BLUE WATERS

SUSTAINED PETASCALE COMPUTING

Performance-oriented Parallel Programming

Integrating Hardware, Middleware, and Applications

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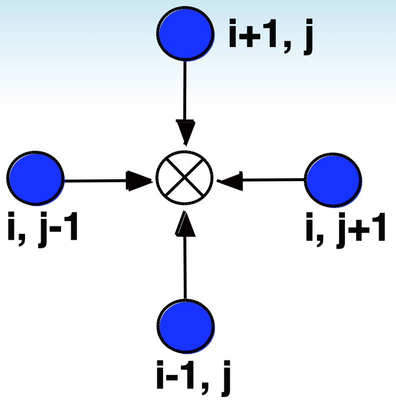
15th SIAM Conference on Parallel Processing for Scientific Computing
SIAG Junior Scientist Prize Award and Lecture

GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION

How to write efficient code?



- Simplified 5-point (2D) stencil
  - Represents other stencils

```
for(int i=1; i<n; ++i)
  for(int j=1; j<n; ++j)
    a[i,j] = b[i,j]+(b[i-1,j]+b[i+1,j]+b[i,j-1]+b[i,j+1])/4.0;
```

3 SLOC

- Simple code, easy to read
  - Very slow to execute → 150 MF/s (peak ~18 GF/s)

Serial Code Transformations

unroll-and-jam, vectorization, prefetch, nt stores, reg blocking, alignment

```
for(int i=1; i<n; ++i)
  for(int j=1; j<n; ++j)
    a[i,j] = b[i,j]+(b[i-1,j]+b[i+1,j]+b[i,j-1]+b[i,j+1])/4.0;
```

3 SLOC

Tuning →

```
for(int ib=1; ib<n+1; ib+=bs)
  for(int jb=1; jb<n+1; jb+=bs)
    for(register int i=ib; i<min(ib+bs, n+1); ++i)
      #pragma ivdep
      for(register int j=jb; j<min(jb+bs,n+1); j+=2) {
        register double x=anew[ind(i,j)]/2.0;
        register double y=anew[ind(i,j+1)]/2.0;
        register double z=anew[ind(i,j+2)]/2.0;
        x = x + (aold[ind(i-1,j)] + aold[ind(i+1,j)] + aold[ind(i,j-1)] + aold[ind(i,j+1)])/8.0;
        y = y + (aold[ind(i-1,j+1)] + aold[ind(i+1,j+1)] + aold[ind(i,j)] + aold[ind(i,j+2)])/8.0;
        z = z + (aold[ind(i-1,j+2)] + aold[ind(i+1,j+2)] + aold[ind(i,j+1)] + aold[ind(i,j+3)])/8.0;
        heat += x + y + z;
        anew[ind(i,j)] = x;
        anew[ind(i,j+1)] = y;
        anew[ind(i,j+2)] = z;
      }
```

121 SLOC

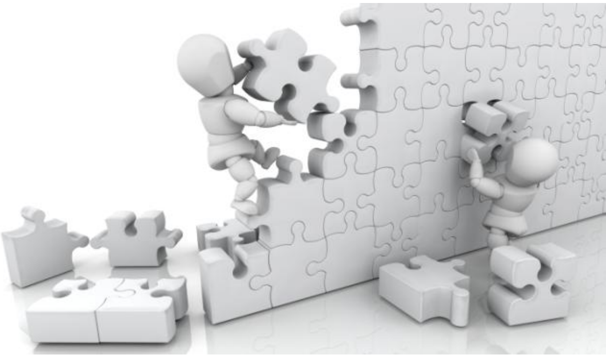
150 MF/s **1.32 GF/s**

- Huge programming effort (5 minutes vs. 5 hours)
  - Very hard to read and change!
  - Not portable (techniques and constants differ!)
- Best automatic compiler optimization (+manual optimization):

GCC 4.6.1	PGCC 11.9	PathCC 4.0.9	CrayC 7.4.4
0.66 GF/s (18%)	0.66 GF/s (16%)	1.22 GF/s (8%)	0.38 GF/s (-35%)

Data collected on Hector/UK

Serial Optimization is well understood



- Follows higher-order principles
  - Autotuning for specific parameters
  - CS help needed to drive the effort
- Compilers improve significantly
  - Optimizations improve performance 10x
  - Humans or domain-specific (auto)tuning beat them[1]
- Parallelism becomes ubiquitous
  - Key question: How do we make parallel programming **as** "easy" as serial programming?

