SURAgrid Support for SCOOP

SURAgrid All Hands Meeting

March 28, 2008

Mission Statement

The purpose of this working group is to

- promote communication between SCOOP and SURAgrid,
- deploy SCOOP models on SURAgrid,
- develop demonstrations for both SCOOP and SURAgrid presentations, and
- develop easy-to-use deployment documentation.

Overall this group works to enable significant, predictive science in the SURA region, for the SURA region.

Working Group formed April, 2007

Coordination & Communication

- Spread across many SCOOP and SURAgrid sites.
- Work together toward a shared understanding of research needs.
- Collaboration is balanced between SURA, SCOOP liaison, SCOOP researchers, and SURAgrid resource owners.
- SURA IT staff are the primary facilitators on the SURAgrid side.
- The liaison provides detail and direction on the upcoming hurricane season modeling timeframes, priorities, modeling requirements, porting materials, new ideas, and so forth.
- Biweekly liaison (Tuesday) and deployment (Thursday) calls.

Liaison group: Luis Bermudez (SURA), Matt Smith (UAH), Mary Fran Yafchak (SURA), Mary Trauner (SURA)

Deployment: Art Vandenberg and Nicole Geiger (GSU), Archit Kulshrestha, Gabrielle Allen, Dan Katz (LSU), Steve Johnson (TAMU), Mary Trauner, Mary Fran Yafchak, Dali Wang (SURA)

The Scenarios

Event-driven: Event-driven mode begins when the National Hurricane Center issues a Forecast Advisory indicating that there is a severe Atlantic storm that may threaten North America. Extreme events (e.g. growing hurricanes) will trigger ensemble calculations that bring all available resources to bear on the immediate needs of hazard response. Facilities to support calculations for up to three simultaneous events are required.

Immediate

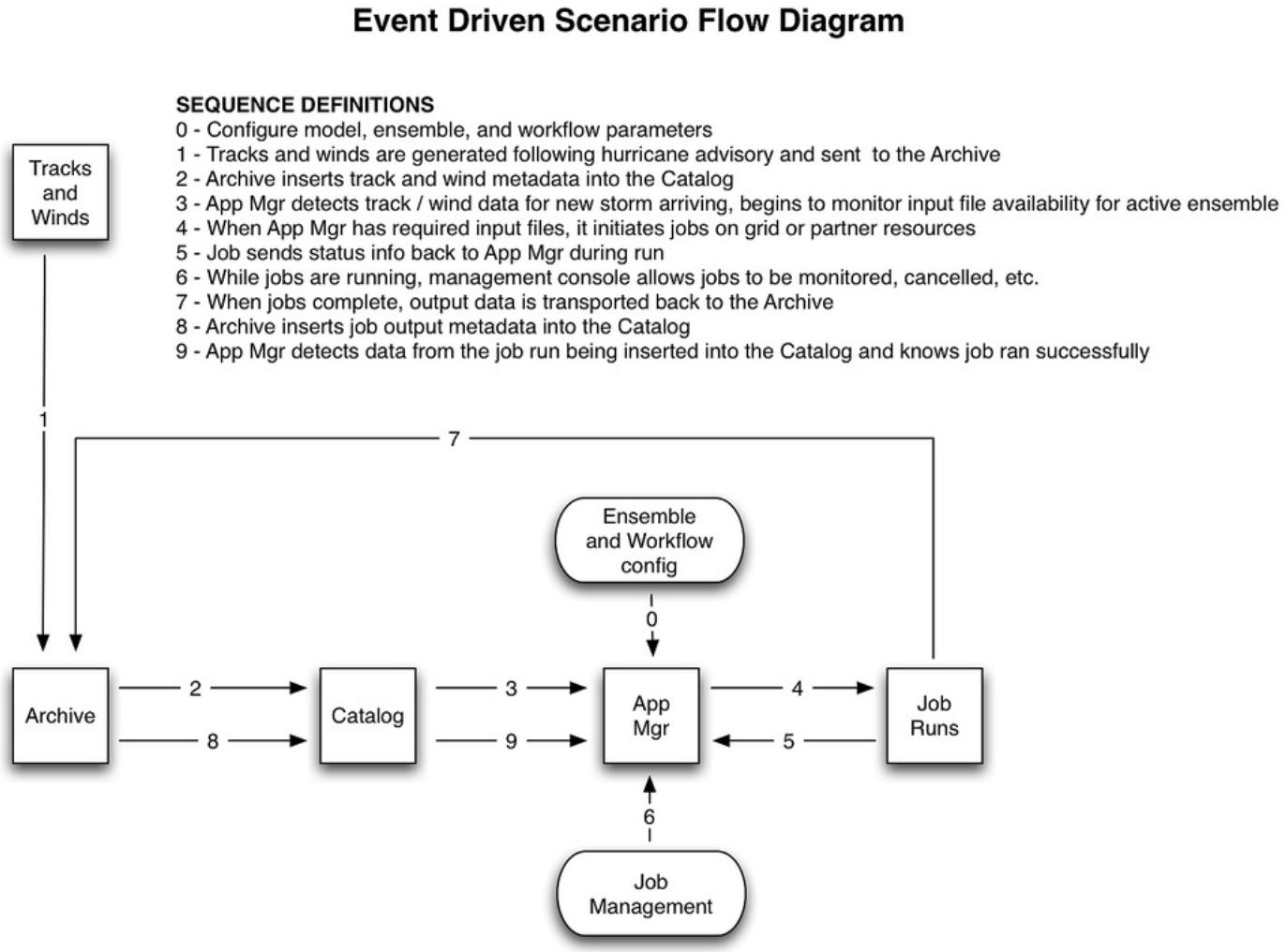
24/7: 24/7 mode is the normal day-to-day ocean observations and forecast models that run within the SCOOP infrastructure which include water level and wave forecasts for the east coast of North America.

