Lecture 21: Parallel Programming Models for Scientific Computing

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Parallel Programming Models

- Multiple classes of models differ in how we think about communication and synchronization among processes or threads.
  - Shared memory
  - Distributed memory
  - Some of each
  - Less explicit
- Shared Memory (really globally addressable)
  - Processes (or threads) communicate through memory addresses accessible to each
- Distributed memory
  - Processes move data from one address space to another via sending and receiving messages
- Multiple cores per node make the shared-memory model efficient and inexpensive; this trend encourages all shared-memory and hybrid models.

Higher-Level Models

- Parallel Languages
  - ♦ UPC
  - ♦ Co-Array Fortran
  - ♦ Titanium
- Abstract, declarative models
  - ♦ Logic-based (Prolog)
  - ♦ Spreadsheet-based (Excel)
- The programming model research problem: Define a model (and language) that
  - ♦ Can express complex computations
  - ♦ Can be implemented efficiently on parallel machines
  - ♦ Is easy to use
- It is hard to get all three
  - ♦ Specialized libraries can implement very high-level, even application-specific models

Writing Parallel Programs

- Parallel programming models are expressed:
  - In libraries callable from conventional languages
  - In languages compiled by their own special compilers
  - In structured comments that modify the behavior of a conventional compiler
- We will survey some of each of these and consider a single example written in each
  - Not an adequate tutorial on any of these approaches
  - Many detailed sources are available
  - Only trying to convey the “flavor” of each approach

Programming Models and Systems

- Not just parallel programming
  - ♦ And not just "classical" programming languages – python, Matlab, multi-lingual programs
- (At least) Two goals
  - ♦ Clear, maintainable programs
    - "Productivity"
  - ♦ Performance
    - Otherwise, you don't need parallelism
- One more requirement
  - ♦ Interoperability with components (library routines) written in other languages
- Most parallel programming systems consist of
  - ♦ A conventional single-threaded model
  - ♦ A parallel coordination layer

Single Threaded Languages

- Fortran, C, C++ (and many others)
  - ♦ No intrinsic parallelism until recently (C11 threads, Fortran coArrays)
  - ♦ Do provide some features for memory hierarchies
- Programming for memory hierarchy
  - ♦ These provide some simple tools that can help the compiler produce better-performing code
- In C/C++
  - ♦ const – Data is not changed
  - ♦ restrict (pointers) – roughly, data is not accessed with a different pointer
- In Fortran
  - ♦ Arguments to routines are *required* to be distinct
    - As if they had C's restrict semantics
    - One of the reasons that Fortran is considered easier to optimize than C
  - ♦ Fortran provides intent as well (IN, OUT, INOUT). IN can help the compiler
- You should *always* use the correct declaration
  - ♦ Compilers continue to improve and to exploit this knowledge
  - ♦ Compiler may also check whether you told the truth
- One more issue - Aligned memory
  - ♦ Some special features require that operands be aligned on double-word (e.g., 16-byte) boundaries

Illustrating the Programming Models

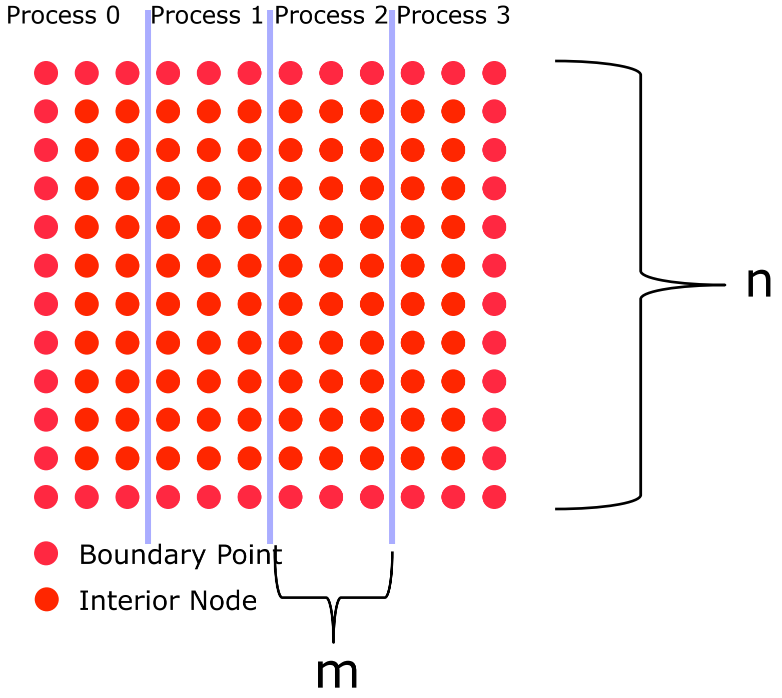
- Learning each programming model takes more than an hour ☺
  - ♦ This section will show samples of programming models, applied to one simple operation (sparse matrix-vector multiply on a regular grid)
  - ♦ For more information, consider
    - Tutorials (e.g., at SC)
    - Taking a parallel programming class covering a specific programming model
    - Reading books on different models

