

Outline

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

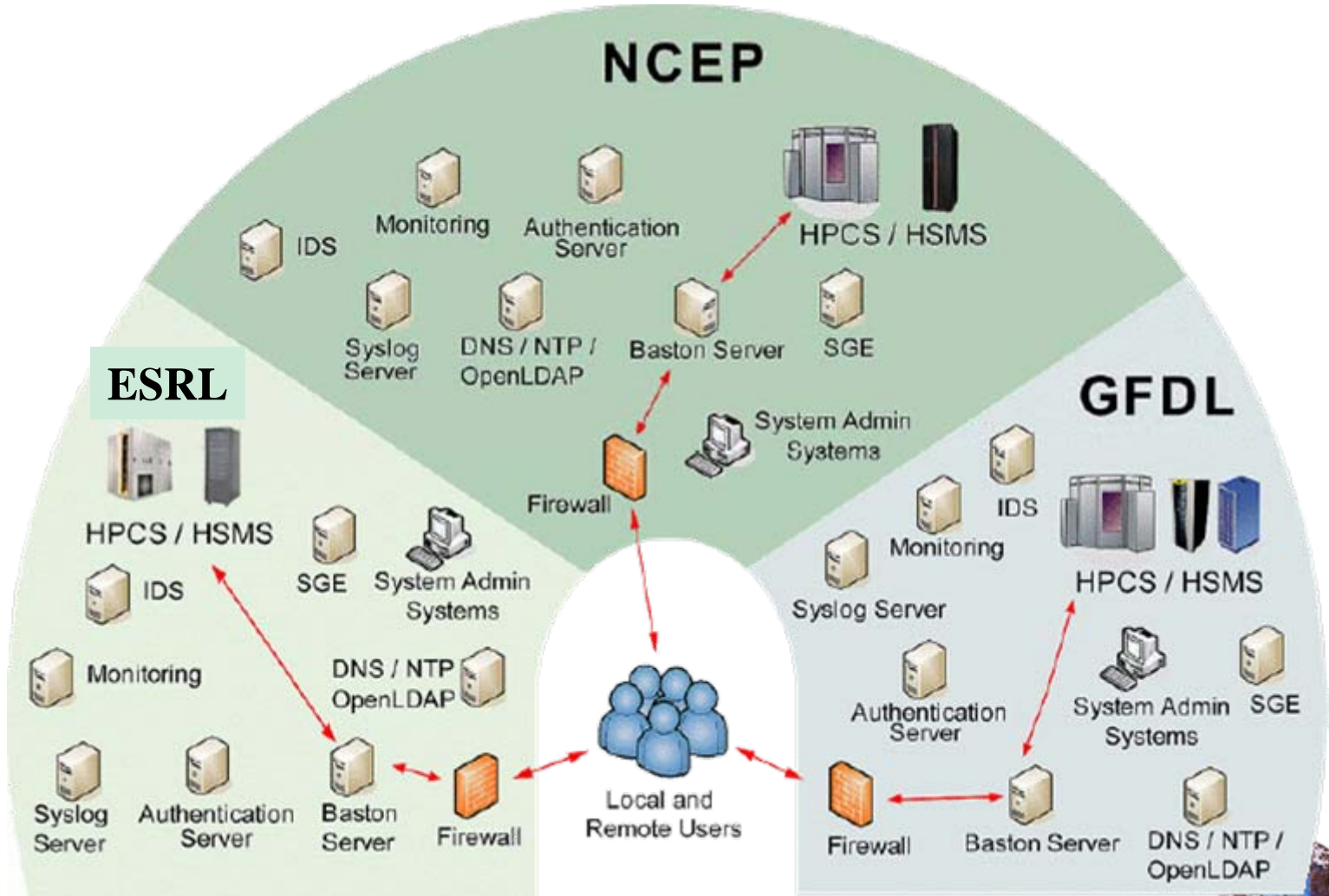
The NOAA Boulder HPC System

October 2006

Use of High Performance Computing
In Meteorology



Merging Toward One Virtual HPC Facility at NOAA

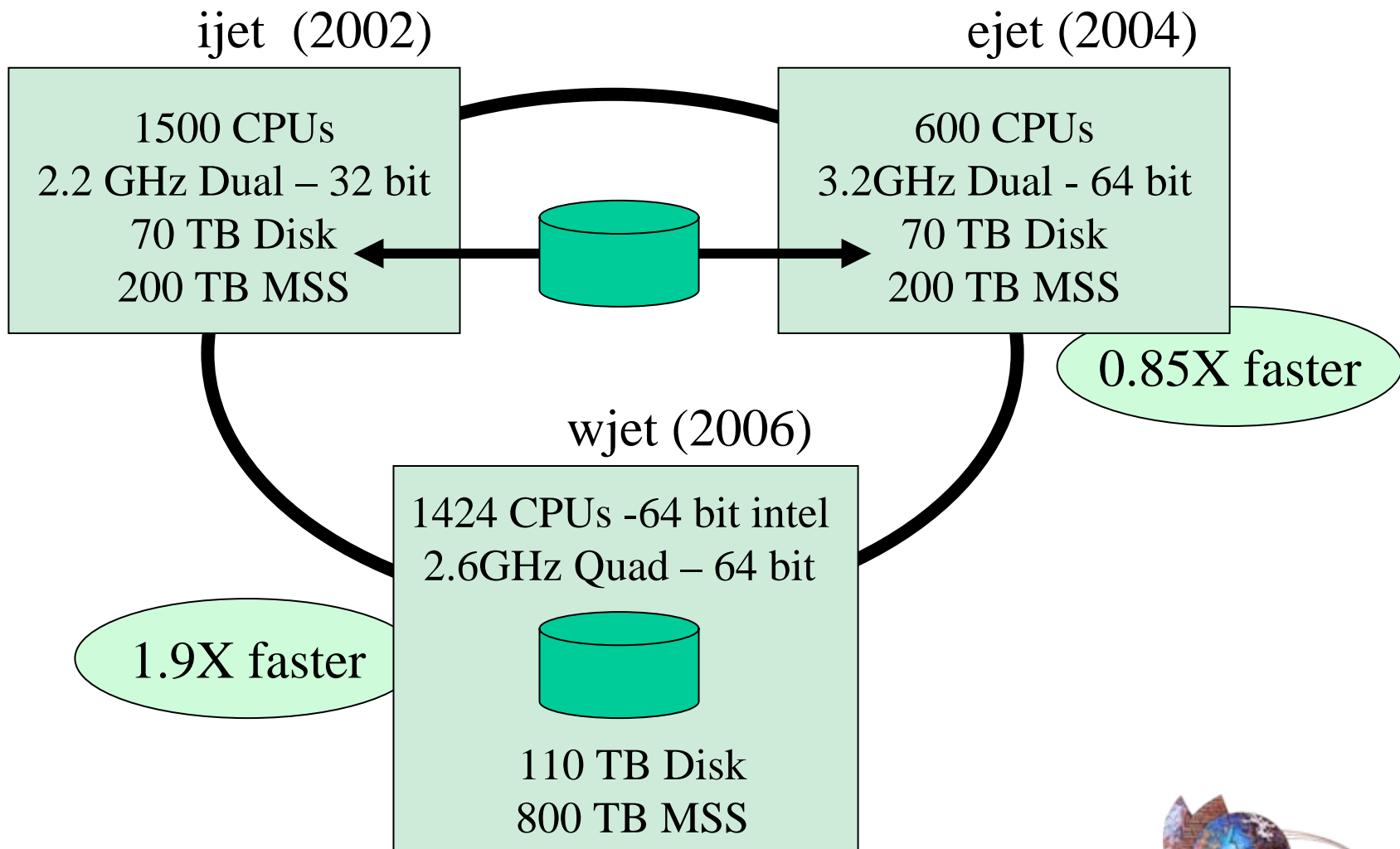


Use of High Performance Computing
In Meteorology

October 2006



ESRL HPC Facility



Use of High Performance Computing
In Meteorology



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 Assimilation 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 Exchange 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

