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Overcoming the Barriers to Sustained Petaflop Performance

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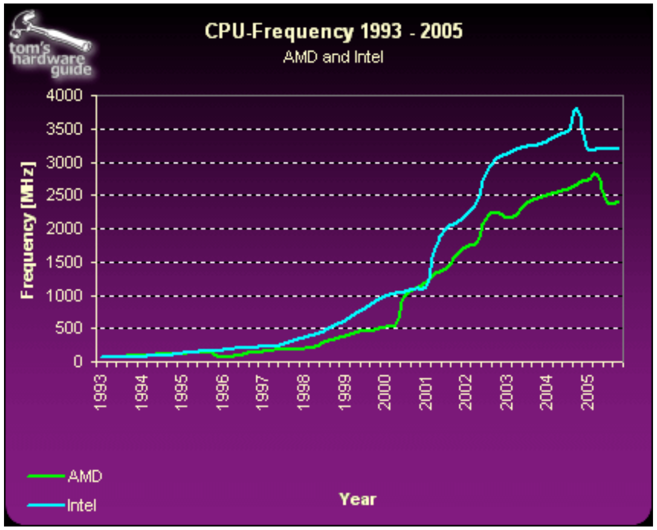
But First…

- Are we too CPU-centric?
- What about I/O?
  - What do applications *need* (not what are they doing)?
  - Will problems with scalable, parallel I/O be what keeps massively parallel machines from succeeding?
    - *Are you sure? How much are you willing to bet? $100M? $200M?*

Where will we get (Sustained) Performance?

