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

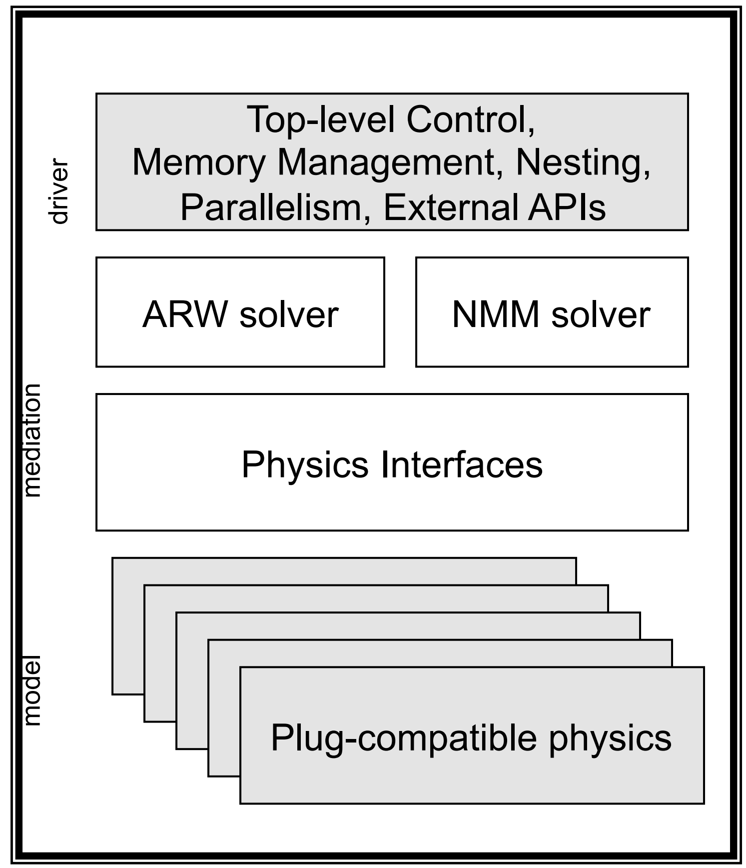
Introduction – WRF Software Characteristics

- 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

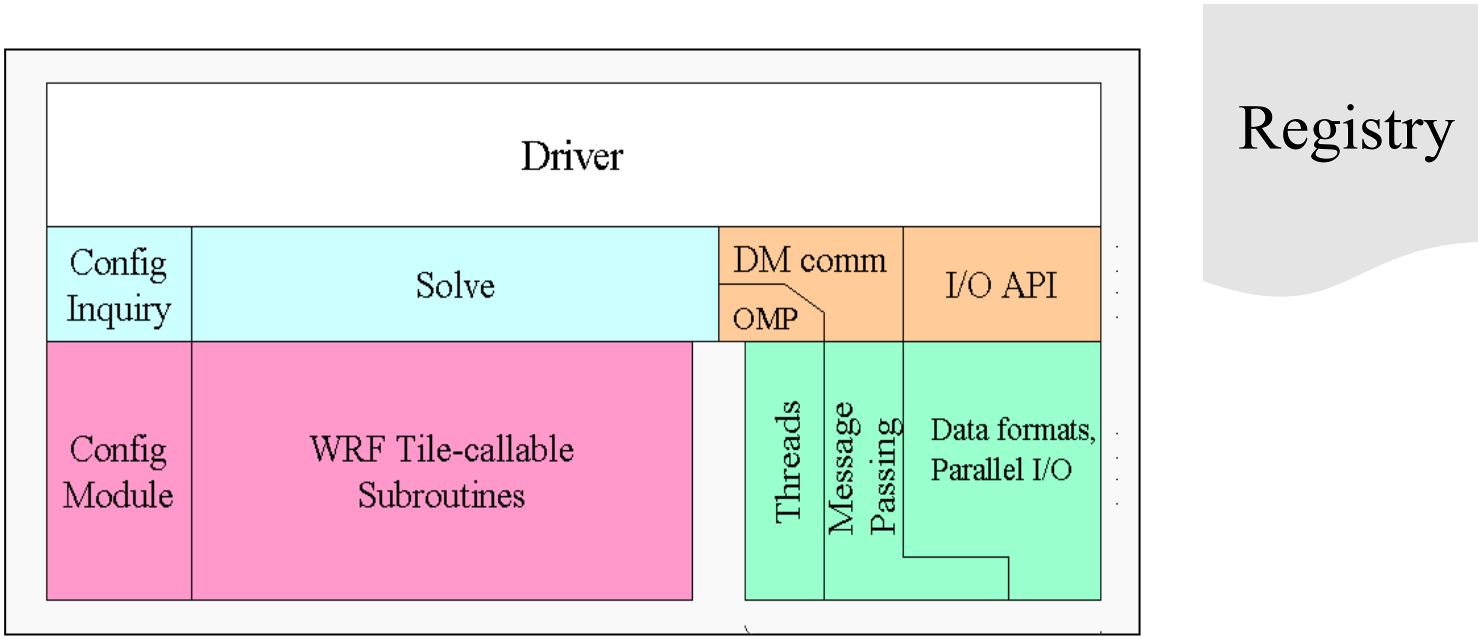
Introduction - WRF Software Framework Overview

