Adaptive MPI
Santos Dumont Supercomputing Summer School 2021

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Outline

Presentation

Parallel Programming Model
  Ideal Features
  Parallel Objects
  Charm++

Adaptive Message Passing Interface
  Introduction
  Communication Optimizations
  Migration

Global Variable Privatization
Where do I come from?

Central America

Costa Rica

is not Puerto Rico
has no standing army since 1949
hosts 6% of world’s biodiversity
produces 98% of its electricity from green sources
Costa Rica High Technology Center
CeNAT

Development through Knowledge
Collaborative Research Projects
Accelerating scientific discovery

Physics

Seismology

Biodiversity

Bioinformatics

Mobility

Epidemics

HPC

Image Analysis
Trainings and Seminars
Advanced Computing Laboratory

Costa Rica HPC School

Costa Rica Big Data School
Parallel Programming Model
Flame Simulation on IPLMCFD Application
Parallel Programming Model
An abstract machine on which parallel programs will execute

- Components:
  - Execution model: how code gets executed
  - Memory model: how data moves between memory hierarchy

- Most parallel systems expose multiple parallel programming models

Copernicus’s heliocentric model
Desirable Features
The HPC Holy Grail

- **Performant**: extracts as much performance as possible from the underlying hardware
- **Productive**: expresses abstract algorithms easily
- **Portable**: can be used on any computer
- **Expressive**: allows a broad range of algorithms
- **Scalable**: the general structure of the code persists as more hardware is used
Implementation
Alternatives for using the model

- **Library:**
  - An API of function calls
  - Library gets linked with the executable; multiple languages

- **Programming Language Extension:**
  - Additional constructs for parallelism
  - Compiler support for translation

- **New Programming Language:**
  - Design of new language grammar
  - Flexibility to include features

*There are only two kinds of languages: the ones people complain about and the ones nobody uses*

Bjarne Stroustrup
Parallel Objects Model
Object-oriented parallel programming

- An application is decomposed into wudus (work and data units)
- Objects are reactive entities: interface of remote methods
- All message-passing operations are nonblocking: *asynchronous method invocation*
- A message-driven execution similar to Active Messages

- Objects know how to serialize/deserialize, also called the pack-unpack (*PUP*) framework
- Goals:
  - Latency hiding
  - Load balancing
  - Adaptivity

"Parallel Objects Model" is an object-oriented parallel programming model. An application is decomposed into work and data units (wudus). Objects act as reactive entities, providing an interface for remote method access. All message-passing operations are nonblocking, allowing for asynchronous method invocation. A message-driven execution similar to Active Messages is facilitated. Objects know how to serialize/deserialize, using the pack-unpack (*PUP*) framework. The goals are:
- Latency hiding
- Load balancing
- Adaptivity
Introspective Runtime System

Smart and automatic decision making

- A thin layer between the application and the machine
- Based on object-based *overdecomposition*: many more objects than processing entities
- Components:
  - Message scheduler
  - Routing tables
  - Load and communication monitoring
Migration

Objects can be relocated

- The underlying system consists of a collection of processing entities (cores, processors, or nodes)
- Objects are distributed among the processing entities
- That assignment may change dynamically if load imbalance arises
- An introspective runtime system detects performance bottlenecks and balances load by moving objects around.
Load Balance

A complex optimization problem

- NP-complete problem: suboptimal, but fast heuristic algorithms
- Goal: avoid overloaded nodes
- Runtime collects load and communication data
- Greedy strategies, graph partitioning
- Runtime system shuffles objects around to avoid overloading
- Dynamic load balance
- Principle of persistence
- Based on PUP framework
Charm++
Actively developed since mid 90s

- Objects are called *chares*
- Chare arrays are the main object collection
- Chares export remote *entry methods*
Global Object Space
Entry methods can be called from anywhere
Global Object Space

Proxy chares channel remote method calls
Charm++ Runtime System
Multiple layers with different abstraction
Charm++ Applications
Span multiple scientific domains
Exercise
Got Charm++?