[1]: Tang et al. "The Pochoir Stencil Compiler" (SPAA 2011)

Parallel 2D Stencil in “six-function” MPI

- Simple 2D stencil

```
// figure out my coordinates (x,y) -- r=x*a+y in the 2d processor array
  int rx = r % px;
  int ry = r / px;
  // figure out my four neighbors
  int north = (ry-1)*px+rx; if(ry-1 < 0)   north = MPI_PROC_NULL;
  int south = (ry+1)*px+rx; if(ry+1 >= py) south = MPI_PROC_NULL;
  int west= ry*px+rx-1;     if(rx-1 < 0)   west = MPI_PROC_NULL;
  int east = ry*px+rx+1;    if(rx+1 >= px) east = MPI_PROC_NULL;
  // decompose the domain
  int bx = n/px; // block size in x
  int by = n/py; // block size in y
  int offx = rx*bx; // offset in x
  int offy = ry*by; // offset in y

  MPI_Request reqs[8];
  double *sbufnorth = (double*)calloc(1,bx*sizeof(double)); // send buffers
  double *sbufsouth = (double*)calloc(1,bx*sizeof(double));
  double *sbufeast = (double*)calloc(1,by*sizeof(double));
  double *sbufwest = (double*)calloc(1,by*sizeof(double));
  double *rbufnorth = (double*)calloc(1,bx*sizeof(double)); // receive buffers
  double *rbufsouth = (double*)calloc(1,bx*sizeof(double));
  double *rbufeast = (double*)calloc(1,by*sizeof(double));
  double *rbufwest = (double*)calloc(1,by*sizeof(double));
  for(int i=0; i<bx; ++i) sbufnorth[i] = aold[ind(i+1,1)]; // pack loop - last valid region
  for(int i=0; i<bx; ++i) sbufsouth[i] = aold[ind(i+1,by)]; // pack loop
  for(int i=0; i<by; ++i) sbufeast[i] = aold[ind(bx,i+1)]; // pack loop
  for(int i=0; i<by; ++i) sbufwest[i] = aold[ind(1,i+1)]; // pack loop
  MPI_Isend(sbufnorth, bx, MPI_DOUBLE, north, 9, comm, &reqs[0]);
  MPI_Isend(sbufsouth, bx, MPI_DOUBLE, south, 9, comm, &reqs[1]);
  MPI_Isend(sbufeast, by, MPI_DOUBLE, east, 9, comm, &reqs[2]);
  MPI_Isend(sbufwest, by, MPI_DOUBLE, west, 9, comm, &reqs[3]);
  MPI_Irecv(rbufnorth, bx, MPI_DOUBLE, north, 9, comm, &reqs[4]);
  MPI_Irecv(rbufsouth, bx, MPI_DOUBLE, south, 9, comm, &reqs[5]);
  MPI_Irecv(rbufeast, by, MPI_DOUBLE, east, 9, comm, &reqs[6]);
  MPI_Irecv(rbufwest, by, MPI_DOUBLE, west, 9, comm, &reqs[7]);
  MPI_Waitall(8, reqs, MPI_STATUS_IGNORE);
  for(int i=0; i<bx; ++i) aold[ind(i+1,0)] = rbufnorth[i]; // unpack loop - into ghost cells
  for(int i=0; i<bx; ++i) aold[ind(i+1,by+1)] = rbufsouth[i]; // unpack loop
  for(int i=0; i<by; ++i) aold[ind(bx+1,i+1)] = rbufeast[i]; // unpack loop
  for(int i=0; i<by; ++i) aold[ind(0,i+1)] = rbufwest[i]; // unpack loop

  heat = 0.0;
  for(int i=1; i<bx+1; ++i) {
    for(int j=1; j<by+1; ++j) {
      anew[ind(i,j)] = anew[ind(i,j)]/2.0 + (aold[ind(i-1,j)] + aold[ind(i+1,j)] + aold[ind(i,j-1)] + aold[ind(i,j+1)])/4.0/2.0;
      heat += anew[ind(i,j)];
    }
  }
```

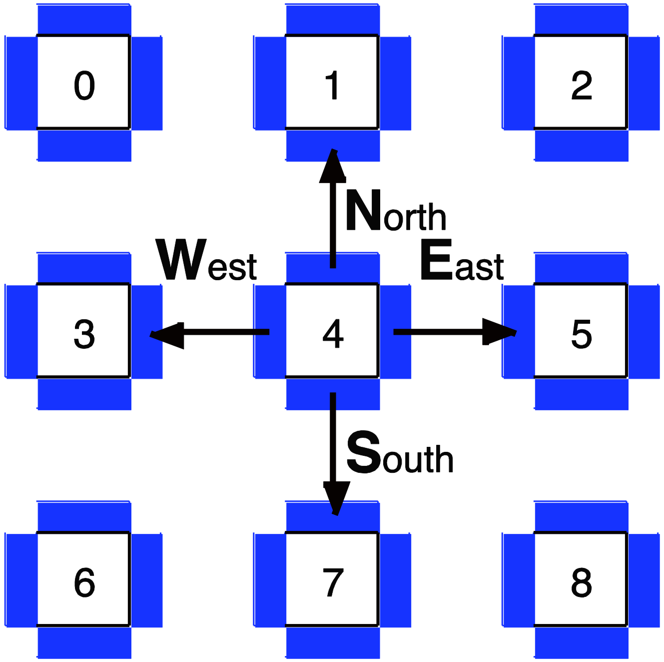
50 SLOC

26% decomposition

26% data movement

20% communication

4.67 GF (P=32)



- Packs and communicates four directions
  - Simple code, easy to read, slow execution

