WRF Software: Code and Parallel Computing

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Outline

- WRF architecture driver, mediation, model
- Need and design for parallelism
- Communication patterns to support parallelism
- Directory structure and file location overview
- Model layer interface
 - The "grid" struct
 - Indices
 - Dereferencing
- I/O

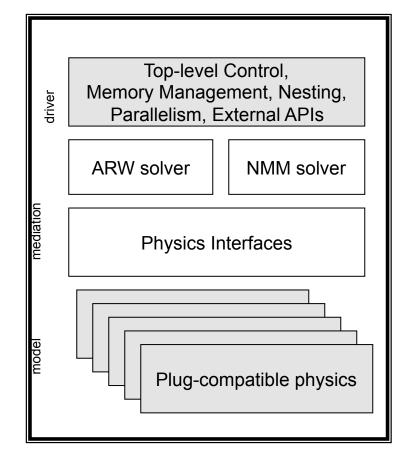
Introduction – WRF Software Characteristics

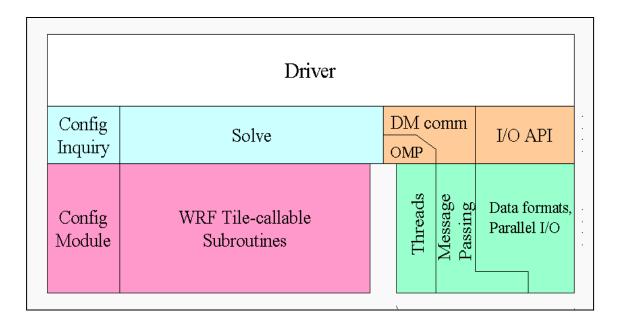
- Developed from scratch beginning around 1998, primarily Fortran and C
- Requirements emphasize flexibility over a range of platforms, applications, users, performance
- WRF develops rapidly. First released Dec 2000
- Supported by flexible efficient architecture and implementation called the WRF Software 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

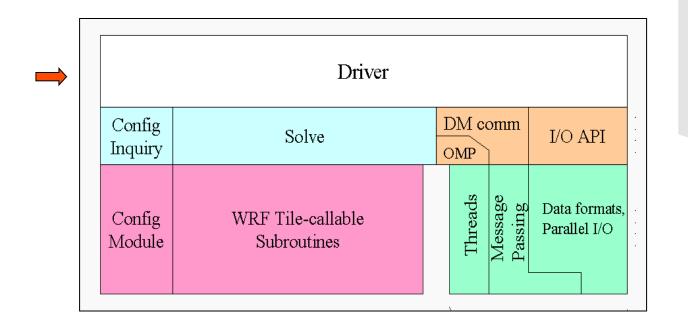
http://mmm.ucar.edu/wrf/WG2/bench/





Registry

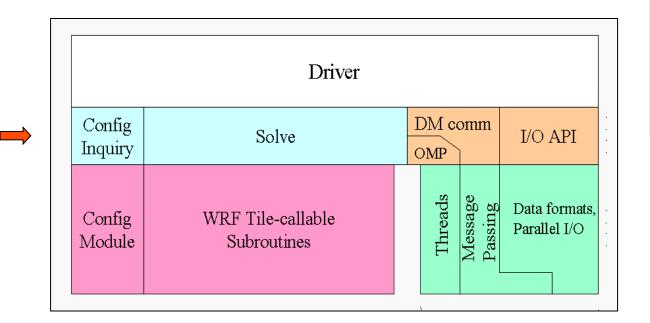
- Hierarchical software architecture
 - Insulate scientists' code from parallelism and other architecture/ implementation-specific details
 - Well-defined interfaces between layers, and external packages for communications, I/O, and model coupling facilitates code reuse and exploiting of community infrastructure, e.g. ESMF.



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

Registry

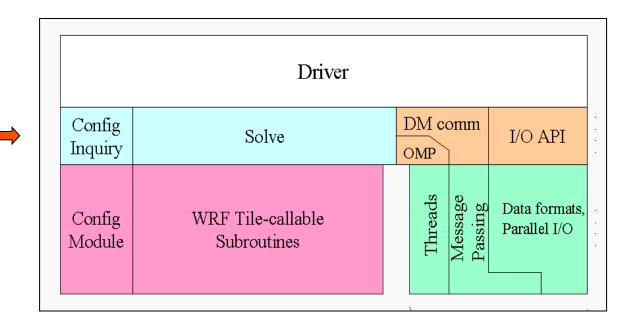
- **Time loop**: top level, algorithms for integration over nest hierarchy



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

Registry

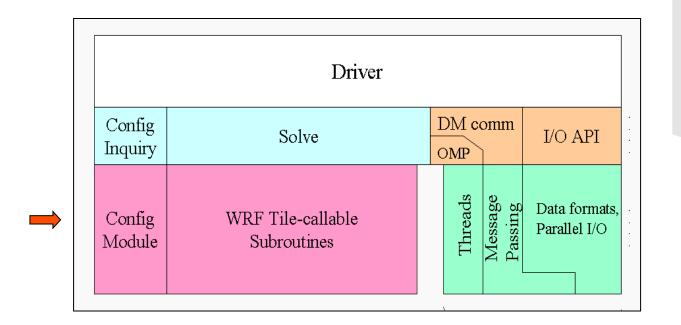
- Nest forcing, interpolation, and feedback routines