- 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/

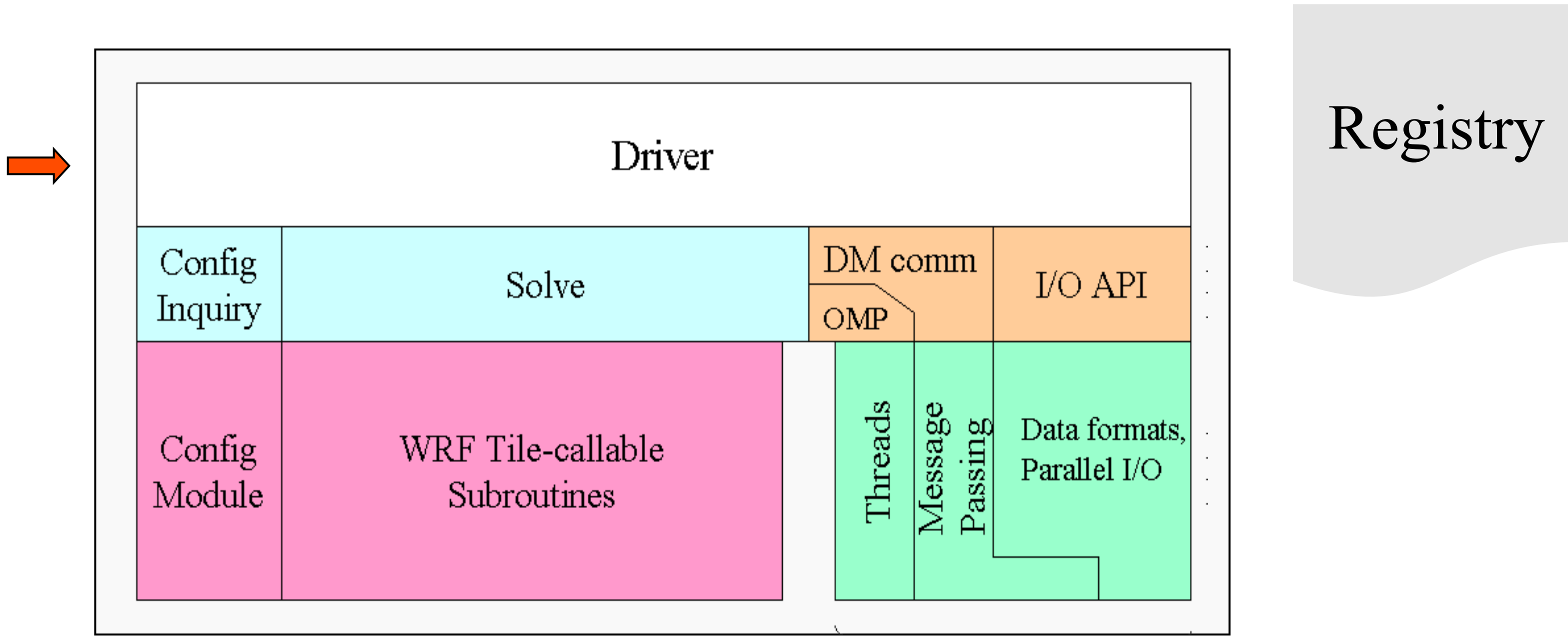


WRF Software Architecture



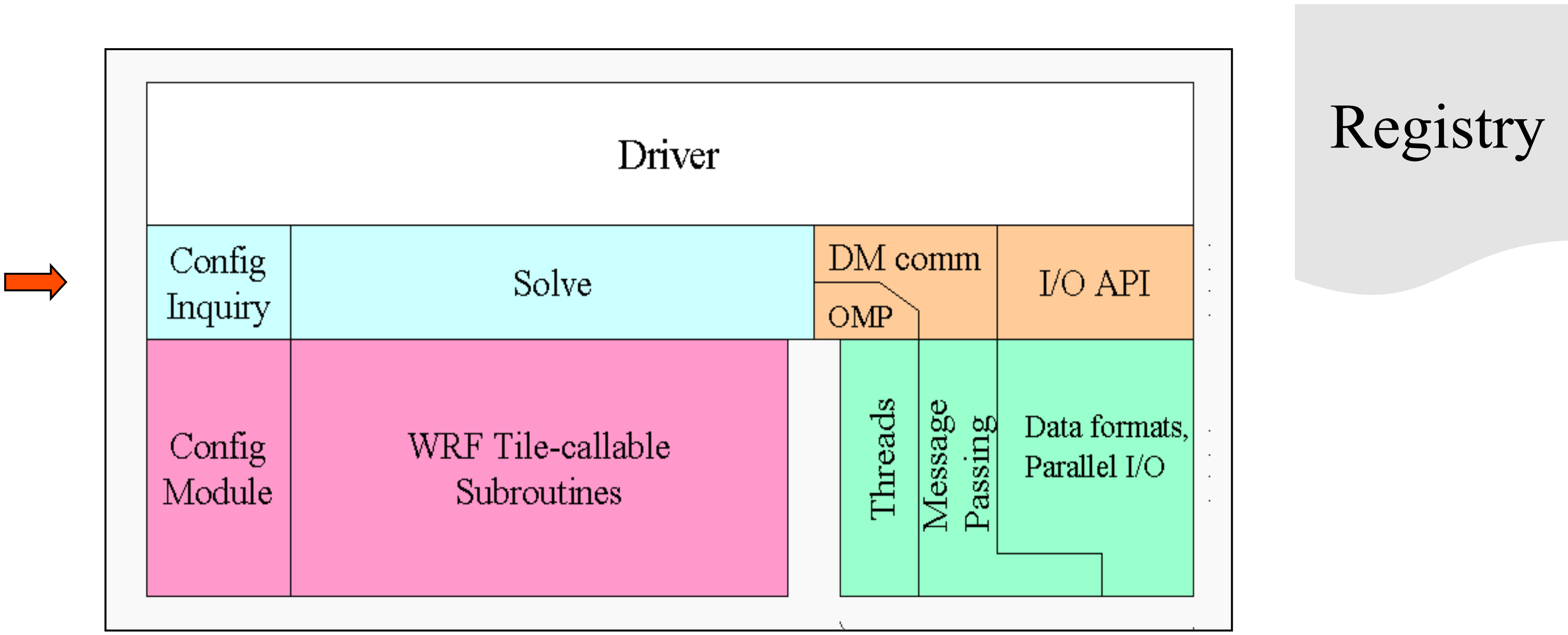
- Hierarchical software architecture
  - Insulate scientists' code from parallelism and other architecture/ implementation-specific details
  - Well-defined interfaces between layers, and external packages for communications, I/O, and model coupling facilitates code reuse and exploiting of community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

WRF Software Architecture



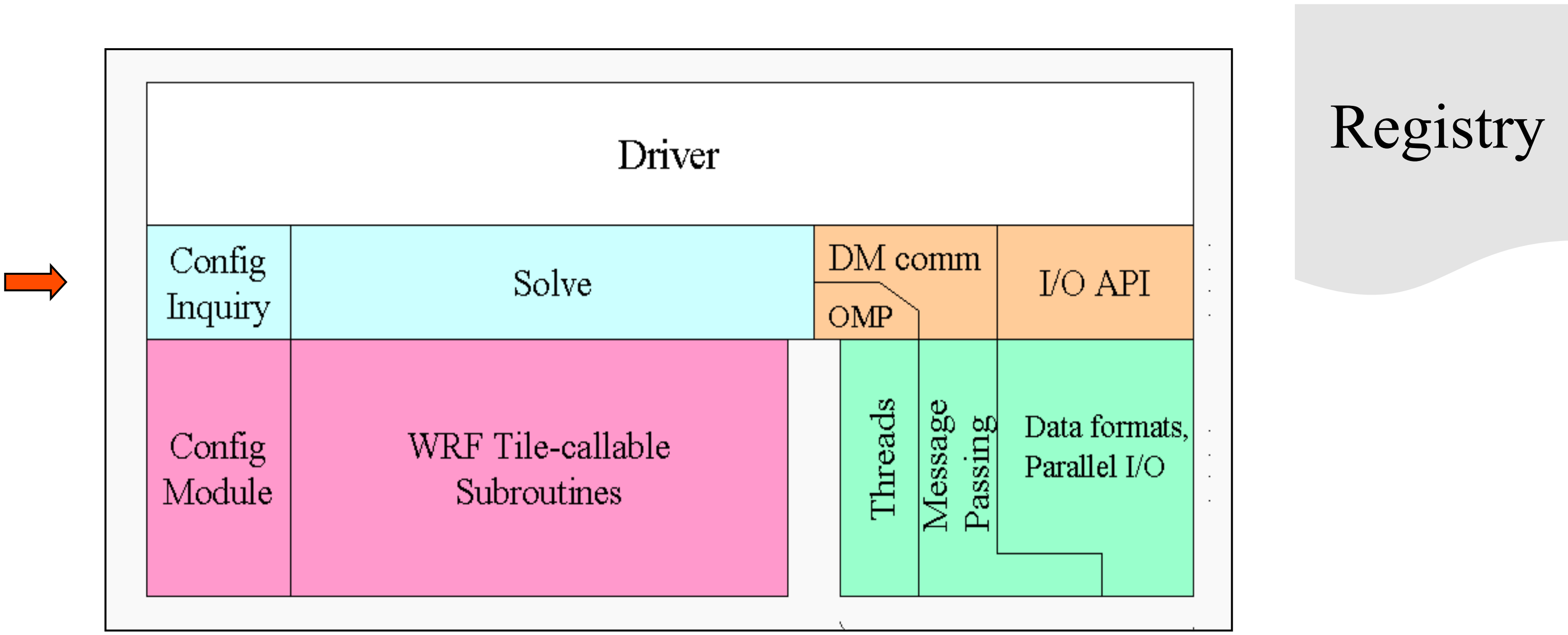
- Driver Layer
  - **Domains**: Allocates, stores, decomposes, represents abstractly as single data objects
  - **Time loop**: top level, algorithms for integration over nest hierarchy

