PROGRAMMING AND OPTIMIZATION FOR INTEL® ARCHITECTURE

Hands-On Workshop (HOW) Series "Deep Dive"

Session 5

Colfax International — *colfaxresearch.com*

2017

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COURSE ROADMAP

- Module I. Programming
  - 01. Intel Architecture and Modern Code – Feb 13
  - 02. Xeon Phi, Coprocessors, Omni-Path – Feb 14
- Module II. Expresssing Parallelism
  - 03. Expressing Parallelism with Vectors – Feb 15
  - 04. Multi-threading with OpenMP – Feb 16
  - 06. Distributed Computing, MPI – Feb 17
- Module III. Optimization
  - 06. Optimization Overview: N-body – Feb 20
  - 07. Scalar tuning, Vectorization – Feb 21
  - 08. Common Multi-threading Problems – Feb 22
  - 09. Multi-threading, Memory Aspect – Feb 23
  - 10. Access to Caches and Memory – Feb 24

February 2017

S	M	T	W	H	F	S
			1	2	3	4
5	6	7	8	9	10	11
12	13	14	15	16	17	18
19	20	21	22	23	24	25
26	27	28				

— Webinar+remote access

HOW SERIES ONLINE

Course page:
colfaxresearch.com/how-17-02

- Slides
- Code
- Video
- Chat

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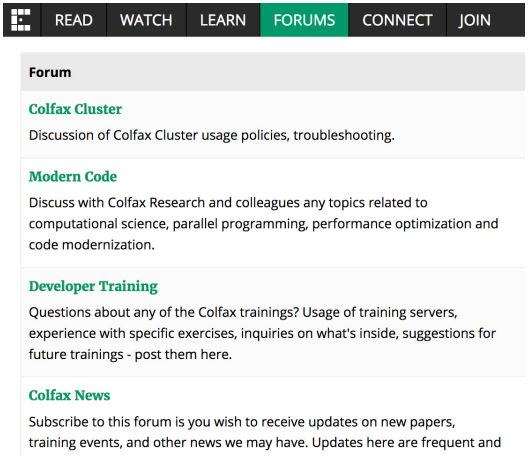
GET YOUR QUESTIONS ANSWERED: CHAT

colfaxresearch.com/how-17-02

GET YOUR QUESTIONS ANSWERED: FORUMS



colfaxresearch.com/discussion

HANDS-ON EXERCISES AND REMOTE ACCESS

- All registrants receive an invitation from cluster@colfaxresearch.com
- Queue-based access to Intel Xeon E5, Intel Xeon Phi (KNC and KNL)
- Can access the cluster the entire 2 weeks of the workshop