- Started at the Parallel Programming Laboratory of the University of Illinois at Urbana-Champaign in the mid 90's by Prof. Laxmikant V. Kalé
- Maintained by Charmworks Inc
- Charm++ official website: http://charmplusplus.org/
- Get latest release version
- Build Charm++ and AMPI on your computer
  - Linux:
    ./build AMPI netlrts-linux-x86_64 --with-production
    --enable-error-checking -j4 -k
  - Mac:
    ./build AMPI netlrts-darwin-x86_64 --with-production
    --enable-error-checking -j4 -k
Adaptive Message Passing Interface
Adaptive Message Passing Interface
An MPI implementation on top of Charm++ runtime system

- Enables Charm++ dynamic features for pre-existing MPI codes
- Each MPI rank is wrapped as a Charm++ chare
- The collection of MPI ranks becomes a chare array
- MPI codes run on Charm++ runtime system
Process Virtualization

AMPI virtualizes MPI ranks

- MPI ranks are implementing as migratable user-level threads rather than OS processes
- Virtualization ratio akin to object overdecomposition

- If one MPI rank is blocked on communication, the scheduler picks other rank to run
AMP Library

AMP virtualizes MPI ranks

- Another MPI implementation, similar to MPICH, OpenMPI, MVAPICH
- Currently compliant with MPI 2.2 standard
- Benefits:
  - Communication/computation overlap
  - Cache benefits to smaller working sets
  - Dynamic load balancing
  - Fault tolerance
  - Lower latency messaging within a process
  - Reuse existing MPI codes and developer skills, but scale them further
- Disadvantages:
  - Some code modifications are required, v.g., global/static variables shared must be privatized
  - Latest MPI functions might not be supported by AMP
Communication Optimizations
Speeding up algorithms

- AMPI overlaps communication of one rank with computation of others scheduled on the same core
- Even blocking calls are executed asynchronously
- Supports non-blocking collectives since before MPI-3.0
- AMPI optimizes for communication locality (i.e. neighbor exchanges)
- Can even load balance based on the application communication graph, to improve communication locality dynamically
Communication Optimizations

Internal communications

AMPI offers lower latency and higher bandwidth than process-based MPIs for messages within a core or node.

- P1: two ranks on the same core
- P2: two ranks on different cores in the same process
Communication Optimizations
Example, OSU MPI latency benchmark

Running on Quartz (Intel Xeon/Omni-Path cluster at LLNL)

- P1: two ranks on the same core
- P2: two ranks on different cores in the same process
Communication Optimizations
Example, OSU MPI latency benchmark
Communication Optimizations
Example, OSU MPI bi-directional bandwidth benchmark
Dynamic Load Balancing

AMPI instructions

- AMPI ranks are migratable across address spaces at runtime

```
• Add a call to AMPI_Migrate(MPI_Info)
• Where info is the following:
  MPI_Info_set(info, ampi_load_balance sync)
```
Dynamic Load Balancing
BRAMS weather simulation code

Isomalloc
Memory allocator

- User-level thread stack + heap
- Reserves globally unique slices of virtual memory on each process for all ranks
- No need for Pack/UnPack routines
- Works on all 64-bit platforms except BGQ and Windows
Dynamic Load Balancing
Example, Harm3D application

- Existing MPI astrophysics code developed by Scott Noble at Tulsa (in collaboration with NCSA)
- Imbalanced case: two black holes (zones) move through the grid with 3x more computational work in buffer zone than in near zone
Dynamic Load Balancing

Example, Harm3D application
Fault Tolerance

Checkpointing ranks

- AMPI ranks can be migrated to persistent storage or in remote memories for fault tolerance
- Storage can be disk, SSD, NVRAM
- Online fault detection and recovery
- Just pass a different MPI_Info to AMPI_Migrate()
  