Daily, possibly scheduled

Retrospective: Retrospective mode is used to visualize and download past storm data.

As needed

The Scenarios



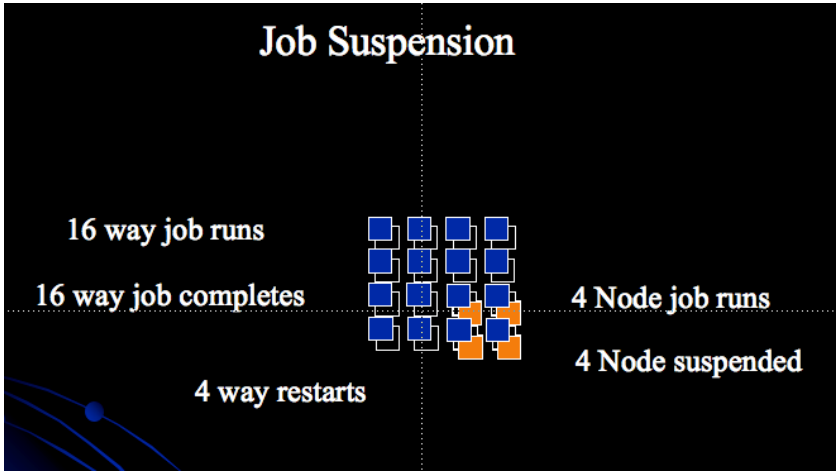
The Scenario Requirements

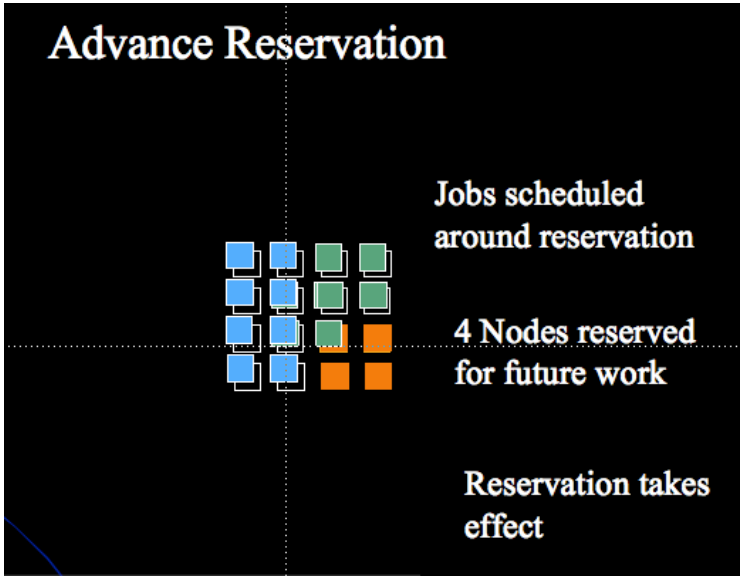
24 x 7: Daily

Retrospective: As needed

Event-driven: Immediate

Loadleveler, Pre-emptive queues



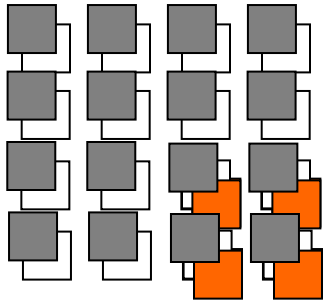


The Scenario Requirements

Job Suspension

16 way job runs

16 way job completes



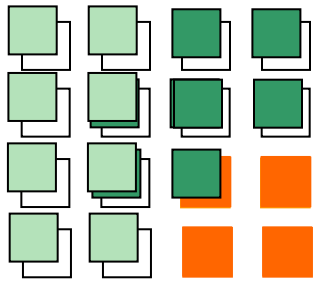
4 Node job runs

4 Node suspended

4 way restarts

The Scenario Requirements

Advance Reservation



Jobs scheduled around reservation

4 Nodes reserved for future work

Reservation takes effect

The Models

ADCIRC Coastal Circulation and Storm Model

ADCIRC is a finite element method shallow water model for computing tidal and storm surge water level and depth-averaged currents associated with these phenomena. Grid