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

Registry

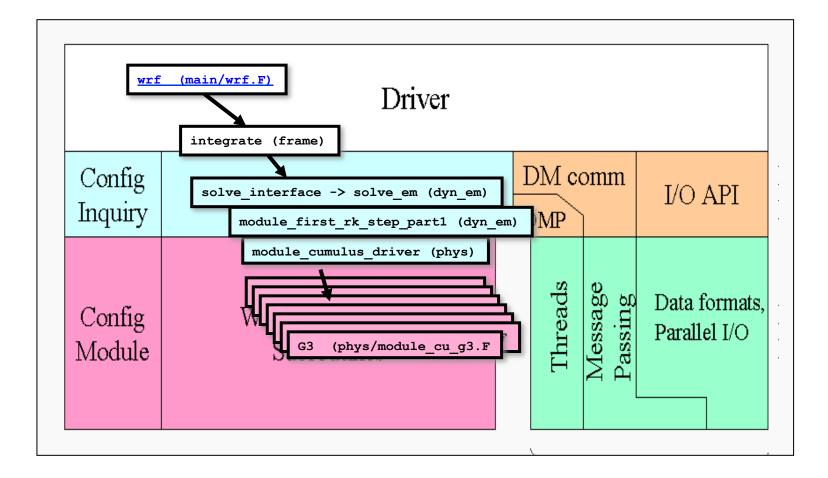
- Dereferences fields in calls to physics drivers and dynamics code
- Calls to message-passing are contained here as part of Solve routine



- 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

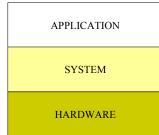
Registry

Call Structure Superimposed on Architecture



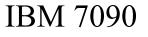


- The 'N' in NWP
- Components
 - Processor
 - A program counter
 - Arithmetic unit(s)
 - Some scratch space (registers)
 - Circuitry to store/retrieve from memory device
 - Cache
 - Memory
 - Secondary storage
 - Peripherals
- The implementation has been continually refined, but the basic idea hasn't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



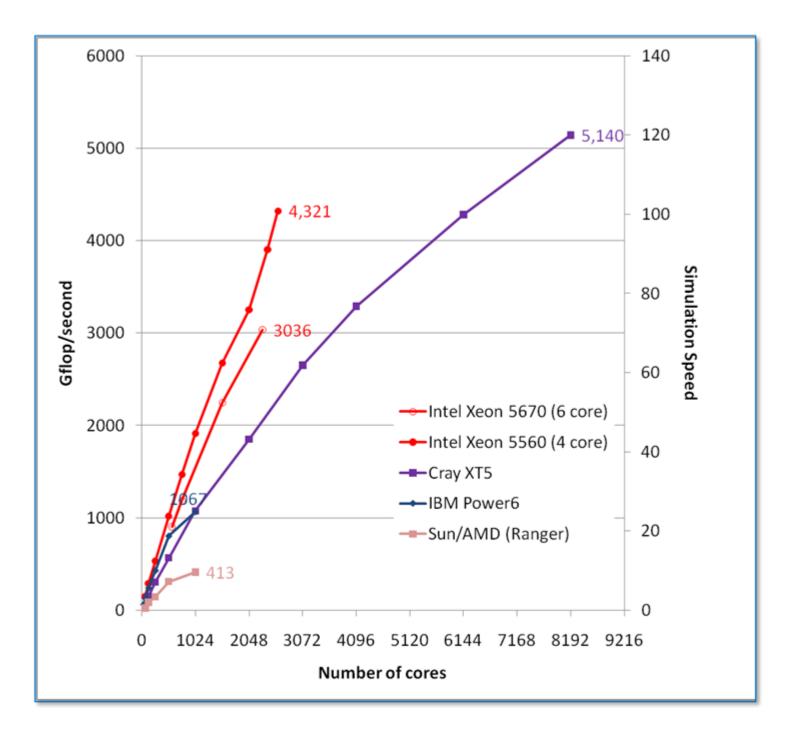
Dual core, 2.6 GHz chip 64-bit floating point precision 20 MB L3

~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

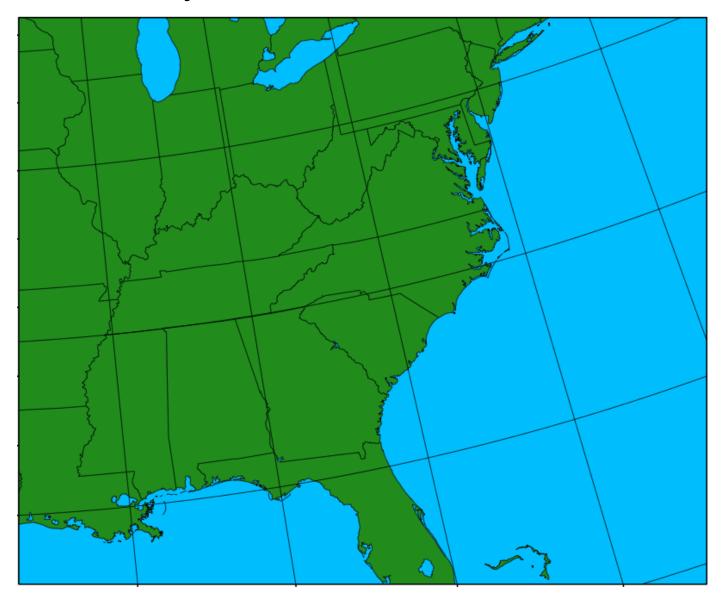
~1,000,000,000,000 flop/s ~2500 procs 48-h,12-km WRF CONUS in under 15 minutes



