Co-Design Via Proxy Applications: MiniMD in Chapel

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SIAM PP14, MS78: Co-Design w/ Proxy Apps and Prog. Abstractions
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What is Chapel?

- **An emerging parallel programming language**
  - Design and development led by Cray Inc.
    - in collaboration with academia, labs, industry
  - Initiated under the DARPA HPCS program

- **A work-in-progress**

- **Chapel's overall goal: Improve programmer productivity**
  - Improve the programmability of parallel computers
  - Match or beat the performance of current programming models
  - Support better portability than current programming models
  - Improve the robustness of parallel codes

Chapel's Implementation

- **Being developed as open source at SourceForge**
- **Licensed as BSD software**
- **A Community Effort**
  - version 1.8 saw 19 developers from 8 organizations and 5 countries
- **Target Architectures:**
  - multicore desktops and laptops
  - commodity clusters and the cloud
  - HPC systems from Cray and other vendors
  - *in-progress:* exascale-era architectures

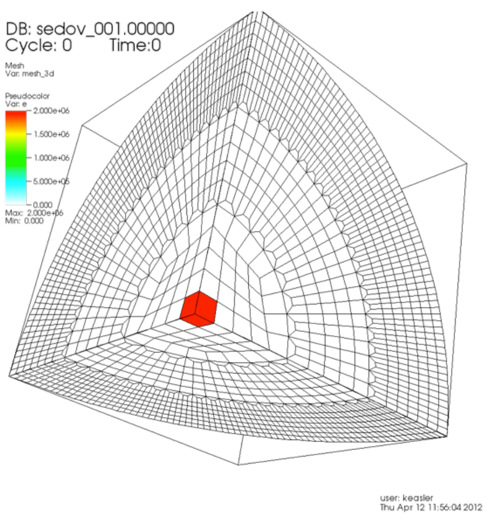
Chapel and Proxy Applications

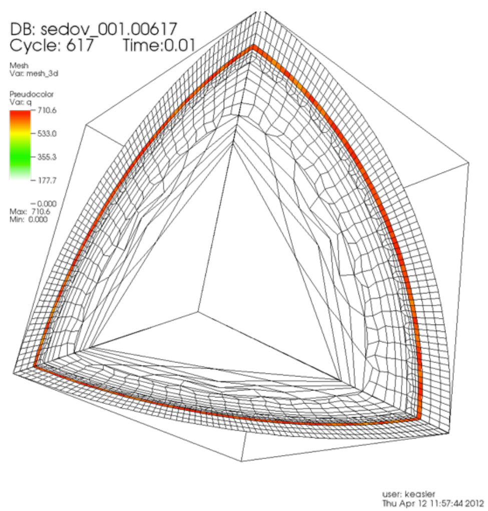
Overall, we like proxy applications a lot

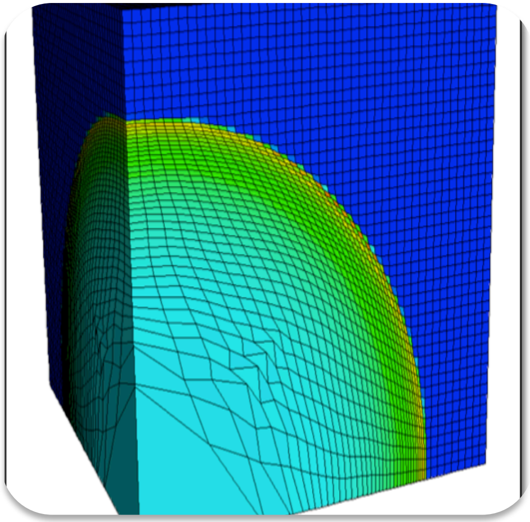
- A chance to compare Chapel productivity/performance to status quo
- Users are more invested in them than traditional benchmarks
  - less likely to say “well, that’s nice, but it says nothing about my work”
  - more likely to wrestle through various design decisions with us
- Form a good basis for discussion between teams with distinct skill sets
  - codesign!
- Larger and more substantive than benchmarks
  - yet, without being overwhelming
- Documentation & reference versions have generally been pretty good

Chapel's First DOE Proxy Application: LULESH

Goal: Solve one octant of the spherical Sedov problem (blast wave) using Lagrangian hydrodynamics for a single material







pictures courtesy of Rob Neely, Bert Still, Jeff Keasler, LLNL

Chapel's First DOE Proxy Application: LULESH

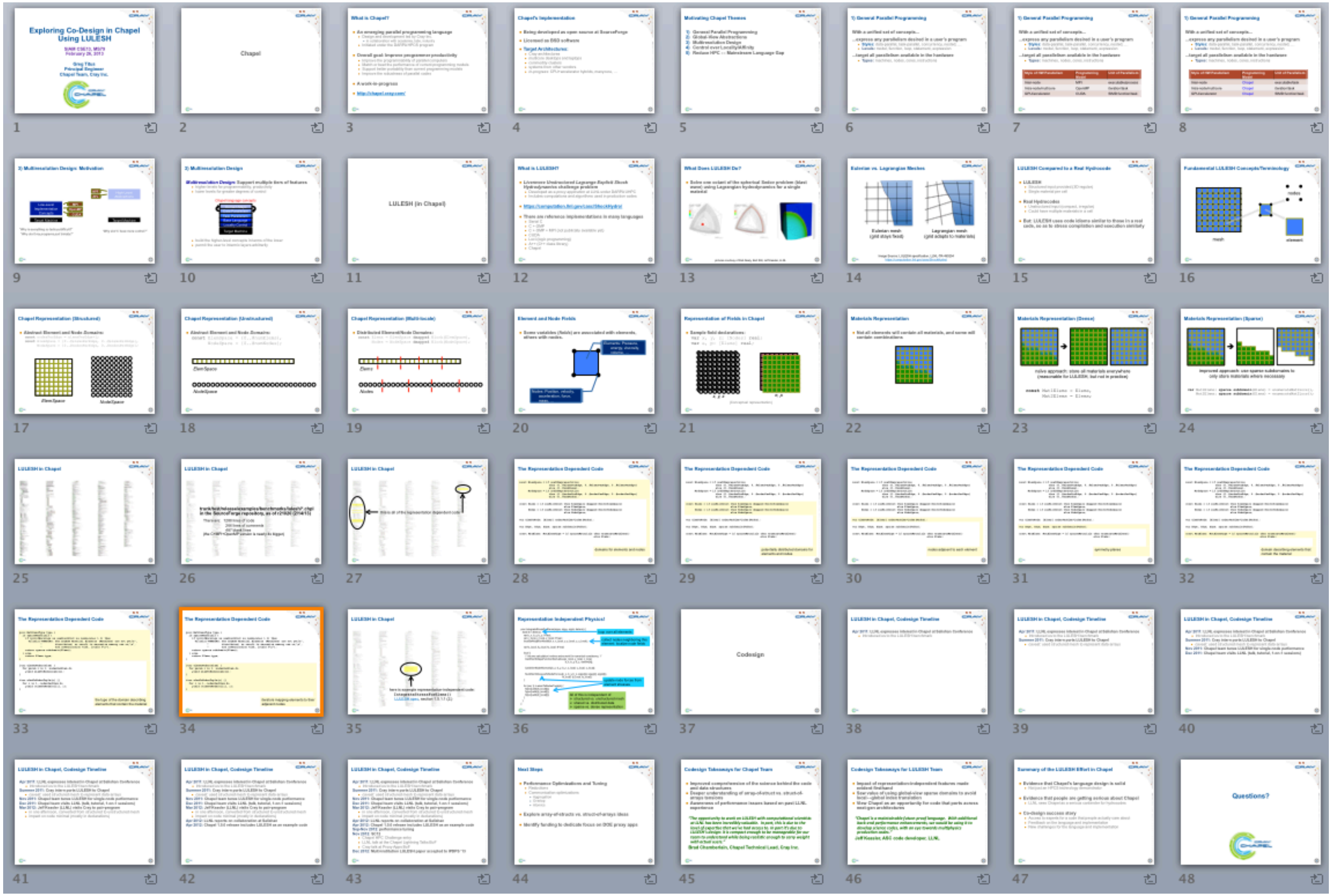
History:

- Idea came about as a result of a Salishan discussion
- Summer intern did a naïve initial port to Chapel in a few weeks
- Chapel team made additional improvements over time
  - Included a productive pair-programming session with LLNL expert
- Now included as an example code in Chapel releases

Remaining work:

- Additional performance tuning work remains
  - Several general Chapel issues
  - Some application-specific (e.g., optimize data distribution for locality)
- Also, need to catch up with LULESH 2.0