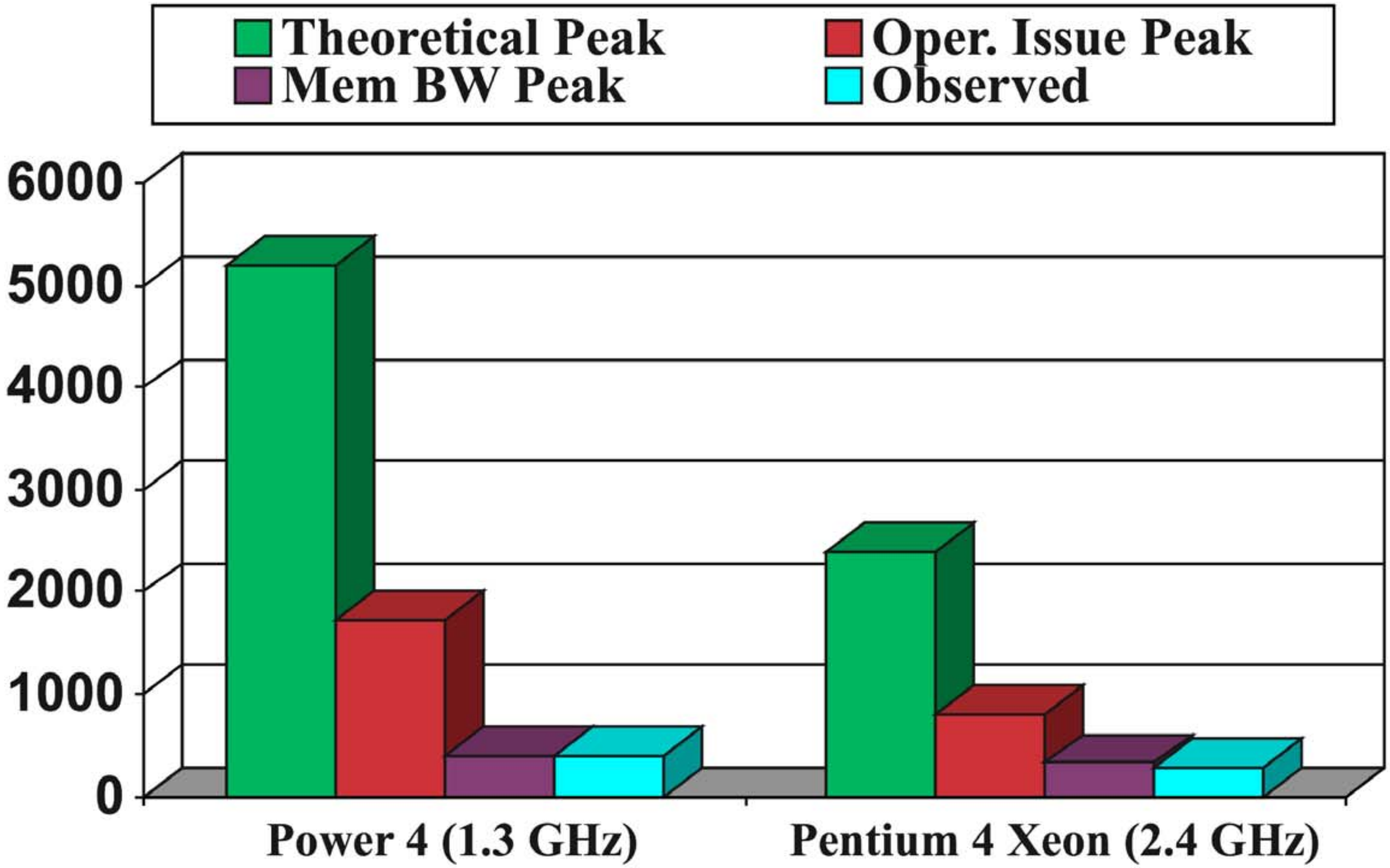


- Algorithms that are a better match for the architectures
- Parallelism at all levels
- Concurrency at all levels
- A major challenge is to realize these approaches in code
  - Most compilers do poorly with important kernels in computational science
  - Three examples - sparse matrix vector product, dense matrix-matrix multiply, flux calculation

