Introduction to parallel Computing

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What is high performance computing ?

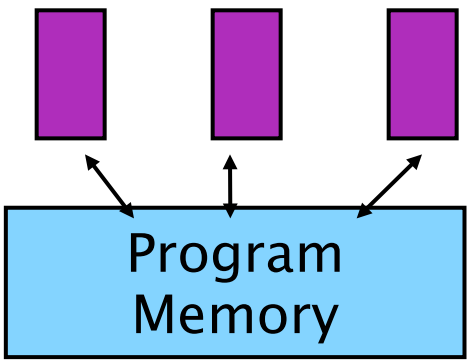
- Large volume numerical calculations : Set up facilites to run large number of codes in an efficient manner.
- Fast and efficient algorithms: Increase the speed of computing by optimizing the algorithm for a particular architecture.
- Highly scalable algorithms: Develop parallel codes that can scale linearly with number of processors .
- Modification of the computing model to allow for the use of recent advances in hardware: Cuda programming for GPU .
- Codes for complex problems: climate modeling , turbulence, protein folding, pattern and speech recognization, structural predictions ..

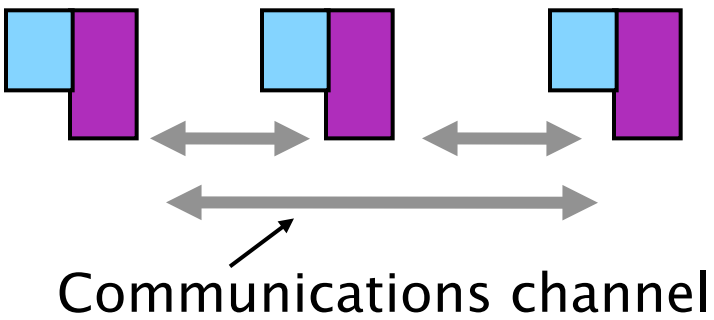
Sequential vs Parallel

- We are used to sequential programming – C, Java, C++, etc. E.g., Bubble Sort, Binary Search, Multiplication, FFT, BLAST, …
- Main idea – Specify the steps in perfect order
- Reality – We are used to parallelism a lot more than we think – as a concept; not for programming
- Methodology – Launch a set of tasks; communicate to make progress. E.g., Sorting 500 answer papers by – making 5 equal piles, have them sorted by 5 people, merge them together.

Main Paradigms: Shared vs Distributed Memory Programming

- Shared Memory – All tasks access the same memory, the same data. *pthreads*
- Distributed Memory – All memory is local. Data sharing is by explicitly transporting data from one task to another (*send-receive* pairs in MPI, e.g.)





- Tasks vs CPUs;
- SMPs vs Clusters

Simple Parallel Program – sorting numbers in a large array A

- Notionally **divide** A into **5** pieces [0..99;100..199;200..299;300..399;400..499].
- **Each part** is sorted by an **independent** sequential algorithm and **left** within its region.

- The resultant parts are merged by simply reordering among **adjacent** parts.

Work Break-down

- Parallel algorithm
- Prefer simple intuitive breakdowns
- Usually highly optimized sequential algorithms are not easily parallelizable
- Breaking work often involves some pre- or post- processing (much like divide and conquer)
- Fine vs large grain parallelism and relationship to communication

Sample OpenMP code

```
!$omp PARALLEL
!$OMP do
 do I=1,n
   y(I)=f(x(I))
Enddo
!$OMP end do
!$omp end PARALLEL
```

- ifort -openmp test.f
- export omp_NUM_THREADS=8
- ./a.out

```
#pragma omp PARALLEL for
for { I==1;I<=m;I++
   y(I)=f(x(I))
}
```

- icc -openmp test.f
- export omp_NUM_THREADS=8
- ./a.out

MPI: What do we need to think about…

- How many people are doing the work. (Degree of Parallelism)
- What is needed to begin the work. (Initialization)
- Who does what. (Work distribution)
- Access to work part. (Data/IO access)
- Whether they need info from each other to finish their own job. (Communication)
- When are they all done. (Synchronization)
- What needs to be done to collate the result.

