# WRF Software: Code and Parallel Computing

John Michalakes, Head WRF Software Architecture

Dave Gill

### **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

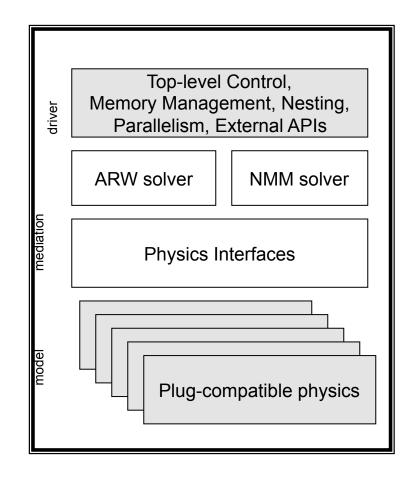
### Introduction – WRF Software Characteristics

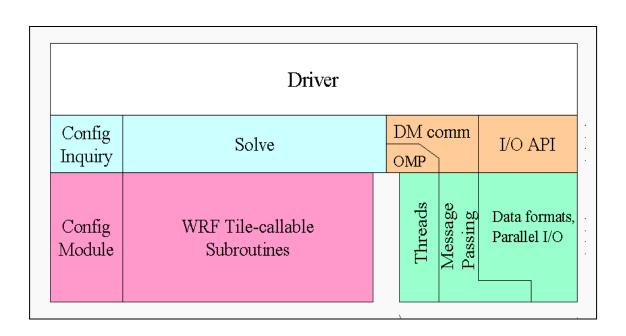
- Developed from scratch beginning around 1998, primarily Fortran and C
- Requirements emphasize flexibility over a range of platforms, applications, users, performance
- WRF develops rapidly. First released Dec 2000
- Supported by flexible efficient architecture and implementation called the WRF Software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

### Introduction - WRF Software Framework Overview

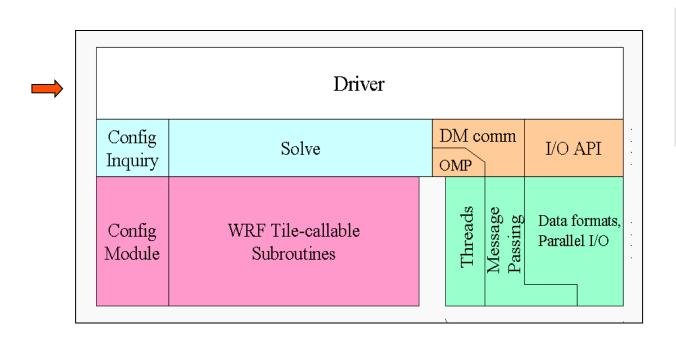
- Implementation of WRF Architecture
  - Hierarchical organization
  - Multiple dynamical cores
  - Plug compatible physics
  - Abstract interfaces (APIs) to external packages
  - Performance-portable
- Designed from beginning to be adaptable to today's computing environment for NWP

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

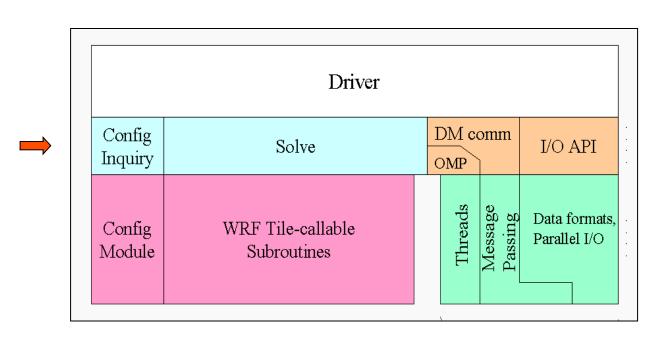




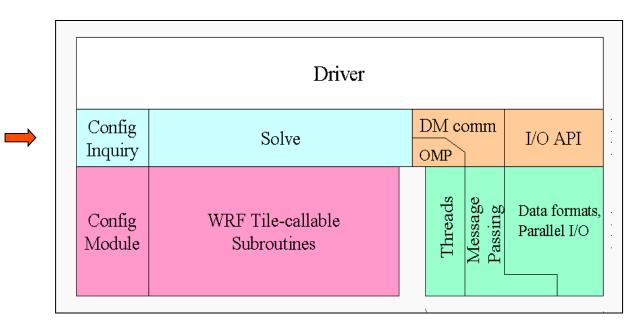
- Hierarchical software architecture
  - Insulate scientists' code from parallelism and other architecture/ implementation-specific details
  - Well-defined interfaces between layers, and external packages for communications, I/O, and model coupling facilitates code reuse and exploiting of community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