§2. DISTRIBUTED COMPUTING

COMPUTING HARDWARE

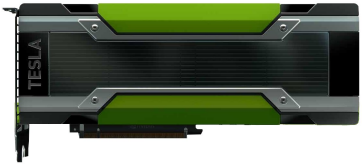
Computing Platforms

Workstations

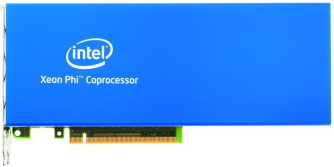
Servers

Clusters

Computing Accelerators



GPGPUs

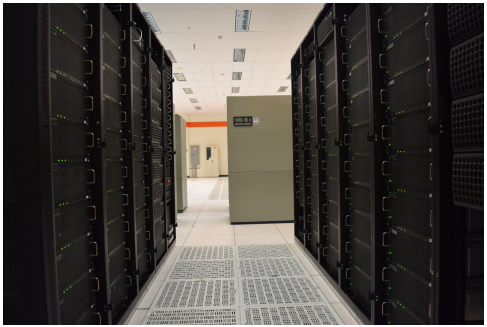


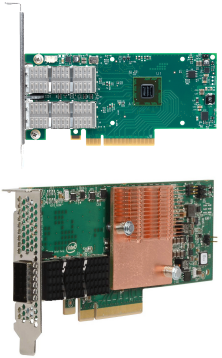
Coprocessors

FPGAs

CLUSTERS

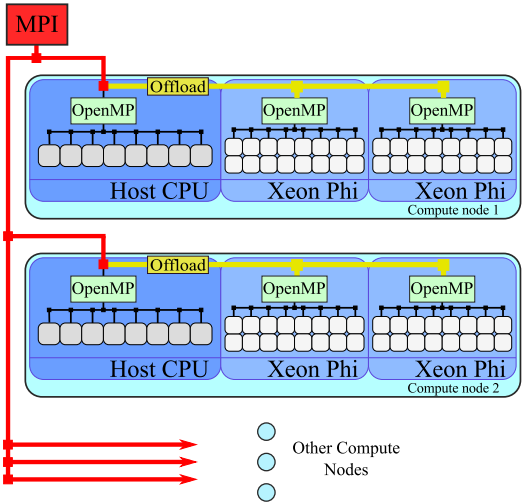
Clusters often use Gigabit Ethernet for administration and InfiniBand or Intel Omni-Path for communication.





SCALING ACROSS A CLUSTER WITH COPROCESSORS

- MPI processes only on CPUs
- Divide data between coprocessors
- Concurrent offload from multiple host threads
- Synchronize data between nodes with MPI



SCALING ACROSS A CLUSTER WITH COPROCESSORS WITH MPI

- MPI processes only on CPUs
- Divide data between coprocessors
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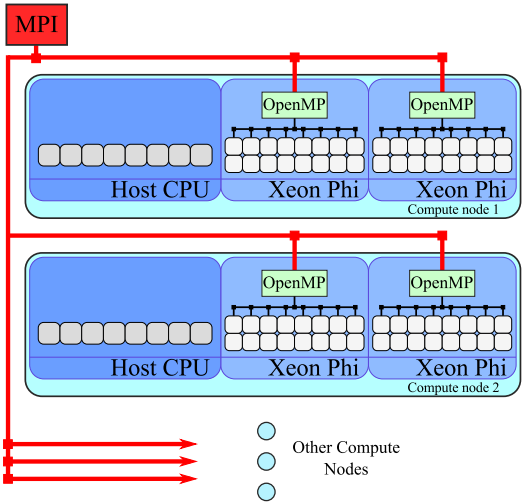
- Synchronize data between nodes with MPI



PARALLEL PROGRAMMING FRAMEWORKS

Data-Parallel :

intrinsics, vector classes, automatic vectorization, array notation, kernels

Shared Memory :

Pthreads, Threading Building Blocks, OpenMP

Message Passing :

TCP/IP, MPI

MPI AND HETEROGENEOUS COMPUTING

STRUCTURE OF MPI APPLICATIONS: HELLO WORLD

```
#include "mpi.h"
#include <cstdio>
int main (int argc, char *argv[]) {
  MPI_Init (&argc, &argv);  // Initialize MPI envirnmnt
  int rank, size, namelen;
  char name[MPI_MAX_PROCESSOR_NAME];
  MPI_Comm_rank (MPI_COMM_WORLD, &rank); // ID of current process
  MPI_Get_processor_name (name, &namelen); // Hostname of node
  MPI_Comm_size (MPI_COMM_WORLD, &size); // Number of processes
  printf ("Hello World from rank %d running on %s!\n", rank, name);
  if (rank == 0) printf("MPI World size = %d processes\n", size);
  MPI_Finalize (); // Terminate MPI environment
}
```

MPICH site contains a list of MPI 3.2 routines

COMPILING AND RUNNING MPI APPLICATIONS ON LOCALHOST

Compilation:

```
u100@c005% mpiicpc -o HelloMPI HelloMPI.cc
```

Command file `mympi`:

```
#PBS -l nodes=1
cd $PBS_O_WORKDIR
mpirun -host localhost -np 2 ./HelloMPI
```

Results:

```
u100@c005% qsub mympi
2000
u100@c005% cat mympi.o2000
Hello World from rank 1 running on c005-n001!
Hello World from rank 0 running on c005-n001!
MPI World size = 2 processes
```

RUNNING MPI APPLICATIONS ON SEVERAL HOSTS

Command file `mydistmpi`:

```
#PBS -l nodes=2
cd $PBS_O_WORKDIR
cat $PBS_NODEFILE
mpirun -machinefile $PBS_NODEFILE ./HelloMPI
```

Results:

```
u100@c005% qsub mydistmpi
2001
u100@c005% cat mydistmpi.o2001
c005-n001
c005-n002
Hello World from rank 1 running on c005-n002!
Hello World from rank 0 running on c005-n001!
MPI World size = 2 processes
```