Realistic Measures of Peak Performance

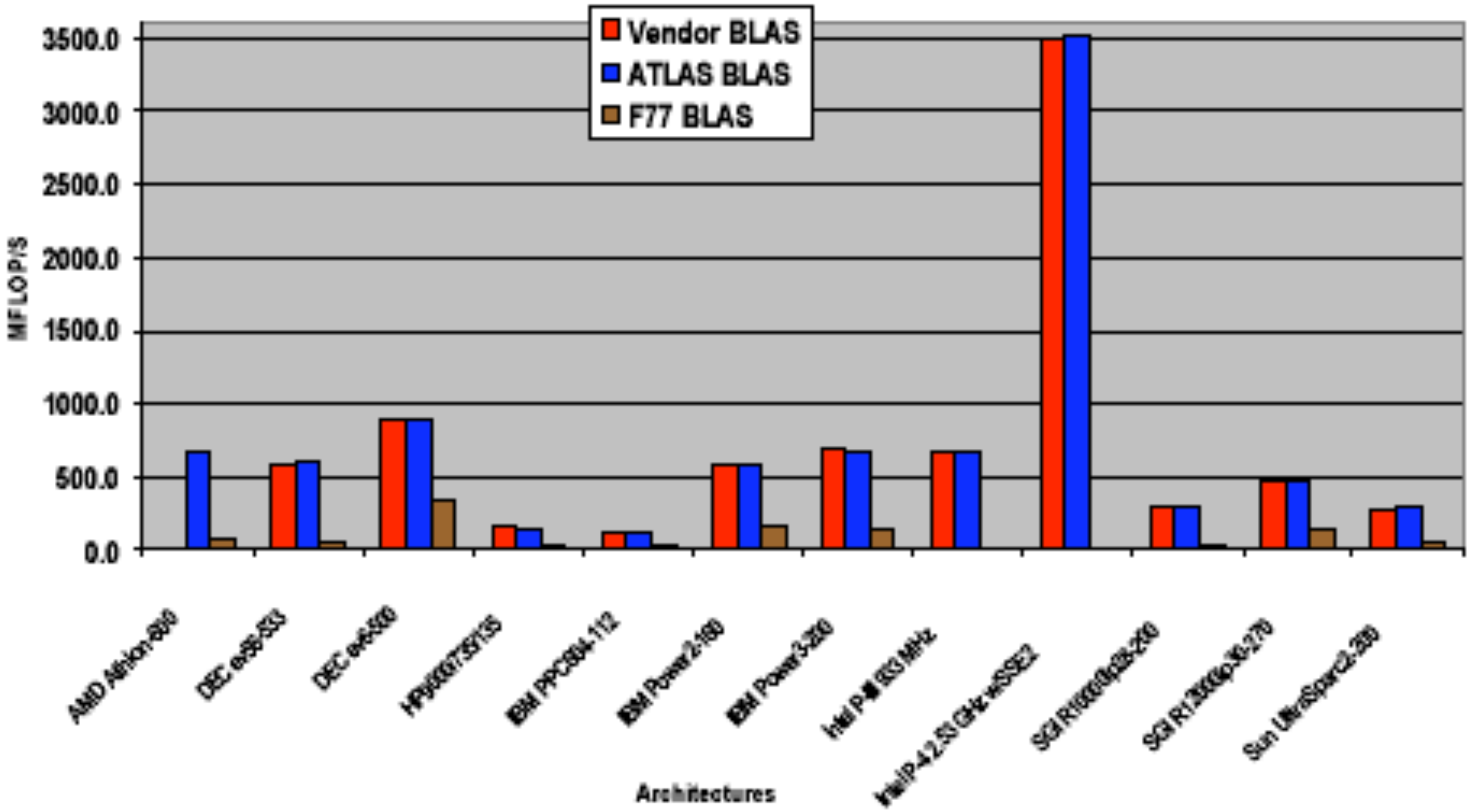
Sparse Matrix Vector Product

One vector, matrix size, m = 90,708, nonzero entries nz = 5,047,120

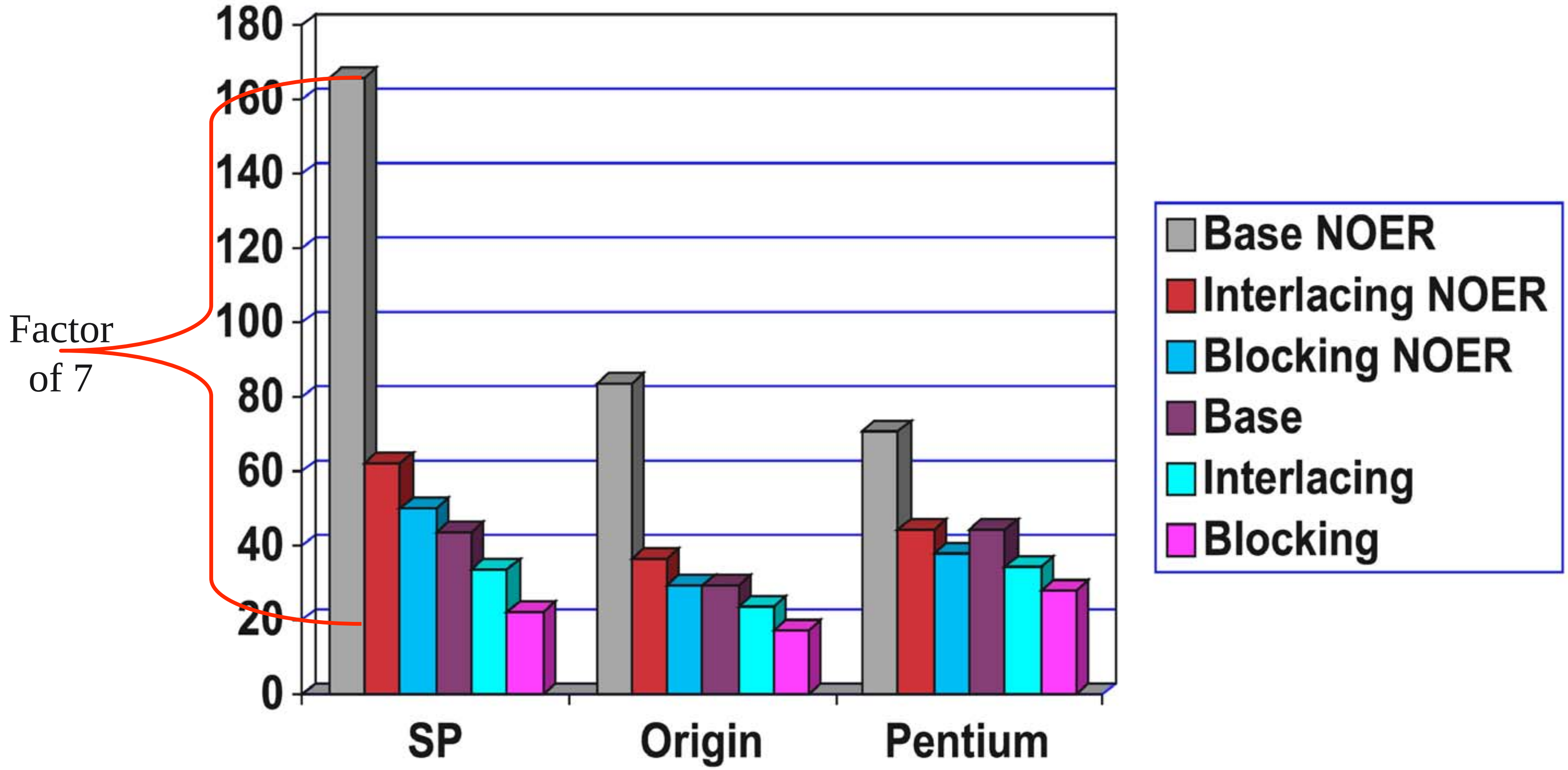


Thanks to Dinesh Kaushik;
ORNL and ANL for compute time

Very Few Compilers do well on DGEMM (n=500)



Effect of code transformations for uni-processor performance



Performance for Real Applications

- Dense matrix-matrix example shows that even for well-studied, compute-bound kernels, compiler-generated code achieves only a small fraction of available performance
  - “Fortran” code uses “natural” loops, i.e., what a user would write for most code
  - Others use multi-level blocking, careful instruction scheduling etc.
- Algorithms design also needs to take into account the capabilities of the system, not just the hardware
  - Example: Cache-Oblivious Algorithms (http://supertech.lcs.mit.edu/cilk/papers/abstracts/abstract4.html)
- Adding concurrency (whether multicore or multiple processors) just adds to the problems

Possible solutions

- Single, integrated system
  - Best choice when it works
    - *Matlab*
- Current Terascale systems and many proposed petascale systems exploit hierarchy
  - Successful at many levels
    - *Cluster hardware*
    - *OS scalability*
  - We should apply this to productivity software
    - *The problem is hard*
    - *Apply classic and very successful Computer Science strategies to address the complexity of generating fast code for a wide range of user-defined data structures.*
- How can we apply hierarchies?
  - One approach is to use libraries
    - *Limited by the operations envisioned by the library designer*
  - Another is to enhance the users ability to express the problem in source code

Annotations

- Aid in the introduction of hierarchy into the software
  - Its going to happen anyway, so make a virtue of it
- Create a “market” or ecosystem in transformation tools
- Longer term issues
  - Integrate annotation language into “host” language to ensure type safety, ensure consistency (both syntactic and semantic), closer debugger integration, additional optimization opportunities through information sharing, …

