



# WRF Data Assimilation System

Michael Kavulich Special thanks to: Xin Zhang, Xiang-Yu Huang

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Many slides are borrowed from WRF software lectures





# WRFDA System – Outline

- Introduction
- WRFDA Software Overview
- Computing Overview





# Introduction – What is WRFDA?

- A data assimilation system for the WRF Model (ARW core)
  - 3D- and 4D-VAR, Ensemble, and Hybrid methods
- Designed to be flexible, portable and easily installed and modified
  - Open-source and public domain
  - Can be compiled on a variety of platforms
  - Part of the WRF Software Framework
- Designed to handle a wide variety of data
  - Conventional observations
  - Radar velocity and reflectivity
  - Satellite (radiance and derived data)
  - Accumulated precipitation



#### **WRF Modeling System Flow Chart**









WRFDA in the WRF Modeling System



### **Blue: Supported by WRFDA team**





# WRFDA System – Outline

- Introduction
- WRFDA Software
- Computing Overview

program da\_wrfvar\_main



```
! in (and broadcasting for distributed memory) configuration data, defining
   ! and initializing the top-level domain, either from initial or restart
   ! data, setting up time-keeping, and then calling the da_solve
  ! routine assimilation. After the assimilation is completed,
  ! the model is properly shut down.
   !-----
  use module symbols util, only : wrfu finalize
  use da_control, only : trace_use, var4d
  use da_tracing, only : da_trace_init, da_trace_report, da_trace_entry, &
     da trace exit
  use da_wrf_interfaces, only : wrf_shutdown, wrf_message, disable_quilting
  use da_wrfvar_top, only : da_wrfvar_init1,da_wrfvar_init2,da_wrfvar_run, &
     da_wrfvar_finalize
#ifdef VAR4D
  use da 4dvar, only : clean 4dvar, da finalize model
#endif
  implicit none
   ! Split initialisation into 2 parts so we can start and stop trace here
  call disable_quilting
  call da_wrfvar_init1
  if (trace_use) call da_trace_init
  if (trace_use) call da_trace_entry("da_wrfvar_main")
  call da_wrfvar_init2
  call da_wrfvar_run
  call da wrfvar finalize
#ifdef VAR4D
  if (var4d) then
     call clean 4dvar
     call da_finalize_model
  end if
#endif
  call wrf_message("*** WRF-Var completed successfully ***")
  if (trace use) call da trace exit("da wrfvar main")
  if (trace_use) call da_trace_report
  call wrfu finalize
  call wrf shutdown
end program da wrfvar main
```

! Purpose: Main program of WRF-Var. Responsible for starting up, reading





### WRFDA Directory structure

arch		
clean	build	
compile >	·	
configure	scripts	
dyn_em		
dyn_exp		
external		
frame		
inc		
main		
Makefile		
phys	README file with information	about WREDA
README . DA		
Registry 👡	Contains modiations more	
run	Comuns registry.var	
share		
test		Legend•
tools	WREDA source	Blue – directory
var 🔶 🚽		Green – script file
	code directory	Grav – other text file





# WRFDA/var Directory structure

build <	Executables built here
convertor	
da 🗧	WRFDA source code contained here
external	Source code for external libraries (CRTM, BUFR, etc.)
gen_be	GEN_BE source code
graphics	
Makefile	
obsproc	OBSPROC source code
README.basics	
README.namelist	More README files with
<b>README.radiance</b>	useful information
run 🔶 🗌	Useful runtime files (mostly for radiance)
scripts	
test 🧲	Data for tutorial cases

Legend: Blue – directory Green – script file Gray – other text file







registry.var

- Hierarchical software architecture
  - Insulate scientists' code from parallelism and other architecture/implementation-specific details
  - Well-defined interfaces between layers, and external packages for communications, I/O.







registry.var

- Registry: an "Active" data dictionary
  - Tabular listing of model state and attributes
  - Large sections of interface code generated automatically
  - Scientists manipulate model state simply by modifying Registry, without further knowledge of code mechanics
  - **registry.var** is the dictionary for WRFDA







#### Registry

- Driver Layer
  - Domains: Allocates, stores, decomposes, represents abstractly as single data objects







Registry

- Minimization/Solver Layer
  - Minimization/Solver routine, choose the function based on the namelist variable, 3DVAR, 4DVAR, FSO or Verification, and choose the minimization algorithm.