SIAM CSE13: Greg Titus Spoke on LULESH



LULESH in Chapel

LULESH in Chapel

1288 lines of source code

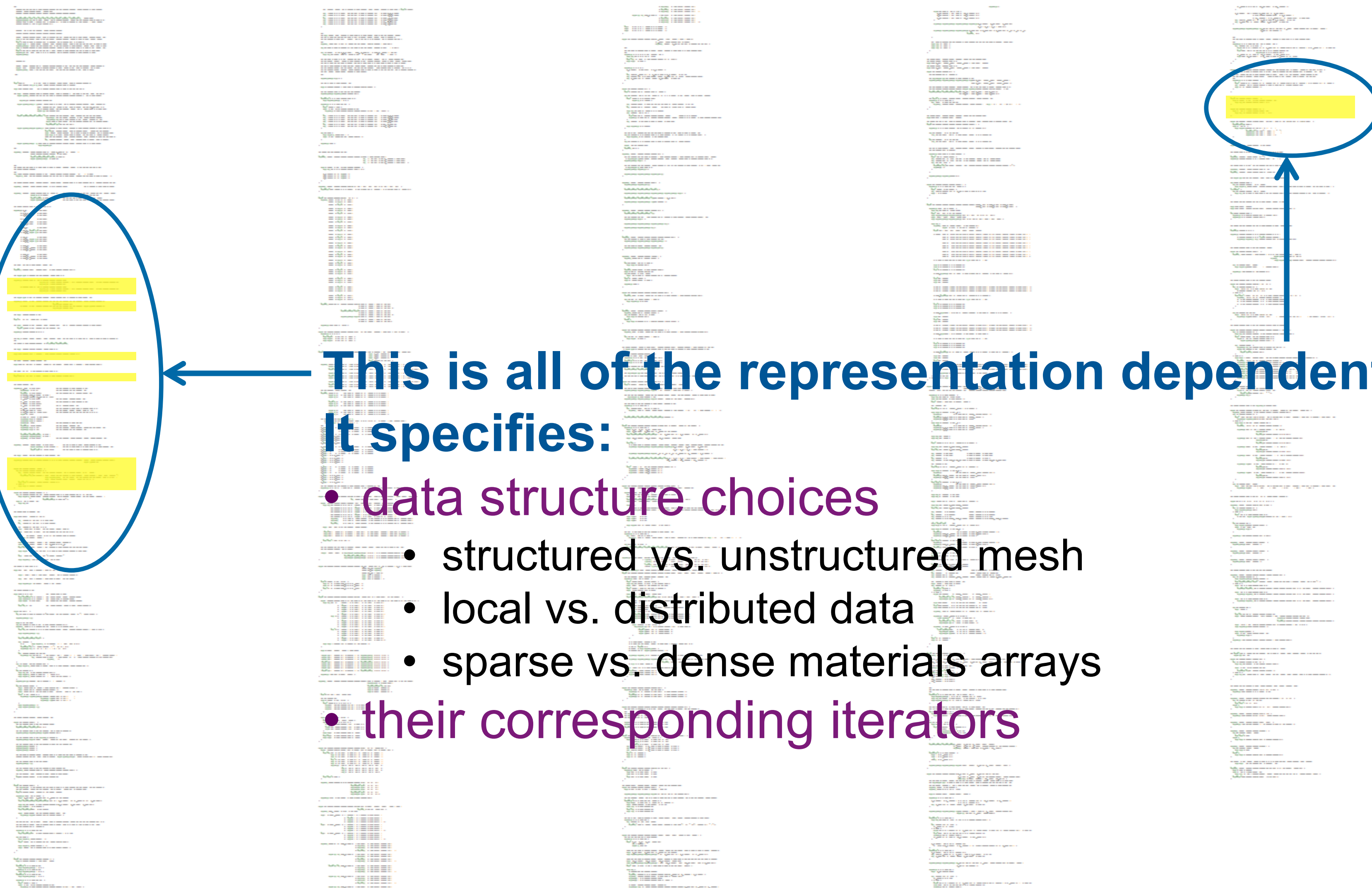
plus 266 lines of comments

487 blank lines

(the corresponding C+MPI+OpenMP version is nearly 4x bigger)

This is trunk/test/release/examples/benchmarks/lulesh/*.chpl in the SourceForge repository, as of r22745 (2/16/14).

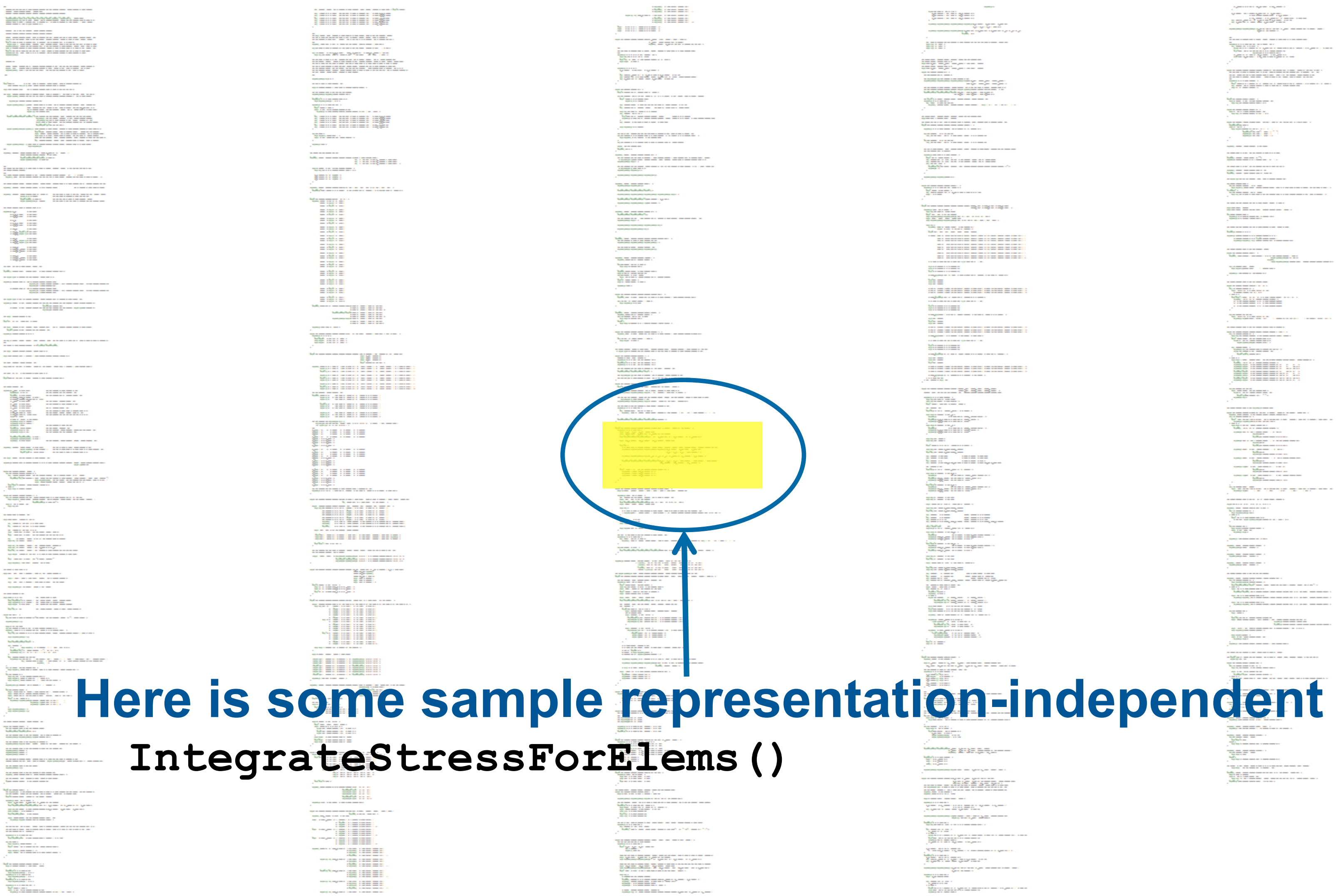
LULESH in Chapel



This is all of the representation dependent code.
It specifies:

- data structure choices
  - structured vs. unstructured mesh
  - local vs. distributed data
  - sparse vs. dense materials arrays
- their corresponding iterators

LULESH in Chapel



Here is some sample representation-independent code

`IntegrateStressForElems()`

Representation-Independent Physics

```
proc IntegrateStressForElems(sigxx, sigyy, sigzz, determ) {
  forall k in Elems {
    var b_x, b_y, b_z: 8*real;
    var x_local, y_local, z_local: 8*real;
    localizeNeighborNodes(k, x, x_local, y, y_local, z, z_local);

    var fx_local, fy_local, fz_local: 8*real;

    local {
      /* Volume calculation involves extra work for numerical consistency. */
      CalcElemShapeFunctionDerivatives(x_local, y_local, z_local,
                                       b_x, b_y, b_z, determ[k]);

      CalcElemNodeNormals(b_x, b_y, b_z, x_local, y_local, z_local);

      SumElemStressesToNodeForces(b_x, b_y, b_z, sigxx[k], sigyy[k], sigzz[k],
                                  fx_local, fy_local, fz_local);
    }

    for (noi, t) in elemToNodesTuple(k) {
      fx[noi].add(fx_local[t]);
      fy[noi].add(fy_local[t]);
      fz[noi].add(fz_local[t]);
    }
  }
}
```

parallel loop over elements

collect nodes neighboring this element; localize node fields

update node forces from element stresses

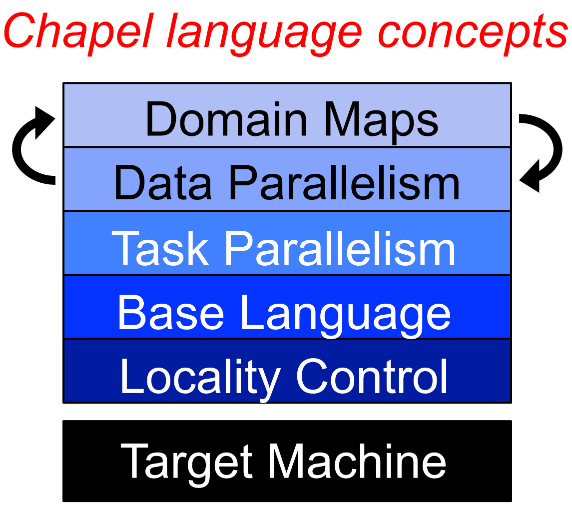
All of this is independent of:

- structured vs. unstructured mesh
- shared vs. distributed data
- sparse vs. dense representation

Multiresolution Design

Multiresolution Design: **Support multiple tiers of features**

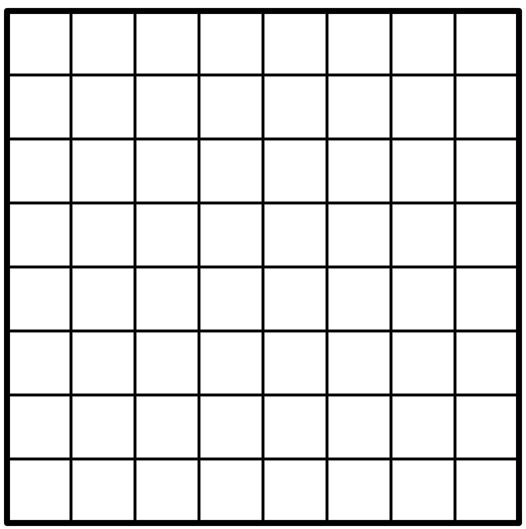
- higher levels for programmability, productivity
- lower levels for greater degrees of control



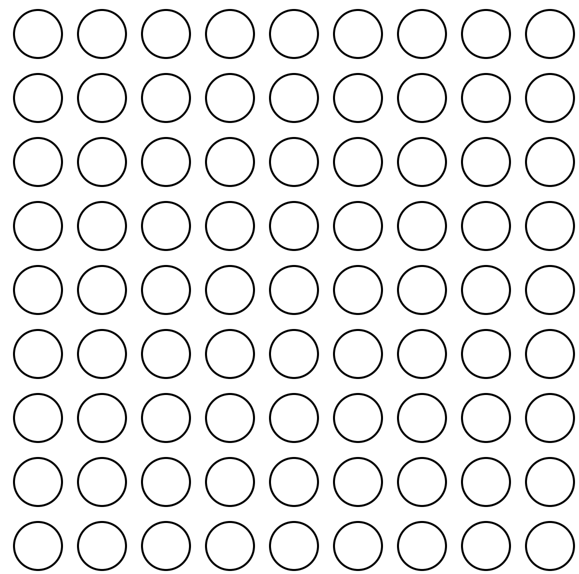
- build the higher-level concepts in terms of the lower
- permit the user to intermix layers arbitrarily

