluster interconnected on top of an overlay network to deploy jobs submitted by users.
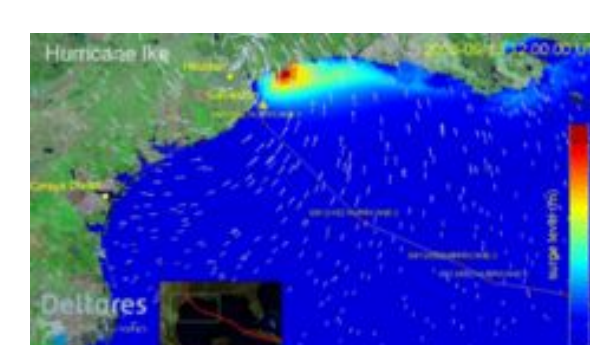
Docker Containers

Containers are isolated, but share OS and, where appropriate, bins/libraries

...result is significantly faster deployment, much less overhead, easier migration, faster restart

Docker is an open platform allowing developers to build, ship, and run, and manage distributed applications in self-contained environments. (credit: http://docker.com)

We designed a dual-container system to separate the scientific application and data, which is hosted on a customized Jupyter Notebook to enable interface data analysis and visualization.
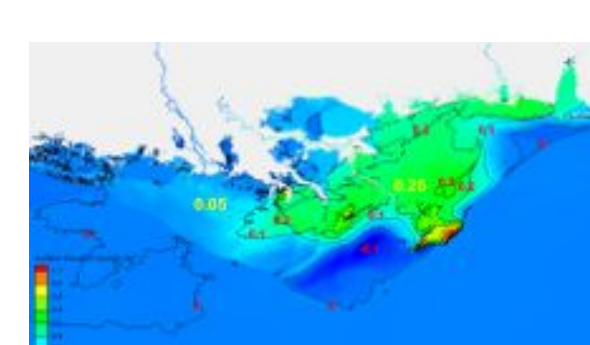
Coastal Model Repository

Delft3D is a flexible integrated modeling suite, which simulates two-dimensional and three-dimensional flow, sediment transport and morphology, waves, water quality and ecology and is capable of handling the interactions between these processes
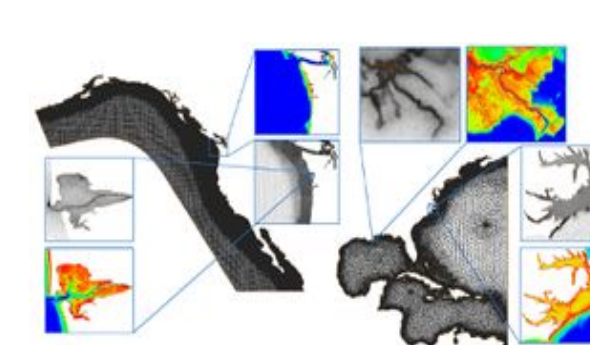
ADCIRC is a system of computer programs for solving time dependent, free surface circulation and transport problems in two and three dimensions. These programs utilize the finite element method in space allowing the use of highly flexible, unstructured grids.
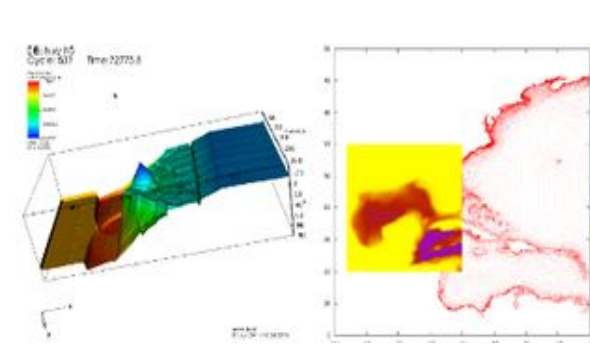
CaFunwave is developed based on the Total Variation Diminishing (TVD) version of the FUNWAVE code, which is a phase-resolving, time-stepping Boussinesq model for ocean surface wave propagation in the near shore.

SWAN is a third-generation wave model that computes random, short-crested wind-generated waves in coastal regions and inland waters.

