John Michalakes, Head WRF Software Architecture
Michael Duda

Dave Gill

Outline

- Introduction
- Computing Overview
- WRF Software Overview

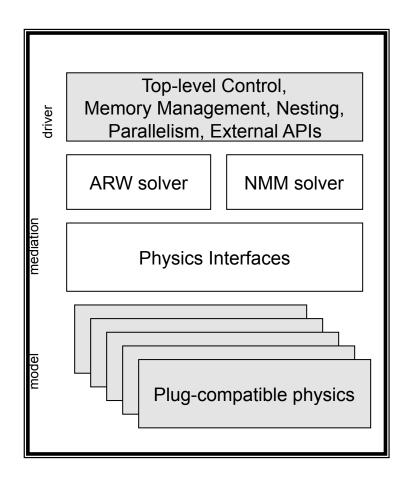
Introduction – WRF Software Characteristics

- 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 v3.3 (April 2011); next release WRF v3.3.1 (August 2011)
- Supported by flexible efficient architecture and implementation called the WRF Software Framework

Introduction - WRF Software Framework Overview

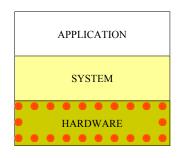
- Implementation of WRF Architecture
 - Hierarchical organization
 - Multiple dynamical cores
 - Plug compatible physics
 - Abstract interfaces (APIs) to external packages
 - Performance-portable
- Designed from beginning to be adaptable to today's computing environment for NWP

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



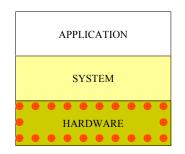
Outline

- Introduction
- Computing Overview
- WRF Software Overview



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

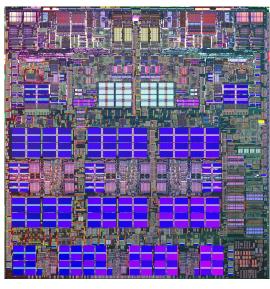
36-bit floating point precision

~144 Kbytes

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

A computer in 2008

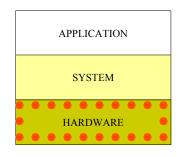




Dual core, 4.7 GHz chip 64-bit floating point precision 1.9 MB L2, 36 MB L3

Upto 16 GB per processor

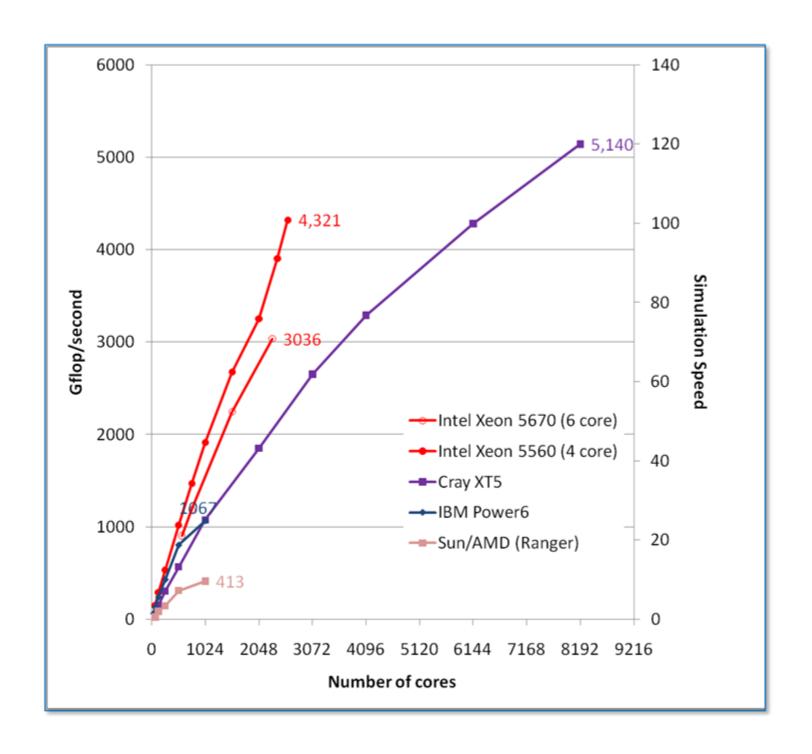
~5,000,000,000 flop/s
48 12km WRF CONUS in 52 Hours