Parallel Optimizations are less understood

- Many techniques are known, applied manually
  - Often with good libraries (PETSc, ScaLAPACK, …)
  - CS needs to drive automation
- Identify necessary optimization techniques
  - Define the right abstractions
  - I will show several examples
- Define composable interfaces
  - CS researchers adapt programs and systems

Optimization Principles for Parallel Programs

1. Serialization/Deserialization of sent/recvd data
2. Optimizing communication patterns
   - Collective operations cf. “Communication BLAS”
3. Communication/computation overlap
   - Pipelining, cf. “Cache prefetch”
4. Synchronization and System Noise
5. Topology mapping
6. Scalable Algorithms and Load Balance
7. Domain Decomposition/Data Distribution

1. Serialization/Deserialization of data

- Network needs contiguous byte stream
  - Often leads to inefficient "manual pack loops"
  - MPI datatypes can avoid copying[1]

```
// figure out my coordinates (x,y) -- r=x*a+y in the 2d processor array
  int rx = r % px;
  int ry = r / px;
  // figure out my four neighbors
  int north = (ry-1)*px+rx; if(ry-1 < 0)   north = MPI_PROC_NULL;
  int south = (ry+1)*px+rx; if(ry+1 >= py) south = MPI_PROC_NULL;
  int west= ry*px+rx-1;     if(rx-1 < 0)   west = MPI_PROC_NULL;
  int east = ry*px+rx+1;    if(rx+1 >= px) east = MPI_PROC_NULL;
  // decompose the domain
  int bx = n/px; // block size in x
  int by = n/py; // block size in y
  int offx = rx*bx; // offset in x
  int offy = ry*by; // offset in y
   MPI_Datatype north_south_type;
   MPI_Type_contiguous(bx, MPI_DOUBLE, &north_south_type);
   MPI_Type_commit(&north_south_type);
   MPI_Datatype east_west_type;
   MPI_Type_vector(by,1,bx+2,MPI_DOUBLE, &east_west_type);
   MPI_Type_commit(&east_west_type);

   MPI_Request reqs[8];
   MPI_Isend(&aold[ind(1,1)] /* north */, 1, north_south_type, north, 9, comm, &reqs[0]);
   MPI_Isend(&aold[ind(1,by)] /* south */, 1, north_south_type, south, 9, comm, &reqs[1]);
   MPI_Isend(&aold[ind(bx,1)] /* east */, 1, east_west_type, east, 9, comm, &reqs[2]);
   MPI_Isend(&aold[ind(1,1)] /* west */, 1, east_west_type, west, 9, comm, &reqs[3]);
   MPI_Irecv(&aold[ind(1,0)] /* north */, 1, north_south_type, north, 9, comm, &reqs[4]);
   MPI_Irecv(&aold[ind(1,by+1)] /* south */, 1, north_south_type, south, 9, comm, &reqs[5]);
   MPI_Irecv(&aold[ind(bx+1,1)] /* west */, 1, east_west_type, east, 9, comm, &reqs[6]);
   MPI_Irecv(&aold[ind(0,1)] /* east */, 1, east_west_type, west, 9, comm, &reqs[7]);
   MPI_Waitall(8, reqs, MPI_STATUS_IGNORE);

   heat = 0.0;
   for(int i=1; i<bx+1; ++i) {
    for(int j=1; j<by+1; ++j) {
      anew[ind(i,j)] = anew[ind(i,j)]/2.0 + (aold[ind(i-1,j)] + aold[ind(i+1,j)] + aold[ind(i,j-1)] + aold[ind(i,j+1)])/4.0/2.0;
      heat += anew[ind(i,j)];
    }
   }
```

24% less SLOC

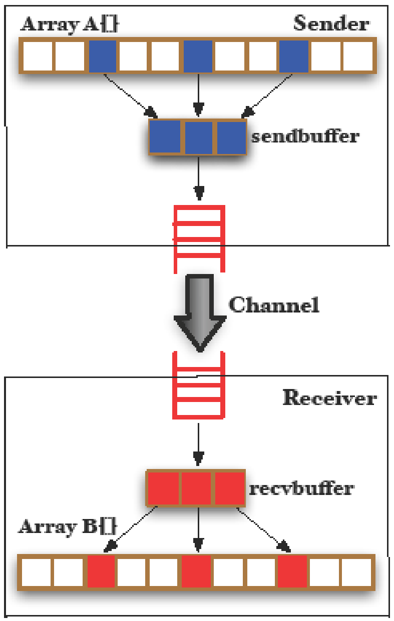
26% decomposition

15% declaration

26% communication

4.67 GF → 5.05 GF

(32 cores, IB)