The Coastal Model Repository (CMR) is targeting cloud and cloud-like architectures to enable quick deployment of coastal models and their working environments. Hosted on Docker Hub, CMR will serve as a community repository for precompiled open source models that are widely used by coastal researchers. CMR will introduce distribution of containerized coastal models, which can run on any cloud-like architecture directly, and with negligible system overhead. (credit: http://hub.docker.com)
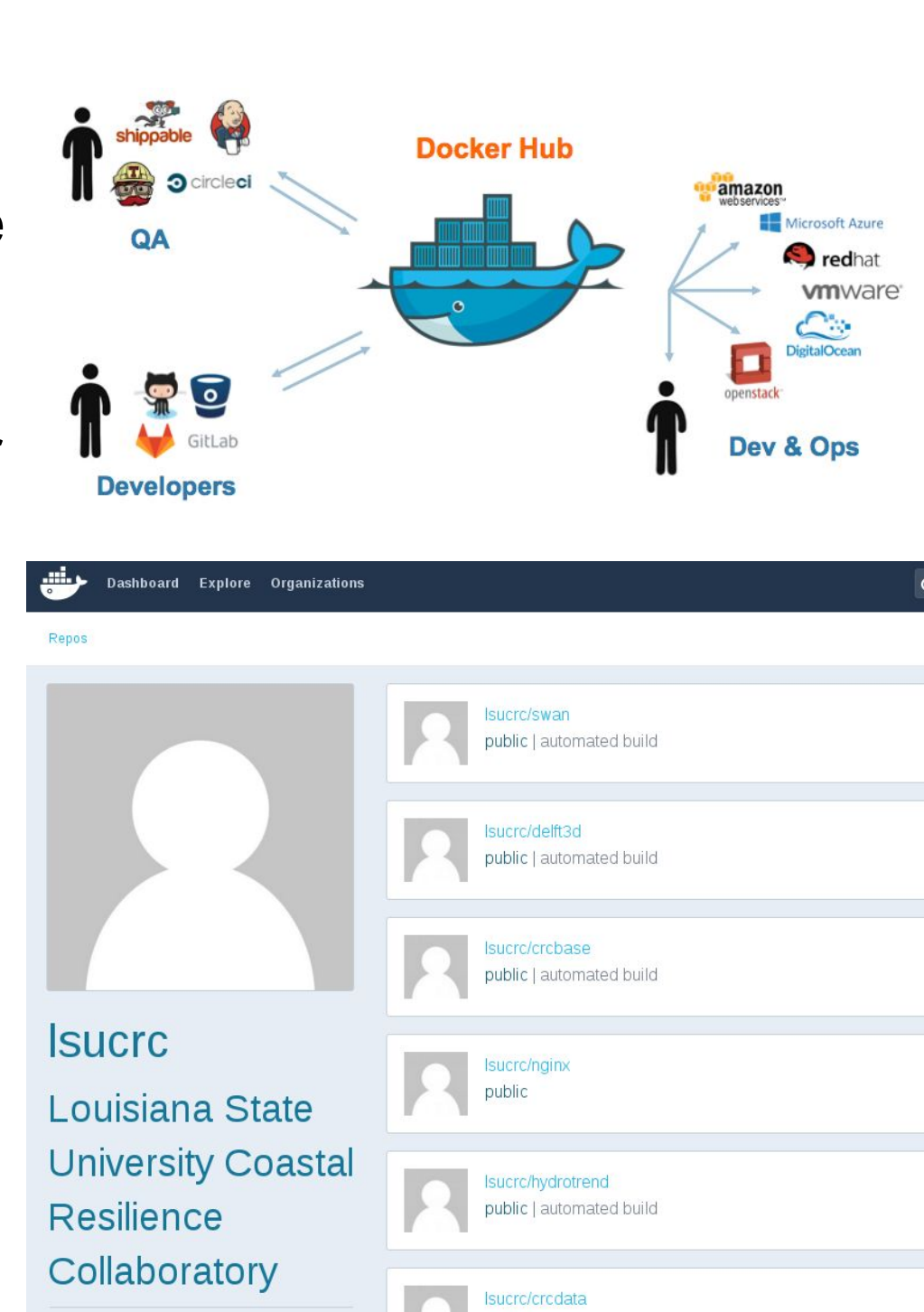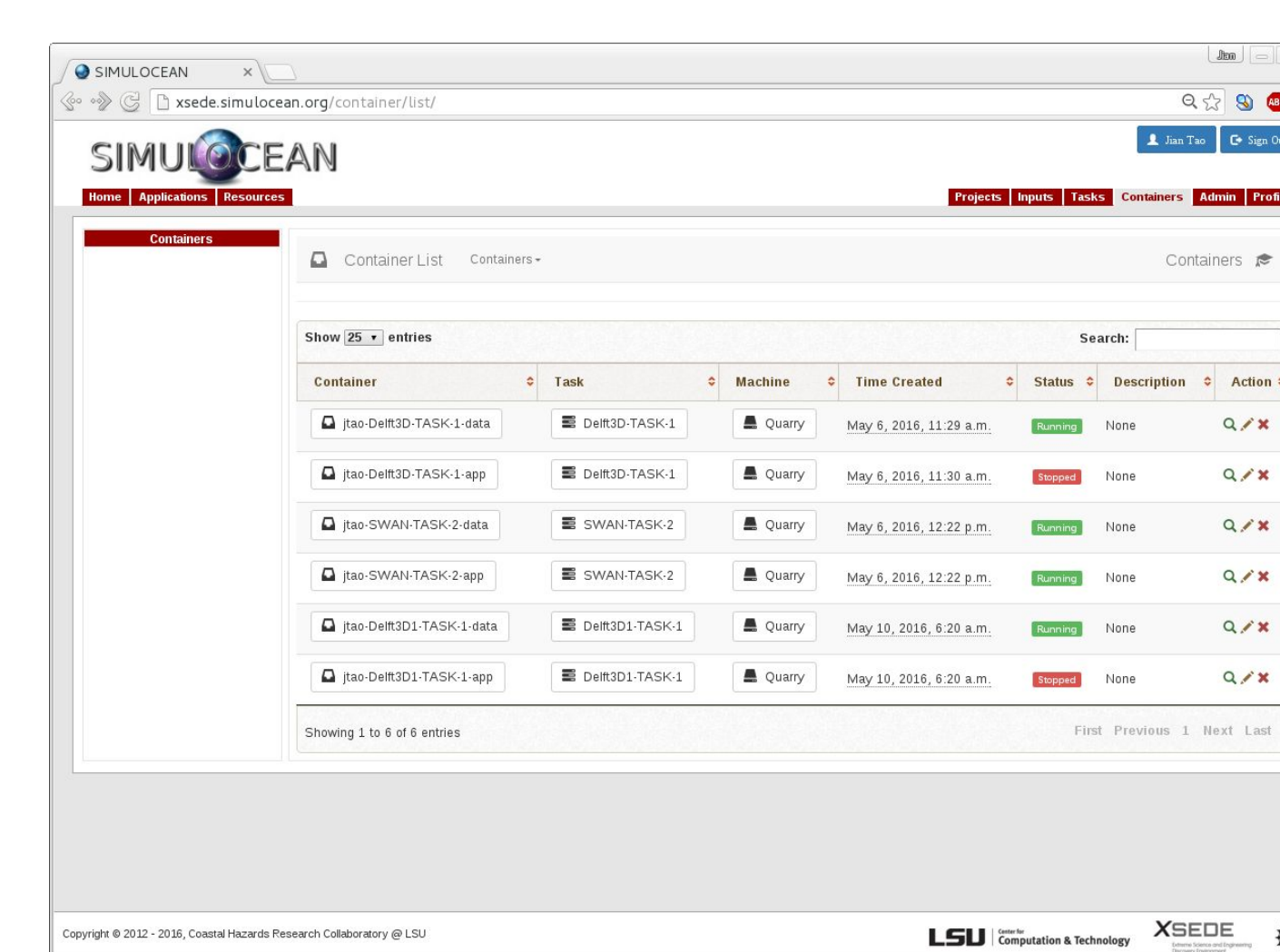
Web Interface
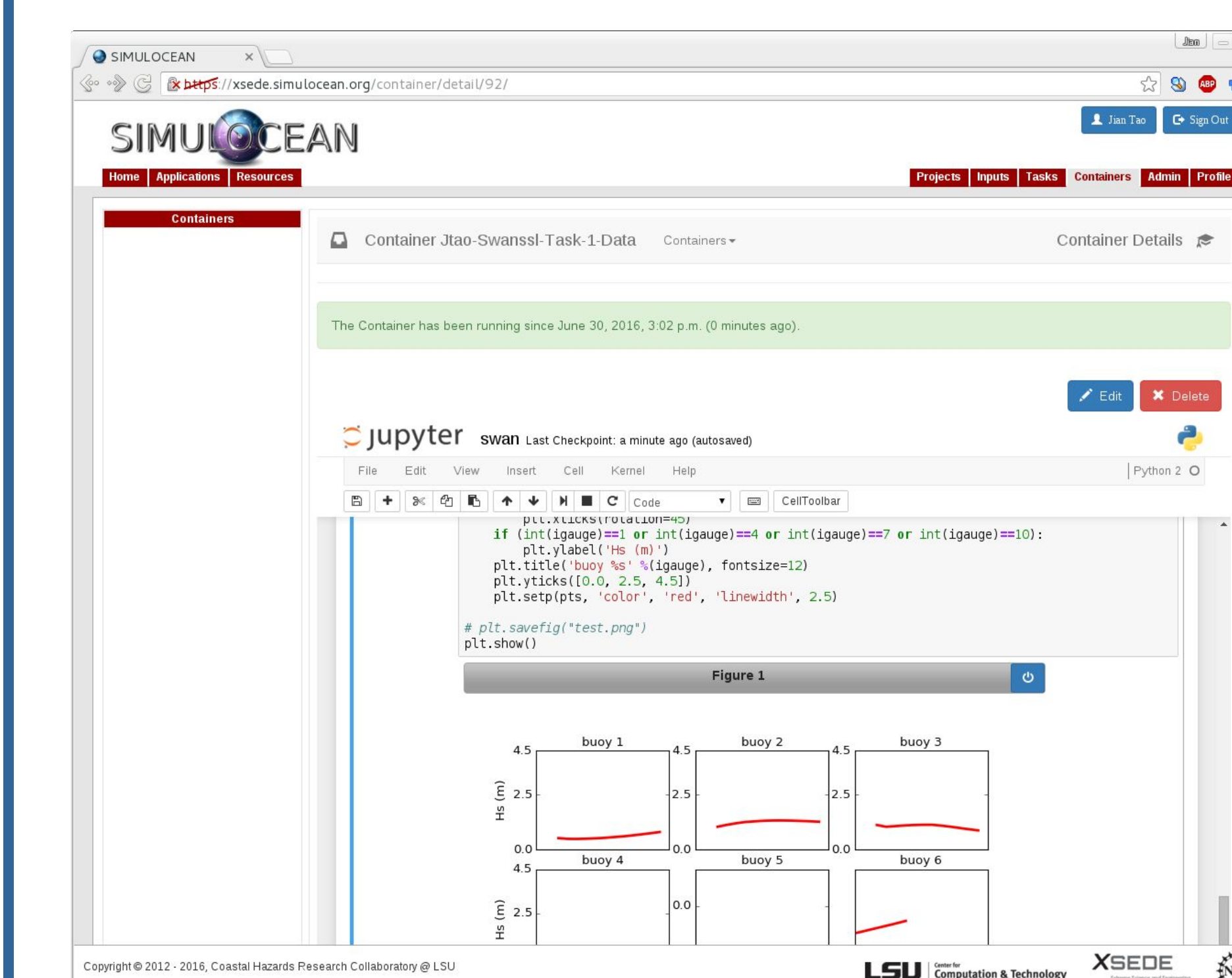

