CHARE ARRAY SECTIONS

Chare Array Review

- Arbitrarily-sized collection of chares
- Every item in the collection has a unique index and proxy
- Can be indexed like an array or by an arbitrary object
- Can be sparse or dense
- Elements may be dynamically inserted and deleted
- Elements can be migrated

Motivation

- 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++
  - A section is a subset of a Chare Array

Section Creation

- Through explicit enumeration:

```
CkVec<CkArrayIndex3D> elems;    // add array indices
  for (int i=0; i<10; i++)
    for (int j=0; j<20; j+=2)
      for (int k=0; k<30; k+=2)
         elems.push_back(CkArrayIndex3D(i, j, k));

CProxySection_Hello proxy =
   CProxySection_Hello::ckNew(helloArrayID,
elems.getVec(), elems.size());
```

Section Creation

- Through index range specification:
- Specify array ID of the base chare array and the inidvidual chare array elements of the array participating in the section

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

Section Class Generation

- Section proxy classes are automatically generated for each chare and group defined in the .ci file
- Placed into decl.h and def.h files

Using Sections

```
CProxySection_Hello proxy;

// section broadcast
proxy.someEntry(...)

//sections are unranked, not allowed
proxy[0].someEntry(...)
```

- For example implementations, see
  - $(CHARM)/examples/charm++/arraysection
  - https://charmplusplus.org/miniApps/#leanmd

Spanning Trees

- CkMulticast implements tree algorithms for multicasts and reductions
  - Messages are routed over a *spanning tree* of the section elements
- Default branching factor is 2,
  - but a different number can be specified while creating a section
  - Add branching factor as a last integer parameter

CkMulticast Messages

- To use CkMulticast library, all multicast messages must inherit from CkMcastBaseMsg
  - CkMcastBaseMsg must be inherited from first
  - No parameter marshalling is allowed in entry methods used as targets of multicast

```
class HiMsg : public CkMcastBaseMsg, public CMessage_HiMsg
{
   public:
   int *data;
        ..
};
```

Reductions: setReductionClient

- An array element can be a member of multiple array sections
  - It is necessary to disambiguate which array section reduction it is participating in each time it contributes to one
- The reduction callback should be set at the time of creation.
  - This callback will be invoked after each reduction is complete

```
CkCallback *cb =  new CkCallback(
                        CkReductionTarget (Cell, reduceForces),
                        thisProxy(thisIndex.x,thisIndex.y,thisIndex.z)));

mySecProxy.setReductionClient(cb);
```

Reductions: CkSectionInfo

- A data structure called "CkSectionInfo" is created by CkMulticastMgr for each array section that the array element belongs to
  - During a section reduction, the array element must pass the CkSectionInfo as a parameter in the contribute()
  - This CkSectionInfo “cookie” can be retrieved from a previous message that was sent through CkMulticastMgr
    - Therefore, you can contribute into a reduction **only** following a broadcast to the same section.

Reductions with CkMulticast

```
CkSectionInfo cookie;

void SayHi(HiMsg *msg)
{   // this is a broadcast to SayHi using
    // the section we want to to contribute to
     //update section cookie every time
     CkGetSectionInfo(cookie, msg);
     int data = thisIndex;
     mcastGrp->contribute(sizeof(int),&data,

         CkReduction::sum_int, cookie);
}
```

Callbacks

- As with array reductions, a callback needs to be specified with each contribute
  - OR a default callback should be specified using setReductionClient

Example: Matrix Multiplication

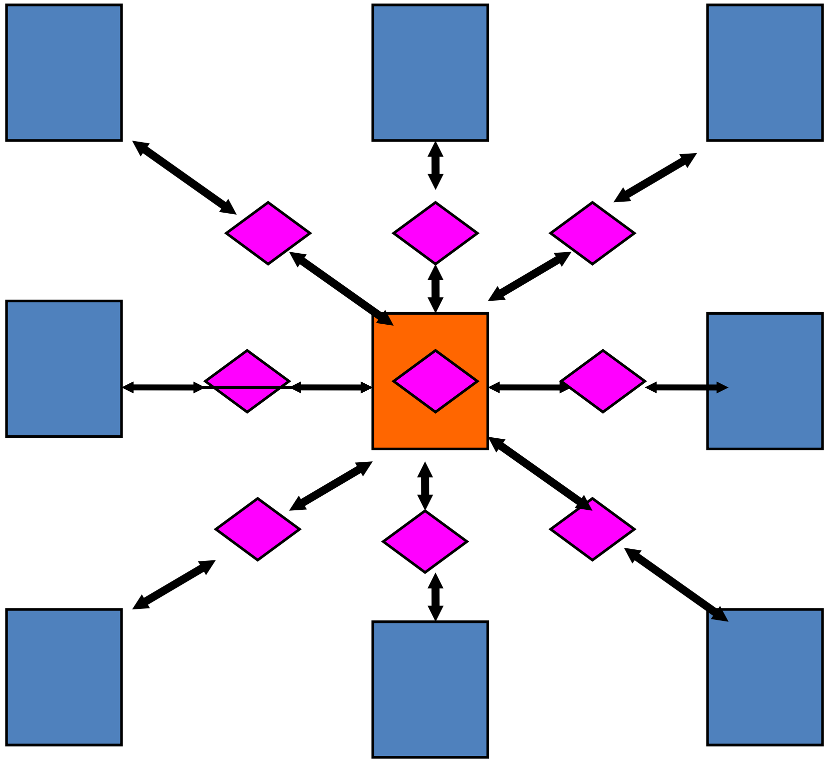
- Inputs: 2D chare arrays A, B of matrix blocks
- Output: 2D chare array C of matrix blocks
- Elements of A and B multicast their blocks to a section comprising a row or column of C
- Exercise: implement algorithm