environments such as SURAgrid are ideal for the ensembles in applications like ADCIRC, which is one of a set included under SCOOP (SURA Coastal Ocean Observing and Prediction) program that is focused on improving predictions of coastal phenomena. Project Partners: University of North Carolina Marine Science, Renaissance Computing Institute (RENCI), MCNC, SAIC.

The Models

WW3 WaveWatch III Ocean Wave Model

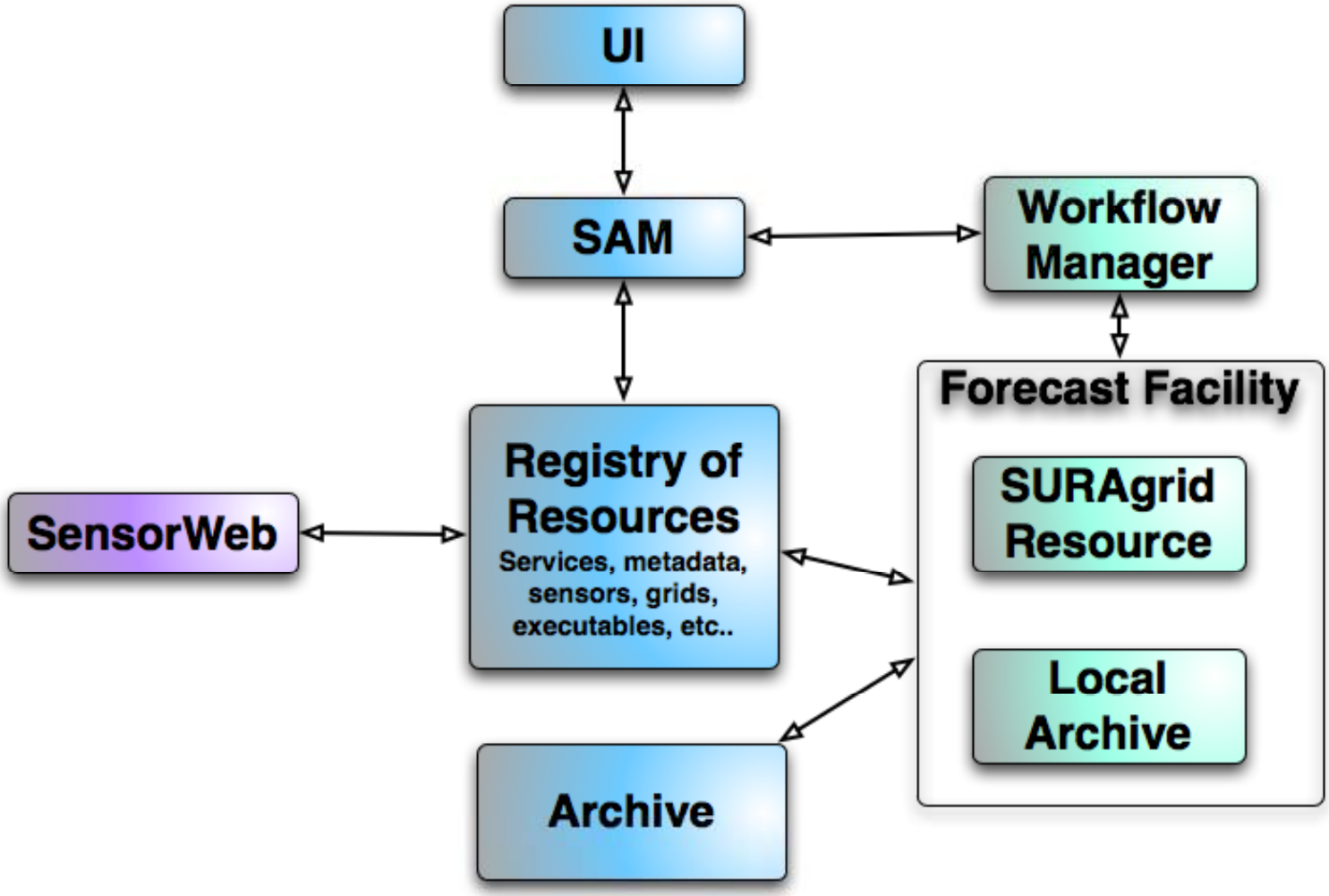
WAVEWATCH III solves the spectral action density balance equation for wavenumber-direction spectra. Grids such as SURAgrid have the potential to greatly improve the ability to distribute Event Driven Wave Watch 3 instances across geographical domains and take advantage of supercomputing resources to process wave model for Hurricane events. Project Partners: Center for Computation and Technology (CCT), Louisiana State University; SCOOP; Bedford Institute of Oceanography.

