Outline

1) **Introduction**
    - Object Design
    - Execution Model
2) Hello World
3) Benefits of Charm++
4) Charm++ Basics
    - Object Collections
5) Overdecomposition
6) Migratability
    - Checkpointing and Resilience
7) Structured Dagger
8) Application Design
9) Performance Tuning
10) Using Dynamic Load Balancing
11) Interoperability
12) Debugging
13) Further Optimization

What is Charm++?

- Charm++ is a generalized approach to writing parallel programs
  - An alternative to the likes of MPI, UPC, GA etc.
  - But not to sequential languages such as C, C++, and Fortran

- Charm++ builds upon a proven approach: objects

- Identify the entities being simulated (say atoms, routers, humans, etc)
- Define the computational tasks being performed (e.g. force computation)
- Create C++ classes to encapsulate them
- Use member functions to interact

- What about processors? Do you really want to worry about them?

Stuff you already know

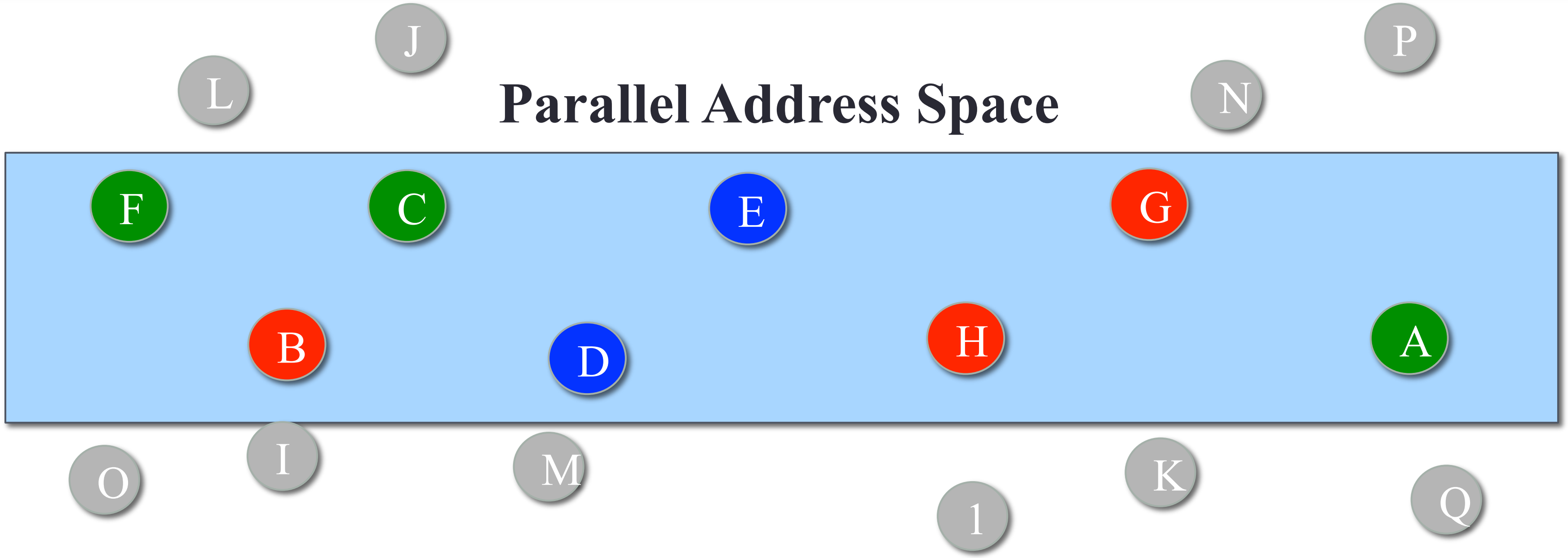
Benefits of Object-based code

- Objects encapsulate data
- Methods represent functionality relevant to that data
- Method invocations can modify / update state of the object / data
- Computation can be expressed in terms of objects interacting via method invocations

- Methods are natural units of sequential computation on object data
- Thoughtful design yields focused methods with single purpose
- Naturally expresses an object’s response to inputs (signals / data)

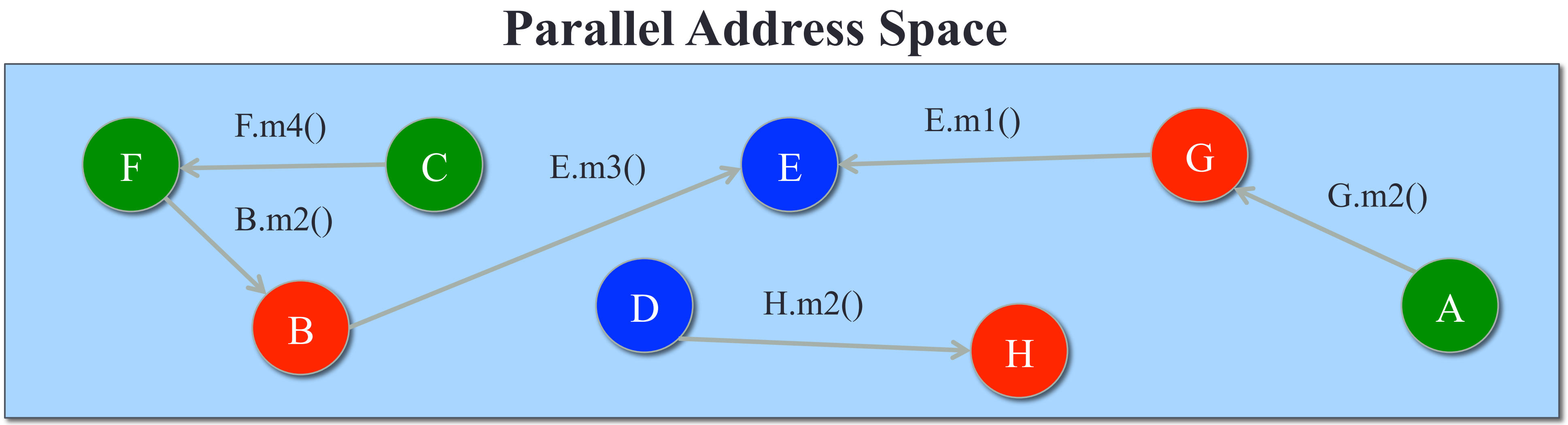
- Nothing new
- It is not about language syntax. It is about program structure

Globally-Visible Objects: Chares



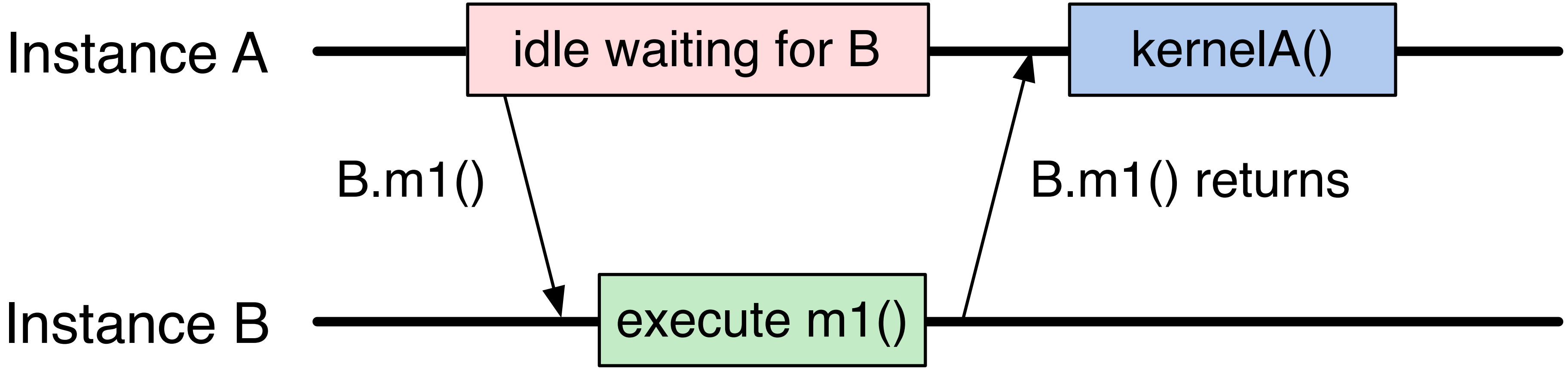
- Certain “special” object *instances* are:
  - first-class citizens in the parallel address space,
  - with unique location-independent names
- Under the hood, the runtime handles locality and provides the mechanisms to promote objects to the parallel space

Globally-Visible Methods: Entry Methods



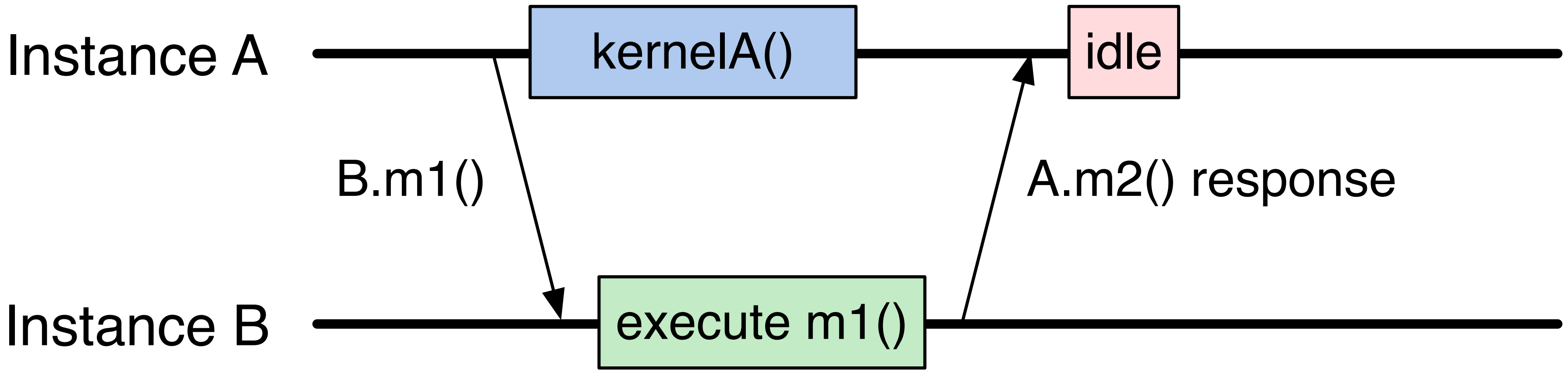
- How can objects communicate across address spaces?
  - Just like a sequential object-oriented language, an object's reference is used to invoke a method
  - In the parallel space, this is a handle that is location transparent
  - A method invocation becomes an act of communication

Method-Driven Asynchronous Communication



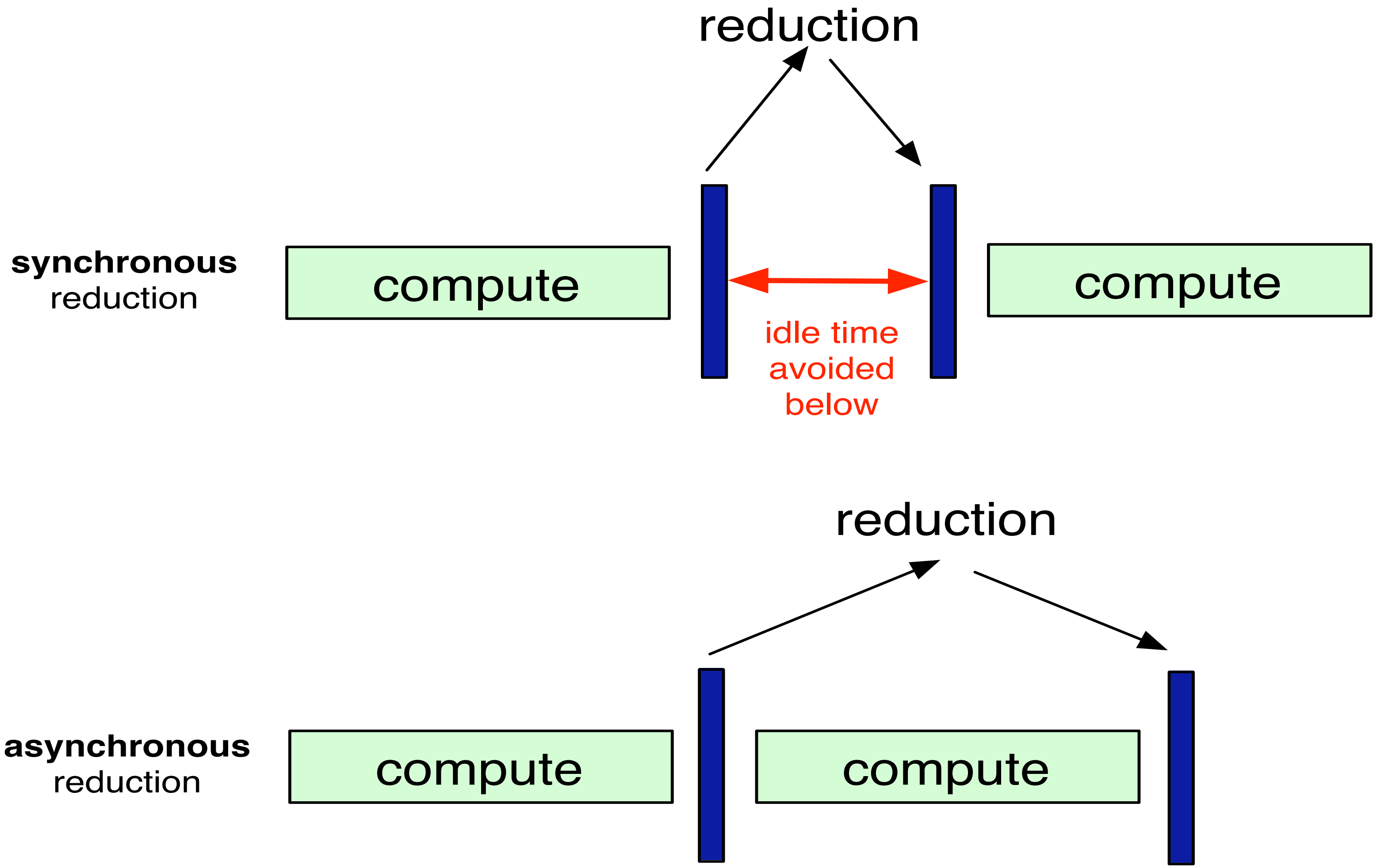
- What happens if an object waits for a return value from a method invocation?
  - Performance
  - Latency
  - Reasoning about correctness

Design Principle: Do not wait for remote completion



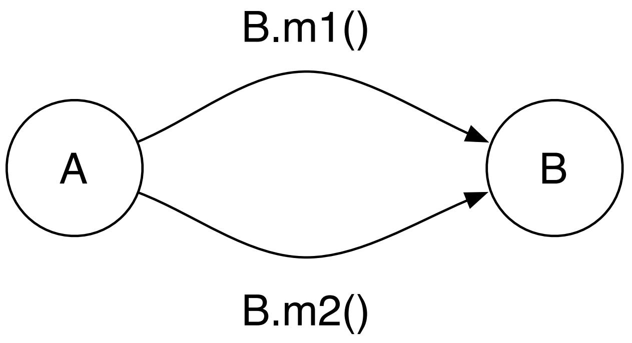
- Hence, method invocations should be asynchronous
  - No return values
- Computations are driven by the incoming data
  - Initiated by the sender or method caller

For example, a reduction



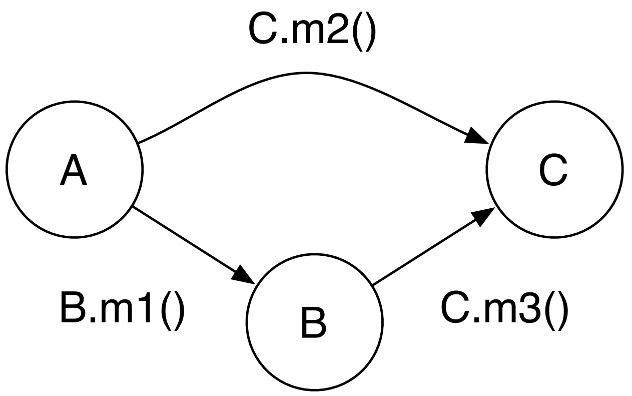
Methods: Natural Units of Sequential Computation

- Methods still have the same sequential semantics
  - Atomicity: methods of the same object do not execute in parallel
- Methods cannot be interrupted or preempted
- Methods interact and update state of an object in the same way
- Method sequencing is what changes from sequential computation



B may observe

m1() m2()
OR
m2() m1()



C may observe

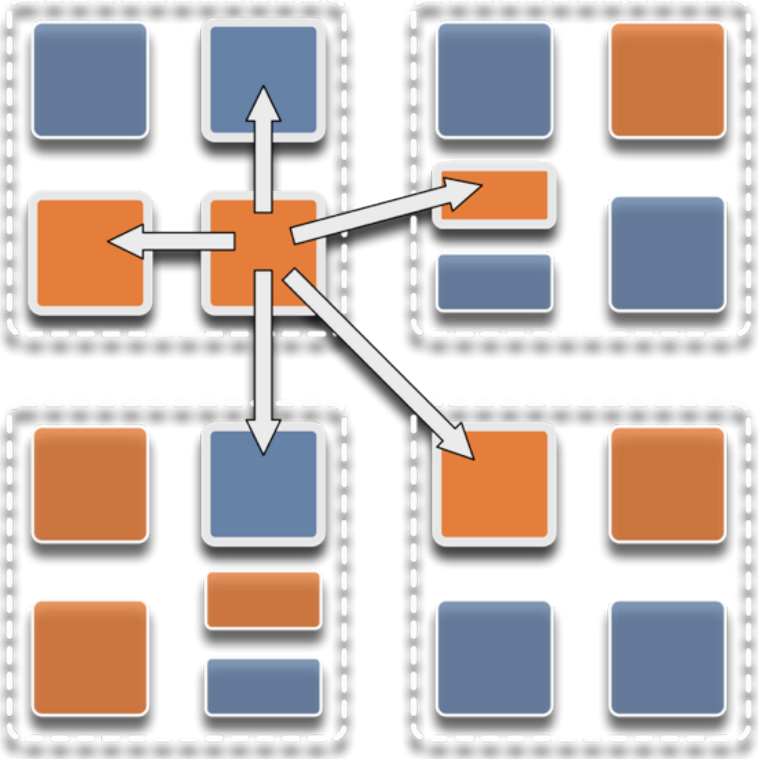
m2() m3()
OR
m3() m2()

Foundational Ideas

- Overdecomposition
- Migratability
- Asynchrony – message-driven execution

Overdecomposition

- Decompose the work units & data units into many more pieces (chares) than execution units
  - Cores/Nodes/..
- Not so hard: we do decomposition anyway



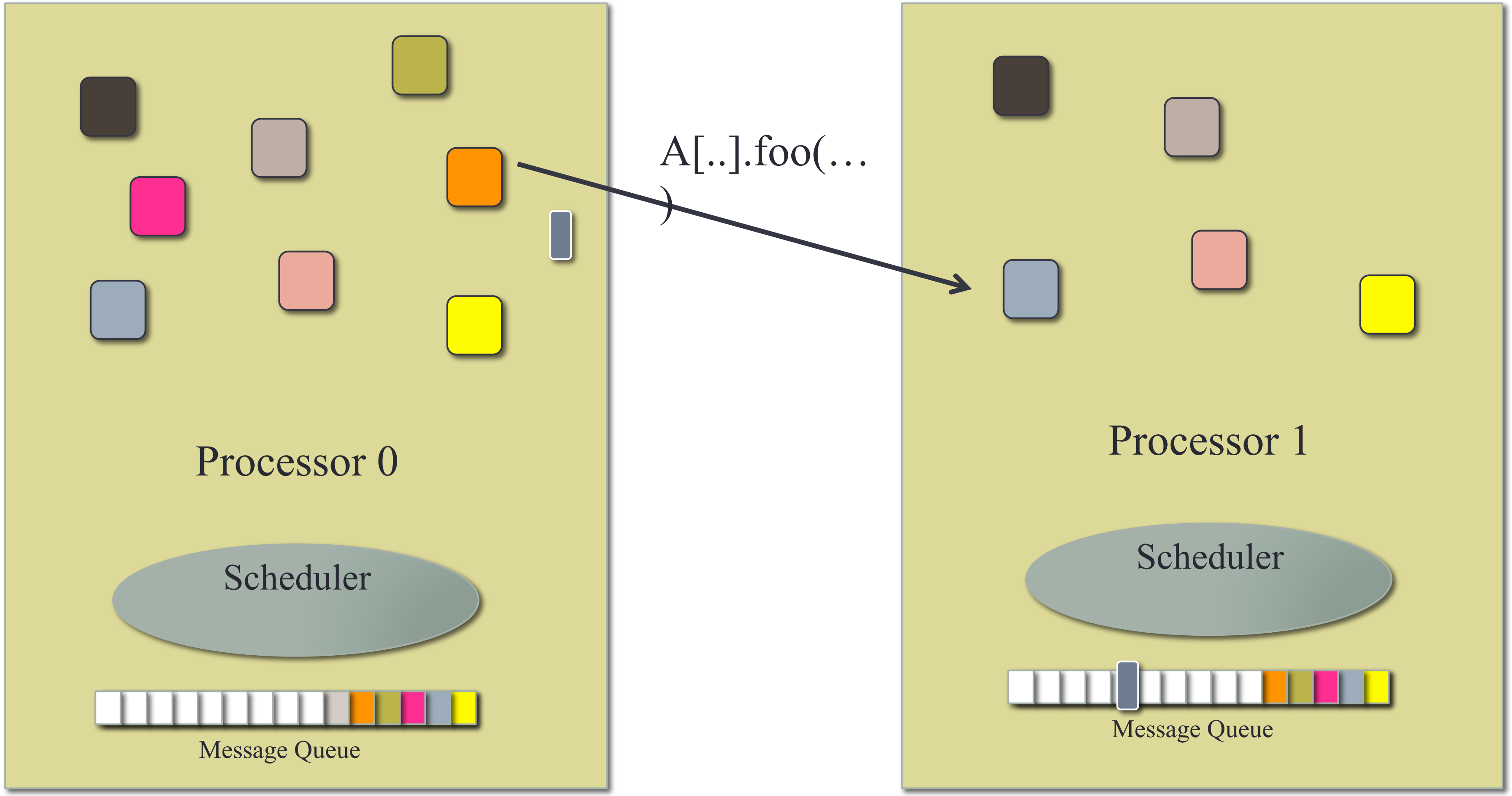
Migratability

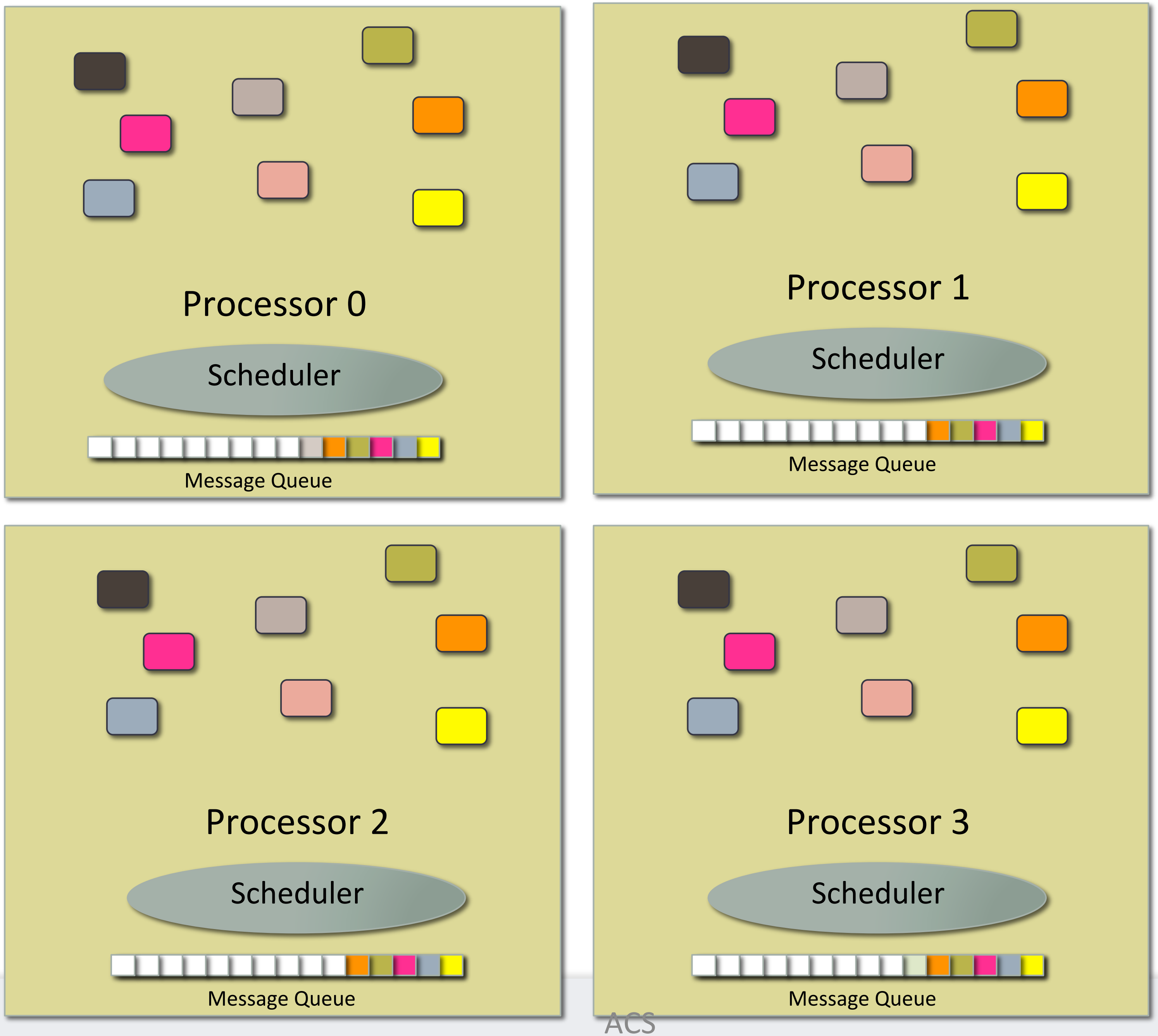
- Allow chares to be migratable at runtime
  - i.e. the programmer or runtime can move them
- Consequences for the app-developer
  - Communication must be addressed to logical units with global names, not to physical processors
  - But this is a good thing
- Consequences for RTS
  - Must keep track of where each chare is
  - Naming and location management

The Asynchronous Execution Model

- Several chares live on a single *PE*
  - For now, think of it as a core (or just “processor”)
- As a result,
  - Method invocations directed at chares on that processor will have to be stored in a pool,
  - And a user-level scheduler will select one invocation from the queue and runs it to completion
  - A PE is the entity that has one scheduler instance associated with it
- Execution is triggered by availability of a “message” (a method invocation)
- When an entry method executes,
  - it may generate messages for other chares
  - the RTS deposits them in the message Q on the target processor