WRF Software Architecture



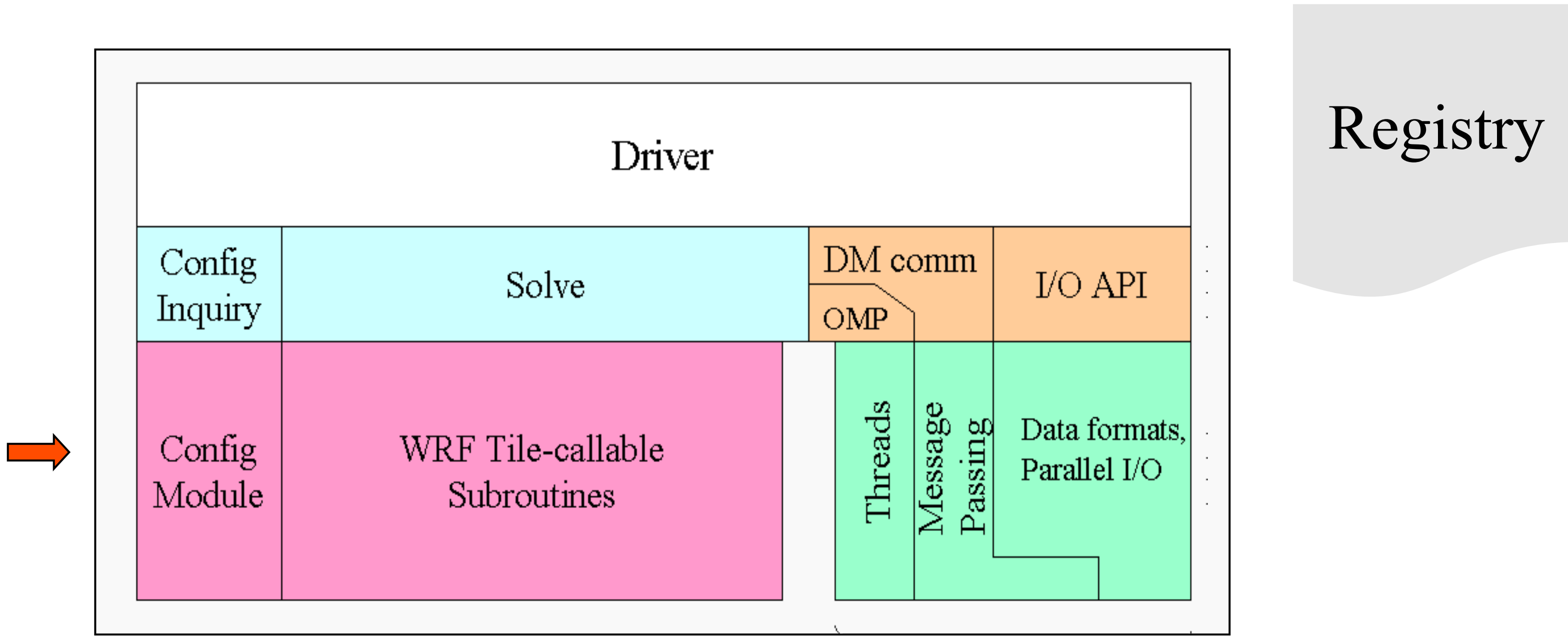
- Mediation Layer
  - Solve routine, takes a domain object and advances it one time step
  - Nest forcing, interpolation, and feedback routines

WRF Software Architecture



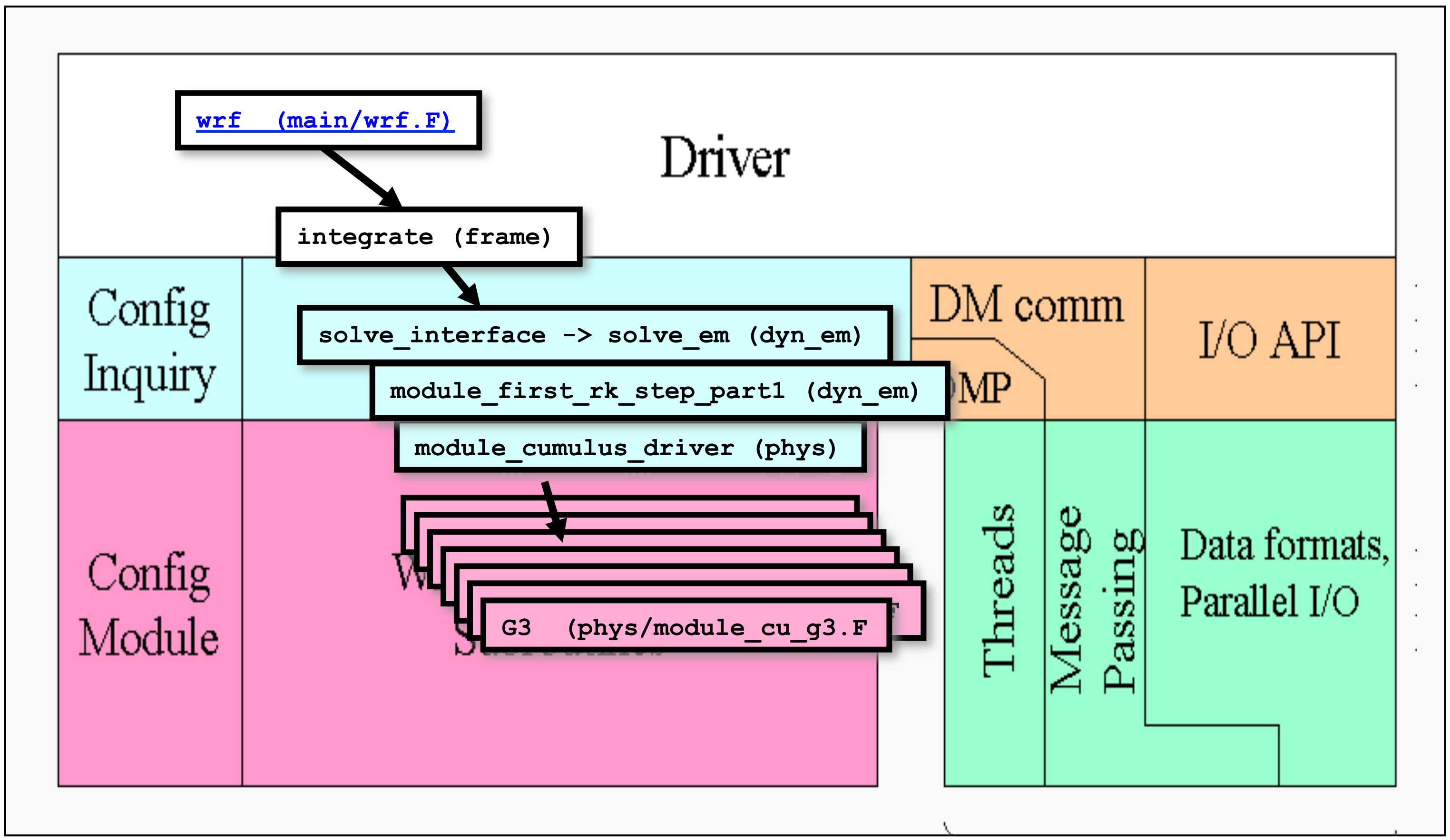
- Mediation Layer
  - The sequence of calls for doing a time-step for one domain is known in Solve routine
  - Dereferences fields in calls to physics drivers and dynamics code
  - Calls to message-passing are contained here as part of Solve routine

