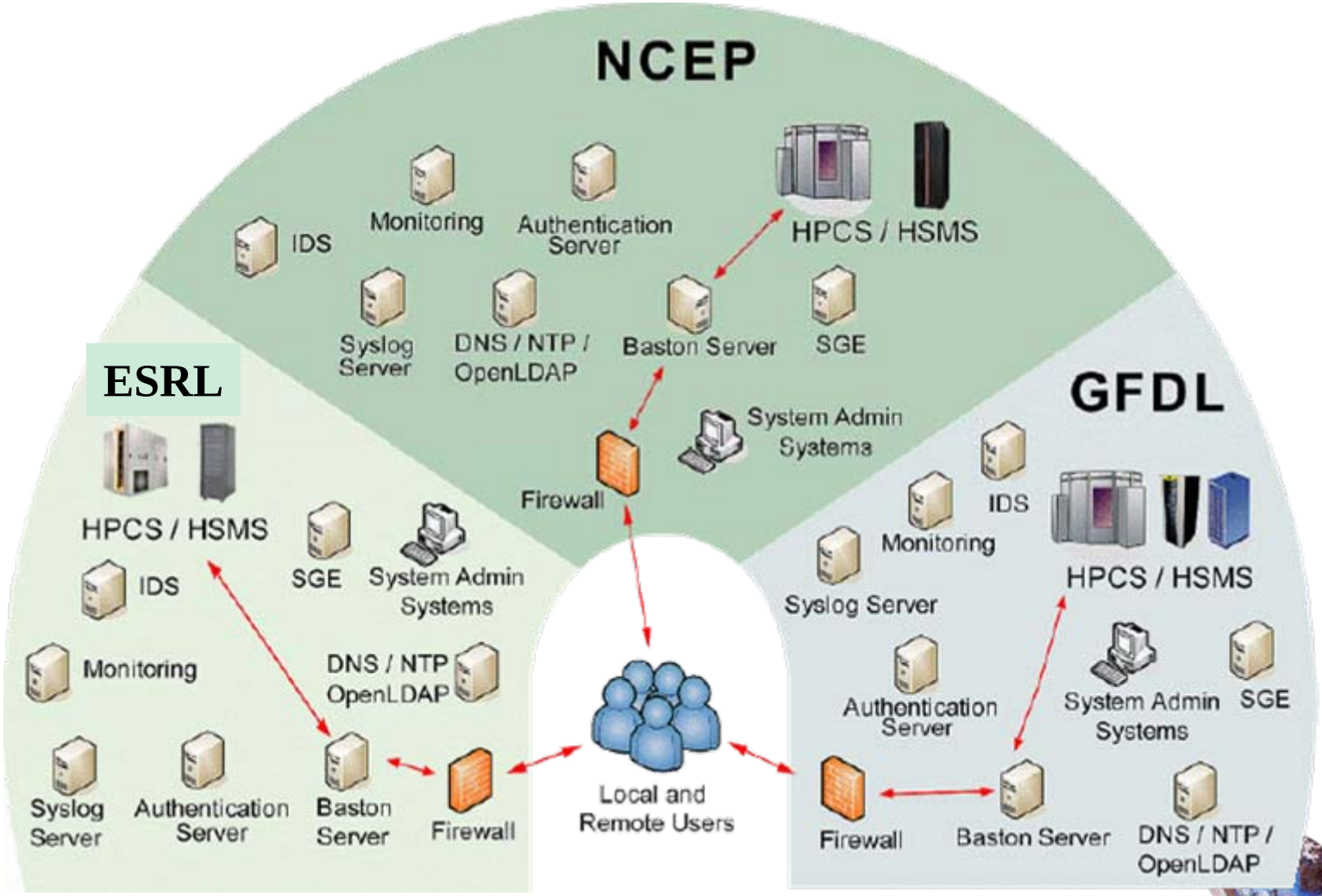
Outline

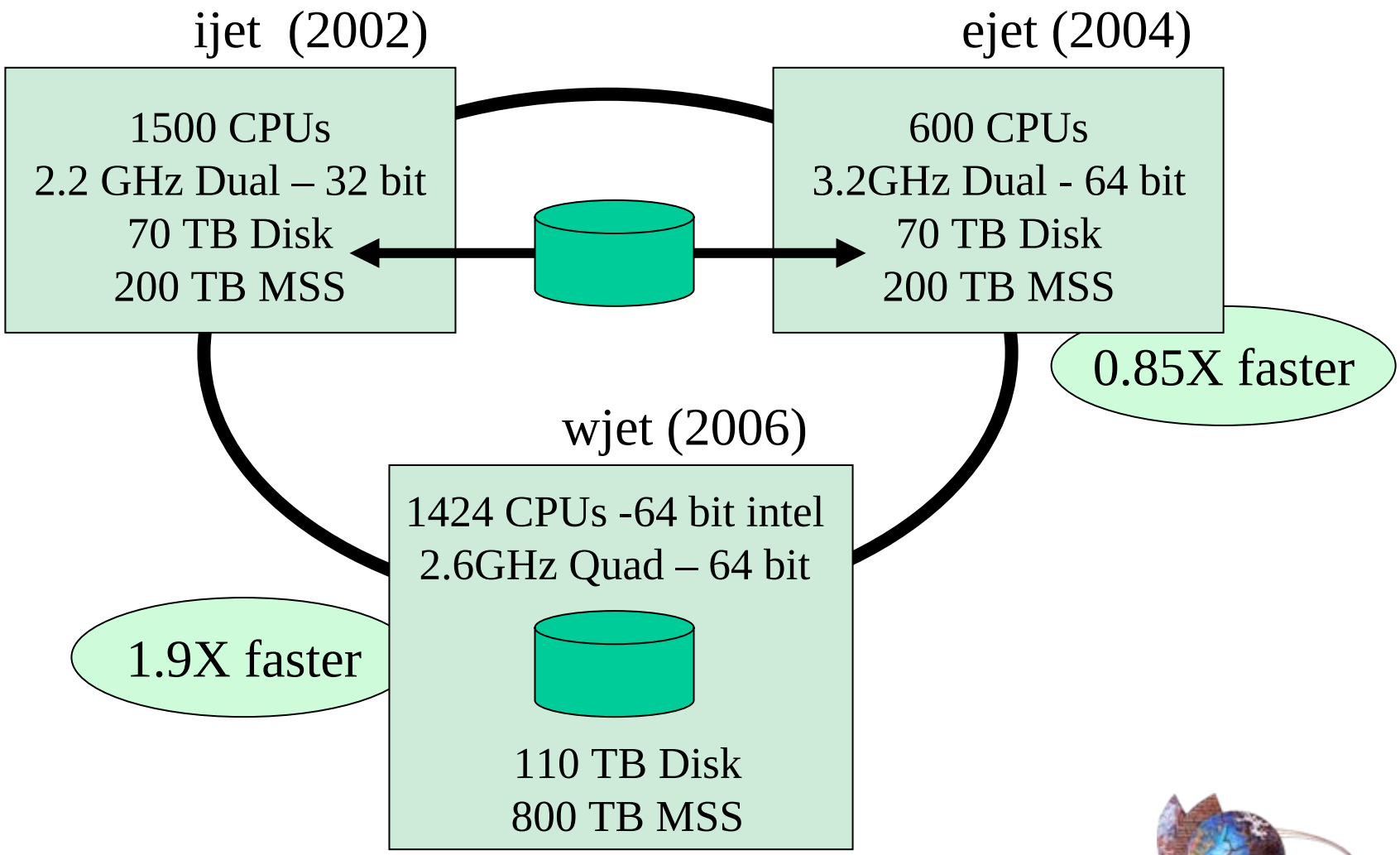
- The NOAA Boulder HPC System
- Parallel Debugging using SMS
- Workflow and Portal Development Activities

The NOAA Boulder HPC System

Merging Toward One Virtual HPC Facility at NOAA



ESRL HPC Facility



Some HPC Projects

- Implementation of the GFDL AM2 Model at CDC
- Properties of Fish Stock-Production Models
- All-Weather Microwave Radiance Assimilation
- Coastal Coupled Air-Sea Modeling
- Regional Climate Impact & Air Quality Experiments
- Global CO2 Assimilation and Flux Estimates
- Climate and Role of the Thermohaline Circulation
- Coastal Remote Sensing
- CSD WRF-Chem model
- Developmental Testbed Center
- ENSO and Beyond
- Studies of Pacific ENSO Variability
- ETL Cloud Model Conversion
- Integrated Feature Oriented Regional Modeling
- Toward an Improved Seasonal Prediction
- Great Lakes Regional Coupled Modeling
- Remote Sensing in Vietnam Waters
- Earth Magnetic Model
- THORPEX Data Assimiliation using NCEP & GFDL Models
- Modelling of ABL Processes over Complex Terrain
- Ensemble Forecasts with Stochastic Radiation
- Mesoscale Ensemble Forecast
- Coastal Modeling
- MMAP Hydrodynamic Model Development
- accounting for model error in ensemble DA
- Creating MODIS Data time series
- 2000 New England Air Quality Study
- Nested Ocean Models for the Northeast Pacific
- Reanalysis Without Radiosondes
- Regional Environmental Modeling
- Stratosphere-Troposphere Exhcange Study
- Predict Seasonal to Decadal Stormtrack Anomalies
- Space Weather Reanalysis
- 2000 Texas Air Quality Study
- WRF-Chem development
- Hybrid ensemble-3DVAR data assimilation on WRF
- WRF Simulations of MCS Rainfall
- Arctic Ocean Modeling and Global Climate Studies

ESRL System Characteristics

- High number of jobs
  - Thousands of jobs strains the SGE scheduler
  - Project allocations but no accounting
    - This will change as system load increases
- Parallel job requirements
  - Many require small number of PEs
  - Some require 100+
  - A few require >256
  - None above 500 PEs but that will be changing

