WRF Software: Code and Parallel Computing

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Outline

- Introduction
- Computing Overview
- WRF Software Overview

Introduction – WRF Software Characteristics

- Developed from scratch beginning around 1998, primarily Fortran and C
- Requirements emphasize flexibility over a range of platforms, applications, users, performance
- WRF develops rapidly. First released Dec 2000; current release WRF v3.5.1 (Sep 2013); next release WRF v3.6 (Apr 2014)
- Supported by flexible efficient architecture and implementation called the WRF Software Framework

Introduction - WRF Software Framework Overview

- Implementation of WRF Architecture
 - Hierarchical organization
 - Multiple dynamical cores
 - Plug compatible physics
 - Abstract interfaces (APIs) to external packages
 - Performance-portable
- Designed from beginning to be adaptable to today's computing environment for NWP

http://mmm.ucar.edu/wrf/WG2/bench/





- The 'N' in NWP
- Components
 - Processor
 - A program counter
 - Arithmetic unit(s)
 - Some scratch space (registers)
 - Circuitry to store/retrieve from memory device
 - Cache
 - Memory
 - Secondary storage
 - Peripherals
- The implementation has been continually refined, but the basic idea hasn't changed much



Hardware has not changed much...

A computer in 1960





6-way superscalar

36-bit floating point precision

 $\sim \! 144 \text{ Kbytes}$

~50,000 flop/s 48hr 12km WRF CONUS in 600 years

A computer in 2013



Dual core, 2.6 GHz chip 64-bit floating point precision 20 MB L3

~5,000,000,000 flop/s 48 12km WRF CONUS in 26 Hours

APPLICATION	
SYSTEM	how we use it has
HARDWARE	

- Fundamentally, processors haven't changed much since 1960
- Quantitatively, they haven't improved nearly enough
 - 100,000x increase in peak speed
 - 100,000x increase in memory size
- We make up the difference with <u>parallelism</u>
 - Ganging multiple processors together to achieve 10^{11-12} flop/second
 - Aggregate available memories of 10^{11-12} bytes

~1,000,000,000,000 flop/s ~250 procs 48-h,12-km WRF CONUS in under 15 minutes



January 2000 Benchmark

- 74x61 grid cells
- 1 hour forecast, 3 minute time step, 20 time step average
- IO exlcuded

Decomposed domain sizesproc count: I-dim x J-dim1: 74x612: 74x314: 37x318: 37x16

16: 19x16 32: 19x8 64: 10x8

January 2000 Benchmark

Processor Count		SM — OpenMP % Efficiency	DM — MPI % Efficiency
1	74x61	100	100
2	74x31	72	98
4	37x31	65	91
8	37x16	31	83
16	19x16	16	70
32	19x8	8	56
64	10x8	3	40



Examples

• 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
 4 MPI processes, each with 4 threads 		
setenv OMP_NUM_THREADS 4	4 threads	4 threads
mpirun -np 4 wrf.exe		
 8 MPI processes, each with 2 threads 		
	1 MPI	1 MPI
setenv OMP_NUM_THREADS 2		
mpirun -np 8 wrf.exe	4 threads	4 threads
 16 MPI processes, each with 1 thread 		

mpirun -np 16 wrf.exe

setenv OMP NUM THREADS 1

Examples

• 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
 4 MPI processes, each with 4 threads 	2 threads	2 threads
setenv OMP_NUM_THREADS 4	2 threads	2 threads
mpirun -np 4 wrf.exe		
 8 MPI processes, each with 2 threads 	2 MPI	2 MPI
setenv OMP_NUM_THREADS 2 mpirun -np 8 wrf.exe	2 threads	2 threads
 16 MPI processes, each with 1 thread 	2 threads	2 threads

setenv OMP_NUM_THREADS 1
mpirun -np 16 wrf.exe

Examples

- 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?
 - 4 MPI processes, each with 4 threads

setenv OMP_NUM_THREADS 4
mpirun -np 4 wrf.exe

- 8 MPI processes, each with 2 threads

setenv OMP_NUM_THREADS 2
mpirun -np 8 wrf.exe

- 16 MPI processes, each with 1 thread

setenv OMP_NUM_THREADS 1
mpirun -np 16 wrf.exe





- WRF can be run serially or as a parallel job
- WRF uses *domain decomposition* to divide total amount of work over parallel processes



Parallelism in WRF: 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 mediation layer solver or physics driver.