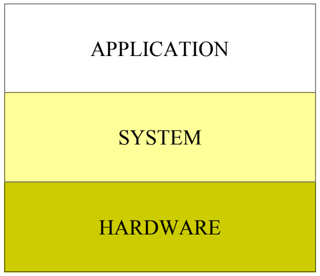
WRF Software Architecture



- 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

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

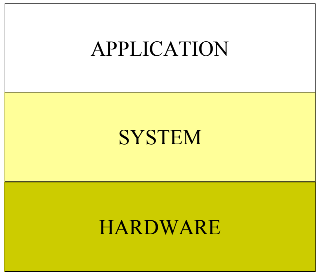
A computer in 2013

Dual core, 2.6 GHz chip

64-bit floating point precision

20 MB L3

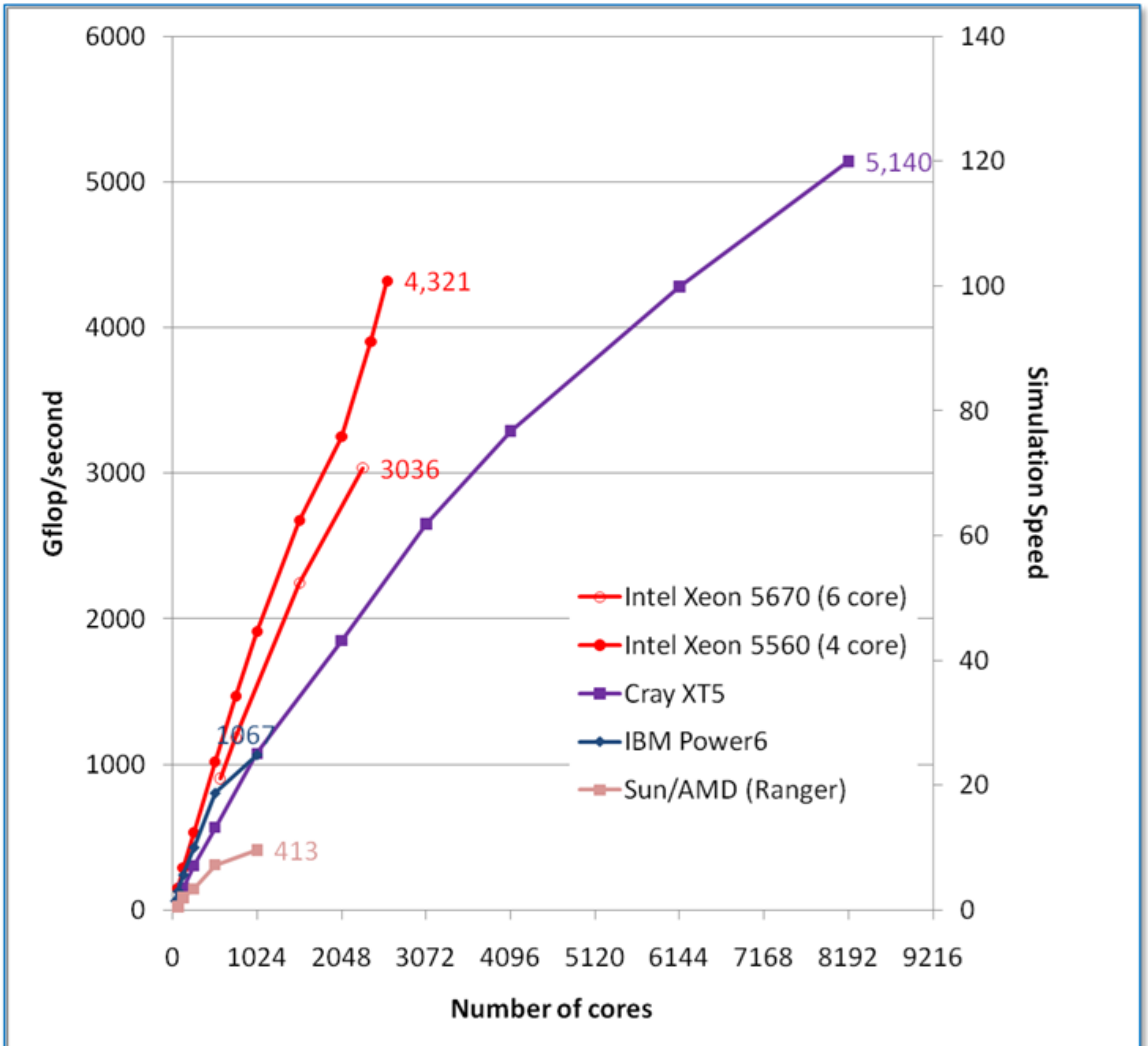
~5,000,000,000 flop/s
48 12km WRF CONUS in 26 Hours



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

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



Gflop/second
Simulation Speed
Number of cores
0
1000
2000
3000
4000
5000
6000
0
20
40
60
80
100
120
140
0
1024
2048
3072
4096
5120
6144
7168
8192
9216
4,321
3036
5,140
1067
413
Intel Xeon 5670 (6 core)
Intel Xeon 5560 (4 core)
Cray XT5
IBM Power6
Sun/AMD (Ranger)

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
```

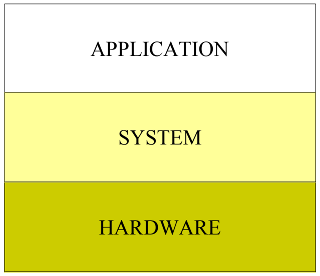
- OpenMP

