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

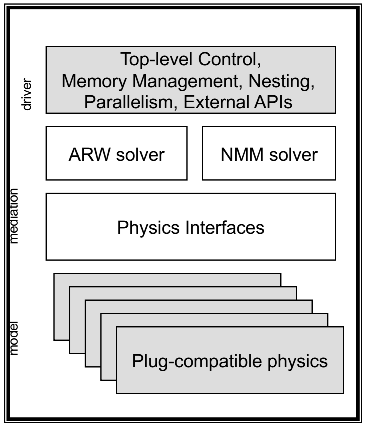
Introduction – WRF Software Characteristics

- 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

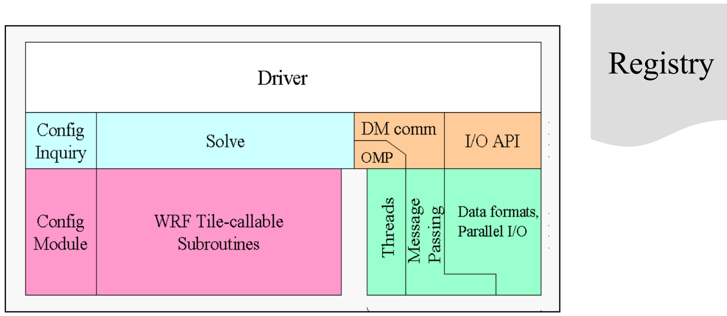
Introduction - WRF Software Framework Overview

- 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/

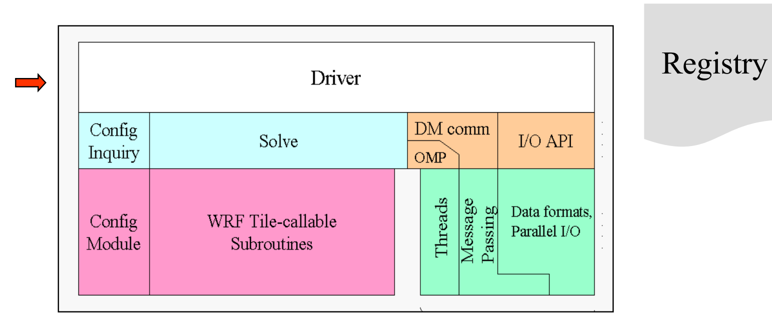


WRF Software Architecture



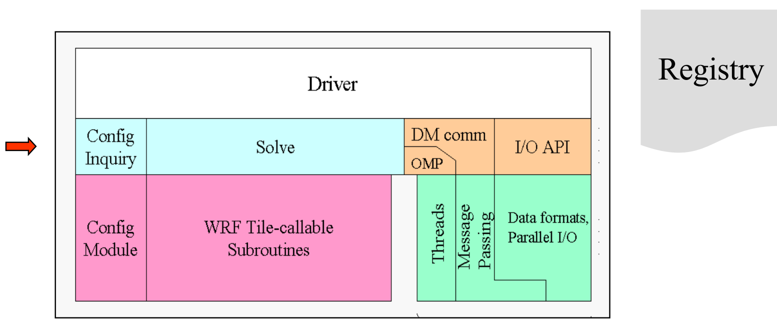
- Hierarchical software architecture
  - Insulate scientists' code from parallelism and other architecture/implementation-specific details
  - Well-defined interfaces between layers, and external packages for communications, I/O, and model coupling facilitates code reuse and exploiting of community infrastructure,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

WRF Software Architecture



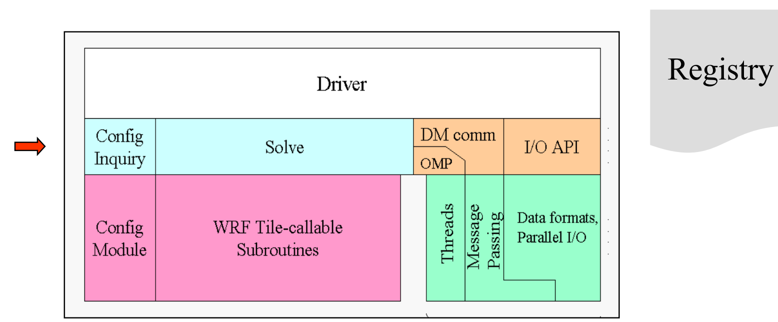
- Driver Layer
  - **Domains**: Allocates, stores, decomposes, represents abstractly as single data objects
  - **Time loop**: top level, algorithms for integration over nest hierarchy