Parallel Debugging using SMS

Scalable Modeling System
1988 - present

Leslie Hart

Tom Henderson

Mark Govett

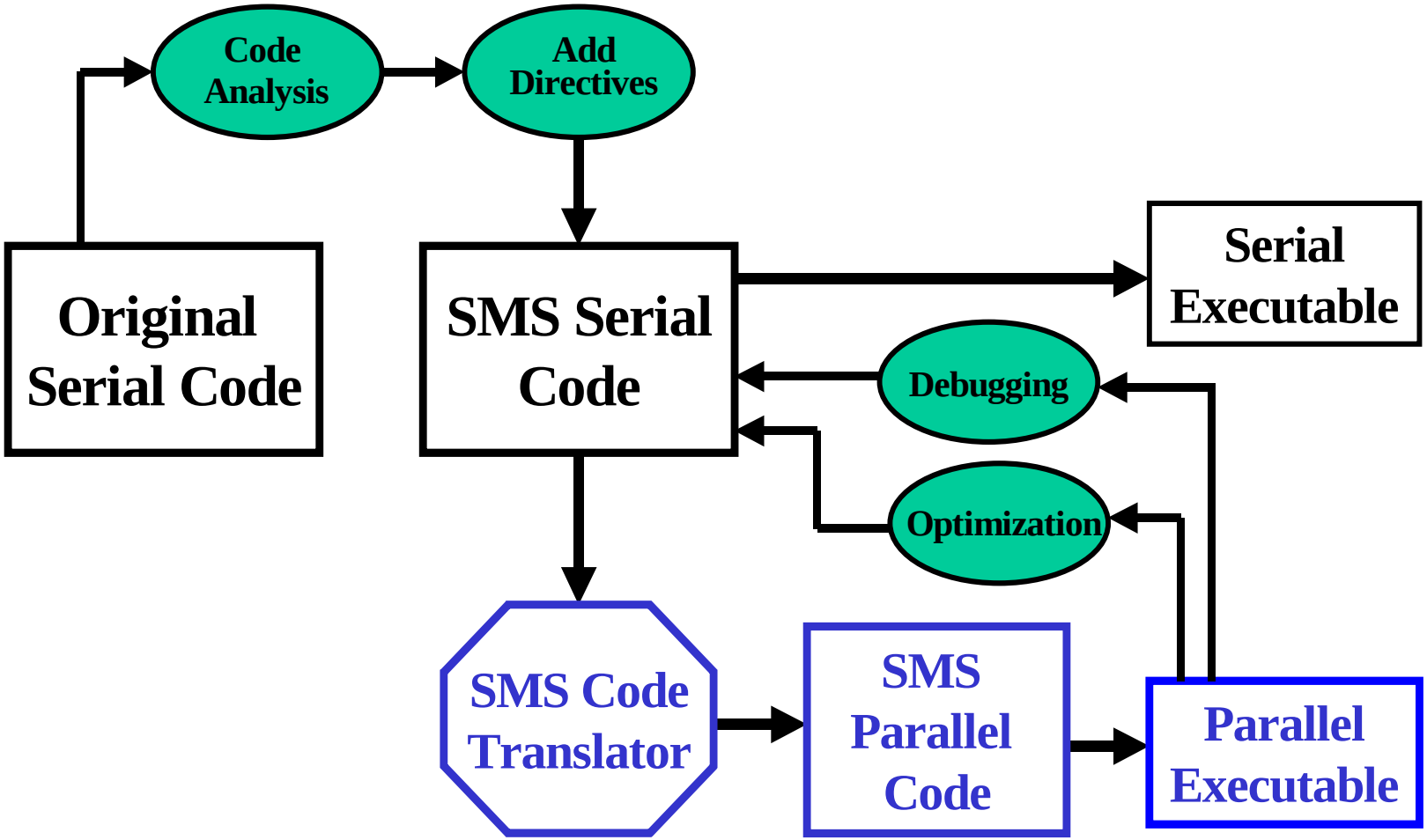
Jacques Middlecoff

Dan Schaffer

SMS Overview

- User adds directives to serial code
- SMS translates directives/serial code into parallel code
- Resulting parallel code runs efficiently on shared or distributed memory machines
- Parallelized many weather, ocean models including RUC, Eta and ROMS, POM
- Powerful debugging directives facilitate parallelization

Code Parallelization with SMS



SMS Debugging Support

- Run serial vs. parallel or parallel vs. parallel (different numbers of processes) and compare results on the fly
  - SMS directive