COMPILING AND RUNNING NATIVE MPI APPLICATIONS ON COPROCESSORS

Compilation

```
u100@c005% mpiicpc -mmic -o HelloMPI.MIC HelloMPI.c
```

Command file `mymic`:

```
#PBS -l nodes=1:coprocessor
cd $PBS_O_WORKDIR
scp HelloMPI.MIC mic0:~/
export I_MPI_MIC=1
mpirun -host mic0 -np 2 ~/HelloMPI.MIC
```

Results:

```
Hello World from rank 1 running on c005-n001-mic0!
Hello World from rank 0 running on c005-n001-mic0!
MPI World size = 2 processes
```

HETEROGENEOUS MPI APPLICATIONS: HOST + COPROCESSORS

Command file `myhet`:

```
#PBS -l nodes=1:coprocessor
cd $PBS_O_WORKDIR
scp HelloMPI.MIC mic0:~/
export I_MPI_MIC=1
mpirun -host localhost -np 1 ./HelloMPI : -host mic0 -np 1 ~/HelloMPI.MIC
```

Results:

```
Hello World from rank 0 running on c005-n001!
Hello World from rank 1 running on c005-n001-mic0!
MPI World size = 2 processes
```

- Specify Xeon executable for host processes
- Specify Xeon Phi executable for coprocessor processes

HETEROGENEOUS MPI APPLICATIONS: MACHINE FILE

Xeon Phi coprocessors may be configured to be IP-addressable on cluster network and share file system paths with hosts.

Machine file `hosts.txt`:

```
c005-n101:1
c005-n102:1
c005-n101-mic0:1
c005-n102-mic0:1
```

Job submission:

```
vega@lyra% export I_MPI_MIC_POSTFIX=.MIC
vega@lyra% mpirun -machinefile hosts.txt ~/Hello
```

- Specify Xeon executable for host processes
- MIC executable obtained by appending `I_MPI_MIC_POSTFIX`

COMPILING AND RUNNING MPI APPLICATIONS

1. Compile and link with the MPI wrapper of the compiler:
   - `mpiicc` for C,
   - `mpiicpc` for C++,
   - `mpiifort` for Fortran 77 and Fortran 95.
2. For Xeon Phi coprocessors (KNC): `I_MPI_MIC=1`
3. Launch with the tool `mpirun`
   - Colon-separated list of hosts (`-host` *hostname*),
   - Alternatively, `-machinefile $PBS_NODEFILE`

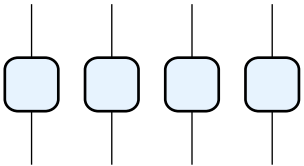
COMMUNICATION PATTERNS

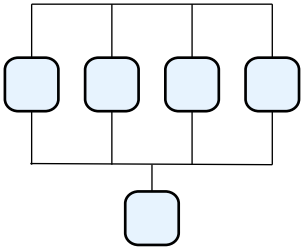
POINT TO POINT COMMUNICATION

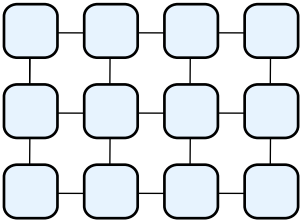
```
1  if (rank == sender) {
2
3   char outgoingMsg[messageLength];
4   strcpy(outgoingMsg, "Hi There!");
5   MPI_Send(&outgoingMsg, messageLength, MPI_CHAR, receiver, tag, MPI_COMM_WORLD);
6
7
8  } else if (rank == receiver) {
9
10  char incomingMsg[messageLength];
11  MPI_Recv (&incomingMsg, messageLength, MPI_CHAR, sender,
12                                                    tag, MPI_COMM_WORLD, &stat);
13  printf ("Received message with tag %d: '%s'\n", tag, incomingMsg);
14
15
16 }
```