MPI program structure

- All MPI programs must follow the same general structure. This structure is outlined as follows:

- include MPI header file
- variable declarations
- initialize the MPI environment

- ...do computation and MPI communication calls...

- close MPI communications

Hello world !!!

```
#include <stdio.h>
#include <mpi.h>
void main (int argc, char *argv[]) {
  int myrank, size;
  MPI_Init(&argc, &argv);                 /* Initialize MPI       */
  MPI_Comm_rank(MPI_COMM_WORLD, &myrank); /* Get my rank
     */
  MPI_Comm_size(MPI_COMM_WORLD, &size);   /* Get the total
                                          number of processors */
  printf("Processor %d of %d: Hello World!\n", myrank, size);
  MPI_Finalize();                         /* Terminate MPI        */
 }
```

- Out put if run with "mpirun -np 4 ./a.out"
- Processor 2 of 4: Hello World!
- Processor 1 of 4: Hello World!
- Processor 3 of 4: Hello World!
- Processor 0 of 4: Hello World!

This program evaluates the trapezoidal rule estimate for an integral of F(x). In this case, F(x) is exp(x) evaluated for the interval of 0 to 1.

```
*   This program requires the following call(s)
*           MPI_Init,   MPI_Comm_rank,  MPI_Comm_size,  MPI_Abort,  MPI_Finalize

main (int argc, char **argv)
{ double  A = 0.0, B = 1.0;
MPI_Init(&argc, &argv);       /* Initialize MPI */
MPI_Comm_rank(MPI_COMM_WORLD, &whoami);/* Find out this processor number */
MPI_Comm_size(MPI_COMM_WORLD, &nworkers); /* Find out the number of processo
DH=(B-A)/nworkers;
if (whoami > NP)  MPI_Abort(MPI_COMM_WORLD, errcode);

T1=A+whoami*DH; T2=A+(whoami+1)*DH; H=(T2-T1)/50.0;

SUM = 0.0;
for (i = 0; i <=49; i++)   SUM = SUM+F(T1+H*i)+F(T1+H*(i+1));
TN = SUM*H;

MPI_Reduce (&TN, &res,1,MPI_DOUBLE, MPI_SUM, 1, MPI_COMM_WORLD);

if(whoami==2)printf("Integral = %10.6f\n",res);

MPI_Finalize(); }
```

An MPI program to simulate the Ising model in two dimensions.

This program demonstrate the usage of mpi grid topology and communication between grid elements.