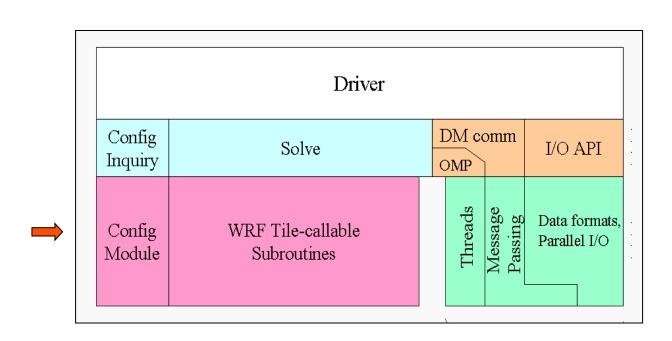
- Driver Layer
  - Domains: Allocates, stores, decomposes, represents abstractly as single data objects
  - Time loop: top level, algorithms for integration over nest hierarchy



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

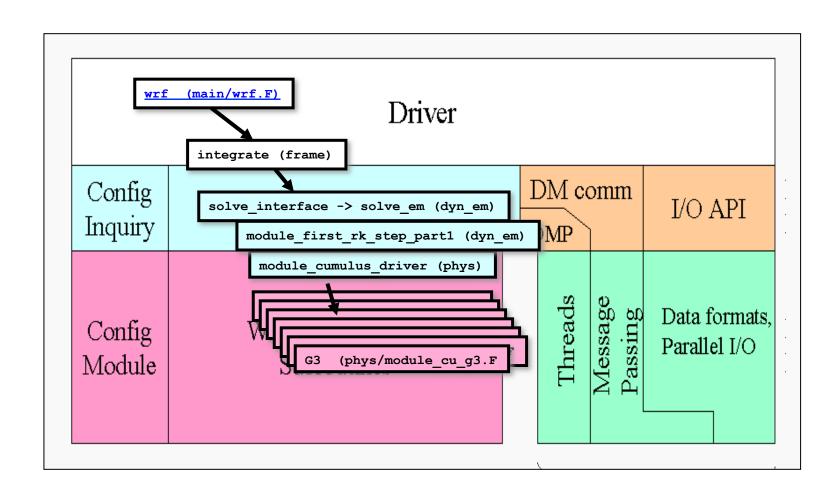


- Mediation Layer
  - The sequence of calls for doing a time-step for one domain is known in Solve routine
  - Dereferences fields in calls to physics drivers and dynamics code
  - Calls to message-passing are contained here as part of Solve routine



- 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



### 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

APPLICATION

**SYSTEM** 

**HARDWARE** 

### Hardware has not changed much...

### A computer in 1960

**IBM** 7090



6-way superscalar

36-bit floating point precision

~144 Kbytes

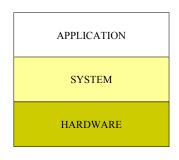
~50,000 flop/s 48hr 12km WRF CONUS in 600 years