October 2006

Use of High Performance Computing
In Meteorology



Scalable Modeling System

1988 - present

Leslie Hart

Tom Henderson

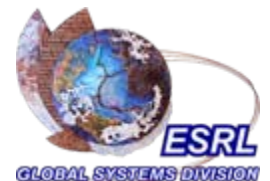
Mark Govett

Jacques Middlecoff

Dan Schaffer

October 2006

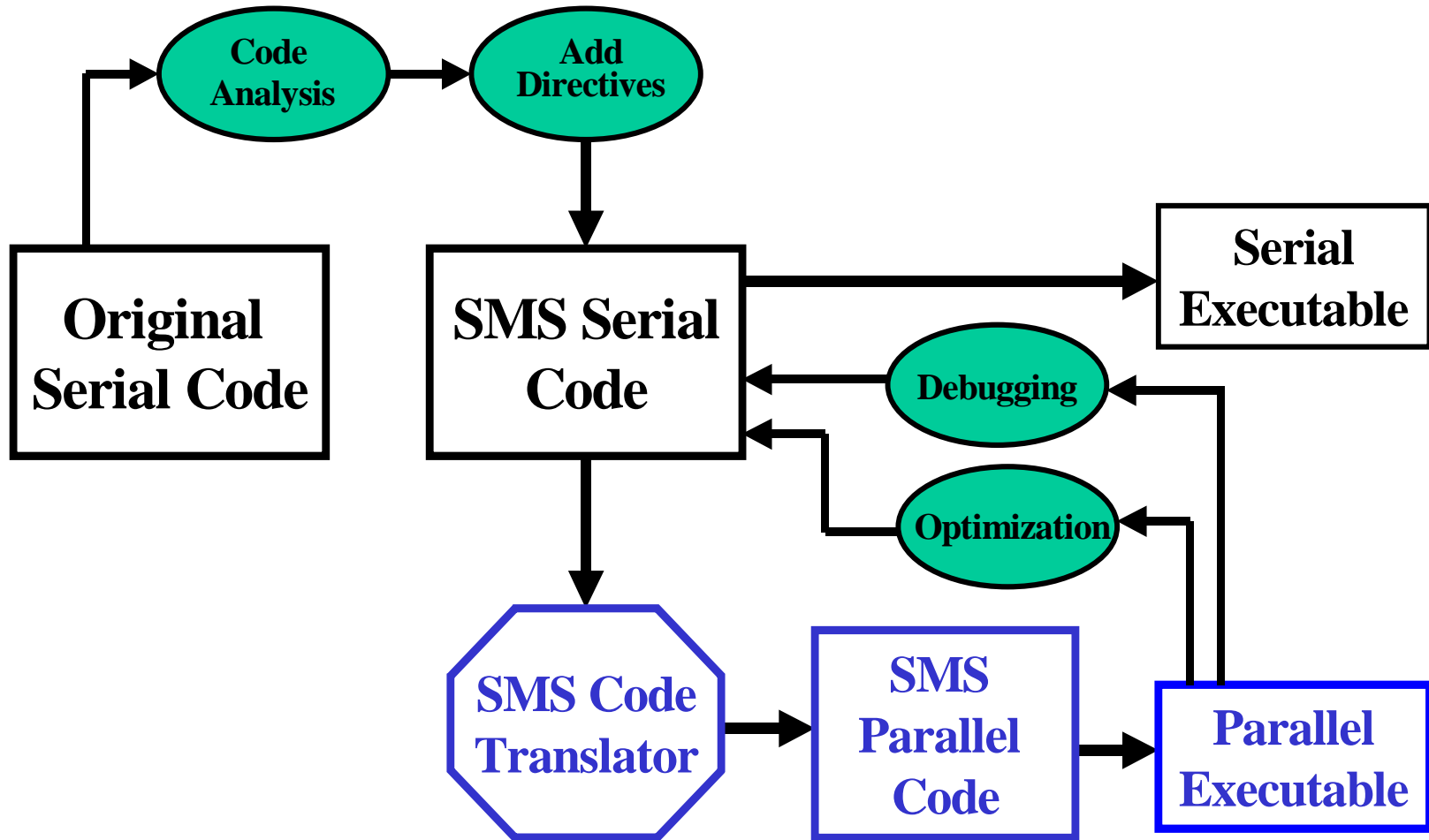
Use of High Performance Computing
In Meteorology



