Performance-oriented Parallel Programming
Integrating Hardware, Middleware, and Applications

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SIAG Junior Scientist Prize Award and Lecture

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How to write efficient code?

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

```java
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;
```

• Simple code, easy to read
• Very slow to execute \( \rightarrow 150 \text{ MF/s} \) \( (\text{peak } \sim 18 \text{ GF/s}) \)
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;

Tuning

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):

<table>
<thead>
<tr>
<th></th>
<th>GCC 4.6.1</th>
<th>PGCC 11.9</th>
<th>PathCC 4.0.9</th>
<th>CrayC 7.4.4</th>
</tr>
</thead>
<tbody>
<tr>
<td>GF/s</td>
<td>0.66</td>
<td>0.66</td>
<td>1.22</td>
<td>0.38</td>
</tr>
<tr>
<td>%</td>
<td>(18%)</td>
<td>(16%)</td>
<td>(8%)</td>
<td>(-35%)</td>
</tr>
</tbody>
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Data collected on Hector/UK

Torsten Hoefler: Performance-oriented Parallel Programming
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
  
  ```c
  // 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
  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
  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\(^1\)

\(^1\): 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

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

```
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

[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\(^1\)

\[\text{MPI\_Datatype\ north\_south\_type;}\]
\[\text{MPI\_Type\ contiguous(bx, MPI\_DOUBLE, &north\_south\_type);}\]
\[\text{MPI\_Type\ commit(&north\_south\_type);}\]
\[\text{MPI\_Datatype\ east\_west\_type;}\]
\[\text{MPI\_Type\ vector(by,1,bx+2,MPI\_DOUBLE, &east\_west\_type);}\]
\[\text{MPI\_Type\ commit(&east\_west\_type);}\]
\[\text{MPI\_Comm\ comm\_new;}\]
\[\text{MPI\_Cart\_create(comm, 2, (bx, by), [0,0], 1, &comm\_new);}\]
\[\text{MPI\_Ineighbor\_alltoallw(sbuf, (1,1,1), [0,0,0,0], (north\_south\_type, east\_west\_type, north\_south\_type, east\_west\_type), rbuf, (1,1,1), [0,0,0,0], (north\_south\_type, east\_west\_type, north\_south\_type, east\_west\_type), comm\_new, &req);}\]

\[\text{heat = 0.0;}\]
\[\text{for(int i=2; i<bx; ++i)}\]
\[\text{for(int j=2; j<by; ++j)}\]
\[\text{anew[ind(i,j)] = anew[ind(i,j)]/2.0 + (aold[ind(i-1,j)] + aold[ind(i+1,j)] + aold[ind(i,j-1)] + aold[ind(i,j+1)])/4.0/2.0;}\]
\[\text{heat += anew[ind(i,j)];}\]
\[\text{MPI\_Wait(&req, MPI\_STATUS\_IGNORE);}\]
\[\text{for(int i=2; i<bx; ++i)}\]
\[\text{for(int j=1; j<by+1; j+=by-1)}\]
\[\text{anew[ind(i,j)] = anew[ind(i,j)]/2.0 + (aold[ind(i-1,j)] + aold[ind(i+1,j)] + aold[ind(i,j-1)] + aold[ind(i,j+1)])/4.0/2.0;}\]
\[\text{heat += anew[ind(i,j)];}\]

30% more SLOC
31% declaration
12% communication

5.11 GF \(
\rightarrow
\) 5.19 GF

- Break computation into pieces and arrange with communication (software pipelining)\(^1\)

\[\text{[1]: Hoefler et al.: “Leveraging Non-blocking Collective Communication […]” (SPAA 2008)}\]
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

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[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\(^1\))

>60% reduction in average dilation!

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

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)

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 \textit{[in progress]}
  • Topology mapping
    • Mapping heuristics (RCM) \textit{[ICS’11]}
• Optimized (asynchronous) Nonblocking Collectives
  • LibNBC \textit{[SC’07]}, kernel-level progression \textit{[EuroPar’11]}
• Optimized neighborhood collectives
  • Group Operation Assembly Language \textit{[ICPP’09]}
• Optimized Routing in HPC networks \textit{[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

```cpp
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];
}
```

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

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

Parallel RandomAccess

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?
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