### A computer in 2013



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

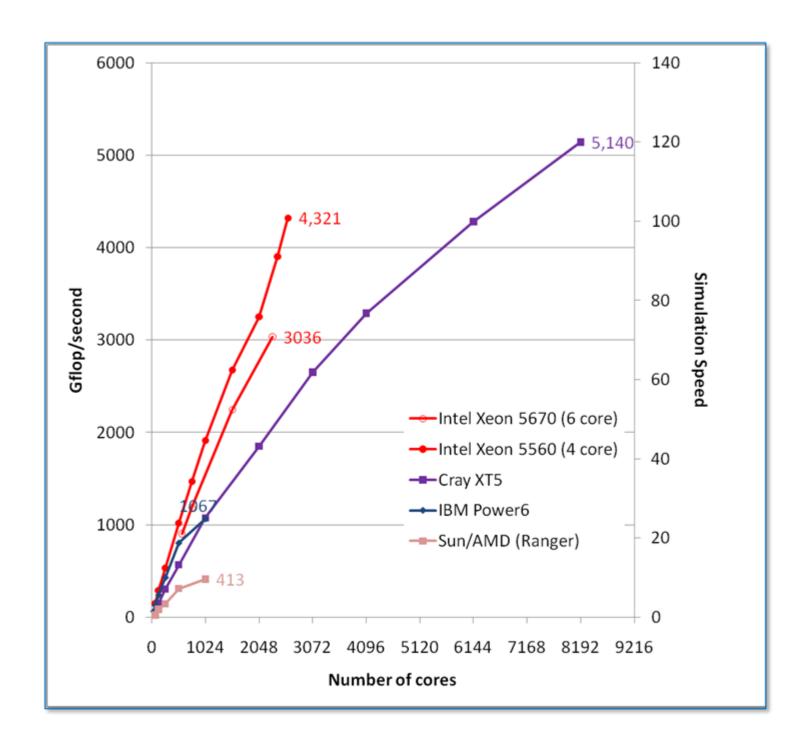
~5,000,000,000 flop/s
48 12km WRF CONUS in 26 Hours



#### ...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 <u>parallelism</u>
  - Ganging multiple processors together to achieve 10<sup>11-12</sup> flop/second
  - Aggregate available memories of 10<sup>11-12</sup> bytes

~1,000,000,000,000 flop/s ~2500 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 sizes proc count: I-dim x J-dim

1: 74x61 2: 74x31 4: 37x31 8: 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

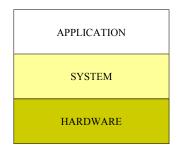
OpenMP

Timing for main on domain 1: 8.56216 elapsed seconds

MPI

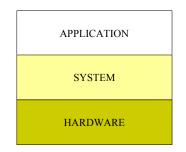
Timing for main on domain 1: 7.36243 elapsed seconds

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



### Application: WRF

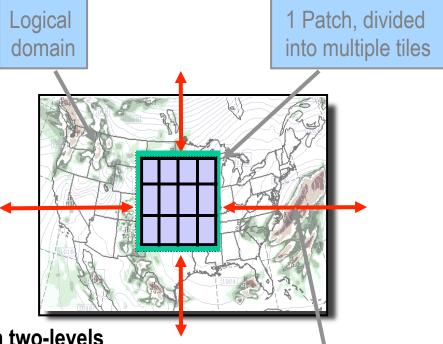
- WRF can be run serially or as a parallel job
- WRF uses *domain decomposition* to divide total amount of work over parallel processes



### 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.

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

### 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.

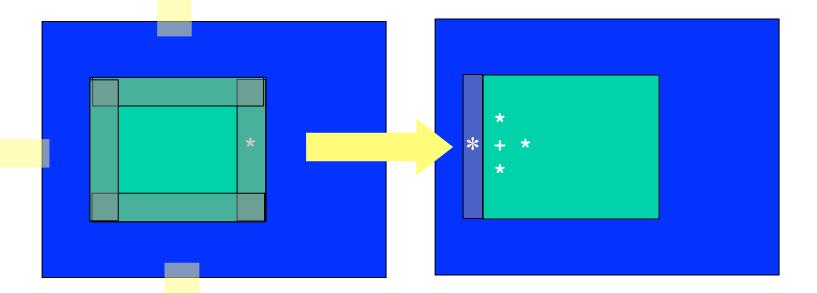
These are *horizontal data dependencies* because the indexed operands may lie in the patch of a neighboring processor. That neighbor's updates to that element of the array won't be seen on this processor.