WRF Software Architecture



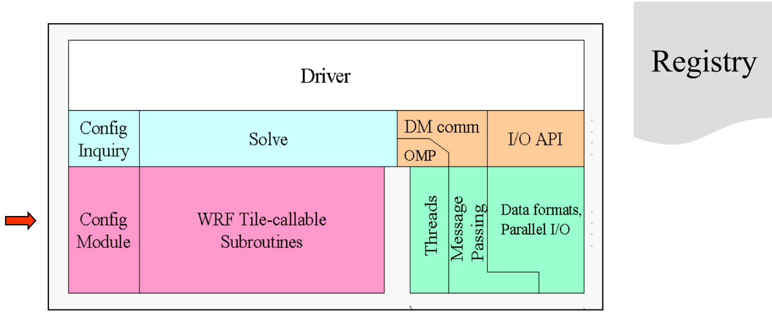
- Mediation Layer
  - Solve routine, takes a domain object and advances it one time step
  - Nest forcing, interpolation, and feedback routines

WRF Software Architecture



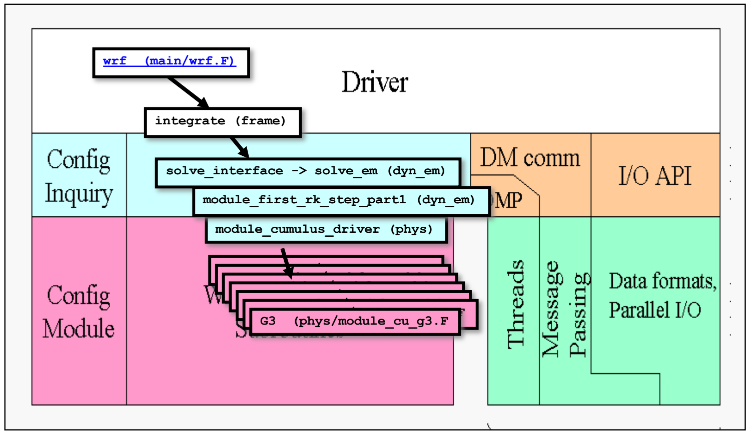
- Mediation Layer
  - The sequence of calls for doing a time-step for one domain is known in Solve routine
  - Dereferences fields in calls to physics drivers and dynamics code
  - Calls to message-passing are contained here as part of Solve routine

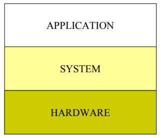
WRF Software Architecture



- 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

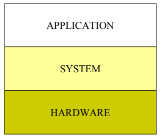
Call Structure Superimposed on Architecture





Hardware: The Computer

- 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

IBM 7090

6-way superscalar

36-bit floating point precision

~144 Kbytes

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

A computer in 2017

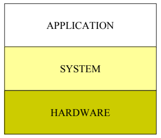
Dual core, 2.3 GHz chip

16 Flops/clock

64-bit floating point precision

20 MB L3

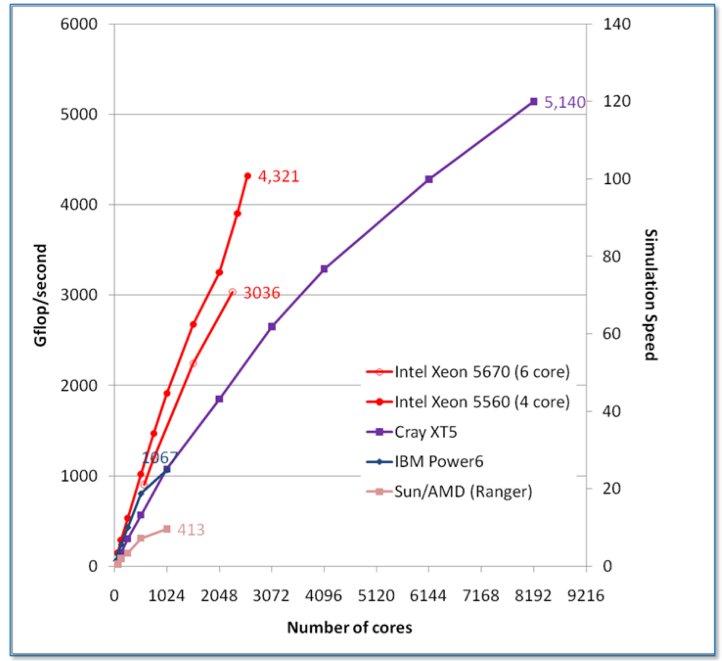
~5,000,000,000 flop/s
48 12km WRF CONUS in 26 Hours



…how we use it has

- 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 parallelism
  - Ganging multiple processors together to achieve $10^{11\text{-}12}$ flop/second
  - Aggregate available memories of $10^{11\text{-}12}$ bytes

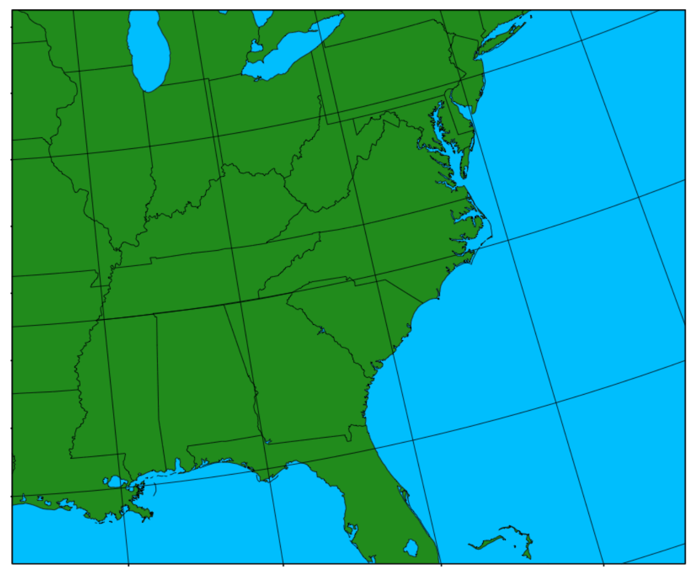
~1,000,000,000,000 flop/s ~2500 procs
48-h,12-km WRF CONUS in under 15 minutes



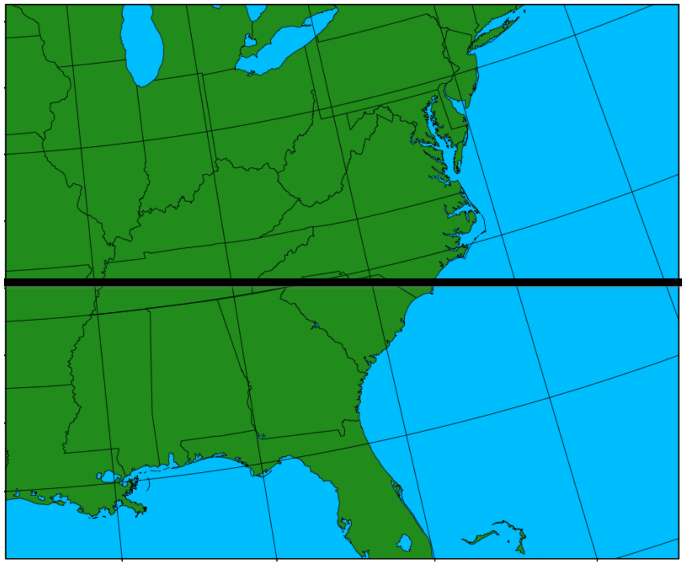
WRF Domain Decomposition

- 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

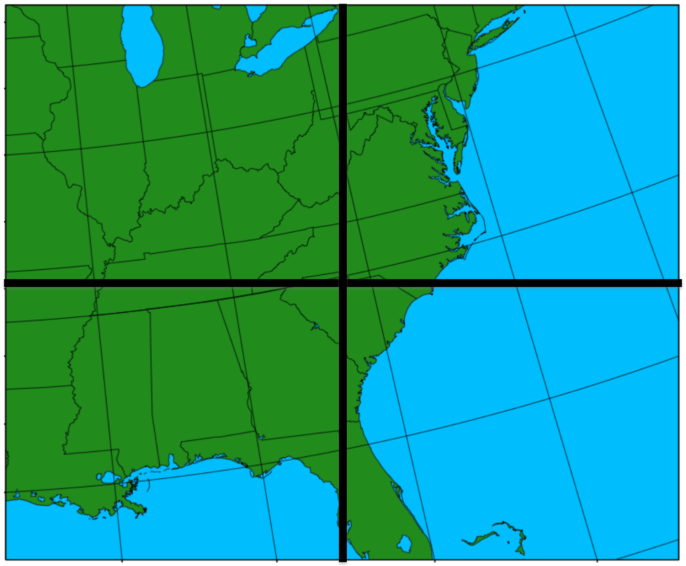
January 2000 Benchmark – 1 task: 74x61



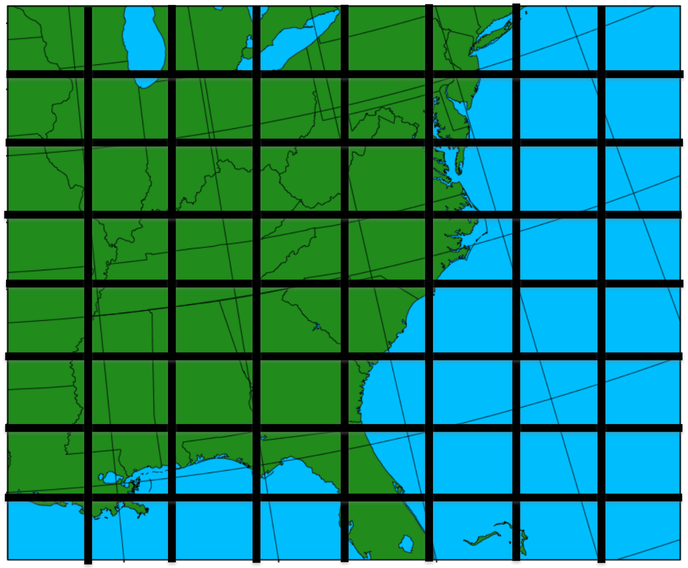
January 2000 Benchmark – 2 tasks: 74x31



January 2000 Benchmark – 4 tasks: 37x31



January 2000 Benchmark – 64 tasks: 10x8

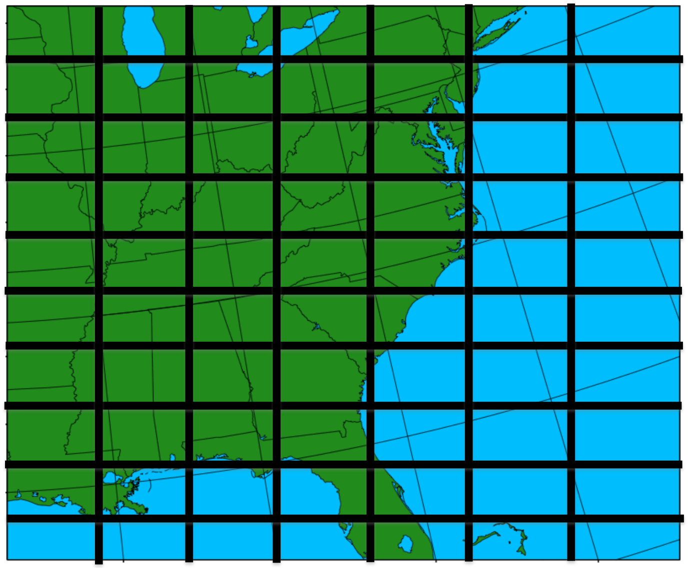


WRF Domain Decomposition

- Users may choose a preferred decomposition (nproc_x, nproc_y)

```
&domains
 nproc_x            =  7
 nproc_y            = 10
```

January 2000 Benchmark – 70 tasks



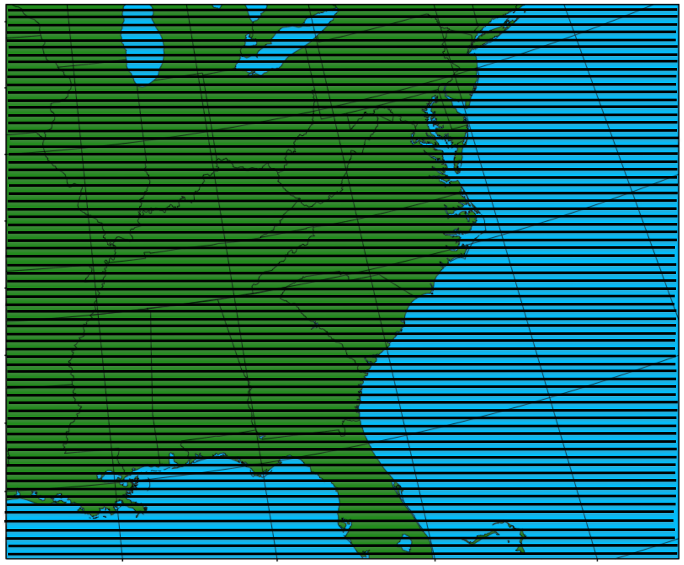
WRF Domain Decomposition

- Users may choose a preferred decomposition (nproc_x, nproc_y)

```
&domains
 nproc_x          =  7
 nproc_y          = 10
```

- Prime numbers and composites with large prime factors are usually to be avoided
- The behavior of 70 vs 71 is quite different

January 2000 Benchmark – 71 tasks



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 increase
- As the computation time gets smaller compared to the communications time, parallel efficiency suffers

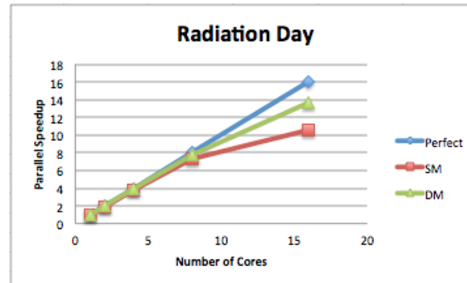
January 2000 Benchmark

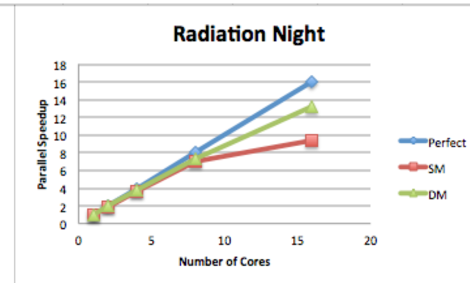
- 74x61 grid cells, 24 hour forecast, 3 minute time step
- IO excluded
- Timing partitioned
  - Local DAY Radiation step (17 time periods)
  - Local NIGHT Radiation step (24 time periods)
  - Not a Radiation step (432 time periods)

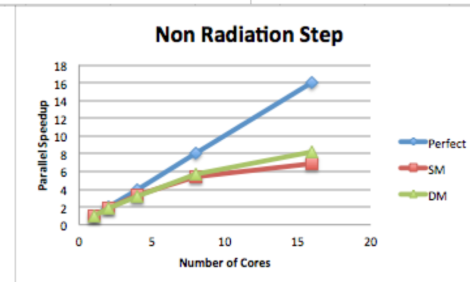
Decomposed domain sizes   proc count: I-dim x J-dim

1: 74x61   2: 74x31   4: 37x31   8: 37x16   16: 19x16

January 2000 Benchmark







January 2000 Benchmark

Radiation Day

Core Count	SM Efficiency	DM Efficiency
1 74x61	100	100
2 74x31	97	100
4 37x31	93	97
8 37x16	91	96
16 19x16	65	85

Avg 5.76 s

Std 0.019 s

n = 17

Radiation Night

Core Count	SM Efficiency	DM Efficiency
1 74x61	100	100
2 74x31	97	100
4 37x31	93	95
8 37x16	88	92
16 19x16	59	83

Avg 2.16 s

Std 0.005 s

n = 24

Not Radiation Timestep

Core Count	SM Efficiency	DM Efficiency
1 74x61	100	100
2 74x31	94	97
4 37x31	84	80
8 37x16	68	71
16 19x16	43	52

Avg 0.39 s

Std 0.012 s

n = 432

January 2000 Benchmark

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

Serial – 1 core, Day radiation step

```
Timing for main on domain   1:    5.77810 elapsed seconds
```

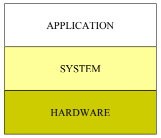
OpenMP – 8 cores, Day radiation step

```
Timing for main on domain   1:    0.83044 elapsed seconds
```

MPI – 16 cores, Day radiation step

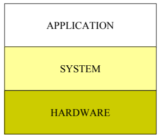
```
Timing for main on domain   1:    0.39633 elapsed seconds
```

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



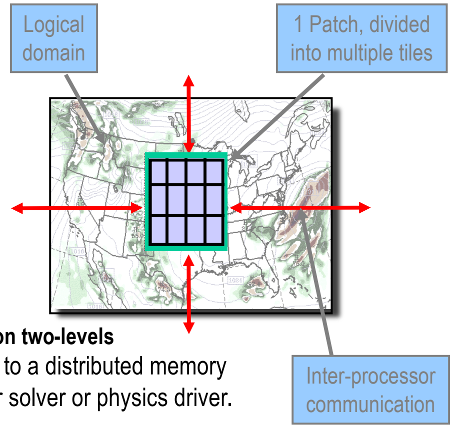
Application: WRF

- 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.

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

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 **rr**, **H1,** and **H2** arrays on right-hand side of assignment.

These are ***horizontal data dependencies*** 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

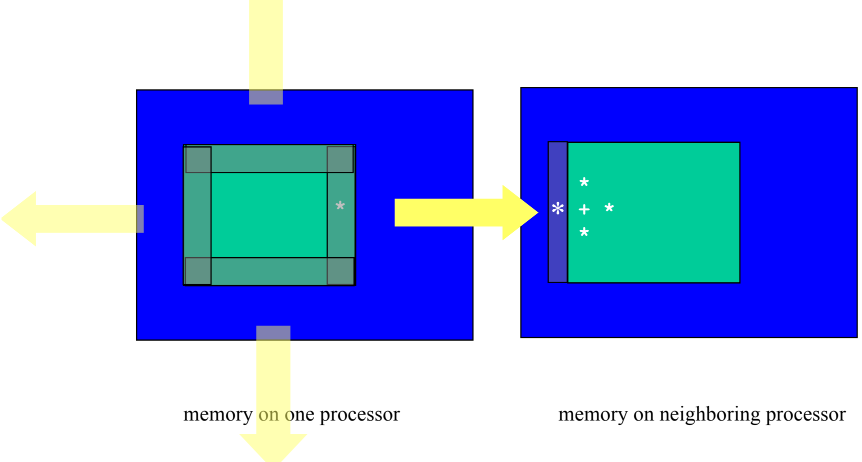
```
                              (module_diffusion.F )

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  ))-         &
            msft(i,j)*(H1avg(i,k+1,j)-H1avg(i,k,j)+                 &
                       H2avg(i,k+1,j)-H2avg(i,k,j)                  &
                                )/dzetaw(k)                         &
           )
   ENDDO
   ENDDO
   ENDDO
 . . .
```

APPLICATION
SYSTEM
HARDWARE

Distributed Memory MPI Communications

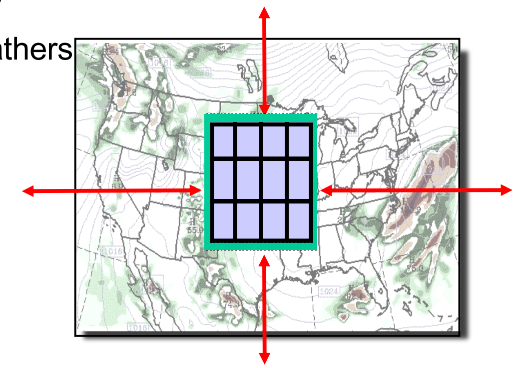
- Halo updates



APPLICATION
SYSTEM
HARDWARE

Distributed Memory (MPI) Communications

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



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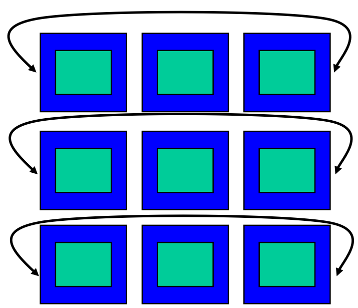

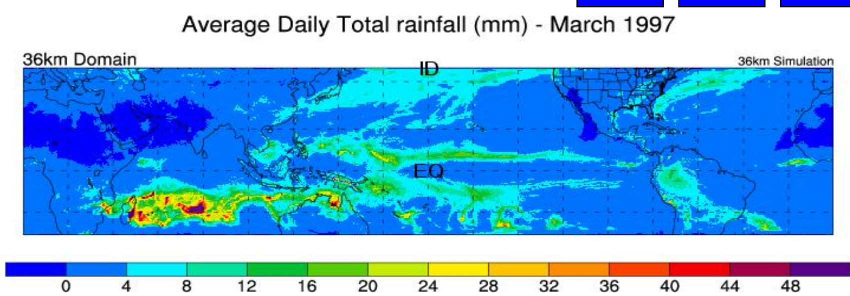

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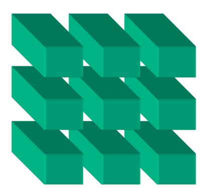
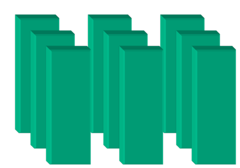
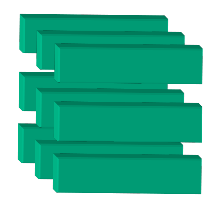


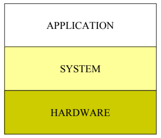
all y on patch



all z on patch



all x on patch



Distributed Memory (MPI) Communications

- Halo updates
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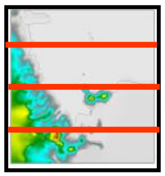
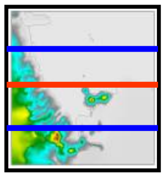
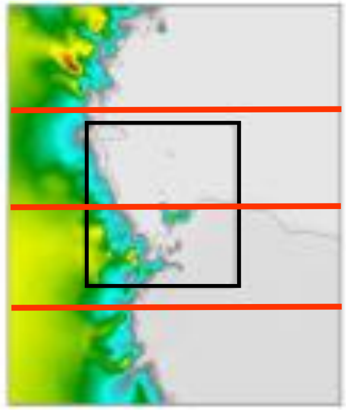
- Nesting scatters/gathers





NEST:2.22 km

INTERMEDIATE: 6.66 km



COARSE
Ross Island
6.66 km

WRF Model Top-Level Directory Structure

WRF Design and Implementation Doc, p 5

DRIVER ● (red)
MEDIATION ● (blue)
MODEL ● (yellow)

```
Makefile
README
README_test_cases
clean
compile        } build scripts
configure
Registry/        CASE input files
arch/            machine build rules
dyn_em/
dyn_nnm/
external/
frame/
inc/           } source code directories
main/
phys/
share/
tools/
run/           } execution directories
test/
```

(dyn_em/, dyn_nnm/, share/: blue; frame/, main/: red; phys/: yellow)

Where are WRF source code files located?

```
$(RM) $@

$(CPP) -I$(WRF_SRC_ROOT_DIR)/inc \
  $(CPPFLAGS) $(OMPCPP) $*.F  > $*.f90

$(FC) -o $@ -c $(FCFLAGS) $(MODULE_DIRS) \
  $(PROMOTION) $(FCSUFFIX) $*.f90
```

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
```

Where are WRF source code files located?

- 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.

Where are WRF source code files located?

- 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

Where are WRF source code files located?

- 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

Where are WRF source code files located?

- 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

Where are WRF source code files located?

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

module_cu_bmj.F	module_cu_camzm.F
module_cu_g3.F	module_cu_gd.F
module_cu_kf.F	module_cu_kfeta.F
module_cu_nsas.F	module_cu_osas.F
module_cu_sas.F	module_cu_tiedtke.F

Where are WRF source code files located?

- Advection
  - WRFV3/dyn_em/module_advect_em.F
- Lateral boundary conditions
  - WRFV3/dyn_em/module_bc_em.F

Where are WRF source code files located?

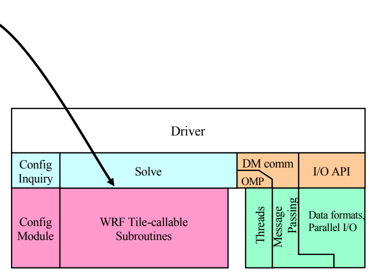
- Compute various RHS terms, pressure gradient, buoyancy, w damping, horizontal and vertical diffusion, Coriolis, curvature, Rayleigh damping
  - WRFV3/dyn_em/module_big_step_utilities_em.F
- All of the sound step utilities to advance u, v, mu, t, w within the small time-step loop
  - WRFV3/dyn_em/module_small_step_em.F

WRF 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

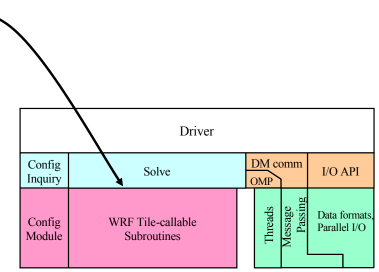
Restrictions on Model Layer subroutines:

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

template for model layer subroutine

```
SUBROUTINE model_subroutine ( &
  arg1, arg2, arg3, … , argn,    &
  ids, ide, jds, jde, kds, kde, &  ! Domain dims
  ims, ime, jms, jme, kms, kme, &  ! Memory dims
  its, ite, jts, jte, kts, kte  )  ! Tile dims

IMPLICIT NONE

! Define Arguments (State and I1) data
REAL, DIMENSION (ims:ime,kms:kme,jms:jme) :: arg1, . . .
REAL, DIMENSION (ims:ime,jms:jme)         :: arg7, . . .
 . . .
! Define Local Data (I2)
REAL, DIMENSION (its:ite,kts:kte,jts:jte) :: loc1, . . .
 . . .
```

WRF Model Layer Interface

template for model layer subroutine

```
. . .
! 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
```

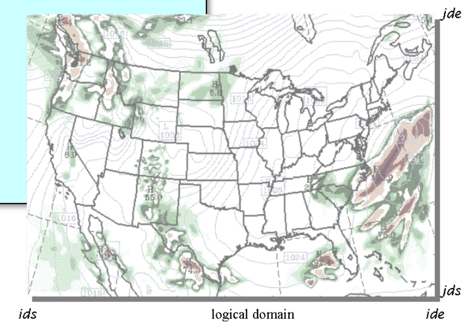
template for model layer subroutine

```
SUBROUTINE model ( &
  arg1, arg2, arg3, … , argn,    &
  ids, ide, jds, jde, kds, kde, & ! Domain dims
  ims, ime, jms, jme, kms, kme, & ! Memory dims
  its, ite, jts, jte, kts, kte  ) ! Tile dims

IMPLICIT NONE

! Define Arguments (S and I1) data
REAL, DIMENSION (ims:ime,kms:kme,jms:jme) :: arg1, . . .
REAL, DIMENSION (ims:ime,jms:jme)         :: arg7, . . .
 . . .
! Define Local Data (I2)
REAL, DIMENSION (its:ite,kts:kte,jts:jte) :: loc1, . . .
 . . .
! Executable code; loops run over tile
! dimensions
DO j = MAX(jts,jds), MIN(jte,jde-1)
  DO k = kts, kte
    DO i = MAX(its,ids), MIN(ite,ide-1)
      loc1(i,k,j) = arg1(i,k,j) + …
    END DO
  END DO
END DO
```

- Domain dimensions
  - Size of logical domain
  - Used for bdy tests, etc.



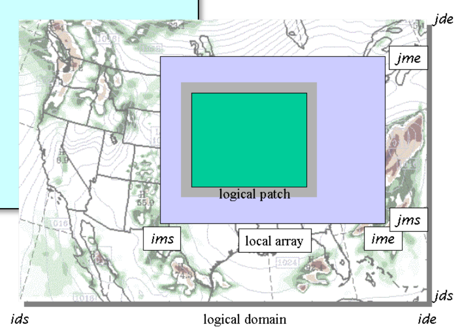
template for model layer subroutine

```
SUBROUTINE model ( &
  arg1, arg2, arg3, … , argn,    &
  ids, ide, jds, jde, kds, kde, & ! Domain dims
  ims, ime, jms, jme, kms, kme, & ! Memory dims
  its, ite, jts, jte, kts, kte  ) ! Tile dims

IMPLICIT NONE

! Define Arguments (S and I1) data
REAL, DIMENSION (ims:ime,kms:kme,jms:jme) :: arg1, . . .
REAL, DIMENSION (ims:ime,jms:jme)         :: arg7, . . .
 . . .
! Define Local Data (I2)
REAL, DIMENSION (its:ite,kts:kte,jts:jte) :: loc1, . . .
 . . .
! Executable code; loops run over tile
! dimensions
DO j = MAX(jts,jds), MIN(jte,jde-1)
  DO k = kts, kte
    DO i = MAX(its,ids), MIN(ite,ide-1)
      loc1(i,k,j) = arg1(i,k,j) + …
    END DO
  END DO
END DO
```

- Domain dimensions
  - Size of logical domain
  - Used for bdy tests, etc.
- Memory dimensions
  - Used to dimension dummy arguments
  - Do not use for local arrays



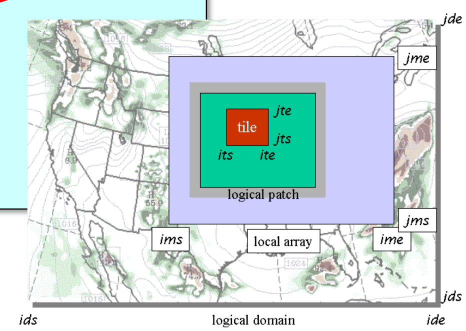
template for model layer subroutine

```
SUBROUTINE model ( &
  arg1, arg2, arg3, … , argn,    &
  ids, ide, jds, jde, kds, kde, & ! Domain dims
  ims, ime, jms, jme, kms, kme, & ! Memory dims
  its, ite, jts, jte, kts, kte  ) ! Tile dims

IMPLICIT NONE

! Define Arguments (S and I1) data
REAL, DIMENSION (ims:ime,kms:kme,jms:jme) :: arg1, . . .
REAL, DIMENSION (ims:ime,jms:jme)         :: arg7, . . .
 . . .
! Define Local Data (I2)
REAL, DIMENSION (its:ite,kts:kte,jts:jte) :: loc1, . . .
 . . .
! Executable code; loops run over tile
! dimensions
DO j = MAX(jts,jds), MIN(jte,jde-1)
  DO k = kts, kte
    DO i = MAX(its,ids), MIN(ite,ide-1)
      loc1(i,k,j) = arg1(i,k,j) + …
    END DO
  END DO
END DO
```

- Domain dimensions
  - Size of logical domain
  - Used for bdy tests, etc.
- Memory dimensions
  - Used to dimension dummy arguments
  - Do not use for local arrays
- Tile dimensions
  - Local loop ranges
  - Local array dimensions



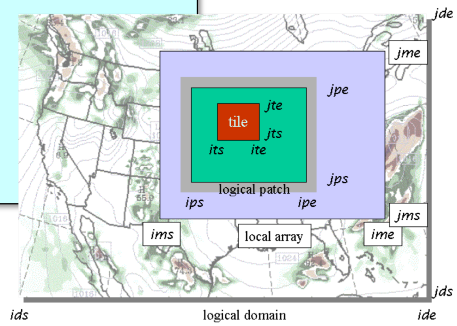
template for model layer subroutine

```
SUBROUTINE model ( &
  arg1, arg2, arg3, … , argn,    &
  ids, ide, jds, jde, kds, kde, &  ! Domain dims
  ims, ime, jms, jme, kms, kme, &  ! Memory dims
  its, ite, jts, jte, kts, kte  )  ! Tile dims

IMPLICIT NONE

! Define Arguments (S and I1) data
REAL, DIMENSION (ims:ime,kms:kme,jms:jme) :: arg1, . . .
REAL, DIMENSION (ims:ime,jms:jme)         :: arg7, . . .
 . . .
! Define Local Data (I2)
REAL, DIMENSION (its:ite,kts:kte,jts:jte) :: loc1, . . .
 . . .
! Executable code; loops run over tile
! dimensions
DO j = MAX(jt,jds), MIN(jte,jde-1)
  DO k = kts, kte
    DO i = MAX(its,ids), MIN(ite,ide-1)
      loc1(i,k,j) = arg1(i,k,j) + …
    END DO
  END DO
END DO
```

- Domain dimensions
  - Size of logical domain
  - Used for bdy tests, etc.
- Memory dimensions
  - Used to dimension dummy arguments
  - Do not use for local arrays
- Tile dimensions
  - Local loop ranges
  - Local array dimensions



- Patch dimensions
  - Start and end indices of local distributed memory subdomain
  - Available from mediation layer (solve) and driver layer; not usually needed or used at model layer

WRF I/O

- 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

WRF I/O

- 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

WRF I/O

- 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)

WRF I/O

- 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

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

Outline

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Hierarchy

Driver
 allocation, time loop

Mediation
 steps for 1 time loop
 call physics
 call dynamics
 handle nesting

Model
 create new values
 tendency terms

Outline

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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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Most developers:
dyn_em
phys

Source is *.F

Post-cpp is *.f90

Physics schemes are a single module

Updates to dependency files for make

Outline

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

Adherence:
parallelism
I/O
initialization

Outline

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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