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

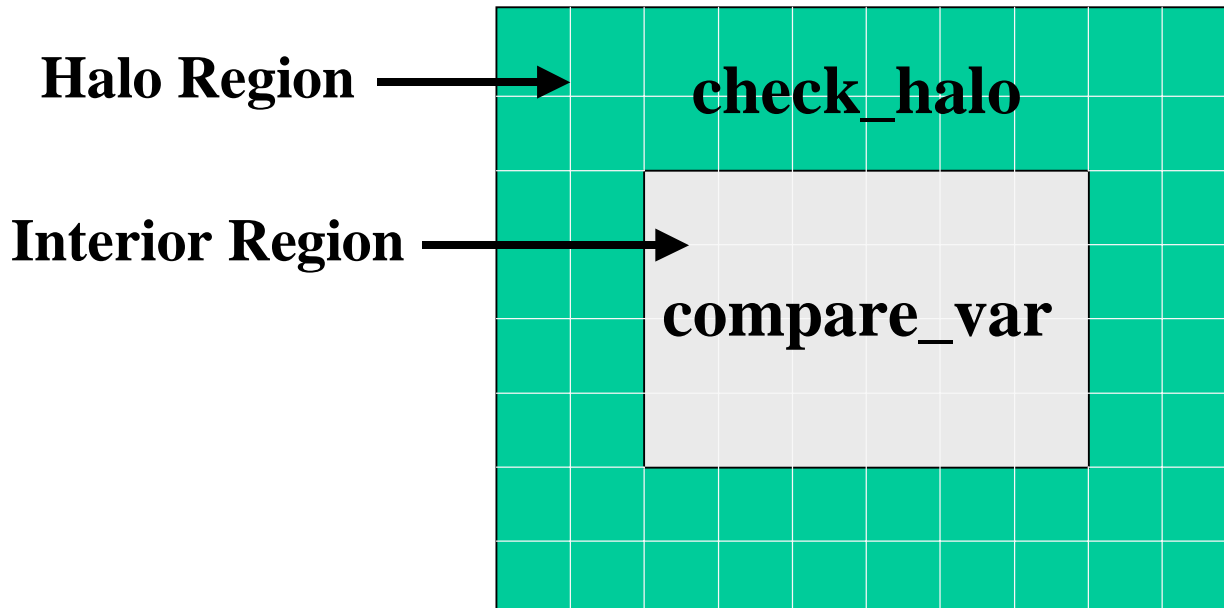
- SMS directive

CSMS\$CHECK_HALO

SMS Debugging Directives

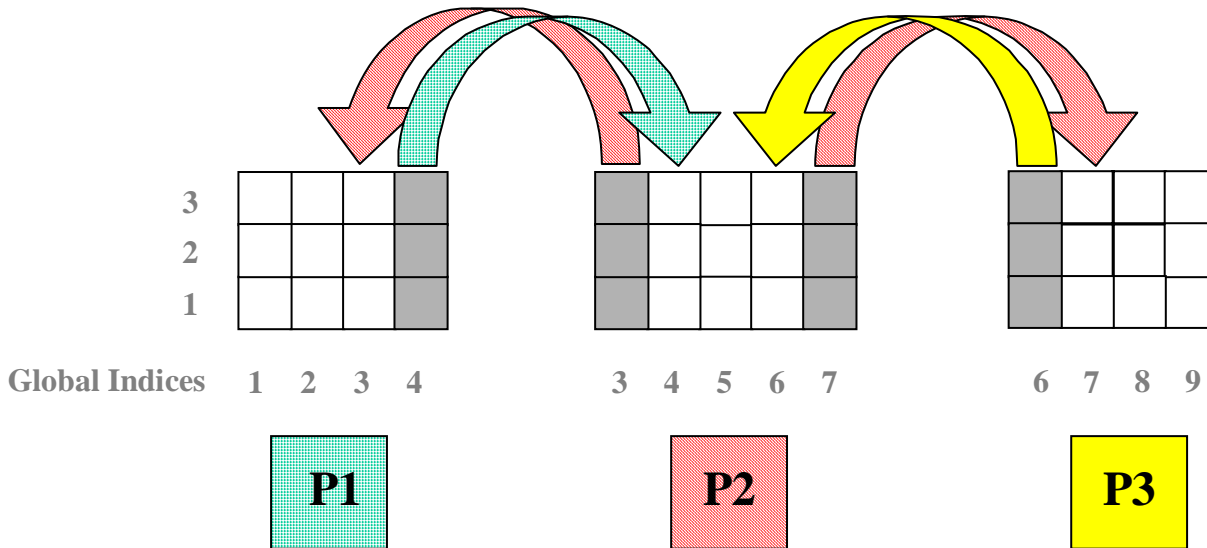
Insert directives in the code to verify
array values are correct