The Execution Model





Processor 0

Scheduler

Message Queue

Processor 1

Scheduler

Message Queue

Processor 2

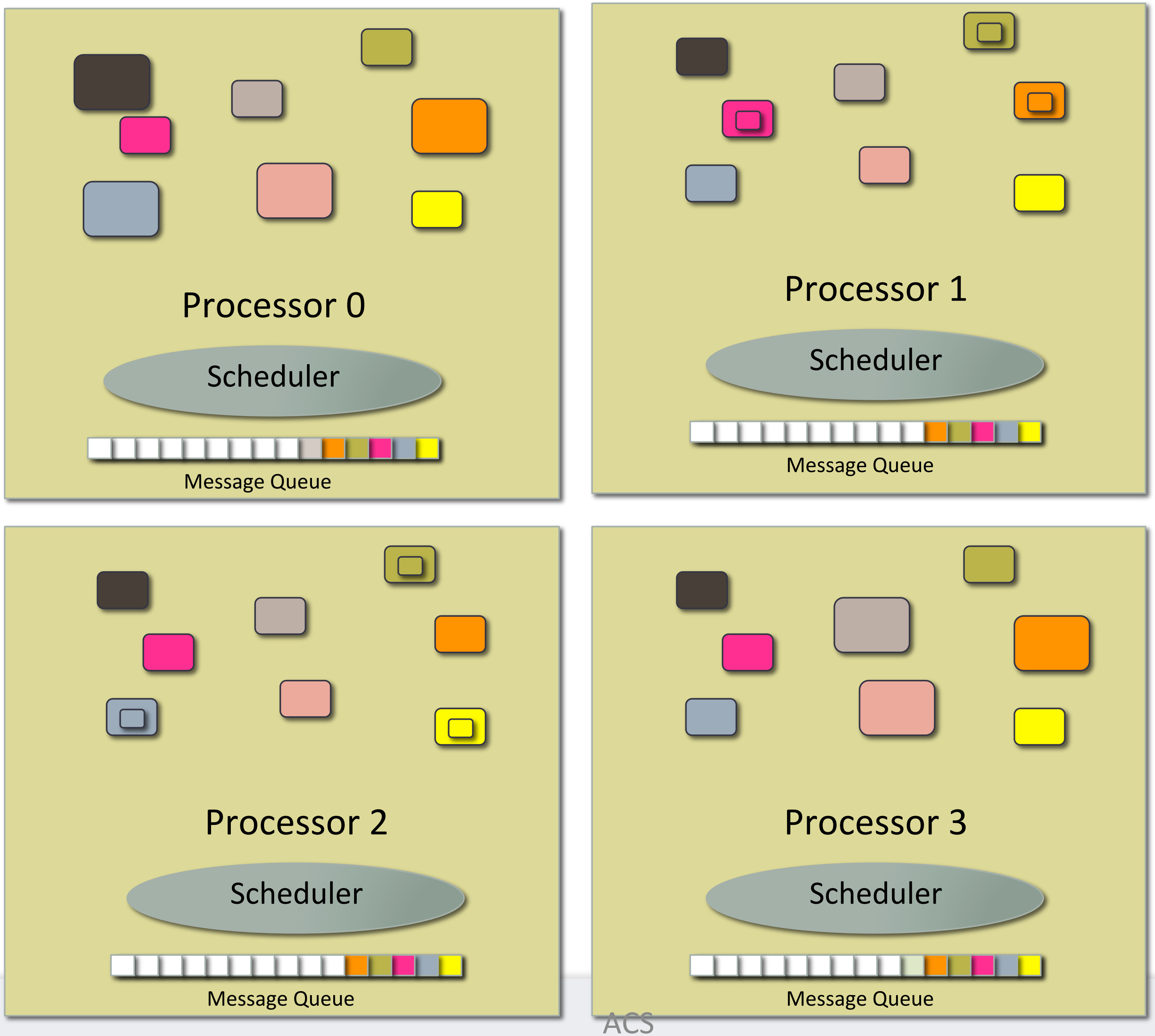
Scheduler

Message Queue

Processor 3

Scheduler

Message Queue



Processor 0

Scheduler

Message Queue

Processor 1

Scheduler

Message Queue

Processor 2

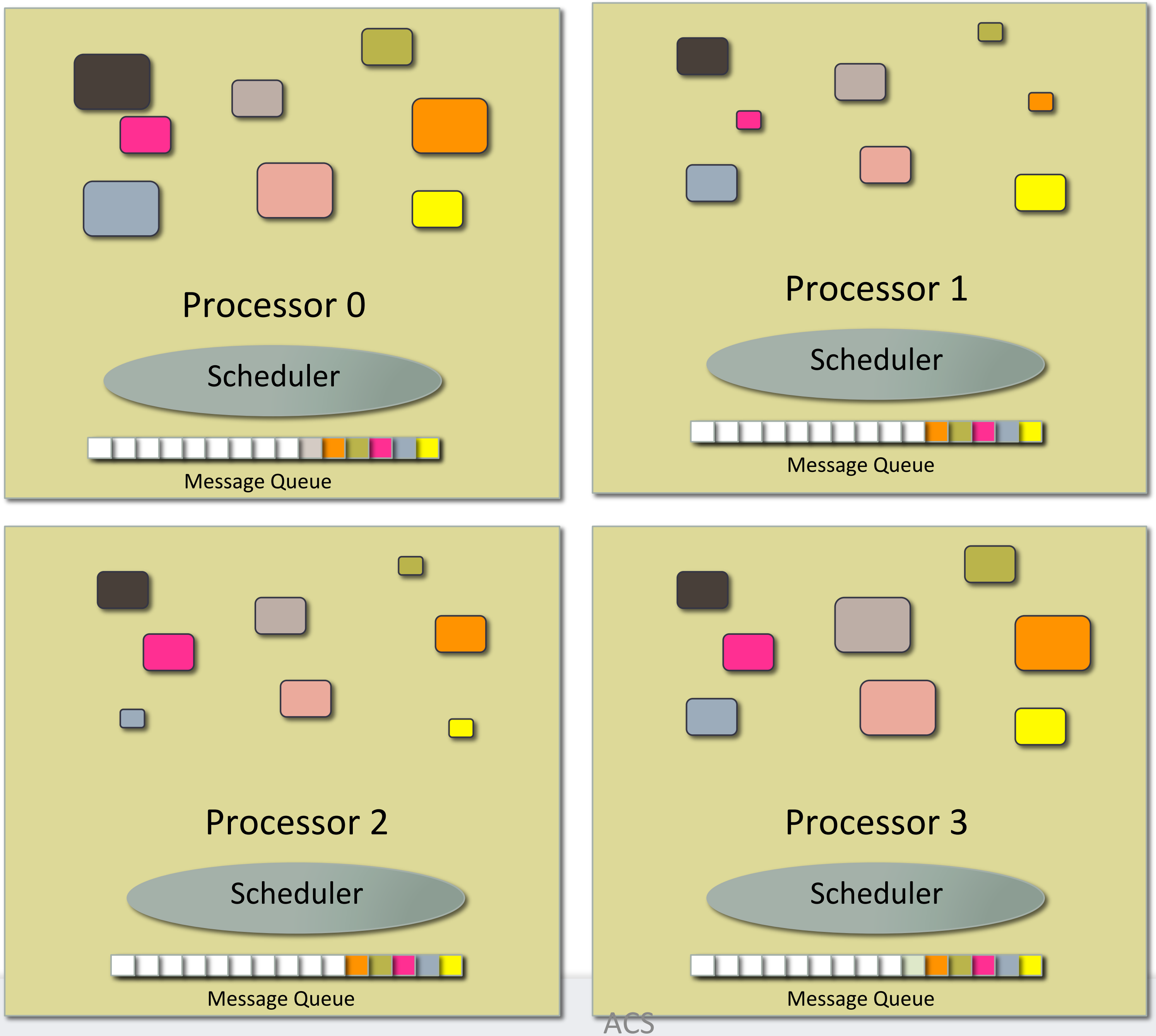
Scheduler

Message Queue

Processor 3

Scheduler

Message Queue



Processor 0

Scheduler

Message Queue

Processor 1

Scheduler

Message Queue

Processor 2

Scheduler

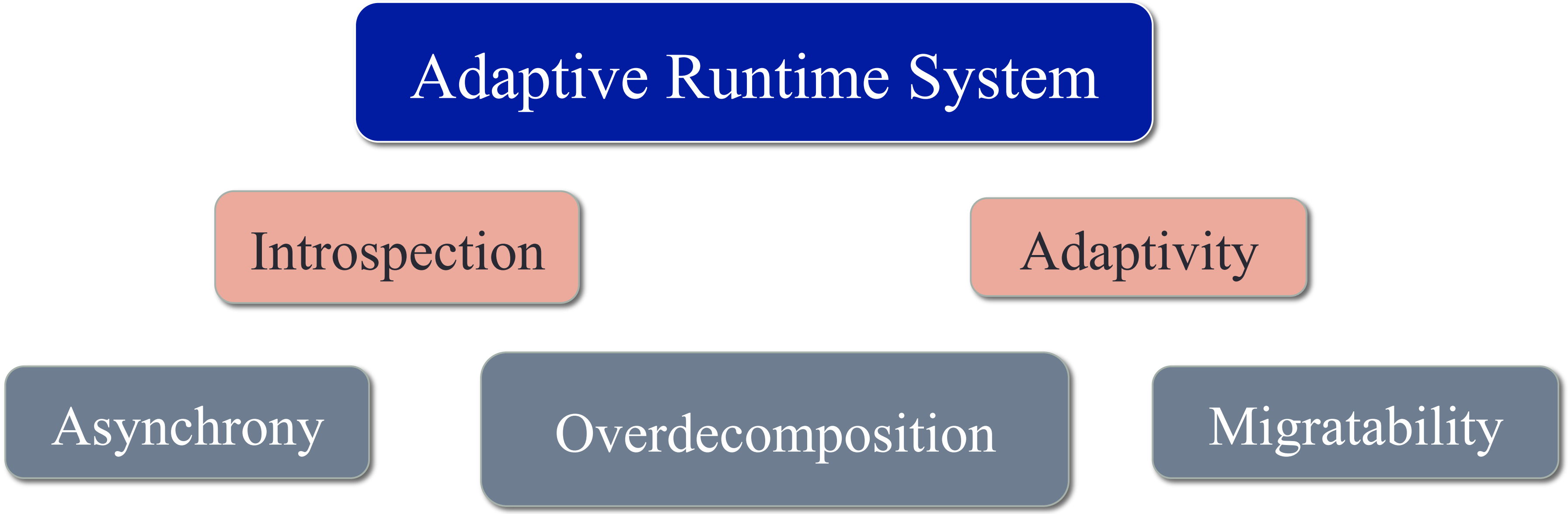
Message Queue

Processor 3

Scheduler

Message Queue

Empowering the RTS



Adaptive Runtime System

Introspection

Adaptivity

Asynchrony

Overdecomposition

Migratability

- The Adaptive RTS can:
  - Dynamically balance loads
  - Optimize communication:
    - Spread over time, async collectives
  - Automatic latency tolerance
  - Prefetch data with almost perfect predictability

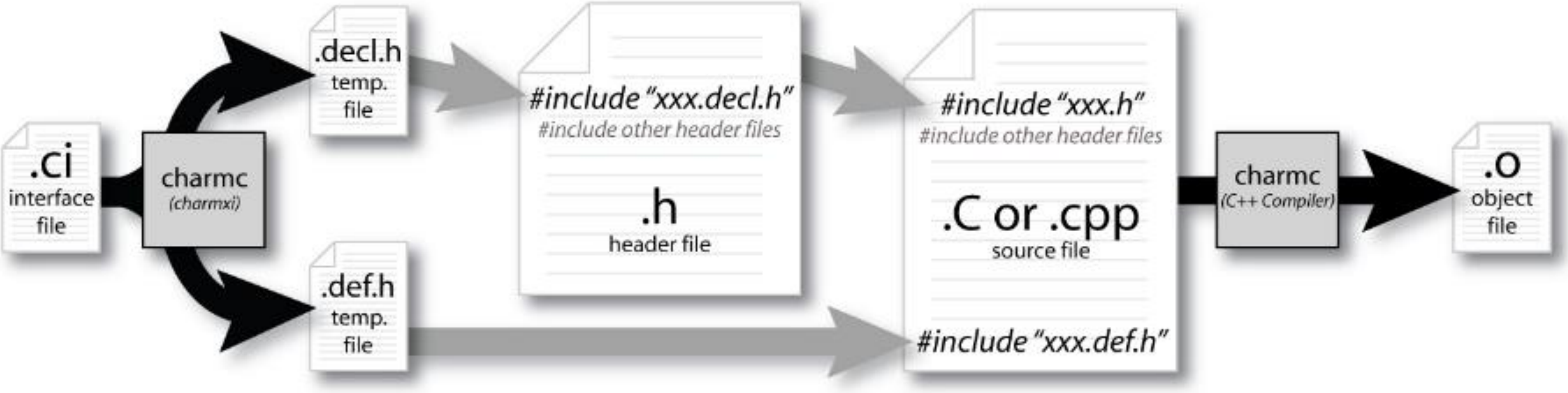
Outline

1) Introduction
    - Object Design
    - Execution Model
2) Hello World
3) Benefits of Charm++
4) **Charm++ Basics**
    - Object Collections
5) Overdecomposition
6) Migratability
    - Checkpointing and Resilience
7) Structured Dagger
8) Application Design
9) Performance Tuning
10) Using Dynamic Load Balancing
11) Interoperability
12) Debugging
13) Further Optimization

Charm++ File Structure

- C++ objects (including Charm++ objects)
  - Defined in regular .h and .C files
- Chare objects, entry methods (asynchronous methods)
  - Defined in .ci file
  - Implemented in the .C file

Compiling a Charm++ Program



Generated Classes

- CProxy_*YourClassName*
  - The type of the proxy handle returned by the constructor
  - For use in method invocations
- CBase_*YourClassName*
  - *YourClassName* should inherit from this

Hello World Example

- hello.ci file

```
mainmodule hello {
 mainchare MyMain {
  entry MyMain(CkArgMsg* m);
 };
};
```

- hello.cpp file

```
#include <stdio.h>
#include "hello.decl.h"
class MyMain : public CBase_MyMain {
 public:
  MyMain(CkArgMsg* m) {
   CkPrintf("Hello World!\n“);
   CkExit();
  };
};
#include "hello.def.h"
```

Charm Interface: Modules

- Charm++ programs are organized as a collection of modules
- Each module defines one or more chares
- The module that contains the *mainchare*, is declared as the mainmodule
- Each module, when compiled, generates two files:

  `MyModule.decl.h` and `MyModule.def.h`

- .ci file

```
module MyModule {
  // ... chare definitions ...
};
```

Charm Interface: Chares

- Chares are parallel objects that are managed by the RTS
- Each chare has a set of *entry methods*, which are asynchronous methods that may be invoked remotely
- The following code, when compiled, generates a C++ class `CBase_MyChare` that encapsulates the RTS object
- This generated class is extended and implemented in the .C file

- .ci file

```
chare MyChare {
  // ... entry method declarations ...
};
```

- .C file

```
class MyChare : public Cbase_MyChare {
  // ...  entry method definitions ...
};
```

Charm Interface: Entry Methods

- Entry methods are C++ methods that can be remotely and asynchronously invoked by another chare
- .ci file

```
entry MyChare(); /* constructor entry method */
entry void foo();
entry void bar(int param);
```

- .C file

```
MyChare::MyChare() { /*... constructor code ...*/ }
MyChare::foo() { /*... code to execute ...*/ }
MyChare::bar(int param) { /*... code to execute ...*/ }
```

Charm Interface: mainchare

- Execution begins with the mainchare's constructor
- The mainchare's constructor takes a pointer to system-defined class `CkArgMsg`
- `CkArgMsg` contains `argv` and `argc`
- The mainchare will typically create some additional chares

Creating a Chare

- A chare declared as `chare MyChare {...};` can be instantiated by the following call:

```
CProxy_MyChare::ckNew(... constructor
                    arguments ...);
```

- To communicate with this class in the future, a *proxy* to it must be retained

```
CProxy_MyChare proxy =
            CProxy_MyChare::ckNew(arg1);
```

Chare Proxies

- A chare's own proxy can be obtained through a special variable `thisProxy`
- Chare proxies can also be passed so chares can learn about others
- In this snippet, `MyChare` learns about a chare instance `main`, and then invokes a method on it:

- .ci file

```
entry void foobar2(CProxy_Main main);
```

- .C file

```
MyChare::foobar2(CProxy_Main main) {
   main.foo();
}
```

Charm Termination

- There is a special system call `CkExit()` that terminates the parallel execution on all processors (but it is called on one processor) and performs the requisite cleanup
- The traditional `exit()` is insufficient because it only terminates one process, not the entire parallel job (and will cause a hang)
- `CkExit()` should be called when you can safely terminate the application (you may want to synchronize before calling this)

Chare Creation Example: .ci file

```
mainmodule MyModule {
   mainchare Main {
      entry Main(CkArgMsg* m);
   };

   chare Simple {
      entry Simple(int x, double y);
   };
};
```

Chare Creation Example: .C file

```
#include "MyModule.decl.h"
class Main : public CBase_Main {
 public:
  Main(CkArgMsg* m) {
    CkPrintf("Hello World!\n");
    double pi = 3.1415;
    CProxy_Simple::ckNew(12, pi);
  };
};
class Simple : public CBase_Simple {
 public:
  Simple(int x, double y) {
    CkPrintf("From chare on %d Area of a circle of radius %d is %g\n“, CkMyPe(), x,y*x*x);
    CkExit();
  };
};
#include "MyModule.def.h"
```

Asynchronous Methods

- Entry methods are invoked by performing a C++ method call on a chare’s proxy

```
CProxy_MyChare proxy =
  CProxy_MyChare::ckNew(/* ... constructor arguments ...*/);

proxy.foo();
proxy.bar(5);
```

- The `foo` and `bar` methods will then be executed with the arguments, wherever the created chare, `MyChare`, happens to live
- The policy is one-at-a-time scheduling (that is, one entry method on one chare executes on a processor at a time)

Asynchronous Methods

- Method invocation is not ordered (between chares, entry methods on one chare, etc.)!
- For example, if a chare executes this code:

```
CProxy_MyChare proxy = CProxy_MyChare::ckNew();
proxy.foo();
proxy.bar(5);
```

- These prints may occur in **any** order

```
MyChare::foo() {
  CkPrintf(" foo executes\n");
}
MyChare::bar(int param) {
  CkPrintf(" bar executes\n");
}
```

Asynchronous Methods

- For example, if a chare invokes the same entry method twice:

```
proxy.bar(7);
proxy.bar(5);
```

- These may be delivered in **any** order

```
MyChare::bar(int param) {
  CkPrintf(“bar executes with %d\n”);
}
```

- Output:

```
bar executes with 5
bar executes with 7
```

OR

```
bar executes with 7
bar executes with 5
```

Asynchronous Example: .ci file

```
mainmodule MyModule {
  mainchare Main {
    entry Main(CkArgMsg *m);
  };
  chare Simple {
    entry Simple(double y);
    entry void findArea(int radius, bool done);
  };
};
```

Does this program execute correctly?

```
struct Main : public CBase_Main {
  Main(CkArgMsg* m) {
    CProxy_Simple sim = CProxy_Simple::ckNew(3.1415);
    for (int i = 1; i < 10; i++) sim.findArea(i, false);
    sim.findArea(10, true);
  };
};
struct Simple : public CBase_Simple {
  double y;
  Simple(double pi) { y = pi; }
  void findArea(int r, bool done) {
    CkPrintf("Area of a circle of radius %d is %f\n" ,r, y*r*r);
    if (done) CkExit();
  }
};
```

Data types and entry methods

- You can pass basic C++ types to entry methods (int, char, bool)
- C++ STL data structures can be passed
- Arrays of basic data types can also be passed like this:

- `.ci` file:

```
entry void foobar(int length, int data[length]);
```

- `.C` file

```
MyChare::foobar(int length, int* data) {
  // ... foobar code ...
}
```

ReadOnly Variables

- Global Constants
- Initialized in MainChare

```
readonly int foo;
readonly CProxy_Main mainProxy;
```

`.C` file: at global scope

```
int foo;
CProxy_Main mainProxy;
```

`.C` file: inside mainchare's constructor

```
foo=2;
mainProxy=thisProxy;
```

Collections of Objects: Concepts

- Objects can be grouped into indexed collections

- Basic examples
  - Matrix block
  - Chunk of unstructured mesh
  - Portion of distributed data structure
  - Volume of simulation space

- Advanced Examples
  - Abstract portions of computation
  - Interactions among basic objects or underlying entities

Collections of Objects

- Structured: 1D, 2D, . . . , 6D
- Unstructured: Anything hashable
- Dense
- Sparse
- Static - all created at once
- Dynamic - elements come and go

Declaring a Chare Array

- .ci file:

```
array [1D] foo {
  entry foo(); // constructor
  // ... entry methods ...
};
array [2D] bar {
  entry bar(); // constructor
  // ... entry methods ...
};
```

- .C file:

```
struct foo : public CBase_foo {
  foo() { }
  foo(CkMigrateMessage*) { }
  // ... entry methods ...
};
struct bar : public CBase_bar {
  bar() { }
  bar(CkMigrateMessage*) { }
};
```

Constructing a Chare Array

- Constructed much like a regular chare
- The size of each dimension is passed to the constructor
- Dimensional parameters are placed after other constructor arguments

```
CProxy_foo::ckNew(…,10);
CProxy_bar::ckNew(…,5, 5);
```

- The proxy may be retained:

```
CProxy_foo myFoo = CProxy_foo::ckNew(…, 10);
```

- The proxy represents the entire array, and may be indexed to obtain a proxy to an individual element in the array

```
myFoo[4].invokeEntry();
```

thisIndex

- 1d: `thisIndex` returns the index of the current chare array element
- 2d: `thisIndex.x` and `thisIndex.y` return the indices of the current chare array element

`.ci` file:

```
array [1D] foo {
  entry foo();
}
```

`.C` file:

```
struct foo : public CBase_foo {
  foo() {
    CkPrintf("  array index = %d",thisIndex);
  }
};
```

Chare Array: Hello Example

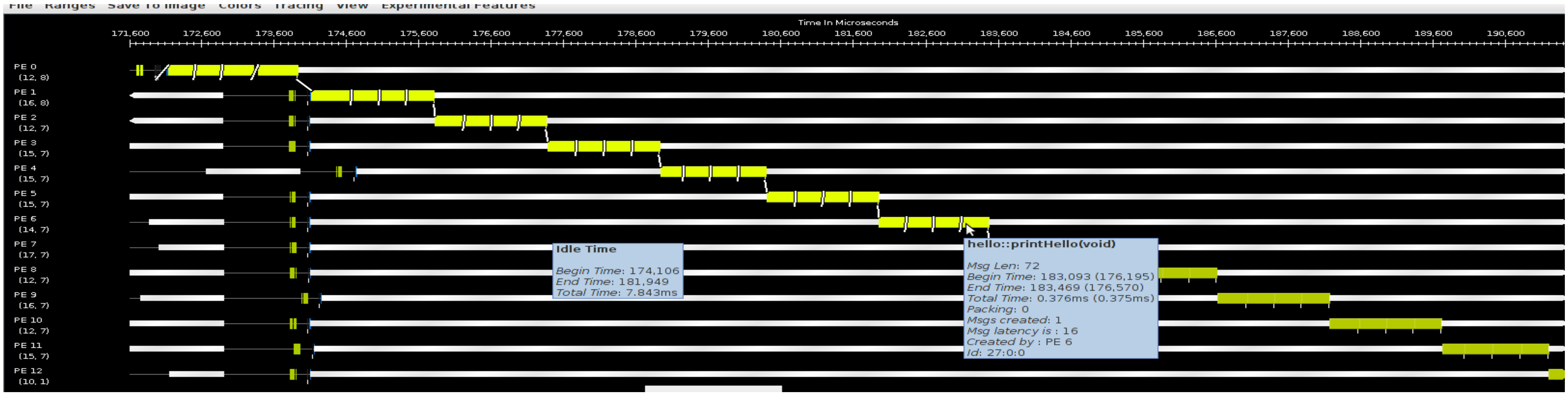
```
mainmodule arr {
  mainchare MyMain {
    entry MyMain(CkArgMsg*);
  }
  array [1D] hello {
    entry hello(int);
    entry void printHello();
  }
}
```

Chare Array: Hello Example

```cpp
#include "arr.decl.h"
struct MyMain : CBase_MyMain {
  MyMain(CkArgMsg* msg) {
    int arraySize = atoi(msg->argv[1]);
    CProxy_hello p = CProxy_hello::ckNew(arraySize, arraySize);
    p[0].printHello();
  }
};
struct hello : CBase_hello {
  hello(int n) : arraySize(n) { }
  void printHello() {
    CkPrintf("PE[%d]: hello from p[%d]\n", CkMyPe(), thisIndex);
    if (thisIndex == arraySize - 1) CkExit();
    else thisProxy[thisIndex + 1].printHello();
  }
  int arraySize;
};
#include "arr.def.h"
```

Hello World Array Projections Timeline View

- Add “`-tracemode projections`” to link line to enable tracing
- Run Projections tool to load trace log files and visualize performance



Idle Time

Begin Time: 174,106
End Time: 181,949
Total Time: 7.843ms

hello::printHello(void)

Msg Len: 72
Begin Time: 183,093 (176,195)
End Time: 183,469 (176,570)
Total Time: 0.376ms (0.375ms)
Packing: 0
Msgs created: 1
Msg latency is : 16
Created by : PE 6
Id: 27:0:0

- `arrayHello` on BG/Q 16 Nodes, mode c16, 1024 elements (4 per process)

Collections of Objects: Runtime Service

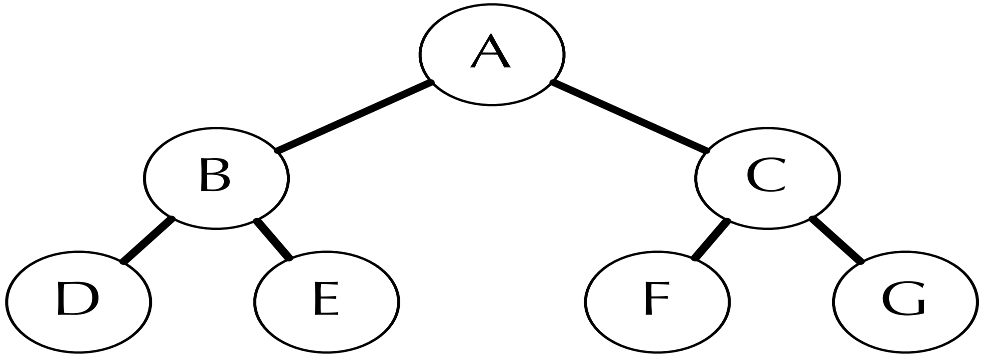
- System knows how to ‘find’ objects efficiently:
  (*collection*, *index*) → *processor*
- Applications can specify a mapping or use simple runtime-provided options (e.g. blocked, round-robin)
- Distribution can be static or dynamic!
- Key abstraction: application logic doesn’t change, even though performance might

Collections of Objects: Runtime Service

- Can develop and test logic in objects separately from their distribution
- Separation in time: make it work, then make it fast
- Division of labor: domain specialist writes object code, computationalist writes mapping
- Portability: different mappings for different systems, scales, or configurations
- Shared progress: improved mapping techniques can benefit existing code

Collective Communication Operations

- Point-to-point operations involve only two objects
- Collective operations that involve a collection of objects
- Broadcast: calls a method in each object of the array
- Reduction: collects a contribution from each object of the array
- A spanning tree is used to send/receive data



Broadcast

- A message to each object in a collection
- The chare array proxy object is used to perform a broadcast
- It looks like a function call to the proxy object
- From the main chare:

```
CProxy_Hello helloArray = CProxy_Hello::ckNew(helloArraySize);
helloArray.foo();
```

- From a chare array element that is a member of the same array:

```
thisProxy.foo();
```

- From any chare that has a proxy p to the chare array

```
p.foo();
```

Reduction

- Combines a set of values: `sum`, `max`, `concat`
- Usually reduces the set of values to a single value
- Combination of values requires an operator
- The operator must be commutative and associative
- Each object calls `contribute` in a reduction

Reduction: Example

```
mainmodule reduction {
  mainchare Main {
    entry Main(CkArgMsg* msg);
    entry [reductiontarget] void done(int value);
  };
  array [1D] Elem {
    entry Elem(CProxy_Main mProxy);
  };
}
```

Reduction: Example

```
#include "reduction.decl.h"
const int numElements = 49;
class Main : public CBase_Main {
 public:
  Main(CkArgMsg* msg) {
    CProxy_Elem::ckNew(thisProxy, numElements);
  }
  void done(int value) {
    CkPrintf("value: %d\n“,value);
    CkExit();
  }
};
class Elem : public CBase_Elem {
 // . . .
};
#include "reduction.def.h"
```

```
class Elem : public CBase_Elem {
 public:
  Elem(CProxy_Main mProxy) {
    int val = thisIndex;
    CkCallback cb(CkReductionTarget(Main, done), mProxy);
    contribute(sizeof(int), &val, CkReduction::sum_int,
cb);
  }
};
```