The Models

UFL CH3D Storm Surge Monitoring System with Grid Appliance

The Curvilinear Hydrodynamics in Three Dimensions (CH3D) application is used to model physical processes in bays, rivers, lakes, and estuaries. CH3D is a circulation model that aids storm surge forecasting and is one of a set of applications included under the SCOOP program. On SURAgrid, CH3D is implemented in combination with the Grid Appliance application, which is a self-configuring virtual machine that contains the IPOP virtual networking package and the NSF/NMI Condor middleware. The retrospective analysis the application duo is used for requires high-throughput, is computationally intensive, and can thus take advantage of the resources available on SURAgrid .

The SCOOP System



Workflow System

The Workflow Manager components handle

- Ensemble Definitions
- Resource Manager
- Scheduling
- Job Controller
- Resource Monitoring
- Process Monitoring
- Transport Monitoring

In general the Workflow Manager

- completes all runs,
- provides job status information,
- runs the workflow on TERAgrid, OSG, and SURAgrid as QoS needs dictate.

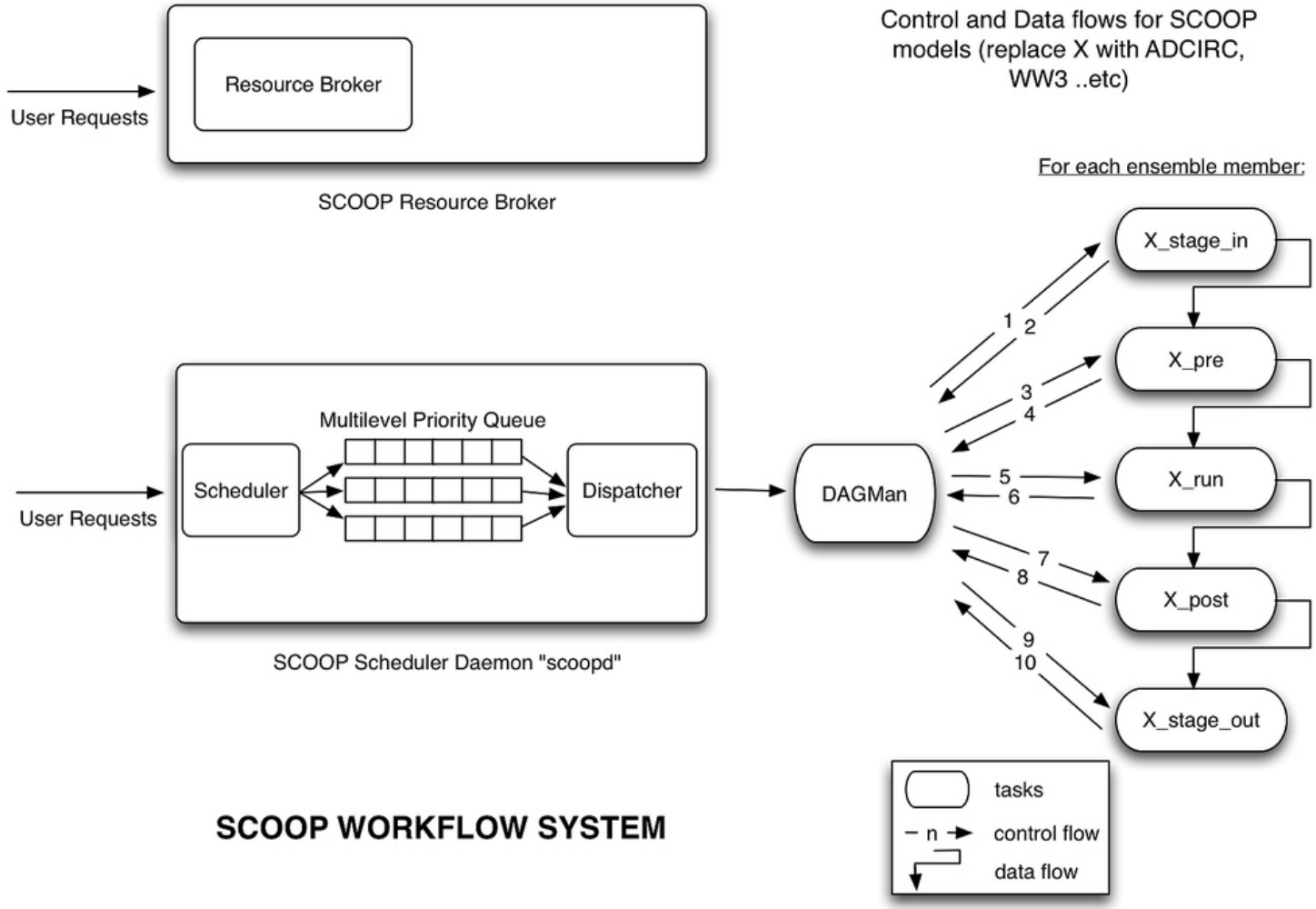
Condor DAGMAN is used for workflow management.