Data Parallelism in LULESH (Structured)

```
const Elems = {0..#elemsPerEdge, 0..#elemsPerEdge},
      Nodes = {0..#nodesPerEdge, 0..#nodesPerEdge};

var determ: [Elems] real;

forall k in Elems { …determ[k]… }
```



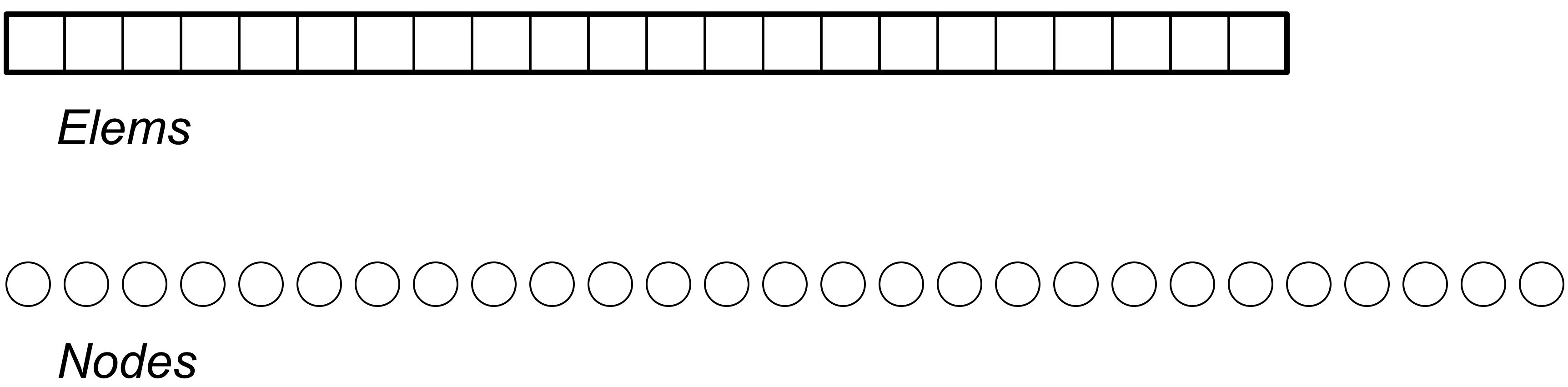
Elems



Nodes

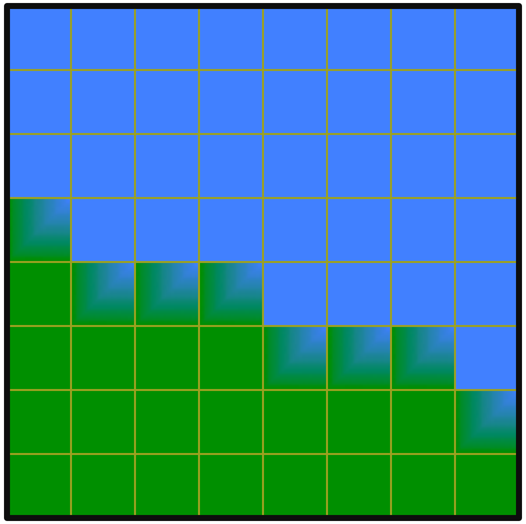
Data Parallelism in LULESH (Unstructured)

```
const Elems = {0..#numElems},
      Nodes = {0..#numNodes};

var determ: [Elems] real;

forall k in Elems { …determ[k]… }
```

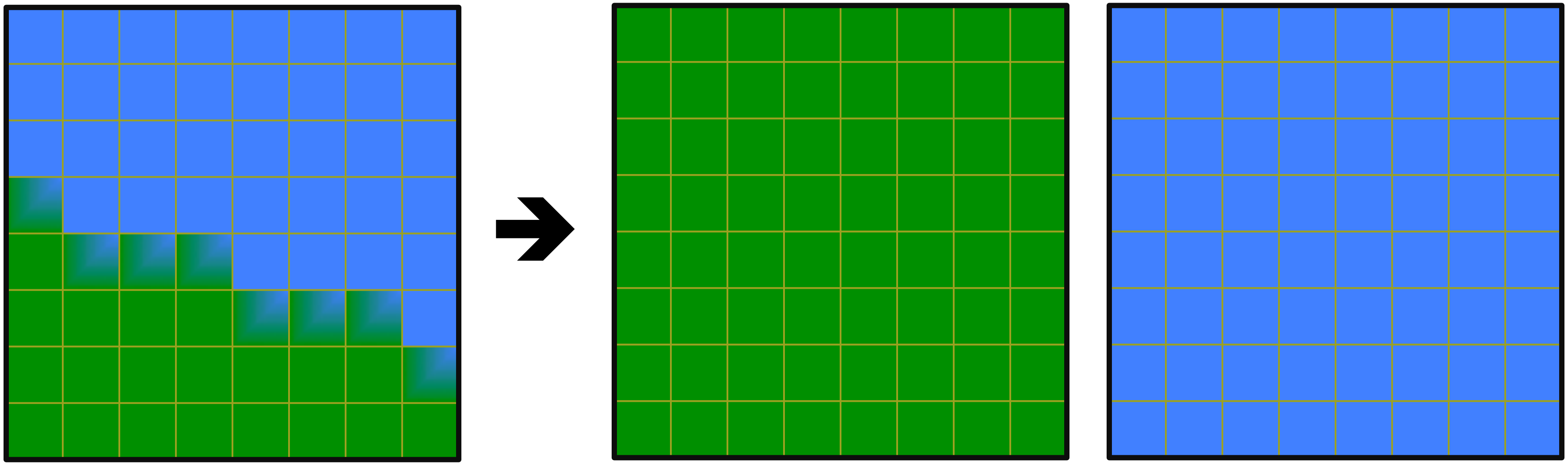


Materials Representation

- Not all elements will contain all materials, and some will contain combinations



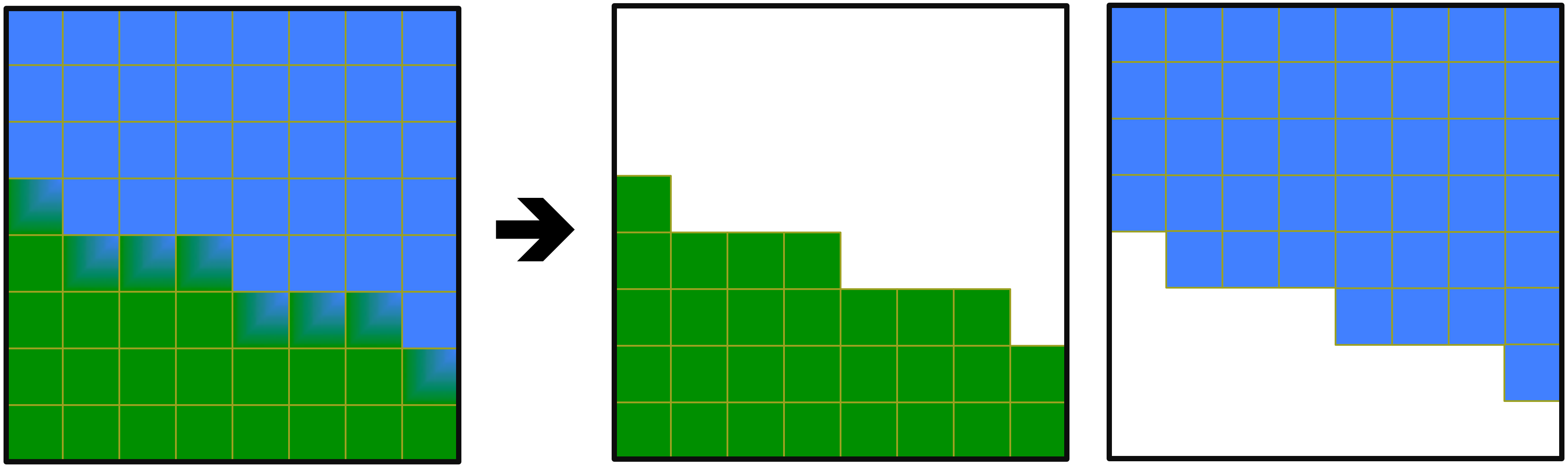
Materials Representation (Dense)



naïve approach: store all materials everywhere
(reasonable for LULESH 1.0, but not in practice)

```
const Mat1Elems = Elems,
      Mat2Elems = Elems;
```

Materials Representation (Sparse)



improved approach: use sparse subdomains to only store materials where necessary

```
var Mat1Elems: sparse subdomain(Elems) = enumerateMat1Locs(),
    Mat2Elems: sparse subdomain(Elems) = enumerateMat2Locs();
```

Data Parallel Iterators: Multiresolution in Action

Q: How are domains and arrays implemented?

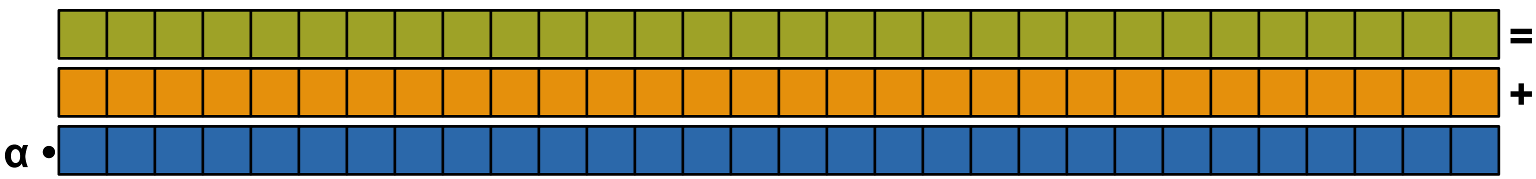
(distributed or local? distributed how? stored in memory how?)

```
const Elems = {0..#numElems},
      Nodes = {0..#numNodes};

var determ: [Elems] real;
```