Task Management
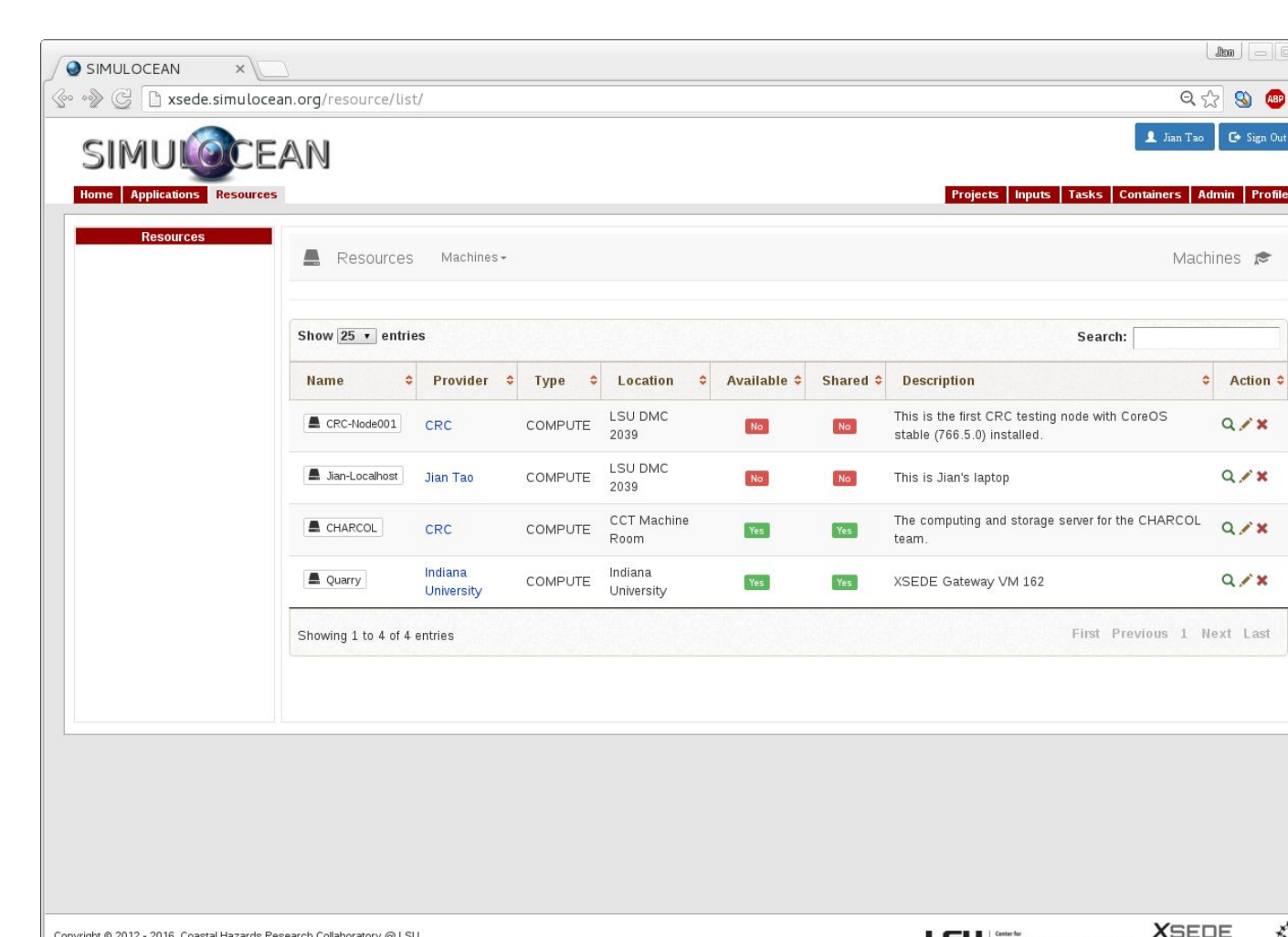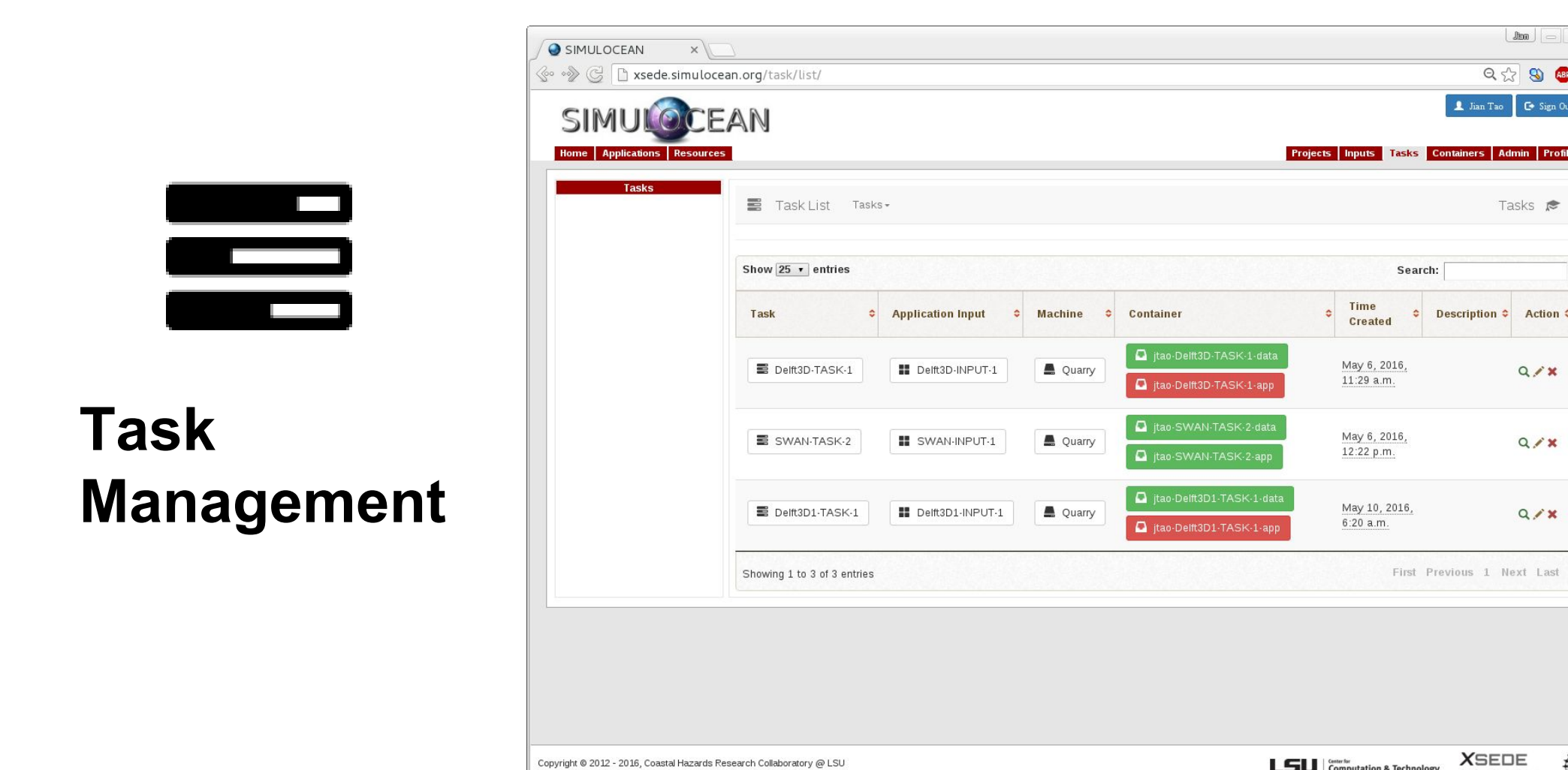
Resource Management

Container Management

Embedded Jupyter Notebook

A customized Jupyter container is created to provide an interactive interface for SIMULOCEAN users for data analysis and visualization. A default Jupyter notebook will be provided for each science application. Users can modify the notebook while the application is still running. Changes to the notebook could be saved and exported for later usage.

Conclusion and Future Work

In this poster, we introduced SIMULOCEAN, a web-based deployment and visualization framework for coastal modeling. The goal of SIMULOCEAN is to help coastal modelers to deploy and analyze coastal models with minimum effort. We will extend our current framework to integrate more widely used coastal models and support job deployment in different HPC environments.

Acknowledgments