Help from Ms. Prathyusha in the preparation of this code is acknowledged.

```
#include <math.h>
#include <mpi.h>
#include <string.h>
#define LENGTH 6        /* system+boundary layer size is LENGTH*LENGTH
#define BUFSIZE (LENGTH-2)*(LENGTH-2)        /* system size*/
#define TEMP   1.0         /* TEMP in units of interaction and k_B */
#define WARM   1000
#define MCS    1250

int    total_energy( int [][LENGTH], int [] , int []);
int    total_mag( int [][LENGTH]); int coordinates[2];

double ran3( long int *); float  fpow (float , float); float  mag_analytic(float);
/* total number of processes "nworkers", identity of each process "rank" */
int          nworkers, rank, NP;
int spin[LENGTH][LENGTH];  int nbr1[LENGTH];  int nbr2[LENGTH];

/* structure defining the variables of the grid topology */
typedef struct GRID_INFO_TYPE{
int p;
MPI_Comm comm;   MPI_Comm row_comm;  MPI_Comm col_comm;
int q;  int my_row;  int my_col;  int my_rank;
}GRID_INFO_TYPE;
```

```
void   print_config (GRID_INFO_TYPE* grid, int [][LENGTH] , int );

/* set up the grid-topology */
void Setup_grid(GRID_INFO_TYPE* grid);

void initialize(GRID_INFO_TYPE* grid, int [][LENGTH], int [] , int []);

void mcmove(GRID_INFO_TYPE* grid, int[][LENGTH] , int [] , int [] );

/* communicate the state of the spins at the boundaries to neighbors */
void boundary(GRID_INFO_TYPE* grid, int[][LENGTH] , int [] , int [] );
```

```
main (int argc, char **argv)
{
/* Allocate memory for the  structure grid */
GRID_INFO_TYPE *grid = (GRID_INFO_TYPE *)malloc(sizeof(GRID_INFO_TYPE));
    /* Initialize MPI */
MPI_Init(&argc, &argv);
    /* Find out this process number */
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    /* Find out the number of processes */
MPI_Comm_size(MPI_COMM_WORLD, &nworkers);

Setup_grid(grid);

   int itime;
   int i;
   int big_energy,E;
   int big_mag,M;
   double E_per_spin;
   double M_per_spin;
   NP=sqrt(nworkers);
   iseed=iseed*(rank+1);
     itime = 0;
     big_energy = 0;
     big_mag = 0;
```

```
/* get started */
   initialize(grid,spin, nbr1, nbr2);
            boundary(grid,spin, nbr1, nbr2);
/* warm up system */
     for (i = 1 ; i <= WARM; i++)
     {   itime = i;
         mcmove(grid,spin, nbr1, nbr2);
         boundary(grid,spin, nbr1, nbr2);  }
/* do Monte Carlo steps and collect stuff for averaging */
     for (i = (WARM + 1) ; i <= MCS; i++)
     {        itime = i;
              mcmove(grid,spin, nbr1, nbr2);
              if(i!=MCS)boundary(grid,spin, nbr1, nbr2);
                 big_mag = big_mag + total_mag(spin);
                 big_energy = big_energy + total_energy(spin,nbr1,nbr2); }
  printf("Mag  %f rank %d time %d\n", 1.0*big_mag/(MCS-WARM), rank, MCS-WARM);
     MPI_Reduce (&big_mag, &M,1,MPI_INT, MPI_SUM, 0, MPI_COMM_WORLD);
/*process 0 adds total magentization from each process to find the net magnetization.
*/
     MPI_Reduce (&big_energy, &E,1,MPI_INT, MPI_SUM, 0, MPI_COMM_WORLD);
     if(rank==0)
     { M_per_spin = (float)M/((MCS - WARM)*(nworkers*(LENGTH-2)*(LENGTH-2)));
       E_per_spin = (float)E/((MCS - WARM)*nworkers*((LENGTH-2)*(LENGTH-2)));}
    print_config(grid, spin, itime );
   MPI_Finalize();  /* exit all MPI functions */ }
```

```
void Setup_grid(GRID_INFO_TYPE* grid){
int dimensions[2];
int periods[2];
int varying_coords[2];
MPI_Comm   localname;

MPI_Comm_size(MPI_COMM_WORLD, (&grid->p)); /* get the total number of
processes */
grid->q=(int)sqrt((double) grid->p);  /* square grid  */
dimensions[0]=dimensions[1]=grid->q;   /* dimension of the grid */
periods[0]=periods[1]=1;  /*  periodic if 1 and non-periodic if 0 */

MPI_Cart_create(MPI_COMM_WORLD, 2, dimensions, periods, 1, &(grid->comm)
create a grid communicator from the "Comm_world" , having dimension 2, reorder
process to processor mapping */

MPI_Comm_rank(grid->comm, &(grid->my_rank));
MPI_Cart_coords(grid->comm, grid->my_rank,2,coordinates);
grid->my_row=coordinates[0];
grid->my_col=coordinates[1];
varying_coords[0]=0;varying_coords[1]=1;
MPI_Cart_sub(grid->comm,varying_coords,&(grid->row_comm));
varying_coords[0]=1;varying_coords[1]=0;
MPI_Cart_sub(grid->comm,varying_coords,&(grid->col_comm));
}
```

```
void initialize(GRID_INFO_TYPE* grid,int spin[][LENGTH], int nbr1[], int nbr2[])
{
 int i, ix, iy,m,n,mt,nt,tag=50; float sd;

  char message[100];

     for (iy = 0 ; iy <LENGTH; iy++) /* start with random spins */
     for (ix = 0 ; ix <LENGTH; ix++)
     { sd=ran3(&iseed);
       if( sd>0.5 )spin[ix][iy] = 1;
       if( sd <= 0.5 )spin[ix][iy] = -1; }

     for (i = 1 ; i < LENGTH-1 ; i++)  /* set up neighbor list */
     {
       nbr1[i] = i - 1;
       nbr2[i] = i + 1;
      }
}
```

```
void print_config(GRID_INFO_TYPE *grid, int spin[][LENGTH] , int itime )
  int ix , iy, i,buf[(LENGTH-2)],buf1[LENGTH-2],tag=147,n,mp,np;
  char fname[30],message[50];
  float cx[1];
  FILE* fpr;
  MPI_Status status;
  if(grid->my_rank!=0)/* if rank is not zero pack all spins into a 1-d array */
  {  i=0;
      for (iy =1  ; iy < LENGTH-1; iy++)    {
      for (ix = 1 ; ix < LENGTH-1; ix++)
         {  buf[i]=spin[iy][ix];  i++; } }
       MPI_Send(buf,BUFSIZE,MPI_INT,0,tag,MPI_COMM_WORLD); /* send it to
process 0 */ }
  else  /* if the rank is zero */
 { fpr=fopen("config","w");  /* open the file */
   for (iy =1  ; iy < LENGTH-1; iy++) /* print the own configuration*/
   { for (ix = 1 ; ix < LENGTH-1; ix++)
     {   fprintf(fpr,"%d \t", spin[iy][ix]); } }
   for (n=1 ; n<nworkers;n++)
   { MPI_Recv(buf1,BUFSIZE,
MPI_INT,n,tag,MPI_COMM_WORLD,MPI_STATUS_IGNORE); /* receive from all other
processes */
      for(i=0; i<(LENGTH-2);i++)
      { for (ix = i*(LENGTH-2) ; ix < (i+1)*(LENGTH-2); ix++)
        { fprintf(fpr,"%d \t", buf1[ix]); }  } }   fclose(fpr);} }
```

```
void mcmove(GRID_INFO_TYPE* grid, int spin[][LENGTH], int nbr1[] , int nbr2[])
{
  int *U1,*D1,*R1,*L1;
/* arrays to recieve the spin configuration from neighbors */
     U1=(int *)malloc(LENGTH*sizeof(int));
     D1=(int *)malloc(LENGTH*sizeof(int));
     R1=(int *)malloc(LENGTH*sizeof(int));
     L1=(int *)malloc(LENGTH*sizeof(int));
   MPI_Status status;
  MPI_Cart_shift(grid->comm,0,-1,&m,&n);
  MPI_Recv(U1,LENGTH, MPI_INT,n,tag,MPI_COMM_WORLD,&status); /* receive U1
buffer with dimension LENGTH of type MPI_INT from process "n" with "tag" */
  MPI_Cart_shift(grid->comm,0,1,&m,&n);
  MPI_Recv(D1,LENGTH, MPI_INT,n,tag,MPI_COMM_WORLD,&status);
  MPI_Cart_shift(grid->comm,1,-1,&m,&n);
  MPI_Recv(L1,LENGTH, MPI_INT,n,tag,MPI_COMM_WORLD,&status);
  MPI_Cart_shift(grid->comm,1,1,&m,&n);
  MPI_Recv(R1,LENGTH, MPI_INT,n,tag,MPI_COMM_WORLD,&status);
  prob1 = exp(-8.0/TEMP);
  prob2 = exp(-4.0/TEMP);
  for (i = 1 ; i < LENGTH-1; i++)
  {  spin[i][0]=U1[i]; spin[i][LENGTH-1]=D1[i]; spin[0][i]=R1[i];  spin[LENGTH-1][i]=L1[i];  }
            free(U1); free(D1); free(L1); free(R1);
```