...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
 - These are too slow and too small for even a moderately large NWP run today
- We make up the difference with <u>parallelism</u>
 - Ganging multiple processors together to achieve 10¹¹⁻¹² flop/second
 - Aggregate available memories of 10¹¹⁻¹² bytes

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



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

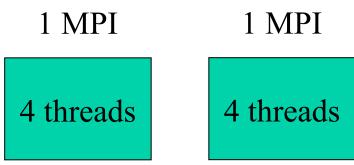
setenv OMP_NUM_THREADS 4
mpirun -np 4 wrf.exe

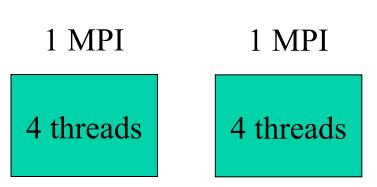
8 MPI processes, each with 2 threads

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





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?

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setenv OMP_NUM_THREADS 4
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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

2 MPI

2 threads

2 threads

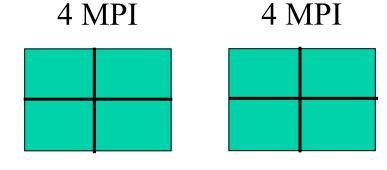
Examples

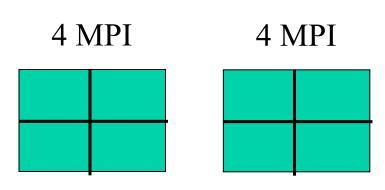
- If the machine consists of 4 nodes, each with 4 processors, how many different ways can you run a job to use all 16 processors?
 - 4 MPI processes, each with 4 threads

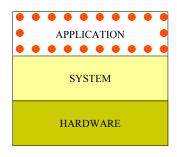
8 MPI processes, each with 2 threads

```
setenv OMP_NUM_THREADS 2
mpirun -np 8 wrf.exe
```

16 MPI processes, each with 1 thread

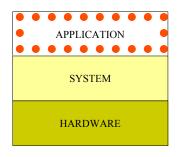






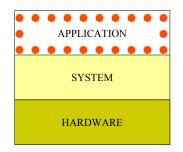
Application: WRF

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



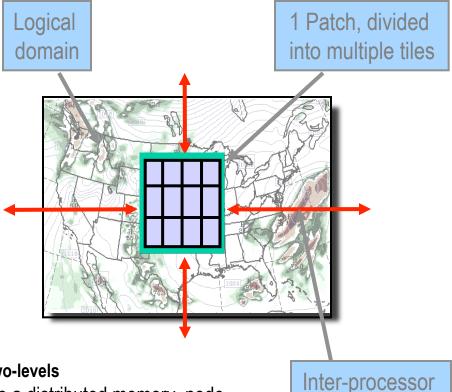
Application: WRF

- The decomposition of the application over processes has two levels:
 - The *domain* is first broken up into rectangular pieces that are assigned to MPI (distributed memory) processes. These pieces are called *patches*
 - The *patches* may be further subdivided into smaller rectangular pieces that are called *tiles*, and these are assigned to *shared-memory threads* within the process.



Parallelism in WRF: Multi-level Decomposition

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



communication

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

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.