Examples of the Challenges

- Fast code for DGEMM (dense matrix-matrix multiply)
  - Code generated by ATLAS omitted to avoid blindness ☺
  - Example code from “Superscalar GEMM-based Level 3 BLAS”, Gustavson et al on the next slide
- PETSc code for sparse matrix operations
  - Includes unrolling and use of registers
  - Code for diagonal format is fast on cache-based systems but slow on vector systems.
    - *Too much code to rewrite by hand for new architectures*
- MPI implementation of collective communication and computation
  - Complex algorithms for such simple operations as broadcast and reduce are far beyond a compiler’s ability to create from simple code

A fast DGEMM (sample)

```
      SUBROUTINE DGEMM ( TRANSA, TRANSB, M, N, K, ALPHA, A, LDA, B, LDB,
     $                   BETA, C, LDC )
 ...
                  UISEC = ISEC-MOD( ISEC, 4 )
                  DO 390 J = JJ, JJ+UJSEC-1, 4
                     DO 360 I = II, II+UISEC-1, 4
                        F11 = DELTA*C( I,J )
                        F21 = DELTA*C( I+1,J )
                        F12 = DELTA*C( I,J+1 )
                        F22 = DELTA*C( I+1,J+1 )
                        F13 = DELTA*C( I,J+2 )
                        F23 = DELTA*C( I+1,J+2 )
                        F14 = DELTA*C( I,J+3 )
                        F24 = DELTA*C( I+1,J+3 )
                        F31 = DELTA*C( I+2,J )
                        F41 = DELTA*C( I+3,J )
                        F32 = DELTA*C( I+2,J+1 )
                        F42 = DELTA*C( I+3,J+1 )
                        F33 = DELTA*C( I+2,J+2 )
                        F43 = DELTA*C( I+3,J+2 )
                        F34 = DELTA*C( I+2,J+3 )
                        F44 = DELTA*C( I+3,J+3 )
                        DO 350 L = LL, LL+LSEC-1
                           F11 = F11 + T1( L-LL+1, I-II+1 )*
     $                                 T2( L-LL+1, J-JJ+1 )
                           F21 = F21 + T1( L-LL+1, I-II+2 )*
     $                                 T2( L-LL+1, J-JJ+1 )
                           F12 = F12 + T1( L-LL+1, I-II+1 )*
     $                                 T2( L-LL+1, J-JJ+2 )
                           F22 = F22 + T1( L-LL+1, I-II+2 )*
     $                                 T2( L-LL+1, J-JJ+2 )
                           F13 = F13 + T1( L-LL+1, I-II+1 )*
     $                                 T2( L-LL+1, J-JJ+3 )
                           F23 = F23 + T1( L-LL+1, I-II+2 )*
     $                                 T2( L-LL+1, J-JJ+3 )
                           F14 = F14 + T1( L-LL+1, I-II+1 )*
     $                                 T2( L-LL+1, J-JJ+4 )
                           F24 = F24 + T1( L-LL+1, I-II+2 )*
     $                                 T2( L-LL+1, J-JJ+4 )
                           F31 = F31 + T1( L-LL+1, I-II+3 )*
     $                                 T2( L-LL+1, J-JJ+1 )
                           F41 = F41 + T1( L-LL+1, I-II+4 )*
     $                                 T2( L-LL+1, J-JJ+1 )
                           F32 = F32 + T1( L-LL+1, I-II+3 )*
     $                                 T2( L-LL+1, J-JJ+2 )
                           F42 = F42 + T1( L-LL+1, I-II+4 )*
     $                                 T2( L-LL+1, J-JJ+2 )
                           F33 = F33 + T1( L-LL+1, I-II+3 )*
     $                                 T2( L-LL+1, J-JJ+3 )
                           F43 = F43 + T1( L-LL+1, I-II+4 )*
     $                                 T2( L-LL+1, J-JJ+3 )
                           F34 = F34 + T1( L-LL+1, I-II+3 )*
     $                                 T2( L-LL+1, J-JJ+4 )
                           F44 = F44 + T1( L-LL+1, I-II+4 )*
     $                                 T2( L-LL+1, J-JJ+4 )
  350                   CONTINUE
 ...
*     End of DGEMM.
*
      END
```