Output

```
value: 1176
Program finished.
```

Outline

1) Introduction
   - Object Design
   - Execution Model
2) Hello World
3) Benefits of Charm++
4) Charm++ Basics
   - Object Collections
5) **Overdecomposition**
6) Migratability
   - Checkpointing and Resilience
7) Structured Dagger
8) Application Design
9) Performance Tuning
10) Using Dynamic Load Balancing
11) Interoperability
12) Debugging
13) Further Optimizations

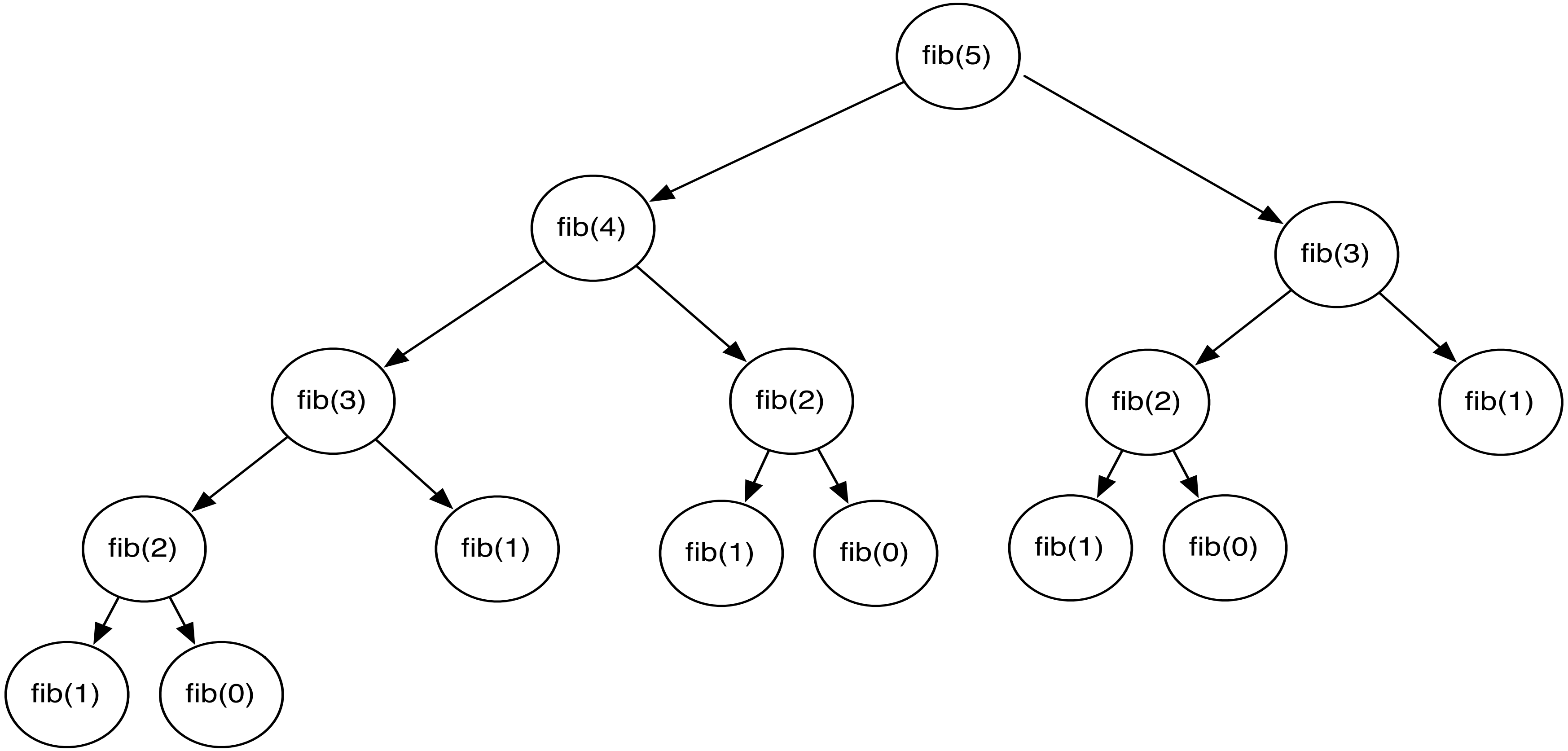
Task Parallelism with Objects

- Divide-and-conquer
  - Each object recursively creates *n* objects that divide the problem into subproblems
  - Each object *t* then waits for all *n* objects to finish and then may ‘combine’ the responses
  - At some point the recursion stops (at the bottom of the tree), and some sequential kernel is executed
  - Then the result is propagated upward in the tree recursively
  - Examples: fibonacci, quicksort, . . .

Fibonacci Example

- Each `Fib` object is a task that performs one of two actions:
  - Creates two new `Fib` objects to compute *fib(n – 1)* and *fib(n – 2)* and then waits for the response, adding up the two responses when they arrive
    - After both arrive, sends a response message with the result to the parent object
    - Or prints the value and exits if it is the root
  - If $n = 1$ or $n = 0$ (passed down from the parent) it sends a response message with n back to the parent object

Fibonacci Execution



Object-based Overdecomposition

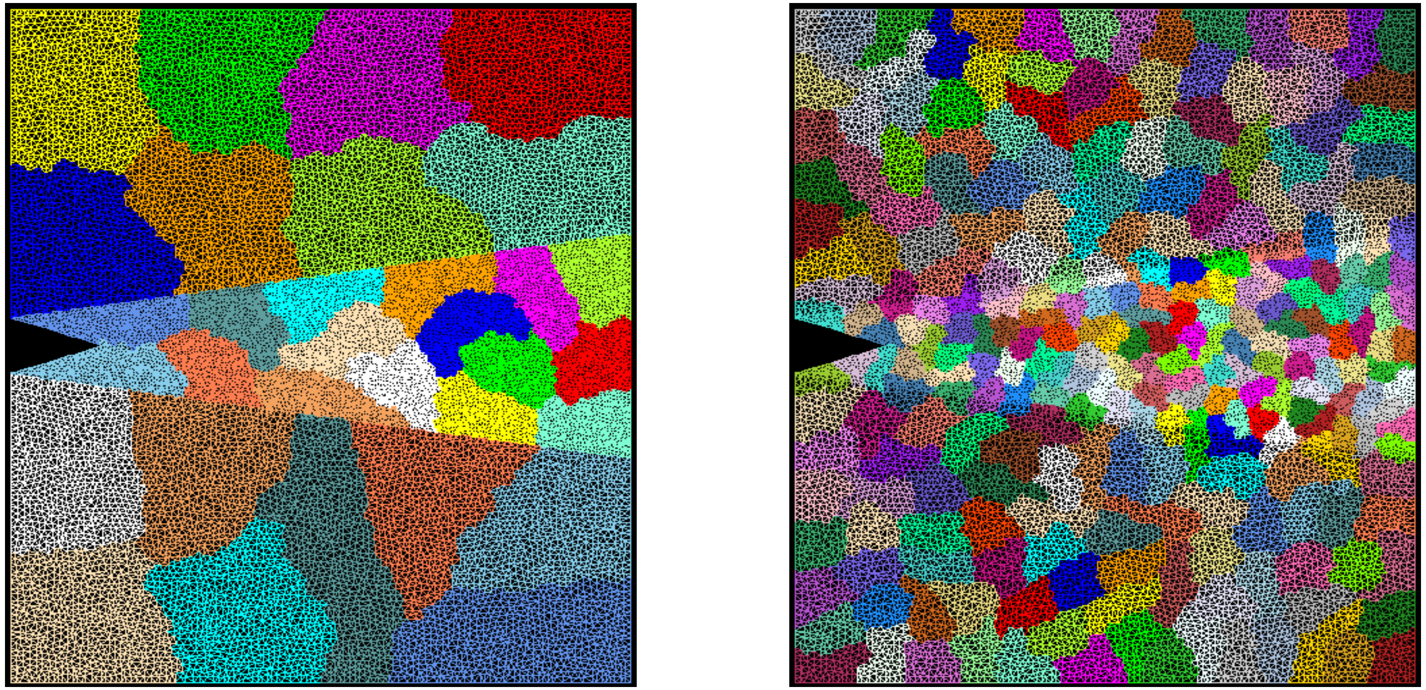
- Charm++ philosophy:
  - Let the programmer decompose their work and data into coarse-grained entities

- It is important to understand what we mean by coarse-grained entities
  - You don’t write sequential programs that some system will auto-decompose
  - You don’t write programs when there is one object for each *float*
  - You consciously choose a grainsize, BUT choose it independent of the number of processors, or parameterize it, so you can tune later

Amdahl's Law and Grainsize

- Original "law":
  - If a program has *K%* sequential section, then speedup is limited to $\frac{100}{K}$
    - If the rest of the program is parallelized completely
- Grainsize corollary:
  - If any individual piece of work is > *K* time units, and the sequential program takes T_{seq},
    - Speedup is limited to $\frac{Tseq}{K}$
- So:
  - Examine performance data via histograms to find the sizes of remappable work units
  - If some are too big, change the decomposition method to make smaller units

Quick Example: Crack Propagation



- Decomposition into 16 chunks (left) and 128 chunks, 8 for each PE (right). The middle area contains cohesive elements. Both decompositions obtained using METIS.
- Pictures: S. Breitenfeld, and P. Geubelle

Overdecomposition and Grainsize

- Common misconception: overdecomposition must be expensive
- (Working) Definition: the amount of computation per potentially parallel event (task creation, enqueue/dequeue, messaging, locking, etc)

Grainsize and Overhead

- What is the ideal grainsize?
- Should it depend on the number of processors?

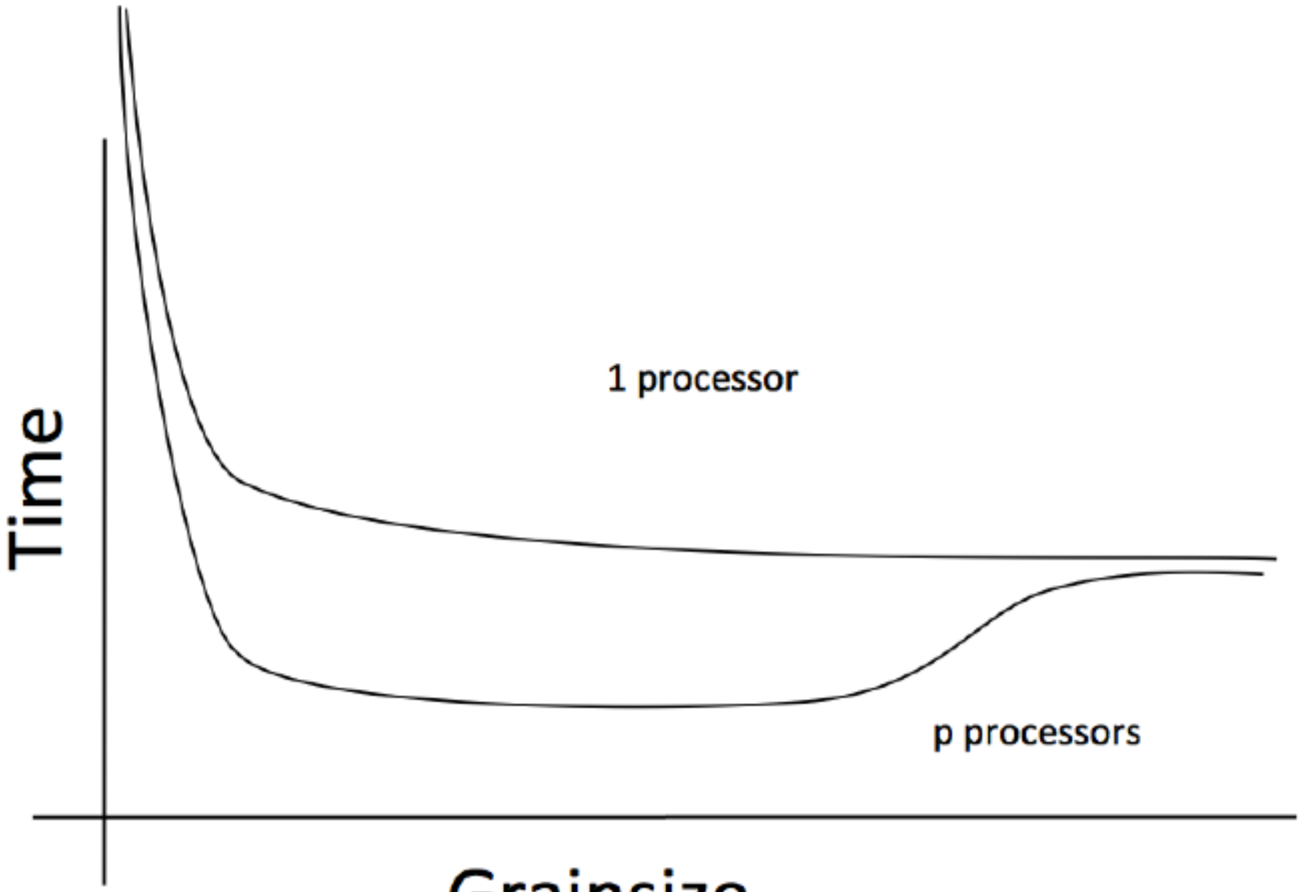
$$T_1 = T\left(1 + \frac{v}{g}\right)$$

$$T_p = \max\left\{g, \frac{T_1}{p}\right\}$$

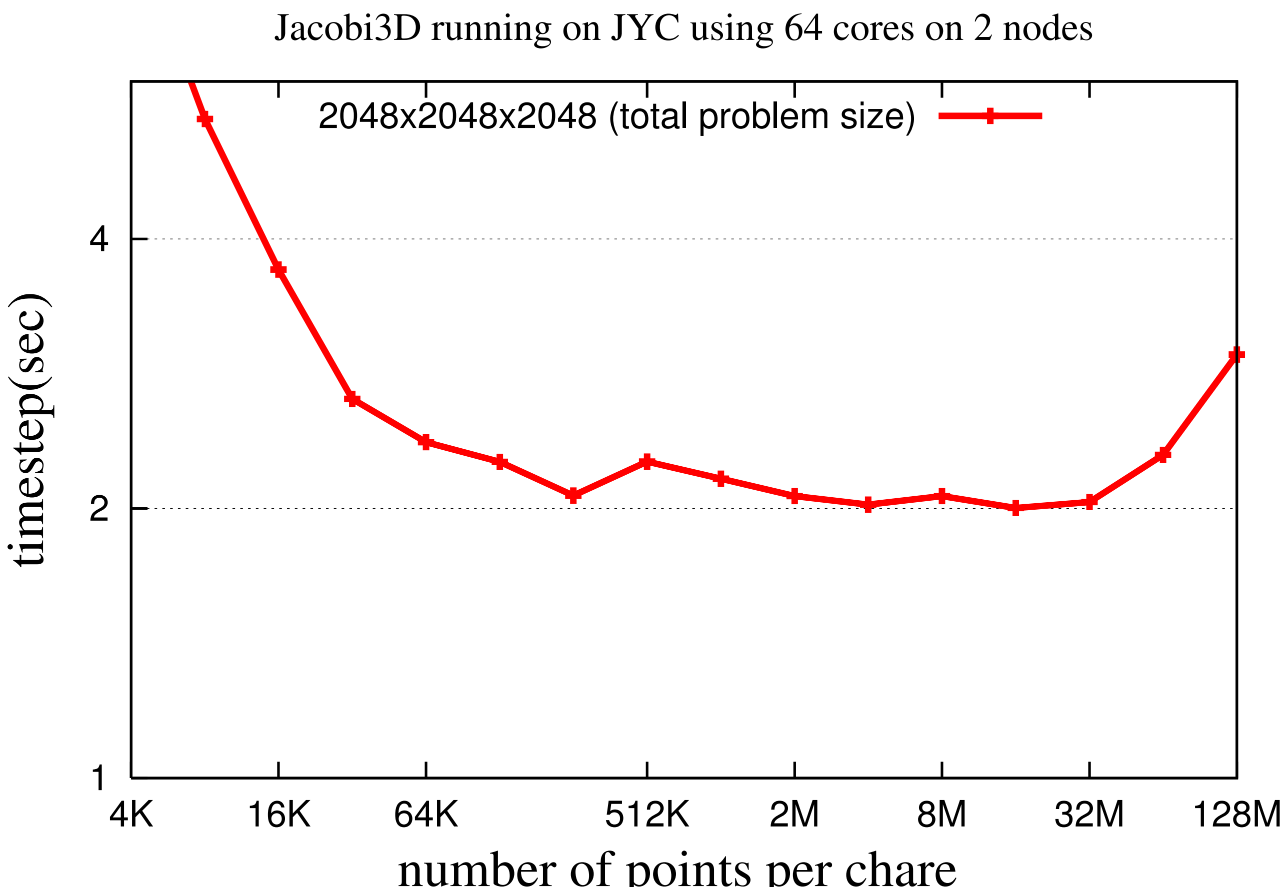
$$T_p = \max\left\{g, \frac{T\left(1 + \frac{v}{g}\right)}{p}\right\}$$

v: overhead per message,
T_p: completion time of processor p
g: grainsize (computation per message)

Grainsize and Scalability

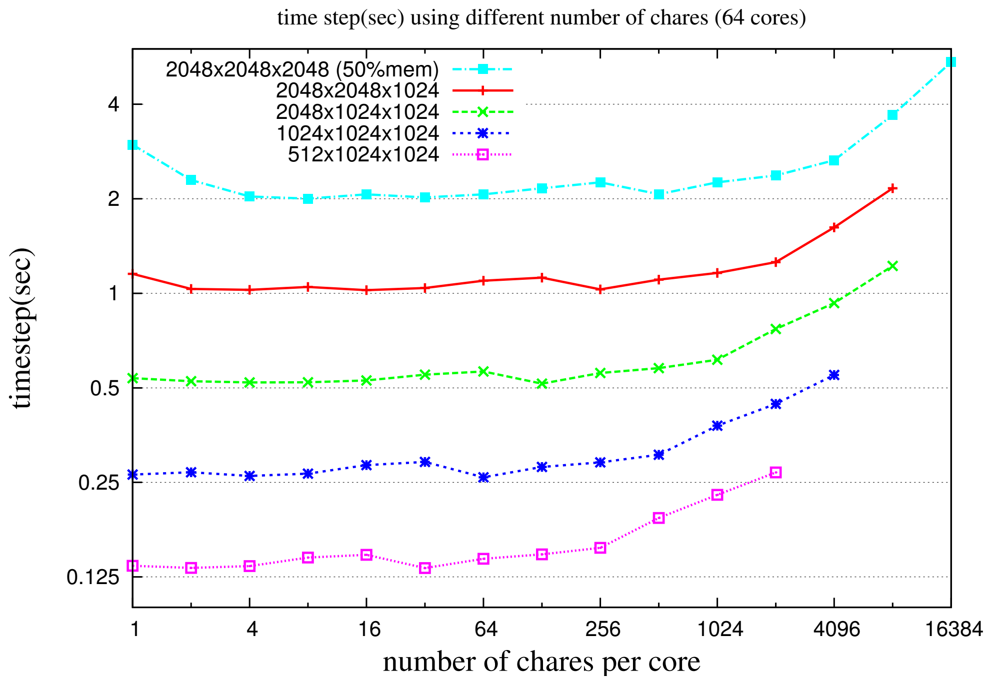


Grainsize Study for Jacobi3D



Grainsize Study for Stencil Computation

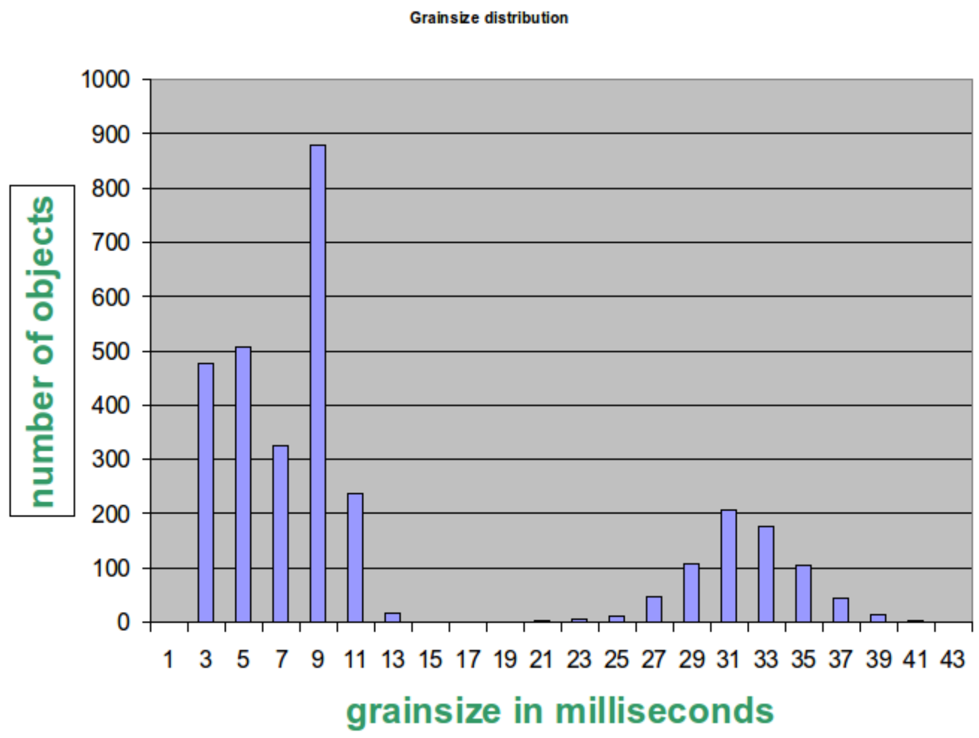
- Blue Waters (JYC), 2 nodes, 32 cores each



Typically, having tens of chares per code is adequate (although reasoning should be based on computation per message)

Grainsize and Load Balancing

How Much Balance Is Possible?

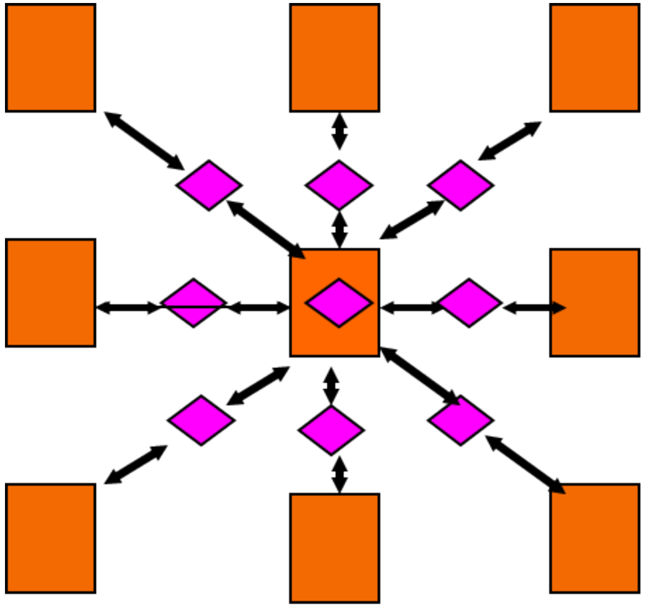


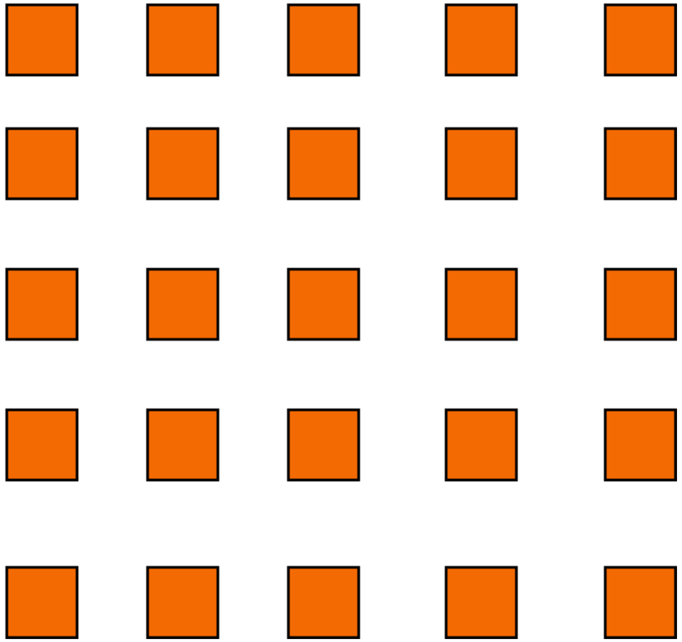
Solution:

Split compute objects that may have too much work, using a heuristic based on number of interacting atoms

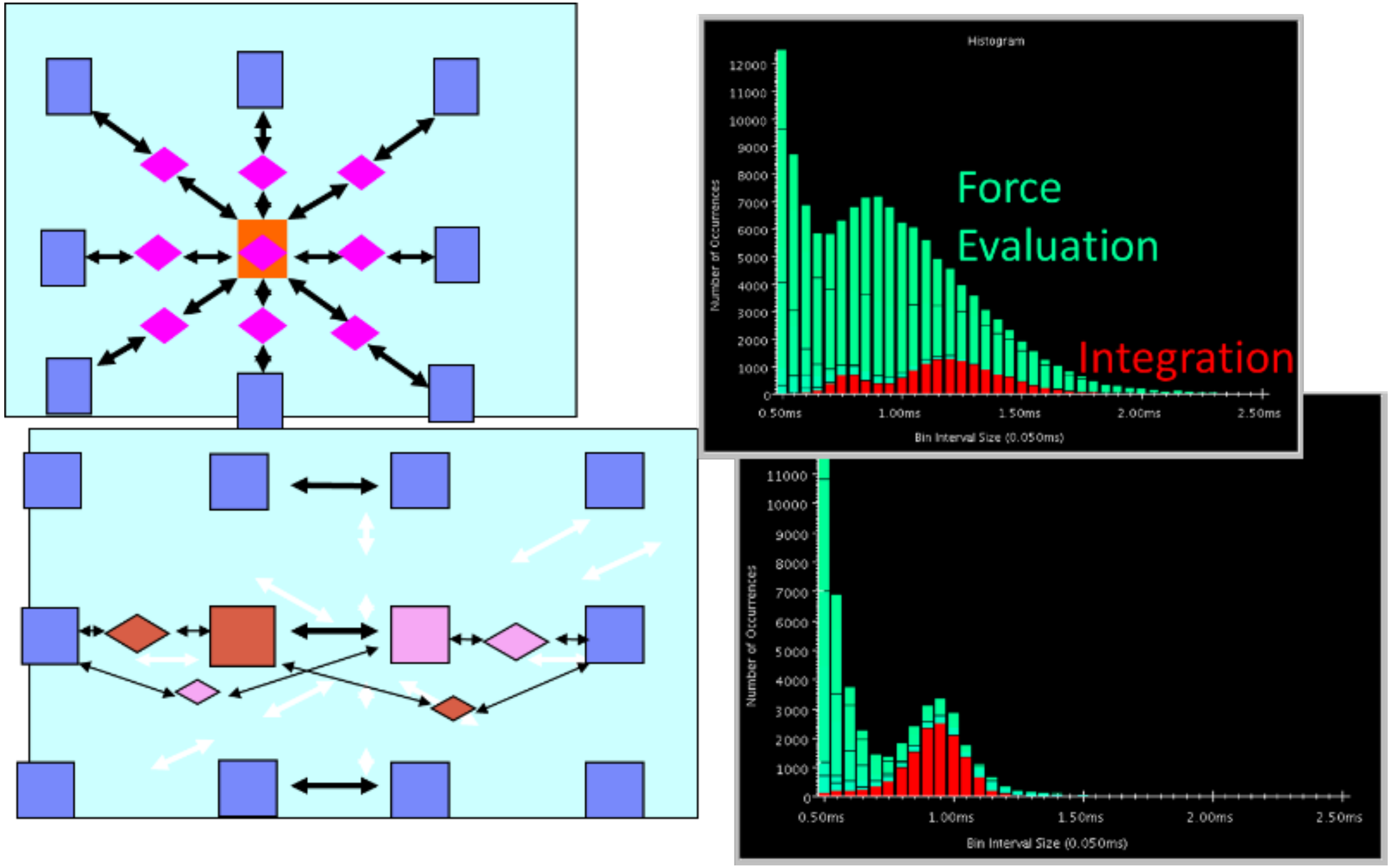
Grainsize For Extreme Scaling

- Strong Scaling is limited by expressed parallelism
  - Minimum iteration time limited by lengthiest computation
    - Largest grains set lower bound
- 1-away generalized to k-away provides fine granularity control