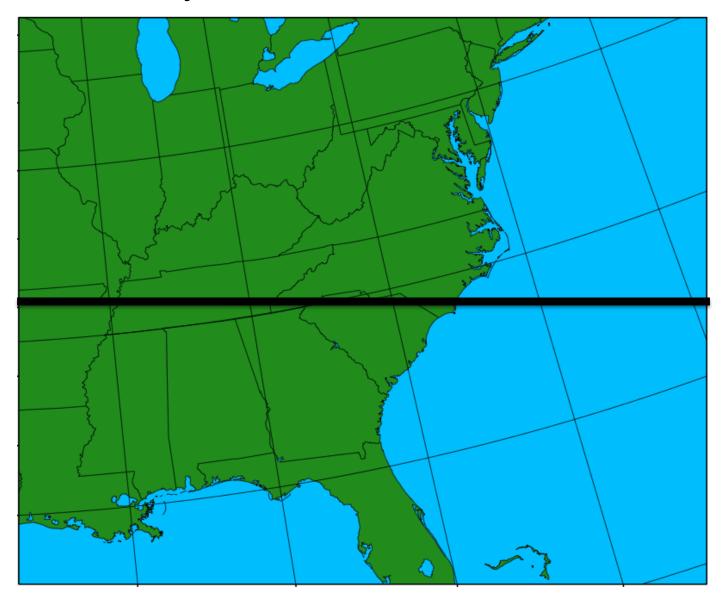
WRF Domain Decomposition

- The WRF model decomposes domains horizontally
- For *n* MPI tasks, the two nearest factors (*n*= *k* * *m*)are selected; the larger is used to decompose the y-direction, the smaller is used to decomposed the x-direction
- Users may choose a preferred decomposition (nproc_x, nproc_y)
- Prime numbers and composites with large prime factors are usually to be avoided
- The behavior of 132 vs 131, and 200 vs 202 are quite different