[1]: Hoefler, Gottlieb: "Parallel Zero-Copy Algorithms […] using MPI Datatypes" (EuroMPI 2010)
Kjolstad, Hoefler, Snir: "[…] Convert Packing Code to Compact Datatypes […]" (PPoPP 2012)

2. Optimizing communication patterns

- Architecture/Network-specific optimization
  - Post send/recv manually in right order
  - Or use neighborhood collectives [MPI-3.0][1]

```
MPI_Datatype north_south_type;
MPI_Type_contiguous(bx, MPI_DOUBLE, &north_south_type);
MPI_Type_commit(&north_south_type);
MPI_Datatype east_west_type;
MPI_Type_vector(by,1,bx+2,MPI_DOUBLE, &east_west_type);
MPI_Type_commit(&east_west_type);

MPI_Comm comm_new;
MPI_Cart_create(comm, 2, {bx, by}, {0,0}, 1, &comm_new);
MPI_Neighbor_alltoallw(sbuf, {1,1,1,1}, {0,0,0,0}, {north_south_type, east_west_type, north_south_type, east_west_type},
          rbuf, {1,1,1,1}, {0,0,0,0}, {north_south_type, east_west_type, north_south_type, east_west_type}, comm_new);

heat = 0.0;
for(int i=1; i<bx+1; ++i) {
  for(int j=1; j<by+1; ++j) {
    anew[ind(i,j)] = anew[ind(i,j)]/2.0 + (aold[ind(i-1,j)] + aold[ind(i+1,j)] + aold[ind(i,j-1)] + aold[ind(i,j+1)])/4.0/2.0;
    heat += anew[ind(i,j)];
  }
```

64% less SLOC

33% declaration

11% communication

5.05 GF → 5.11 GF

  - Declare the communication topology like a type
    - Optimizations possible in the library

[1]: Hoefler, Traeff: “Sparse Collective Operations for MPI” (HIPS 2009)

3. Communication/computation overlap

- Utilize the machine efficiently (no wait cycles)
  - Often done manually for simple problems
  - Nonblocking collectives provide huge benefit[1]

```
MPI_Datatype north_south_type;
MPI_Type_contiguous(bx, MPI_DOUBLE, &north_south_type);
MPI_Type_commit(&north_south_type);
MPI_Datatype east_west_type;
MPI_Type_vector(by,1,bx+2,MPI_DOUBLE, &east_west_type);
MPI_Type_commit(&east_west_type);

MPI_Comm comm_new;
MPI_Cart_create(comm, 2, {bx, by}, {0,0}, 1, &comm_new);
MPI_Ineighbor_alltoallw(sbuf, {1,1,1,1}, {0,0,0,0}, {north_south_type, east_west_type, north_south_type, east_west_type},
          rbuf, {1,1,1,1}, {0,0,0,0}, {north_south_type, east_west_type, north_south_type, east_west_type}, comm_new, &req);

heat = 0.0;
for(int i=2; i<bx; ++i)
  for(int j=2; j<by; ++j) {
    anew[ind(i,j)] = anew[ind(i,j)]/2.0 + (aold[ind(i-1,j)] + aold[ind(i+1,j)] + aold[ind(i,j-1)] + aold[ind(i,j+1)])/4.0/2.0;
    heat += anew[ind(i,j)];
  }

MPI_Wait(&req, MPI_STATUS_IGNORE);

for(int i=2; i<bx; ++i)
  for(int j=1; j < by+1; j+=by-1) {
    anew[ind(i,j)] = anew[ind(i,j)]/2.0 + (aold[ind(i-1,j)] + aold[ind(i+1,j)] + aold[ind(i,j-1)] + aold[ind(i,j+1)])/4.0/2.0;
    heat += anew[ind(i,j)];
  }
```