NAMD: 2-AwayX Example

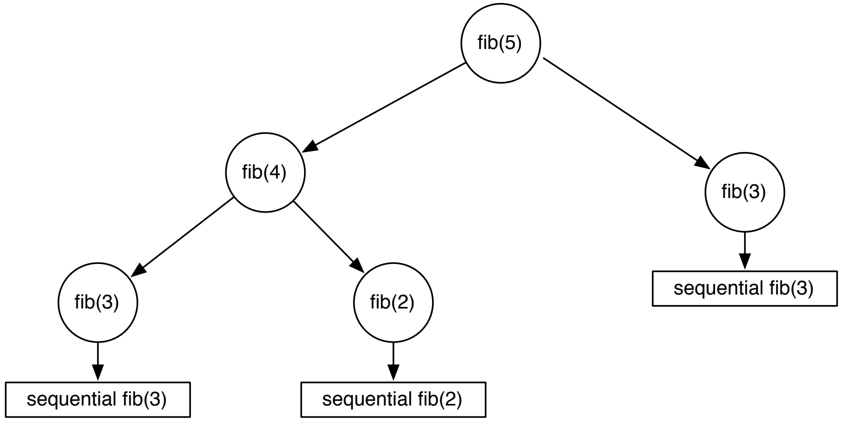


Rules of thumb for grainsize

- Make it as small as possible, as long as it amortizes the overhead
- More specifically, ensure:
  - *Average* grainsize is greater than *kv* (say *10v*)
  - No single grain should be allowed $\frac{T}{p}$ to be too large
    - Must be smaller than , but actually we can express it as: p
    - Must be smaller than *kmv* (say *100v*)
- Important corollary:
  - You can be at close to optimal grainsize without having to think about *p*, the number of processors
- $kv < g < mkv$ $(10v < g < 100v)$

Grainsize for Fibonacci Example

- Set a sequential threshold in the computational tree
  - Past this threshold (i.e. when n < threshold), instead of constructing two new chares, compute the fibonacci sequentially



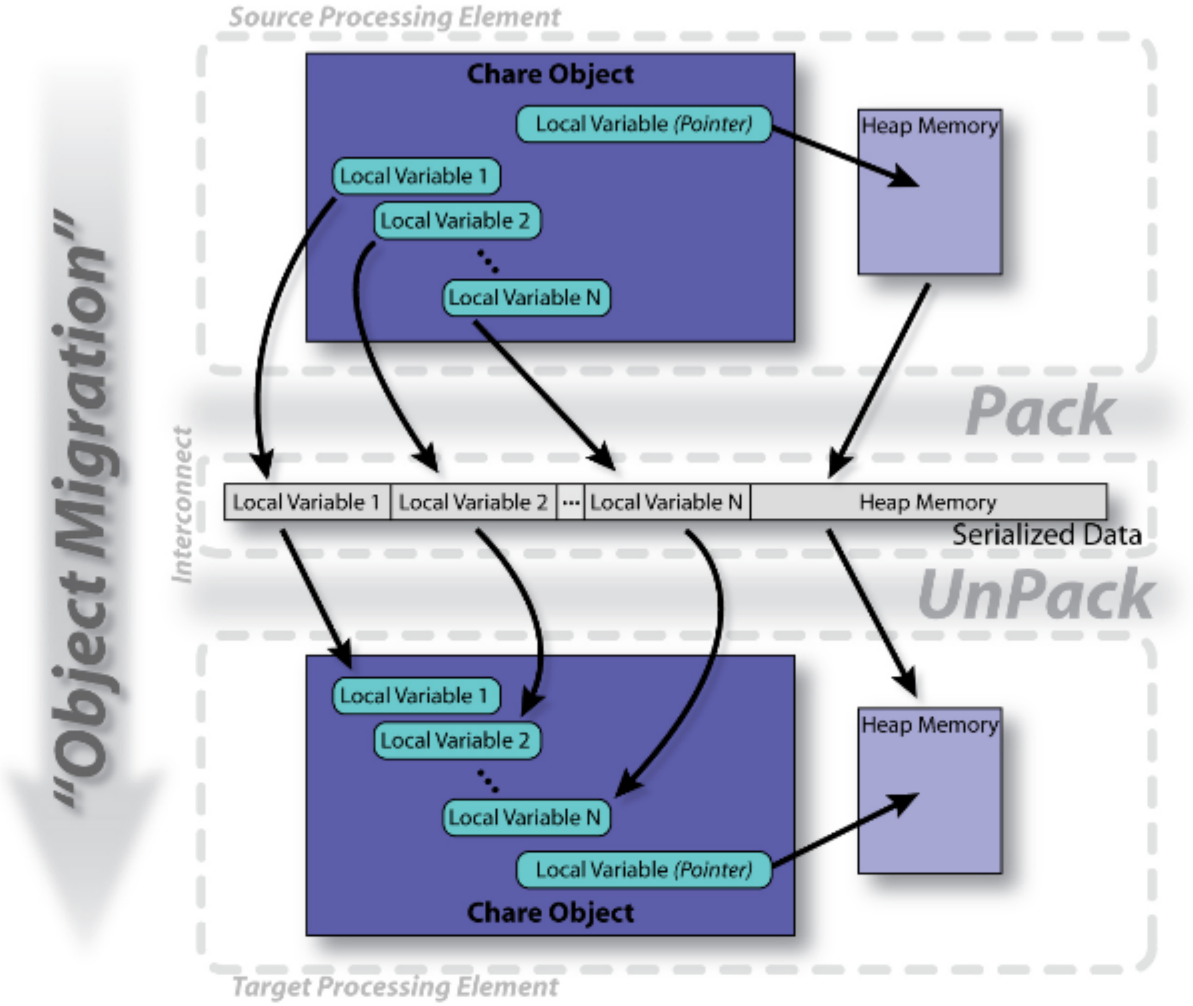
- Setting the grainsize limit at 4 (which is too small, but good for illustration)
- The internal nodes of the tree do very little work, but
- The coarser grains now amortize the cost of the fine-grained chares

Outline

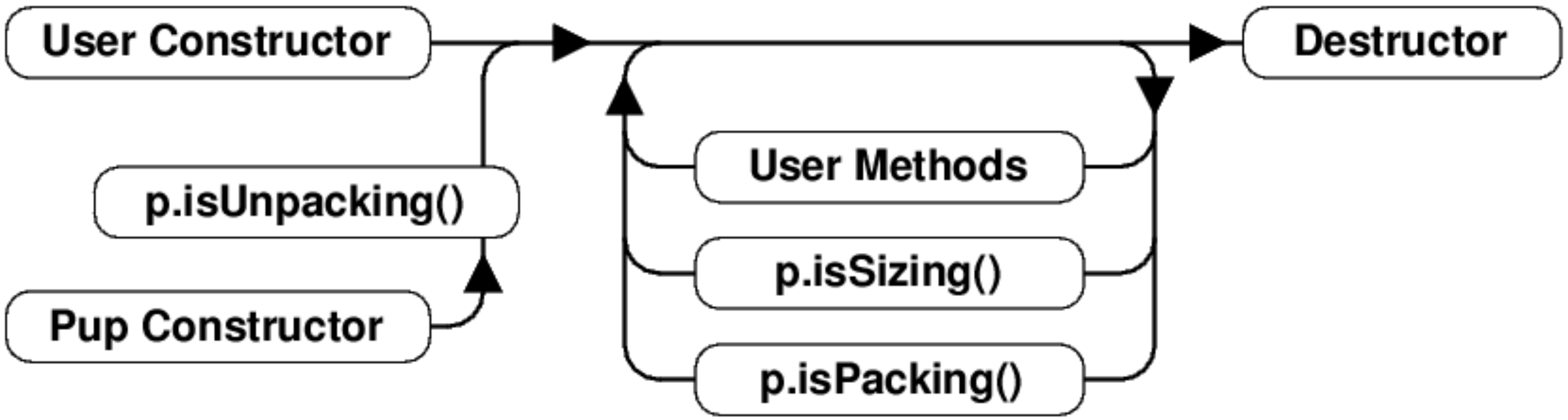
1) Introduction
   - Object Design
   - Execution Model
2) Hello World
3) Benefits of Charm++
4) Charm++ Basics
   - Object Collections
5) Overdecomposition
6) **Migratability**
   - Checkpointing and Resilience
7) Structured Dagger
8) Application Design
9) Performance Tuning
10) Using Dynamic Load Balancing
11) Interoperability
12) Debugging
13) Further Optimizations

Object Serialization Using PUP:
The **P**ack/**U**n**P**ack Framework

The PUP Process



PUP Usage Sequence



- Migration out:
  - ckAboutToMigrate
  - Sizing
  - Packing
  - Destructor
- Migration in:
  - Migration constructor
  - UnPacking
  - ckJustMigrated

Writing a PUP routine

```
class MyChare :
 public CBase_MyChare {
  int a;
  float b;
  char c;
  float localArray[SIZE];
};
```

```
void pup(PUP::er &p) {
  p | a;
  p | b;
  p | c;
  p(localArray, SIZE);
}
```

Writing a PUP routine

```
class MyChare :
 public CBase_MyChare {
  int heapArraySize;
  float *heapArray;
  MyClass *pointer;
};
```

```
void pup(PUP::er &p) {
  p | heapArraySize;
  if (p.isUnpacking()) {
    heapArray =
      new float[heapArraySize];
  }
  p(heapArray, heapArraySize);
  bool isNull = !pointer;
  p | isNull;
  if (!isNull) {
    if(p.isUnpacking())
      pointer = new MyClass();
    p | *pointer;
  }
}
```

PUP: Pitfalls

- If variables are added to an object, update the PUP routine
- If the object allocates data on the heap, copy it recursively, not just the pointer
- Remember to allocate memory while unpacking
- Sizing, Packing, and Unpacking must scan the variables in the same order
- Test PUP routines with `+balancer RotateLB`

Fault Tolerance in Charm++/AMPI

- Four Approaches:
  - Disk-based checkpoint/restart
  - In-memory double checkpoint/restart
  - Experimental: Proactive object evacuation
  - Experimental: Message-logging for scalable fault tolerance
- Common Features:
  - Easy checkpoint
  - Migrate-to-disk leverages object-migration capabilities
  - Based on dynamic runtime capabilities
  - Can be used in concert with load-balancing schemes

Checkpointing to the file system : Split Execution

- The common form of checkpointing
  - The job runs for 5 hours, then will continue at the next allocation another day!
- The existing Charm++ infrastructure for chare migration helps
- Just "migrate" chares to disk
- The call to checkpoint the application is made in the main chare at a synchronization point

```
CkCallback cb(CkIndex_Hello::SayHi(),helloProxy);
CkStartCheckpoint("log",cb);


> ./charmrun hello +p4 +restart log
```

Code to Use Load Balancing

- Write PUP method to serialize the state of a chare
- Insert `if(myLBStep) AtSync();` call at natural barrier
- Implement `ResumeFromSync()` to resume execution
  - Typically, `ResumeFromSync` contribute to a reduction

Using the Load Balancer

- link a LB module
  - `-module <strategy>`
  - RefineLB, NeighborLB, GreedyCommLB, others
  - EveryLB will include all load balancing strategies
- compile time option (specify default balancer)
  - `-balancer RefineLB`
- runtime option
  - `+balancer RefineLB`

Outline

1) Introduction
   - Object Design
   - Execution Model
2) Hello World
3) Benefits of Charm++
4) Charm++ Basics
   - Object Collections
5) Overdecomposition
6) Migratability
   - Checkpointing and Resilience
7) **Structured Dagger**
8) Application Design
9) Performance Tuning
10) Using Dynamic Load Balancing
11) Interoperability
12) Debugging
13) Further Optimization

Chares are reactive

- The way we described Charm++ so far, a chare is a reactive entity:
  - If it gets this method invocation, it does this action,
  - If it gets that method invocation then it does that action
  - But what does it do?
  - In typical programs, chares have a life-cycle
- How to express the life-cycle of a chare in code?
  - Only when it exists
    - i.e. some chars may be truly reactive, and the programmer does not know the life cycle
  - But when it exists, its form is:
    - Computations depend on remote method invocations, and completion of other local computations
    - A DAG (Directed Acyclic Graph)!

Fibonacci Example

```
mainmodule fib {
  mainchare Main {
    entry Main(CkArgMsg* m);
  };

  chare Fib {
    entry Fib(int n, bool isRoot, CProxy_Fib parent);
    entry void respond(int value);
  };
};
```

Fibonacci Example

```
class Main : public CBase_Main {
 public:
  Main(CkArgMsg*m) {
    CProxy_Fib::ckNew(atoi(m- >argv[1]), true,
CProxy_Fib());
  }
};
class Fib : public CBase_Fib {
 public:
  CProxy_Fib parent;
  bool isRoot;
  int result, count;
  Fib(int n, bool isRoot_, CProxy_Fib parent_)
  : parent(parent_), isRoot(isRoot_),
result(0), count(2) {
    if (n < 2) respond(n);
    else {
      CProxy_Fib::ckNew(n -1, false, thisProxy);
      CProxy_Fib::ckNew(n -2, false, thisProxy);
    }
  }
  void respond(int val);
};
```

```
void Fib::respond(int val) {
  result += val;
  if (-- count == 0 || n < 2) {
    if (isRoot) {
      CkPrintf(“Fibonacci number is: %d\n", result);
      CkExit();
    } else {
      parent.respond(result);
      delete this;
    }
  }
}
```

Consider Fibonacci Chare

- The Fibonacci chare gets created
- If it's not a leaf,
  - It fires two chares
  - When both children return results (by calling `respond`):
    - It can compute my result and send it up, or print it
  - But in our example, this logic is hidden in the flags and counters . . .
    - This is simple for this simple example, but . . .
  - Let's look at how this would look with a little notational support

Structured Dagger

The when construct

- The `when` construct
  - Declare the actions to perform when a message is received
  - In sequence, it acts like a blocking receive

```
entry void someMethod() {
  when entryMethod1(parameters) { /* block2 */}
  when entryMethod2(parameters) { /* block3 */}
};
```

Structured Dagger

The `serial` construct

- The `serial` construct
  - A sequencial block of C++ code in the .ci file
  - The keyword `serial` means that the code block will be executed without interruption/preemption, like an entry method
  - Syntax `serial <optionalString> { /* C++ code */ }`
    - The `<optionalString>` is used for identifying the `serial` for performance analysis
  - Serial blocks can access all members of the class they belong to
- Examples (.ci file):

```
entry void method1(parameters) {
  serial {
    thisProxy.invokeMethod(10);
    callSomeFunction();
  }
};
```

```
entry void method2(parameters) {
  serial "setValue" {
    value = 10;
  }
};
```

Structured Dagger

Sequence

```
entry void someMethod() {
  serial { /* block1 */}
  when entryMethod1(parameters) serial { /* block2 */}
  when entryMethod2(parameters) serial { /* block3 */}
};
```

- Sequence
  - Sequentially execute `/* block1 */`
  - Wait for `entryMethod1` to arrive, if it has not, return control back to the Charm++ scheduler, otherwise, execute `/* block2 */`
  - Wait for `entryMethod2` to arrive, if it has not, return control back to the Charm++ scheduler, otherwise, execute `/* block3 */`

Structured Dagger

The when construct

- Execute `/* further code */` when `myMethod` arrives

```
when myMethod(int param1, int param2)
  { /* further code */ }
```

- Execute `/* further code */` when `myMethod1` and `myMethod2` arrive

```
when myMethod1(int param1, int param2),
     myMethod2(bool param3)
  { /* further code */ }
```

- Which is almost the same as this:

```
when myMethod1(int param1, int param2) {
  when myMethod2(bool param3)
    { /* further code */ }
}
```

Structured Dagger

Boilerplate

- Structured Dagger can be used in any entry method (except for a constructor)
  - Can be used in a `mainchare` , `chare` , or `array`
- For any class that has Structured Dagger in it you must insert:
  - The Structured Dagger macro: `[ClassName]_SDAG_CODE`

Structured Dagger

Declaration Syntax

The `.ci` file:

```
[mainchare,chare,array] MyFoo {
        entry void method(/* parameters */){
    // ... structured dagger code here ...
  };
  // ...
}
```

The `.cpp` file:

```
class MyFoo : public CBase_MyFoo {
  MyFoo_SDAG_Code /* insert SDAG macro */
 public:
  MyFoo() { }
};
```

Fibonacci with Structured Dagger

```
chare Fib {
    entry Fib(int n, bool isRoot, CProxy_Fib parent);
    entry void calc(int n) {
      if (n < THRESHOLD) serial { respond(seqFib(n)); }
      else {
        serial {
          CProxy_Fib::ckNew(n -1, false, thisProxy);
          CProxy_Fib::ckNew(n -2, false, thisProxy);
        }
        when response(int val)
          when response(int val2)
            serial { respond(val + val2); }
      }
    };
    entry void response(int);
};
```

Fibonacci with Structured Dagger

```
#include " fib.decl.h"
#define THRESHOLD 10
class Main : public CBase_Main {
 public:
  Main(CkArgMsg*m) { CProxy_Fib::ckNew(atoi(m- >argv[1]), true, CProxy_Fib()); }
};
class Fib : public CBase_Fib {
 public:
  Fib_SDAG_CODE
  CProxy_Fib parent; bool isRoot;
  Fib(int n, bool isRoot_, CProxy_Fib parent_):parent(parent_), isRoot(isRoot_)
    { calc(n); }
  int seqFib(int n) { return (n < 2) ? n : seqFib(n -1) + seqFib(n -2); }
  void respond(int val) {
    if (!isRoot) {
      parent.response(val);
      thisProxy.ckDestroy();
    } else {
      CkPrintf(" Fibonacci number is: %d\n", val);
      CkExit();
    }
  }
};
#include " fib.def.h"
```

Structured Dagger

The when construct

- What is the sequence?

```
when myMethod1(int param1, int param2) {
  when myMethod2(bool param3),
       myMethod3(int size, int arr[size]) /* sdag block1 */
  when myMethod4(bool param4) /* sdag block2 */
}
```

- Sequence:
  - Wait for `myMethod1` , upon arrival execute body of `myMethod1`
  - Wait for `myMethod2` and `myMethod3` , upon arrival of both, execute `/* sdag block1 */`
  - Wait for `myMethod4` , upon arrival execute `/* sdag block2 */`
- Question: if `myMethod4` arrives first what will happen?

Structured Dagger

The when construct

- The `when` clause can wait on a certain reference number
- If a reference number is specified for a `when` , the first parameter for the `when` must be the reference number
- Semantic: the `when` will “block” until a message arrives with that reference number

```
when method1[100](int ref, bool param1)
  /* sdag block */

serial {
  proxy.method1(200, false); /* will not be delivered to the when */
  proxy.method1(100, true); /* will be delivered to the when */
}
```

Structured Dagger

The `if-then-else` construct

- The `if-then-else` construct:
  - Same as the typical C if-then-else semantics and syntax

```
if (thisIndex.x == 10) {
  when method1[block](int ref, bool someVal) /* code block1 */
} else {
  when method2(int payload) serial {
    // ...           some C++ code
  }
}
```

Structured Dagger

The `for` construct

- The `for` construct:
  - Defines a sequenced `for` loop (like a sequential C for loop)
  - Once the body for the *i*th iteration completes, the $i + 1$ iteration is started

```
for (iter = 0; iter < maxIter; ++iter) {
  when recvLeft[iter](int num, int len, double data[len])
    serial { computeKernel(LEFT, data); }
  when recvRight[iter](int num, int len, double data[len])
    serial { computeKernel(RIGHT, data); }
}
```

- `iter` must be defined in the class as a member

```
class Foo : public CBase_Foo {
 public: int iter;
};
```

Structured Dagger

The `while` construct

- The `while` construct:
  - Defines a sequenced `while` loop (like a sequential C while loop)

```
while (i < numNeighbors) {
  when recvData(int len, double data[len]) {
    serial { /* do something */}
    when method1() /* block1 */
    when method2() /* block2 */
  }
  serial { i++; }
}
```

Structured Dagger

The `overlap` construct

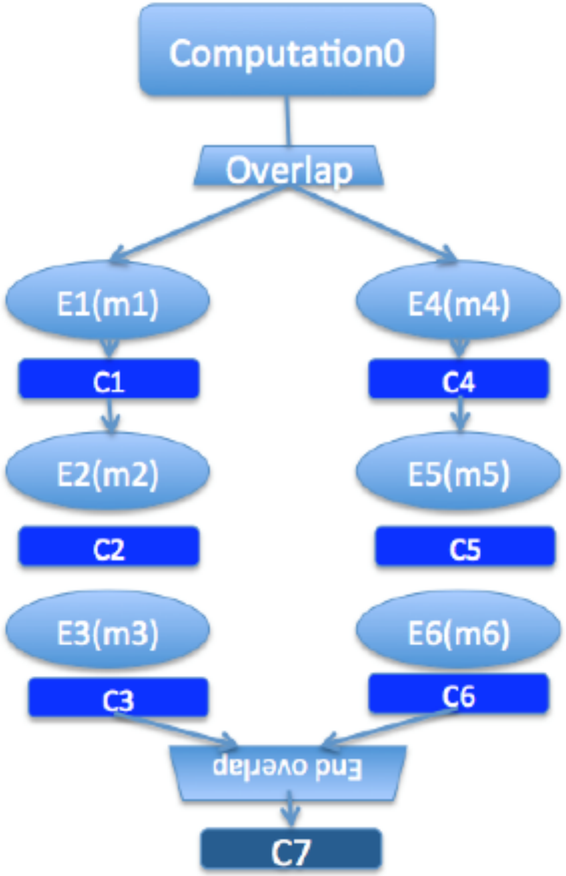
- By default, Structured Dagger defines a sequence that is followed sequentially
- `overlap` allows multiple independent clauses to execute in any order
- Any constructs in the body of an `overlap` can happen in any order
- An `overlap` finishes in sequence when all the statements in it are executed
- Syntax: `overlap {  /* sdag constructs */ }`

What are the possible execution sequences?

```
serial { /* block1 */}
overlap {
  serial { /* block2 */}
  when entryMethod1[100](int ref_num, bool param1) /* block3 */
  when entryMethod2(char myChar) /* block4 */
}
serial { /* block5 */}
```

Illustration of a long “overlap”

- Overlap can be used to get back some of the asynchrony within a chare
  - ➢But it is constrained
  - ➢Makes for more disciplined programming,
    - ★ with fewer race conditions



Structured Dagger

The `forall` construct

- The `forall` construct:
  - Has “do-all” semantics: iterations may execute an any order
  - Syntax:

    `forall [<ident>] (<min> : <max>, <stride>) <body>`
  - The range from `<min>` to `<max>` is inclusive

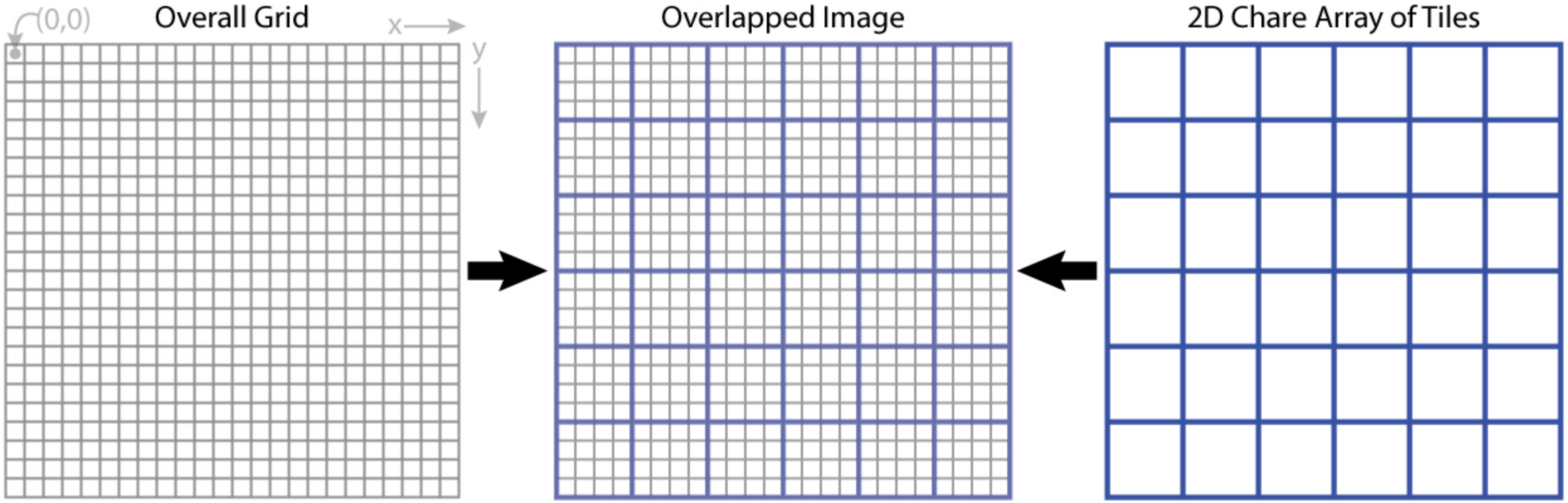
```
forall [block] (0 : numBlocks-1, 1) {
  when method1[block](int ref, bool someVal) /* code block1 */
}
```

- Assume `block` is declared in the class as `public: int block;`

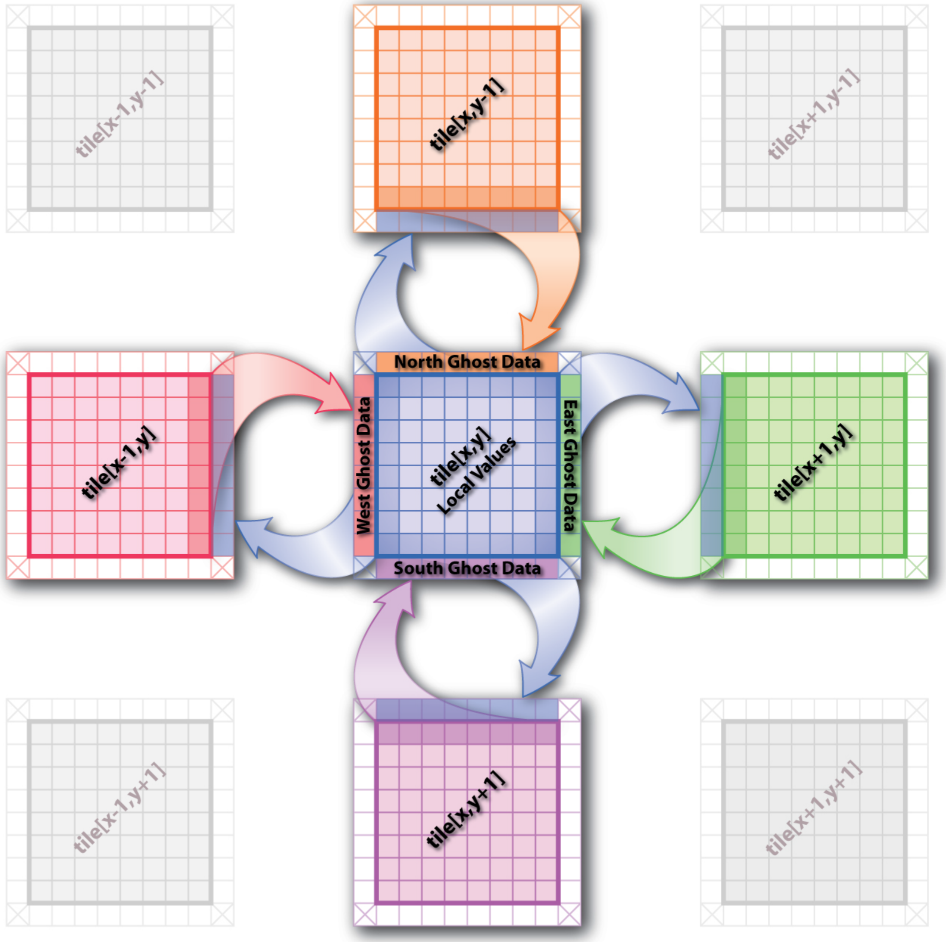
Stencil Codes

- Iterative applications where array elements are updated according to some fixed pattern.
- Used in computational simulations, solving partial differential equations, Jacobi kernel, GaussSeidel method, image processing applications etc.
- Can be 2D or 3D