  ```
  MPI_Info_set(info1, ampi_checkpoint, in_memory)
  MPI_Info_set(info2, ampi_checkpoint, to_file=dir_name)
  ```
Fault Tolerance

Example

PlasComCM: iteration = 95, dt = 0.870094D-02, time = 0.835290D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
PlasComCM: iteration = 97, dt = 0.870094D-02, time = 0.843991D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
PlasComCM: iteration = 98, dt = 0.870094D-02, time = 0.852692D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
PlasComCM: iteration = 99, dt = 0.870094D-02, time = 0.861393D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
PlasComCM: iteration = 100, dt = 0.870094D-02, time = 0.870094D+00, cfl = 0.500000D+00, maxT = 0.298000D+03

[0] Checkpoint started
[0] Checkpoint finished in 0.455819 seconds
PlasComCM: iteration = 101, dt = 0.870094D-02, time = 0.878795D+00, cfl = 0.500000D+00, maxT = 0.298000D+03

1. Checkpoint
Fault Tolerance

Example

PlasComCM: iteration = 96, dt = 0.870094D-02, time = 0.835290D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
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PlasComCM: iteration = 102, dt = 0.870094D-02, time = 0.887496D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
PlasComCM: iteration = 103, dt = 0.870094D-02, time = 0.896197D+00, cfl = 0.500000D+00, maxT = 0.298000D+03

Socket closed before recv.
Socket 4 failed

1. Checkpoint

2. Failure
Fault Tolerance

Example

PlasComCM: iteration = 95, dt = 0.870094D-02, time = 0.835290D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
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PlasComCM: iteration = 103, dt = 0.870094D-02, time = 0.896197D+00, cfl = 0.500000D+00, maxT = 0.298000D+03

Socket closed before recv.
Socket 4 failed

Charmrun finished launching new process in 1.153346 seconds
Charmrun says Processor 1 failed on Node 1
[1] Restarting after crash
[1] Restart finished in 0.458689 seconds at 0.463579.
PlasComCM: iteration = 101, dt = 0.870094D-02, time = 0.878795D+00, cfl = 0.500000D+00, maxT = 0.298000D+03

1. Checkpoint
2. Failure
3. Recover
4. Resume execution
Fault Tolerance

Example

PlasComCM: iteration = 96, dt = 0.870094D-02, time = 0.835290D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
PlasComCM: iteration = 97, dt = 0.870094D-02, time = 0.843991D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
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Charmrun finished launching new process in 1.153346 seconds
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PlasComCM: iteration = 101, dt = 0.870094D-02, time = 0.878795D+00, cfl = 0.500000D+00, maxT = 0.298000D+03

CharmLB> RefineLB: PE [0] starting at 69.353145
CharmLB> RefineLB: PE [0] #Objects migrating: 7
CharmLB> RefineLB: PE [0] finished at 69.355673 duration 0.002528 s

PlasComCM: iteration = 102, dt = 0.870094D-02, time = 0.887496D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
PlasComCM: iteration = 103, dt = 0.870094D-02, time = 0.896197D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
PlasComCM: iteration = 104, dt = 0.870094D-02, time = 0.904898D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
PlasComCM: iteration = 105, dt = 0.870094D-02, time = 0.913599D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
PlasComCM: iteration = 106, dt = 0.870094D-02, time = 0.922300D+00, cfl = 0.500000D+00, maxT = 0.298000D+03
PlasComCM: iteration = 107, dt = 0.870094D-02, time = 0.931001D+00, cfl = 0.500000D+00, maxT = 0.298000D+03

1. Checkpoint
2. Failure
3. Recover
4. Resume execution
5. Load balance
No Virtualization

Example

Load imbalance appears during point-to-point messaging and in MPI_Allreduce each timestep
No Virtualization

Example

Communication/computation cycles mean the network is underutilized most of the time
Virtualization 8x

Example

Most of the idle time due to point-to-point messaging and MPI_Allreduce is now hidden by computation.
Virtualization and Load Balancing