PARALLEL PATTERNS

Common parallel patterns call for collective communication

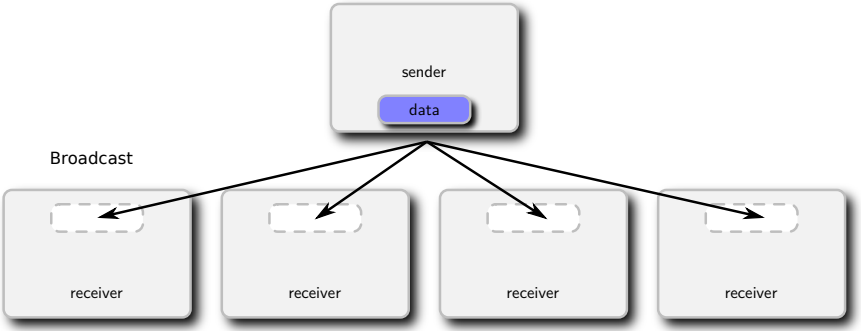






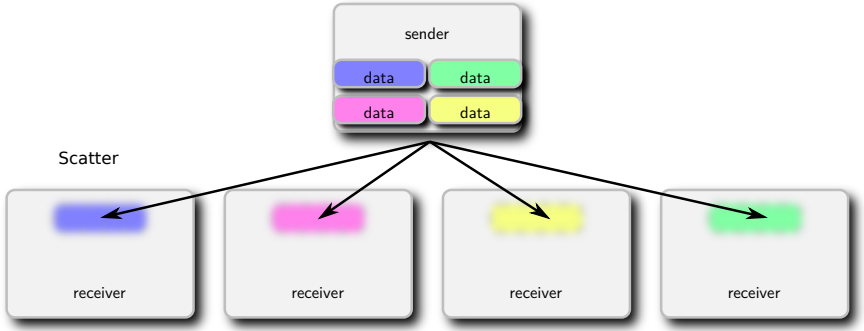
COLLECTIVE COMMUNICATION: BROADCAST

```
1 int MPI_Bcast( void *buffer, int count, MPI_Datatype datatype,
2     int root, MPI_Comm comm );
```



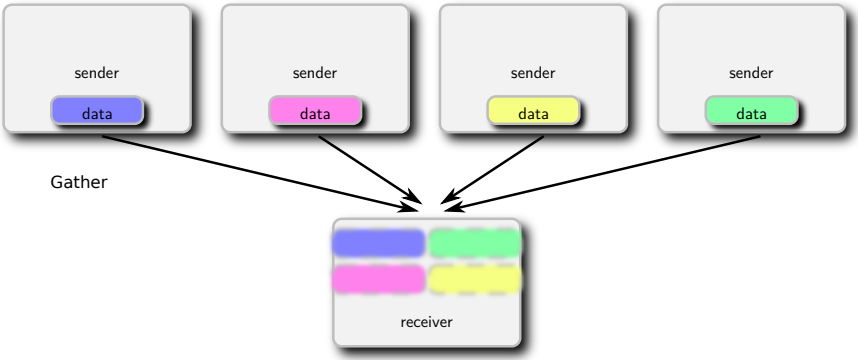
COLLECTIVE COMMUNICATION: SCATTER

```
int MPI_Scatter(void *sendbuf, int sendcnt, MPI_Datatype sendtype, void *recvbuf,
    int recvcnt, MPI_Datatype recvtype, int root, MPI_Comm comm);
```



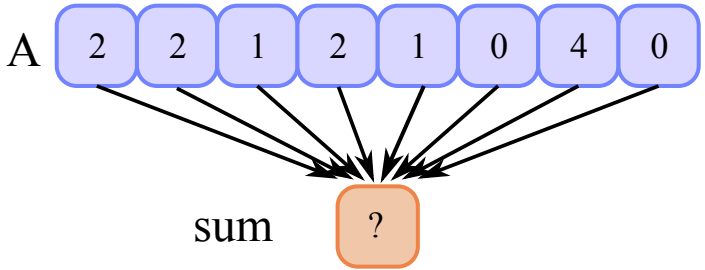
COLLECTIVE COMMUNICATION: GATHER

```
1 int MPI_Gather(void *sendbuf, int sendcnt, MPI_Datatype sendtype,
2     void *recvbuf, int recvcnt, MPI_Datatype recvtype, int root, MPI_Comm comm);
```



COLLECTIVE COMMUNICATION: REDUCTION

```
int MPI_Reduce(void *sendbuf, void *recvbuf, int count, MPI_Datatype datatype,
    MPI_Op op, int root, MPI_Comm comm);
```

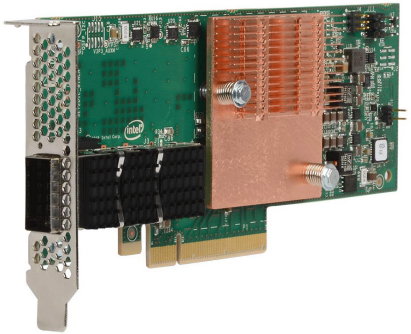


Available reducers: max/min, minloc/maxloc, sum, product, AND, OR, XOR (logical or bitwise).