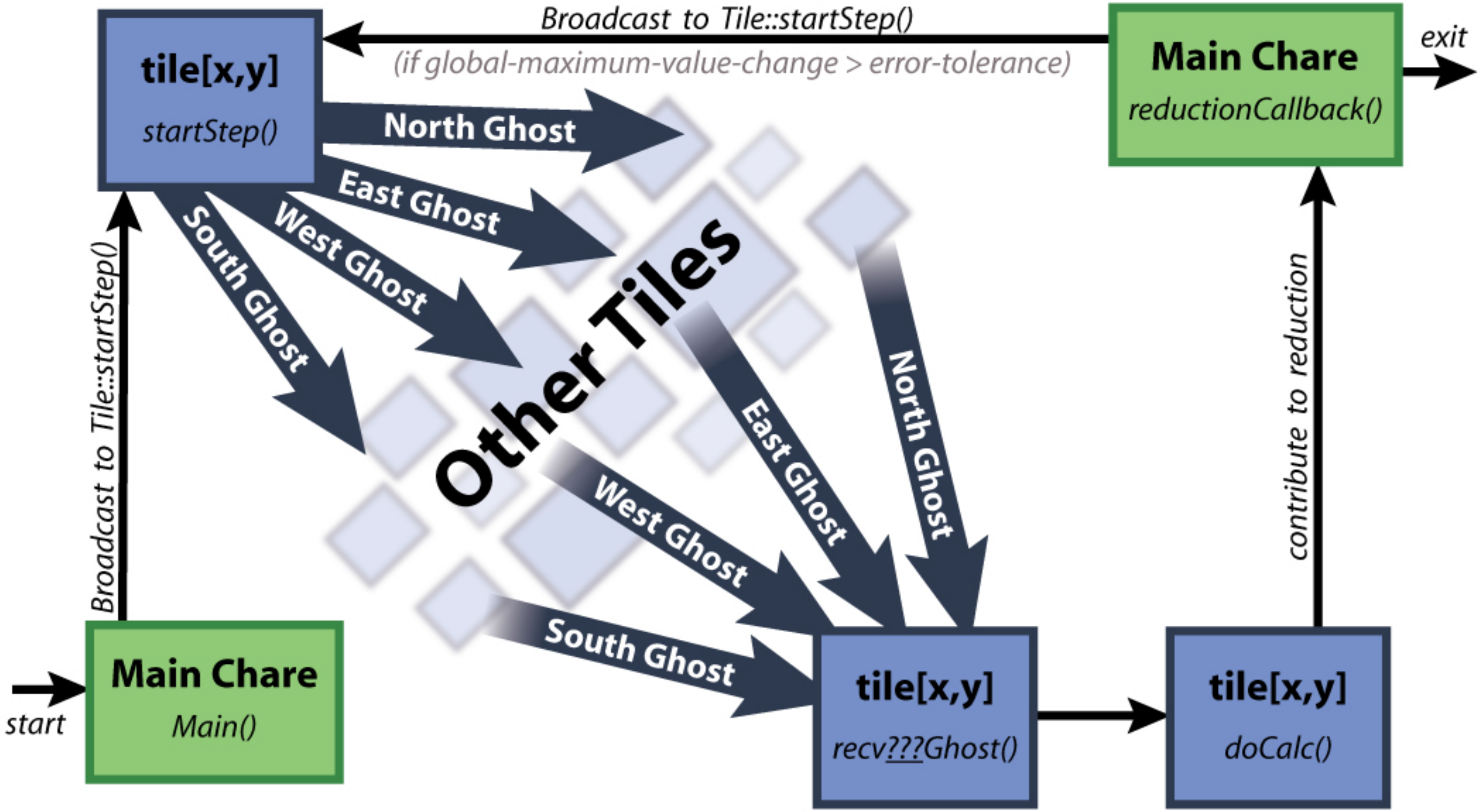
5-point Stencil



5-point Stencil



5-point Stencil



Jacobi: .ci file

```
mainmodule jacobi2d {
  mainchare Main {
    entry Main(CkArgMsg *m);
    entry void done(int iterations);
  };
  array [2D] Jacobi {
    entry Jacobi(CProxy_Main);
    entry void updateGhosts(int ref, int dir, int w, double gh[w]);
    entry [reductiontarget] void checkConverged(bool result);
    entry void run() {
      // ... main loop (next slide) ...
    };
  };
};
```

Jacobi: .ci file

```
while (!converged) {
  serial {
    copyToBoundaries();
    int x = thisIndex.x, y = thisIndex.y;
    int bdX = blockDimX, bdY = blockDimY;
    thisProxy(wrapX(x-1),y).updateGhosts(iter, RIGHT, bdY, rightGhost);
    thisProxy(wrapX(x+1),y).updateGhosts(iter, LEFT, bdY, leftGhost);
    thisProxy(x,wrapY(y-1)).updateGhosts(iter, TOP, bdX, topGhost);
    thisProxy(x,wrapY(y+1)).updateGhosts(iter, BOTTOM, bdX, bottomGhost);
    freeBoundaries();
  }
  for (remoteCount = 0; remoteCount < 4; remoteCount++)
    when updateGhosts[iter](int ref, int dir, int w, double buf[w]) serial {
      updateBoundary(dir, w, buf);
    }
  serial {
    double error = computeKernel();
    int conv = error < DELTA;
    CkCallback cb(CkReductionTarget(Jacobi, checkConverged), thisProxy);
    contribute(sizeof(int), &conv, CkReduction::logical_and, cb);
  }
  when checkConverged(bool result)
    if (result) serial { mainProxy.done(iter); converged = true; }
  serial { ++iter; }
};
```

Jacobi: .ci file (with **asynchronous** reductions)

```
entry void run() {
  while (!converged) {
    serial {
      copyToBoundaries();
      int x = thisIndex.x, y = thisIndex.y;
      int bdX = blockDimX, bdY = blockDimY;
      thisProxy(wrapX(x-1     ),y).updateGhosts(iter, RIGHT, bdY, rightGhost);
      thisProxy(wrapX(x+1),y).updateGhosts(iter, LEFT, bdY, leftGhost);
      thisProxy(x,wrapY(y-1     )).updateGhosts(iter, TOP, bdX, topGhost);
      thisProxy(x,wrapY(y+1)).updateGhosts(iter, BOTTOM, bdX, bottomGhost);
      freeBoundaries();
    }
    for (remoteCount = 0; remoteCount < 4; remoteCount++)
      when updateGhosts[iter](int ref, int dir, int w, double buf[w]) serial {
        updateBoundary(dir, w, buf);
      }
    serial {
      double error = computeKernel();
      int conv = error < DELTA;
      if (iter % 5 == 1)
        contribute(sizeof(int), &conv, CkReduction::logical_and,
                   CkCallback(CkReductionTarget(Jacobi, checkConverged), thisProxy));
      }
      if (++iter % 5 == 0)
        when checkConverged(bool result)
          if (result) serial { mainProxy.done(iter); converged = true; }
  }
};
```

Example

- Consider the following problem:
  - A large number of key-value pairs are distributed on several (hundred) processors (or chares)
  - Each chare needs to get some subset of these values before they can proceed to the next phase of the computation
  - The set of keys needed are not known in advance: they are determined based on the input data

Structured dagger version

```
entry void retrieveValues {
  for (i = 0; i < n; i++) serial {
    keys[i] = // compute i'th key;
    keyValueProxy[keys[i] / B].requestValue(keys[i], thisProxy, i);
  }
```

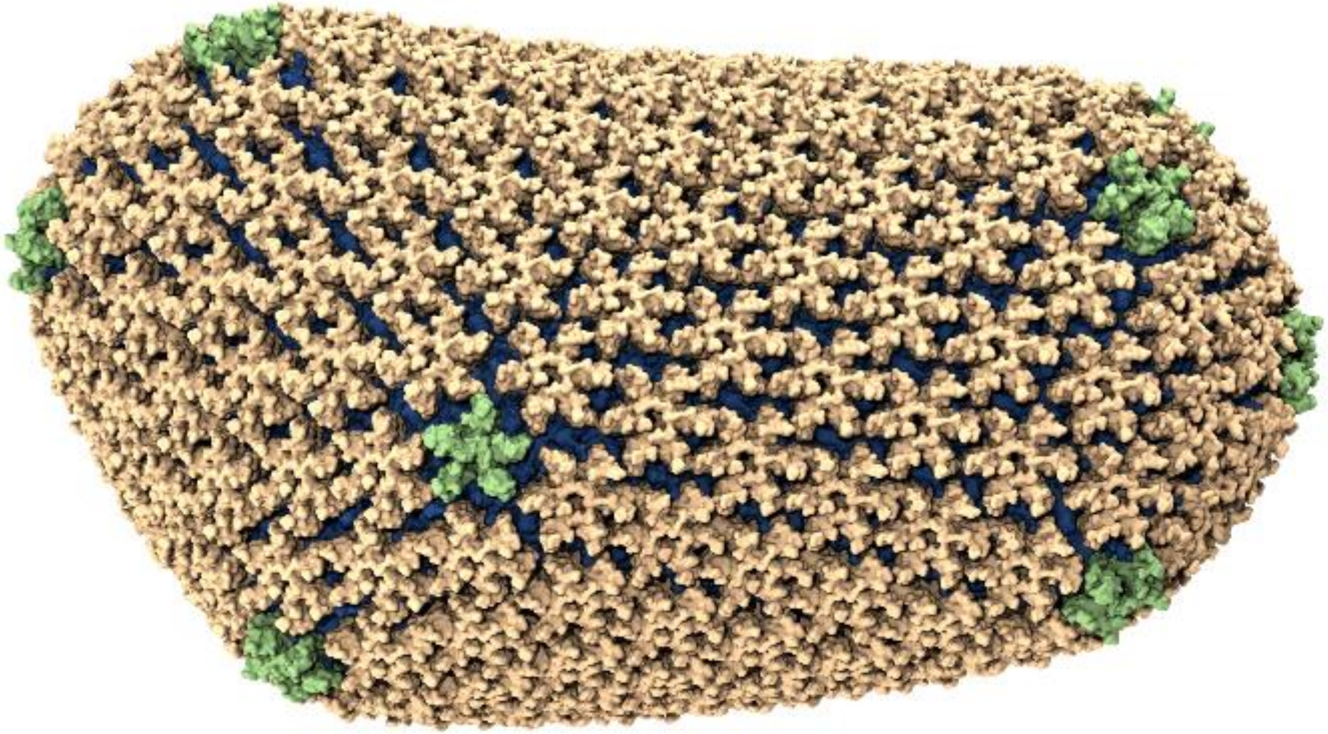
```
  for (i = 0; i < n; i++)
    when response(int i, ValueType value)
      serial { values[i] = value; }
  };
// next phase of computation that uses the keys and values.
```

```
KeyValueClass::requestValue(int key, CProxy_Client c, int ref) {
  ValueType v = localTable[key];
  c.response(ref, v);
}
```

Outline

1) Introduction
    - Object Design
    - Execution Model
2) Hello World
3) Benefits of Charm++
4) Charm++ Basics
    - Object Collections
5) Overdecomposition
6) Migratability
    - Checkpointing and Resilience
7) Structured Dagger
8) **Application Design**
9) Performance Tuning
10) Using Dynamic Load Balancing
11) Interoperability
12) Debugging
13) Further Optimization

NAMD

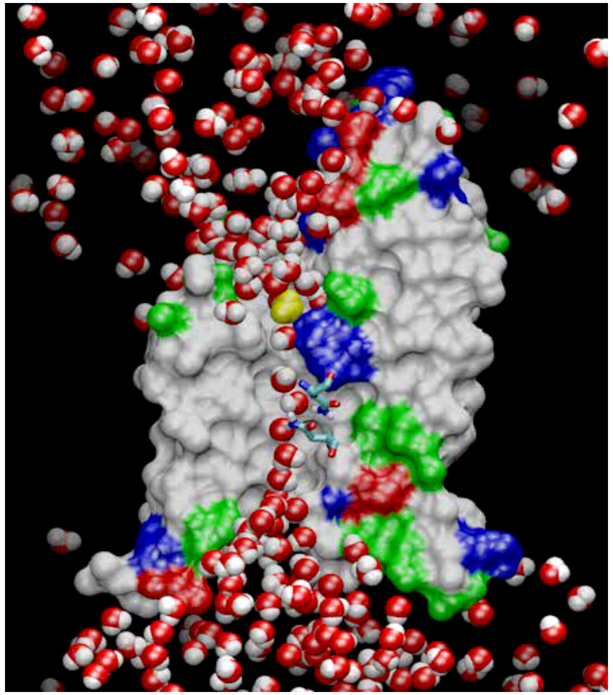


- Ground-breaking Nature article on the structure of the HIV capsid

Molecular Dynamics in NAMD

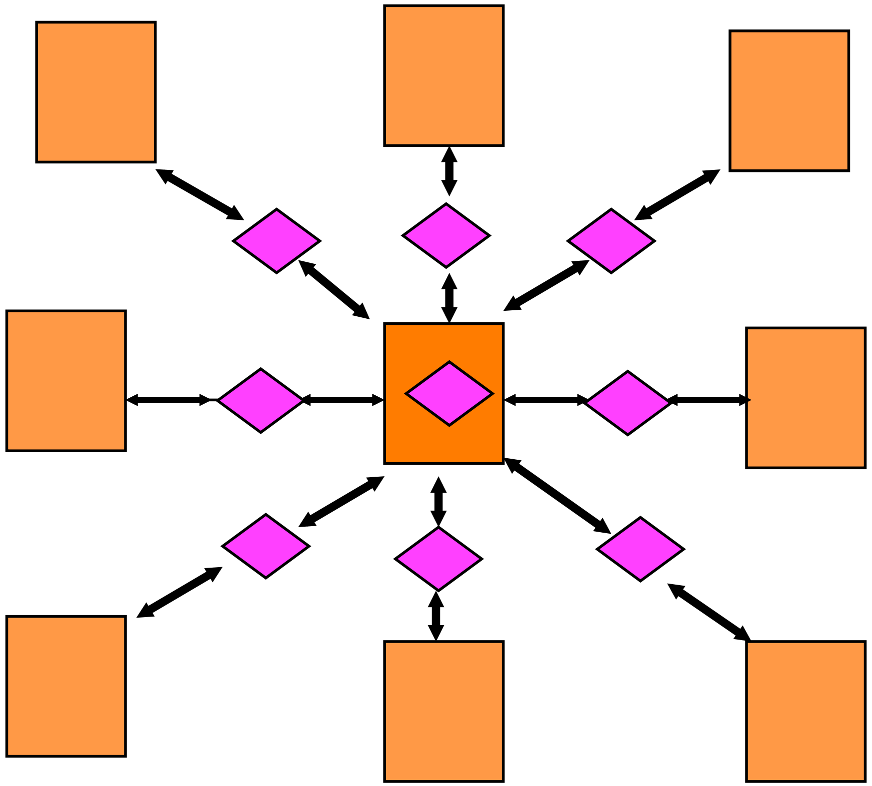
- Collection of charged atoms, with bonds
  - Newtonian mechanics
  - Relatively small amount of atoms (100K – 10M)
- Calculate forces on each atom
  - Bonds
  - Non-bonded: electrostatic and van der Waals
    - Short-distance: every timestep
    - Long-distance: using PME (3D FFT)
    - Multiple Time Stepping : PME every 4 timesteps
- Calculate velocities and advance positions
- Challenge: femtosecond time-step, millions needed!

Collaboration with K. Schulten, R. Skeel, and coworkers



Object Based Parallelization for MD

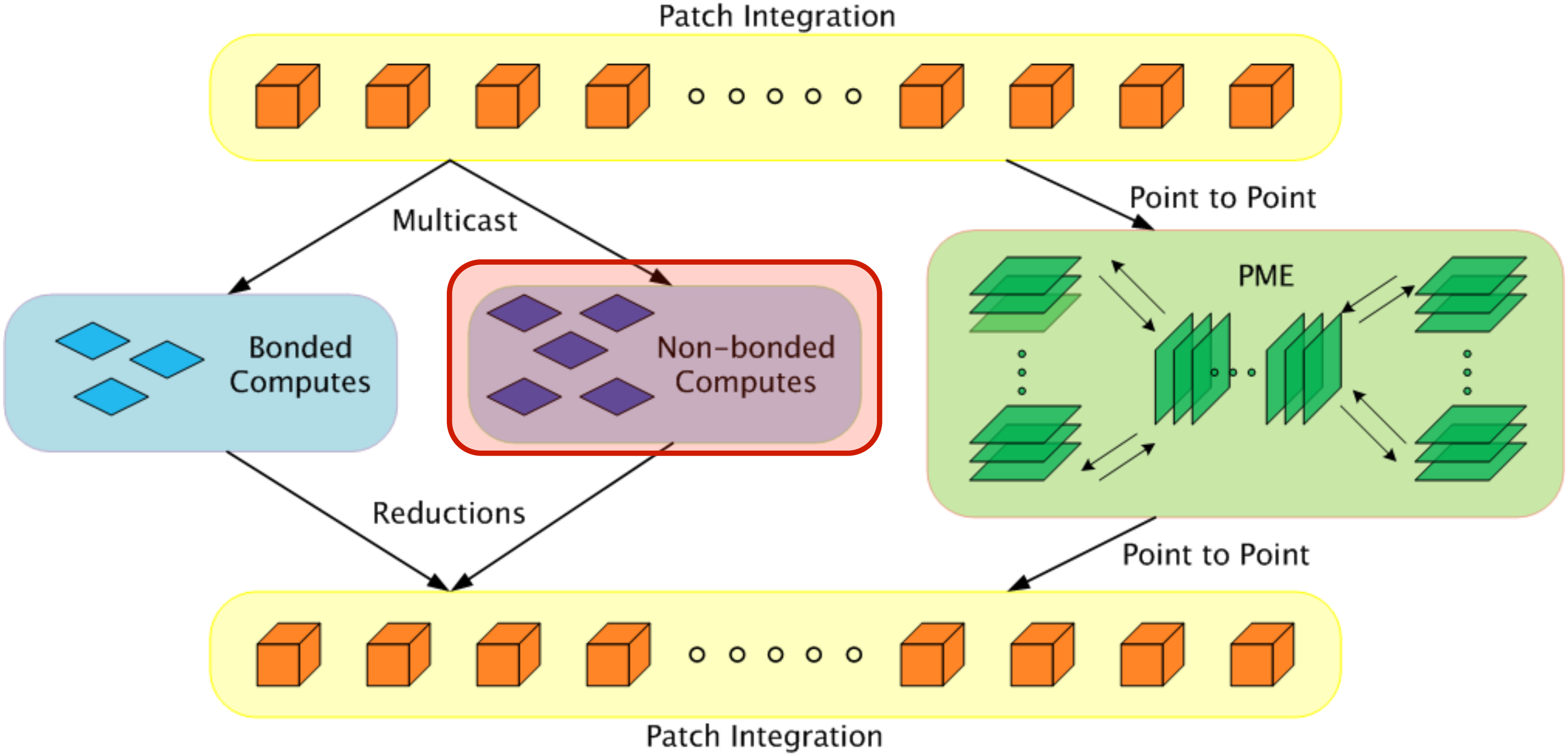
Force Decomposition + Spatial Decomposition



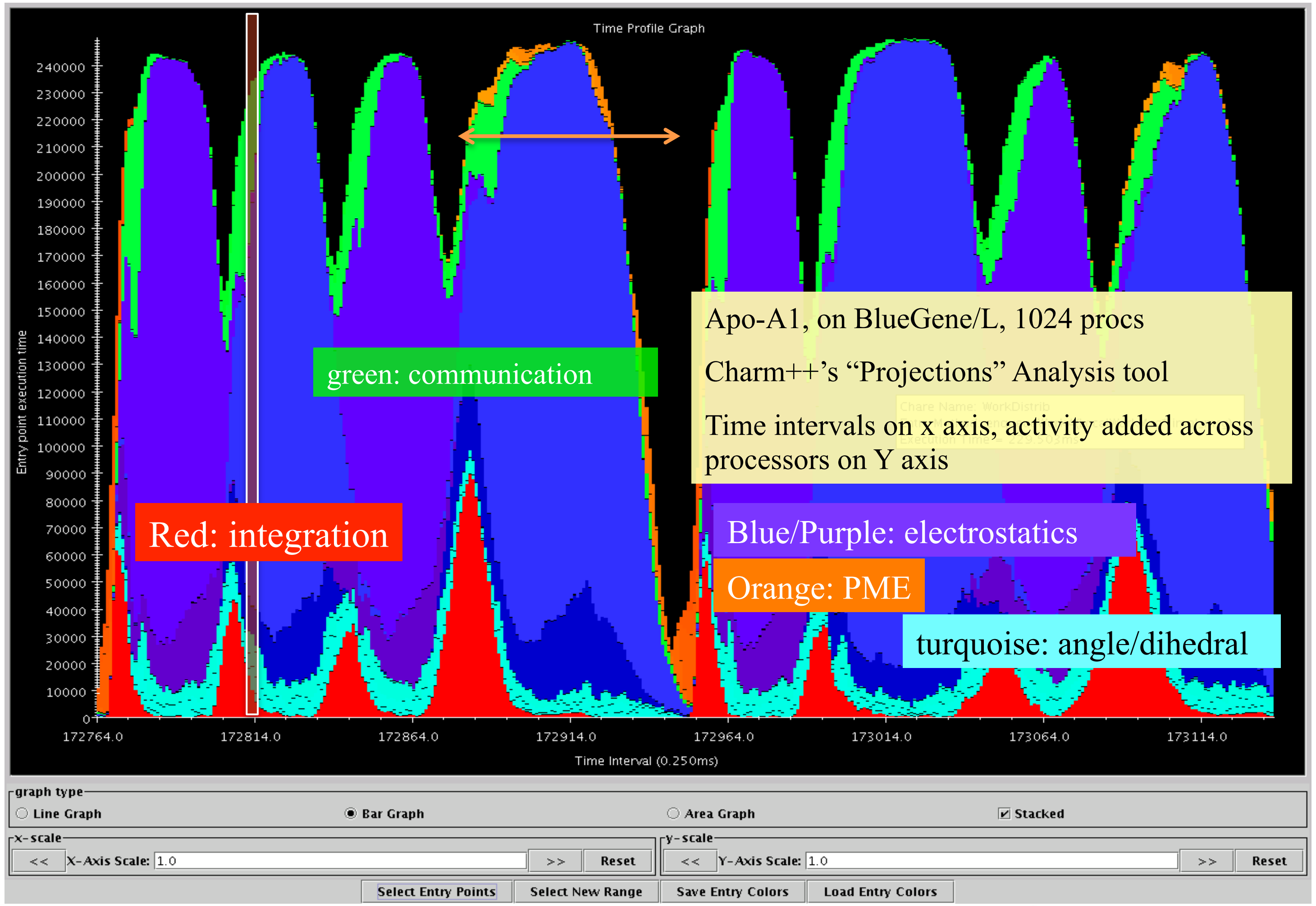
- Now, we have many objects to load balance:
  - Each diamond can be assigned to any proc.
  - Number of diamonds (3D): 14*Number of Patches
- 2-away variation:
  - Half-size cubes
  - Communicate only with neighbors
  - 5 x 5 x 5 interactions
- 3-away interactions:
  - 7 x 7 x 7

NAMD Parallelization Using Charm++

The computation is decomposed into “natural” objects of the application, which are assigned to processors by Charm++ RTS



NAMD Projections



Apo-A1, on BlueGene/L, 1024 procs

Charm++'s "Projections" Analysis tool

Time intervals on x axis, activity added across processors on Y axis

green: communication

Red: integration

Blue/Purple: electrostatics

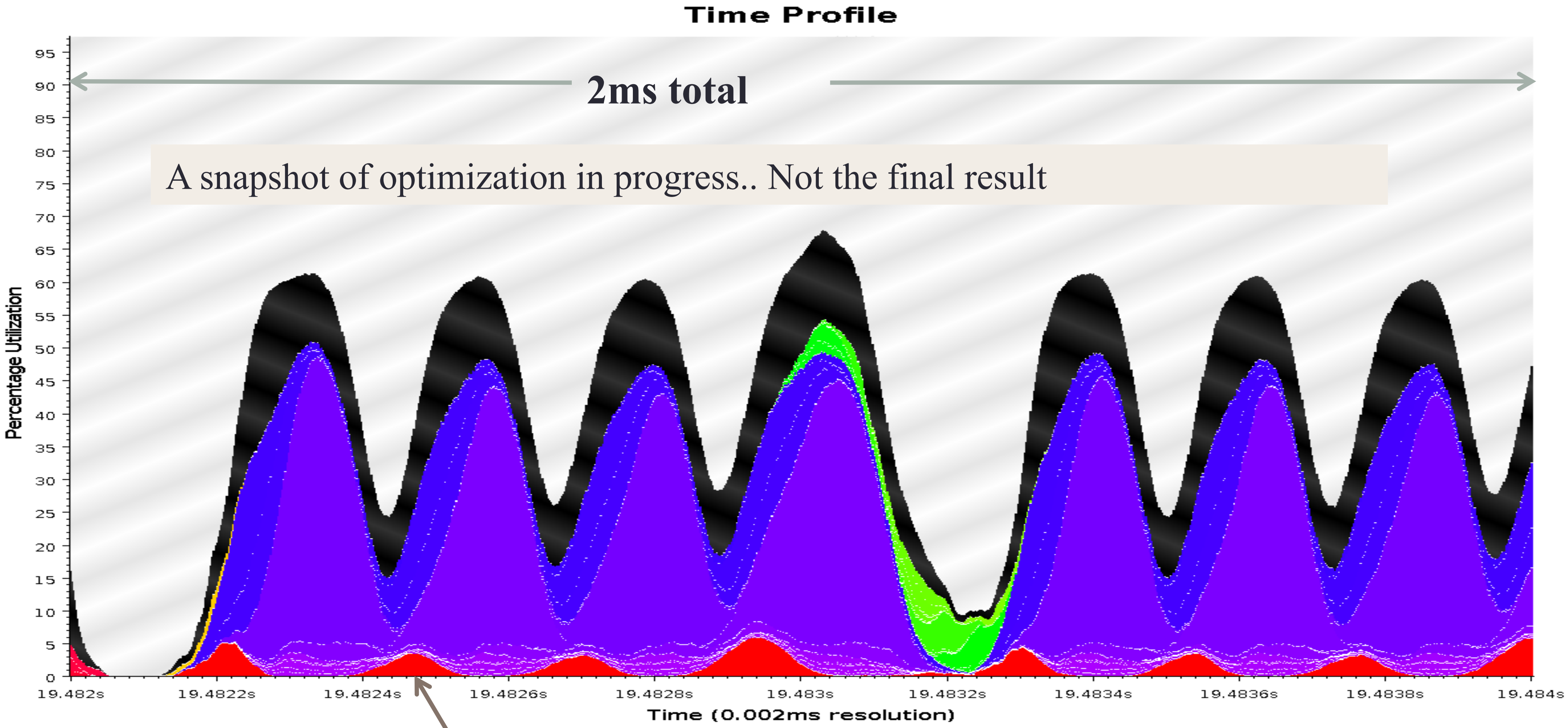
Orange: PME

turquoise: angle/dihedral

Time

Time Profile of ApoA1 on Power7 PERCS

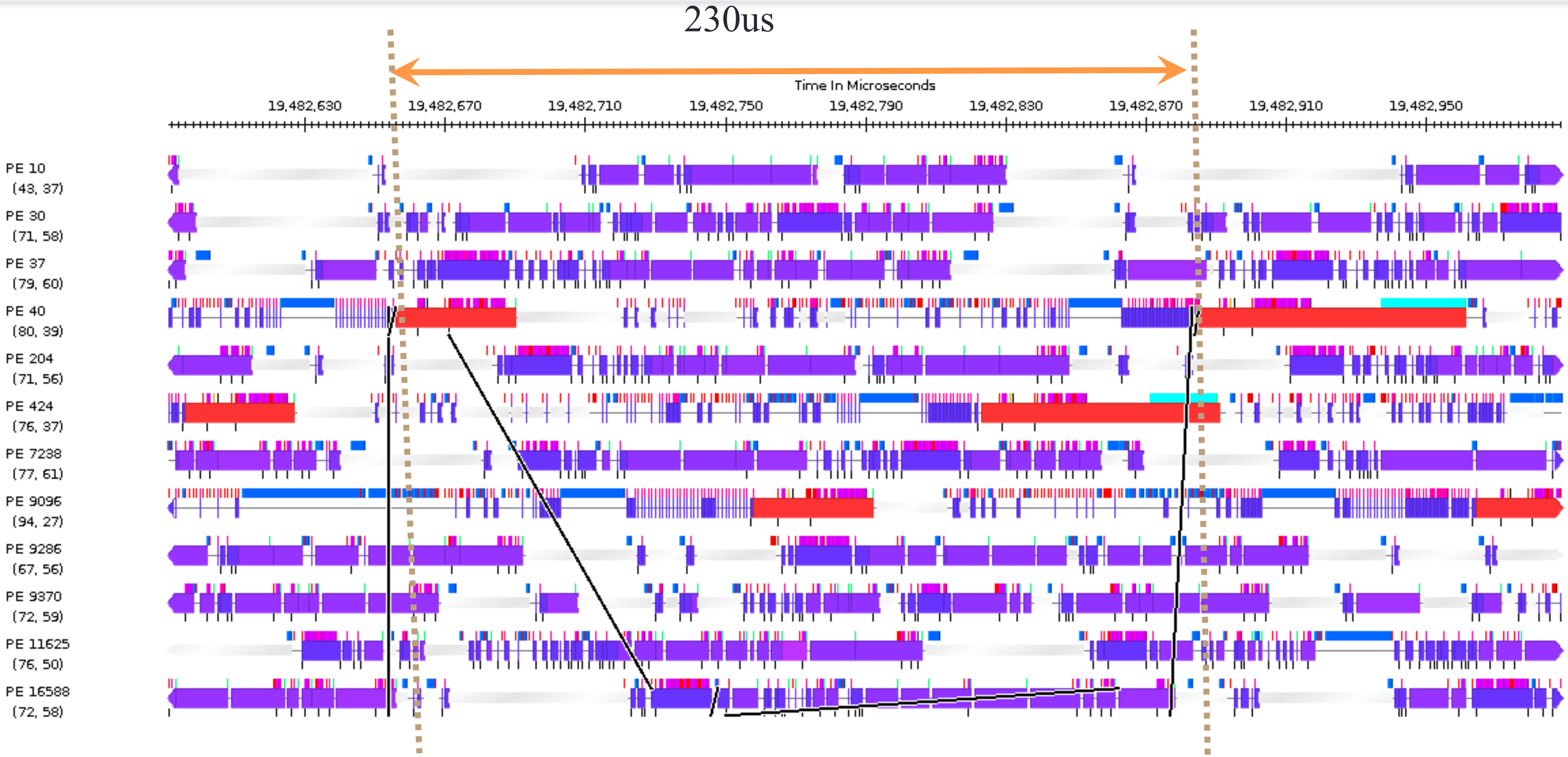
92,000 atom system, on 500+ nodes (16k cores)