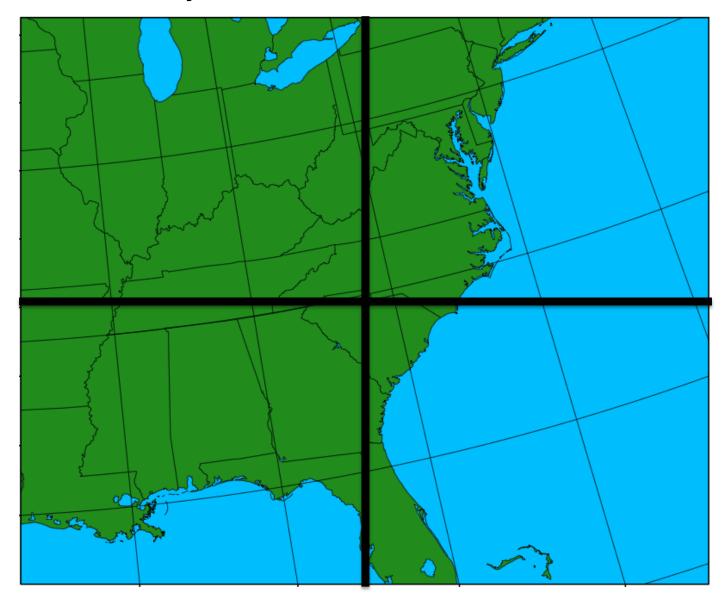
January 2000 Benchmark – 1 task: 74x61



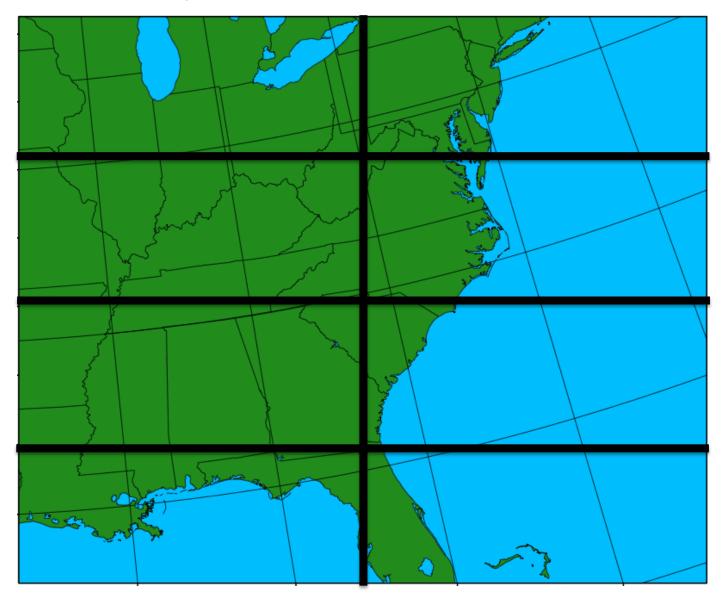
January 2000 Benchmark – 2 tasks: 74x31



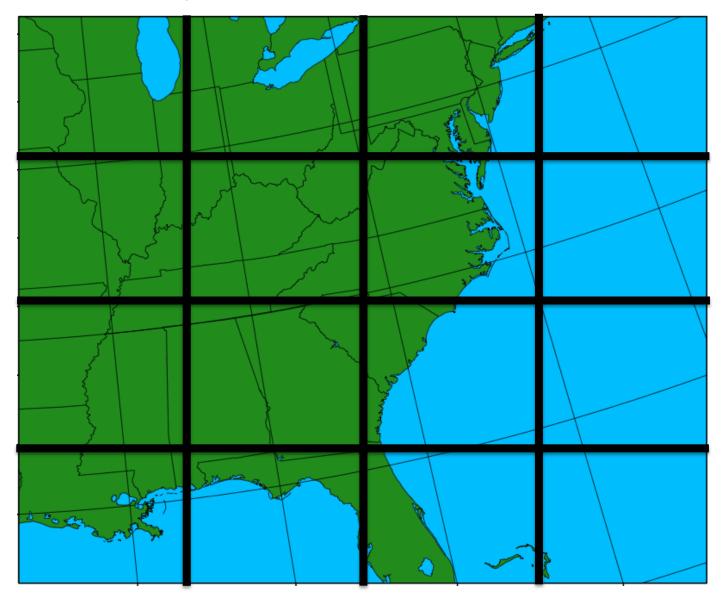
January 2000 Benchmark – 4 tasks: 37x31



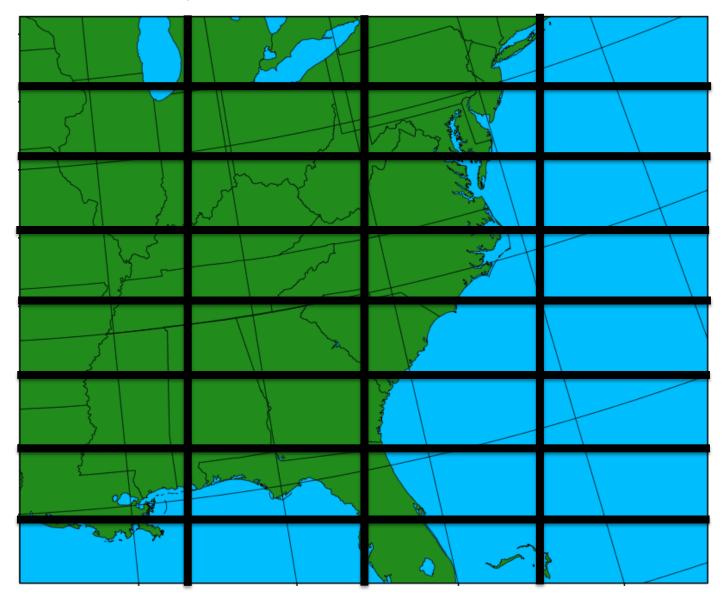
January 2000 Benchmark – 8 tasks: 37x16



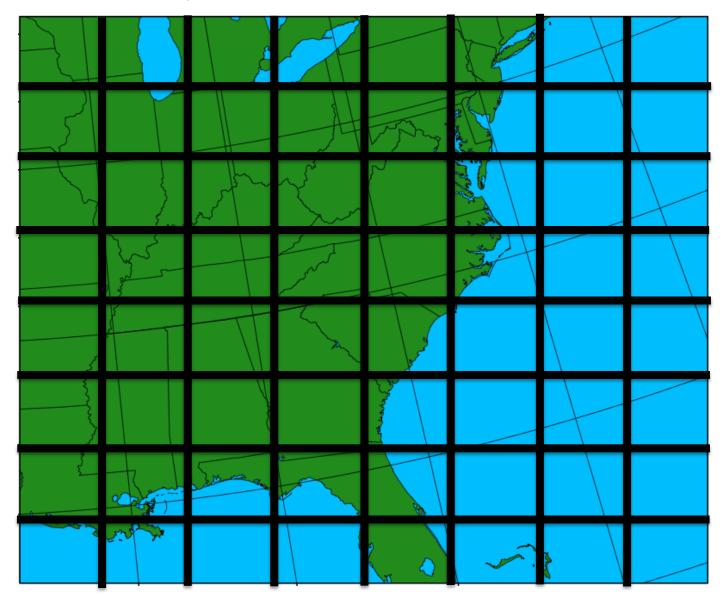
January 2000 Benchmark – 16 tasks: 19x16



January 2000 Benchmark – 32 tasks: 19x8



January 2000 Benchmark – 64 tasks: 10x8



WRF Domain Decomposition

- As you increase the number of total MPI tasks, you reduce the amount of work inside of each MPI task
- The amount of time to process communication between MPI tasks tends to be *at best* constant
- As more MPI tasks are involved, more contention for hardware resources due to communication is likely
- As the computation time gets smaller compared to the communications time, parallel efficiency suffers

January 2000 Benchmark

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

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

January 2000 Benchmark

WRF timing estimates may be obtained from the model print-out
 Serial

Timing for main on domain 1: 32.16074 elapsed seconds
OpenMP

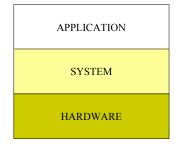
Timing for main on domain 1: 8.56216 elapsed seconds

Timing for main on domain 1: 7.36243 elapsed seconds

• Get enough time steps to include "day-time" radiation, and to have the microphysics "active" for better estimates

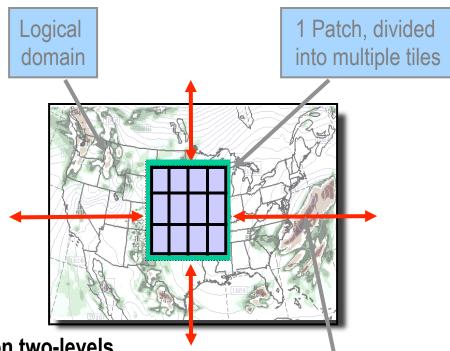


- WRF can be run serially or as a parallel job
- WRF uses *domain decomposition* to divide total amount of work over parallel processes