30% more SLOC

31% declaration

12% communication

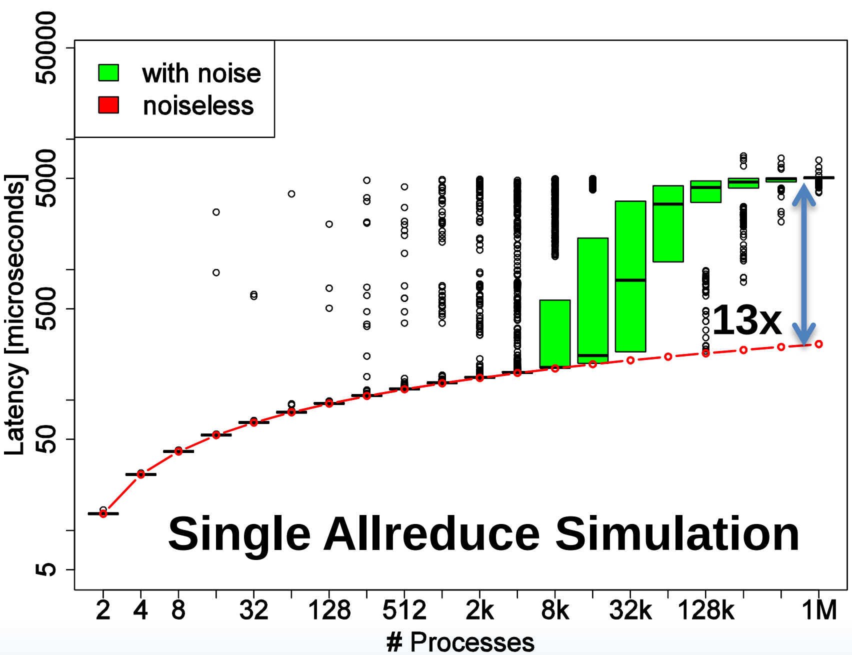
5.11 GF → 5.19 GF

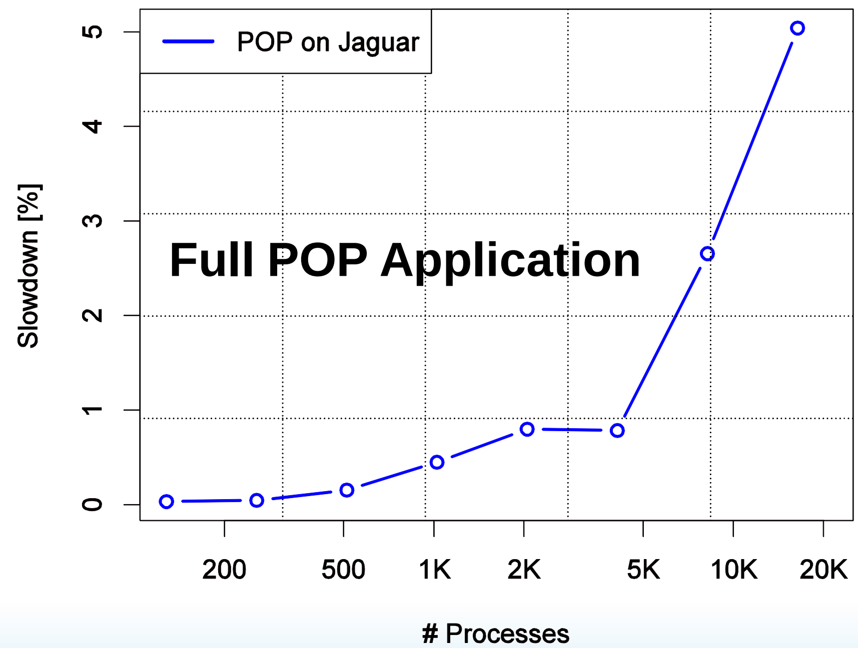
  - Break computation into pieces and arrange with communication (software pipelining)[1]

[1]: Hoefler et al.: "Leveraging Non-blocking Collective Communication […]" (SPAA 2008)

4. Synchronization and System Noise

- Small nondeterministic delays in processes can lead to **huge** delays in parallel applications
  - Depends on the shape and distribution of delays[1]