A snapshot of optimization in progress.. Not the final result

Overlapped steps, as a result of asynchrony

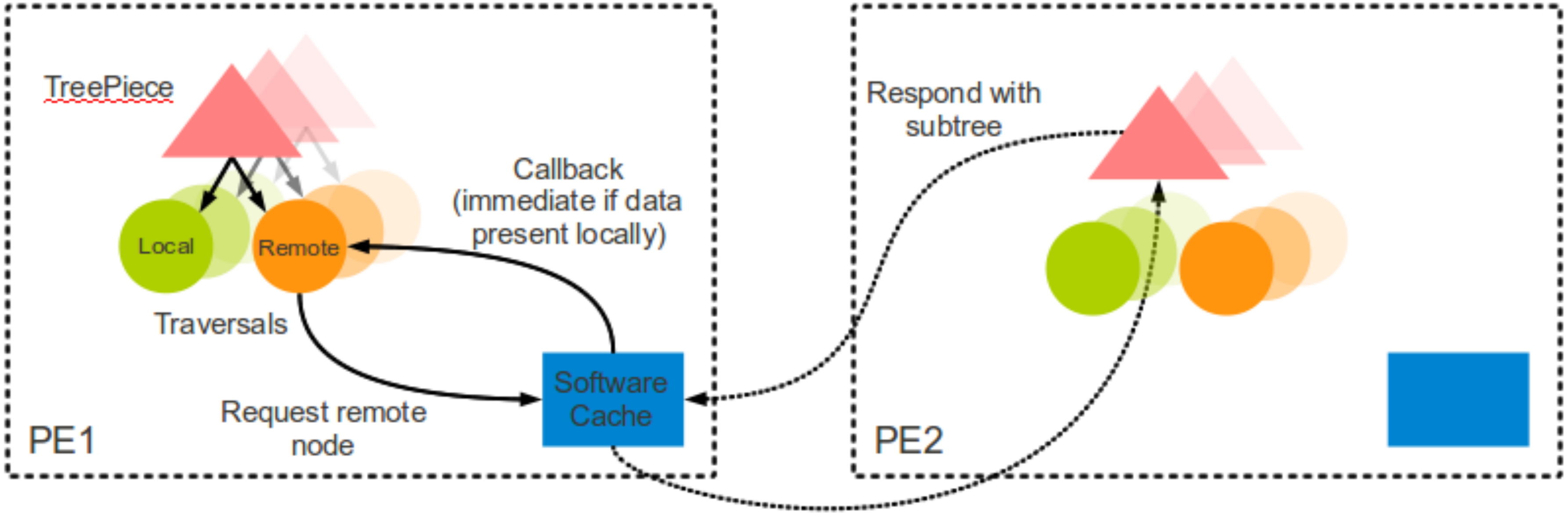
Timeline of ApoA1 on Power7 PERCS



ChaNGa: Parallel Gravity

- Collaborative project (NSF)
  - with Tom Quinn, Univ. of Washington
- Evolution of Universe and Galaxy Formation
- Gravity, gas dynamics
- Barnes-Hut tree codes
  - Oct tree is natural decomposition
  - Geometry has better aspect ratios, so you open up fewer nodes
  - But is not used because it leads to bad load balance
  - Assumption: one-to-one map between sub-trees and PEs
  - Binary trees are considered better load balanced
- With Charm++: Use Oct-Tree, and let Charm++ map subtrees to processors

ChaNGa: Control Flow



TreePiece

Local

Remote

Traversals

Callback (immediate if data present locally)

Request remote node

Software Cache

PE1

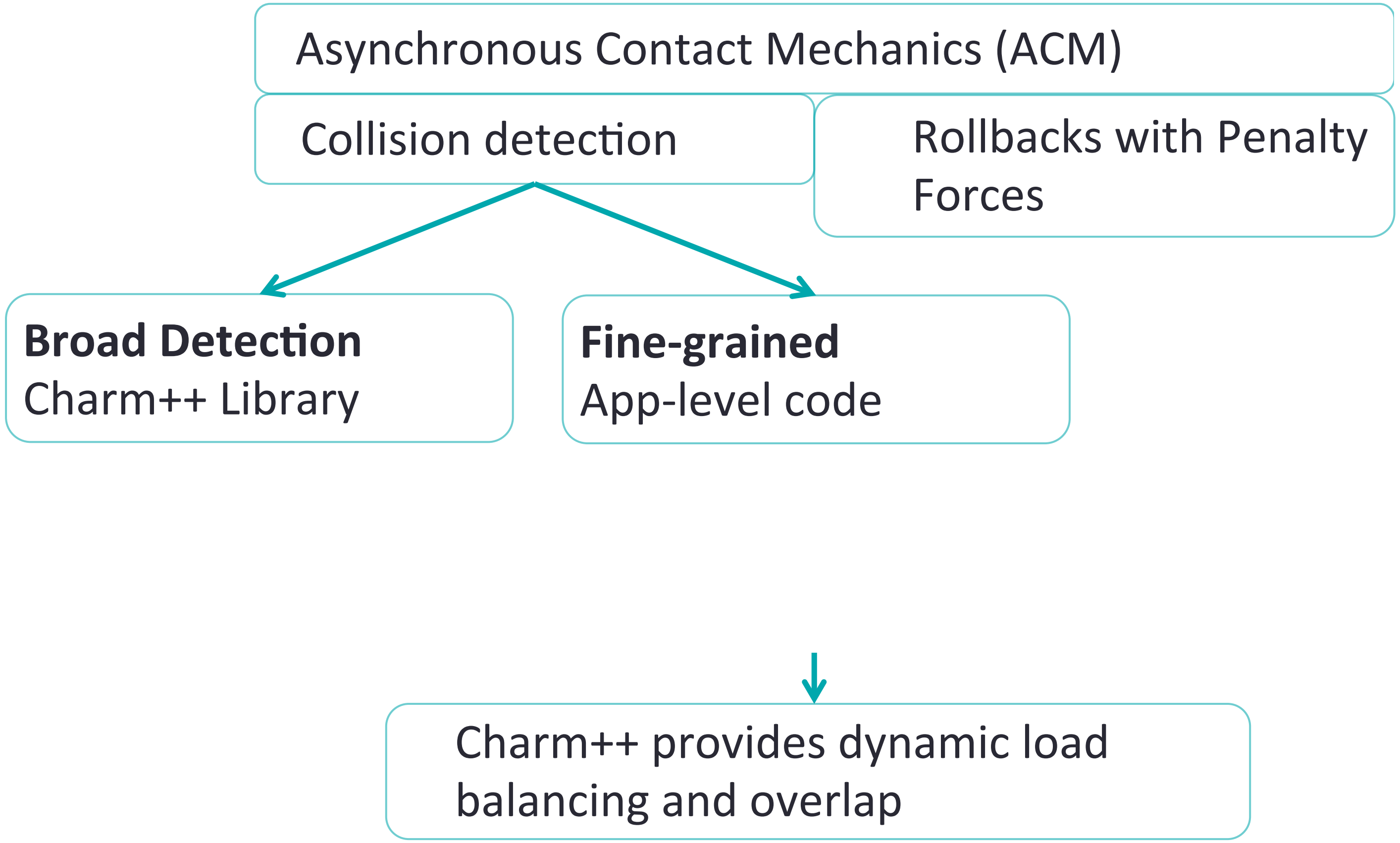
Respond with subtree

PE2

Send request message to owner TreePiece if data not present locally

Cloth Simulation: Disney Research

Collaboration between Rasmus and my student Xiang Ni



Asynchronous Contact Mechanics (ACM)

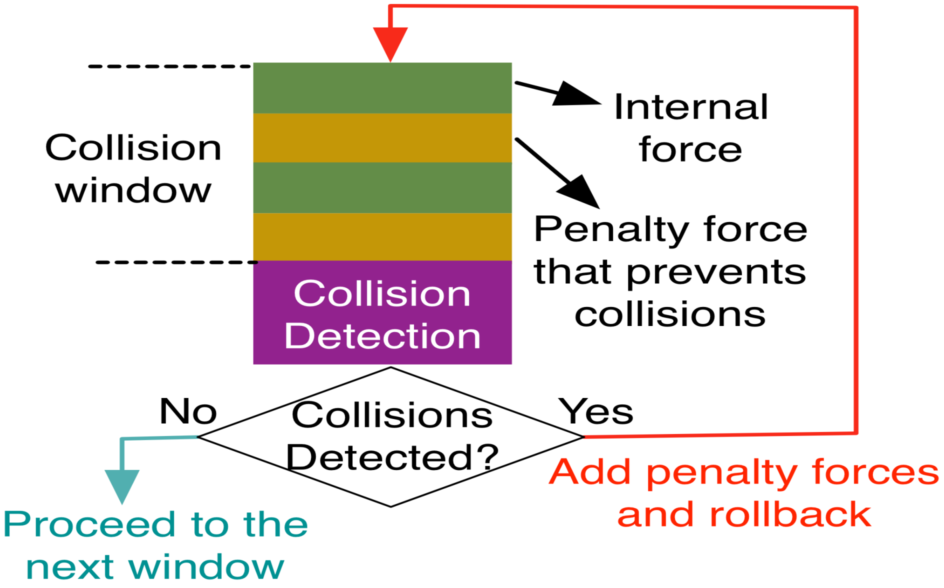
Collision detection

Rollbacks with Penalty Forces

Broad Detection
Charm++ Library

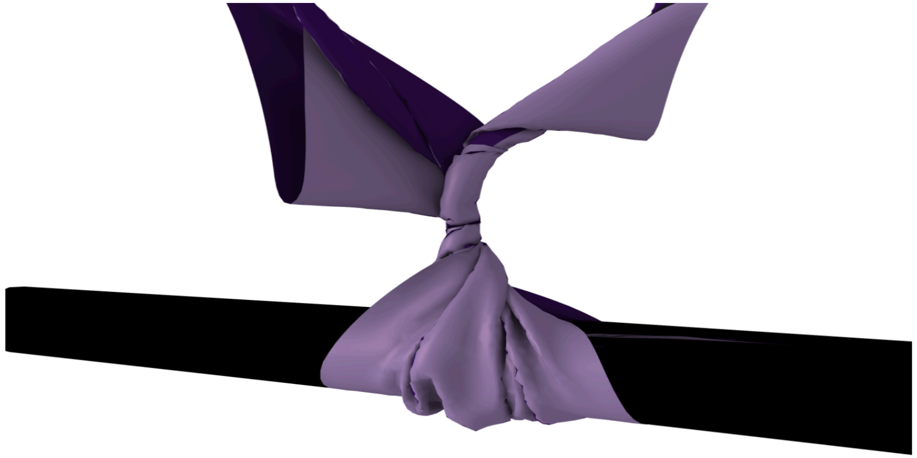
Fine-grained
App-level code

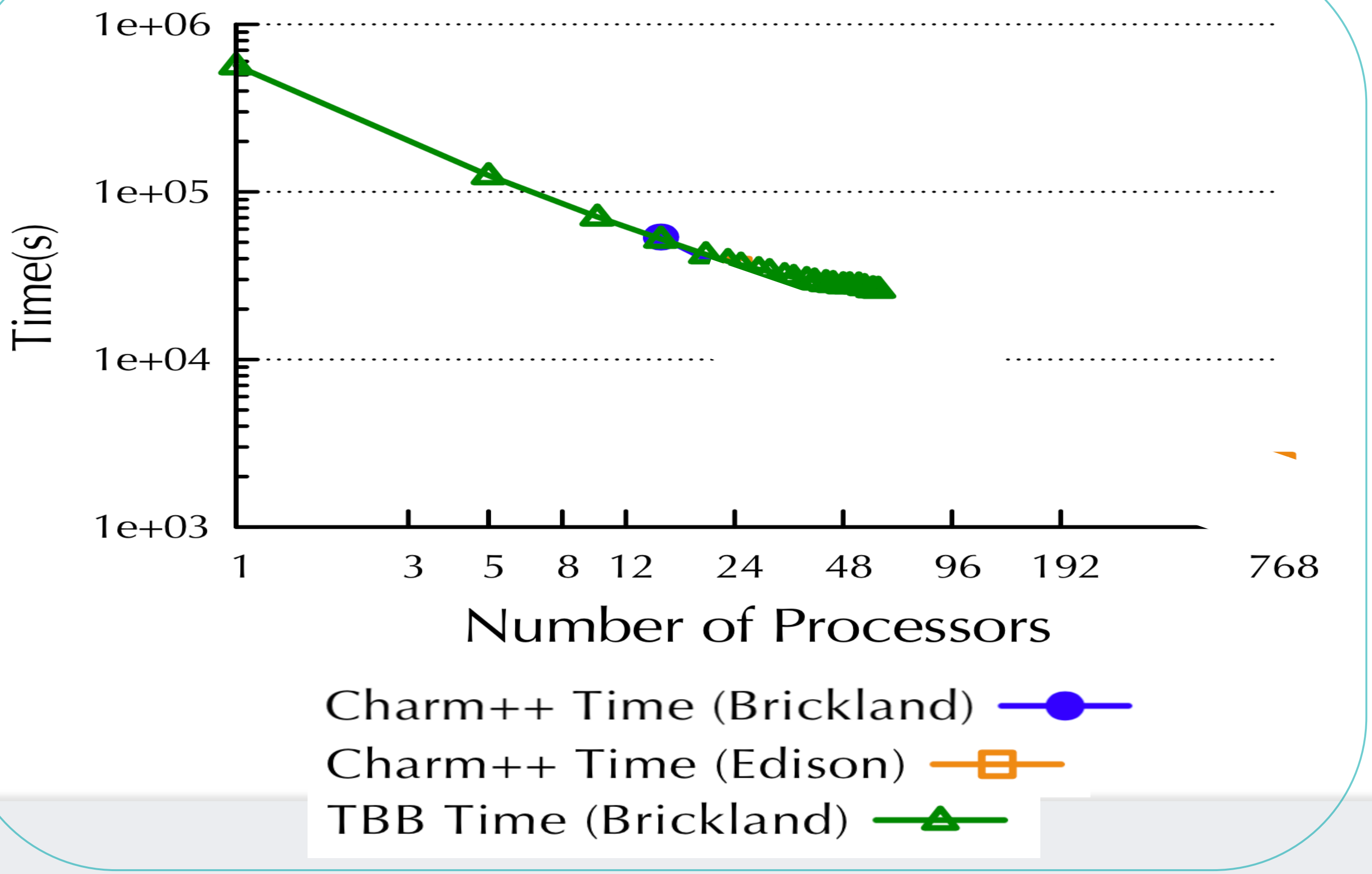
Charm++ provides dynamic load balancing and overlap



Cloth Simulation: Disney Research

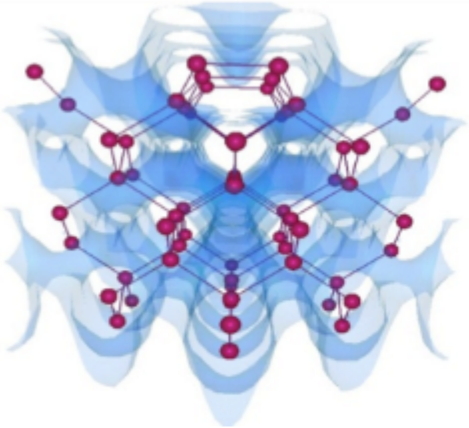
“Twister”



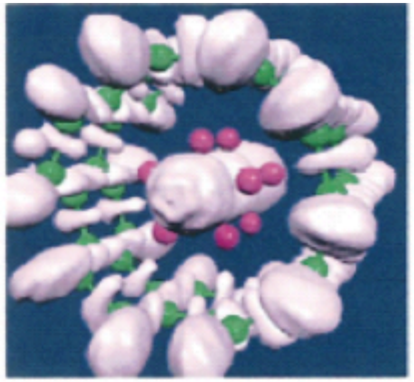


OpenAtom: MD with quantum effects

- Much more fine-grained:
  - Each electronic state is modeled with a large array
- Collaboration with:
  - G. Martyna (IBM)
  - M. Tuckerman (NYU)
- Using Charm++ virtualization, we can efficiently scale small (32 molecule) systems to thousands of processors

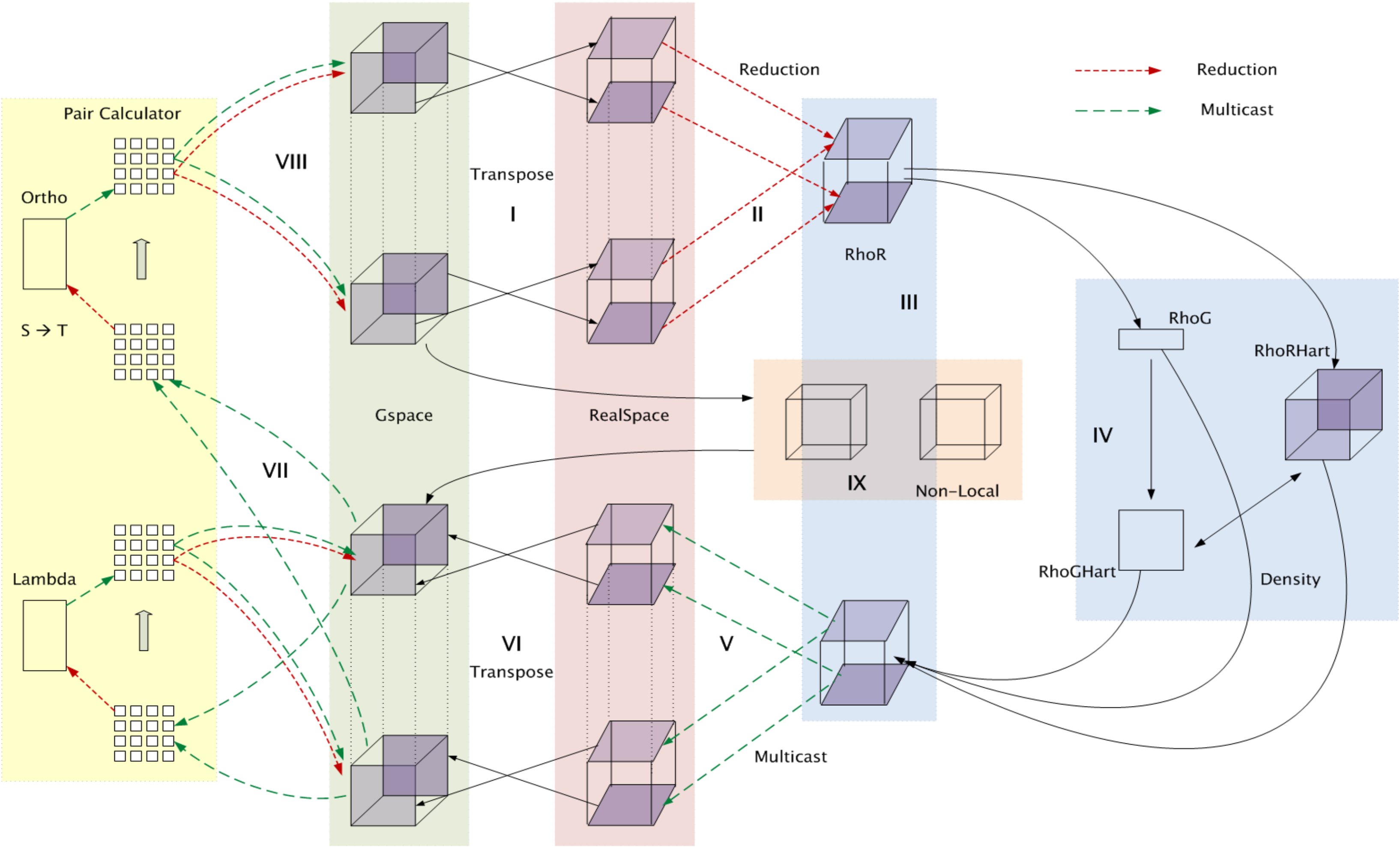


Semiconductor Surfaces

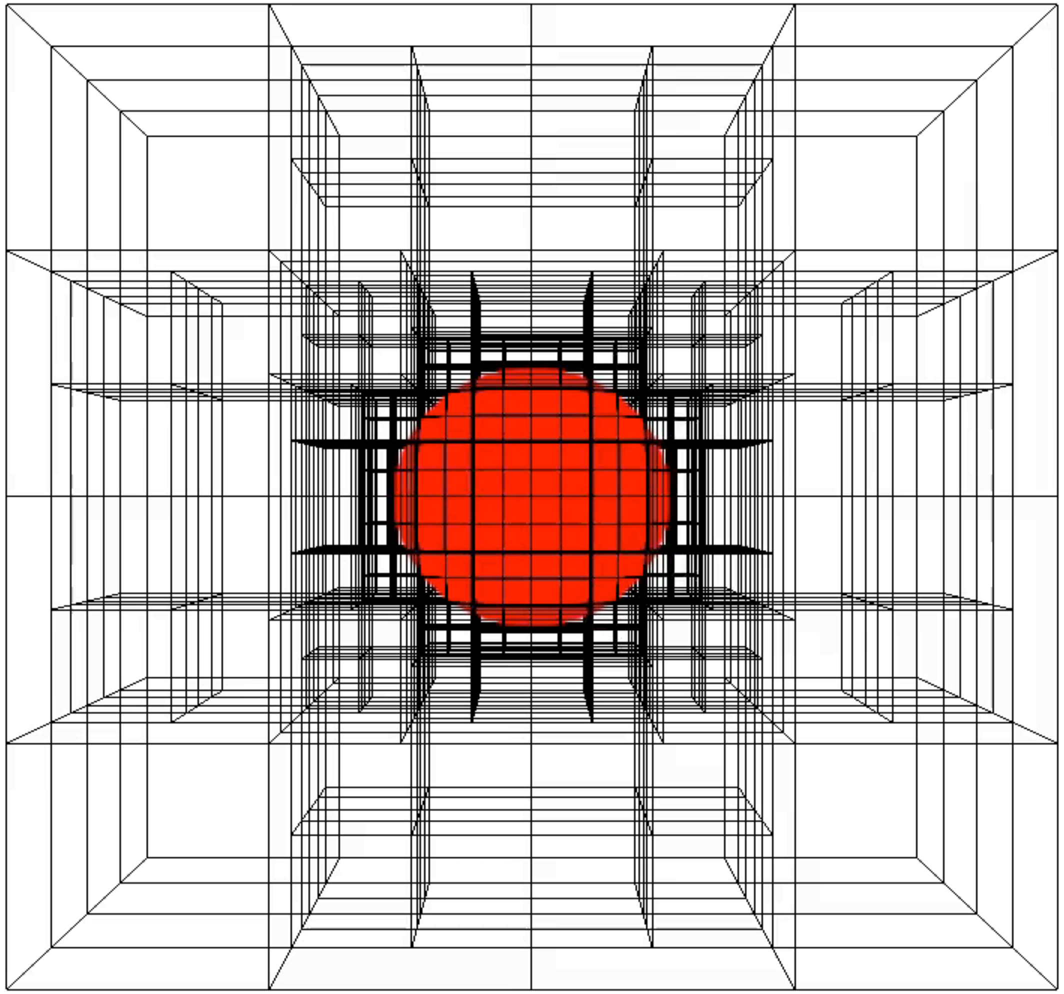


Nanowires

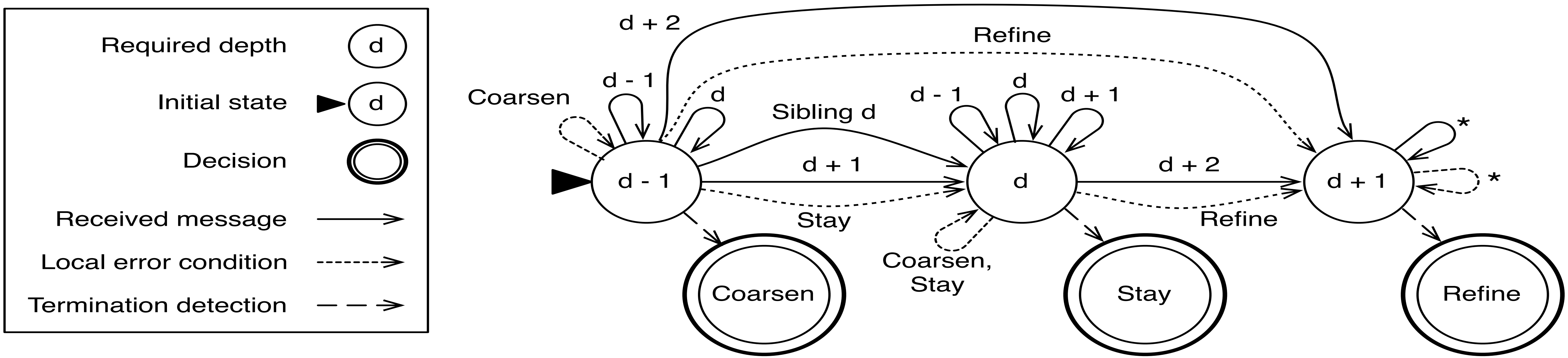
OpenAtom: Decomposition and Computation Flow