Registry

- Observation Layer
  - Observation interfaces: contains the gradient and cost function calculation subroutines for each type of observations.





# Call Structure Superimposed on Architecture

da\_sound.f90(da\_sound)





### WRFDA broken down by process











### Input files: Namelist

- File name: namelist.input
- Specifies Input/Output options, domain details, types of observations to assimilate and how to assimilate them
- Allows user great flexibility to change the usage of WRFDA without having to recompile
- A large number (>1000) of namelist options govern the running of WRFDA; however, users will typically only be concerned with setting a few dozen of these
- More details can be found in the User's Guide





# Input files: x<sub>b</sub> (background)

- File name: fg
- Can be either a WRF input file created by WPS and real.exe, or a WRF output file from a forecast.



# Input files: y (observations) and R (observation errors)

- File name: ob.ascii, amsua.bufr, ob01.rain, etc.
- WRFDA accepts a wide variety of observations in several different formats
  - OBSPROC ASCII format (surface, sounding, GPS, etc.)
  - PREPBUFR format (surface, sounding, etc.)
  - BUFR format (radiance)
  - Other ASCII format (radar, precipitation)
- Observation errors are either provided in the observation file, or standard errors (file name: obserr.txt) are used.





# Input files: B (background error)

- File name: be.dat
- This is a binary file containing background error information
  - cv\_options=3 NCEP background error formulation
    - File provided with WRFDA code
    - Not recommended: should be used with caution
  - cv\_options=5 NCAR background error formulation
    - File created using gen\_be utility
    - Recommended option
  - cv\_options=6; Multivariate Background Error (MBE) statistics
    - Not officially supported



### WRFDA broken down by process







### **Read namelist**









### Read namelist

- Read user-specified options from namelist.input
- Set default values for options *not* specified in the namelist
- Perform consistency checks between namelist options

#### Calling order:

da\_wrfvar\_main ==> call da\_wrfvar\_init1, da\_wrfvar\_init2 ==> call initial\_config

#### Calling subroutines:

da\_wrfvar\_main.f90 ==> da\_wrfvar\_init1.inc, da\_wrfvar\_init2.inc ==> module\_configure.F



### Set up framework









### Set up framework

- Utilize WRF Software Framework distributed memory capability to allocate and configure the domain
- Allocate needed memory, initializes domain and tile dimensions, etc.
- Create output files

#### Calling order:

da\_wrfvar\_main ==> call da\_wrfvar\_init2 ==> call alloc\_and\_configure\_domain da\_wrfvar\_main ==> call da\_wrfvar\_run.inc ==> call da\_wrfvar\_interface ==> call da\_solve ==> call da\_solve\_init

### Calling subroutines:

da\_wrfvar\_main.f90 ==> da\_wrfvar\_init2.inc ==> module\_domain.F da\_wrfvar\_main.f90 ==> da\_wrfvar\_run.inc ==> da\_wrfvar\_interface.inc ==> da\_solve.inc ==> da\_solve\_init.inc



### Set up background









### Set up background

- Read the first-guess file
- Extract fields used by WRFDA
- Create background FORTRAN 90 derived data type **xb**, etc.

### Calling order:

da\_wrfvar\_main ==> call da\_wrfvar\_init2 ==> call da\_med\_initialdata\_input da\_wrfvar\_main ==> call da\_wrfvar\_run ==> call da\_wrfvar\_interface ==> call da\_solve ==> call da\_setup\_firstguess

### Calling subroutines:

da\_wrfvar\_main.f90 ==> da\_wrfvar\_init2.inc ==> da\_med\_initialdata\_input.inc da\_wrfvar\_main.f90 ==> da\_wrfvar\_run.inc ==> da\_wrfvar\_interface.inc ==> da\_solve.inc ==> da\_setup\_firstguess.inc