Workflow System

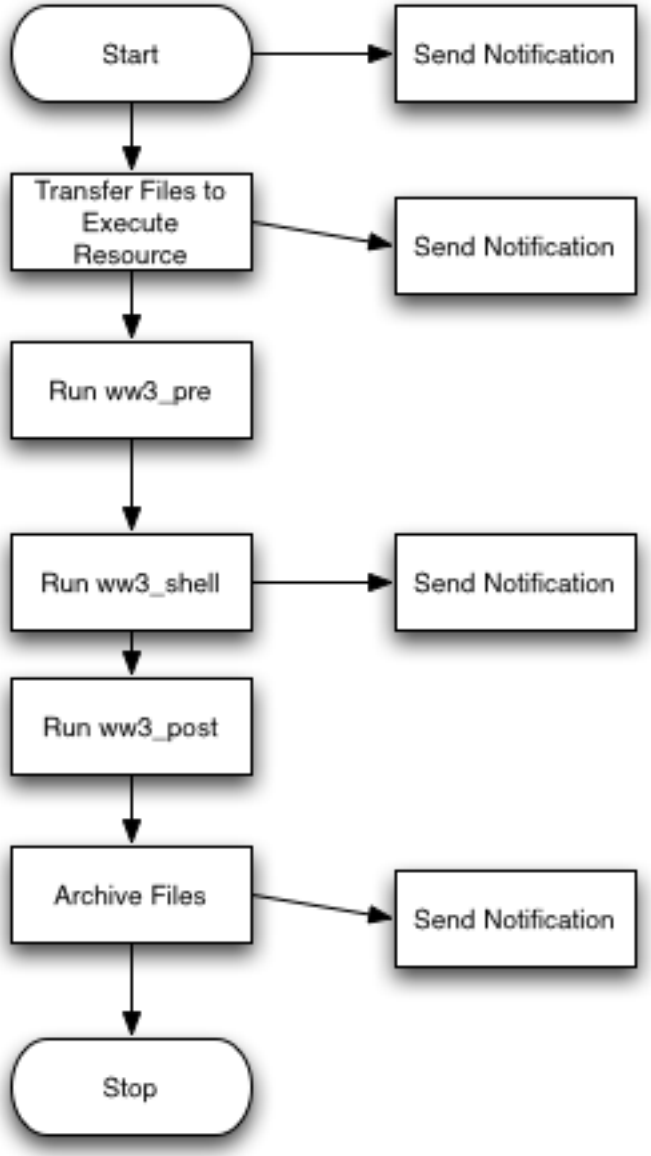
Ensemble Description File (EDF)

```
<?xml version="1.0"?>
<ensembledescription name="Default_Ensemble_2007" lastModified="2007-08-28
+09:00">
  <storm num="12" name="Katrina" date="2005-08-28+09:00"/>
  <ensemble size="10" creationTime="2007-04-24+12:29" lengthForecastHrs="120">
    <member id="1" urgency="1" priority="1">
      <track>p01</track>
      <model>WW3</model>
      <forcing>ANA</forcing>
      <region>Gulf</region>
      <config>0.2</config>
      <hotstart>No</hotstart>
      <comment></comment>
    </member>
    <member id="2" urgency="1" priority="2">
      <track>p02</track>
      <model>WW3</model>
      <forcing>ANA</forcing>
      <region>Gulf</region>
      <config>0.2</config>
      <hotstart>No</hotstart>
      <comment></comment>
    </member>
    <member id="3" urgency="1" priority="3">
      <track>p03</track>
      <model>WW3</model>
      <forcing>ANA</forcing>
```

Workflow System



The WW3 Example Workflow



The Model Requirements

ADCIRC

- Hardware
  - X86-based Linux systems, preferably a cluster but would technically work with a single node, albeit much slower. Prefer >= 2.0 Ghz CPU and >= 2.0 GB of RAM per node at a minimum, and >= 1 GB of free disk space.
- Software
  - MPICH-1.2.x
  - Batch scheduler
  - Globus, including pre-web-services components GRAM and MDS
  - PBS utilities for Globus for job submission and queue status reporting

The Model Requirements

WW3

Hardware

24x7 runs: for each event, on IBM p575, per track
linear from 16 to 256 processors
on 16 processors = 30 minutes
34 tracks/storm (5-day simulation) = 17 hrs/storm
3 simultaneous storms = 51 hours