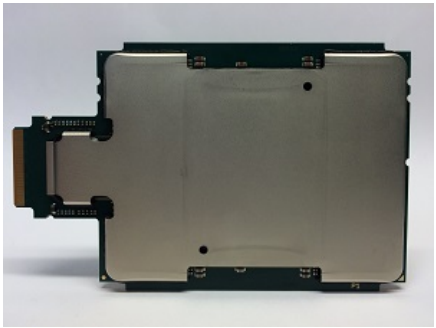
INTEL OMNI-PATH ARCHITECTURE

INTEL'S HPC COMMUNICATION FABRIC

Intel Omni-Path Architecture - low-latency, high-bandwidth, scalable communication fabric for HPC applications.



Discrete

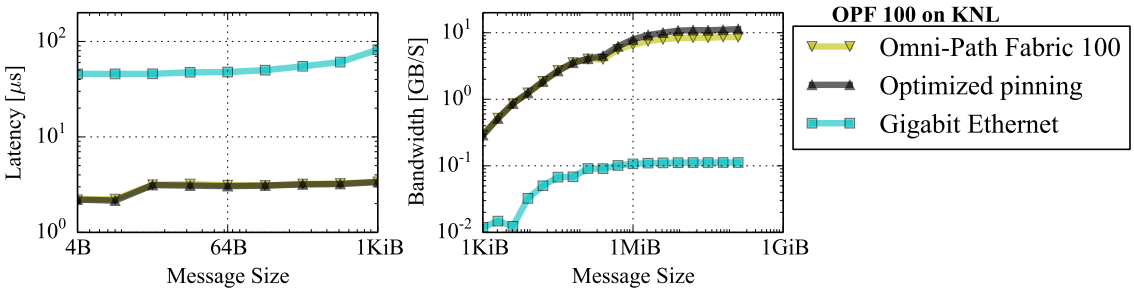


Integrated

INTEL OMNI-PATH FABRIC 100 WITH INTEL XEON PHI PROCESSORS (KNL)

Switching between OPA and 1GbE on Colfax Cluster:

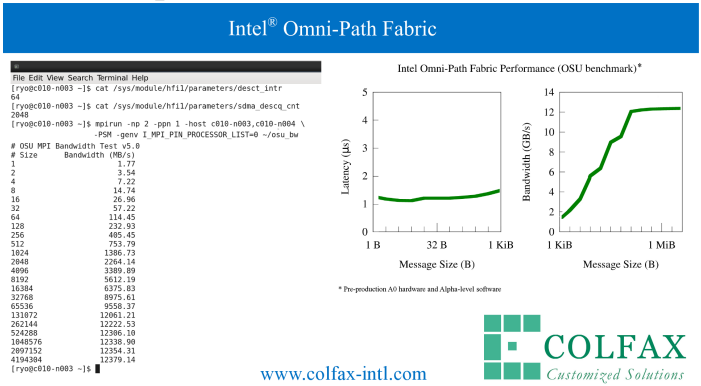
```
I_MPI_FABRICS=tmi mpirun -machinefile $PBS_NODEFILE IMB-MPI1 PingPong
I_MPI_FABRICS=tcp mpirun -machinefile $PBS_NODEFILE IMB-MPI1 PingPong
```



Optimal pinning `I_MPI_PIN_PROCESSOR_LIST=7` may be done automatically by a future version of Intel MPI

INTEL OMNI-PATH FABRIC 100 WITH INTEL XEON PROCESSORS

First generation: 100 Gbps bandwidth, ≈ 1 microsecond latency



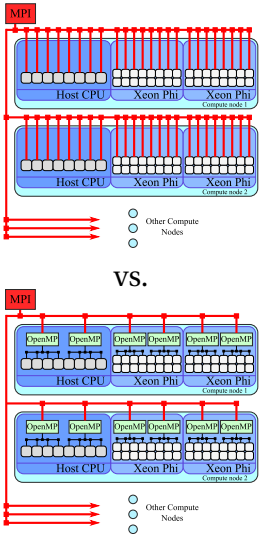
- Rely on MPI for platform-independent communication
- Intel MPI: set `I_MPI_FABRICS=tmi`.