*portion of a decomposed array
owned by a single process*

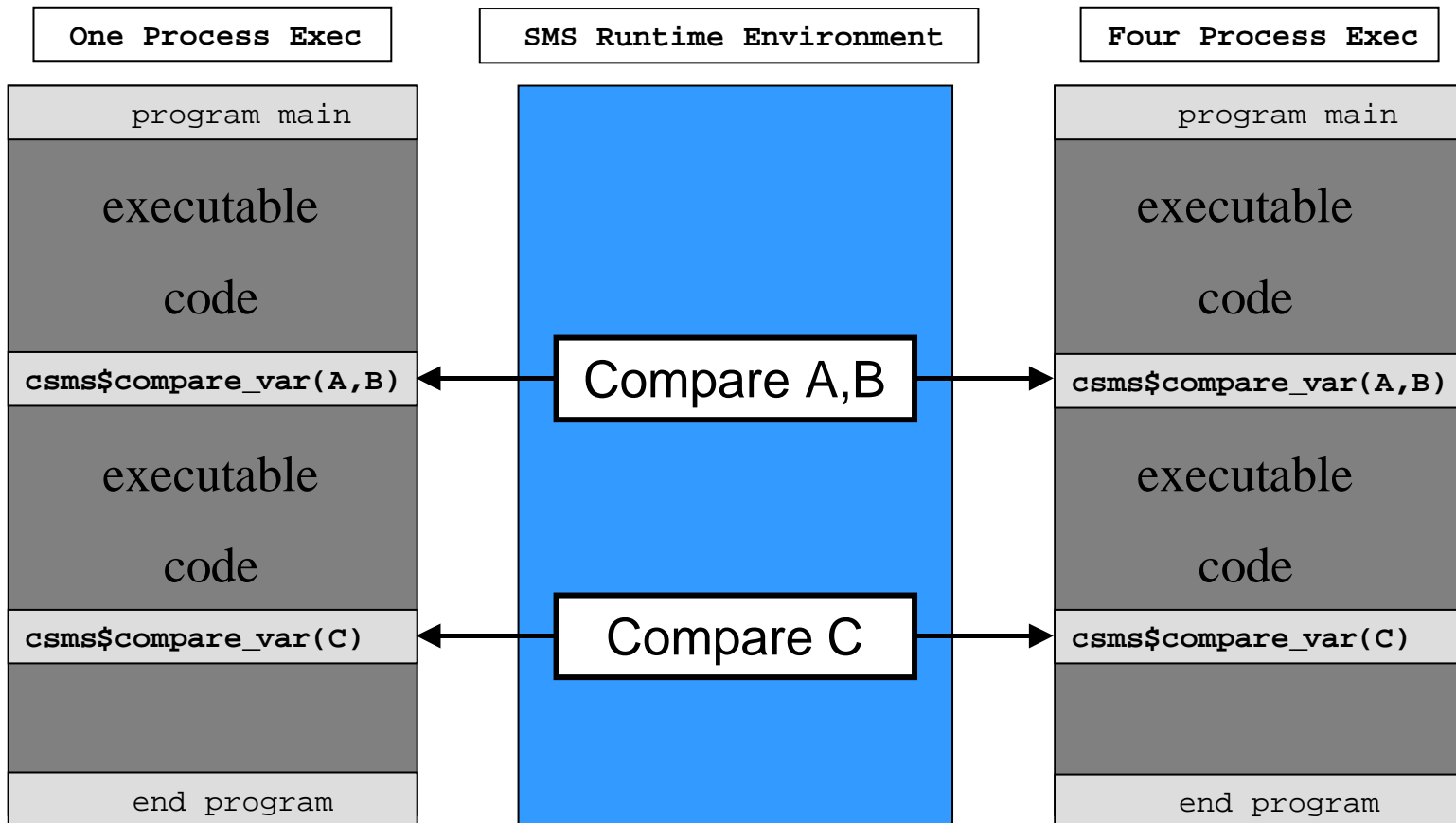


CSMS\$CHECK_HALO

□ interior region data
■ halo region data



CSMS\$COMPARE_VAR



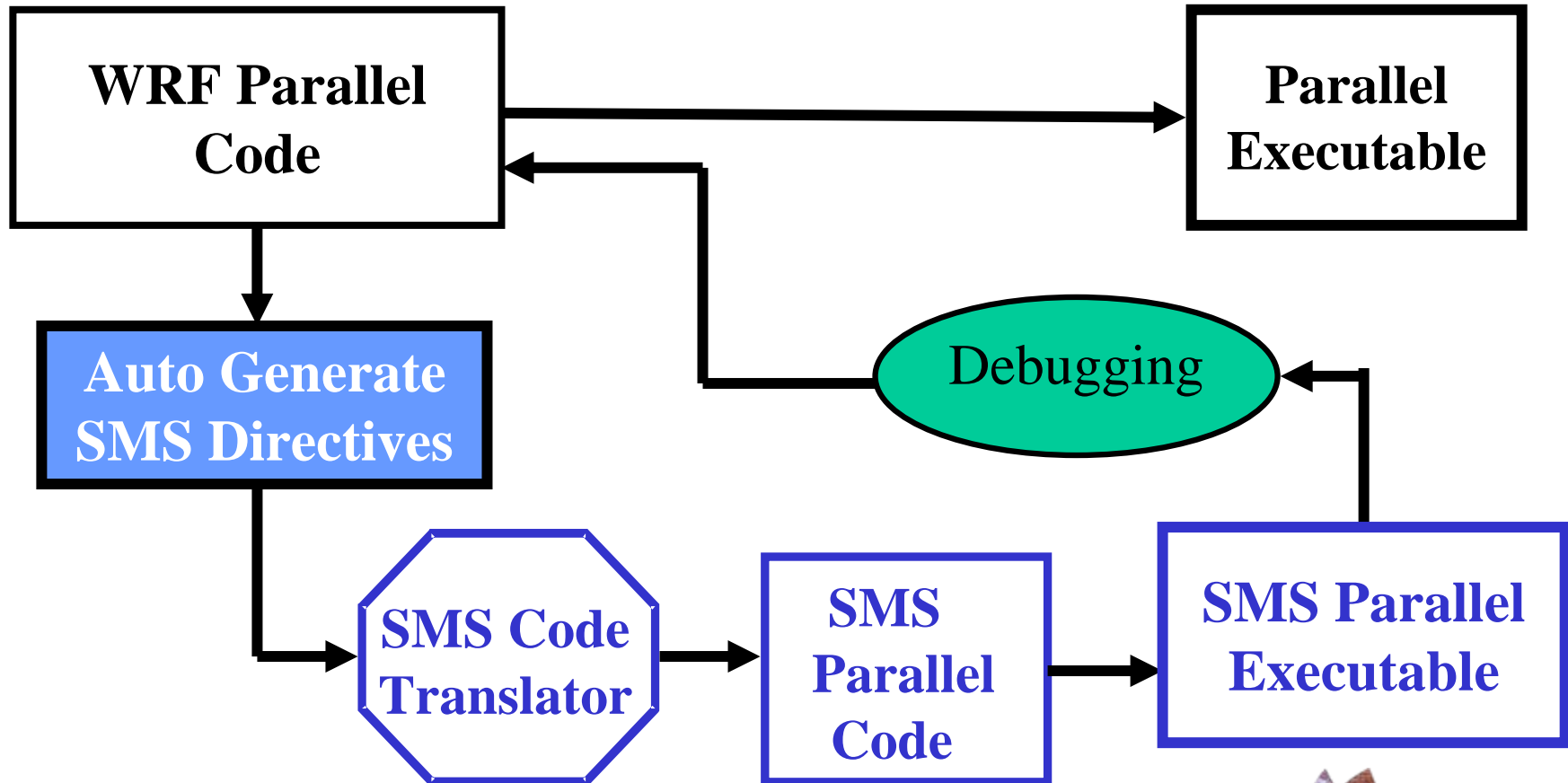
Parallel Debugging Support for WRF

(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
Dan Schaffer
Jeff Smith