Structured AMR miniApp



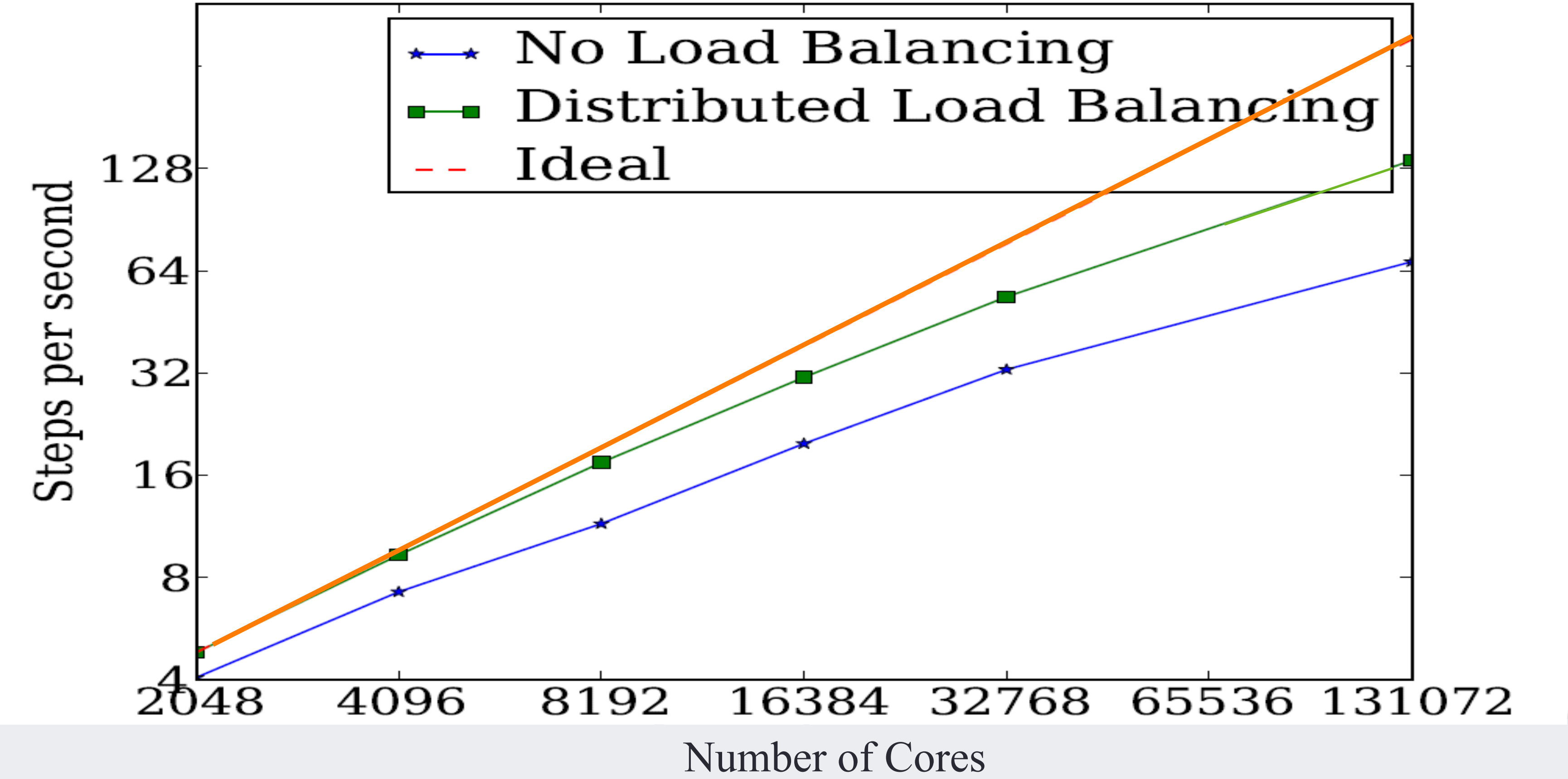
Structured AMR: State Machine



Structured AMR: Performance

Testbed: IBM BG/Q Mira
Cray XK/6 Titan

Advection Benchmark
First order method in 3d-space



Outline

1) Introduction
   - Object Design
   - Execution Model
2) Hello World
3) Benefits of Charm++
4) Charm++ Basics
   - Object Collections
5) Overdecomposition
6) Migratability
   - Checkpointing and Resilience
7) Structured Dagger
8) Application Design
9) **Performance Tuning**
10) Using Dynamic Load Balancing
11) Interoperability
12) Debugging
13) Further Optimization

Performance Analysis Using Projections

- Instrumentation and measurement
  - Link program with `-tracemode projections OR summary`
  - Trace data is generated automatically during run
  - User events can be easily inserted as needed
- Projections: visualization and analysis
  - Scalable tool to analyze up to 300,000 log files
  - A rich set of tool features: time profile, time lines, usage profile, histogram, extrema tool
  - Detect performance problems: load imbalance, grain size, communication bottleneck, etc

Using Projections

- Aggregated performance viewing tools
  - Time profile
  - Histogram
  - Communication over time
- Processor level granularity tools
  - Overview
  - Timeline
- Derived/processed data tools
  - Extrema analysis: identifies outliers
  - Noise miner: highlights probable interference

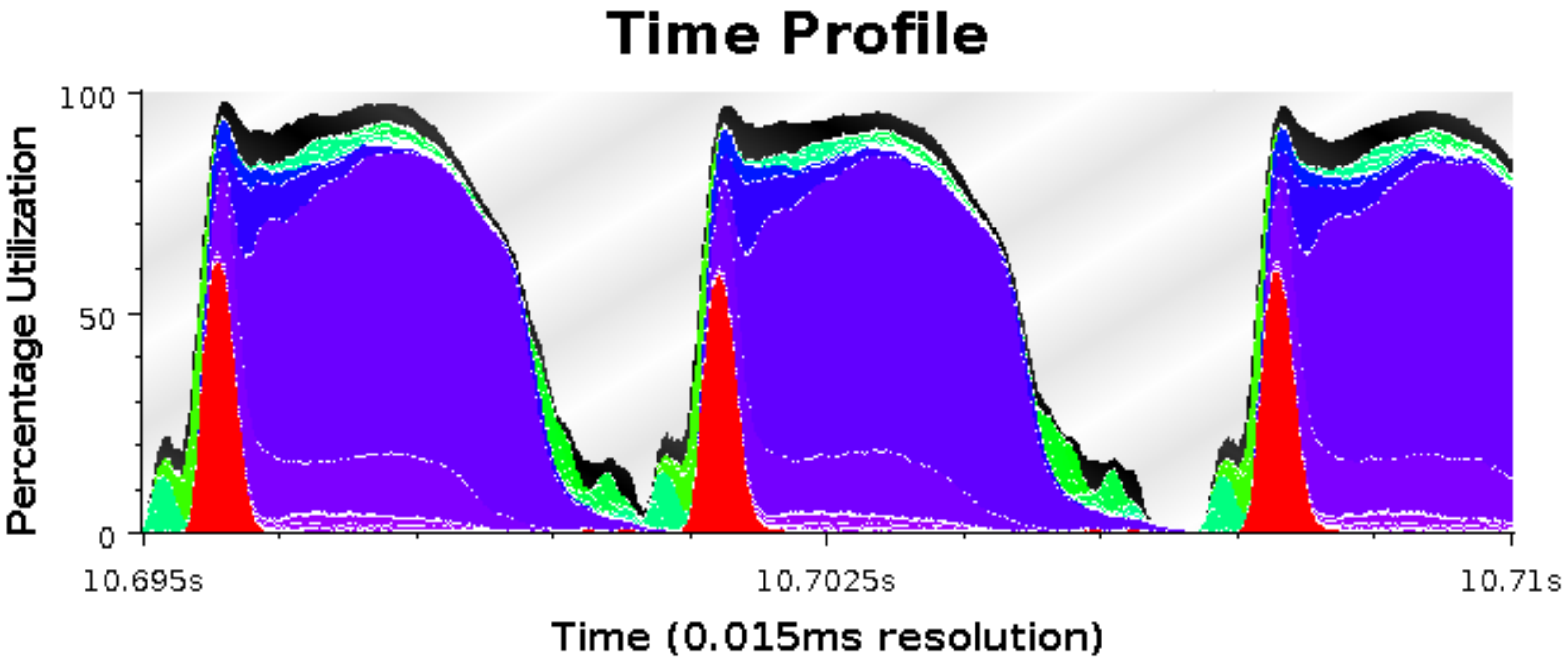
Problem Identification

- Load imbalance
  - Time profile: lower CPU usage
  - Extrema analysis tool:
    - Least idle processors
  - Load the over-loaded processors in Timeline
  - Histogram: grain size issues

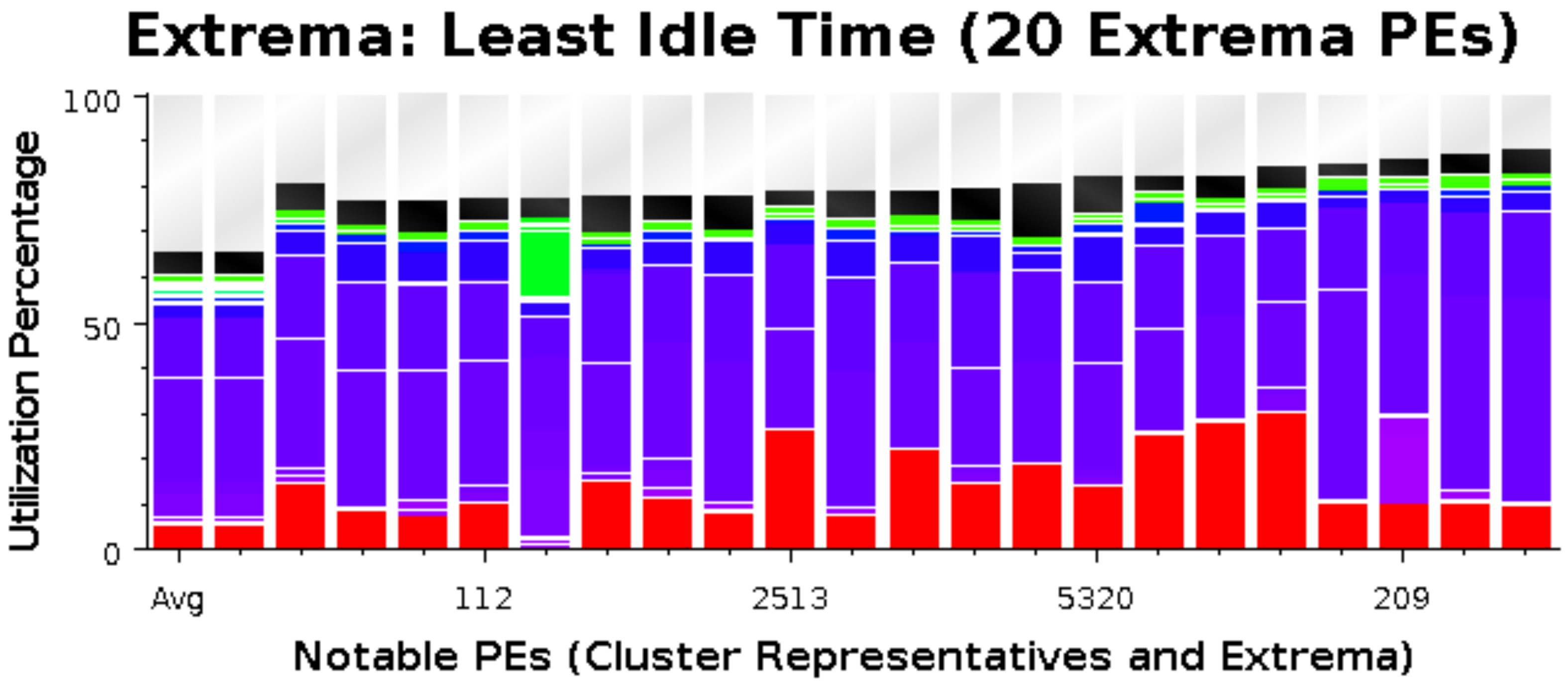
Using Projections

- Example Demonstration
  - Trying to identify the next performance obstacle for NAMD
    - Running on 8192 processors, with 1 million atom simulation
    - Jaguar Cray XK6
    - Test scenario: with PME every step

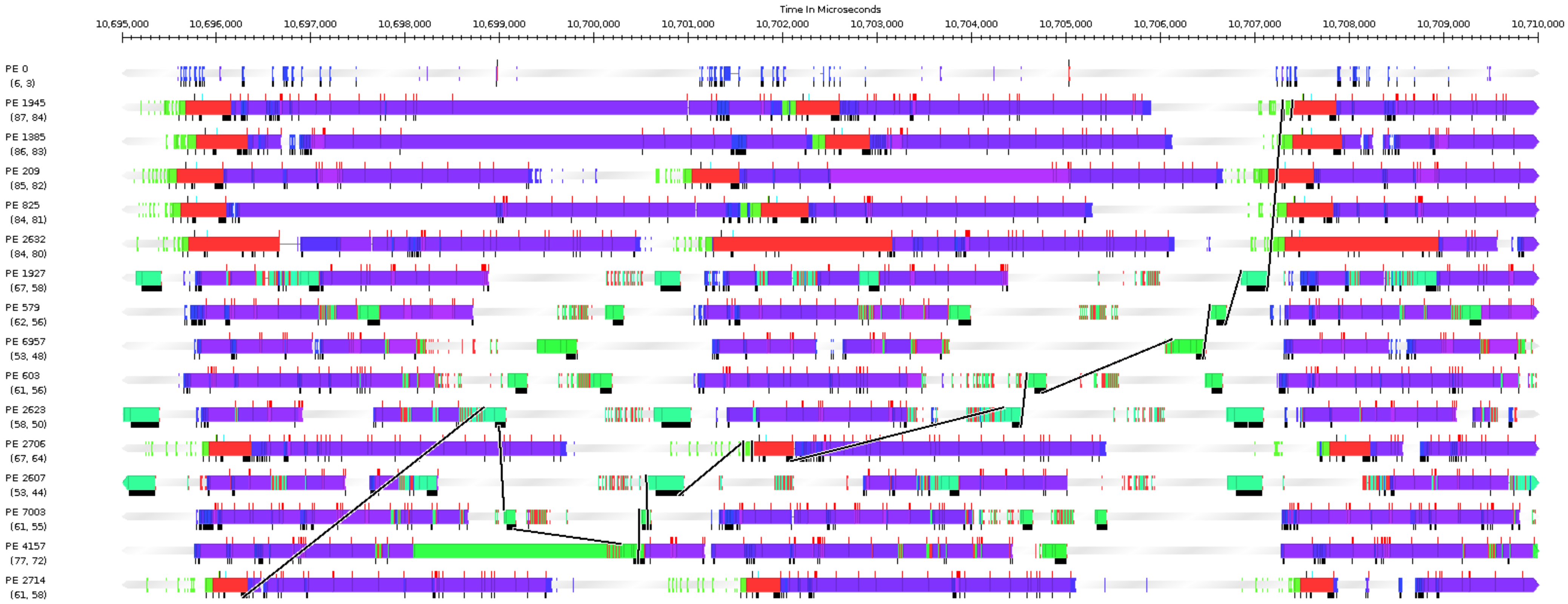
Time Profile



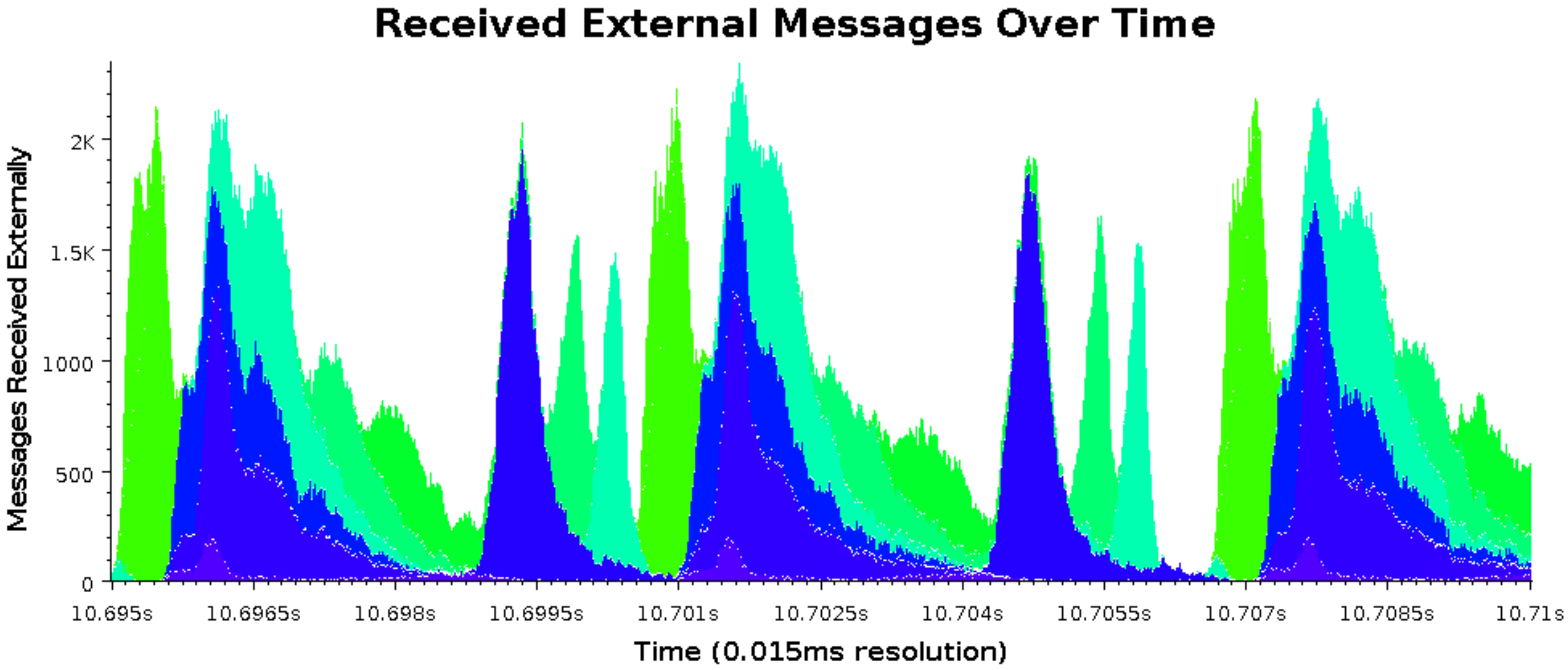
Extrema Tool for Least Idle Processors



Timeline with Message Back Tracing



Communication over Time for all Processors



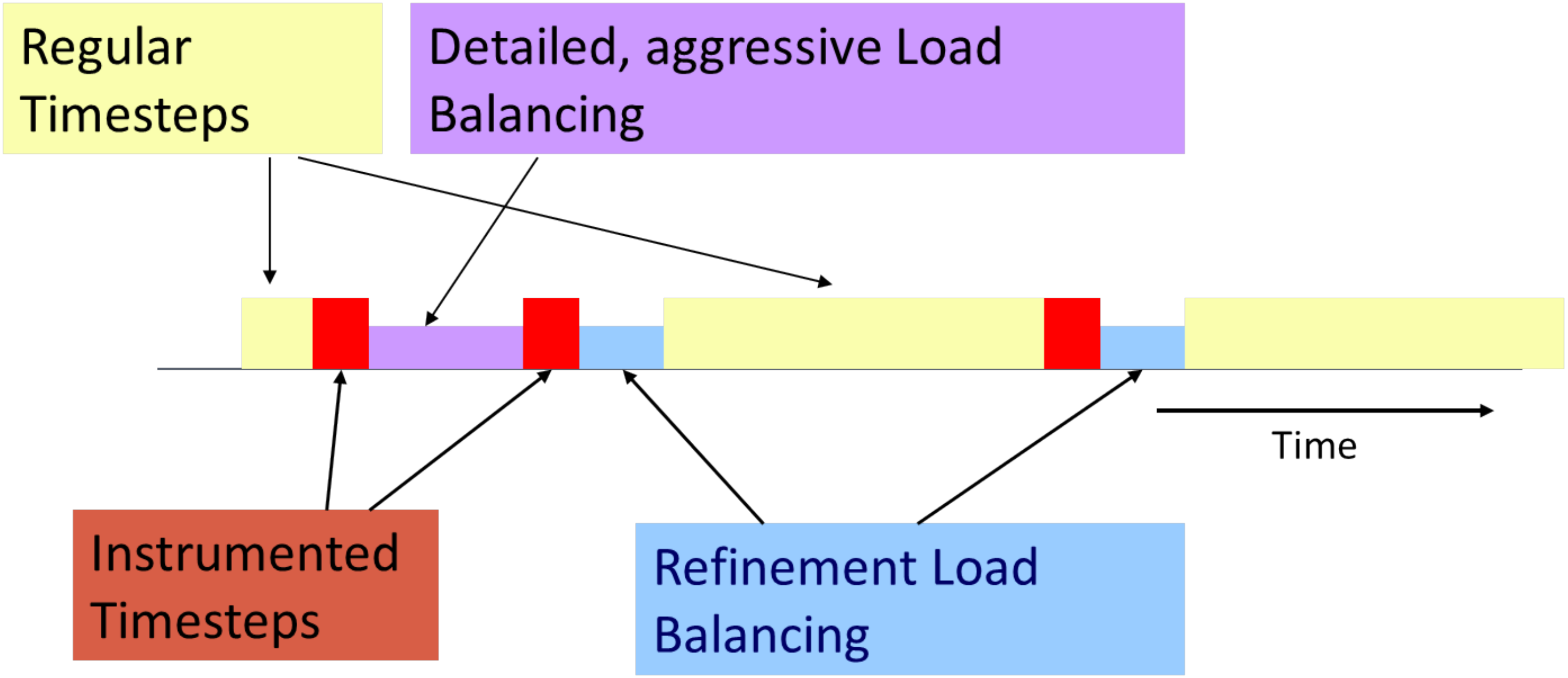
Outline

1) Introduction
   - Object Design
   - Execution Model
2) Hello World
3) Benefits of Charm++
4) Charm++ Basics
   - Object Collections
5) Overdecomposition
6) Migratability
   - Checkpointing and Resilience
7) Structured Dagger
8) Application Design
9) Performance Tuning
10) **Using Dynamic Load Balancing**
11) Interoperability
12) Debugging
13) Further Optimization

Measurement Based Load Balancing

- Principle of persistence: In many CSE applications, computational loads and communication patterns tend to persist, even in dynamic computations
- Therefore, recent past is a good predictor of near future
- Charm++ provides a suite of load-balancers
- Periodic measurement and migration of objects

Typical Load Balancing Steps



Regular Timesteps

Detailed, aggressive Load Balancing

Instrumented Timesteps

Refinement Load Balancing

Time

Code to Use Load Balancing

- Write PUP method to serialize the state of a chare
- Insert `if(myLBStep) AtSync();` and call at a natural barrier
- Implement `ResumeFromSync()` to resume execution
  - Typical `ResumeFromSync` contribute to a reduction

- link a LB module
  - `-module <strategy>`
  - RefineLB, NeighborLB, GreedyCommLB, others
  - EveryLB will include all load balancing strategies
- compile time option (specify default balancer)
  - `-balancer RefineLB`
- runtime option
  - `+balancer RefineLB`

Example: Stencil

```
while (!converged) {
  serial {
    int x = thisIndex.x, y = thisIndex.y, z = thisIndex.z;
    copyToBoundaries();
    thisProxy(wrapX(x - 1), y, z).updateGhosts(i, RIGHT, dimY, dimZ, right);
    /*  ...similar calls to send the 6 boundaries... */
    thisProxy(x, y, wrapZ(z + 1)).updateGhosts(i, FRONT, dimX, dimY, front);
  }
  for (remoteCount = 0; remoteCount < 6; remoteCount++) {
    when updateGhosts[i](int i, int d, int w, int h, double b[w*h])
      serial { updateBoundary(d, w, h, b); }
  }
  serial {
    int c = computeKernel() < DELTA;
    CkCallback cb(CkReductionTarget(Jacobi, checkConverged), thisProxy);
    if (i % 5 == 1) contribute(sizeof(int), &c, CkReduction::logical_and, cb);
  }

  if (++i % 5 == 0) {
    when checkConverged(bool result) serial {
      if (result) { mainProxy.done(); converged = true; }
    }
  }
```

Example: Stencil

```
while (!converged) {
  serial {
    int x = thisIndex.x, y = thisIndex.y, z = thisIndex.z;
    copyToBoundaries();
    thisProxy(wrapX(x - 1), y, z).updateGhosts(i, RIGHT, dimY, dimZ, right);
    /*  ...similar calls to send the 6 boundaries... */
    thisProxy(x, y, wrapZ(z + 1)).updateGhosts(i, FRONT, dimX, dimY, front);
  }
  for (remoteCount = 0; remoteCount < 6; remoteCount++) {
    when updateGhosts[i](int i, int d, int w, int h, double b[w*h])
      serial { updateBoundary(d, w, h, b); }
  }
  serial {
    int c = computeKernel() < DELTA;
    CkCallback cb(CkReductionTarget(Jacobi, checkConverged), thisProxy);
    if (i % 5 == 1) contribute(sizeof(int), &c, CkReduction::logical_and, cb);
  }
  if (i % lbPeriod == 0) { serial { AtSync(); } when ResumeFromSync() {} }
  if (++i % 5 == 0) {
    when checkConverged(bool result) serial {
      if (result) { mainProxy.done(); converged = true; }
    }
  }
```

Golden Rule of Load Balancing

Fallacy: objective of load balancing is to minimize variance in load across processors

Example:

- 50,000 tasks of equal size, 500 processors:
- A: All processors get 99, except last 5 gets 100 + 99 = 199
- OR, B: All processors have 101, except last 5 get 1

Identical variance, but situation A is much worse!

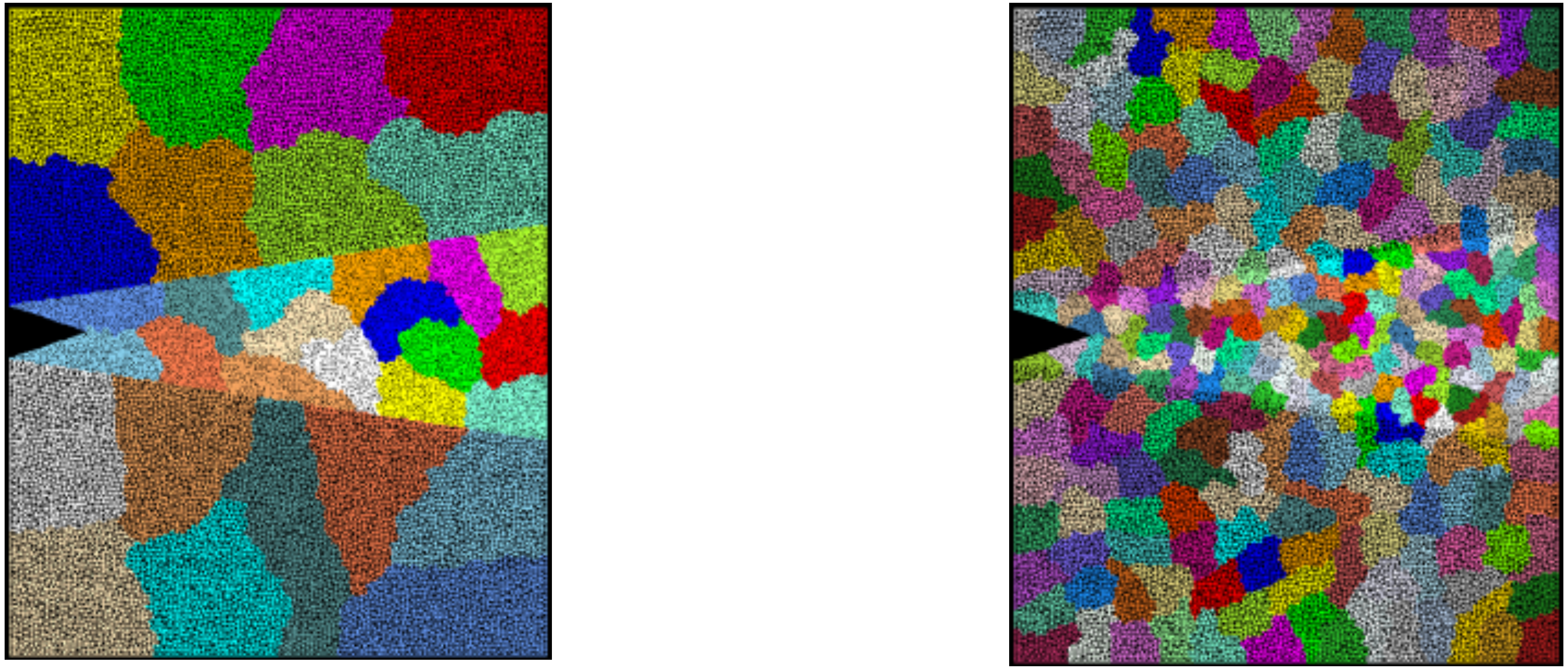
Golden Rule: It is ok if a few processors idle, but avoid having processors that are overloaded with work

Finish time = max_i(Time on processor *i)*

excepting data dependence and communication overhead issues

The speed of any group is the speed of slowest member of that group.