Inter-processor communication

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

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

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.

```
(module diffusion.F )
```

```
SUBROUTINE horizontal_diffusion_s (tendency, rr, var, . . .
```

```
DO j = jts,jte
DO k = kts, ktf
DO i = its, ite
   mrdx=msft(i,j)*rdx
   mrdy=msft(i,j)*rdy
   tendency(i,k,j)=tendency(i,k,j)-
                                                                 &
         (mrdx*0.5*((rr(i+1,k,j)+rr(i,k,j))*H1(i+1,k,j)-
                                                                 S
                    (rr(i-1,k,i)+rr(i,k,i))*H1(i,k,i))+
                                                                 3
         mrdy*0.5*((rr(i,k,j+1)+rr(i,k,j))*H2(i,k,j+1)-
                                                                 &
                    (rr(i,k,j-1)+rr(i,k,j)) * H2(i,k,j)) -
                                                                 3
         msft(i,j) * (Hlavg(i,k+1,j) - Hlavg(i,k,j) +
                                                                 2
                     H2avq(i,k+1,j)-H2avq(i,k,j)
                                                                 &
                              )/dzetaw(k)
                                                                 &
ENDDO
ENDDO
```

ENDDO

APPLICATION
SYSTEM
HARDWARE

Halo updates



memory on one processor

memory on neighboring processor

APPLICATION	
SYSTEM	
HARDWARE	

- Halo updates
- Periodic boundary updates
- Parallel transposes
- Nesting scatters/gathers



APPLICATION
SYSTEM
HARDWARE

- Halo updates
- Periodic boundary updates
- Parallel transposes
- Nesting scatters/gathers



Average Daily Total rainfall (mm) - March 1997



APPLICATION
SYSTEM
HARDWARE

- Halo updates
- Periodic boundary updates
- Parallel transposes
- Nesting scatters/gathers



all y on patch



all z on patch



all x on patch

APPLICATION
SYSTEM
HARDWARE

- Halo updates
- Periodic boundary updates
- Parallel transposes

Nesting scatters/gathers







COARSE Ross Island 6.66 km

NEST:2.22 km

INTERMEDIATE: 6.66 km

Review – Computing Overview



Outline

- Introduction
- Computing Overview
- WRF Software Overview



Registry

- 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, and model coupling facilitates code reuse and exploiting of community infrastructure, e.g. ESMF.



Registry

- Driver Layer
 - Domains: Allocates, stores, decomposes, represents abstractly as single data objects
 - Time loop: top level, algorithms for integration over nest hierarchy



- Mediation Layer
 - Solve routine, takes a domain object and advances it one time step

Registry

- Nest forcing, interpolation, and feedback routines



- Mediation Layer
 - The sequence of calls for doing a time-step for one domain is known in Solve routine

Registry

- Dereferences fields in calls to physics drivers and dynamics code
- Calls to message-passing are contained here as part of Solve routine



- Model Layer
 - Physics and Dynamics: contains the actual WRF model routines are written to perform some computation over an arbitrarily sized/ shaped, 3d, rectangular subdomain

Registry

Call Structure Superimposed on Architecture



WRF Software Overview

- Architecture
- Directory structure
- Model Layer Interface
- Data Structures
- I/O

WRF Model Top-Level Directory Structure

WRF Design and Implementation Doc, p 5 DRIVER MEDIATION MODEL



\$(CITTEROD) \$ (OFFICIT) \$.1 > \$.150
\$(FC) -0 \$@ -c \$(FCFLAGS) \$(MODULE_DIRS) \
\$(PROMOTION) \$(FCSUFFIX) \$*.f90

\$(CPPFLAGS) \$(OMPCPP) \$*.F > \$*.f90

\$(CPP) -I\$(WRF_SRC_ROOT_DIR)/inc \

\$(RM) \$@

Where are WRF source code files located?

Where are WRF source code files located?

cpp -C -P file.F > file.f90
gfortran -c file.f90

Where are WRF source code files located?