The Poisson Problem

- Simple elliptic partial differential equation
- Occurs in many physical problems
    - ♦ Fluid flow, electrostatics, equilibrium heat flow
- Many algorithms for solution
- We illustrate a sub-optimal one, since it is easy to understand and is typical of a data-parallel algorithm

Jacobi Iteration (Fortran Ordering)

- Simple parallel data structure



- Processes exchange columns with neighbors
- Local part declared as xlocal(n,0:m+1)

The Computation

- These details are not important to showing the different programming systems, but may make some things clearer
- Approximation is

$$\frac{u(x+h,y)+u(x-h,y)-4u(x,y)+u(x,y+h)+u(x,y-h)}{h^2}=f(x,y)$$

$$4u(x,y)=\big(u(x+h,y)+u(x-h,y)+u(x,y+h)+u(x,y-h)\big)-h^2 f(x,y)$$

u(x,y+h) becomes u(i,j+1) etc.

Serial Fortran Version

```
real u(0:n,0:n), unew(0:n,0:n), f(1:n, 1:n), h

 ! Code to initialize f, u(0,*), u(n:*), u(*,0), and
 ! u(*,n) with g

 h = 1.0 / n
 do k=1, maxiter
   do j=1, n-1
     do i=1, n-1
       unew(i,j) = 0.25 * ( u(i+1,j) + u(i-1,j) + &
                            u(i,j+1) + u(i,j-1) - &
                            h * h * f(i,j) )
     enddo
   enddo
   ! code to check for convergence of unew to u.
   ! Make the new value the old value for the next iteration
   u = unew
 enddo
```

Adding SMP Parallelism

- We've seen how to use OpenMP for data parallelism in lecture17
- Here we'll see it in Fortran
  - ♦ Since Fortran has no anonymous blocks, special comments (directives) are used to mark the blocks
- Note data placement is not controlled, so performance is hard to get except on machines with real shared memory

OpenMP Version

```
  real u(0:n,0:n), unew(0:n,0:n), f(1:n-1, 1:n-1), h

   ! Code to initialize f, u(0,*), u(n:*), u(*,0),
   ! and u(*,n) with g

   h = 1.0 / n
   do k=1, maxiter
!$omp parallel
!$omp do
     do j=1, n-1
       do i=1, n-1
         unew(i,j) = 0.25 * ( u(i+1,j) + u(i-1,j) + &
                     u(i,j+1) + u(i,j-1) - &
                     h * h * f(i,j) )
       enddo
     enddo
!$omp enddo
     ! code to check for convergence of unew to u.

     ! Make the new value the old value for the next iteration
     u = unew
!$omp end parallel
   enddo
```

MPI

- The Message-Passing Interface (MPI) is a standard library interface specified by the MPI Forum
- It implements the message passing model, in which the sending and receiving of messages combines both data movement and synchronization. Processes have separate address spaces.
- Send(data, destination, tag, comm) in one process matches Receive(data, source, tag, comm) in another process, at which time data is copied from one address space to another
- Data can be described in many flexible ways
- SendReceive can be used for exchange
- Callable from Fortran-77, Fortran, C (and hence C++) as specified by the standard
  - ♦ Other bindings (Python, Java) available, non-standard