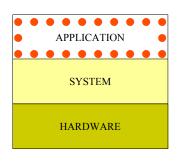
Following is an example code fragment that requires communication between patches

Signs in code

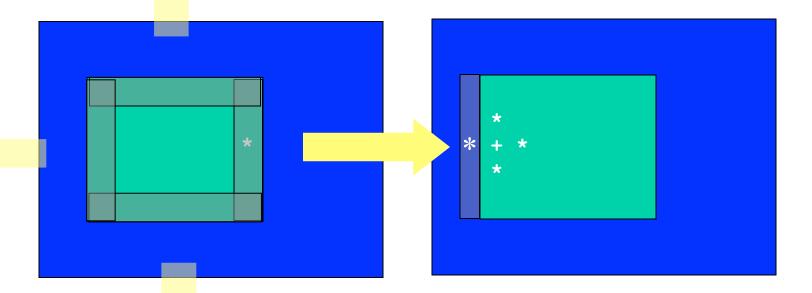
Note the tell-tale +1 and -1 expressions in indices for **rr**, **H1**, and **H2** arrays on right-hand side of assignment.

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.

```
(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)-
                                                                 æ
           (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))-
                                                                 æ
           msft(i,j)*(Hlavg(i,k+1,j)-Hlavg(i,k,j)+
                       H2avg(i,k+1,j)-H2avg(i,k,j)
                                )/dzetaw(k)
   ENDDO
   ENDDO
   ENDDO
```

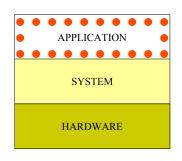


Halo updates

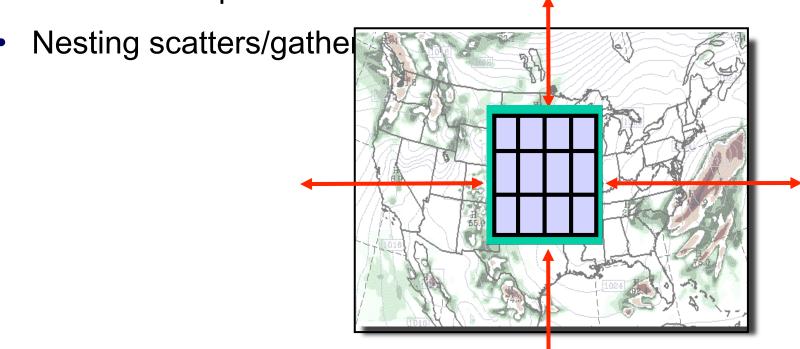


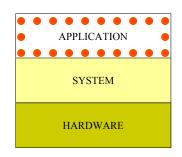
memory on one processor

memory on neighboring processor

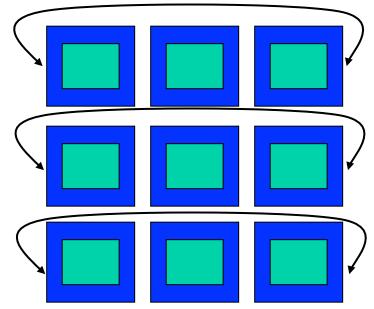


- Halo updates
- Periodic boundary updates
- Parallel transposes

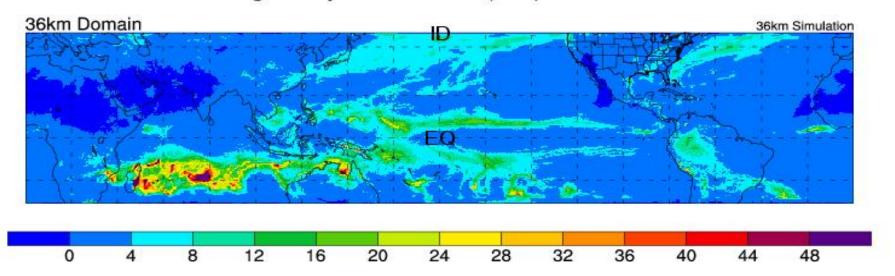


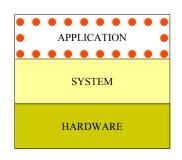


- Halo updates
- Periodic boundary updates
- Parallel transposes
- Nesting scatters/gathers