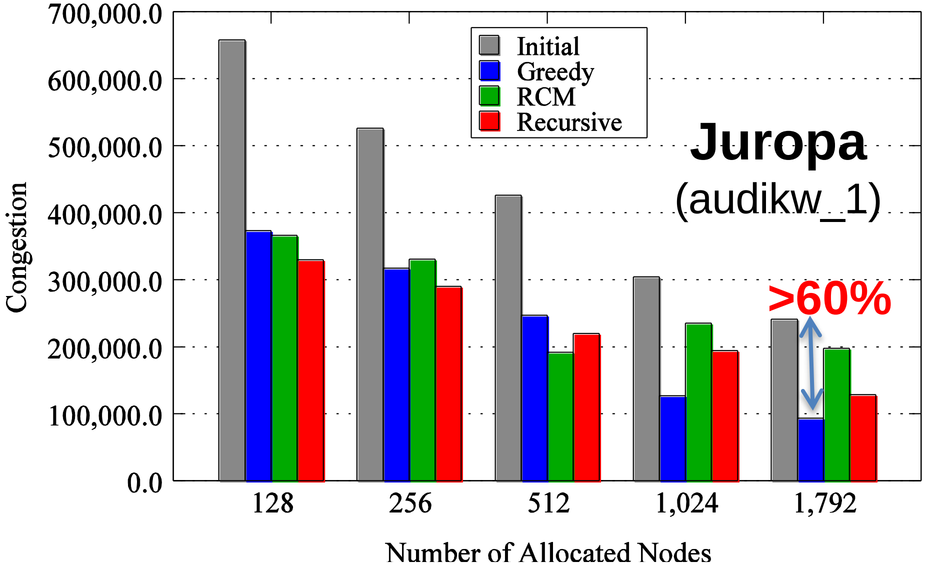


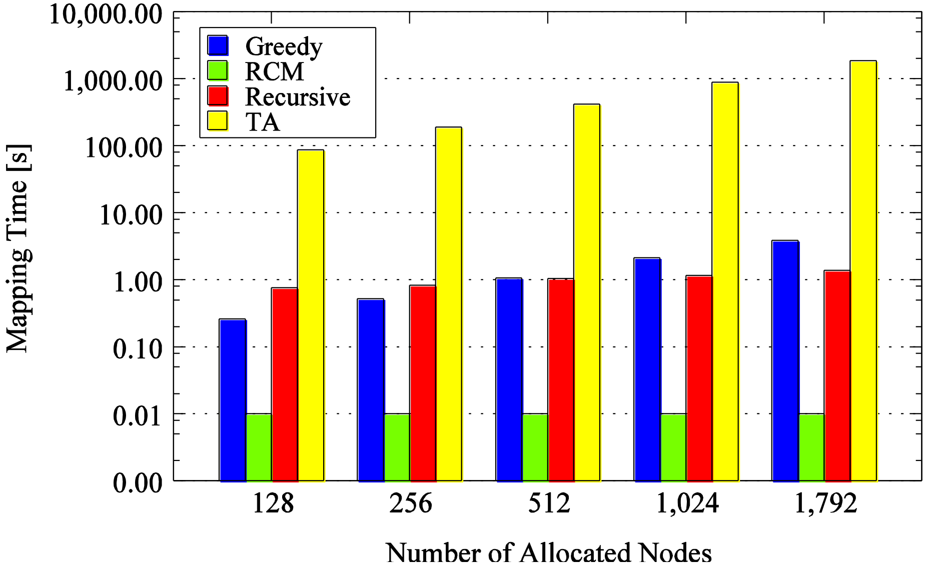


[1]: Hoefler et al.: "Characterizing the Influence of System Noise […]" (SC'10 Best Paper)

5. Topology mapping

- Low-degree physical networks and low-degree application communication networks
  - Good mappings increase performance (NP hard[1])





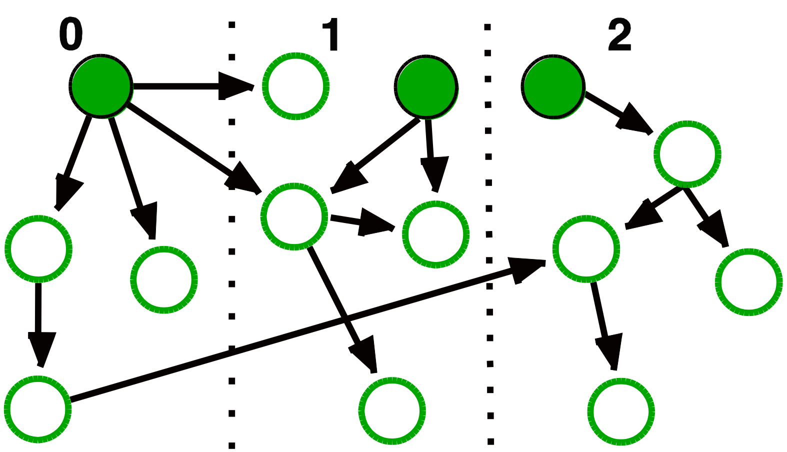
>50% reduction in average dilation!