Software

Globus, including pre-Web services components Gram and Grid FTP
Fortran 90 compilers and libraries
mpi / openmp bindings for fortran 90
latest compatible python versions (2.3 and greater)
Perl
Netcdf utilities (Libraries, ncdump, ncgen)

The Model Requirements

CH3D

- Hardware
  - SGI3400, SGI300, SGI2000, SUN, Intel-based systems, and Beowulf clusters) with a variety of operating systems (Unix, Linux, and Windows)
  - 512 MB of memory
- Software
  - Globus
  - Condor
  - Fortran 90

SURAgrid Deployments To Date

2006 Hurricane Season

- TAMU, ULL, UAH added to the ADCIRC resource pool for 24x7 and event-driven runs. ODU verified but not added.
- ULL added to the CH3D resource pool for 24x7 and event-driven runs.
- SURAgrid objectives: Helped define and develop overall SURAgrid application deployment and user documentation

2007 Hurricane Season

- WW3 deployed on first-available IBMs on SURAgrid (GSU, TAMU, LSU) for event-driven runs (also demo'd at SC07)
- SURAgrid objectives: Provided focus for IBM integration efforts and exploration of proprietary features for application support

2008 Hurricane Season

Support for multiple models…

- Continue WW3, “refresh” ADCIRC & CH3D

…on as many SURAgrid resources as possible,

- Re-verify resources already in use and expand number supporting *each model*
- [Your resource here?]

but scenarios to be supported are still TBD

SURAgrid objectives:

- Increase application activity on SURAgrid
- Continue to refine application deployment process
- Further inform development of authX, user account management and accounting
- Understand policy and support requirements for various “levels of service (e.g., the scenarios)