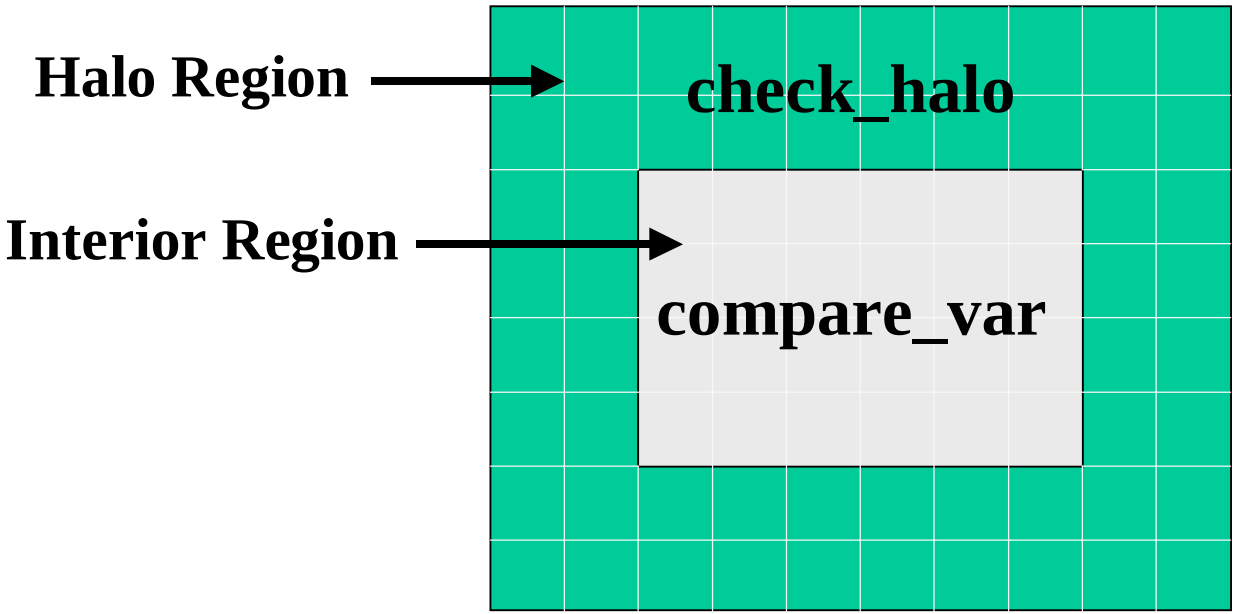
    CSMS$COMPARE_VAR
  - "Bitwise-exact" summations required
    - Round-off error can mask bugs
- Check halo regions
  - SMS directive