INTER-OPERATION WITH OPENMP

HYBRID MPI+OPENMP

Using OpenMP inside of MPI processes:

- Reduces the memory footprint
- Decreases the number of MPI ranks, which reduces communication
- May incur thread synchronization overhead
- Optimal number of threads in MPI processes must be established empirically



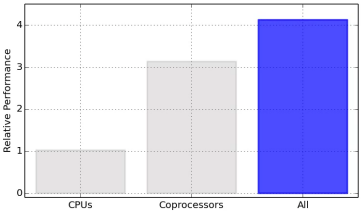
HYBRID MPI+OPENMP

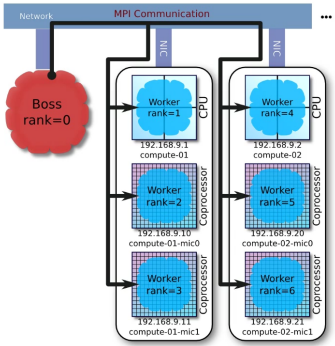
- MPI pins processes to cores and sets OpenMP affinity for them.
- To tune pinning: `I_MPI_PIN`, `I_MPI_PIN_DOMAIN`
- To diagnose process pinning: `I_MPI_DEBUG=4`
- For MPI calls from multiple OpenMP threads, use `-mt_mpi`
- More information in the MPI Reference Manual

LOAD BALANCING

ASIAN OPTION PRICING: HETEROGENEOUS CLUSTERING

Heterogeneous Clustering with Homogeneous Code:
Asian Option Pricing



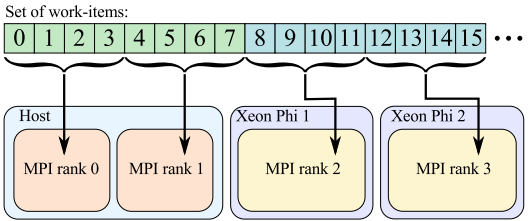


COLFAX
Customized Solutions

http://xeonphi.com/papers/heterogeneous

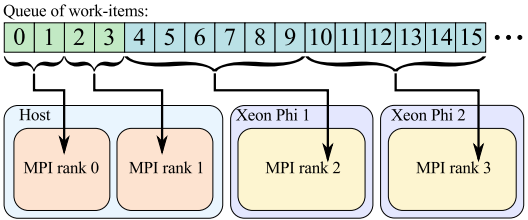
HETEROGENEOUS CALCULATION WITHOUT LOAD BALANCING

```
1  const double optionsPerProcess = double(nOptions)/double(mpiWorldSize);
2  const int myFirstOption = int(optionsPerProcess*(myRank));
3  const int myLastOption  = int(optionsPerProcess*(myRank+1));
4
5  // Static, even load distribution: assign options to ranks
6  for (int i = myFirstOption; i < myLastOption; i++)
7    ComputeOptionPayoffs(option[i], payoff[i]);
```