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)-
                                                                 3
                    (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)
                                                                 3
                              )/dzetaw(k)
                                                                 3
ENDDO
```

ENDDO

ENDDO

```
(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)-
                                                                 3
                    (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)
                                                                 3
                              )/dzetaw(k)
                                                                 3
ENDDO
ENDDO
```

ENDDO

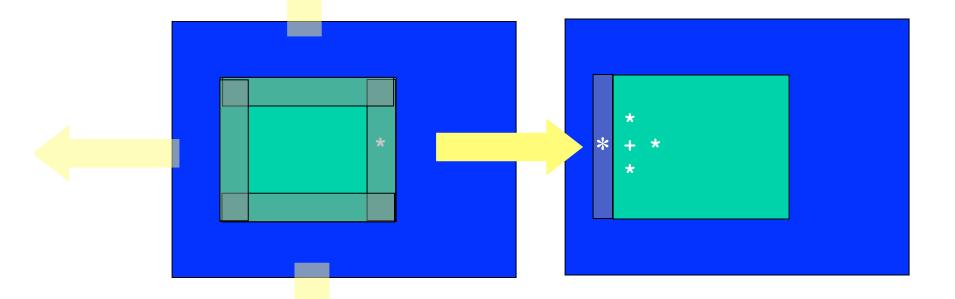
```
(module diffusion.F )
SUBROUTINE horizontal diffusion s (tendency, rr, var, . . .
  DO j = jts,jte
   DO k = kts, ktf
   DO i = its, ite
      mrdx=msft(i,j)*rdx
      mrdy=msft(i,j)*rdy
      tendency(i,k,j) =tendency(i,k,j) -
                                                                   &
            (mrdx*0.5*((rr(i+1,k,j)+rr(i,k,j))*H1(i+1,k,j)-
                                                                   &
                       (rr(i-1,k,j)+rr(i,k,j))*H1(i,k,j)+
                                                                   £
            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)
                                                                   3
                                 )/dzetaw(k)
                                                                   3
```

ENDDO ENDDO

ENDDO

APPLICATION
SYSTEM
HARDWARE

Halo updates

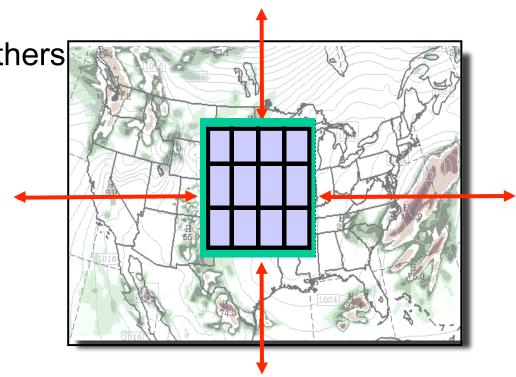


memory on one processor

memory on neighboring processor

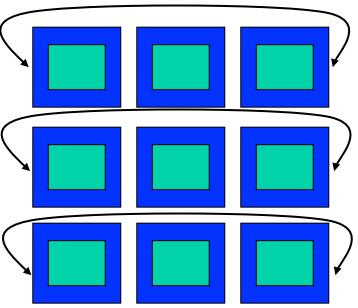
APPLICATION