A: Via domain maps…

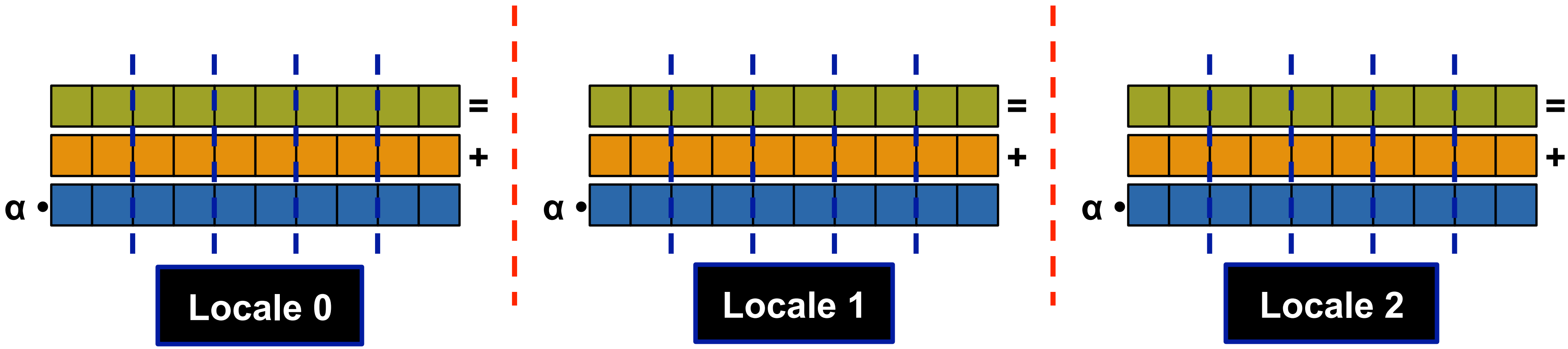
Domain Maps: Concept

Domain maps are "recipes" that instruct the compiler how to map the global view of a computation…



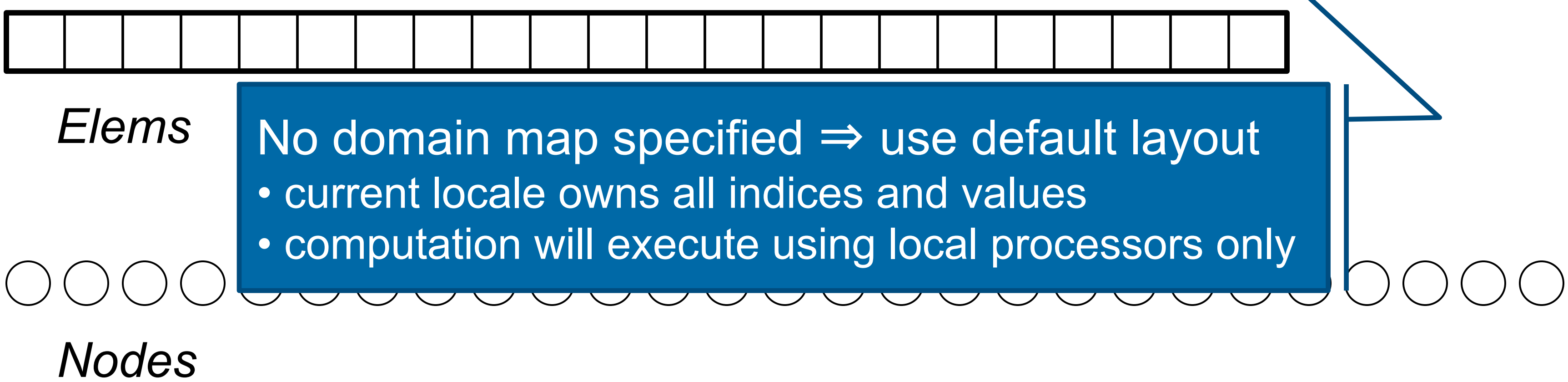

```
A = B + alpha * C;
```

…to the target locales' memory and processors:



LULESH Data Structures (local)

```
const Elems = {0..#numElems},
      Nodes = {0..#numNodes};

var determ: [Elems] real;

forall k in Elems { … }
```

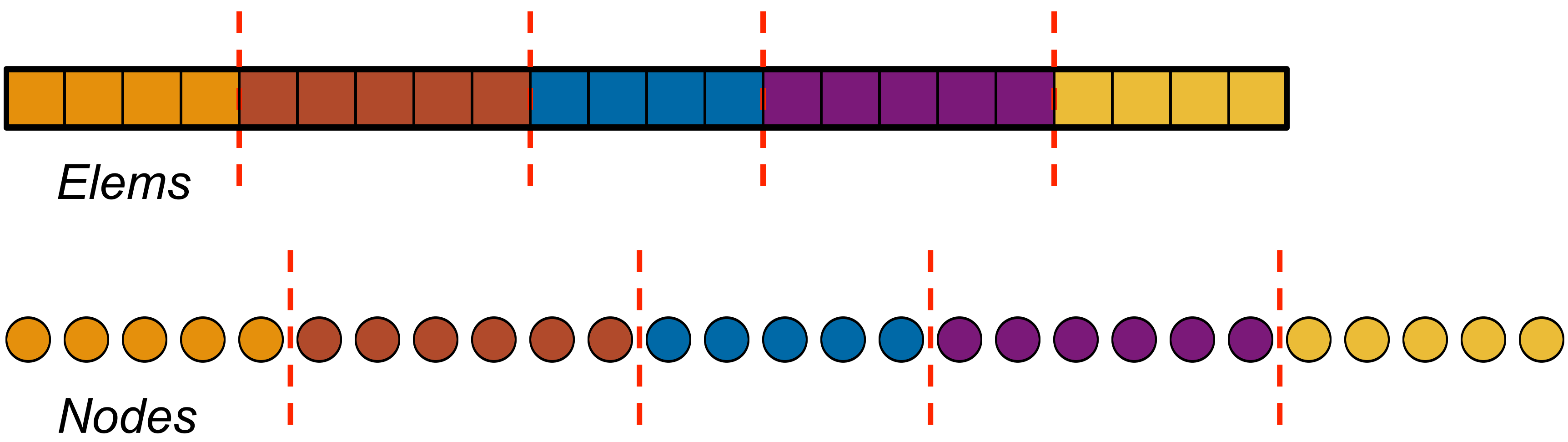


No domain map specified ⇒ use default layout

- current locale owns all indices and values
- computation will execute using local processors only

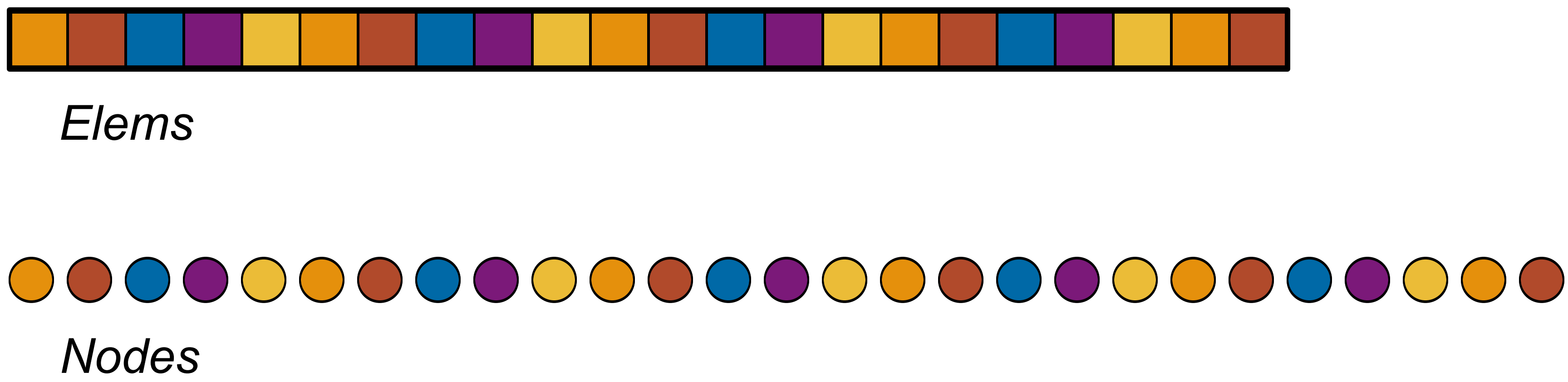
LULESH Data Structures (distributed, block)

```
const Elems = {0..#numElems} dmapped Block(…),
      Nodes = {0..#numNodes} dmapped Block(…);

var determ: [Elems] real;

forall k in Elems { … }
```



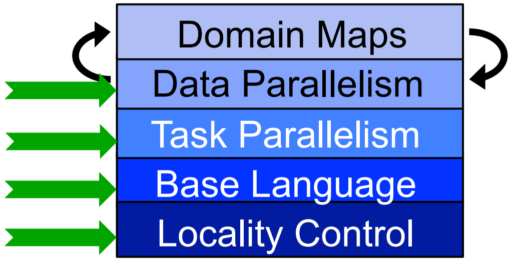
LULESH Data Structures (distributed, cyclic)

```
const Elems = {0..#numElems} dmapped Cyclic(…),
      Nodes = {0..#numNodes} dmapped Cyclic(…);

var determ: [Elems] real;

forall k in Elems { … }
```



Chapel's Domain Map Philosophy

1. **Chapel provides a library of standard domain maps**
   - to support common array implementations effortlessly
2. **Advanced users can write their own domain maps in Chapel**
   - to cope with shortcomings in our standard library



3. **Chapel's standard domain maps are written using the same end-user framework**
   - to avoid a performance cliff between "built-in" and user-defined cases

Support compile-time reconfiguration

```
const ElemSpace = if use3DRepresentation
                    then {0..#elemsPerEdge, 0..#elemsPerEdge, 0..#elemsPerEdge}
                    else {0..#numElems},
      NodeSpace = if use3DRepresentation
                    then {0..#nodesPerEdge, 0..#nodesPerEdge, 0..#nodesPerEdge}
                    else {0..#numNodes};


const Elems = if useBlockDist then ElemSpace dmapped Block(ElemSpace)
                              else ElemSpace,
      Nodes = if useBlockDist then NodeSpace dmapped Block(NodeSpace)
                              else NodeSpace;


const MatElems: MatElemsType = if useSparseMaterials then enumerateMatElems()
                                                     else Elems;


proc MatElemsType type {
  if useSparseMaterials then
    return sparse subdomain(Elems);
  else
    return Elems.type;
}
```

MiniMD Study

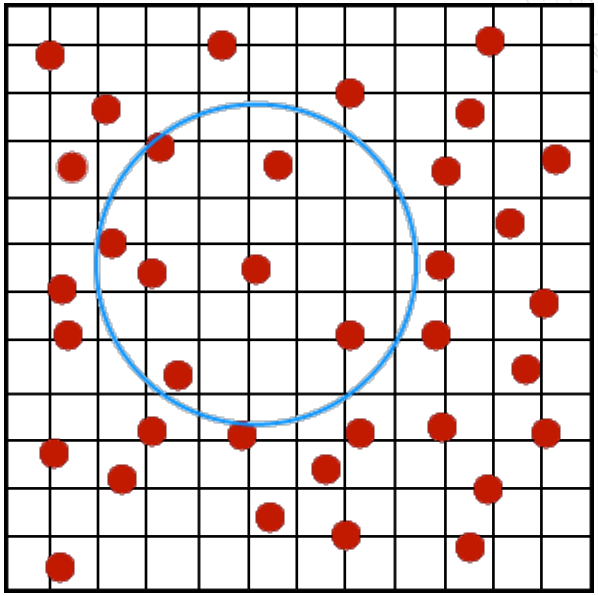
What is MiniMD?