    CSMS$CHECK_HALO

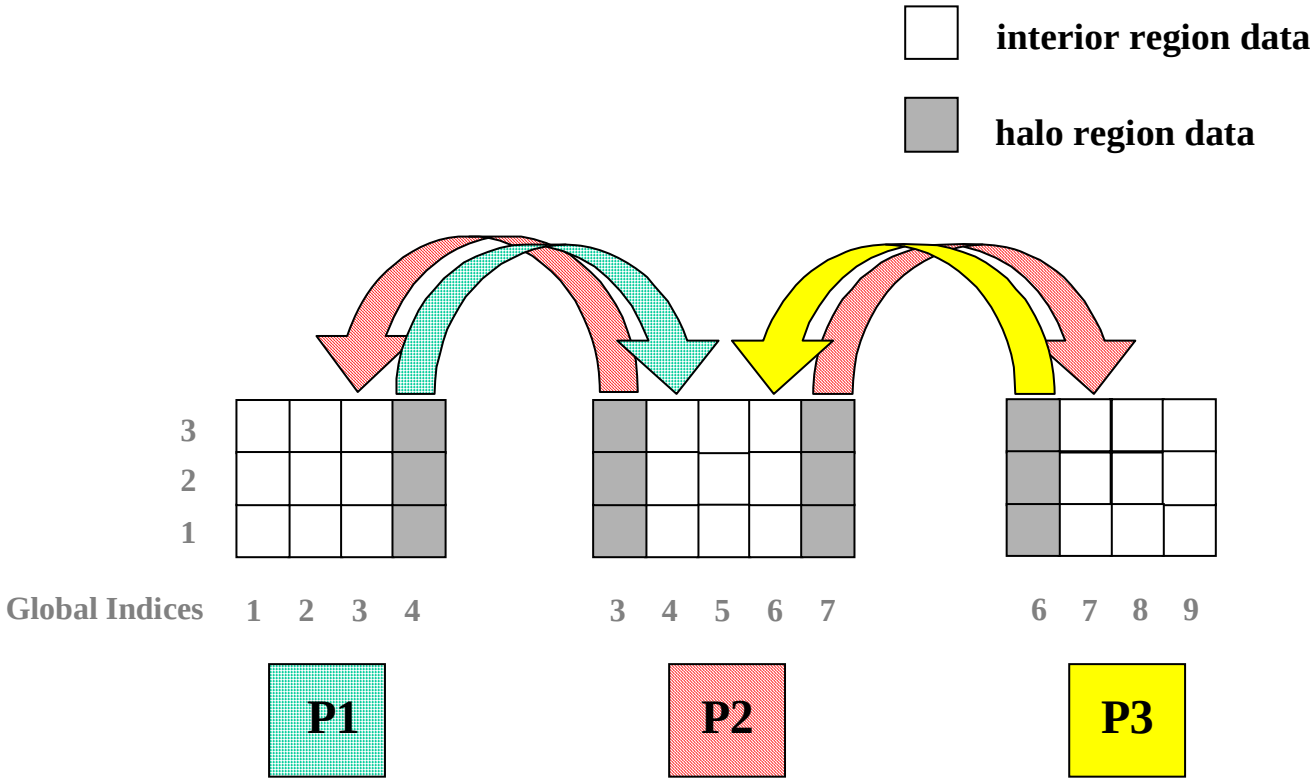
SMS Debugging Directives

Insert directives in the code to verify
array values are correct

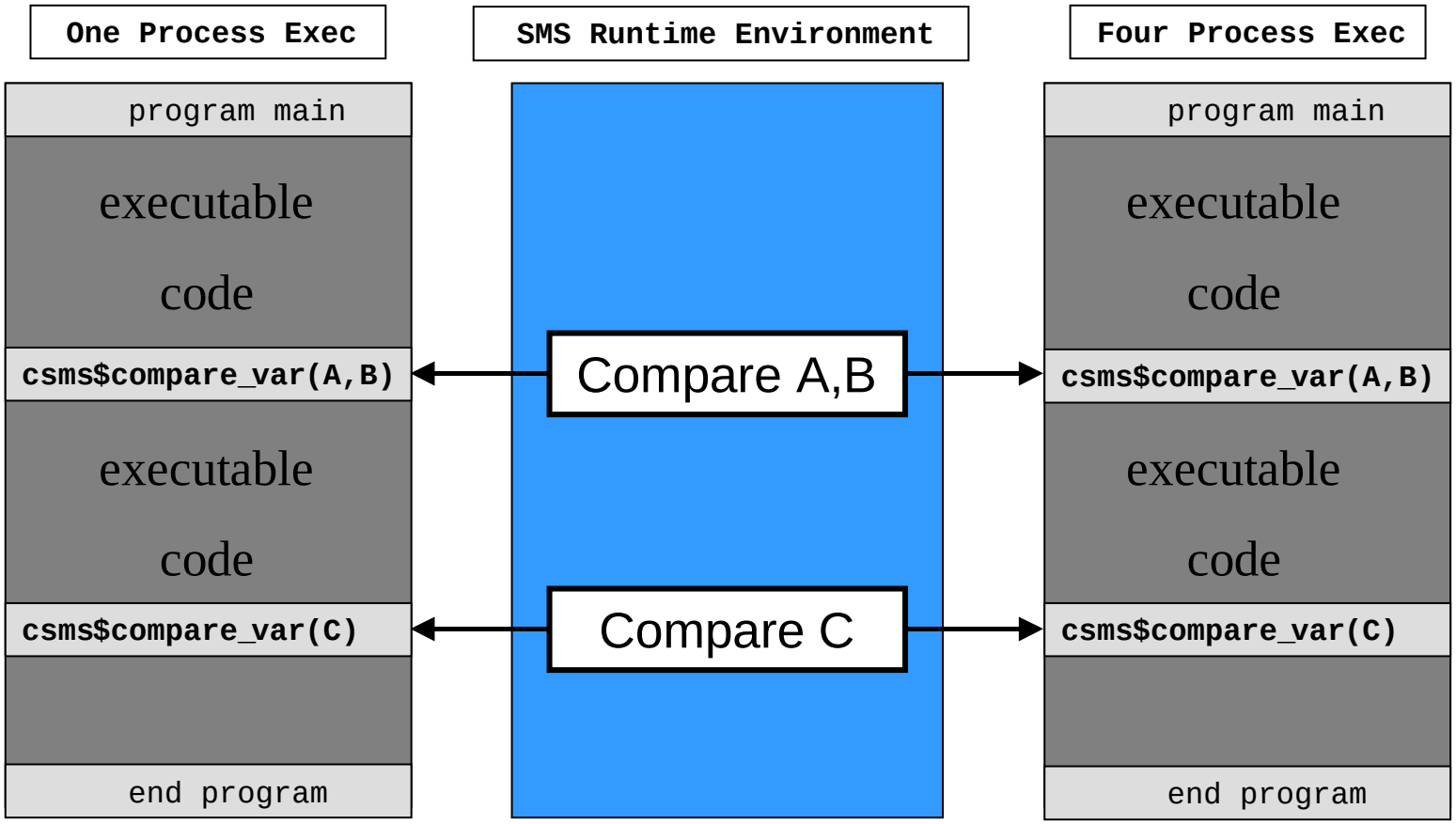
portion of a decomposed array
owned by a single process



