Optimization and Scalability Hands-on Lab

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Introduction to Parallel Computing

Setup

- Login to Stampede:
  - **`ssh username@stampede.tacc.utexas.edu`**
- Untar the lab files:
  - **`cd`**
  - **`tar xvf ~train00/parallel_opt_lab.tar`**
- Change directories and ls to see the files:
  - **`cd parallel_opt_lab`**
  - **`ls`**
- You should see both C and F90 versions of the code

A simple 2D problem

$$f'(x,y,t) = \frac{df(x,y,t)}{dx} = \frac{f(x+\Delta x,y,t) - f(x-\Delta x,y,t)}{2\Delta x}$$

$$f(x,y,t+1) = f(x,y,t) + \epsilon f'(x,y,t)$$

- No particular physical process
- Structure is similar to many explicit codes
  - Calculate the derivative of f
  - Update f
  - Update neighbor boundary values
  - Start again

The Partitioning Scheme

- For clarity we will use a 1D partitioning scheme
- Lines 35-48 (C) and 38-50 (F90) define the 1D virtual topology we will use
- Periodic boundary conditions are embedded in the Cartesian topology
- This allows us to employ “left” and “right” as well defined directions for the MPI exchange

Data Exchange Optimization

- Focus on the main loop starting on line 69 (C, F90) of the code.
- There are several ways to optimize the data exchange between tasks
- Think back to the concepts presented and find at least one way to improve the overall execution time of the code
- Make any changes you need to the code to improve its current performance, but always keep a copy of the original
- Towards the end of the Lab I will explain two different ways to speed up the exchange, but give it your best shot!
- Extra points if your best code is better than mine ☺

Getting started

- Choose the C or the F90 version of the lab
- Make a personal copy that you will modify later

  cp ./exchange_1d.c ./exchange_opt.c
  cp ./exchange_1d.f90 ./exchange_opt.f90
- Compile the current version of the code

  mpicc ./exchange_1d.c –o original
  mpif90 ./exchange_1d.f90 –o original
- Start an interactive session on Stampede
- Run the code using 10 processors and record the timings it gives you when done

  ibrun –n 10 –o 0 ./original
- Now try to beat that time by modifying exchange_opt.c!

I feel kind of lost with this lab…

- Don’t panic! And keep reading…
- If you are not use to coding with MPI this lab can be a little hard.
- There are two proposed solutions already coded in the “proposed_solutions” directory.
- The next four slides explain what was done in the two proposed solutions and why.
- Feel free to simply compile the “solution” versions and compare the execution timings.
- Make sure you understand WHY the proposed solutions are faster than the original.

Optimization and Scalability

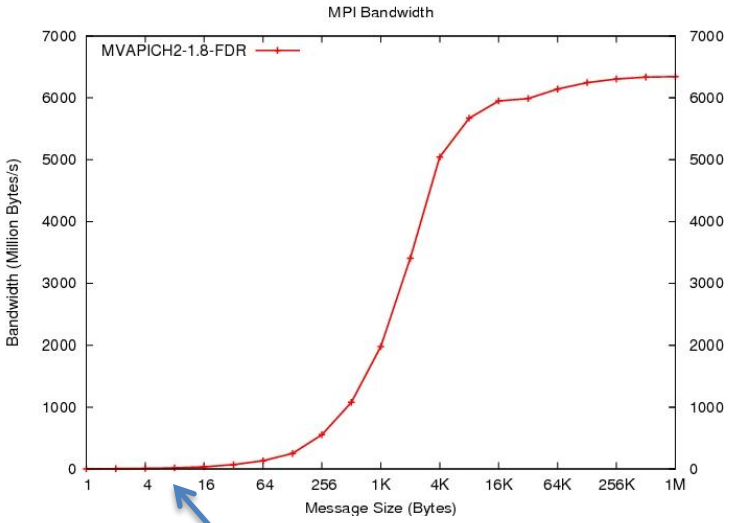
PROPOSED SOLUTION

Original Code

```
// Send to right, receive from left
for( j = 0; j < NY; j++ ){
   sendBuf[0] = f[NX][j];
   MPI_Irecv( recvBuf, 1, MPI_DOUBLE, left, …);
   MPI_Send( sendBuf, 1, MPI_DOUBLE, right, …);
   MPI_Wait( &request, &status );
   f[0][j] = recvBuf[0];
}
```

```
// Send to left, receive from right
for( j = 0; j < NY; j++ ){
   sendBuf[0] = f[1][j];
   MPI_Irecv( recvBuf, 1, MPI_DOUBLE, right, …);
   MPI_Send( sendBuf, 1, MPI_DOUBLE, left, …);
   MPI_Wait( &request, &status );
   f[NX+1][j] = recvBuf[0];
}
```

- One message for each data item to exchange in each direction
- Message size is 8 Bytes



Tiny effective bandwidth !!!

Optimized Code (1)

```
// Send to right, receive from left
for( j = 0; j < NY; j++ ) sendBuf[j] = f[NX][j];

MPI_Irecv( recvBuf, NY, MPI_DOUBLE, left,  … );
MPI_Send(  sendBuf, NY, MPI_DOUBLE, right, … );
MPI_Wait( &request, &status );

for( j = 0; j < NY; j++ ) f[0][j] = recvBuf[j];
```

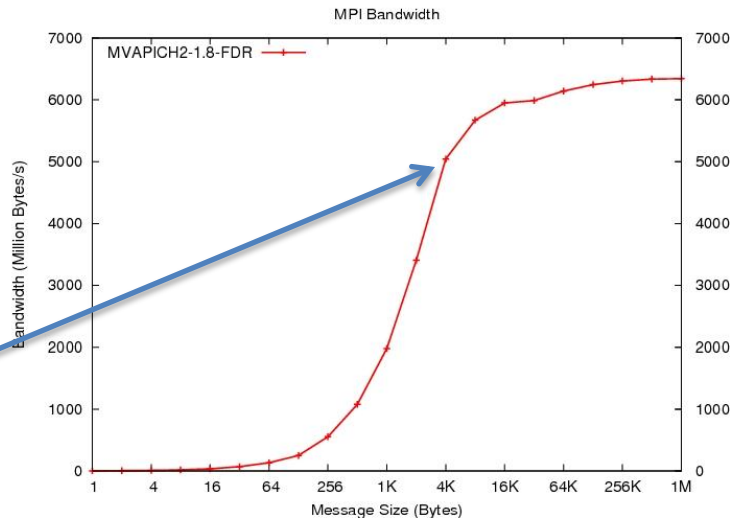
```
// Send to left, receive from right
for( j = 0; j < NY; j++ ) sendBuf[j] = f[1][j];

MPI_Irecv( recvBuf, NY, MPI_DOUBLE, right, … );
MPI_Send(  sendBuf, NY, MPI_DOUBLE, left, … );
MPI_Wait( &request, &status );

for( j = 0; j < NY; j++ ) f[NX+1][j] = recvBuf[j];
```

- Pack data to be sent to the right
- Single exchange with packed data
- Unpack data received from left
- Repeat for the left to right exchange
- Message size is 4 KB

Large effective bandwidth increase



Optimized Code (2)

```
for( j = 0; j < NY; j++ ){
    sendBufRight[j] = f[NX][j];
    sendBufLeft[j] = f[1][j];
}

MPI_Irecv( recvBufLeft, NY, MPI_DOUBLE, left,…);
MPI_Irecv( recvBufRight, NY, MPI_DOUBLE, right,…);
MPI_Isend( sendBufRight, NY, MPI_DOUBLE, right,…);
MPI_Isend( sendBufLeft, NY, MPI_DOUBLE, left …);
MPI_Waitall( 4, request, status );

for( j = 0; j < NY; j++ ){
    f[0][j] = recvBufLeft[j];
    f[NX+1][j] = recvBufRight[j];
}
```

- Pack data to send to both left and right
- Non-blocking data exchange
- Unpack data

- Uses bi-directional capability of IB

Significant effective bandwidth increase