- **"Mini Molecular Dynamics"**
  - A proxy application from Sandia's Mantevo group
  - Representative of key idioms from real applications
  - ~5000 lines of C++/MPI
    - ~2000 lines in Chapel

- **Molecular Dynamics?**
  - Computing physical properties like energy, pressure, and temperature for a simulated space containing moving atoms

- **Interesting in that it's the first stencil code we've had a chance to focus on in Chapel**

Store atoms in spatial bins



- **Given a bunch of atoms…**

```
record atom {
  var vel, force, position : 3*real;
}
```

- **Sort atoms into bins based on spatial position**

```
const binSpace = {1..12, 1..12};
var perBinSpace = {1..8};
var bins: [binSpace] [perBinSpace] atom;
```

- **Use cutoff to restrict number of atoms to compute against**
  - Reduces complexity from $O(n^2)$ to $\sim O(n)$

Compute forces between atoms

```
forall bin in bins {
  for atom in bin {
    for neighbor in atom.neighbors {
      if distance(atom, neighbor) < cutoff {
        updateForces(atom, neighbor);
      }
    }
  }
}
```

Now let's go to distributed memory…

Distributing Bins in C++/MPI

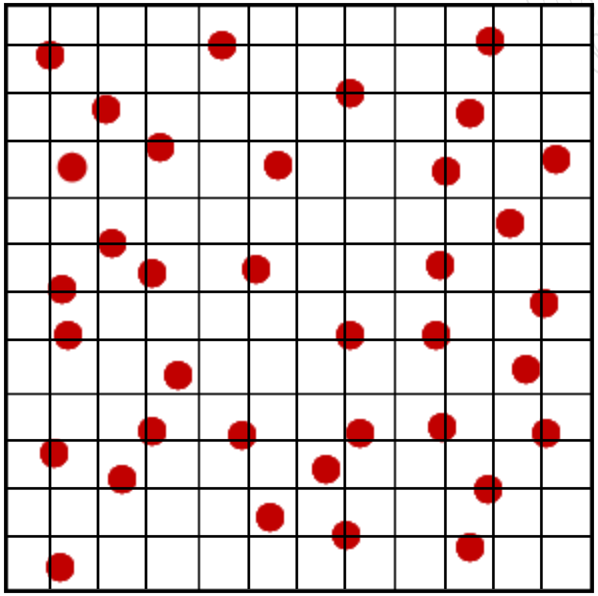
```
while(ipx <= nprocs) {
    if(nprocs % ipx == 0) {
      nremain = nprocs / ipx;
      ipy = 1;

      while(ipy <= nremain) {
        if(nremain % ipy == 0) {
          ipz = nremain / ipy;
          surf = area[0] / ipx / ipy +
                 area[1] / ipx / ipz +
                 area[2] / ipy / ipz;

          if(surf < bestsurf) {
            bestsurf = surf;
            procgrid[0] = ipx;
            procgrid[1] = ipy;
            procgrid[2] = ipz;
          }
        }

        ipy++;
      }
    }

    ipx++;
  }
```

```
 int reorder = 0;
  periods[0] = periods[1] = periods[2] = 1;

  MPI_Cart_create(MPI_COMM_WORLD, 3, procgrid,
                  periods, reorder, &cartesian);
  MPI_Cart_get(cartesian, 3, procgrid, periods,
               myloc);
  MPI_Cart_shift(cartesian, 0, 1, &procneigh[0][0],
                 &procneigh[0][1]);
  MPI_Cart_shift(cartesian, 1, 1, &procneigh[1][0],
                 &procneigh[1][1]);
  MPI_Cart_shift(cartesian, 2, 1, &procneigh[2][0],
                 &procneigh[2][1]);

for(int idim = 0; idim < 3; idim++)
    for(int i = 1; i <= need[idim]; i++, iswap += 2) {
      MPI_Cart_shift(cartesian, idim, i,
                     &sendproc_exc[iswap],
                     &sendproc_exc[iswap + 1]);
      MPI_Cart_shift(cartesian, idim, i,
                     &recvproc_exc[iswap + 1],
                     &recvproc_exc[iswap]);
    }
```

+ Hundreds of lines of additional MPI setup

Distributing Bins in Chapel

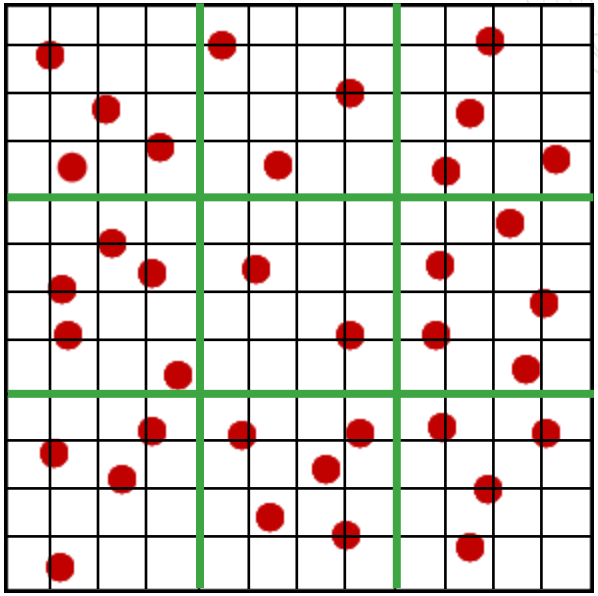
```
record atom {
  var vel, force, position : 3*real;
}
```



```
const binSpace = {1..12, 1..12};
var perBinSpace = {1..8};
var bins : [binSpace] [perBinSpace] atom;
```

Distributing Bins in Chapel

```
record atom {
  var vel, force, position : 3*real;
}
```



```
const binSpace = {1..12, 1..12} dmapped Block(…);
var perBinSpace = {1..8};
var bins : [binSpace] [perBinSpace] atom;
```

Compute forces between atoms (dist. mem.)

Runtime distributes work across locales and handles communication of data

```
forall bin in bins {
  for atom in bin {
    for neighbor in atom.neighbors {
      if distance(atom, neighbor) < cutoff {
        updateForces(atom, neighbor);
      }
    }
  }
}
```

There must be a catch…?

Yes, performance! (today, at least)

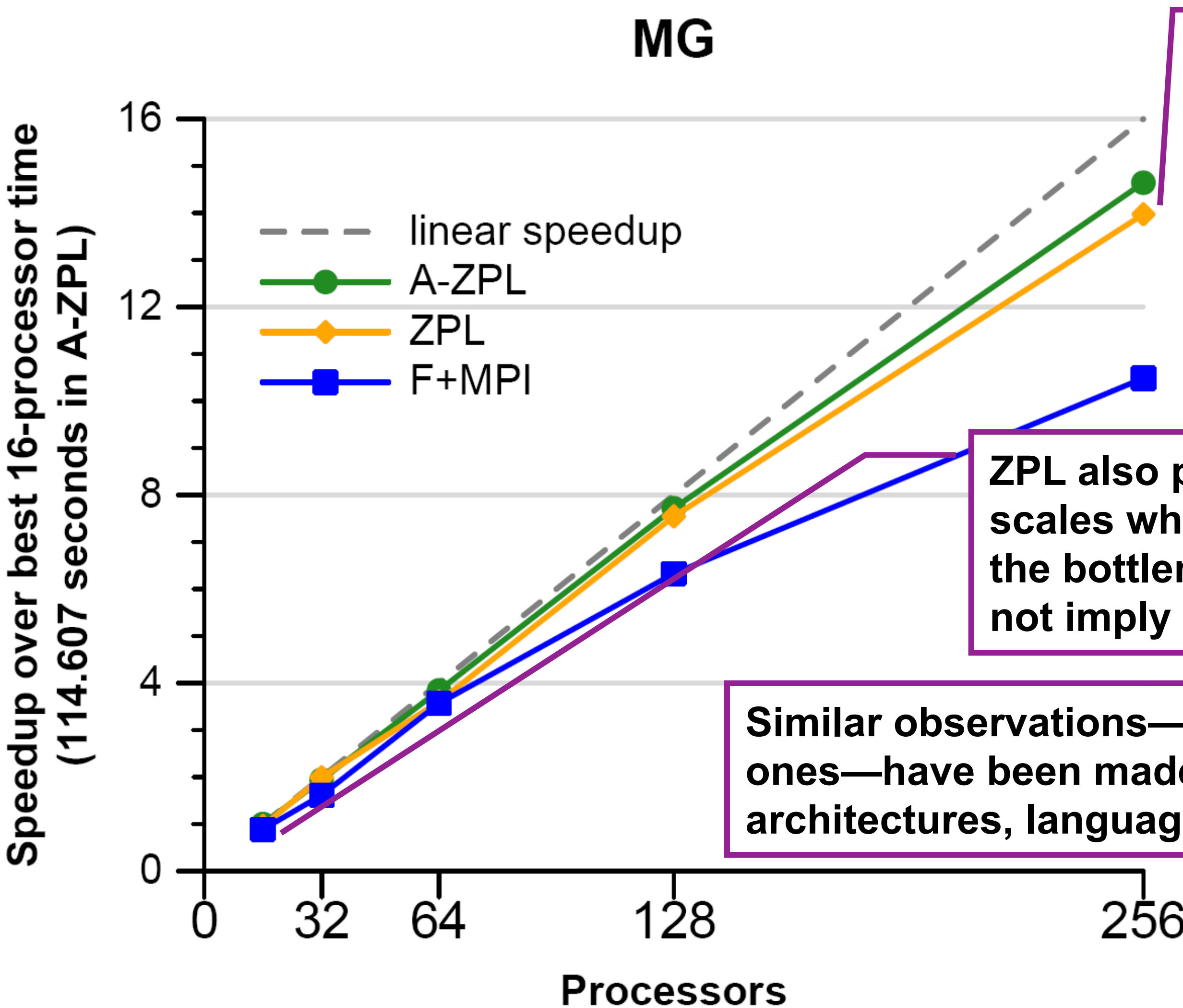
- Chapel communication currently tends to be fine-grain, demand-driven
- Stencils really want to move slabs of data between neighbors
  - This is why stencils and MPI have had a positive feedback cycle

- **Chapel was designed for good support for stencils…**
  - See, for example, Richard Barrett's CUG 2007 talk

  …and for good stencil performance
  - Based on previous work in ZPL which outperformed F+MPI for stencils

- **Yet, stencils have not been a focus of our efforts to date**
  - Sadly, HPCS milestones and HPCC have not required them…

NAS MG Speedup: ZPL vs. Fortran + MPI



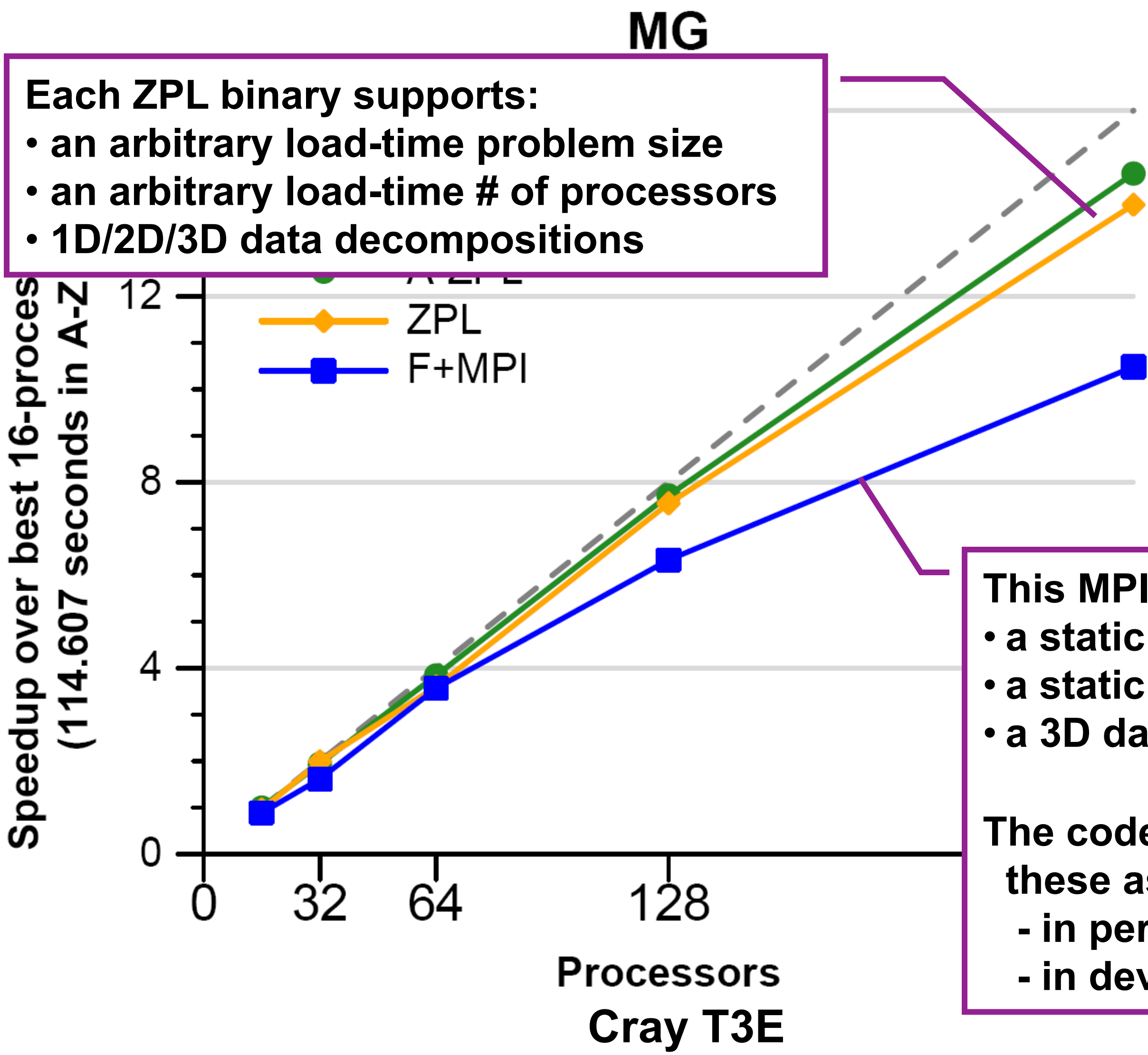
Cray T3E

ZPL scales better than MPI since its communication is expressed in an implementation-neutral way; this permits the compiler to use SHMEM on this Cray T3E but MPI on a commodity cluster

ZPL also performs better at smaller scales where communication is not the bottleneck ⇒ new languages need not imply performance sacrifices

Similar observations—and more dramatic ones—have been made using more recent architectures, languages, and benchmarks

Generality Notes

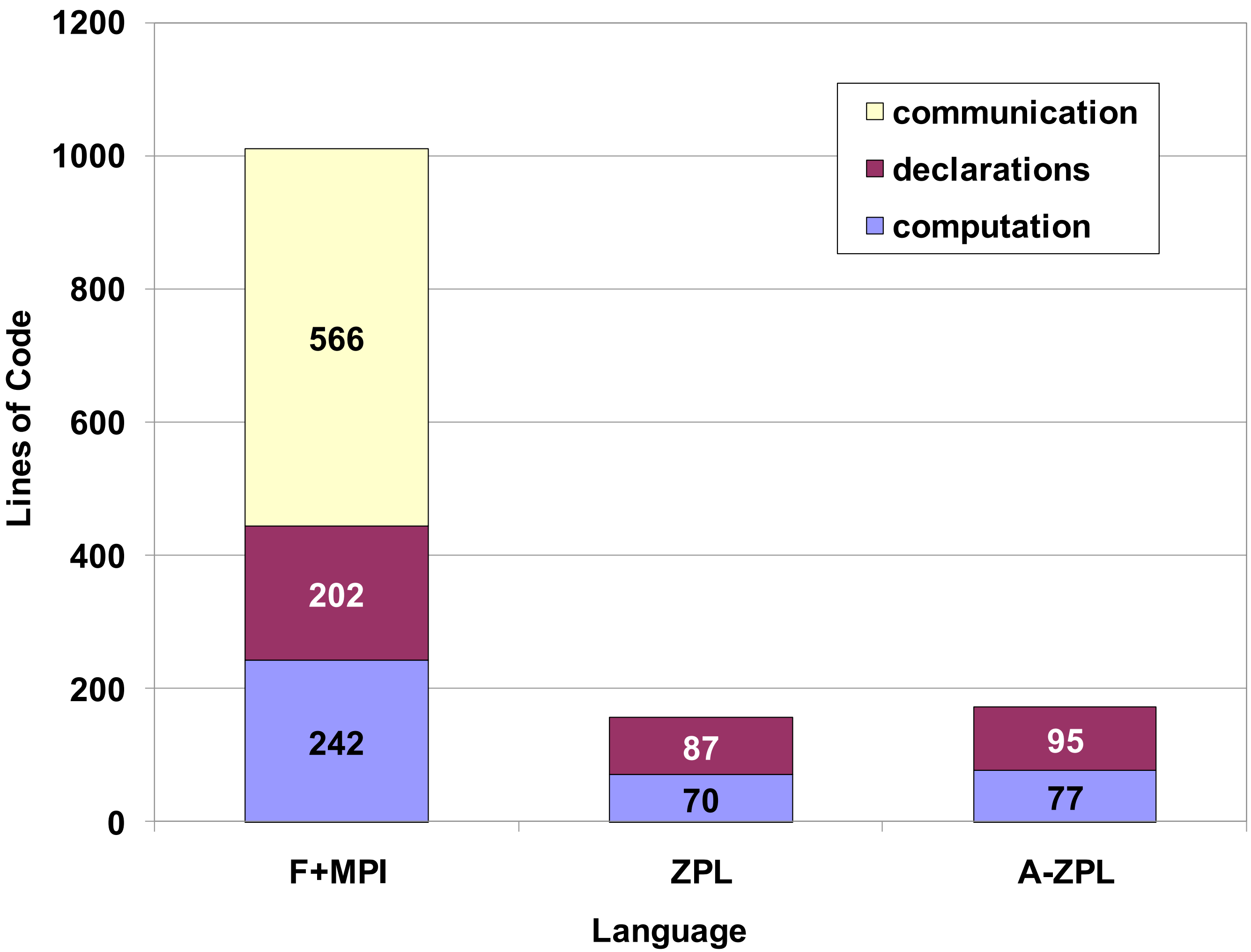


Each ZPL binary supports:
- **an arbitrary load-time problem size**
- **an arbitrary load-time # of processors**
- **1D/2D/3D data decompositions**

This MPI binary only supports:
- **a static 2**_k_ problem size**
- **a static 2**_j_ # of processors**
- **a 3D data decomposition**

The code could be rewritten to relax these assumptions, but at what cost?
- **in performance?**
- **in development effort?**

Code Size

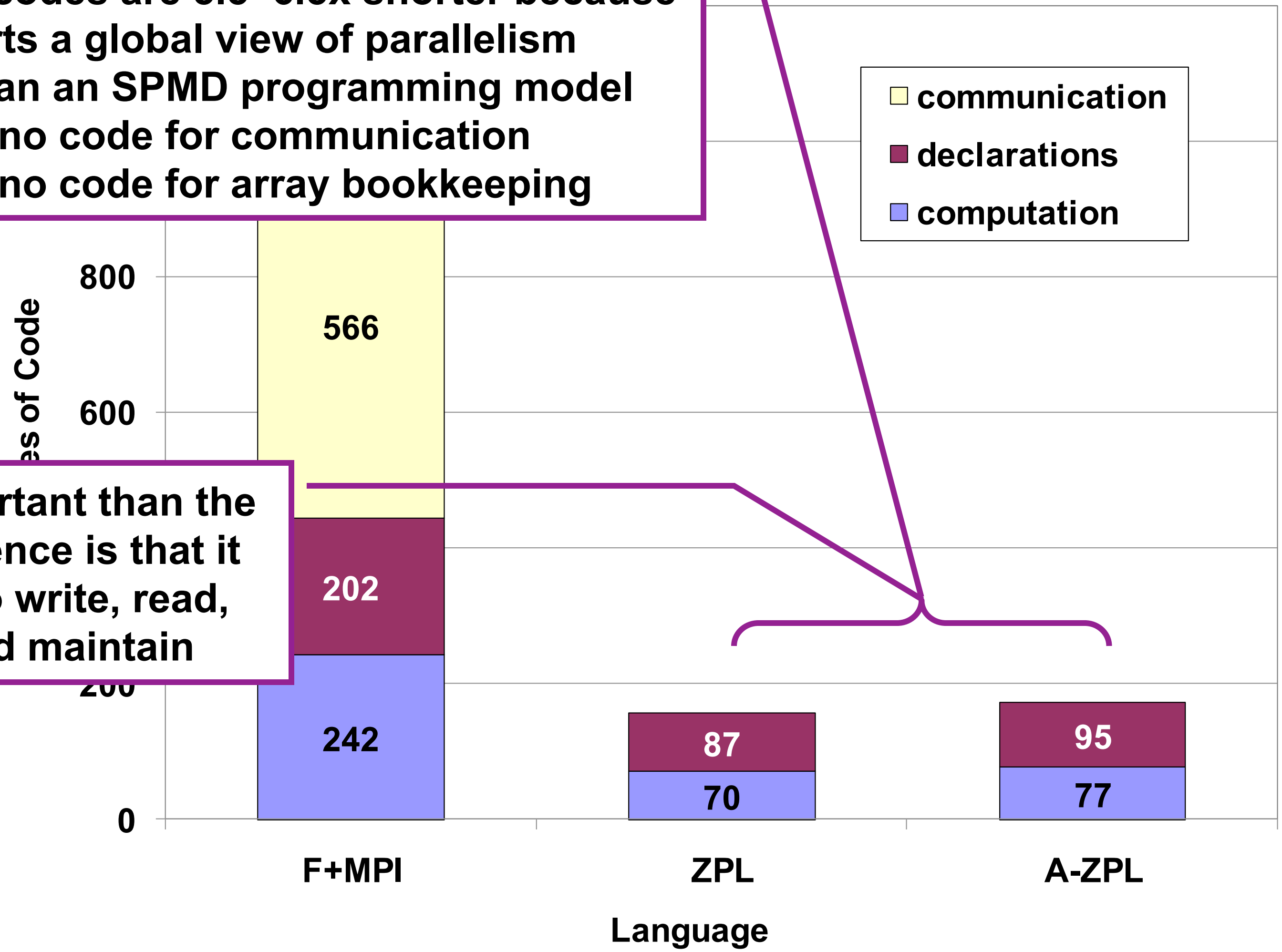


1200
1000
800
600
400
200
0
Lines of Code
communication
declarations
computation
566
202
242
87
70
95
77
F+MPI
ZPL
A-ZPL
Language

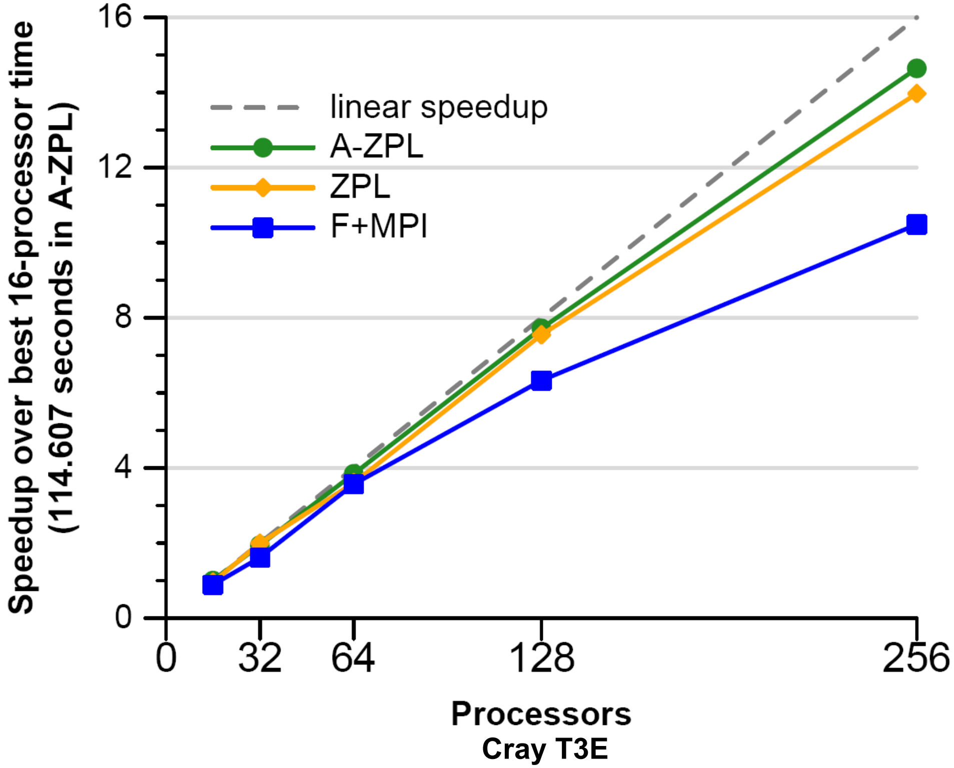
Code Size Notes

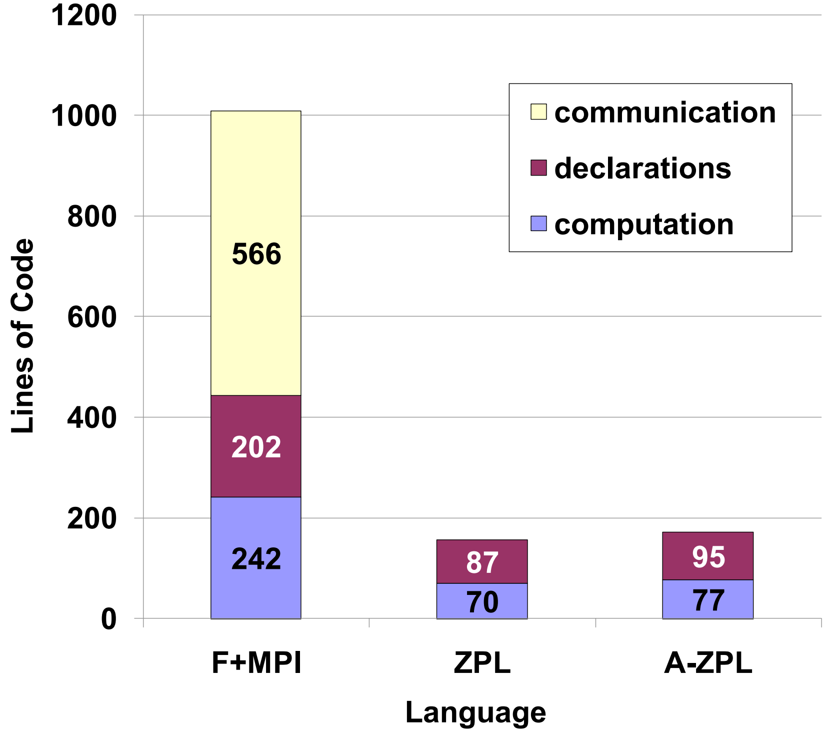
- the ZPL codes are 5.5–6.5x shorter because it supports a global view of parallelism rather than an SPMD programming model
  - ⇒ little/no code for communication
  - ⇒ little/no code for array bookkeeping

More important than the size difference is that it is easier to write, read, modify, and maintain



High-level languages can benefit Productivity





- more programmable, flexible
- able to achieve competitive performance
- more portable by leaving low-level details to the compiler

As ZPL, So Chapel?

ZPL-like results should be achievable by Chapel as well

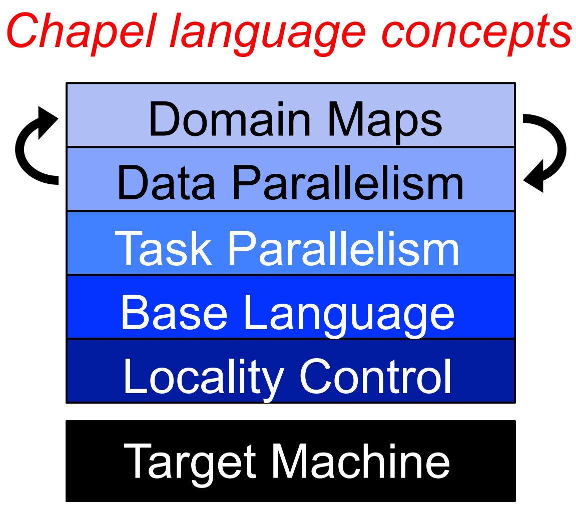
- Chapel's data parallel features are based on ZPL's

Yet, Chapel lags ZPL precisely because of the generality introduced via abstractions like domain maps

- ZPL, like C and Fortran, "owned" its array format and operations
- Chapel permits it to be specified flexibly by the end-user
- Ultimately, similar performance should be achievable, but we started out with a significant disadvantage, and are still catching up

So what's an impatient HPC programmer to do?

Use Chapel's Multiresolution Features…

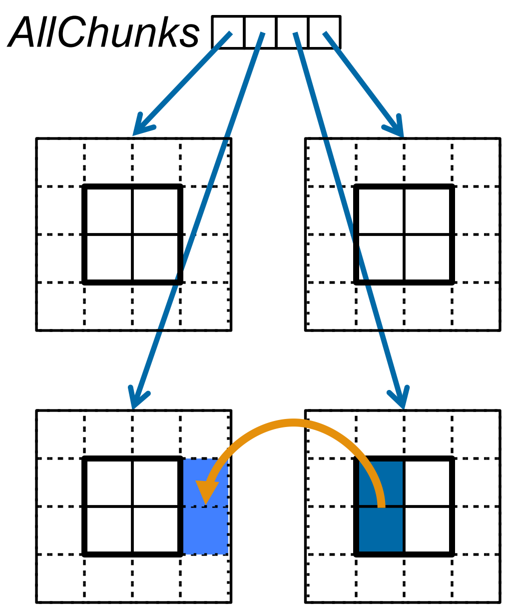


Use Chapel's Multiresolution Features…

1) Ben wrote an explicit version of MiniMD

- SPMD + manually fragmented data structures as in an MPI code

```
class Chunk {…}
var AllChunks: [LocaleSpace] Chunk;

coforall loc in Locales do
  on loc {
    var myChunk = new Chunk(…);
    AllChunks[here.id] = myChunk;
    updateFluff(myChunk);
    forall bin in myChunk …
  }
```



- of course, because of Chapel's PGAS model, communication was expressed using array slicing rather than message passing

Use Chapel's Multiresolution Features…

2) Then he refactored that logic into a *Stencil* domain map:

- an extension of *Block* supporting fluff and boundary conditions

```
const binSpace = {1..12, 1..12} dmapped Stencil(…);
var perBinSpace = {1..8};
var bins : [binSpace] [perBinSpace] atom;
```

…with user-callable routines to update these values

```
bins.updateFluff();
forall bin in bins {
  for atom in bin {
    for neighbor in atom.neighbors {
      if distance(atom, neighbor) < cutoff {
        updateForces(atom, neighbor);
      }
    }
  }
}
```

To browse MiniMD in Chapel

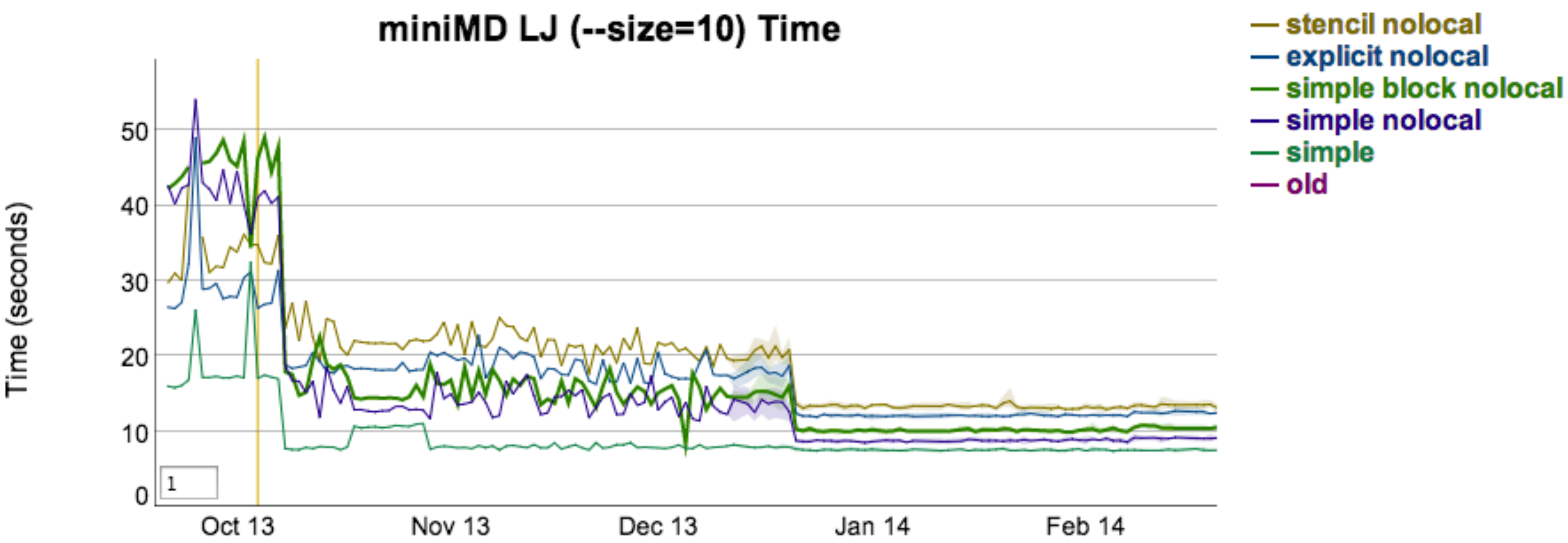
- **See examples/benchmarks/miniMD/ in the Chapel release**
- **Or, point browser to:**

  http://svn.code.sf.net/p/chapel/code/trunk/test/release/examples/benchmarks/miniMD

- **You'll find two versions of the code:**
  - **version 1:** supports three approaches via compiler options:
    - single-locale (shared memory)
    - naïve multi-locale: uses Block distribution
    - Stencil-Block multi-locale: uses Ben's custom distribution
  - **version 2:** explicit SPMD version

Next Steps

- **Presently:**
  - working on single-locale optimizations to benefit most Chapel codes



Next Steps

- **Presently:**
  - working on single-locale optimizations to benefit most Chapel codes
- **Short-term:**
  - Detailed review of code for performance/elegance improvements
  - Performance studies, comparisons, and optimizations
  - Merge Stencil domain map capabilities into Block
- **Longer-term:**
  - Have Chapel compiler automatically insert calls to update fluff
    - (reproduce ZPL analysis and optimization within Chapel)

A Closing Note on Chapel's Productivity

Ben…

- an undergraduate
- with no significant parallel programming experience
- no Chapel experience
- no MiniMD experience

…wrote 4 elegant versions of MiniMD in ~13 weeks

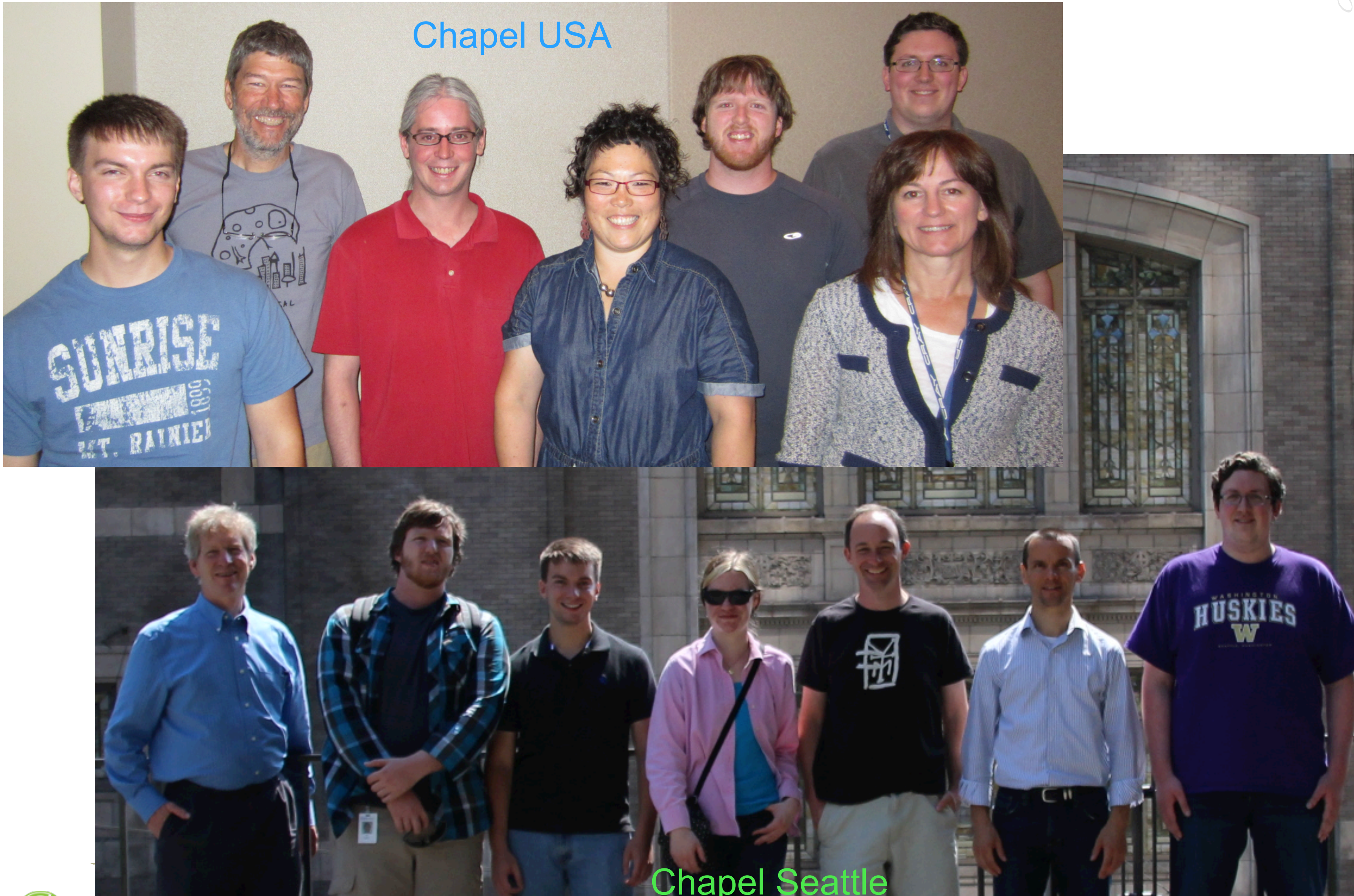
- **2 weeks:** learned Chapel, miniMD, **wrote single-locale transliteration**
- **2 weeks:** edited for Chapel style based on feedback from team
- **2 weeks:** performance improvements and **Block multi-locale version**
- **3 weeks: explicitly distributed version**
- **2.5 weeks:** wrote the **Stencil distribution version** (and the dist. itself)
- **1.5 weeks:** merged single-locale, Block, and Stencil versions into one
  - select between them with a compiler flag

Summary

- **Proxy apps are great**
  - LULESH and MiniMD are particularly good examples

- **Initial Chapel ports of LULESH and MiniMD are available**
  - Chapel's programmability goals are being met
  - more work required on performance optimizations and tuning

The Cray Chapel Team (Summer 2013)



Chapel…

…is a collaborative effort — join us!

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For More Information: Online Resources

Chapel project page: http://chapel.cray.com

- overview, papers, presentations, language spec, …

Chapel SourceForge page: https://sourceforge.net/projects/chapel/

- release downloads, public mailing lists, code repository, …

Mailing Aliases:

- chapel_info@cray.com: contact the team at Cray
- chapel-announce@lists.sourceforge.net: announcement list
- chapel-users@lists.sourceforge.net: user-oriented discussion list
- chapel-developers@lists.sourceforge.net: developer discussion
- chapel-education@lists.sourceforge.net: educator discussion
- chapel-bugs@lists.sourceforge.net: public bug forum

For More Information: Suggested Reading

Overview Papers:

- *The State of the Chapel Union* [slides], Chamberlain, Choi, Dumler, Hildebrandt, Iten, Litvinov, Titus. CUG 2013, May 2013.
  - *a high-level overview of the project summarizing the HPCS period*
- *A Brief Overview of Chapel*, Chamberlain (pre-print of a chapter for *A Brief Overview of Parallel Programming Models*, edited by Pavan Balaji, to be published by MIT Press in 2014).
  - *a more detailed overview of Chapel's history, motivating themes, features*

Blog Articles:

- *[Ten] Myths About Scalable Programming Languages*, Chamberlain. IEEE Technical Committee on Scalable Computing (TCSC) Blog, (https://www.ieeetcsc.org/activities/blog/), April-November 2012.
  - *a series of technical opinion pieces designed to rebut standard arguments against the development of high-level parallel languages*

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