CSMS$CHECK_HALO



CSMS$COMPARE_VAR



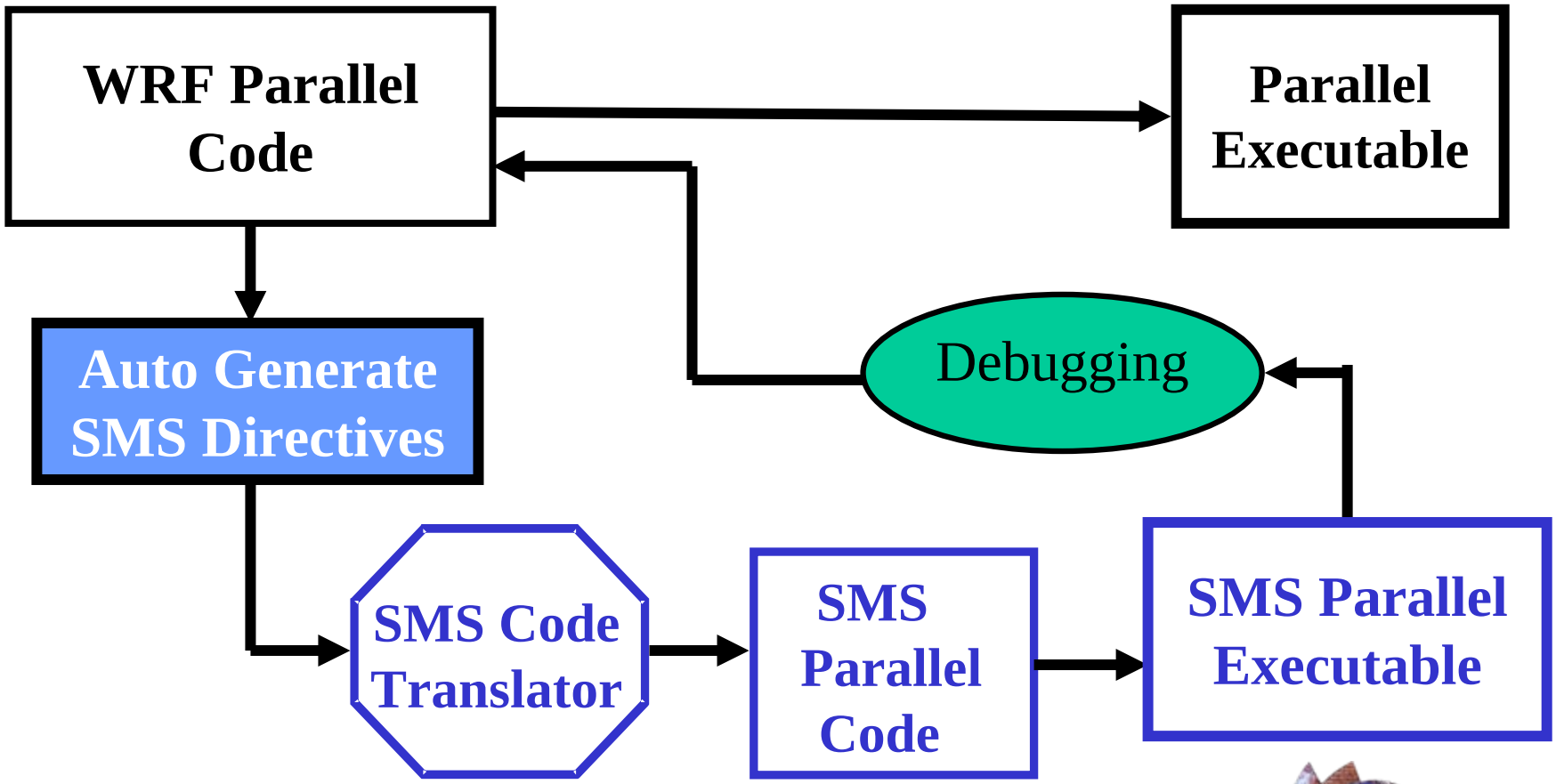
Parallel Debugging Support for WRF

(Govett, Schaffer, Henderson)

- Utilize SMS debugging directives
- Link SMS run-time libraries with WRF
- Build a tool to automatically insert debugging directives in the code
  - where variables that have been updated
  - where horizontal dependencies exist

Status: Work is in progress

SMS Debugging Support for WRF



Workflow and Portal Development

Mark Govett
Chris Harrop
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Jeff Smith

Workflow and Portal Development

- Motivation
  - Developmental Testbed Center (DTC)
    - Collaboration between NOAA, NCEP, ESRL and NCAR, others
    - to evaluate and transfer new modeling capabilities
  - Support Model Development and Observing System Testing
    - Costly systems to build, deploy, and maintain
    - More complex models harder to evaluate

A Typical Scenario at the DTC

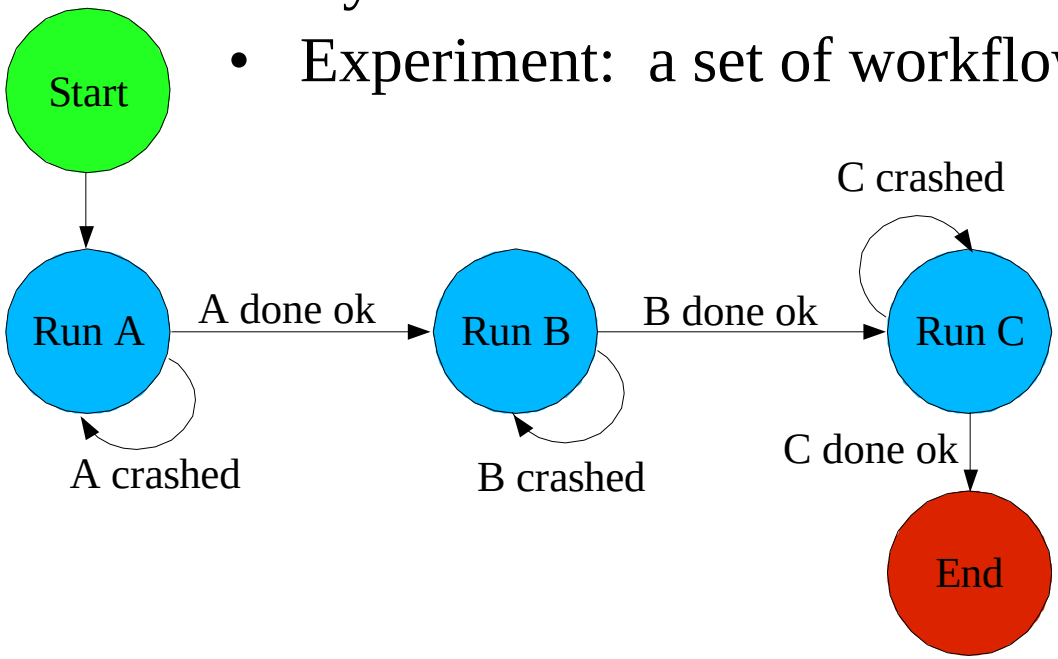
- Investigate the sensitivity of WRF-ARW to the choices of upper dampening depth and cooeficient
- Testing
  - many subtle variations are frequently tried for a single date.
  - Once a couple promising configurations were identified, more extensive tests are run
    - 4 – 30 day seasonal runs, three comparisons, two model variants.
    - Each run takes ~ 7 hours to complete