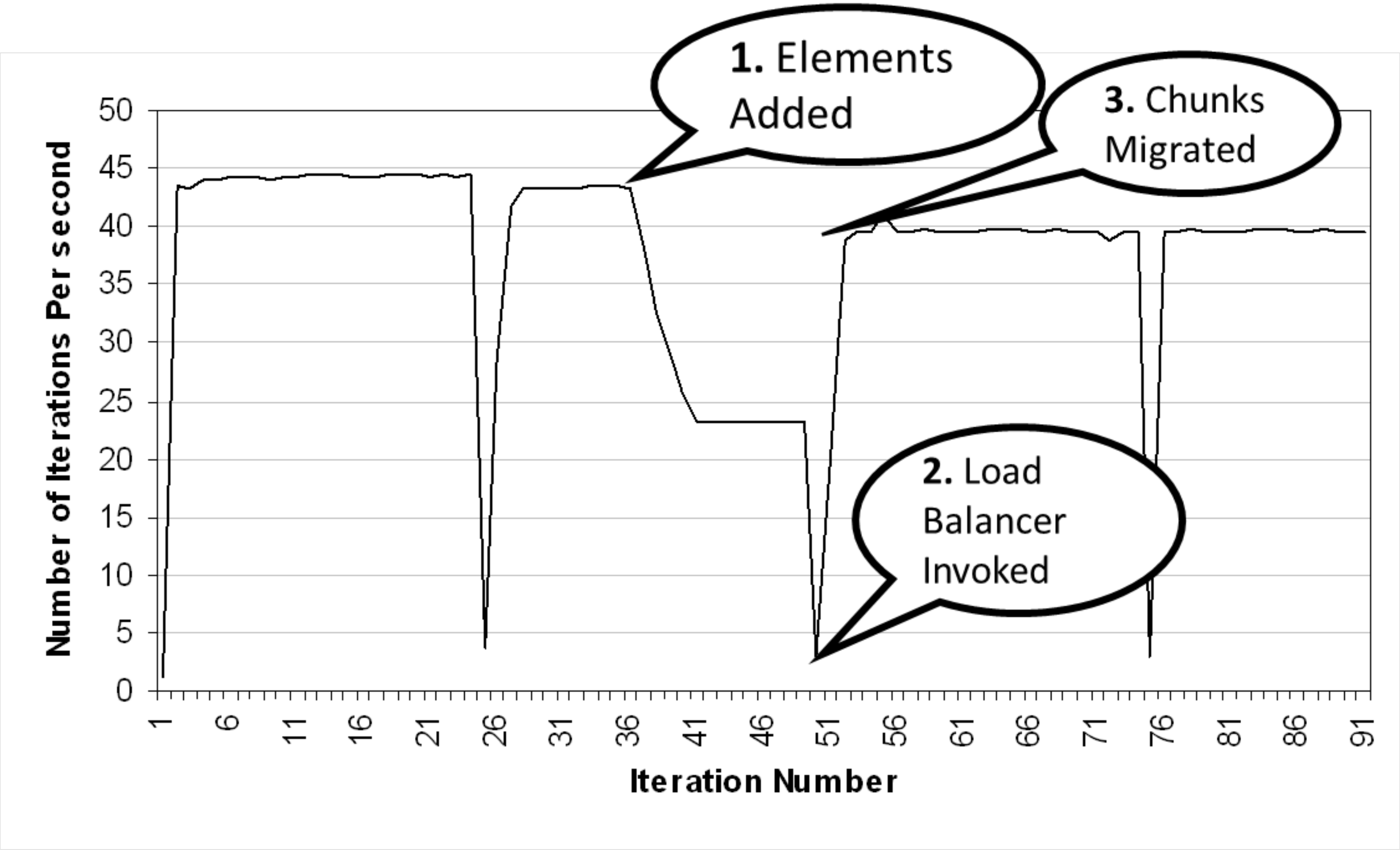
Crack Propagation



Decomposition into 16 chunks (left) and 128 chunks, 8 for each PE (right). The middle area contains cohesive elements. Both decompositions obtained using Metis. Pictures: S. Breitenfeld and P. Geubelle

As computation progresses, crack propagates, and new elements are added, leading to more complex computations in some chunks

Load Balancing Crack Propagation



1. Elements Added

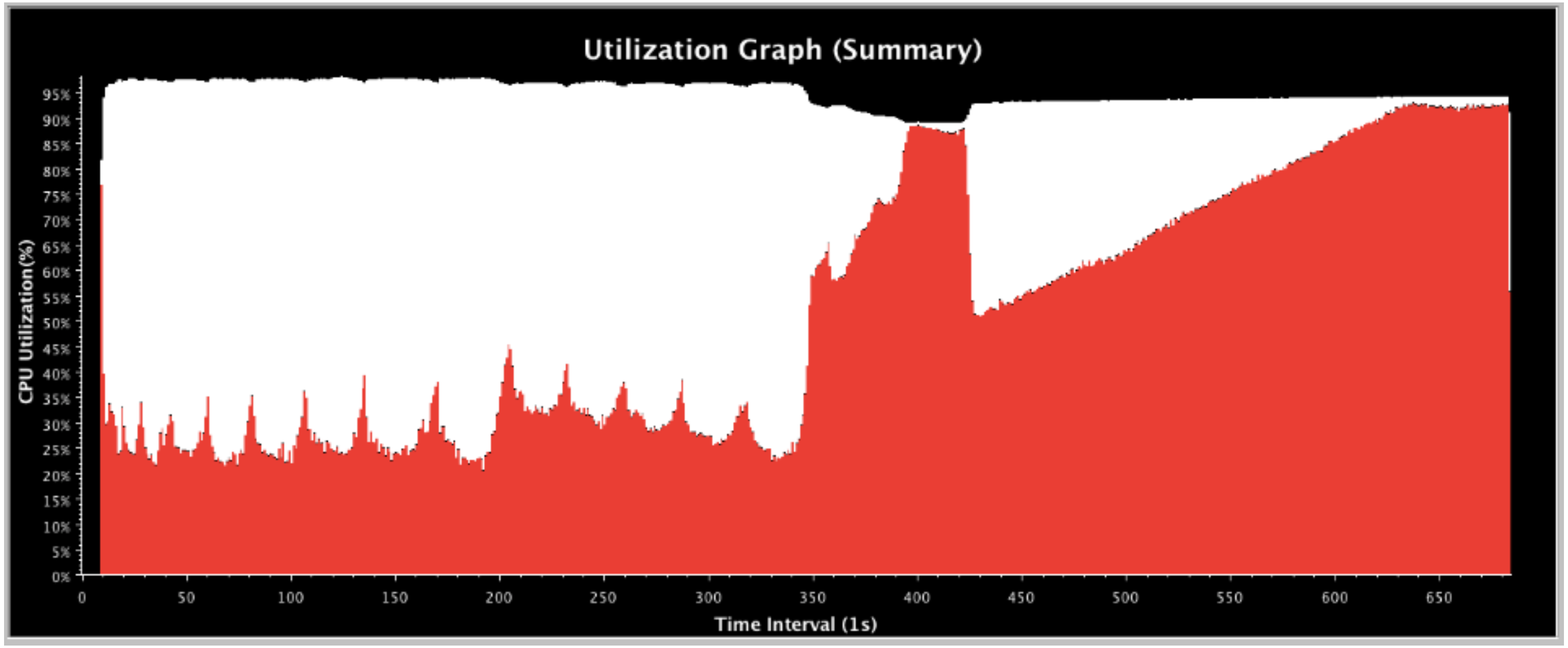
2. Load Balancer Invoked

3. Chunks Migrated

MetaBalancer - When and how to load balance?

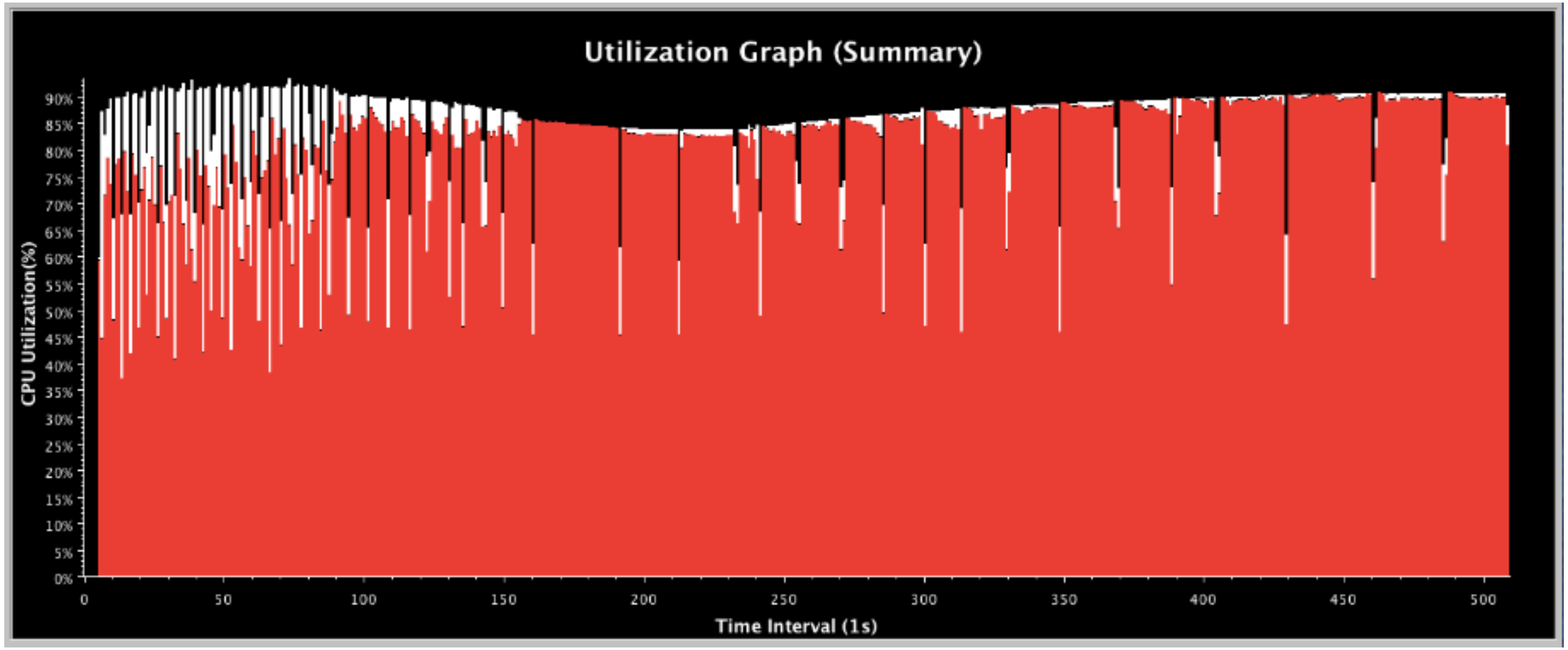
- Difficult to find the optimum load balancing period
  - Depends on the application characteristics
  - Depends on the machine the application is run on
- Monitors the application continuously and predicts behavior.
- Decides when to invoke which load balancer.
- Command line argument - +MetaLB

Fractography with No Load Balancing



- Large variation in processor utilization
- Low utilization leading to resource wastage

Metabalancer Utilization Graph for Fractography



Outline

1) Introduction
    - Object Design
    - Execution Model
2) Hello World
3) Benefits of Charm++
4) Charm++ Basics
    - Object Collections
5) Overdecomposition
6) Migratability
    - Checkpointing and Resilience
7) Structured Dagger
8) Application Design
9) Performance Tuning
10) Using Dynamic Load Balancing
11) **Interoperability**
12) Debugging
13) Further Optimization

Adaptive MPI

- MPI implemented on top of Charm++
- Each MPI process implemented as a user-level thread embedded in a chare
- Overdecompose to obtain communication-computation overlap between threads
- Supports migration, load balancing, fault tolerance and other Charm++ functionality
- Use cases - Rocstar, BRAMS, NPB, Lulesh, XPACC, etc
- Build with AMPI as target and compile using ampi* compilers

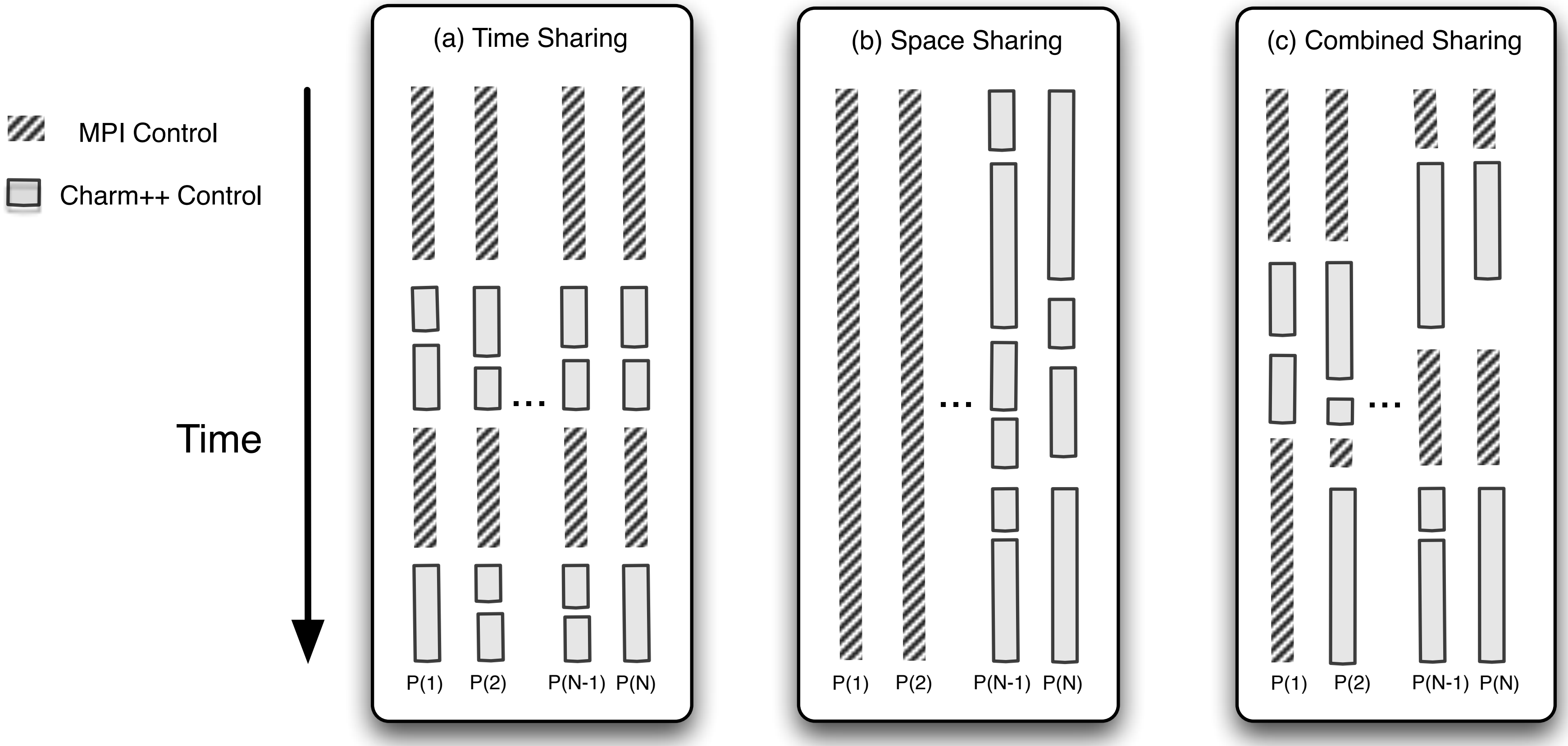
```
./build AMPI net-linux-x86_64 --with-production --enable-tracing -j8
```

```
ampiCC myAMPIpgm.C -o myAMPIpgm
```

Charm++ - MPI Interoperability

- Any library written in Charm++ can be called from MPI
- Charm++ resides in the same memory space as the MPI program
- Control transfer between MPI and Charm++ analogous to the control transfer between a program and an external library being used by the program

Interoperability Modes



Example Code Flow

```
MPI_Init(argc,argv); // initialize MPI
// Do MPI related work here
```

```
// Create comm to be used by Charm++
MPI_Comm_split(MPI_COMM_WORLD, myRank % 2, myRank, newComm);
CharmLibInit(newComm,argc,argv) // Initialize Charm++ over my communicator
```

```
if (myRank % 2)
  StartHello(); // invoke Charm++ library on one set
else
  // do MPI work on other set
```

```
kNeighbor(); // Invoke Charm++ library on both sets individually
CharmLibExit(); // Destroy Charm++
```

Enabling Interoperability

- Add interface functions that can be called from MPI, and triggers Charm++ RTS

```
void StartHello(int elems)
  if (CkMyPe() == 0) {
    CProxy MainHello mainhello =
      CProxy MainHello::ckNew(elems);
  }
  StartCharmScheduler();
}
```

- Use CkExit to return the control back to MPI
- Include *mpi-interoperate.h* in MPI and Charm++ code

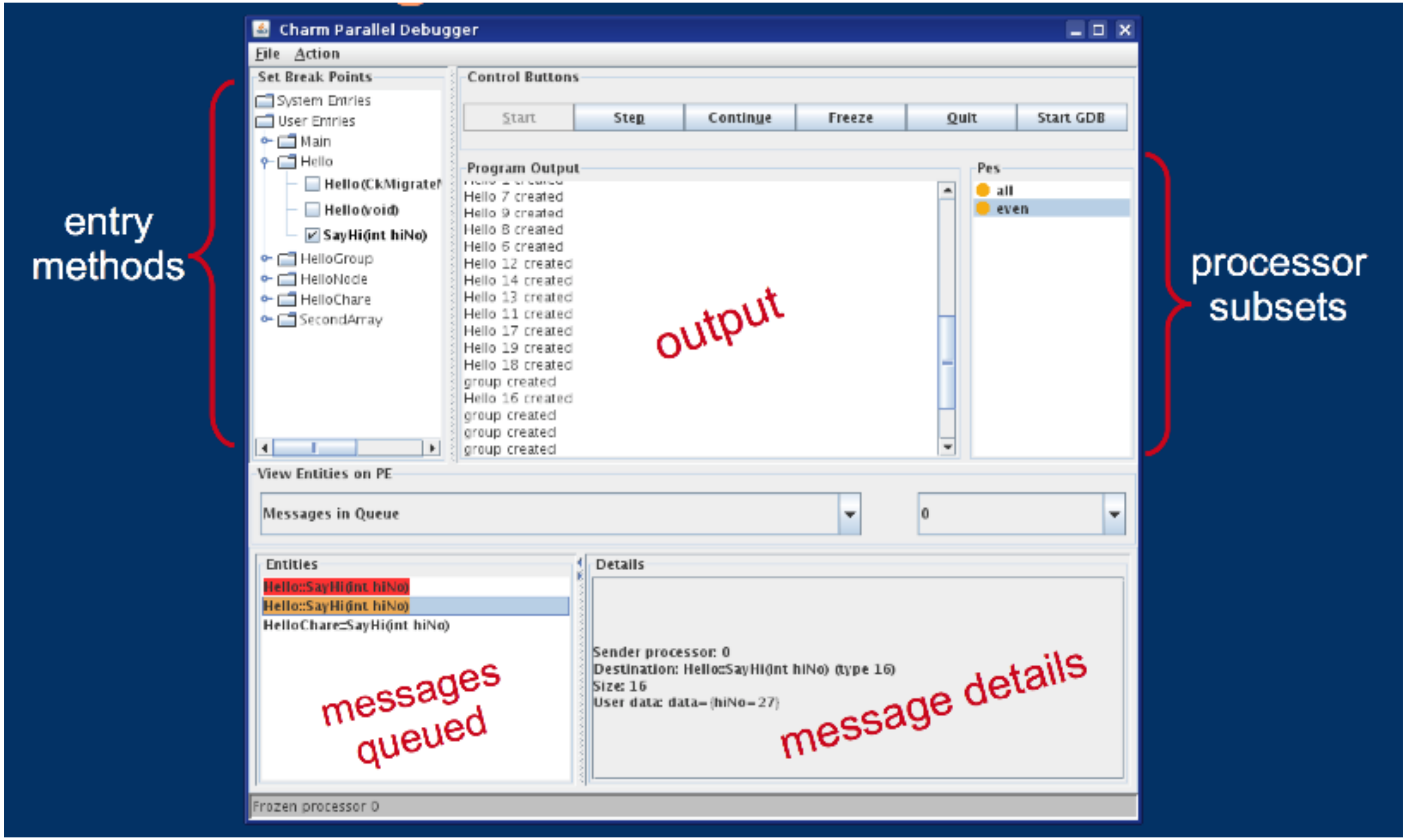
Outline

1) Introduction
    - Object Design
    - Execution Model
2) Hello World
3) Benefits of Charm++
4) Charm++ Basics
    - Object Collections
5) Overdecomposition
6) Migratability
    - Checkpointing and Resilience
7) Structured Dagger
8) Application Design
9) Performance Tuning
10) Using Dynamic Load Balancing
11) Interoperability
12) **Debugging**
13) **Further Optimization**

Debugging Parallel Applications

- It can be very difficult
- The typical “printf” strategy may be insufficient
- Using gdb
  - Very easy with Charm++!
  - Just run the application with the ++debug command line parameter and a gdb window for each PE will open through X (and can be forwarded)
    - Not very scalable
- We have developed a scalable tool for debugging Charm++ applications
  - It’s interactive
  - Allows you to change message order to find bugs!
  - “What-if” scenarios can be explored using provisional message delivery
  - Memory can be tracked to find memory leaks

CharmDebug



```
Hello 7 created
Hello 9 created
Hello 8 created
Hello 6 created
Hello 12 created
Hello 14 created
Hello 13 created
Hello 11 created
Hello 17 created
Hello 19 created
Hello 18 created
group created
Hello 16 created
group created
group created
group created
```

Sender processor: 0
Destination: Hello::SayHi(int hiNo) (type 16)
Size: 16
User data: data={hiNo=27}

entry methods

output

processor subsets

messages queued

message details

Additional features

- Quiescence detection
- Map objects for explicit initial placement of chare array elements
- Messages
- Groups
- Node-Groups
- Entry Method Attributes
- Threaded Methods, futures, sync methods…
- Sections
- Writing your own dynamic load balancers

Quiesence Detection

- What if determining global termination of an application is difficult?
- Mechanism to detect completion - Quiesence!
- From any chare, invoke

  CkStartQD(CkCallback(CkIndex_Main::finished(), mainProxy));
- Runs in background, waits for all outstanding messages to be consumed.
- Invokes the callback when quiesence is detected.

Controlling Placement: Map Objects

- In some applications, load patterns don’t change much as computation progresses
  - You, the programmer, may want to control which chare lives on which processors
  - This is also true when load may evolve over time, but you want to control initial placement of chares
- The feature in Charm++ for this purpose is **called Map Objects**

Messages

- Avoids extra copy
- Can be custom packed
- Reusable
- Useful for transfer of complex data structures
- It provides explicit control for the application over allocation, reuse, and scope
- Encapsulates variable size quantities
- Execution order of messages in the queue can be prioritized

Groups

- Like a chare-array with one chare per PE
- Encapsulate processor local data
- May access the local member as a regular C++ object
- In .ci file,

```
group ExampleGroup {
  // Interface specifications as for normal chares
  // For instance, the constructor ...
  entry ExampleGroup(parameters1);
  // ... and an entry method
  entry void someEntryMethod(parameters2);
};
```

- No difference in .h and .C file definitions

Node Groups

- A chare-array with one chare per node
  - In non-smp mode groups and node groups are same
- No difference in .h and .C
- Creation and usage same as others
- An entry method on a node-group member may be executed on any PE of the node
- Concurrent execution of two entry methods of a node-group member may happen
  - Use `[exclusive]` for entry methods which are unsuitable for reentrance safety

Customizing Entry Method Attributes

- `threaded` executed using separate thread
  - each thread has a stack, and may be suspended, for sync methods or futures
  - to set stacks size use +stacksize < size in bytes >
- `sync` - returns a value
- `inline` entry method invoked immediately if destination chare on same PE
  - blocking call
- `reductiontarget` target of an array reduction
  - Takes parameter marshaled arguments
- `notrace` not traced for projections

Customizing Entry Methods

- `expedited` entry method skips the priority-based message queue in Charm++ runtime
- `nokeep` message belongs to Charm
- `exclusive` mutual exclusion on execution of entry methods on node-groups
- `python` can be called from python scripts

Sections

- It is often convenient to define subcollections of elements within a chare array
  - Example: rows or columns of a 2D chare array
  - One may wish to perform collective operations on the subcollection (e.g. broadcast, reduction)
- Sections are the standard subcollection construct in Charm++

```
CProxySection_Hello proxy =
  CProxySection_Hello::ckNew(helloArrayID, 0, 9, 1, 0, 19, 2, 0, 29, 2);
```

Threaded methods

- Any method that calls a sync method must be able to suspend:
  - Needs to be declared as a `threaded` method
  - A threaded method of a chare C
    - Can suspend, without blocking the processor
    - Other chares can then be executed
    - Even other methods of chare C can be executed
- Low level thread operations for advanced users:
  - `CthThread CthSelf()`
  - `CthAwaken(CthThread t)`
  - `CthYield()`
  - `CthSuspend()`

`sync` methods

- Synchronous as opposed to asynchronous
- They return a value - always a `message` type
- Other than that, just like any other entry method:

In the interface file:

```
entry [sync] MsgData *f(double A[2*m], int m);
```

In the C++ file:

```
MsgData *f(double X[], int size) {
  // ...
  m = new MsgData(..);
  // ...
  return m;
}
```

Customized Load Balancers

- Statistics collected by Charm

```
struct LDStats { // load balancing database
  ProcStats *procs; // statistics of PEs
  int count;
  int n_objs;
  int n_migrateobjs;
  LDObjData *objData; // info regarding chares
  int n_comm;
  LDCommData *commData; // communication information
  int *from_proc, *to_proc; // residence of chares
}
```

- Use LDStats, ProcArray and ObjGraph for processor load and communication statistics
- *work* is the function invoked by Charm RTS to perform load balancing

Conclusion

- Charm++ is a production-ready parallel programming system
- Program mostly in C++
- Very powerful runtime system
  - Dynamic load balancing
  - Automatic overlap of computation and communication
  - Fault tolerance built in
- Topics we did not cover:
  - Many different types of load balancers
  - Threaded methods in detail
  - Futures
  - Accelerator support
  - Topology aware communication strategies
- More information on `http://charm.cs.illinois.edu/`