Example: LeanMD

- Lennart-Jones Dynamics
- We have a 3D array of Cells
- And a 6D array of cell-pairs
  – (also called “compute” objects in the leanmd miniApp at https://charmplusplus.org/miniApps/#leanmd)

Object Based Parallelization for MD:

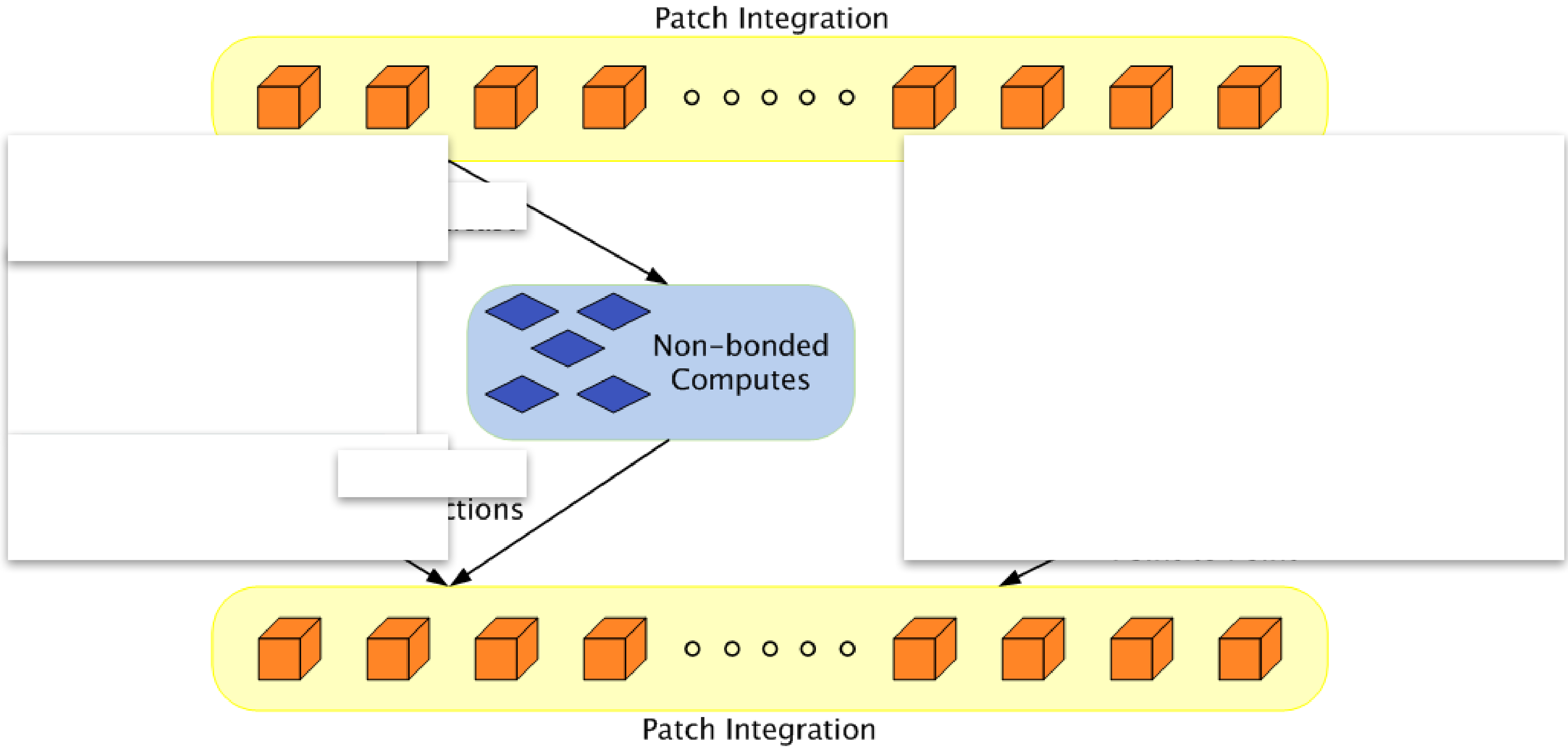
Force Decomposition + Spatial Decomposition