DTC Requirements

- Need to thoroughly test and evaluate models (user)
  - More complex models, configurations
  - Higher density data sets
  - More observational platforms
- Need to reliably manage the model runs (Workflow Manager)
- Need remote access to NOAA HPC systems (Portal)
- Need a clean way to manage code, scripts and configurations (Portal)
  - Repeat runs, compare configurations
- Need to evaluate results using verification and visualization capabilities

Workflow Manager

- Task: A single unit of computation
- Workflow: a set of tasks and their inter-dependencies
- Cycle: a workflow instantiated for a single date
- Experiment: a set of workflows run over a set of dates



Run Dates

2006020100
2006020112
2006020200
2006020212

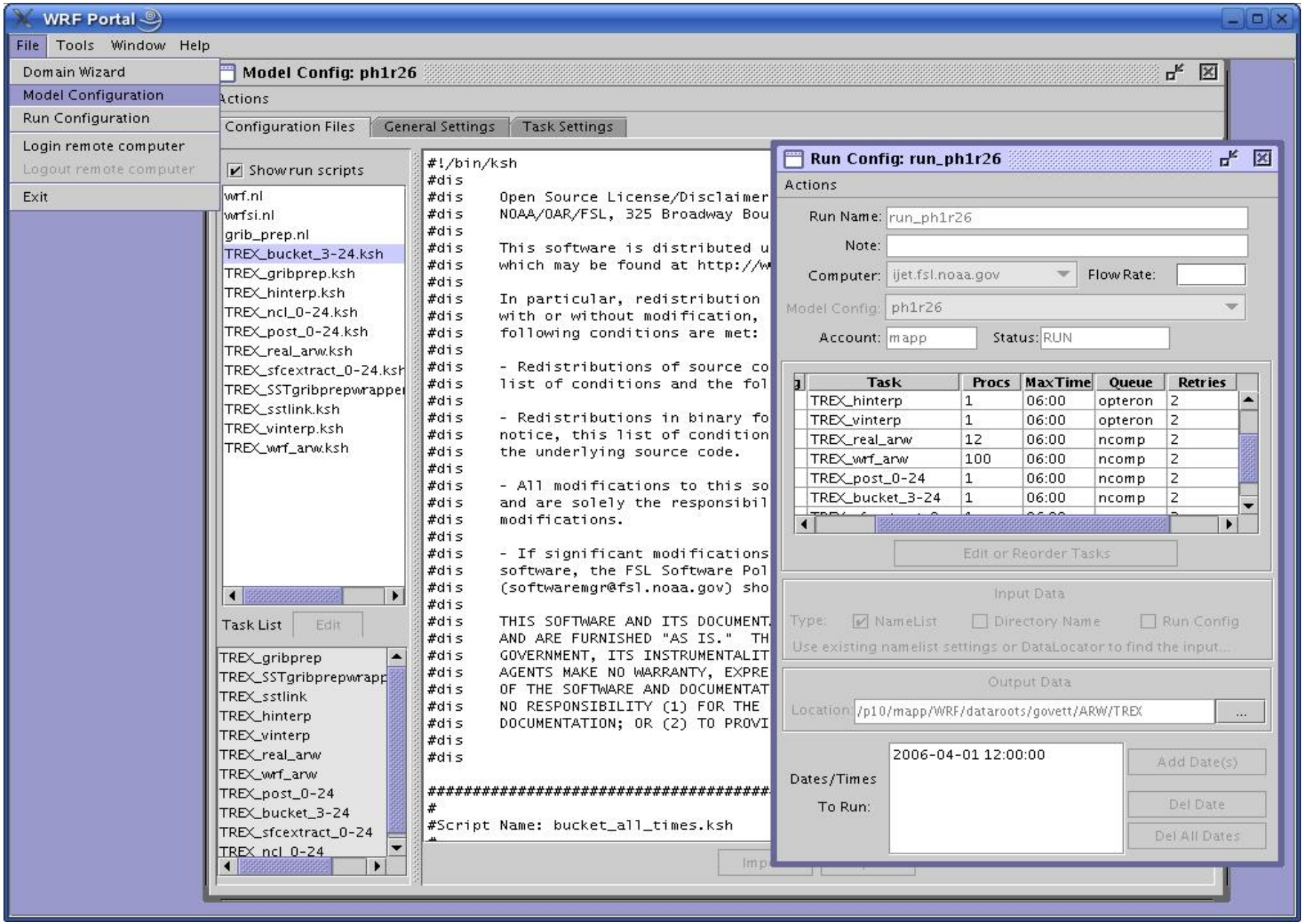
Workflow Manager

- Manages tasks running on a system
  - Automated detection of and recovery from system faults
    - Workflow can automatically resume after extended outages
  - Automatically retry tasks that have failed
  - Throttle option controls the number of tasks that can run simultaneously
  - Flow rate limits the number of cycles running at a time