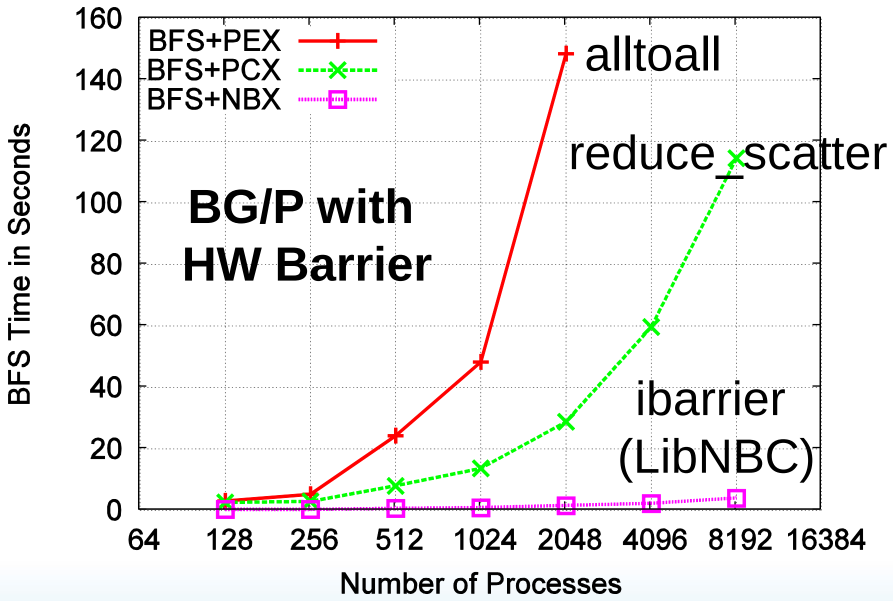
asymptotically faster!

[1]: Hoefler, Snir: "Generic Topology Mapping Strategies […]" (ICS 2011)

6. Scalable Algorithms and Load Balance

- Termination detection (TD) is an important problem
- DSDE[1] is a special case of 1-level TD:
  - Sparse exchange, knowledge only at sender

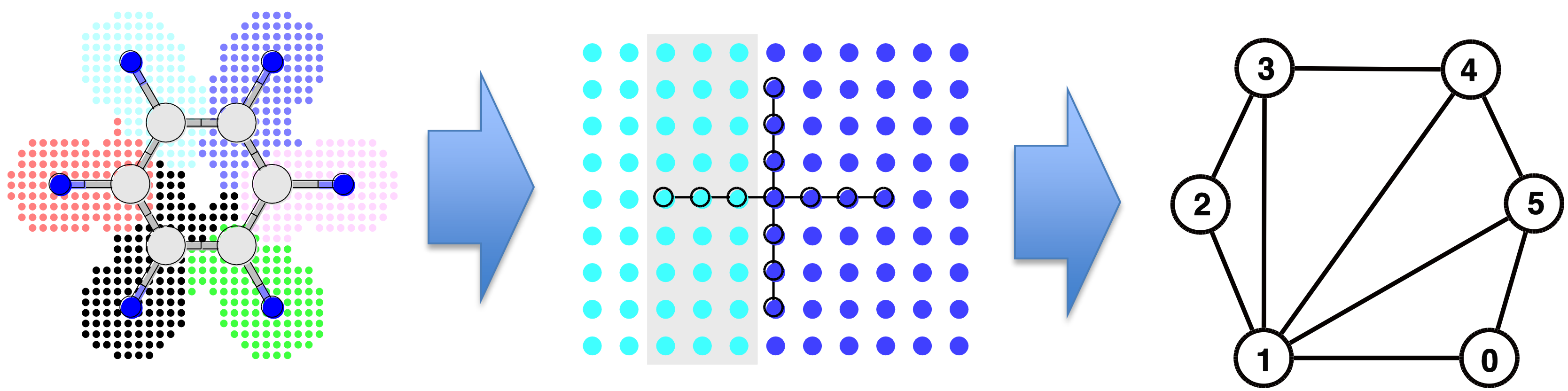




[1]: Hoefler et al.: "Scalable Communication […] for Dynamic Sparse Data Exchange" (PPoPP 2010)

7. Domain Decomposition/Data Distribution

- Most important but also hard (NP hard)
  - Good heuristics exist (METIS, SCOTCH, Chaco, …)
  - Use in conjunction with topology mapping (MPI-2.2)



MPI 2.2

Hoefler et al.: "The Scalable Process Topology Interface of MPI 2.2" (CCPE 2010)

The Optimization Space is Large

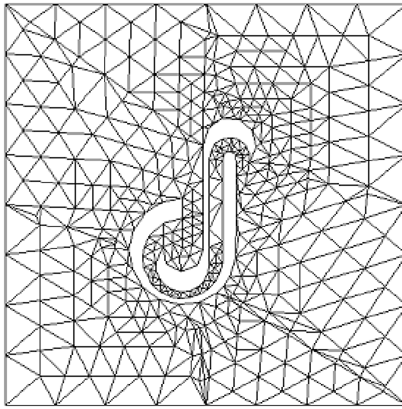
- All criteria are (performance) composable in layers!
- The **right** abstractions and declarations are key
  - Enable CS systems people (like me) to optimize malleable applications
  - Specify as much as possible statically
- Automatic composition: DSLs
  - PBGL / AP (C++ templates)
  - PMTL (C++ templates)
  - … many more!