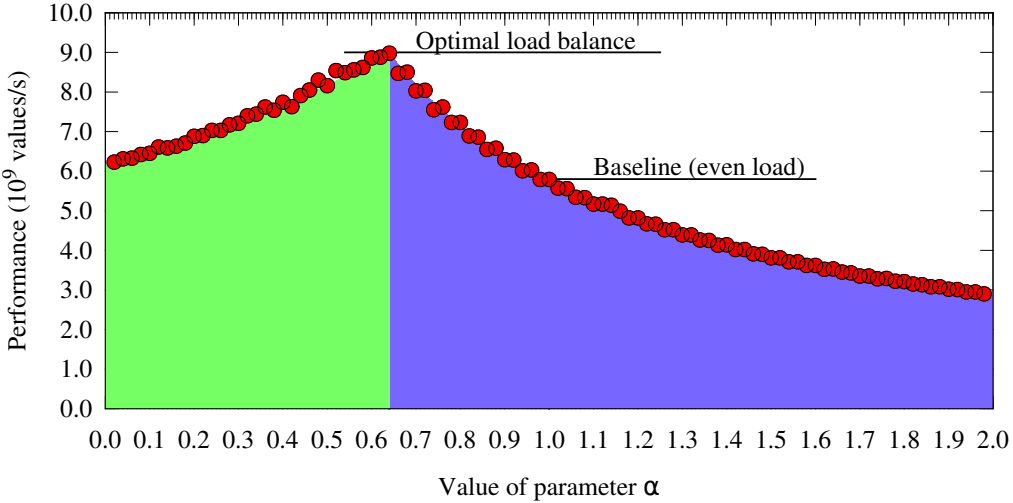


STATIC LOAD BALANCING

```
1 if (rankTypes[myRank] == 0) { // I am a MIC-based rank
2   double optionsPerProc = double(lastOptForCPUs)/double(cpuRanks.size());
3   myFirstOpt = int(optionsPerProc*(myGroupRank));
4   myLastOpt  = int(optionsPerProc*(myGroupRank+1.0));
5 } else { // I am a CPU-based rank
6   double optionsPerProc = double(nOpts-lastOptForCPUs)/double(micRanks.size());
7   myFirstOpt=lastOptForCPUs+int(optionsPerProc*(myGroupRank));
8   myLastOpt=lastOptForCPUs+int(optionsPerProc*(myGroupRank+1.0)); }
```

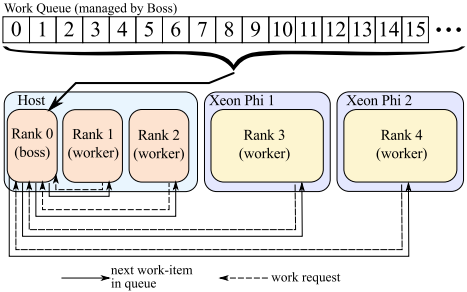


STATIC LOAD BALANCING: PARAMETER TUNING

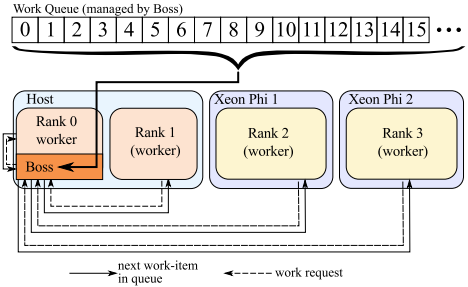


DYNAMIC LOAD BALANCING

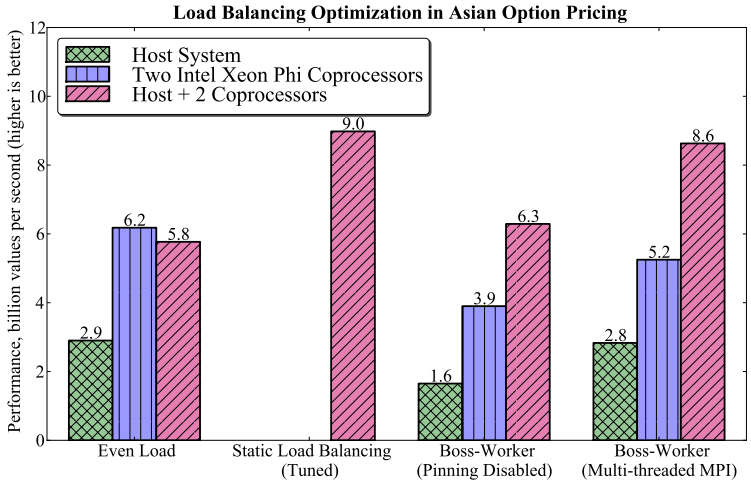
```
1  if (myRank == 0) // Boss's branch
2    DistributeWork(nOptions, option, mpiWorldSize);
3  else // Workers' branch
4    ReceiveWork(option, payoff, myRank);
```



or



PERFORMANCE WITH DIFFERENT SCHEDULING MODES



Refer to the book for explanation on the last two results.