### **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,i)+rr(i,k,i))*H1(i,k,i))+
           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)*(Hlavg(i,k+1,j)-Hlavg(i,k,j)+
                       H2avq(i,k+1,j)-H2avq(i,k,j)
                                )/dzetaw(k)
   ENDDO
   ENDDO
   ENDDO
```

### Distributed Memory MPI Communications

Halo updates

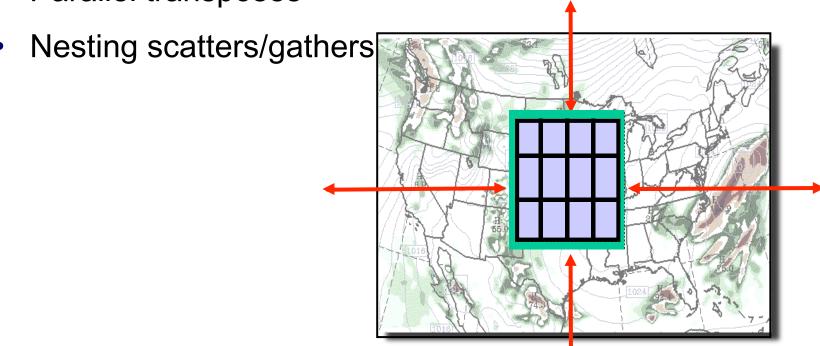


memory on one processor

memory on neighboring processor

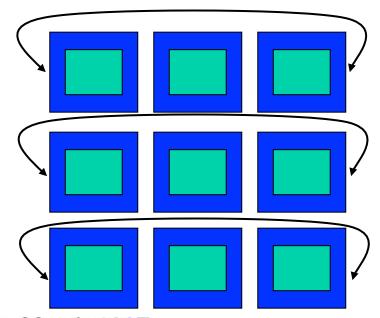
## Distributed Memory (MPI) Communications

- Halo updates
- Periodic boundary updates
- Parallel transposes

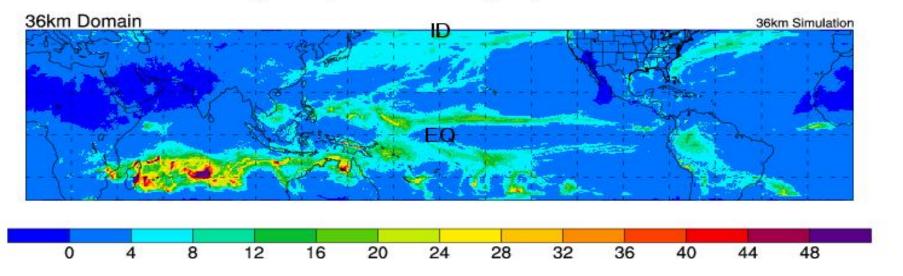


## Distributed Memory (MPI) Communications

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

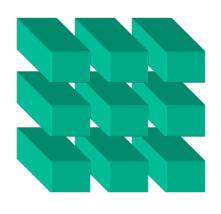


Average Daily Total rainfall (mm) - March 1997

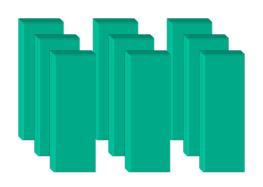


## Distributed Memory (MPI) Communications

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



all y on patch



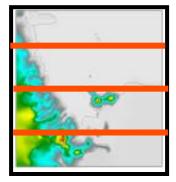
all z on patch



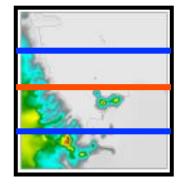
all x on patch

## Distributed Memory (MPI) Communications

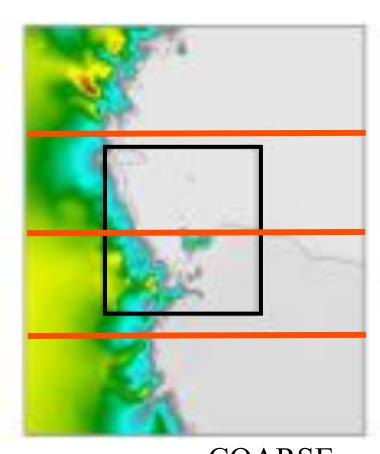
- Halo updates
- Periodic boundary updates
- Parallel transposes
- Nesting scatters/gathers



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
MEDIATION
MODEL

Makefile README README test cases clean build compile scripts configure CASE input files Registry/ machine build rules arch/ dyn em/ dyn nnm/ source external/ frame/ code inc/ directories main/ phys/ share/ tools/ execution run/ directories test/