Work at the System or Implementation Level

- Implement abstractions!
  - SerDes with Datatypes
    - Datatype "JIT" Compiler *[in progress]*
  - Topology mapping
    - Mapping heuristics (RCM) *[ICS'11]*
  - Optimized (asynchronous) Nonblocking Collectives
    - LibNBC *[SC'07],* kernel-level progression *[EuroPar'11]*
  - Optimized neighborhood collectives
    - Group Operation Assembly Language *[ICPP'09]*
  - Optimized Routing in HPC networks *[IPDPS'11]*

Work at the Interface to static Applications

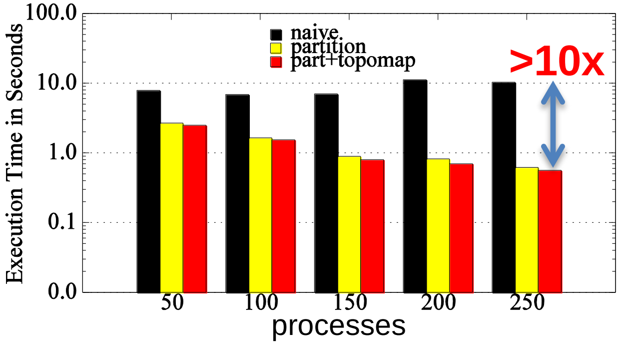
- Matrix Template Library - Linear Algebra
  - Automatic partitioning, load balancing, topology mapping, serial optimizations, neighborhood collectives



Parallel LU

```
for (std::size_t k= 0; k < num rows(LU)−1; k++) {
  if(abs(LU[k][k]) <= eps) throw matrix singular();
  irange r(k+1, imax); // Interval [k+1, n−1]
  LU[r][k] /= LU[k][k];
  LU[r][r] −= LU[r][k] * LU[k][r];
}
```

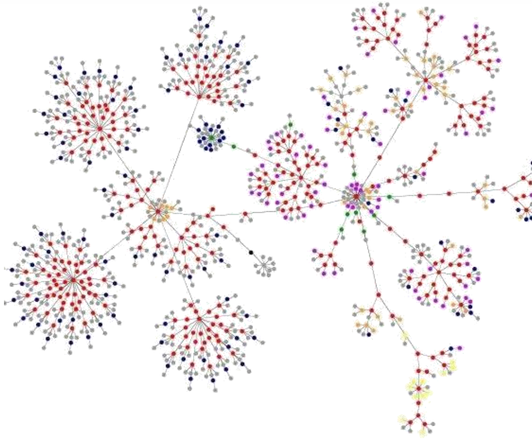
Single MatVec (Idoor) Partitioning/Topology Mapping



Gottschling, Hoefler: “Productive Parallel Linear Algebra Programming […] “ (CCGrid 2012)

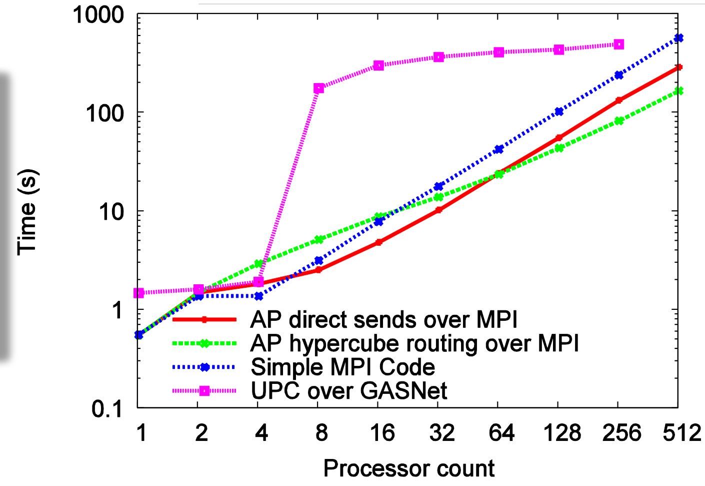
Work at the Interface to dynamic Applications

- Active Pebbles - Graph Programming
  - Automatic overlap, coalescing, active routing, termination detection, vectorized handlers



Parallel RandomAccess

```
struct update_handler {
  bool operator()(uint64_t ran) const
  { table[ran % (N/P)] ^= ran; } // update to table
};
```



Willcock, Hoefler et al.: “Active Pebbles: Parallel Programming for Data-Driven Applications “ (ICS’11)

Summary & Conclusions

- Is parallel programming as “easy” as serial programming? – No(t yet)
  - We made some progress (still far to go)
- Communication and network become issue → network-centric programming
- New languages can and will help
  - But they shall never ignore the past (MPI)
- Domain-specific languages can isolate problems
  - How does a good general parallel language look like?

Collaborators, Acknowledgments & Support

- Marc Snir, Bill Gropp, Bill Kramer
- Andrew Lumsdaine, J. Willcock, N. Edmonds
- Peter Gottschling
- Students: T. Schneider, J. Domke, C. Siebert
- Sponsored by: