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

ijet (2002)

- 1500 CPUs
- 2.2 GHz Dual – 32 bit
- 70 TB Disk
- 200 TB MSS

ejet (2004)

- 600 CPUs
- 3.2 GHz Dual - 64 bit
- 70 TB Disk
- 200 TB MSS

wjet (2006)

- 1424 CPUs -64 bit intel
- 2.6GHz Quad – 64 bit
- 110 TB Disk
- 800 TB MSS

0.85X faster

1.9X faster

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

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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

Original Serial Code -> Code Analysis -> Add Directives

SMS Serial Code

SMS Serial Code 

SMS Code Translator

SMS Parallel Code 

Parallel Executable

Serial Executable

Debugging 

Optimization
SMS Debugging Support

• Run serial vs. parallel or parallel vs. parallel (different numbers of processes) and compare results on the fly
  – SMS directive
    \texttt{CSMS\$COMPARE\_VAR}
  – "Bitwise-exact" summations required
    • Round-off error can mask bugs

• Check halo regions
  – SMS directive
    \texttt{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

Halo Region

check_halo

Interior Region

compare_var
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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

WRF Parallel Code

Auto Generate SMS Directives

SMS Code Translator

Debugging

SMS Parallel Code

SMS Parallel Executable

Parallel Executable
Workflow and Portal Development

Mark Govett
Chris Harrop
Dan Schaffer
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 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

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