Example

The communication of each virtual rank is overlapped with the computation of others scheduled on the same core.
Virtualization 8x

Example

- Communication is spread over the whole timestep
- Peak network bandwidth used is reduced by 3x
AMI Code
Compiling and running

- To compile an AMPI program:
  charm/bin/ampicc pgm pgm.o
- For migratability, link with: -memory isomalloc
- For LB strategies, link with: -module CommonLBs
- To run an AMPI job, specify the number of virtual processes (+vp)
  .charmrun +p 1024 ./pgm
  .charmrun +p 1024 ./pgm +vp 16384
  .charmrun +p 1024 ./pgm +vp 16384 +balancer RefineLB
Exercise
Compiling and running

Steps:

1. Build and run the LULESH mini-app on AMPI
2. Experiment with varying degrees of virtualization (ranks/core)
3. Add calls to create MPI_Info for LB and to AMPI_Migrate()
   
   MPI_Info_create(&info);
   
   MPI_Info_set(info, "ampi_load_balance", "sync");

4. Experiment with dynamic load balancing (frequency, strategy)

Get started:
AMPi is distributed with Charm++, and is already built in the pre-installed directory
Global Variable Privatization
Global Variable Privatization

AMPI virtualizes the ranks of MPI_COMM_WORLD

- Ranks are implemented as user-level threads rather than OS processes
- Is this safe?

```c
int rank, size;
int main (int argc, char *argv[])
{
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);

    MPI_Barrier(MPI_COMM_WORLD);

    if(rank == 0) MPI_Send(..);
    else if (rank == 1) MPI_Recv(...);
    MPI_Finalize();
}
```
Global Variable Privatization
Unsafe code without modification

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Conclusion

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Global Variable Privatization

Recap

- AMPI virtualizes the ranks of MPI_COMM_WORLD
- It is unsafe to use a mutable global state:
  - Global state: global and static variables that can be modified
  - Mutable: written multiple times
- Rule:
  If global/static variables are written-once (or read-only) to same value across all ranks, they are safe. Otherwise, they are unsafe.
Global Variable Privatization
How to make an existing code safe for AMPI virtualization?

- For new codes, this is easy: avoid mutable global state
- For existing codes, how should we safely virtualize them?
  - Avoid using mutable global/static variables, or refactor to avoid them
  - Tag declarations of unsafe variable as `thread_local`
  - AMPI supports privatizing these to each rank at runtime:
    ```
    ampicc -tlsglobals
    ```
  - Other approaches possible, but either less portable or still under development
Global Variable Privatization

Manual encapsulation

- Method of refactoring an application to not use mutable global/static state
  - One-time refactoring with minor but pervasive changes, can be done by novice programmers
  - Can keep non-mutable variables at global scope
  - Results in a portable program that can be run with both MPI and AMPI

- Kinds of unsafe global/static variables:
  - C/C++: non-const globally scoped variables, static variables
  - Fortran: non-PARAMETER variables that are COMMON, SAVE, or MODULE
Global Variable Privatization
Example

```c
int rank, size;

int main (int argc, char *argv[]){
    initMPI(argc, argv);
    doWork();
}

int initMPI(int argc, char *argv[]){
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
}
```
Global Variable Privatization

Solution

```c
int size;

int main (int argc, char *argv[]){
    int rank;
    initMPI(argc, argv, &rank);
    doWork(rank);
}

int initMPI(int argc, char *argv[], int *rank){
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
}
```
AMPI Privatization
Manual encapsulation

In applications with many global variables, it is often easier to define a new structure or derived type that contains all the mutable global variables:

- Can do this hierarchically within each module first, then define one top-level structure that contains a type for each module
- Can safely ignore PARAMETERs or const global data
- Benefit: only pass one extra argument to each function that uses one or many global variables
Thread-Local Storage (TLS) provides per-thread copies of memory
  ▶ C/C++11 provide standard support for thread_local attribute
  ▶ Fortran has no standard support for TLS, though OpenMP has threadprivate
AMI provides support for privatizing TLS variables to its user-level threads
  ▶ Only change necessary is tagging global variable declarations with TLS attribute
  ▶ Runtime overhead is switching the TLS pointer at each ULT context switch
  ▶ Currently requires gcc/gfortran and Linux
Other approaches for AMPI Privatization