INTEL MPI PERFORMANCE SNAPSHOT

USING INTEL MPI PERFORMANCE SNAPSHOT

Part of Intel Trace Analyzer and Collector (ITAC), invoke with `-mps` argument of `mpirun`:

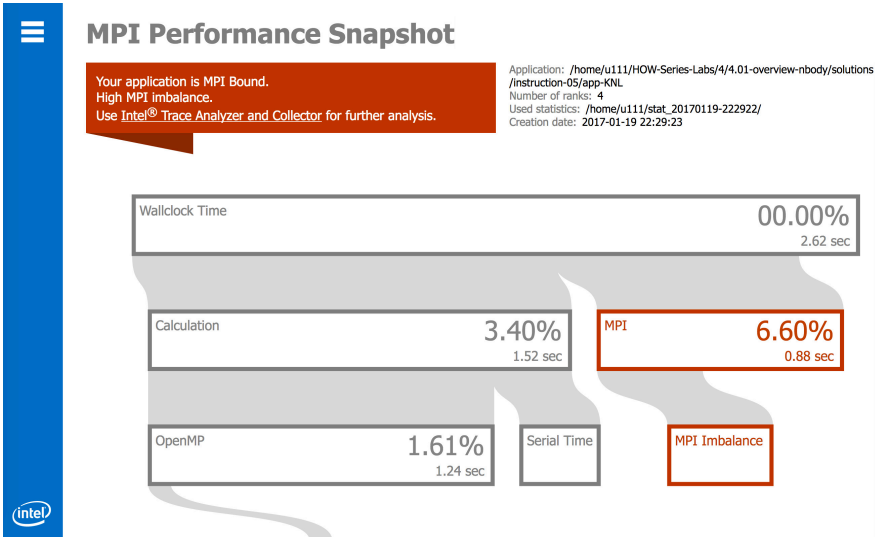
```
#PBS -l nodes=4

cd $PBS_O_WORKDIR
source /opt/intel/itac_latest/bin/mpsvars.sh
mpirun -mps -machinefile $PBS_NODEFILE ./myApplication
```

Produces `stat_*` directory with `.bin` files in it. Analyze them with `mps`.

```
u111@c005% ls ./stat_*
/home/u111/myproject/stat_20170119-222922:
stat-0.bin  stat-1.bin  stat-2.bin  stat-3.bin
u111@c005% mps stat_20170119-222922
u111@c005% mps -g stat_20170119-222922
```

READING INTEL MPI PERFORMANCE SNAPSHOT



§3. SUMMARY

MPI CONCEPTS AND FUNCTIONS

Communication modes – (non-)blocking, (a)synchronous, ready mode

Message buffers – application, system, user space

Communicators, Groups – creation, manipulation, usage

Data types – built-in, derived

Collective communication – patterns

Hybrid programming – co-existence with threads: safety, performance

One-sided communication – remote memory access

Click for links from the MPI Forum.
More information in our book and MPI tutorial from the LLNL

SUMMARY ON MPI

- Framework for distributed-memory programming
- Hides from developer complexity of programming a variety of fabrics
- Collective communication may use functions of the fabric
- Intel Omni-Path Architecture is a native solution for Xeon Phi
- Intel tool for tuning load balance, communication: ITAC

Next session: performance optimization: overview, case study

NEW PROJECT: MC^2 SERIES

Webinars on performance optimization by computational scientists

MC² Series

Posted on February 10, 2017 in MC² Series, Training

In Modern Code Contributed Talks, or MC² Series, experts in computational disciplines share their experience. Register for these ongoing webinars to learn the performance optimization methods used in real-life applications.

Would you like to contribute a talk? Contact us. Scholarship is available in the form of access to a diverse collection of powerful computing platforms.

MC² 001: Astrophysics, Hydrodynamics

Speaker: Dr. Fabio Baruffa, Leibniz Supercomputing Centre
Title: Performance Optimization of SPH Algorithms for Multi/Many-Core Architectures
Date: March 7, 2017 at 17:00-18:00 GMT (convert)

More Information

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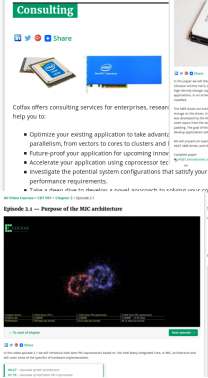

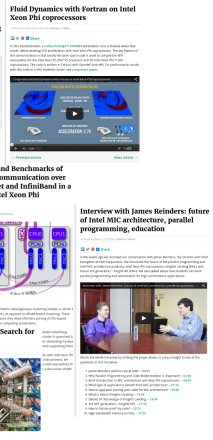

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