• The most important command is the "find" command. If there is an error in the model output, you can find that location in the source code with the **find** command.

cd WRFV3

find . -name *.F -exec grep -i "Flerchinger" {} \; -print
- All of the differences between the .F and .f90 files are due to the included pieces that are manufactured by the Registry.
- These additional pieces are all located in the WRFV3/inc directory.
- For a serial build, almost 450 files are manufactured.
- Usually, most developers spend their time working with physics schemes.

- The "main" routine that handles the calls to all of the physics and dynamics:
 WRFV3/dyn_em/solve_em.F
- This "solver" is where the tendencies are initialized to zero, some pre-physics terms are computed, and the time stepping occurs
- The calls to the physics schemes are made from a further call down the call tree — dyn_em/module_first_rk_step_part1.F

- Inside of solve_em and first_rk_step_part1, all of the data is located in the "grid" structure: grid%ht.
- The dimensions in solve_em and first_rk_step_part1 are "d" (domain), and "m" (memory):

ids, ide, jds, jde, kds, kde

ims, ime, jms, jme, kms, kme

- The "t" (tile) dimensions are computed in first_rk_step_part1 and passed to all drivers.
- WRF uses global indexing

- If you are interested in looking at physics, the WRF system has organized the files in the WRFV3/phys directory.
- In WRFV3/phys, each type of physics has a driver:

module_cumulus_driver.Fcumodule_microphysics_driver.Fmpmodule_pbl_driver.Fblmodule_radiation_driver.Framodule_surface_driver.Fsf

• The subgrid-scale precipitation (*_cu_*.F)

module_cu_bmj.F module_cu_g3.F module_cu_kf.F module_cu_nsas.F module_cu_sas.F

module_cu_camzm.F
module_cu_gd.F
module_cu_kfeta.F
module_cu_osas.F
module_cu_tiedtke.F

• Advection

WRFV3/dyn_em/module_advect_em.F

• Lateral boundary conditions WRFV3/dyn_em/module_bc_em.F

- Compute various RHS terms, pressure gradient, buoyancy, w damping, horizontal and vertical diffusion, Coriolis, curvature, Rayleigh damping WRFV3/dyn_em/module_big_step_utilities_em.F
- All of the sound step utilities to advance u, v, mu, t, w within the small time-step loop WRFV3/dyn_em/module_small_step_em.F

WRF Software Overview

- Architecture
- Directory structure
- Model Layer Interface
- Data Structures
- I/O

WRF Model Layer Interface – The Contract with Users

All state arrays passed through argument list as simple (not derived) data types

Domain, memory, and run dimensions passed unambiguously in three dimensions

Model layer routines are called from mediation layer (physics drivers) in loops over tiles, which are multi-threaded



WRF Model Layer Interface – The Contract with Users

Restrictions on Model Layer subroutines:

No I/O, communication

No stops or aborts Use wrf_error_fatal

No common/module storage of decomposed data

Spatial scope of a Model Layer call is one "tile"



WRF Model Layer Interface

```
SUBROUTINE driver for some physics suite (
!$OMP DO PARALLEL
  DO ij = 1, numtiles
     its = i start(ij) ; ite = i end(ij)
      jts = j start(ij) ; jte = j end(ij)
     CALL model subroutine (arg1, arg2, . . .
           ids , ide , jds , jde , kds , kde ,
           ims , ime , jms , jme , kms , kme ,
           its , ite , jts , jte , kts , kte )
  END DO
END SUBROUTINE
```

WRF Model Layer Interface



WRF Model Layer Interface



```
! Executable code; loops run over tile
! dimensions
DO j = jts, MIN(jte,jde-1)
DO k = kts, kte
DO i = its, MIN(ite,ide-1)
loc1(i,k,j) = arg1(i,k,j) + ...
END DO
END DO
END DO
```



ids

logical domain







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Driver Layer Data Structures: Domain Objects

- Driver layer
 - All data for a domain is an object, a domain derived data type (DDT)
 - The domain DDTs are dynamically allocated/deallocated
 - Linked together in a tree to represent nest hierarchy; root pointer is head_grid, defined in frame/module_domain.F
 - Supports recursive depth-first traversal algorithm (frame/ module_integrate.F)



 Every Registry defined state, 11, 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.