```
Timing for main on domain   1:    8.56216 elapsed seconds
```

- MPI

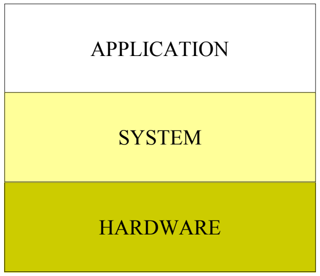
```
Timing for main on domain   1:    7.36243 elapsed seconds
```

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

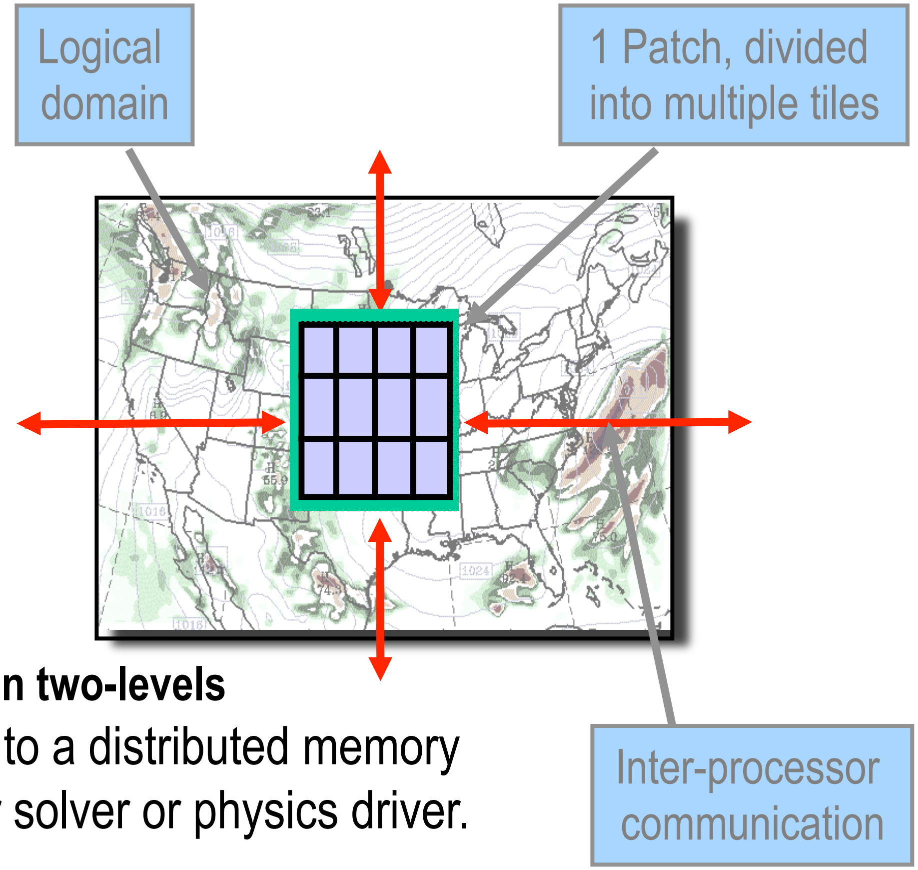


Application: WRF

- 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.

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

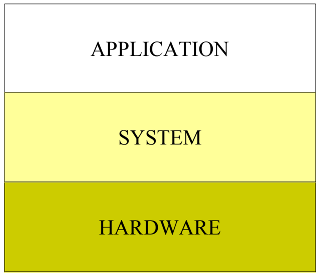
Note the tell-tale +1 and –1 expressions in indices for **rr**, **H1,** and **H2** arrays on right-hand side of assignment.

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

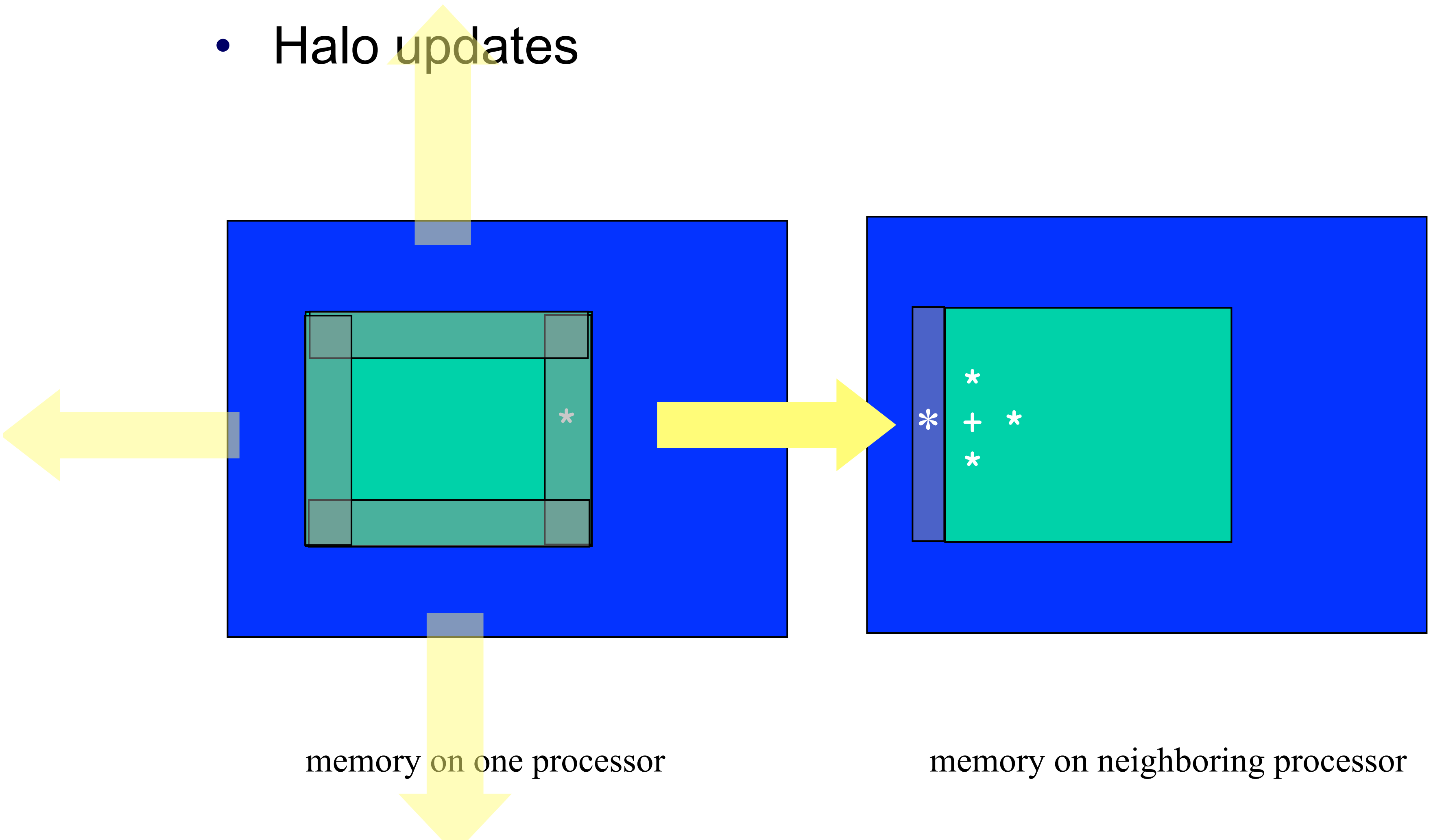
(module_diffusion.F)

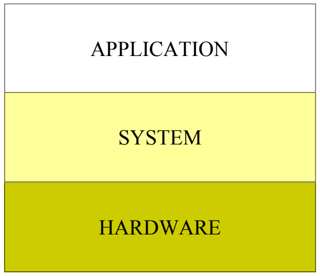
```
SUBROUTINE horizontal_diffusion_s (tendency, rr, var, . . .
. . .
   DO j = jts,jte
   DO k = kts,ktf
   DO i = its,ite
      mrdx=msft(i,j)*rdx
      mrdy=msft(i,j)*rdy
      tendency(i,k,j)=tendency(i,k,j)-                                    &
           (mrdx*0.5*((rr(i+1,k,j)+rr(i,k,j))*H1(i+1,k,j)-               &
                      (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
 . . .
```



Distributed Memory MPI Communications

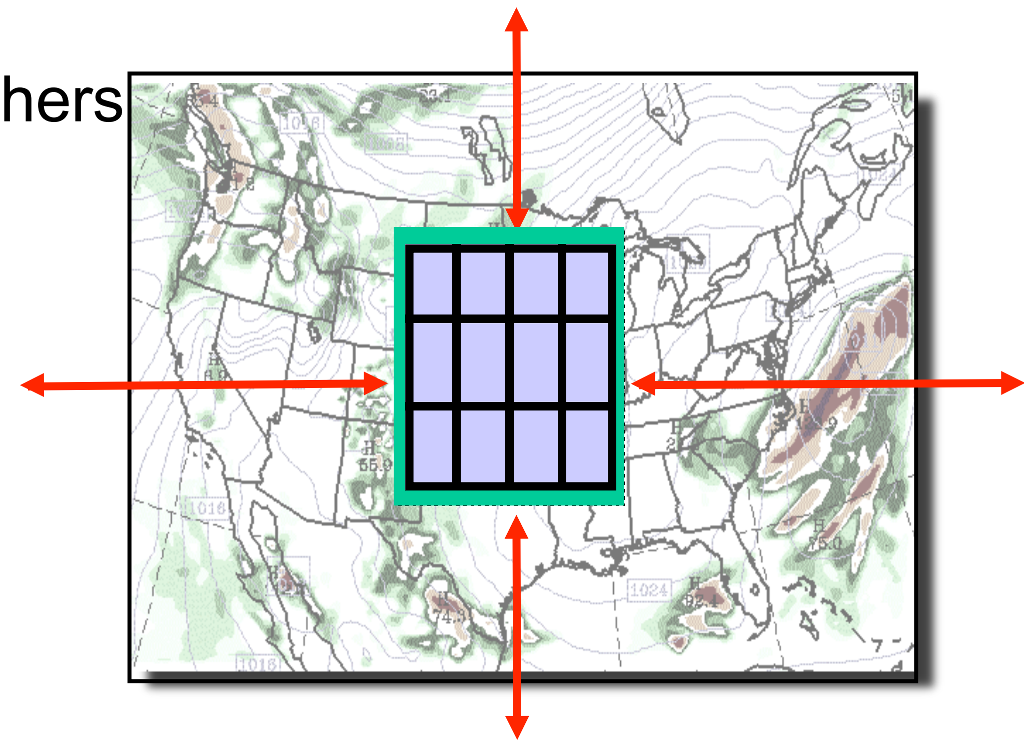
- Halo updates

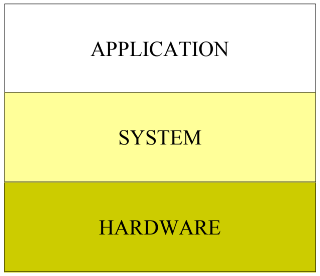




Distributed Memory (MPI) Communications

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





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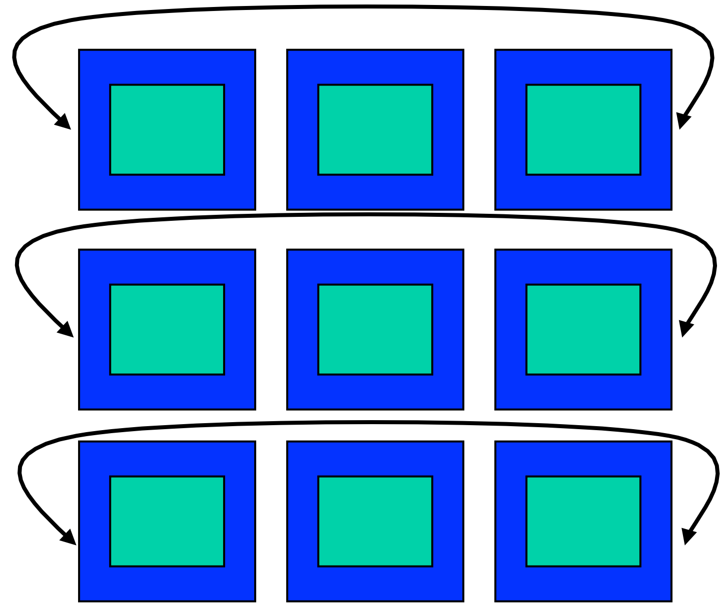

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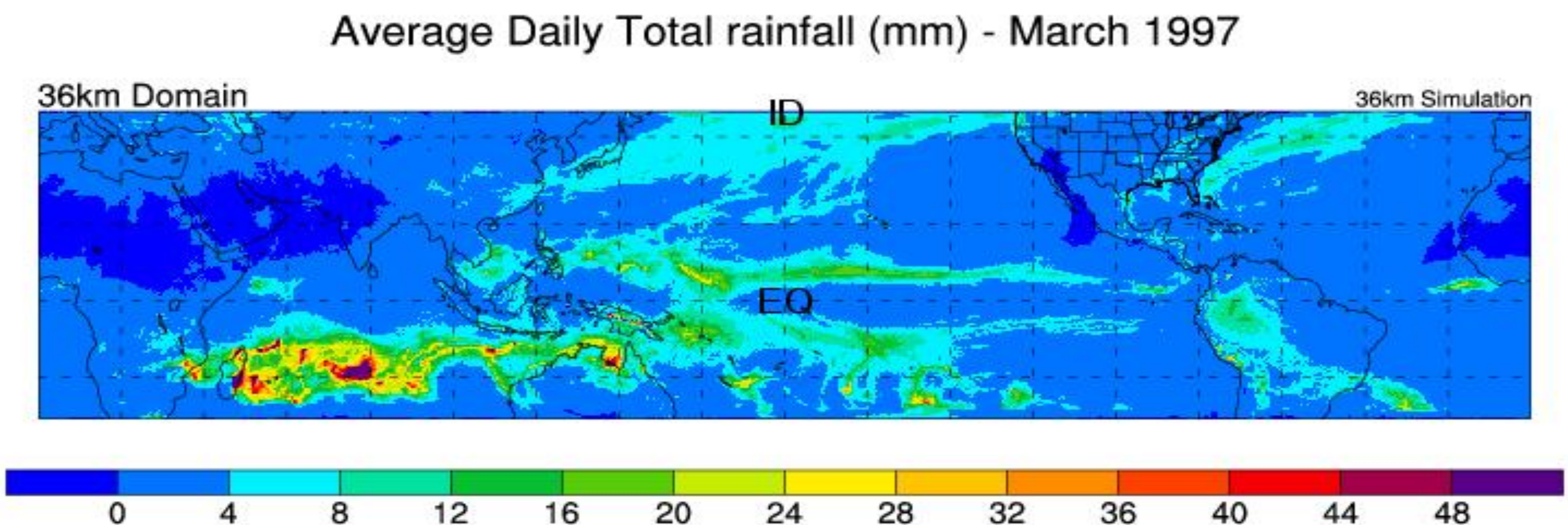

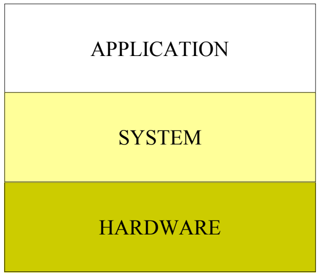

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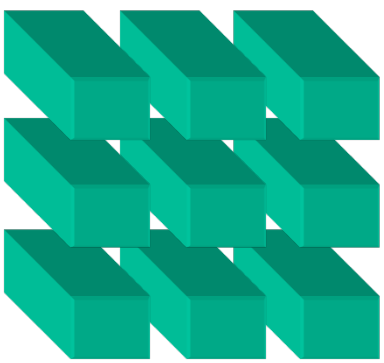
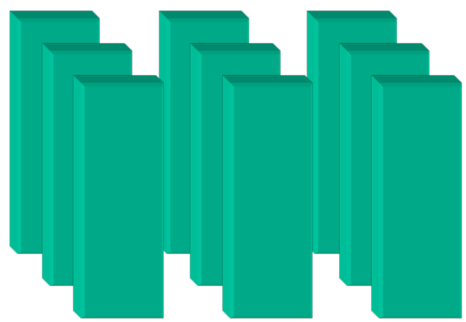
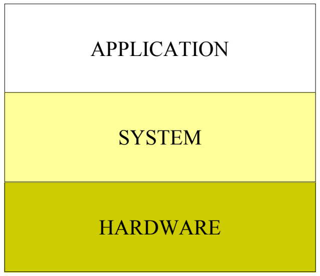


all y on patch



all z on patch

all x on patch



Distributed Memory (MPI) Communications

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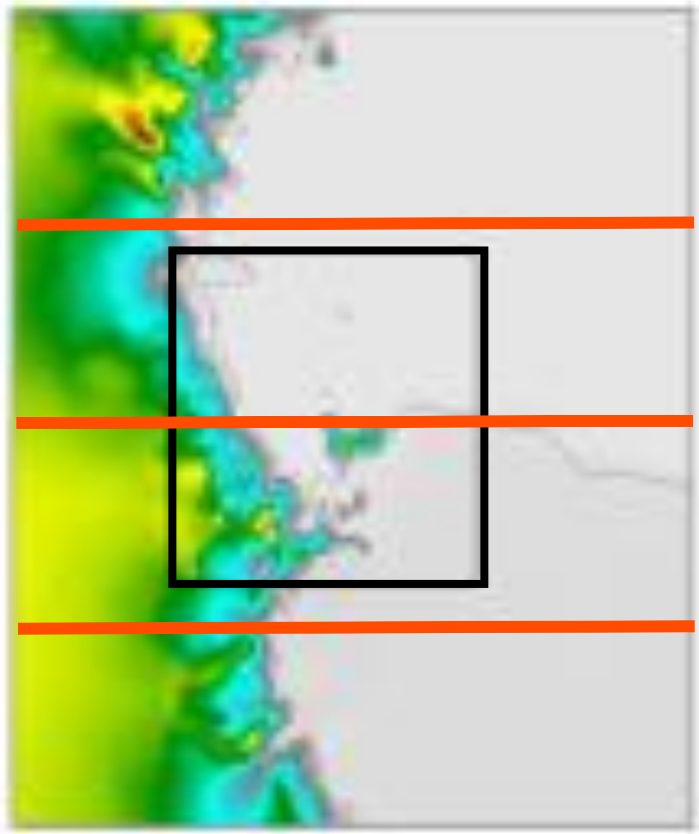
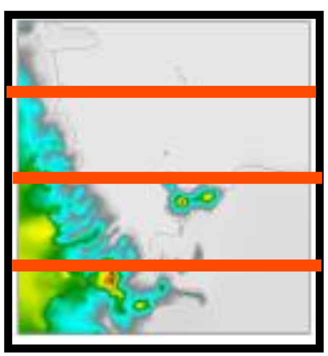
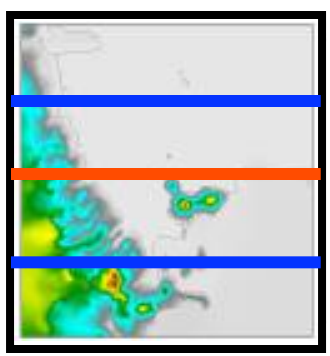


COARSE
Ross Island
6.66 km



NEST:2.22 km



INTERMEDIATE: 6.66 km

WRF Model Top-Level Directory Structure

WRF Design and Implementation Doc, p 5

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