SYSTEM
HARDWARE

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

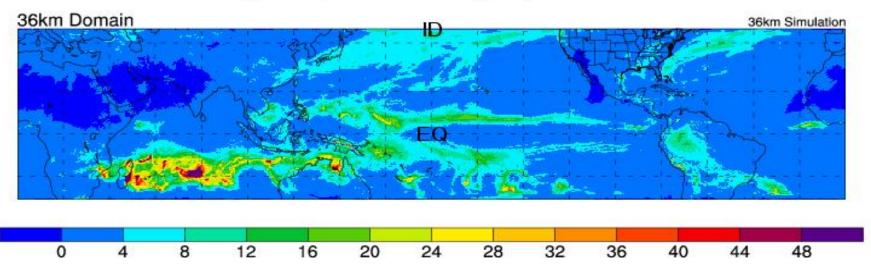


APPLICATION
SYSTEM
HARDWARE

- Halo updates
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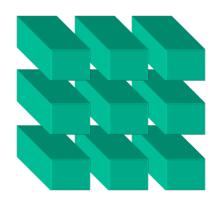


Average Daily Total rainfall (mm) - March 1997

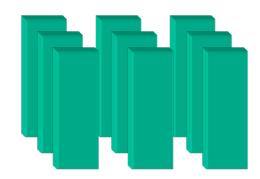


APPLICATION
SYSTEM
HARDWARE

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



all y on patch



all z on patch

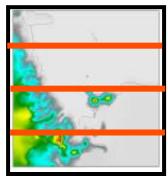


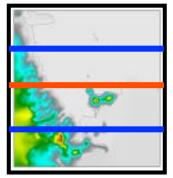
all x on patch

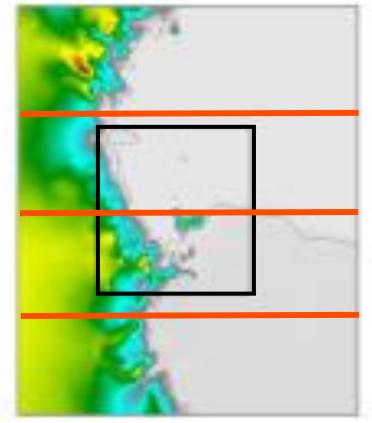
APPLICATION
SYSTEM
HARDWARE

Distributed Memory (MPI) Communications

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







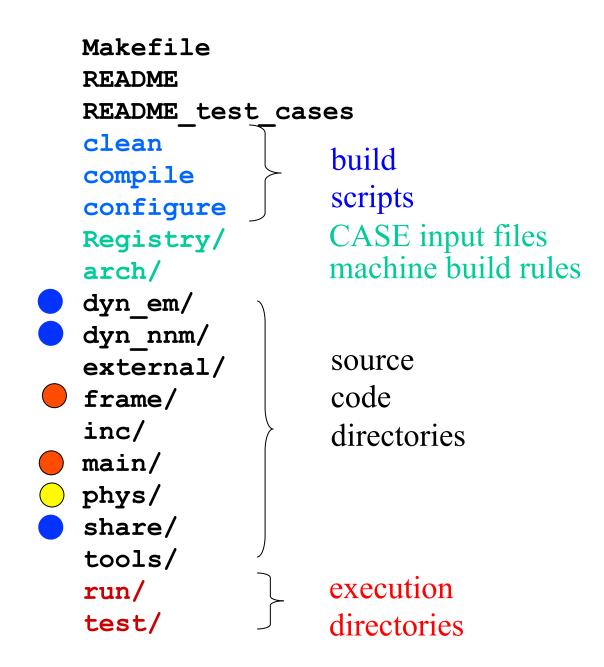
COARSE Ross Island 6.66 km

NEST:2.22 km

INTERMEDIATE: 6.66 km

WRF Model Top-Level Directory Structure

WRF Design and Implementation Doc, p 5 DRIVER MEDIATION MODEL



\$(FC) -o \$@ -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?

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

• 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 most of 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.F	CU
module_microphysics_driver.F	mp
module_pbl_driver.F	bl
module_radiation_driver.F	ra
module_surface_driver.F	sf

• 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 timestep loop

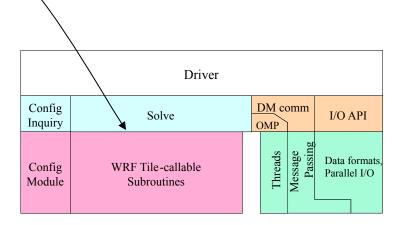
WRFV3/dyn_em/module_small_step_em.F

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

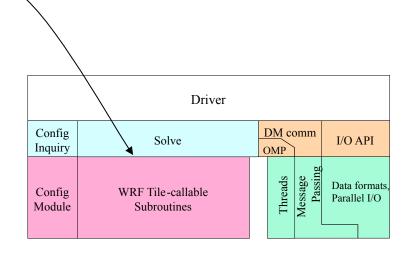
Restrictions on Model Layer subroutines:

No I/O, communication

No stops or aborts Use wrf_error_fatal

No common/module storage of decomposed data

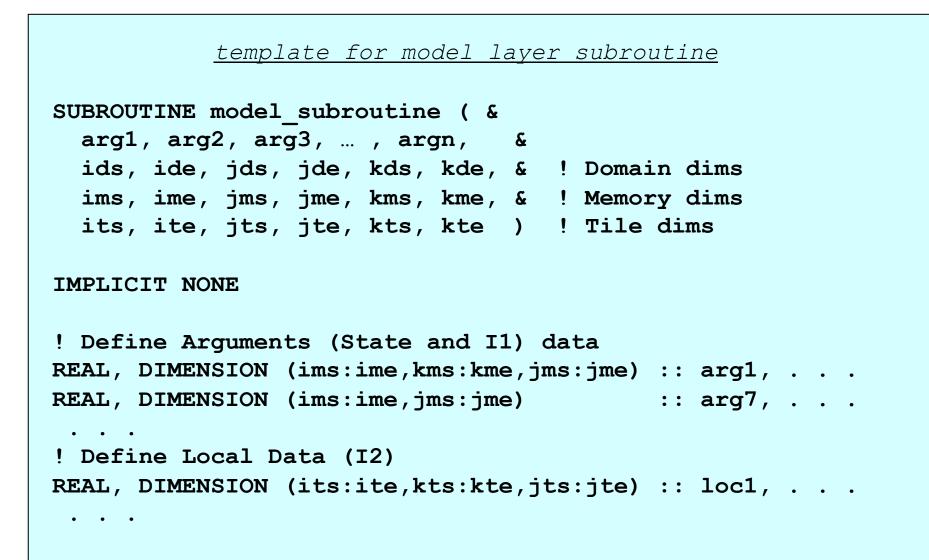
Spatial scope of a Model Layer call is one "tile"



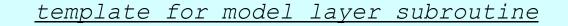
WRF Model Layer Interface