- 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
  - – 5x5x5 interactions
- –3-away interactions: 7x7x7

Parallelization Using Charm++

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



LJdynamics - Cell

```
 entry void run() {
        for(stepCount = 1; stepCount <= finalStepCount; stepCount+
+) {
            atomic { sendPositions(); }
            for(forceCount=0; forceCount < inbrs; forceCount++)
               when receiveForces[stepCount](int iter, vec3
                                                  forces[n], int n)
            atomic { addForces(forces); }
            atomic { updateProperties(); }
             if ((stepCount %  MIGRATE_STEPCOUNT) == 0) {
               atomic { sendParticles(); }
               when statements for receiving particles from
neighbors
            }
        }//end of for loop
        atomic {
            contribute(0, CkReduction::NULL,
              CkCallback(CkReductionTarget(Main,done),mainProxy));
        }
}//end of run
```

LJdynamics - Pair

```
entry void run() {
   for(stepCount = 1; stepCount <= finalStepCount; stepCount++) {
   if (thisIndex.x1==thisIndex.x2 &&
thisIndex.y1==thisIndex.y2 &&
       thisIndex.z1==thisIndex.z2)
             when calculateForces[stepCount](ParticleData *data)
                atomic { selfInteract(data); }
  else {
      when calculateForces[stepCount]   (ParticleData *data)
           atomic { bufferedData = data; }
      when calculateForces[stepCount](ParticleData *data)
           atomic { interact(data); }
        }
     // contribute/send forces to the cells involved
    }//enf of for loop
};//end of run
```

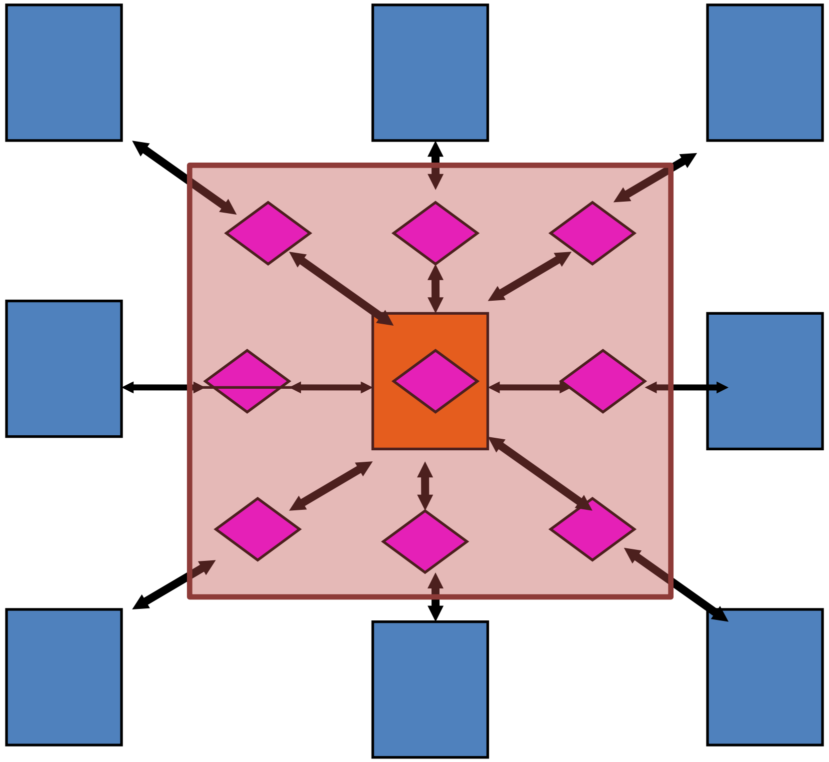
Using section in sendPositions

- Especially useful if you are using a 2-away formulation:
  - There are 5x5x5 = 125 pairs to which each cell must send its coordinates
    - Same data to everyone, so it is a Multicast
- This happens repeatedly, every iteration
  - At load balancing time the locations of pairs may change, but the *set* is the same
- So, each cell sets up its own section of pairs
- Each pair is a member of two [or one] sections

Expressing in Charm++

- Two chare arrays:
  - Cells: a 3D array of chares
  - Pairs: one object for each "neighboring" chare
- What is the dimensionality of *"pairs"*?
  - Idea 1: make it a 3D array.. Does it work?
  - Idea 2: Make it a 1D array,
    - Explicitly assign indices to chares: the pair object between Cells[2,3,4] and Cells[2,3,5] is Pairs[someIndex].
  - Idea 3: Make it a 6D array
    - Pairs[2,3,4,2,3,5]
    - But: (a) it is sparse and
    - (b) symmetry? Do we also have Pairs[2,3,5,2,3,4]
    - Use only one of them.. (say "smaller" in dictionary order)

Object Based Parallelization for MD (with sections)



- All pairs in the box constitute a section for the central proc:
  - Central chare uses CkMulticast for optimized broadcasts to this section
  - Without CkMulticast, it would have been point-to-point sends for all
  - Reductions are used across the section to aggregate results for force calculation