```
Makefile
README
README_test_cases
clean
compile
configure
Registry/
arch/
dyn_em/
dyn_nnm/
external/
frame/
inc/
main/
phys/
share/
tools/
run/
test/
```

- clean, compile, configure — build scripts
- Registry/ — CASE input files
- arch/ — machine build rules
- dyn_em/ (MEDIATION), dyn_nnm/ (MEDIATION), external/, frame/ (DRIVER), inc/, main/ (DRIVER), phys/ (MODEL), share/ (MEDIATION), tools/ — source code directories
- run/, test/ — execution directories

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 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

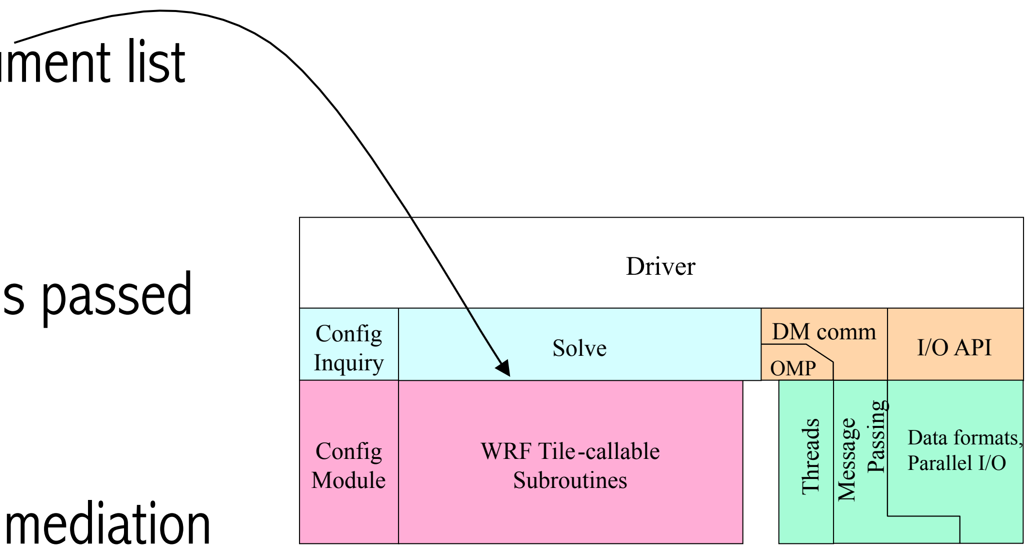
  WRFV3/dyn_em/module_small_step_em.F

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

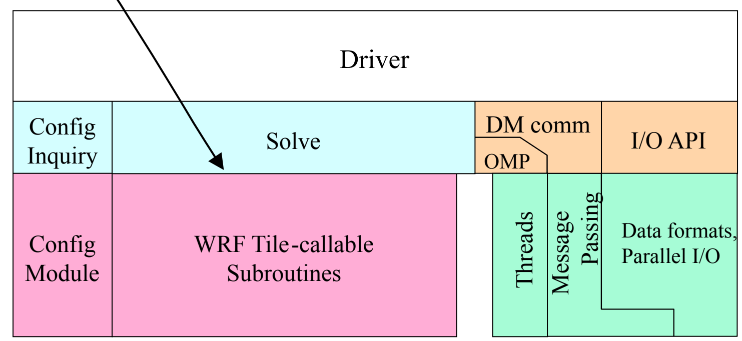
Restrictions on Model Layer subroutines:

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
```