```
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
```

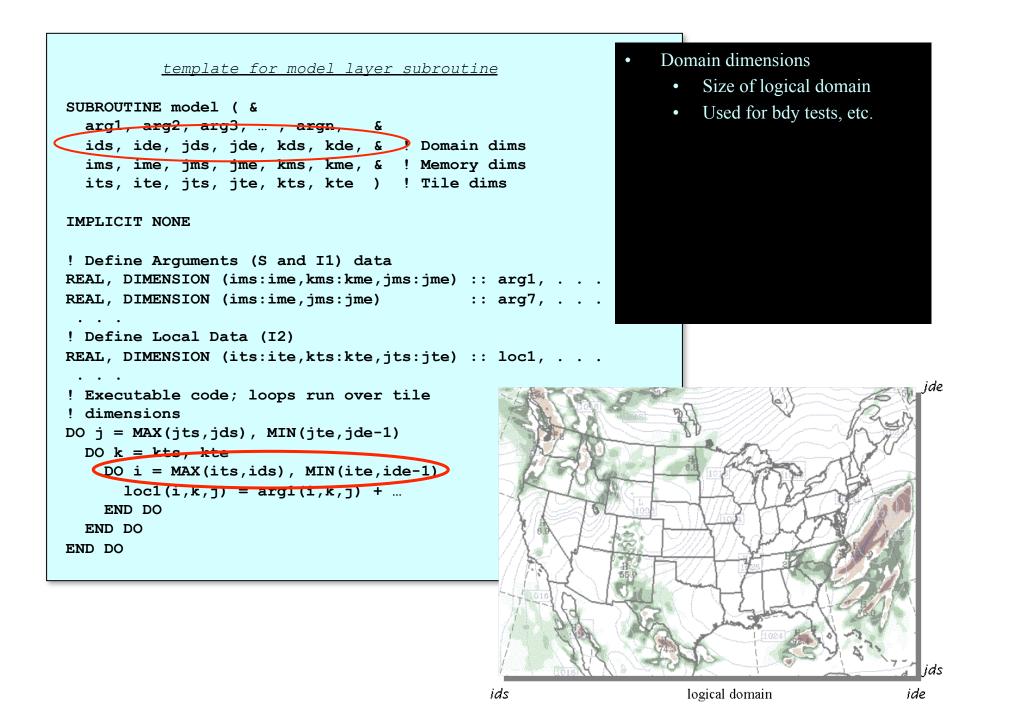
WRF Model Layer Interface

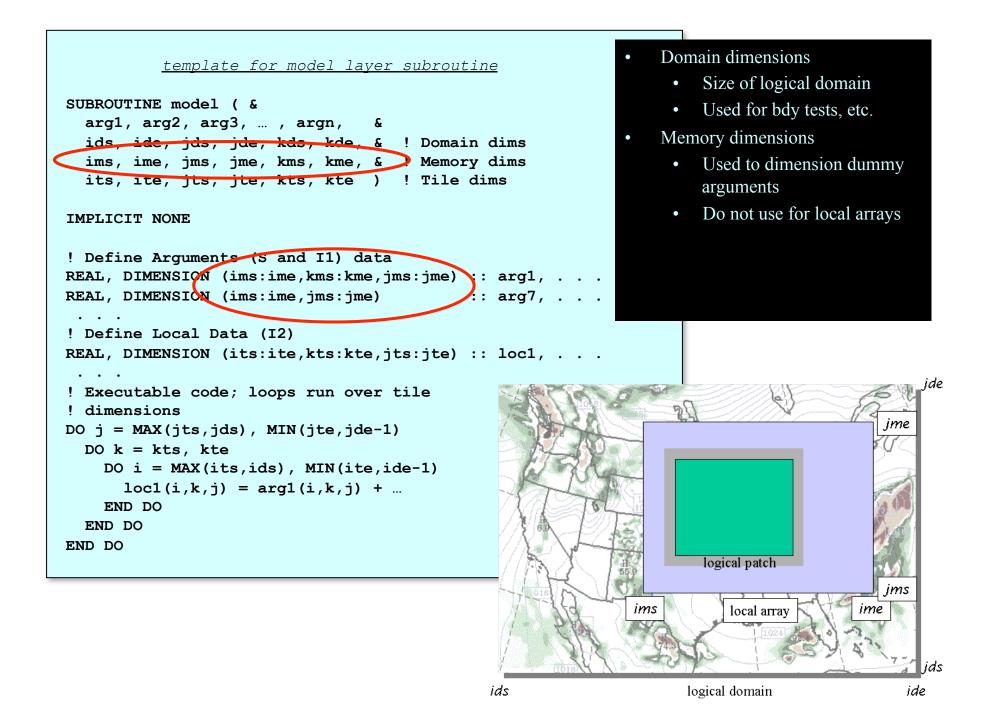


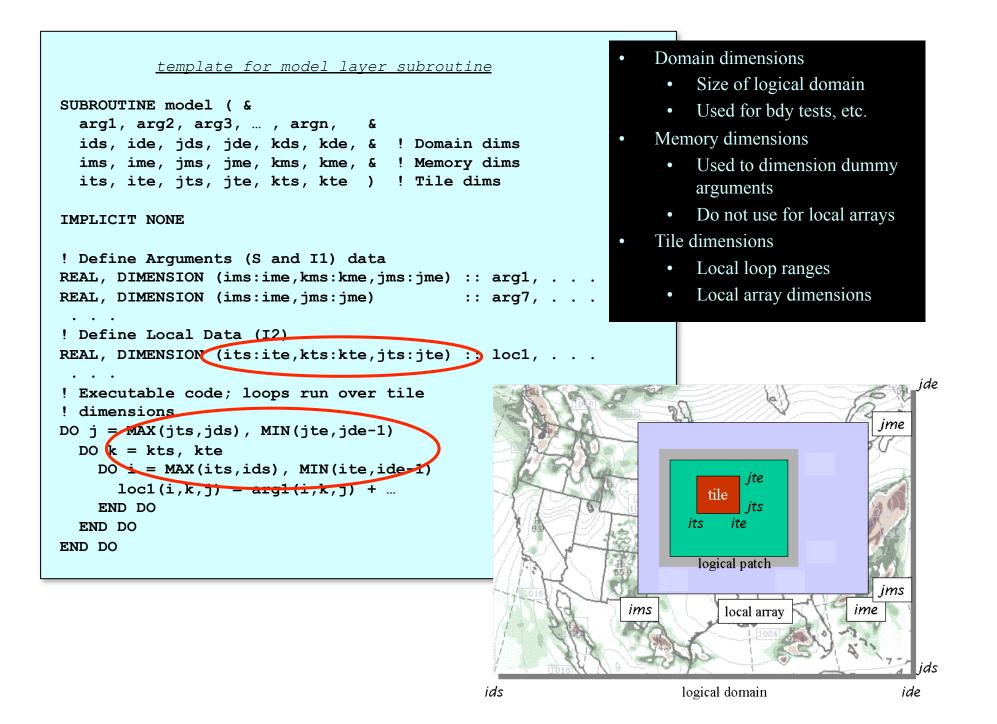
WRF Model Layer Interface

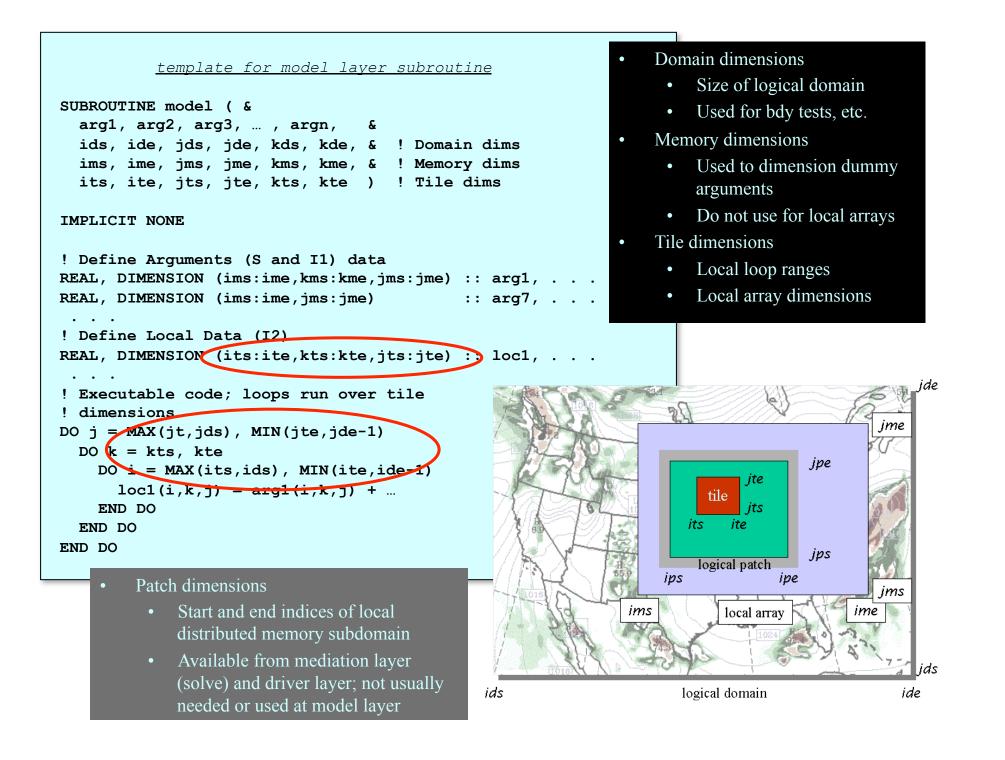