Simple MPI Version

```
use mpi
 real u(0:n,js-1:je+1), unew(0:n,js-1:je+1)
 real f(1:n-1, js:je), h
 integer nbr_down, nbr_up, status(MPI_STATUS_SIZE), ierr

 ! Code to initialize f, u(0,*), u(n:*), u(*,0), and
 ! u(*,n) with g

 h = 1.0 / n
 do k=1, maxiter
   ! Send down
   call MPI_Sendrecv( u(1,js), n-1, MPI_REAL, nbr_down, k &
                  u(1,je+1), n-1, MPI_REAL, nbr_up, k, &
                  MPI_COMM_WORLD, status, ierr )
   ! Send up
   call MPI_Sendrecv( u(1,je), n-1, MPI_REAL, nbr_up, k+1, &
                  u(1,js-1), n-1, MPI_REAL, nbr_down, k+1,&
                  MPI_COMM_WORLD, status, ierr )
   do j=js, je
     do i=1, n-1
       unew(i,j) = 0.25 * ( u(i+1,j) + u(i-1,j) + &
                       u(i,j+1) + u(i,j-1) - &
                       h * h * f(i,j) )
     enddo
   enddo
   ! code to check for convergence of unew to u.
   ! Make the new value the old value for the next iteration
   u = unew
 enddo
```

HPF

- HPF is a specification for an extension to Fortran 90 that focuses on describing the **distribution of data among processes** in structured comments.
- Thus an HPF program is also a valid Fortran-90 program and can be run on a sequential computer
- All communication and synchronization if provided by the compiled code, and hidden from the programmer
- No longer in much use, though some variations in use in Japan

HPF Version

```
   real u(0:n,0:n), unew(0:n,0:n), f(0:n, 0:n), h
!HPF$ DISTRIBUTE u(:,BLOCK)
!HPF$ ALIGN unew WITH u
!HPF$ ALIGN f WITH u

    ! Code to initialize f, u(0,*), u(n:*), u(*,0),
    ! and u(*,n) with g

    h = 1.0 / n
    do k=1, maxiter
      unew(1:n-1,1:n-1) = 0.25 * &
                ( u(2:n,1:n-1) + u(0:n-2,1:n-1) + &
                  u(1:n-1,2:n) + u(1:n-1,0:n-2) - &
                     h * h * f(1:n-1,1:n-1) )
      ! code to check for convergence of unew to u.
      ! Make the new value the old value for the next iteration

      u = unew
    enddo
```

The PGAS Languages

- PGAS (Partitioned Global Address Space) languages attempt to combine the convenience of the global view of data with awareness of data locality
  - ♦ Co-Array Fortran, an extension to Fortran-90, and now part of Fortran 2008
  - ♦ UPC (Unified Parallel C), an extension to C
  - ♦ Titanium, a parallel version of Java

Co-Array Fortran

- SPMD – Single program, multiple data
- Replicated to a number of images
- Images have indices 1,2, …
- Number of images fixed during execution
- Each image has its own set of local variables
- Images execute asynchronously except when explicitly synchronized
- Variables declared as co-arrays are accessible of another image through set of array subscripts, delimited by [ ] and mapped to image indices by the usual rule
- Intrinsics: this_image, num_images, sync_all, sync_team, flush_memory, collectives such as co_sum
- Critical construct

CAF Version

```
real u( 0:n,js-1:je+1,0:1)[*], f (0:n,js:je), h
integer np, myid, old, new
np = NUM_IMAGES()
myid = THIS_IMAGE()
new = 1
old = 1-new
! Code to initialize f, and the first and last columns of u on the extreme
! processors and the first and last row of u on all processors
 h = 1.0 / n
 do k=1, maxiter
  if (myid .lt. np) u(:,js-1,old)[myid+1] = u(:,je,old)
  if (myid .gt. 0) u(:,je+1,old)[myid-1] = u(:,js,old)
  call sync_all
  do j=js,je
    do i=1, n-1
      u(i,j,new) = 0.25 * ( u(i+1,j,old) + u(i-1,j,old) + &
                            u(i,j+1,old) + u(i,j-1,old) - &
                            h * h * f(i,j) )
    enddo
  enddo
  ! code to check for convergence of u(:,:,new) to u(:,:,old).
  ! Make the new value the old value for the next iteration
  new = old
  old = 1-new
enddo
```

UPC

- UPC is an extension of C with shared and local addresses
- Provides some simple distributions, similar to HPF
- Available on some large-scale systems
  - Including Blue Waters