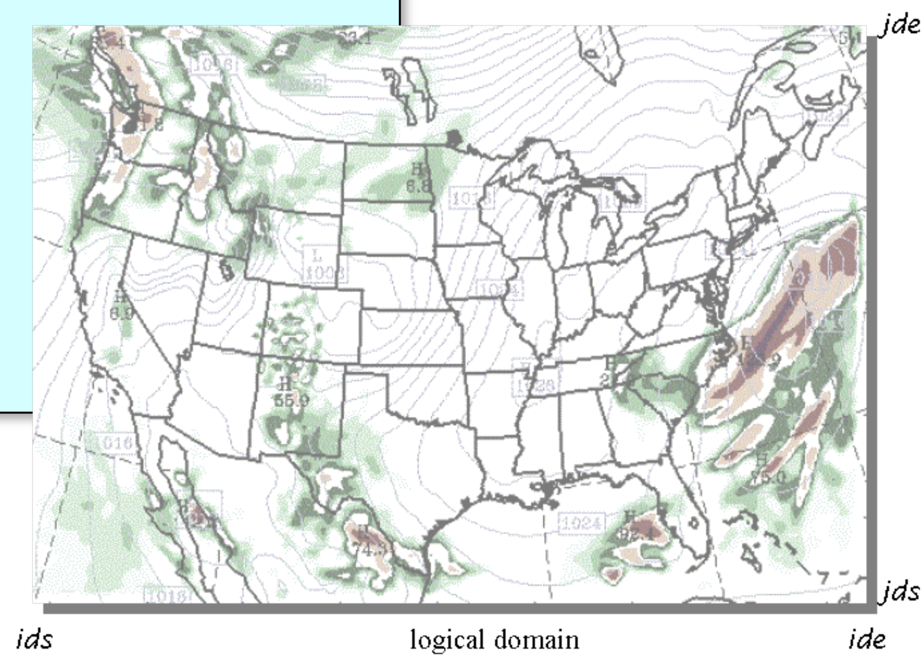
template for model layer subroutine

```
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.



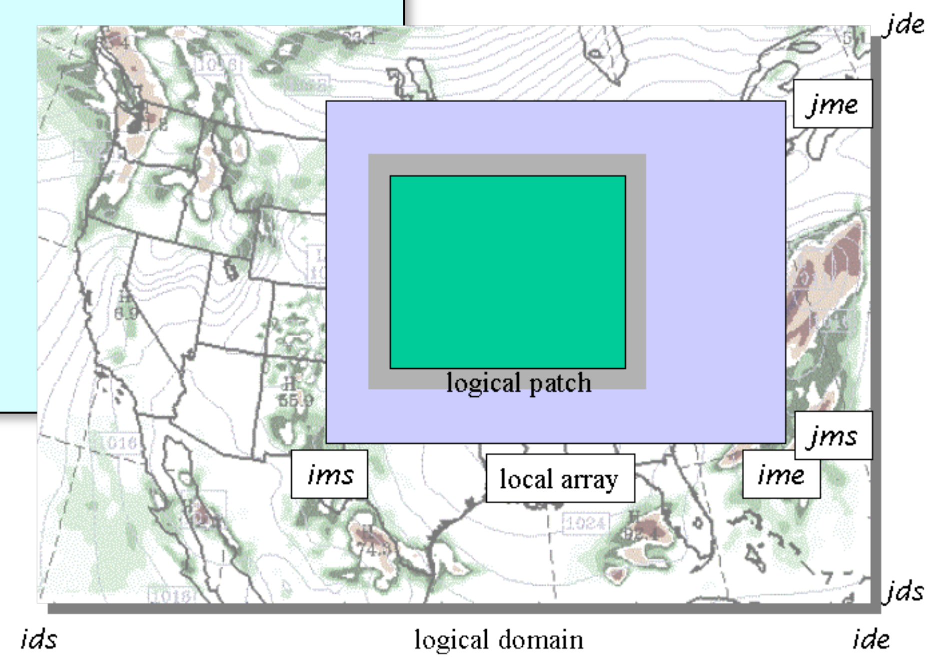
template for model layer subroutine