```
! Executable code; loops run over tile
! dimensions
DO j = jts, MIN(jte,jde-1)
DO k = kts, kte
DO i = its, MIN(ite,ide-1)
loc1(i,k,j) = arg1(i,k,j) + ...
END DO
END DO
END DO
```









- Streams (similar to Fortran units): 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"
 - Non-chemistry: use history streams 13-22, 24
 - Chemistry: use history streams 20, 21, 22, 24

- 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

```
Example 1: Add output without recompiling
• Edit the namelist.input file, the time_control namelist record
iofields_filename = "myoutfields.txt" (MAXDOM)
io_form_auxhist24 = 2 (choose an available stream)
auxhist24_interval = 10 (MAXDOM, every 10 minutes)
• Place the fields that you want in the named text file myoutfields.txt
+:h:24:RAINC, RAINNC
• Where "+" means ADD this variable to the output stream, "h" is the history
stream, and "24" is the stream number
```

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- Need and design for parallelism
- Communication patterns to support
 parallelism
- Directory structure and file location overview
- Model layer interface
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- I/O

Hierarchy

Driver allocation, time loop

Mediation

steps for 1 time loop call physics call dynamics handle nesting

Model

create new values tendency terms

- WRF architecture driver, mediation, model
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Even relatively small domains benefit from parallelism

Two types: DM — MPI, patches SM — OpenMP, tiles

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HALO – nearest neighbor

PERIOD – supporting periodic lateral boundaries

XPOSE – transpose (usually for FFTs)

NEST - intermediate domain

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- I/O

Most developers: dyn_em phys

Source is *.F

Post-cpp is *.f90

Physics schemes are a single module

Updates to dependency files for make

- WRF architecture driver, mediation, model
- Need and design for parallelism
- Communication patterns to support
 parallelism
- Directory structure and file location overview
- Model layer interface
 - The "grid" struct
 - Indices
 - Dereferencing
- I/O

The contract with developers concerning the model layer interface is important.

Adherence: parallelism I/O initialization

- WRF architecture driver, mediation, model
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Use history stream numbers from 13 to 22, 24

Chemistry 20, 21, 22, 24

Always put in an io_form and an interval in the namelist.input file for each stream