### Set up observations and error









# Set up observations and error

- Read in observations
- Assign observational error
- Create observation FORTRAN 90 derived data type **ob**
- Domain and time check

### Calling order:

da\_wrfvar\_main ==> call da\_wrfvar\_run ==> call da\_wrfvar\_interface ==> call da\_solve ==> call da\_setup\_obs\_structures **Calling subroutines:** 

da\_wrfvar\_main.f90 ==> da\_wrfvar\_run.inc ==> da\_wrfvar\_interface.inc ==> da\_solve.inc ==> da\_setup\_obs\_structures.inc



### Set up background error









# Set up background error

- Reads in background error statistics from be.dat
- Extracts necessary quantities: eigenvectors, eigenvalues, lengthscales, regression coefficients, etc.
- Creates background error FORTRAN 90 derived data type be
- Reference :Online BE Documents

### Calling order:

da\_wrfvar\_main ==> call da\_wrfvar\_run ==> call da\_wrfvar\_interface ==> call da\_solve ==>call da\_setup\_background\_errors Calling subroutines:

da\_wrfvar\_main.f90 ==> da\_wrfvar\_run.inc ==> da\_wrfvar\_interface.inc ==> da\_solve.inc ==> da\_setup\_background\_errors.inc



### Calculate y - H(x)









# Calculate y - H(x) (Innovation)

- Calculate model equivalent of observations through interpolation and variable transformations
- Compute observation minus first guess (y H(x)) value
- Create innovation vector FORTRAN 90 derived data type *iv*

### Calling order:

da\_wrfvar\_main ==> call da\_wrfvar\_run ==> call da\_wrfvar\_interface ==>

call da\_solve ==>call da\_get\_innov\_vector, da\_allocate\_y

#### Calling subroutines:

da\_wrfvar\_main.f90 ==> da\_wrfvar\_run.inc ==> da\_wrfvar\_interface.inc ==> da\_solve.inc ==>da\_get\_innov\_vector.inc, da\_allocate\_y.inc



### **Minimize cost function**









# Minimize cost function

- Use conjugate gradient method
  - Initializes analysis increments to zero
  - Computes cost function (if desired)
  - Computes gradient of cost function
  - Uses gradient of the cost function to calculate new value of analysis control variable
- Increment this process until specified minimization is achieved

### Calling order:

da\_wrfvar\_main ==> call da\_wrfvar\_run ==> call da\_wrfvar\_interface ==> call da\_solve ==>call da\_minimise\_cg Calling subroutines:

da\_wrfvar\_main.f90 ==> da\_wrfvar\_run.inc ==> da\_wrfvar\_interface.inc ==> da\_solve.inc ==> da\_minimise\_cg.inc

Further reading: Shewchuk, Jonathan Richard, 1994. An Introduction to the Conjugate Gradient Method Without the Agonizing Pain (http://www.cs.cmu.edu/~quake-papers/painless-conjugate-gradient.pdf)


#### **Compute analysis**









### Compute analysis

- Convert control variables to model space analysis increments
- Calculate analysis = first-guess + analysis increment
- Perform consistency checks (e.g., remove negative humidity)

#### Calling order:

da\_wrfvar\_main ==> call da\_wrfvar\_run ==> call da\_wrfvar\_interface ==> call da\_solve ==>call da\_transfer\_xatoanalysis Calling subroutines:

 $da_wrfvar\_main.f90 ==> da_wrfvar\_run.inc ==> da\_wrfvar\_interface.inc ==> da\_solve.inc ==> da\_transfer\_xatoanalysis.inc ==> da\_vrfvar\_run.inc ==> da\_wrfvar\_interface.inc ==> da\_solve.inc ==> da\_transfer\_xatoanalysis.inc ==> da\_vrfvar\_run.inc ==> da\_vrfvar\_interface.inc ==> da\_solve.inc ==> da\_vrfvar\_run.inc ==> da\_vrfvar\_interface.inc ==> da\_solve.inc ==> da\_vrfvar\_vrn.inc ==> da\_vrfvar\_interface.inc ==> da\_solve.inc ==> da\_vrfvar\_vrn.inc ==> da\_vrfvar\_vrfvar\_vrn.inc ==> da\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfv$ 