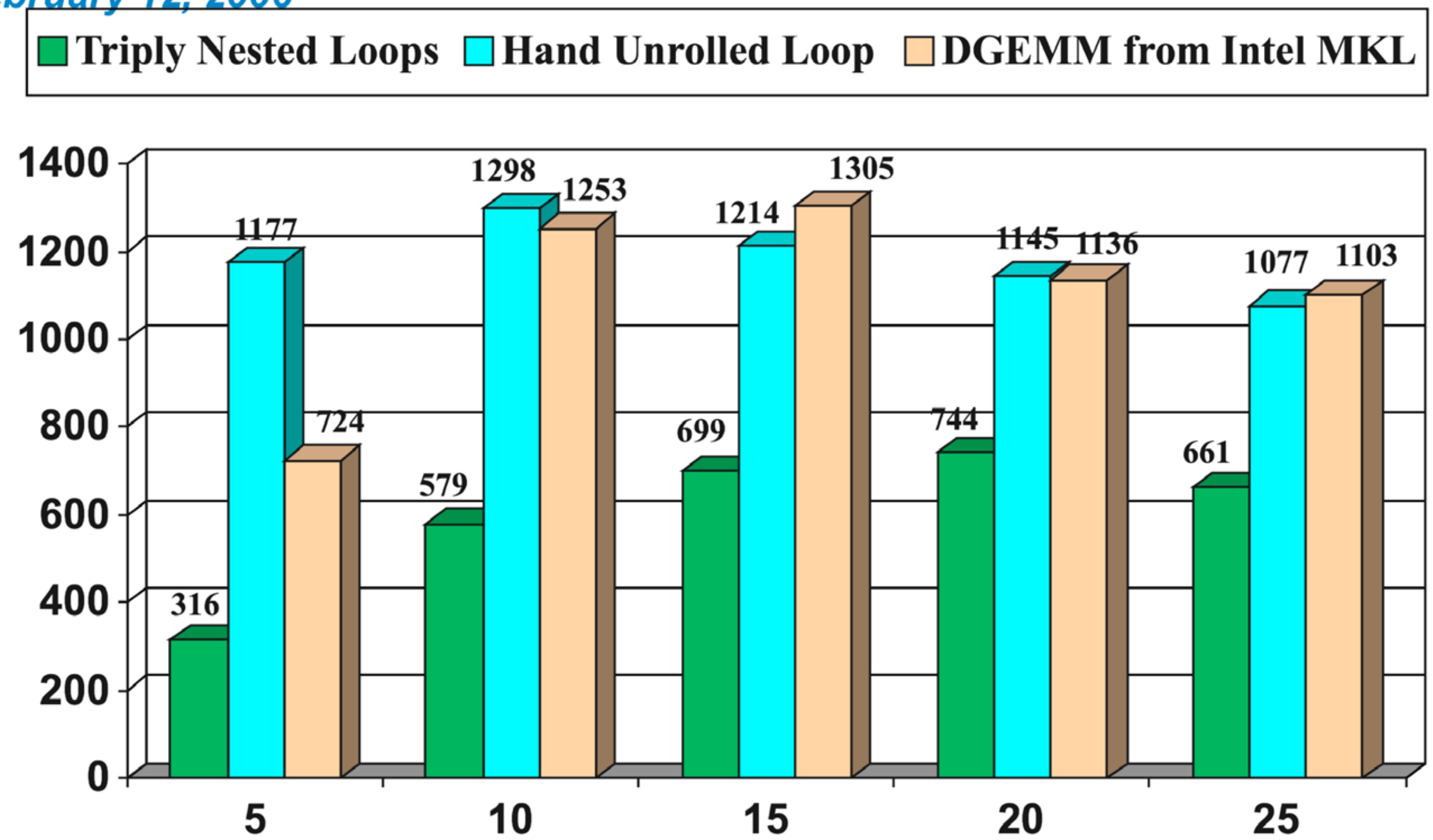
Note: This is just part of DGEMM!