DO THE MC SPIN FLIP MOVES

```
void boundary(GRID_INFO_TYPE* grid, int spin[][LENGTH], int nbr1[] , int nbr2[])
{     U2=(int *)malloc(LENGTH*sizeof(int));     D2=(int *)malloc(LENGTH*sizeof(int));
     R2=(int *)malloc(LENGTH*sizeof(int));  L2=(int *)malloc(LENGTH*sizeof(int));
/* put  the spins at the left, right, up and down boundaries into separate arrays */
     for (i = 1 ; i < LENGTH-1 ; i++)
 {  U2[i]=spin[i][1];  D2[i]=spin[i][LENGTH-2];  L2[i]=spin[1][i];  R2[i]=spin[LENGTH-2][i]; }

/*send the boundary arrays to appropriate neighbor process
Remeber 0 is up and down and  1 is left and right.  */

      MPI_Cart_shift(grid->comm,0,-1,&m,&n); /* find the neighbor process down the
current one */
      MPI_Send(U2,LENGTH, MPI_INT,n,tag,MPI_COMM_WORLD); /* send U2 buffer
with dimension LENGTH of type MPI_INT to  process "n" with "tag" */
      MPI_Cart_shift(grid->comm,0,1,&m,&n);
      MPI_Send(D2,LENGTH, MPI_INT,n,tag,MPI_COMM_WORLD);
      MPI_Cart_shift(grid->comm,1,1,&m,&n);
      MPI_Send(R2,LENGTH, MPI_INT,n,tag,MPI_COMM_WORLD);
      MPI_Cart_shift(grid->comm,1,-1,&m,&n);
      MPI_Send(L2,LENGTH, MPI_INT,n,tag,MPI_COMM_WORLD);

            free(U2);              free(D2);       free(L2);   free(R2);
}
```