#### **Calculate diagnostics**









### Calculate diagnostics

- Output  $\mathbf{y} H(\mathbf{x}_b)$ ,  $\mathbf{y} H(\mathbf{x}_a)$  statistics for all observation types and variables
- Compute x<sub>a</sub> x<sub>b</sub> (analysis increment) statistics for all model variables and levels
- Statistics include minimum, maximum (and their locations), mean and standard deviation.

#### Calling order:

da\_wrfvar\_main ==> call da\_wrfvar\_run ==> call da\_wrfvar\_interface ==> call da\_solve ==>call da\_transfer\_xatoanalysis Calling subroutines:

 $da_wrfvar\_main.f90 ==> da_wrfvar\_run.inc ==> da\_wrfvar\_interface.inc ==> da\_solve.inc ==> da\_transfer\_xatoanalysis.inc ==> da\_vrfvar\_run.inc ==> da\_wrfvar\_interface.inc ==> da\_solve.inc ==> da\_transfer\_xatoanalysis.inc ==> da\_vrfvar\_run.inc ==> da\_vrfvar\_interface.inc ==> da\_solve.inc ==> da\_vrfvar\_run.inc ==> da\_vrfvar\_interface.inc ==> da\_solve.inc ==> da\_vrfvar\_vrn.inc ==> da\_vrfvar\_interface.inc ==> da\_solve.inc ==> da\_vrfvar\_vrn.inc ==> da\_vrfvar\_vrfvar\_vrn.inc ==> da\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfv$ 



#### **Outer loop**









### Outer loop

- An outer loop is a method of iterative assimilation to maximize contributions from observations non-linearly related to the control variables (e.g., GPS refractivity, Doppler radial velocity)
  - After the previous steps, the analysis  $\mathbf{x}_a$  is used as the new first guess
  - The cost function minimization and diagnostic steps are repeated

### This can be repeated up to ten times Calling order:

da\_wrfvar\_main ==> call da\_wrfvar\_run ==> call da\_wrfvar\_interface ==> call da\_solve

#### Calling subroutines:

da\_wrfvar\_main.f90 ==> da\_wrfvar\_run.inc ==> da\_wrfvar\_interface.inc ==> da\_solve.inc



#### Write analysis









### Write analysis

• Write analysis file in native WRF format.

#### Calling order:

da\_wrfvar\_main ==> call da\_wrfvar\_run ==> call da\_wrfvar\_interface ==> call da\_solve ==>call da\_transfer\_xatoanalysis Calling subroutines:

 $da_wrfvar\_main.f90 ==> da_wrfvar\_run.inc ==> da_wrfvar\_interface.inc ==> da\_solve.inc ==> da\_transfer\_xatoanalysis.inc ==> da\_vrfvar\_run.inc ==> da\_wrfvar\_interface.inc ==> da\_solve.inc ==> da\_transfer\_xatoanalysis.inc ==> da\_vrfvar\_run.inc ==> da\_vrfvar\_interface.inc ==> da\_solve.inc ==> da\_vrfvar\_run.inc ==> da\_vrfvar\_interface.inc ==> da\_solve.inc ==> da\_vrfvar\_vrn.inc ==> da\_vrfvar\_interface.inc ==> da\_solve.inc ==> da\_vrfvar\_vrn.inc ==> da\_vrfvar\_vrfvar\_vrn.inc ==> da\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfvar\_vrfv$ 













### Clean up

- Deallocate dynamically-allocated arrays, structures, etc.
- Timing information
- Clean end to WRFDA

#### Calling order:

da\_wrfvar\_main ==> call da\_wrfvar\_run ==> call da\_wrfvar\_interface ==> call da\_solve da\_wrfvar\_main ==> call da\_wrfvar\_finalize

#### Calling subroutines:

da\_wrfvar\_main.f90 ==> da\_wrfvar\_run.inc ==> da\_wrfvar\_interface.inc ==> da\_solve.inc da\_wrfvar\_main.f90 ==> da\_wrfvar\_finalize.inc



#### WRFDA broken down by process









### **Output files: Diagnostics**

- File names: grad\_fn, jo, qcstat\_conv\*, statistics, etc.
- There will be a number of diagnostics files output by WRFDA
  - Many will end in .0000, .0001, etc.; these are diagnostics specific to each processor used
  - Many will also contain a \_01; these files will appear for each outer loop as \_02, \_03, etc.
- More or fewer output files can be specified by certain namelist options





# Output files: **x**<sub>a</sub> (analysis)

- File name: wrfvar\_output
- This is the model output in WRF native format. This file can be used directly for research purposes, or used to initialize a WRF forecast



# Cycling mode

- Because WRFDA takes WRF forecast files as input, the system can naturally be run in cycling mode
- WRFDA initializes a WRF forecast, the output of which is fed back into WRFDA to initialize another WRF forecast
- Requires boundary condition updating





NESL

#### WRFDA in the WRF Modeling System



Further reading: User's Guide, Chapter 6, section "Updating WRF Boundary Conditions"





### WRFDA System – Outline

- Introduction
- WRFDA Software Overview
- Computing Overview



### WRFDA Parallelism



- WRFDA can be run serially or as a parallel job
- WRFDA uses *domain decomposition* to divide total amount of work over parallel processes
- The decomposition of the application over processes has two levels:
  - The *domain* is first broken up into rectangular pieces that are assigned to MPI (distributed memory) processes. These pieces are called *patches*
  - The *patches* may be further subdivided into smaller rectangular pieces that are called *tiles*, and these are assigned to *shared-memory threads* within the process.



#### Parallelism in WRFDA: Multi-level Decomposition



- Single version of code for efficient execution on:
  - Distributed-memory
  - Shared-memory (SMP)
  - Clusters of SMPs
  - Vector and microprocessors

Model domains are decomposed for parallelism on two-levels

*Patch:* section of model domain allocated to a distributed memory node, this is the scope of a minimization layer solver.

*Tile:* section of a patch allocated to a shared-memory processor within a node; this is also the scope of a observation layer subroutine.

Distributed memory parallelism is over patches; shared memory parallelism is over tiles within patches

1 Patch, divided into multiple tiles

HARDWARE

Inter-processor communication





#### Distributed Memory Communications

When Needed?	Communication is required between patches when a horizontal index is incremented or decremented on the right-hand-side of an assignment.
Why?	On a patch boundary, the index may refer to a value that is on a different patch.
	Following is an example code fragment that requires communication between patches
Signs in code	Note the tell-tale +1 and -1 expressions in indices for <b>rr</b> , <b>H1</b> , and <b>H2</b> arrays on right-hand side of assignment.
	These are <i>horizontal data dependencies</i> because the indexed operands may lie in the patch of a neighboring processor. That neighbor's updates to that element of the array won't be seen on this processor.





#### **Distributed Memory Communications**

(da\_transfer\_xatowrf.inc)

```
subroutine da_transfer_xatowrf(grid)
...
do k=kts,kte
    do j=jts,jte+1
        do i=its,ite+1
            u_cgrid(i,j,k)=0.5*(grid%xa%u(i-1,j ,k)+grid%xa%u(i,j,k))
            v_cgrid(i,j,k)=0.5*(grid%xa%v(i ,j-1,k)+grid%xa%v(i,j,k))
            end do
        end do
    end do
    end do
    end do
```





#### **Distributed Memory Communications**

(da\_transfer\_xatowrf.inc)





### Distributed Memory (MPI) Communications



Halo updates



memory on one processor

memory on neighboring processor



## Grid Representation in Arrays

- Increasing indices in WRFDA arrays run
  - West to East (X, or I-dimension)
  - South to North (Y, or J-dimension)
  - Bottom to Top (Z, or K-dimension)
- Storage order in WRFDA is IJK, but for WRF, it is IKJ (ARW) and IJK (NMM)
- Output data has grid ordering independent of the ordering inside the WRFDA model





### Grid Representation in Arrays

- The extent of the logical or *domain* dimensions is always the "staggered" grid dimension. That is, from the point of view of a non-staggered dimension (also referred to as the ARW "mass points"), there is always an extra cell on the end of the domain dimension
- In WRFDA, the minimization is on A-grid (non-staggered grid). The wind components will be interpolated from A-grid to C-grid (staggered grid) before they are output





### WRFDA I/O

- Streams: pathways into and out of model
  - Input
    - fg is the name of the input
    - wrfvar\_output is the name of output
  - Boundary
    - Only needed for 4DVAR.





- Carriery
  - WRFDA is designed to be an easy-to-use data assimilation system for use with the WRF model
  - WRFDA is designed within the WRF Software Framework for rapid development and ease of modification
  - WRFDA can be run in parallel for quick assimilation of large amounts of data





# Appendix – WRFDA Resources

- WRFDA users page
  - http://www.mmm.ucar.edu/wrf/users/wrfda
  - Download WRFDA source code, test data, related packages and documentation
  - Lists WRFDA news and developments
- Online documentation
  - <u>http://www.mmm.ucar.edu/wrf/users/docs/user\_guide\_V3/u</u>
     <u>sers\_guide\_chap6.htm</u>
  - Chapter 6 of the WRF Users' Guide; documents installation of WRFDA and running of various WRFDA methods
- WRFDA user services and help desk
  - wrfhelp@ucar.edu





# Appendix – Derived Data Structures

- Driver layer
  - All data for a domain is an object, a domain derived data type (DDT)
  - The domain DDT is dynamically allocated/deallocated
  - Only one DDT is allowed in WRFDA; it is head\_grid, defined in frame/module\_domain.F
  - WRFDA doesn't support nested domains.



 Every Registry defined state, I1, and namelist variable is contained inside the DDT (locally known as a grid of type domain), where each node in the tree represents a separate and complete 3D model domain/nest.





# Appendix – Derived Data Structures

- cvt
  - Real type array to store the control variables
  - It is an all-ZERO array during the first outer loop and will be updated at the end of each outer loop
- xhat
  - Real type array to store the control variables
  - It stores the control variables for each inner loop.
- be
  - It is used to store the background error covariance.





## Appendix – Derived Data Structures

- iv
  - Stores the innovations for each observational type y Hx
- ob
  - Stores the observations y
- re
  - Store the residual  $\mathbf{y} \mathbf{H}(\mathbf{x} + \Delta \mathbf{x})$





### Appendix – WRFDA structure

- Primarily written in Fortran and C
- Part of the WRF Software Framework
  - Hierarchical organization
  - Multiple functions
  - Plug observation type interface
  - Abstract interfaces (APIs) to external packages
  - Performance-portable





# Appendix – Parallel Computing Terms (Hardware)

• Processor:



- A device that reads and executes instructions in sequence from a memory device, producing results that are written back to a memory device
- **Node**: One memory device connected to one or more processors.
  - Multiple processors in a node are said to share-memory and this is "shared memory parallelism"
  - They can work together because they can see each other's memory
  - The latency and bandwidth to memory affect performance



# Appendix – Parallel Computing Terms (Hardware)

• **Cluster**: Multiple nodes connected by a network



- The processors attached to the memory in one node can not see the memory for processors on another node
- For processors on different nodes to work together they must send messages between the nodes. This is "distributed memory parallelism"
- Network:
  - Devices and wires for sending messages between nodes
  - Bandwidth a measure of the number of bytes that can be moved in a second
  - Latency the amount of time it takes before the first byte of a message arrives at its destination



# Appendix – Parallel Computing Terms (Software)

#### • Process:



- A set of instructions to be executed on a processor
- Enough state information to allow process execution to stop on a processor and be picked up again later, possibly by another processor
- Processes may be lightweight or heavyweight
  - Lightweight processes, e.g. shared-memory threads, store very little state; just enough to stop and then start the process
  - Heavyweight processes, e.g. UNIX processes, store a lot more (basically the memory image of the job)



# Appendix – Parallel Computing Terms (Software)

- Every job has at least one heavy-weight *process*.
  - A job with more than one heavy-weight process is a distributed-memory parallel job
  - Even on the same node, heavyweight processes do not share memory
- Within a heavyweight process you may have some number of lightweight processes, called *threads*.
  - Threads are shared-memory parallel; only threads in the same memory space can work together.
  - A thread never exists by itself; it is always inside a heavy-weight process.
- Heavy-weight processes are the vehicles for distributed memory parallelism
- Threads (light-weight processes) are the vehicles for shared-memory parallelism







# Appendix – Parallel Computing in WRFDA context

 Since the process model has two levels (heavyweight and light-weight = MPI and OpenMP), the decomposition of the application over processes has two levels:

SYSTEM

- The *domain* is first broken up into rectangular pieces that are assigned to heavy-weight processes. These pieces are called *patches*
- The *patches* may be further subdivided into smaller rectangular pieces that are called *tiles*, and these are assigned to *threads* within the process.


#### Appendix – Parallel Computing APIs

- Message Passing Interface MPI, referred to as the communication layer
- MPI is used to start up and pass messages between multiple heavyweight processes
  - The **mpirun** command controls the number of processes and how they are mapped onto nodes of the parallel machine
  - Calls to MPI routines send and receive messages and control other interactions between processes
  - <u>http://www.mcs.anl.gov/mpi</u>







# Appendix – Parallel Computing APIs

 OpenMP is used to start up and control threads within each process



- Directives specify which parts of the program are multithreaded
- OpenMP environment variables determine the number of threads in each process
- <u>http://www.openmp.org</u>
- OpenMP is usually activated via a compiler option
- MPI is usually activated via the compiler name
- The number of **processes** (number of MPI processes times the number of threads in each process) usually corresponds to the number of **processors**
- In general, WRFDA should not be run with shared memory!





• If the machine consists of 4 nodes, each with 4 processors, how many different ways can you run a job to use all 16 processors?

	1 MPI	1 MPI
<pre>- 4 MPT processes, each with 4 threads setenv OMP_NUM_THREADS 4 mpirun -np 4 da_wrfvar.exe</pre>	4 threads	4 threads
<ul> <li>8 MPI processes, each with 2 threads</li> </ul>	1 MPI	1 MPI
setenv OMP_NUM_THREADS 2 mpirun -np 8 da_wrfvar.exe	4 threads	4 threads
- To WPT processes, each with T thread		

setenv OMP\_NUM\_THREADS 1
mpirun -np 16 da\_wrfvar.exe





 If the machine consists of 4 nodes, each with 4 processors, how many different ways can you run a job to use all 16 processors?

	2 MPI	2 MPI
<ul> <li>4 MPI processes, each with 4 threads</li> </ul>	2 threads	2 threads
setenv OMP_NUM_THREADS 4	2 threads	2 threads
mpirum mpiruu_wrrvur.ckc		
<ul> <li>8 MPI processes, each with 2 threads</li> </ul>	2 MPI	2 MPI
setenv OMP_NUM_THREADS 2 mpirun -np 8 da_wrfvar.exe	2 threads	2 threads
<ul> <li>16 MPI processes, each with 1 thread</li> </ul>		2 uneaus

setenv OMP\_NUM\_THREADS 1
mpirun -np 16 da\_wrfvar.exe





 If the machine consists of 4 nodes, each with 4 processors, how many different ways can you run a job to use all 16 processors?







- Note, since there are 4 nodes, we can never have fewer than 4 MPI processes because nodes do not share memory
- What happens on this same machine for the following?

setenv OMP\_NUM\_THREADS 8
mpirun -np 32 da\_wrfvar.exe



#### Distributed Memory (MPI) Communications



- Halo updates
- Parallel transposes





#### Distributed Memory (MPI) Communications



- Halo updates
- Parallel transposes



all y on patch



all z on patch



all x on patch





#### Review – Computing Overview

			Distributed Memory Parallel		Shared Memory Parallel
APPLICATION (WRF)	Domain	contains	Patches	contain	Tiles
SYSTEM (UNIX, MPI, OpenMP)	Job	contains	Processes	contain	Threads
HARDWARE Processors, Memories, Wires)	Cluster	contains	Nodes	contain	Processors



# Appendix – WRFDA/var/da Directory structure



Main WRFDA Program (driver):

da\_main

# WRFDA Subroutines (mediation layer)

da\_4dvar da\_control da\_etkf da\_define\_structures da\_dynamics da\_grid\_definitions da\_interpolation da\_minimisation da\_physics da\_setup\_structures da\_varbc da\_vtox\_transforms

#### OBSERVATION TYPES

da\_airep da\_airsr da\_bogus da\_buoy da\_geoamv da\_gpspw da\_gpsref da\_metar da\_mtgirs da\_pilot da\_polaramv da\_polaramv da\_pseudo

da\_qscat

da\_radar

da\_radiance

da\_rain

da\_satem

da\_ships

da\_sound

da\_ssmi

da\_synop

da\_tamdar





# Appendix – WRFDA History

- Developed from MM5 3DVar beginning around 2002, first version (2.0) released December 2003
- Developed and supported by WRFDA group of MMM, part of NESL
- Requirements emphasize flexibility over a range of platforms, applications, users, performance
- Current release WRFDA v3.5 (April 2013)
- Shares the WRF Software Framework





$$J(x) = \frac{1}{2} (x - x^{b})^{\mathrm{T}} \mathbf{B}_{0}^{-1} (x - x^{b}) + \frac{1}{2} (y_{0} - H(x))^{\mathrm{T}} \mathbf{R}^{-1} (y_{0} - H(x))$$

- Model background (x<sup>b</sup>)
- Background error (B<sub>0</sub>)
- Observations  $(y_0)$  and their associated error statistics (**R**)
- Minimize this cost function (J(x)) to find the analysis  $(x^a)$
- Run forecast, repeat for cycling mode





$$J(x) = \frac{1}{2} (x - x^{b})^{\mathrm{T}} \mathbf{B}_{0}^{-1} (x - x^{b}) + \frac{1}{2} (y_{0} - H(x))^{\mathrm{T}} \mathbf{R}^{-1} (y_{0} - H(x))$$

- Model background  $(x^b)$  is the "first guess" of the atmospheric state before data assimilation
- The background can be provided by WPS and real.exe, or a full WRF forecast





$$J(x) = \frac{1}{2} (x - x^{b})^{\mathrm{T}} \mathbf{B}_{0}^{-1} (x - x^{b}) + \frac{1}{2} (y_{0} - H(x))^{\mathrm{T}} \mathbf{R}^{-1} (y_{0} - H(x))$$

- Background error covariance (B<sub>0</sub>) describes the relationship between different errors in the background
- Arguably the most important ingredient to a successful forecast
- Several options available:
  - cv\_options=3; generic NCEP Background Error model
    - This is recommended for testing and debugging <u>only</u>
  - cv\_options=5; the NCAR Background Error model
    - The default and recommended BE formulation
    - Requires gen\_be (learned in later presentation)
  - cv\_options=6; Multivariate Background Error (MBE) statistics
    - Not officially supported





$$J(x) = \frac{1}{2} (x - x^{b})^{\mathrm{T}} \mathbf{B}_{0}^{-1} (x - x^{b}) + \frac{1}{2} (y_{0} - H(x))^{\mathrm{T}} \mathbf{R}^{-1} (y_{0} - H(x))$$

- Observations (y<sub>0</sub>) and their associated errors (R) are essential to any data assimilation process
- WRFDA can assimilate a wide variety of observations
  - Conventional observations
    - Includes radiosonde, ships, surface, etc.
    - Should be in LITTLE\_R format for ingest into OBSPROC
  - Satellite radiance data
    - Can assimilate data from dozens of instruments
    - Assimilated directly in BUFR format
    - Requires radiative transfer model (CRTM or RTTOV)
- Radar velocity and reflectivity, accumulated precipitation, others