October 2006

Use of High Performance Computing
In Meteorology



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

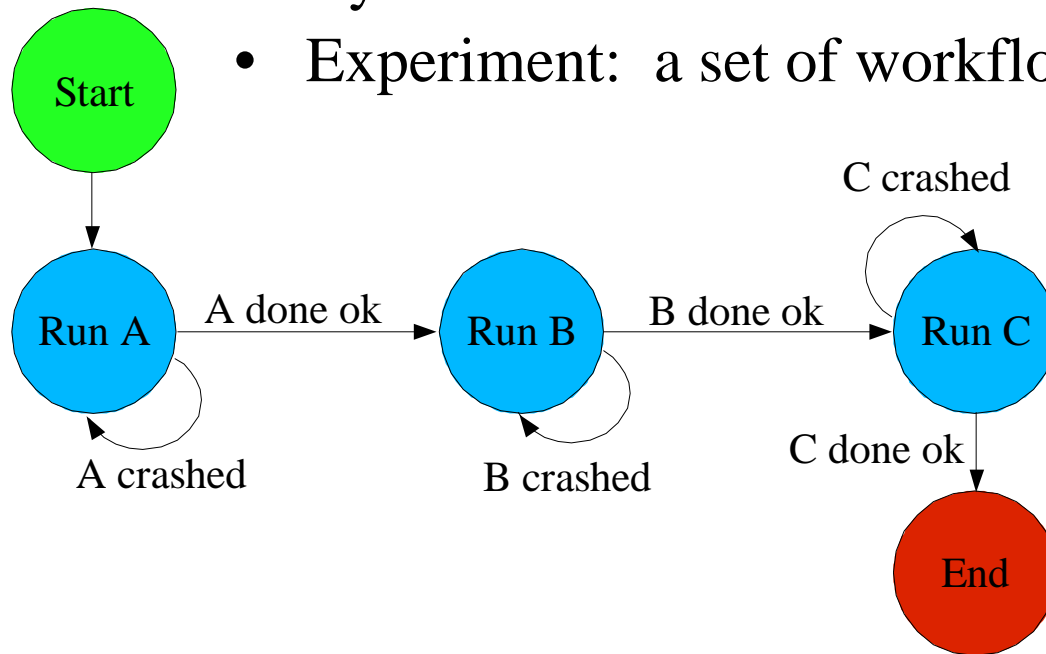
- Investigate the sensitivity of WRF-ARW to the choices of upper dampening depth and coefficient
- Testing
 - many subtle variations are frequently tried for a single date.
 - Once a couple promising configurations were identified, more extensive tests are run
 - 4 – 30 day seasonal runs, three comparisons,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



<u>Run Dates</u>
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

The screenshot displays the WRF Portal interface with the following components:

- Menu Bar:** File, Tools, Window, Help
- Left Panel:**
 - Domain Wizard
 - Model Configuration
 - Run Configuration
 - Login remote computer
 - Logout remote computer
 - Exit
- Model Config: ph1r26**
 - Configuration Files
 - General Settings
 - Task Settings
 - Showrun scripts
 - Task List (with Edit button)
- Script Content:**

```
#!/bin/ksh
#dis
#dis Open Source License/Disclaimer
#dis NOAA/OAR/FSL, 325 Broadway Bou
#dis
#dis This software is distributed u
#dis which may be found at http://w
#dis
#dis In particular, redistribution
#dis with or without modification,
#dis following conditions are met:
#dis
#dis - Redistributions of source co
#dis list of conditions and the fol
#dis
#dis - Redistributions in binary fo
#dis notice, this list of condition
#dis the underlying source code.
#dis
#dis - All modifications to this so
#dis and are solely the responsibil
#dis modifications.
#dis
#dis - If significant modifications
#dis software, the FSL Software Pol
#dis (softwaremgr@fsl.noaa.gov) sho
#dis
#dis THIS SOFTWARE AND ITS DOCUMENT
#dis AND ARE FURNISHED "AS IS." TH
#dis GOVERNMENT, ITS INSTRUMENTALIT
#dis AGENTS MAKE NO WARRANTY, EXPRE
#dis OF THE SOFTWARE AND DOCUMENTAT
#dis NO RESPONSIBILITY (1) FOR THE
#dis DOCUMENTATION; OR (2) TO PROVI
#dis
#####
#
#Script Name: bucket_all_times.ksh
#
```
- Run Config: run_ph1r26**
 - Run Name: run_ph1r26
 - Note:
 - Computer: ijet.fsl.noaa.gov
 - Flow Rate:
 - Model Config: ph1r26
 - Account: mapp
 - Status: RUN
 - Task List Table:

Task	Procs	MaxTime	Queue	Retries
TREX_hinterp	1	06:00	opteron	2
TREX_vinterp	1	06:00	opteron	2
TREX_real_arw	12	06:00	ncomp	2
TREX_wrf_arw	100	06:00	ncomp	2
TREX_post_0-24	1	06:00	ncomp	2
TREX_bucket_3-24	1	06:00	ncomp	2

Additional Run Config details:

- Input Data:
 - Type: NameList Directory Name Run Config
 - Use existing namelist settings or DataLocator to find the input...
- Output Data:
 - Location: /p10/mapp/WRF/dataroots/govett/ARW/TREX
 - Dates/Times: 2006-04-01 12:00:00
 - To Run: [Add Date(s), Del Date, Del All Dates]

WRF Portal: Workflow Monitoring

Monitor Runs

Search Criteria

Run between ... Model Cfg ▼

And ... Note

Status ▼ Computer ▼

Run Config	Date	Status	Run Time	Model Config	
run_ph1r2-NMM	2006-04-16 00:00:00.0	ERROR	15:11	ph1r2-NMM	/p10/t
testARW_run	2006-04-02 12:00:00.0	DONE	00:23	multirunARW	/p10/t
testARW_run	2006-04-02 00:00:00.0	DONE	00:22	multirunARW	/p10/t
savetest	2006-04-01 12:00:00.0	NOT_RUN		ph1r22_savetest	/p10/t
run_ph1r26	2006-04-01 12:00:00.0	DONE	08:18	ph1r26	/p10/t
run_ph1r22	2006-04-01 12:00:00.0	DONE	08:12	ph1r22	/p10/t
testARW_run	2006-04-01 12:00:00.0	DONE	00:16	multirunARW	/p10/t
testARW_run	2006-04-01 00:00:00.0	DONE	00:14	multirunARW	/p10/t

Details for Run Config: 'run_ph1r26' on 2006-04-01 12:00:00.0

Task	Job ID	Job Started	Run Time	Est. Time	Status	
TREX_gribprep	7454114	2006-10-18 10:07 GMT-07:00	00:01	00:01	done	▲
TREX_SSTgribpr...	7454113	2006-10-18 10:07 GMT-07:00	00:01		done	
TREX_sstlink	7454159	2006-10-18 10:10 GMT-07:00	00:01		done	
TREX_hinterp	7454169	2006-10-18 10:11 GMT-07:00	00:01	00:01	done	
TREX_vinterp	7454193	2006-10-18 10:15 GMT-07:00	00:07	00:07	done	
TREX_real_arw	7454267	2006-10-18 10:24 GMT-07:00	00:04	00:04	done	
TREX_wrf_arw	7454306	2006-10-18 10:50 GMT-07:00	04:58	04:58	done	
TREX_post_0-24	7454996	2006-10-18 15:50 GMT-07:00	00:34	00:34	done	▼

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