Introduction to Parallel Computing. Michael Skuhersky vex@mit.edu. What is Parallel Computing? â— Wikipedia says: â€œParallel computing is a form of computation in which many calculations are carried out simultaneouslyâ€. â— Speed measured in FLOPS. What is Parallel Computing? (cont.) How can this be useful?Â Main Granularity Paradigms. â— Granularity: the ratio of computation to communication. â— 3 approaches to parallelism, depending on what kind of problem you need to solve. Embarrassingly Parallel. â— No effort required to separate tasks â— Tasks do not depend on, or communicate. with, each other. â— Examples: Mandlebrot, Folding@home, Password brute-forcing, Bitcoin Mining! Introduction to Parallel Computing. Table of Contents. Abstract. Overview. What is Parallel Computing? Why Use Parallel Computing? Concepts and Terminology. von Neumann Computer Architecture.Â Overview. What is Parallel Computing? Traditionally, software has been written for serial computation: To be run on a single computer having a single Central Processing Unit (CPU) â€¢ Parallel computing: use of multiple processors or computers working together on a common task. â€“ Each processor works on its section of the problem â€“ Processors can exchange information. Grid of Problem to be solved. y. CPU #1 works on this area of the problem exchange.

PDF | On Jan 1, 1994, V. Kumar and others published Introduction to parallel computing. Design and analysis of algorithms | Find, read and cite all the research you need on ResearchGate.Â Since the parallel prefix computation runs in O(log k) steps for k values, obviously the entire time cost can be improved to O(n log k) steps by using k threads. The first thread treats ST [6] and the second thread works on ST [5]. In Step 3, the head position becomes 7, and now all k = 3 threads actively execute operations for ST [7], ST [6], and ST [5] respectively. It should be noted that finally in Step 3 the content of ST [5] is completely determined while those of ST [7] and ST [6] are partially computed and not yet determined. Given a web graph, compute the page rank of each node. Use MPI - vineethshankar/pagerank.Â Join GitHub today. GitHub is home to over 50 million developers working together to host and review code, manage projects, and build software together. Sign up. master. pagerank/Introduction to Parallel Computing, Second Edition-Ananth Grama, Anshul Gupta, George Karypis, Vipin Kumar.pdf. Go to file. Go to file T. Parallel Computing â€“ It is the use of multiple processing elements simultaneously for solving any problem. Problems are broken down into instructions and are solved concurrently as each resource which has been applied to work is working at the same time. Advantages of Parallel Computing over Serial Computing are as follows: It saves time and money as many resources working together will reduce the time and cut potential costs. It can be impractical to solve larger problems on Serial Computing. It can take advantage of non-local resources when the local resources are finite. Serial Computing â€¨w