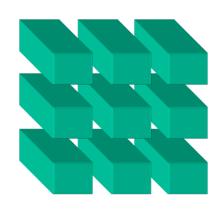


Average Daily Total rainfall (mm) - March 1997

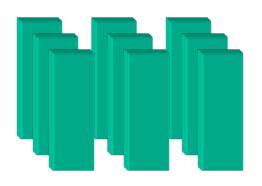




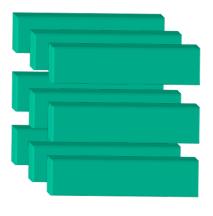
- Halo updates
- Periodic boundary updates
- Parallel transposes
- Nesting scatters/gathers



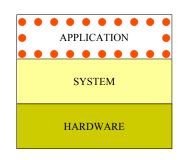
all y on patch



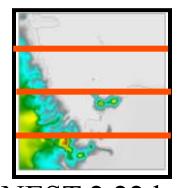
all z on patch



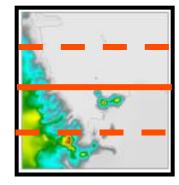
all x on patch



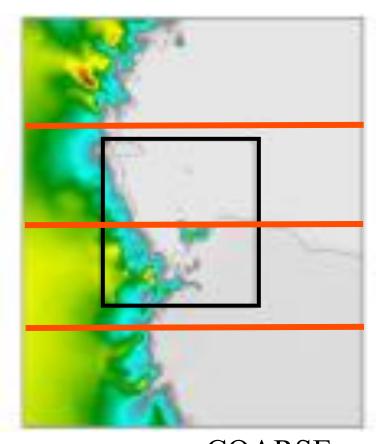
- Halo updates
- Periodic boundary updates
- Parallel transposes
- Nesting scatters/gathers



NEST:2.22 km



INTERMEDIATE: 6.66 km



COARSE Ross Island 6.66 km

Review – Computing Overview

Distributed Memory Parallel Shared Memory Parallel

APPLICATION (WRF)

SYSTEM (UNIX, MPI, OpenMP)

HARDWARE (Processors, Memories, Wires)

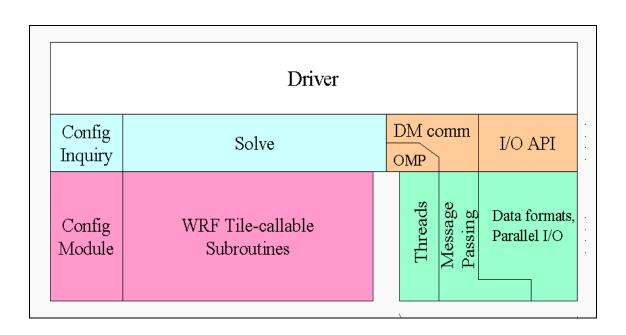
Domain	contains	Patches	contain	Tiles
Job	contains	Processes	contain	Threads
Cluster	contains	Nodes	contain	Processors

Outline

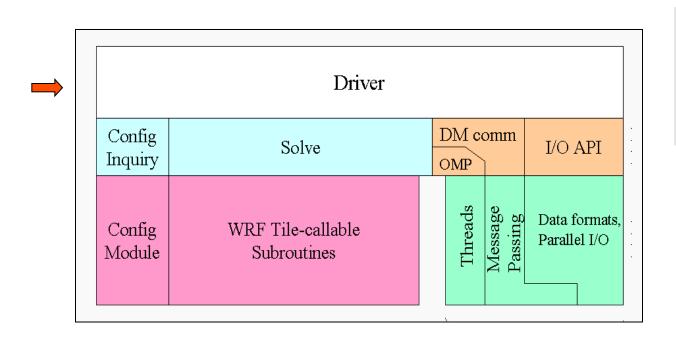
- Introduction
- Computing Overview
- WRF Software Overview

