



WRF Data Assimilation System: Software and Compilation

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WRFDA System – Outline

NSD

- Introduction
- Compiling the code
- WRFDA software structure
- Computing overview





- A data assimilation system for the WRF Model (ARW core)
 - 3D- and 4D-VAR, FGAT, 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

WRFDA in WRF Modeling System





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





WRFDA in the WRF Modeling System



Blue: Supported by WRFDA team



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Compiling – What is needed?

NSF

- WRFDA has similar system requirements to WRF
 - Can be run on a wide variety of UNIX and Linux-based systems
 - Linux/Mac, desktops/laptops, clusters with UNIX-based OS
- WRFDA computational requirements depend on your task
 - Running a small 3DVAR case may take less than 1GB of RAM
 - Large 4DVAR cases may require hundreds of GB
- A supported C and Fortran compiler
 - ifort/icc
 - gfortran/gcc
 - pgf90/pgcc
- Some have known problems; see <u>http://www2.mmm.ucar.edu/wrf/users/wrfda/known-</u> problems.html#compilers

Compiling – What is needed?

NSF

- Similar to WRF, there are required and optional libraries
 - netCDF C/fortran libraries are required, and must be downloaded and built by the user
 - http://www.unidata.ucar.edu/downloads/netcdf/index.jsp
 - MPI libraries, such as MPICH, are required for running WRFDA in parallel
 - For radiance assimilation, a radiative transfer model is needed:
 - CRTM, the Community Radiative Transfer Model, is included with the WRFDA source code
 - RTTOV is provided by EUMETSAT/NWC SAF, and must be downloaded and built separately
 - https://nwpsaf.eu/deliverables/rtm/rtm_rttov11.html
 - BUFR libraries are required for reading PREPBUFR or radiance BUFR files, but they are included in WRFDA and built automatically



Compiling – Getting the source code



- Visit the WRFDA download website:
 - <u>http://www2.mmm.ucar.edu/wrf/users/wrfda/download/get_source.html</u>
- Click "New Users" and fill out the registration form, (registration is free), or
- Click "Returning users" and enter your email if you have previously registered to download a WRF product
- Download the latest tar file (Version 3.7)
- Unzip (gunzip WRFDA_V3.7.tar.gz) and un-tar (tar -xvf
 WRFDA_V3.7.tar) the code package
- You should see a directory named "WRFDA"; this is the WRFDA source code



WRFDA Directory structure

<pre>arch clean compile configure dyn_em dyn_exp external frame inc main</pre>	build scripts	
phys README.DA	README file with informat	ion about WRFDA
	Contains registry.var	
share		
test		Legend:
tools		Blue – directory
var	code directory	Green – script file Gray – other text file

NSF



WRFDA/var Directory structure



build <	Executables built here	
convertor	- WRFDA main source code contained here	
da	- Source code for external libraries (CRTM RUFR etc.)	
external	<i>GEN_BE</i> source code	
gen_be <		
graphics		
Makefile		
obsproc	- OBSPROC source code	
README.basics	More DEADME files with	
README.namelist	More READINE Jues with	
README.radiance	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 ¹²



WRFDA/var/da Directory structure



Main WRFDA Program (driver):		da_ma	in
WRFDA Subroutines (mediation layer)		OBSERVATION TYPES	
da 4dvar		da airep	da pseudo
da control		da airsr	da qscat
daetkf		 da_bogus	
da_define_structures		da_buoy	da_radiance
da_dynamics		da_geoamv	da_rain
da_grid_definitions		da_gpspw	da_satem
da_interpolation		da_gpsref	da_ships
da_minimisation		da_metar	da_sound
da_physics		da_mtgirs	da_ssmi
da_setup_structures		da_pilot	da_synop
da_varbc		da_polaramv	da_tamdar
da_vtox_transforms		da_profiler	



Compiling – Preparing the environment

- As mentioned before, some libraries are required for WRFDA, and some are optional depending what you are using WRFDA for
 - netCDF is required; you should set an environment variable to specify where the netCDF libraries are built on your system:
 - setenv NETCDF full_path_for_NETCDF
- If you plan on doing radiance assimilation, you will need CRTM or RTTOV. WRFDA can be built with either or both
 - The CRTM source code is included in the WRFDA package, use setenv CRTM 1 to build it
 - To use RTTOV, set an environment variable specifying where RTTOV is built on your system:
 - setenv RTTOV full_path_for_RTTOV
- To build faster, if your computer has the gnu make utility, you can set the environment variable J to build the code in parallel
 - setenv J "-j 4" (will build on 4 processors)



Compiling – Building the WRFDA code



- Two scripts must be run to build the code:
- configure asks for some information about your machine and how you want to build the code, and generates a configure.wrf file
- ./configure wrfda

```
> ./configure wrfda
checking for per15... no
checking for perl... found /usr/bin/perl (perl)
Will use NETCDF in dir: /usr/local/netcdf-3.6.3-gfortran
PHDF5 not set in environment. Will configure WRF for use without.
Will use 'time' to report timing information
$JASPERLIB or $JASPERINC not found in environment, configuring to build without grib2 I/0...
Please select from among the following Linux x86 64 options:
                            3. (dmpar)
  1. (serial)
               2. (smpar)
                                         4. (dm+sm)
                                                      PGI (pgf90/gcc)
  5. (serial)
              6. (smpar) 7. (dmpar)
                                                      PGI (pgf90/pgcc): SGI MPT
                                         8. (dm+sm)
                                                      PGI (pgf90/gcc): PGI accelerator
  9. (serial)
              10. (smpar) 11. (dmpar)
                                         12. (dm+sm)
              14. (smpar) 15. (dmpar)
 13. (serial)
                                        16. (dm+sm)
                                                      INTEL (ifort/icc)
```

• Select the option that is best for your purposes



Compiling – Building the WRFDA code

- Two scripts must be run to build the code:
- compile compiles all the code for the settings you specified

./compile all_wrfvar >& compile.wrfda.log

• Depending on your machine and what options you have selected, compilation can take less than 5 minutes up to an hour. For example, gfortran compiles WRFDA quite quickly, while intel compilers take longer to build (but the executables will run faster)



Compiling – review compiled code

- When the compilation script is completed, you should see the message "build completed:" followed by the date and time.
- The script does not automatically check to make sure all executables were successfully built; You will need to check manually
- There should be 44 executables built all together: 43 in the WRFDA/var/build directory, and WRFDA/var/obsproc/obsproc.exe
- In all likelihood, you will not use most of these directly: the majority of them are called by scripts for various diagnostic packages

Compiling – review executables

- These are the executables you will most likely be using:
- da_wrfvar.exe
 - The main WRFDA executable: this program will perform the actual data assimilation/minimization
- obsproc.exe
 - The executable for OBSPROC, the observation pre-processor for text-based observation formats
- da_update_bc.exe
 - The executable for UPDATE_BC; used for updating boundary conditions after assimilation and during cycling runs



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WRFDA Software – Architecture



Registry.wrfvar

- 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.



WRFDA Software – Architecture



Registry.wrfvar

- 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 main dictionary for WRFDA
 - registry.var is combined at compile time with Registry.EM_COMMON.var and others to produce Registry.wrfvar, which contains all of the registry definitions used by WRFDA



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WRFDA Software – Architecture

	Variable	Variable	Namelist
	type	name	name
rconfig	n integer	rttov_emis_atlas_ir	namelist,wrfvar14
rconfig	n integer	rttov_emis_atlas_mw	namelist,wrfvar14
rconfig	y integer	rtminit_print	namelist,wrfvar14
rconfig	y integer	rtminit_nsensor	namelist,wrfvar14
rconfig	y integer	rtminit_platform	namelist,wrfvar14
rconfig	y integer	rtminit_satid	namelist,wrfvar14
rconfig	n integer	rtminit_sensor	namelist,wrfvar14
rconfig	n integer	rad_monitoring	namelist,wrfvar14
rconfig	real	thinning_mesh	namelist,wrfvar14
rconfig	f logical	thinning	namelist,wrfvar14
rconfig	f logical	read_biascoef	namelist,wrfvar14
rconfig	f logical	biascorr	namelist,wrfvar14
rconfig	f logical	biasprep	namelist,wrfvar14
rconfig	f logical	rttov_scatt	namelist,wrfvar14
rconfig	f logical	write_profile	namelist,wrfvar14
rconfig	f logical	write_jacobian	namelist,wrfvar14
rconfig	f logical	qc_rad	namelist,wrfvar14
rconfig	f logical	write_iv_rad_ascii	namelist,wrfvar14
rconfig	f logical	write_oa_rad_ascii	namelist,wrfvar14
rconfig	f logical	write_filtered_rad	namelist,wrfvar14
rconfig	f logical	use_error_factor_rad	namelist,wrfvar14
rconfig	f logical	use_landem	namelist,wrfvar14
rconfig	f logical	use_antcorr	namelist,wrfvar14
rconfig	f logical	use_mspps_emis	namelist,wrfvar14
rconfig	f logical	use_mspps_ts	namelist,wrfvar14

size Default value

Variable

0 1 11 \\ - "rttov emis atlas ir" 11 11 - "rttov emis atlas mw" 1 0 11 11 11 \\ 1 1 - "rtminit print" 11.11 11 \\ 1 - "rtminit nsensor" 1 11 11 max instruments -1 - "rtminit platform" max instruments -1.0 - "rtminit satid" - "rtminit sensor" max instruments -1.0 max instruments 0 - "rad monitoring" - "thinning mesh" max instruments 60.0 .true. - "thinning " 11 11 1 - "read biascoef" 11 \\ 1 .false. 11 11 .false. - "biascorr" 11 \\ 1 11 11 .false. - "biasprep" 1 11 11 11 \\ .false. - "rttov scatt" 11 \\ 1 11 11 .false. - "write profile" 11 \\ 11 11 1 .false. - "write jacobian" 1 11 11 11 \\ - "qc rad" 11 \\ 1 .true. 11 11 .false. - "write iv rad ascii" 1 11 11 11 \\ .false. - "write oa rad ascii" 11 11 11 \\ 1 - "write filtered rad" .false. 11 \\ 11 11 1 - "use error factor rad" .false. 11 \\ 11 11 1 .false. 1 - "use landem" 11 11 11 \\ max instruments .false. - "use antcorr" max instruments .false. - "use mspps emis" max instruments .false. - "use mspps ts"

registry.var

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- WRFDA Software Architecture Registry Driver DM comm Config Solve I/O API Inquiry OMP Message Passing Threads Data formats. Config DA obs type-callable Parallel I/O Subroutine Module
 - Driver Layer
 - **Domains**: Allocates, stores, decomposes, represents abstractly as single data objects

WRFDA Software – Architecture



- 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





WRFDA Software – Architecture



• Observation Layer

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

Registry







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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 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.
- However, WRFDA does not support shared memory parallelism! So distributed memory is what I will cover here.



Parallelism in WRFDA: Multi-level Decomposition





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 rr, H1, and H2 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



Halo (contains information about adjacent patch)



Distributed Memory Communications



Halo (contains information about adjacent patch)



- 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





- 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 (nonstaggered grid). The wind components will be interpolated from A-grid to C-grid (staggered grid) before they are output, to conform with standard WRF format





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



Appendix – WRFDA Resources

NSF

- WRFDA users page
 - <u>http://www2.mmm.ucar.edu/wrf/users/wrfda</u>
 - Download WRFDA source code, test data, related packages and documentation
 - Lists WRFDA news and developments
- Online documentation
 - <u>http://www2.mmm.ucar.edu/wrf/users/docs/user_guide_V</u> <u>3/users_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 – WRFDA History

- Developed from MM5 3DVar beginning around 2002, first version (2.0) released December 2003
- 4DVAR capability added in 2008, made practical with parallelism starting with Version 3.4 (April 2012)
- Developed and supported by WRFDA group of the Mesoscale and Microscale Meteorology Lab of NCAR
- Requirements emphasize flexibility over a range of platforms, applications, users, performance
- Current release WRFDA v3.7 (April 2015)
- Shares the WRF Software Framework



WRFDA and J



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

- Model background $(\mathbf{X}_{\mathbf{b}})$
- Background error (**B**)
- Observations (y_0) and their associated error statistics (\mathbf{R})
- Minimize this cost function (J(x)) to find the analysis (X)
- Run forecast, repeat for cycling mode



WRFDA broken down by process









Input files



namelist.input

- fg
- ob.ascii, amsua.bufr, ob01.rain, etc
- be.dat

- The input file where the user specifies the different options for a WRFDA run. This allows user great flexibility to change the usage of WRFDA without having to recompile
- "First guess"; can be either a WRF input file created by WPS and real.exe, or a WRF output file from a forecast.
- WRFDA accepts a wide variety of observations in several different formats, which will be described in later talks
- This is a binary file containing background error information; it can be generated using the GEN_BE utility, which will be described in a later talk



WRFDA broken down by process







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



- 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



- 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

- 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





- 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*
- Specifics of background error in WRFDA be covered in more detail in a later talk

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
```



Minimize cost function



- Use conjugate gradient method
 - Initializes analysis increments to zero
 - Computes cost function
 - 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



- 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



Calculate diagnostics



- Output $\mathbf{y} H(\mathbf{x}_b)$, $\mathbf{y} H(\mathbf{x}_a)$ statistics for all observation types and variables
- Compute $\mathbf{x}_a \mathbf{x}_b$ (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
```



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 100 times, though only a few should be necessary

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

Further reading: Rizvi et al., 2008 (http://www.mmm.ucar.edu/wrf/users/workshops/WS2008/abstracts/P5-03.pdf)



Write analysis



• Write analysis file in native WRF format (netCDF).

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



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



- 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**_a (analysis)

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