Automatic ELF Global Offset Table swapping

Benefits:
- Full automation, no developer effort
- Already implemented in AMPI

Limitations:
- Requires ELF binary format
- Requires disabling linker optimizations in ld v2.23+
- It does not handle static variables
- Runtime overhead proportional to the number of global variables
Other approaches for AMPI Privatization

icc mpc-privatize

Benefits:
- Full automation, no developer effort

Limitations:
- Requires icc, or patched version of gcc
- Not yet supported by AMPI
Other approaches for AMPI Privatization

Process-in-Process library

Benefits:
- Full automation, no developer effort, no compiler support needed

Limitations:
- Requires patched version of glibc
- Requires dynamic linking of application and libraries with globals
- Not yet implemented in AMPI
Additional concerns for AMPI-izing Fortran codes:

- Fortran program main must be renamed subroutine MPI_Main
- Fortran command line argument parsing must be done with AMPI extension routines similar to Fortran2003 standard routines
- Implicit SAVE variables are static and can be hard to identify
- Use of AUTOMATIC arrays can bloat the ULT stack size
- Must use OpenMP threadprivate attribute for TLS declarations
Exercise

Manual privatization with single data structure

```c
int myrank;
double xyz[100];

void subA();
int main(int argc, char** argv){
    int i;
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
    for(i=0; i<100; i++)
        xyz[i] = i + myrank;
    subA();
    MPI_Finalize();
}

void subA(){
    int i;
    for(i=0; i<100; i++)
        xyz[i] = xyz[i] + 1.0;
}
```
Exercise

Solution

```c
int main(int argc, char** argv){
    int i,ierr;
    struct shareddata *c;
    MPI_Init(&argc, &argv);
    c = (struct shareddata*)malloc(sizeof(struct shareddata));
    MPI_Comm_rank(MPI_COMM_WORLD, &(c->myrank));
    for(i=0;i<100;i++)
        c->xyz[i] = i + c->myrank;
    subA(c);
    MPI_Finalize();
}

void subA(struct shareddata *c){
    int i;
    for(i=0;i<100;i++)
        c->xyz[i] = c->xyz[i] + 1.0;
}
```
Exercise
FORTRAN code

Goal: Learn how to privatize an existing (Fortran) MPI code using two privatization techniques:

- Manual encapsulation
- TLS globals

MiniGhost: a mini-application from the Mantevo suite:

- Fortran90 MPI stencil code
- Contains multiple global and static variables, across multiple modules
- Mix of read-only, and written-once, and mutable variables
Exercise

FORTRAN code

1. Identify the global variables in MiniGhost
2. Only declared in 2 files: MG_CONSTANTS.F and MG_OPTIONS.F
3. Classify them as mutable, written-once, or read-only
4. Privatize mutable global variables using OpenMP threadprivate:
5. Compile with ampif90 -tlsglobals option
6. Run with different degrees of virtualization

```
INTEGER :: VARIABLE
!$omp threadprivate(VARIABLE)
```
1. AMPI Tutorial:  

2. AMPI Research Papers:  
https://charm.cs.illinois.edu/papers

3. AMPI applications:  
git clone https://charm.cs.illinois.edu/gerrit/benchmarks/ampi-benchmarks
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- AMPI Tutorial by Parallel Programming Lab of University of Illinois at Urbana-Champaign
Concluding Remarks

AMPI provides the dynamic RTS support of Charm++ with the familiar API of MPI

- Overdecomposition
- Communication optimizations
- Dynamic load balancing
- Automatic fault tolerance
- Checkpoint/restart
- OpenMP runtime integration