```
$(RM) $@
```

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

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

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.Fcumodule_microphysics_driver.Fmpmodule_pbl_driver.Fblmodule_radiation_driver.Framodule_surface_driver.Fsf
```

The subgrid-scale precipitation (\*\_cu\_\*.F)

module\_cu\_bmj.Fmodule\_cu\_camzm.Fmodule\_cu\_g3.Fmodule\_cu\_gd.Fmodule\_cu\_kf.Fmodule\_cu\_kfeta.Fmodule\_cu\_nsas.Fmodule\_cu\_osas.Fmodule\_cu\_sas.Fmodule\_cu\_tiedtke.F

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

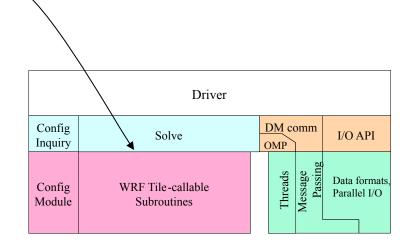
 All of the sound step utilities to advance u, v, mu, t, w within the small time-step loop WRFV3/dyn\_em/module\_small\_step\_em.F

### **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**

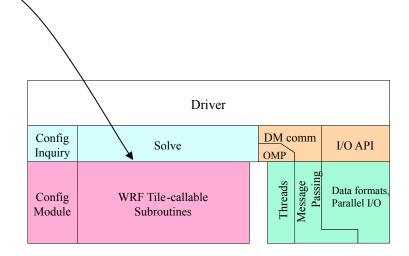
# Restrictions on Model Layer subroutines:

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, . . .
```

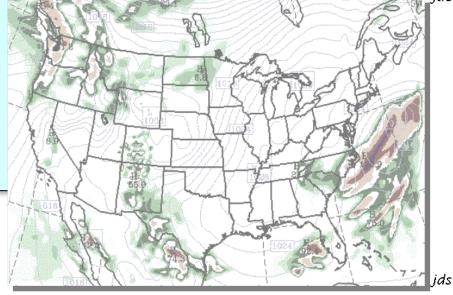
### **WRF Model Layer Interface**

```
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) = argi(i,k,j) + ...
    END DO
  END DO
END DO
```

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

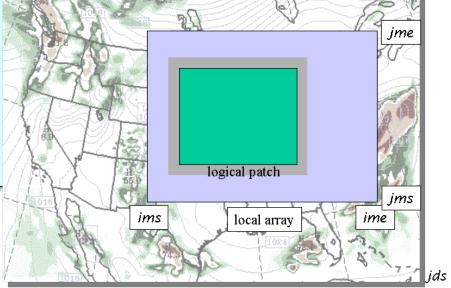


ids logical domain ide

#### 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, 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

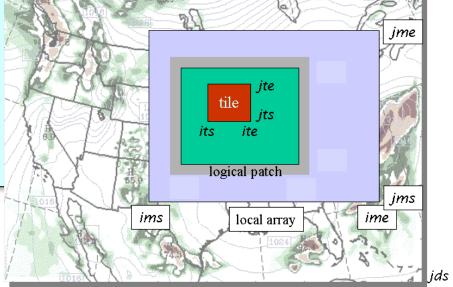
ide

#### 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



ids logical domain

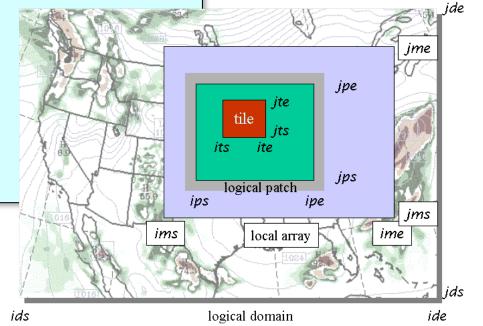
ide

```
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
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REAL, DIMENSION (ims:ime, jms:jme) :: arg7, . . .
! Define Local Data (I2)
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! 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
```

template for model layer subroutine

- 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



- 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**

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- Need and design for parallelism
- Communication patterns to support parallelism
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  - Indices
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