UPC Version

```
#include <upc.h>
#define n 1024
shared [*] double u[n+1][n+1];
shared [*] double unew[n+1][n+1];
shared [*] double f[n][n];
int main() {
   int maxiter = 100;
   //  Code to initialize f, u(0,*), u(n:*), u(*,0), and
   //  u(*,n) with g
   double h = 1.0 / n;
   for (int k=0; k < maxiter; k++) {
     for (int i=1; i < n; i++) {
       upc_forall (int j=1; j < n; j++; &unew[i][j]) {
         unew[i][j] = 0.25 * ( u[i+1][j] + u[i-1][j] +
                        u[i][j+1] + u[i][j-1] -
                        h * h * f[i][j] );
       }
     }
     upc_barrier;
     // code to check for convergence of unew to u.
     // Make the new value the old value for the next iteration
     for (int i = 1; i < n; i++) {
       upc_forall(int j = 1; j < n; j++; &u[i][j]) {
         u[i][j] = unew[i][j];
       }
     }
   }
}
```

Global Operations

- Example: checking for convergence
- In our case, it means computing

$$\|u - unew\|_2^2$$

Locally, sum((u(i,j)-unew(i,j))**2)

- Then sum up the contributions across each processing element (node/ process/thread)
- Often called a "global" sum

Serial Version

```
real u(0:n,0:n), unew(0:n,0:n), twonorm

! ...
  twonorm = 0.0
  do j=1, n-1
    do i=1, n-1
      twonorm = twonorm + (unew(i,j) - u(i,j))**2
    enddo
  enddo
  twonorm = sqrt(twonorm)
  if (twonorm .le. tol) ! ... declare convergence
```

MPI Version

```
use mpi
real u(0:n,js-1:je+1), unew(0:n,js-1:je+1), twonorm, &
                  twonorm_local
integer ierr

! ...

twonorm_local = 0.0
  do j=js, je
    do i=1, n-1
      twonorm_local = twonorm_local + &
                      (unew(i,j) - u(i,j))**2
    enddo
  enddo
  call MPI_Allreduce(twonorm_local, twonorm, 1, &
              MPI_REAL, MPI_SUM, MPI_COMM_WORLD, ierr)
  twonorm = sqrt(twonorm)
  if (twonorm .le. tol) ! ... declare convergence
```

HPF Version

```
    real u(0:n,0:n), unew(0:n,0:n), twonorm
!HPF$ DISTRIBUTE u(:,BLOCK)
!HPF$ ALIGN unew with u
!HPF$ ALIGN f with u

 ! ...
      twonorm = sqrt ( &
              sum ( (unew(1:n-1,1:n-1) - &
                              u(1:n-1,1:n-1))**2) )
      if (twonorm .le. tol) ! ... declare convergence
    enddo
```

OpenMP Version

```
real u(0:n,0:n), unew(0:n,0:n), twonorm, ldiff

   ! ..
      twonorm = 0.0
!$omp parallel
!$omp do private(ldiff,i) reduction(+:twonorm)
      do j=1, n-1
        do i=1, n-1
          ldiff = (unew(i,j) - u(i,j))**2
          twonorm = twonorm + ldiff
        enddo
      enddo
!$omp enddo
!$omp end parallel
      twonorm = sqrt(twonorm)
    enddo
```

The HPCS languages

- DARPA funded three vendors to develop next-generation languages for programming next-generation petaflops computers
  - Fortress (Sun, before Sun acquired by Oracle)
  - X10 (IBM)
  - Chapel (Cray)
- All are global-**view** languages, but also with some notion for expressing locality, for performance reasons.
  - They are more abstract than UPC and CAF in that they do not have a fixed number of processes.
- Sun's DARPA funding was discontinued, and the Fortress project made public. See http://projectfortress.java.net
- Work continues at Cray (chapel.cray.com) and IBM (x10-lang.org)

Other Issues and Approaches

- Programming accelerators (GPGPUs)
  - OpenCL, OpenACC, CUDA
- Annotations, autotuning
- Domain Specific Languages (DSLs) and embedded DSLs
- Integrated Development Environments (Eclipse)
- Automating code optimization and tuning (Annotations, Autotuning)

For More Information

- Using MPI (3rd edition)
- Using Advanced MPI
- Using OpenMP

To Find Out…

- Find out what programming systems are available on your platforms. Look for
  - MPI
  - UPC
  - CoArray Fortran (as a separate language)
  - Fortran 2008 including coArrays
  - SHMEM