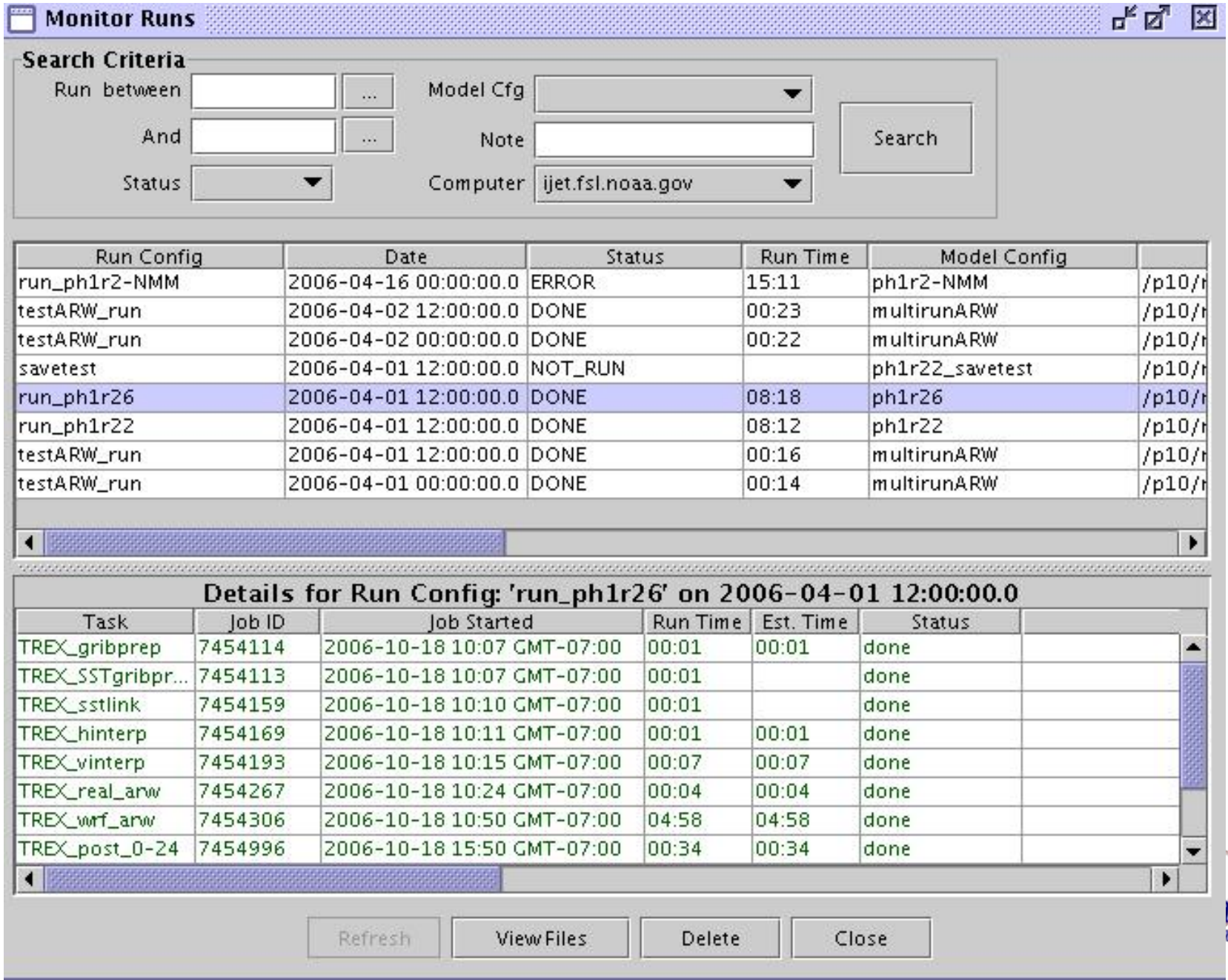
WRF Portal Development

- Java Web-Start Application
- Beta-testing at the DTC
- Key Features
  - Define Tasks
    - Users can select and edit their own scripts, namelists, executables, etc
  - Define and configure workflows
  - Monitor experiment while running
  - Analyze results, diagnose errors

WRF Portal: Workflow Configuration



WRF Portal: Workflow Monitoring



Conclusion

- ESRL is working on a variety of HPC projects to which address new advancements in HPC including:
  - Java application to manage model development
  - Porting codes to new HPC systems
  - Debugging tool to simplify parallel code development and maintenance