```
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



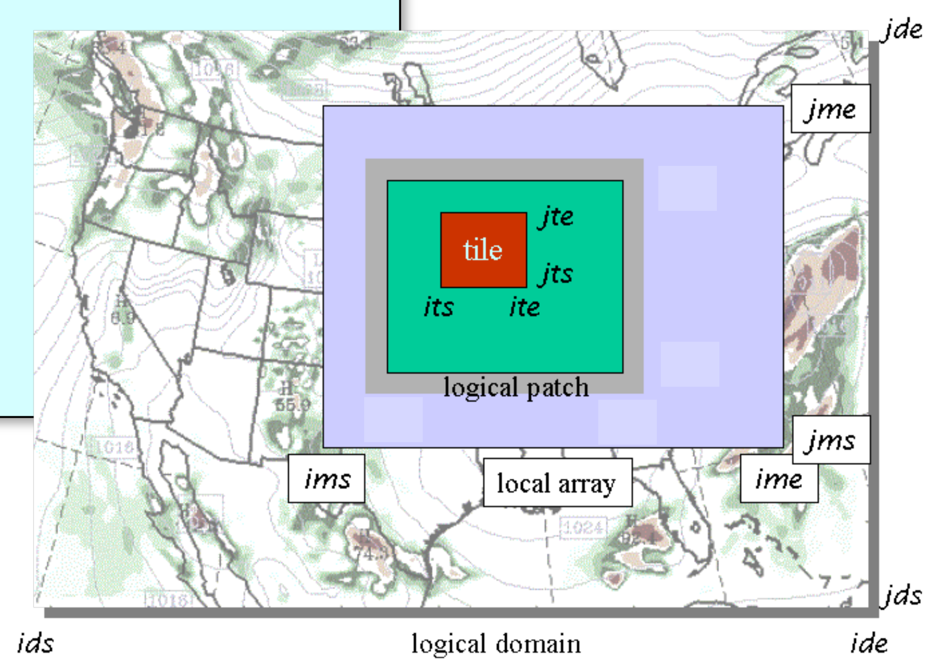
template for model layer subroutine

```
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

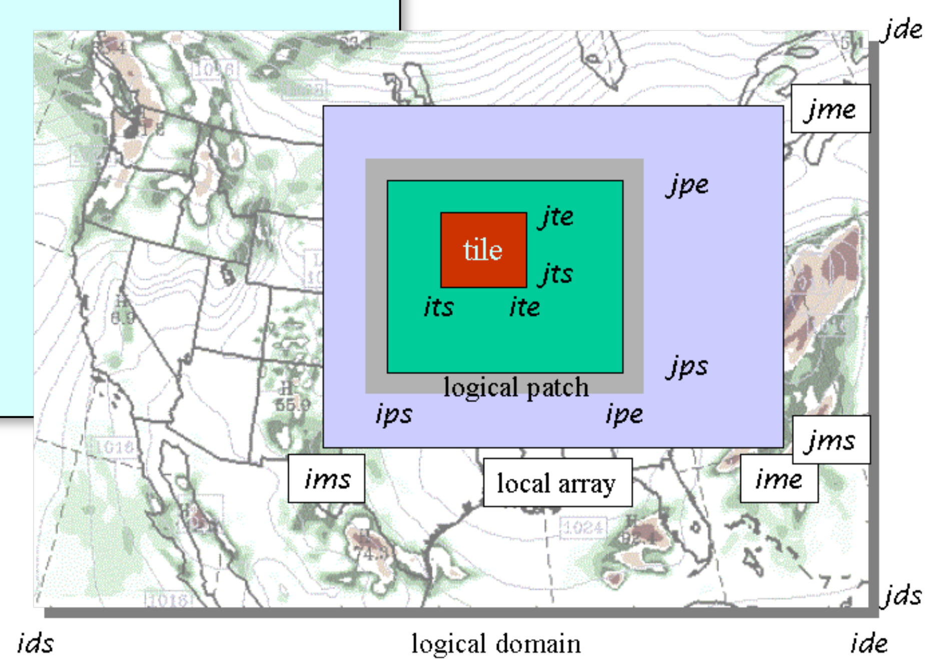
```
SUBROUTINE model ( &
  arg1, arg2, arg3, … , argn,    &
  ids, ide, jds, jde, kds, kde, &  ! Domain dims
  ims, ime, jms, jme, kms, kme, &  ! Memory dims
  its, ite, jts, jte, kts, kte  )  ! Tile dims

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: 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”

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

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