WRF Software Overview

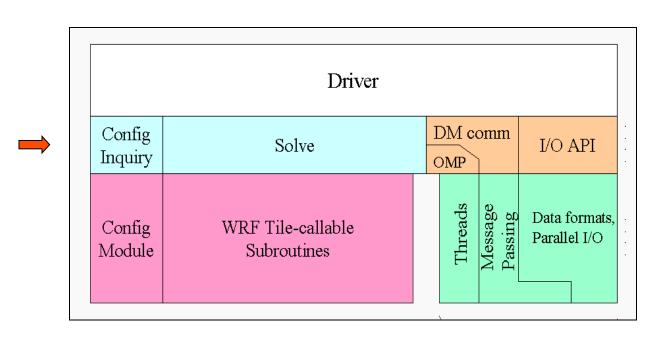
- Architecture
- Directory structure
- Model Layer Interface
- Data Structures
- I/O



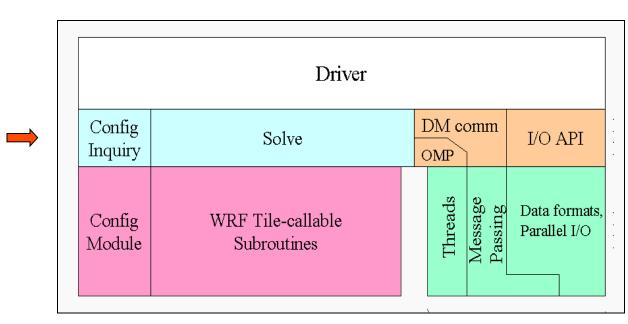
- Hierarchical software architecture
 - Insulate scientists' code from parallelism and other architecture/ implementation-specific details
 - Well-defined interfaces between layers, and external packages for communications, I/O, and model coupling facilitates code reuse and exploiting of community infrastructure,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



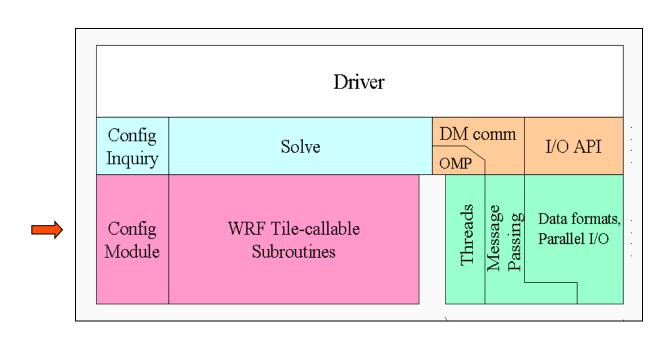
- Driver Layer
 - Domains: Allocates, stores, decomposes, represents abstractly as single data objects
 - Time loop: top level, algorithms for integration over nest hierarchy



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



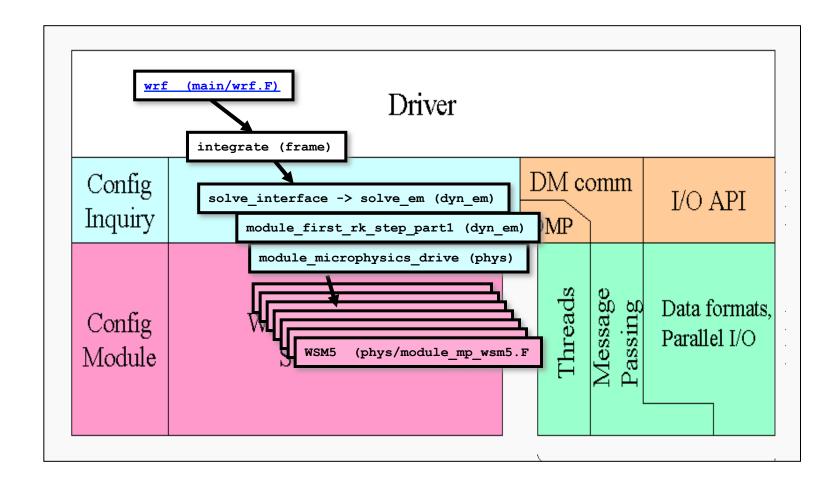
- Mediation Layer
 - The sequence of calls for doing a time-step for one domain is known in Solve routine
 - Dereferences fields in calls to physics drivers and dynamics code
 - Calls to message-passing are contained here as part of Solve routine