Model Layer Data Structures: F77

- Model layer
 - All data objects are scalars and arrays of simple types only
 - Virtually all passed in through subroutine argument lists
 - Non-decomposed arrays and "local to a module" storage are permitted with an initialization at the model start

Mediation Layer Data Structures: Objects + F77

- Mediation layer
 - One task of mediation layer is to dereference fields from DDTs
 - Therefore, sees domain data in both forms, as DDT and as individual fields which are components of the DDTs
- The name of a data type and how it is referenced differs depending on the level of the architecture

- WRF Data Taxonomy
 - State data
 - Intermediate data type 1 (I1)
 - Intermediate data type 2 (I2)
 - Heap storage (COMMON or Module data)

WRF Data Taxonomy

- State data
- Intermediate data type 1 (I1)

Defined in the Registry

- Intermediate data type 2 (I2)
- Heap storage (COMMON or Module)

- WRF Data Taxonomy
 - State data

|--|

- the physics Intermediate data type 2 (I2)
- subroutines Heap storage (COMMON or Module) on the

stack

 WRF Data Taxonomy State data 	Defined in the module top, typically
 Intermediate data type 1 (I1) 	look-up tables
 Intermediate data type 2 (I2) 	and routine
– Heap storage (COMMON or Module)	
	NO HORIZ
	DECOMPOSED
	DATA!
	Common
	blocks must
	not leave the
	Module.

Mediation/Model Layer Data Structures: State Data

- Duration: Persist between start and stop of a domain
- Represented as fields in domain data structure
 - Memory for state arrays are dynamically allocated, only big enough to hold the local subdomain's (ie. patch's) set of array elements
 - Always **memory** dimensioned
 - Declared in Registry using **state** keyword
- Only state arrays can be subject to I/O and Interprocessor communication

Mediation/Model Layer Data Structures: 11 Data

- Persist for the duration of a single time step in solve
- Represented as fields in domain data structure
 - Memory for I1 arrays are dynamically allocated, only big enough to hold the local subdomain's (ie. patch's) set of array elements
 - Always **memory** dimensioned
 - Declared in Registry using **11** keyword
 - Typically tendency fields computed, used, and discarded at the end of every time step
 - Are not used to impact I1 variables on a child domain

Model Layer Data Structures: I2 Data

- Persist for the duration of a call of the physics routine
- NOT contained within the DDT structure (no declarations in the Registry)
 - Memory for I2 arrays are dynamically allocated on subroutine entry, and automatically deallocated on exit
 - Local, intermediate dummy variables required for physics computations
 - If I2 arrays, then they are always **tile** dimensioned
 - Not declared in the Registry, not communicated, no IO, not passed back to the solver, do not exist (retain their previous value) between successive physics calls

Grid Representation in Arrays

- Increasing indices in WRF 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 WRF is IKJ (ARW), but this is a WRF Model convention, not a restriction of the WRF Software Framework (provides cache coherency, but long vectors possible)
- Output data has grid ordering independent of the ordering inside the WRF 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 nonstaggered dimension (also referred to as the "mass points"), there is always an extra cell on the end of the domain dimension

WRF Software Overview

- Architecture
- Directory structure
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• I/O

- Streams: pathways into and out of model
- Can be thought of as files, though that is a restriction
 - History + auxiliary output streams (10 and 11 are reserved for nudging)
 - Input + auxiliary input streams (10 and 11 are reserved for nudging)
 - Restart, boundary, and a special DA in-out stream
 - Currently, 24 total streams
 - Use the large values and work down to stay away from "used"

- Attributes of streams
 - Variable set
 - The set of WRF state variables that comprise one read or write on a stream
 - Defined for a stream at compile time in Registry
 - Format
 - The format of the data outside the program (e.g. NetCDF), split
 - Specified for a stream at run time in the namelist

- Attributes of streams
 - Additional namelist-controlled attributes of streams
 - Dataset name
 - Time interval between I/O operations on stream
 - Starting, ending times for I/O (specified as intervals from start of run)

- Attributes of streams
 - Mandatory for stream to be used:
 - Time interval between I/O operations on stream
 - Format: io_form

Outline - Review

- Introduction
 - WRF started 1998, clean slate, Fortran + C
 - Targeted for research and operations
- WRF Software Overview
 - Hierarchical software layers
 - Patches (MPI) and Tiles (OpenMP)
 - Strict interfaces between layers
 - Contract with developers
 - I/O