Why not just

```
do i=1,n
   do j=1,m
      c(i,j) = 0
      do k=1,p
         c(i,j) = c(i,j) + a(i,k)*b(k,j)
     enddo
  enddo
enddo
```

*Performance of Matrix-Matrix Multiplication (MFlops/s vs. n2; n1 = n2; n3 = n2*n2)*

Intel Xeon 2.4 GHz, 512 KB L2 Cache, Intel Compilers at –O3 (Version 8.1), February 12, 2006



Observations

- Much use of mechanical transformations of code to achieve better performance
  - Compilers do not do this well
    - *Too many other demands on the compiler*
- Use of carefully crafted algorithms for specific operations such as allreduce, matrix-matrix multiply
  - Far more challenging than the performance transformations
- Increasing acceptance of some degree of automation in creating code
  - ATLAS, PhiPAC, TCE
  - Source-to-source transformation systems
    - *E.g., ROSE, Aspect Oriented Programming (asod.net)*

Key Observations

- 90/10 rule
  - current languages adequate for 90% of code
  - 10% of code causes 90% of trouble
- Memory hierarchy issues a major source of problems
  - Significant effort is put into relatively mechanical transformations of code
  - Other transformations are avoided because of their negative impact on the readability and maintainability of the code.
    - *Example is loop fusion for routines that sweep over a mesh to apply different physics. Fusion, needed to reduce memory bandwidth requirements, breaks modularity of routines written by different groups.*
- Coordination of distributed data structures another major source of problems
  - But the need for performance encourages a global/local separation
    - *Reflected in PGAS languages*
- New languages may help, but not anytime soon
  - New languages will never be the entire solution
  - Applications need help now

One Possible Approach

- Use annotations to augment existing languages
  - Not a new approach; used in HPF, OpenMP, others
  - Some applications already use this approach for performance portability
    - *WRF weather code*
- Annotations do have limitations
  - Fits best when most of the code is independent of the parts affected by the annotations
  - Limits optimizations that are available to approaches that augment the language (e.g., telescoping languages)
- But they also have many advantages…

Annotations example: STREAM triad.c for BG/L

```
void triad(double *a, double *b, d
{
  int i;
  double ss = 1.2;
  /* --Align;;var:a,b,c;; */
  for (i=0; i<n; i++)
    a[i] = b[i] + ss*c[i];
 /* --end Align */
}
```

```
void triad(double *a, double *b, double *c, int n)
{
#pragma disjoint (*c,*a,*b)
  int i;
  double ss = 1.2;
  /* --Align;;var:a,b,c;; */
 if ( ((int)(a) | (int)(b) | (int)(c)) & 0xf == 0) {
   __alignx(16,a);
   __alignx(16,b);
   __alignx(16,c);
  for (i=0;i<n;i++) {
    a[i] = b[i] + ss*c[i];
 }
 }
 else {
    for (i=0;i<n;i++) {
        a[i]=b[i] + ss*c[i];
 }
  /* --end Align */
}
```

Simple annotation example: STREAM triad.c on BG/L

Size	No Annotations (MB/s)	Annotations (MB/s)	
10	1920.00	2424.24	
100	3037.97	6299.21	
1000	3341.22	8275.86	2.5X
10000	1290.81	3717.88	
50000	1291.52	3725.48	
100000	1291.77	3727.21	2.9X
500000	1291.81	1830.89	
1000000	1282.12	1442.17	
2000000	1282.92	1415.52	
5000000	1290.81	1446.48	1.12X

Summary

- Provide tools to help computational scientists build transportable, high-performance applications by working *with*, not against the compiler
- Enable an ecosystem so that tools can compete
  - Enables and rewards research and development
- Lowers the barrier to introducing more complex data structures and algorithms

- And don't forget the I/O!