- 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

Call Structure Superimposed on Architecture

module microphysics driver (phys)



WRF Software Overview

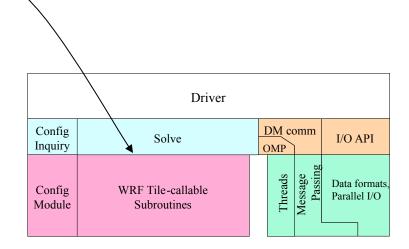
- Architecture
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WRF Model Layer Interface – The Contract with Users

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

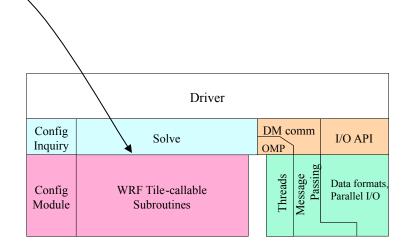
Restrictions on Model Layer subroutines:

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

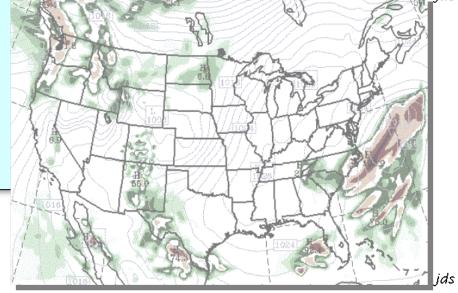
```
template for model layer subroutine

! Executable code; loops run over tile
! dimensions
DO j = 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
```

```
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.



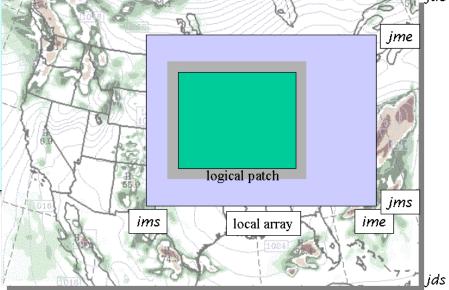
logical domain

ide

ids

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,:: arg7, . . . REAL, DIMENSION (ims:ime,jms:jme) ! 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, kteDO 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



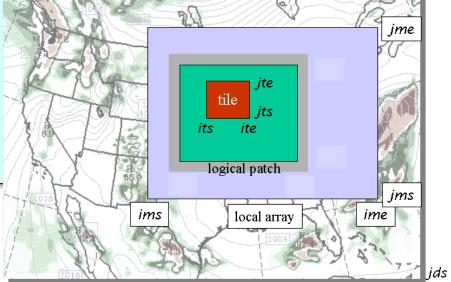
ids

logical domain

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) = argl(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

ide



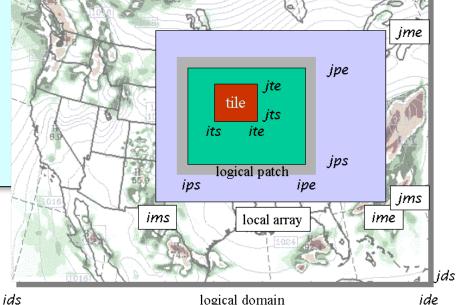
logical domain

ids

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) = argl(i,k,j) + ...END DO END DO END DO 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

- 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



WRF Software Overview

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

WRF I/O

- Streams: pathways into and out of model
 - 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 Var stream

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)

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
 - Data Structures
 - I/O