A User’s View of OpenMP: The Good, The Bad, and The Ugly

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But First:
MPI Fact and Fiction

- MPI requires buffering
  - False. MPI was specifically designed to avoid buffering
  - A few implementations need work (sometime in the OS)
- MPI requires n^2 buffers for n processes
  - False, but most implementations need work
- MPI defined in the 80's
  - MPI Forum's first meeting was in January 1993
- MPI was derived from PVM
  - MPI emerged from a broad consensus of message-passing vendors, researchers, and users.
- MPI thread safety
  - MPI (the standard) was designed to *allow* thread-safe implementations but not require them (performance tradeoffs)
  - MPI_Init_thread (MPI-2) allows an application to request and discover the level of thread safety (4 levels defined)

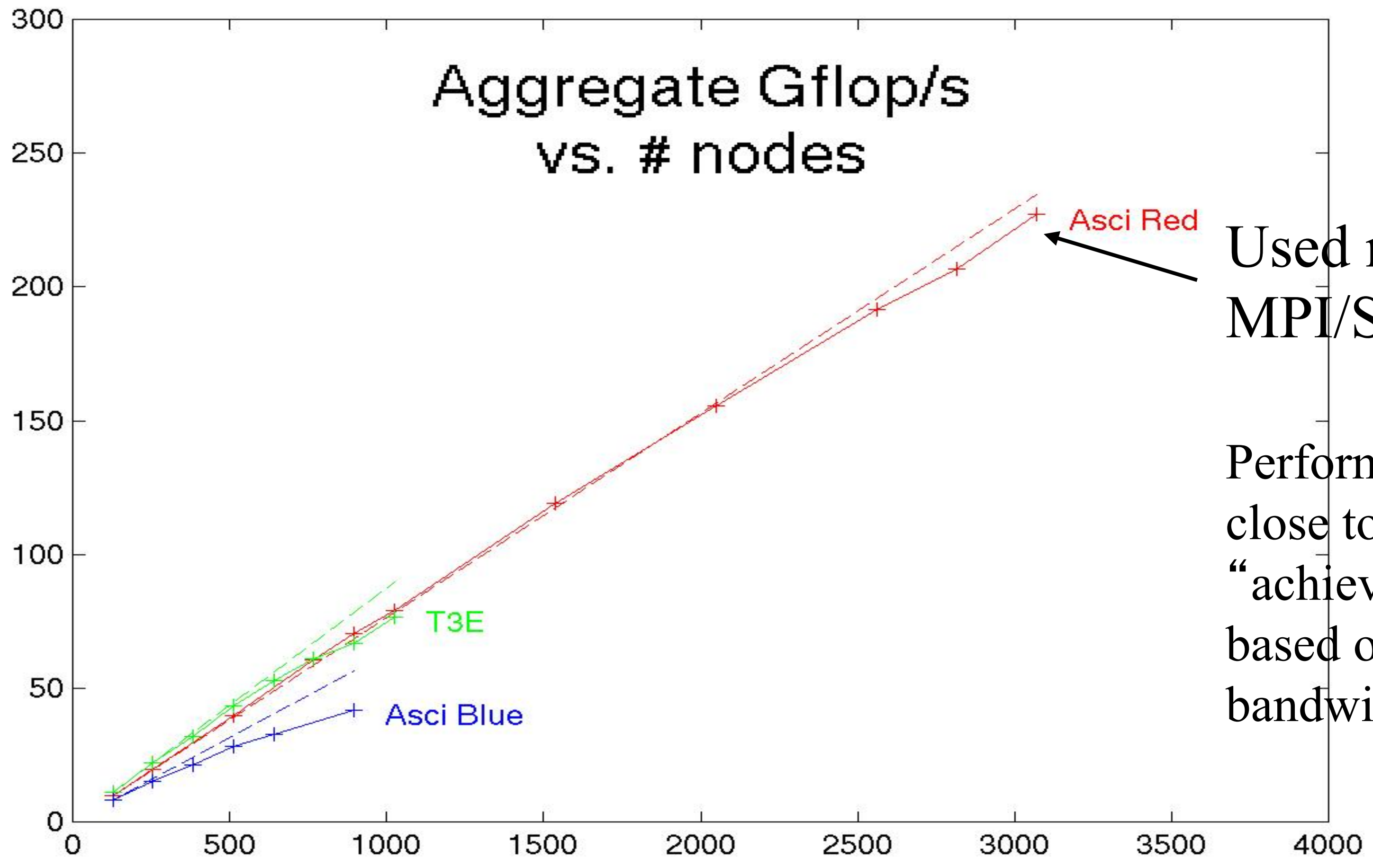
Outline

- The Good
  - Successful use of incremental parallelism
  - (Relatively) easy realization of better algorithms
- The Not so Good
  - Limitations in OpenMP impacted code
  - OpenMP version 2 fixes some (Thanks!)
- The Bad
  - Lack of effective support for modularity and libraries
  - Incorrect programs (that run) are too easy to write
- The Ugly
  - Implementation Issues
  - Mixed C and Fortran applications

What We've Done

- Fun3d-PETSc (1999 Gordon Bell winner)
- Tetrahedral vertex-centered unstructured grid code developed by W. K. Anderson (NASA LaRC) for steady compressible and incompressible Euler and Navier-Stokes equations (with one-equation turbulence modeling)
- Used in airplane, automobile, and submarine applications for analysis and design
- Standard discretization is 2nd-order Roe for convection and Galerkin for diffusion
- Original code used Newton-Krylov solver with global point-block-ILU preconditioning
- Parallel version uses Newton-Krylov-Schwarz, with domain-induced point-block ILU preconditioning

Fun3d Performance



Used mixed MPI/SMP model

Performance close to "achievable peak" based on memory bandwidth

Primary PDE Solution Kernels

loop

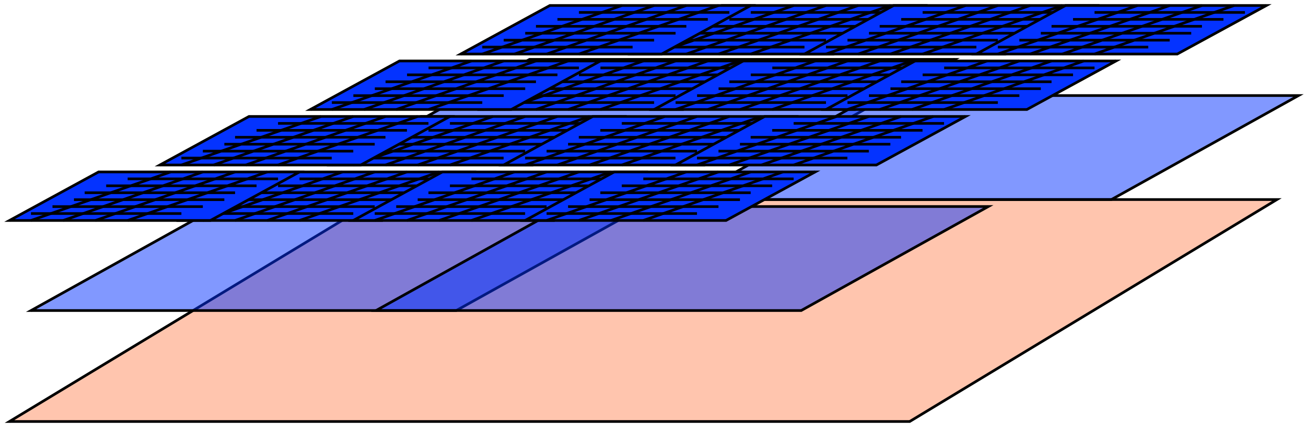
- Vertex-based loops
  - ♦ State vector and auxiliary vector updates
- Edge-based “stencil op” loops
  - ♦ Residual evaluation
  - ♦ Approximate Jacobian evaluation
  - ♦ Jacobian-vector product (often replaced with matrix-free form, involving residual evaluation)
- Sparse, narrow-band recurrences
  - ♦ Approximate factorization and back substitution
- Vector inner products and norms
  - ♦ Orthogonalization/conjugation
  - ♦ Convergence progress and stability checks

task

- **Preconditioned linear (and nonlinear) solution**

Multi-level Numerical Methods

- Domain Decomposition Preconditioner
  - ♦ Efficient method *independent* of parallelism
  - ♦ Multilevel method is a good match to multilevel memory hierarchy without sacrificing convergence rate



Leads to an efficient algorithm for solving nonlinear PDEs:

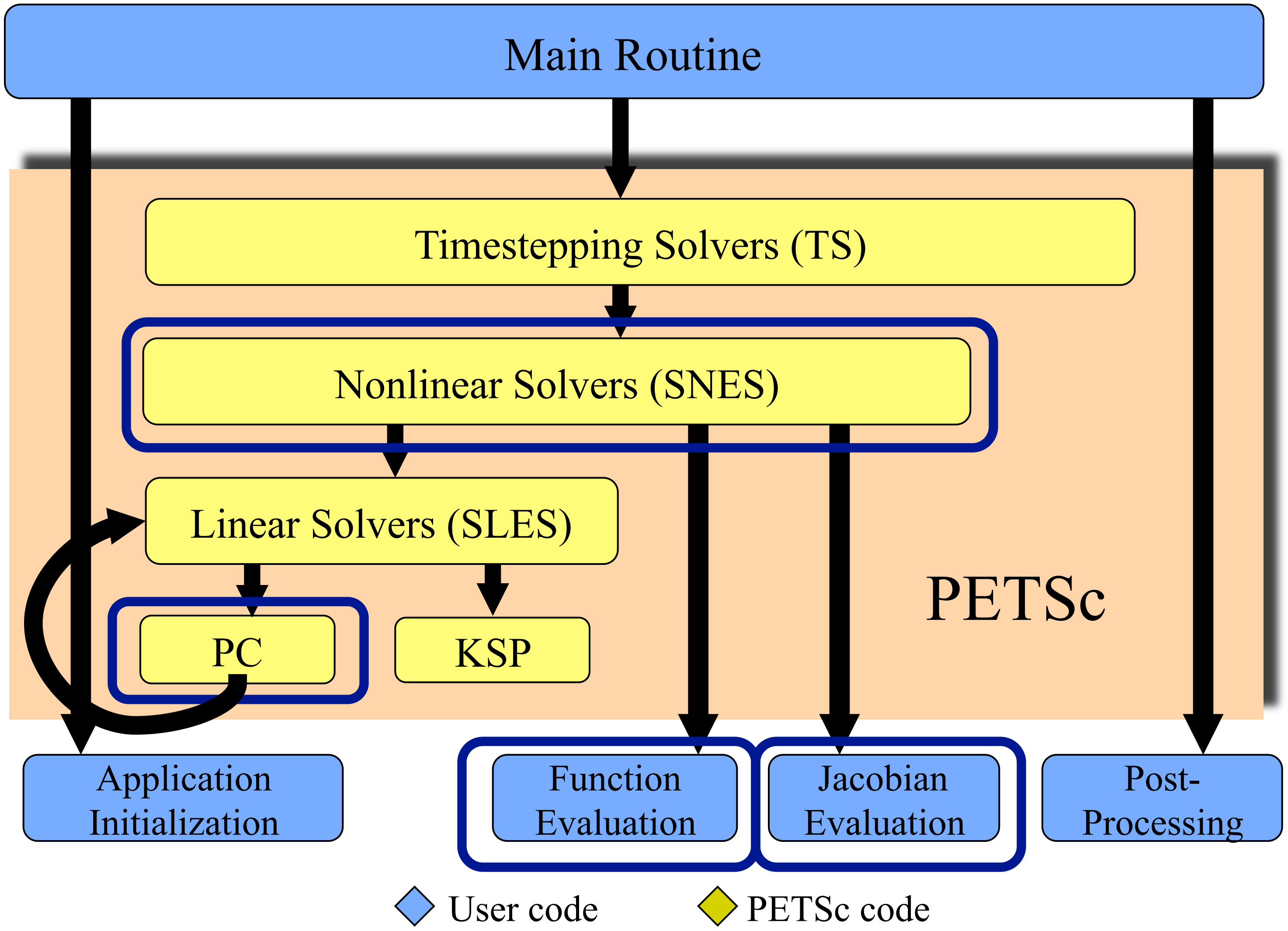
Time-Implicit Newton-Krylov-Schwarz Method

```
for (l = 0; l < n_time; l++) {                                  # n_time ~ 50
    select time step
    for (k = 0; k < n_Newton; k++) {                            # n_Newton ~ 1
      compute nonlinear residual and Jacobian
        for (j = 0; j < n_Krylov; j++) {                        # n_Krylov ~ 50
          forall (i = 0; i < n_Precon ; i++) {
              solve subdomain problems concurrently
          } // End of loop over subdomains
          perform Jacobian-vector product  ←
          enforce Krylov basis conditions
          update optimal coefficients
          check linear convergence
        } // End of linear solver
      perform DAXPY update
      check nonlinear convergence
    } // End of nonlinear loop
} // End of time-step loop
```

Leaf
Recursion

This is implemented in a parallel library…

Separation of Concerns: User Code/PETSc Library



Background of PETSc

- Developed by Gropp, Smith, McInnes & Balay (ANL) to support research, prototyping, and production parallel solutions of operator equations in message-passing environments
- Distributed data structures as fundamental objects—index sets, vectors/gridfunctions, and matrices/arrays
- Iterative linear and nonlinear solvers, combinable modularly and recursively, and extensibly
- Portable, and callable from C, C++, Fortran
- Uniform high-level API, with multi-layered entry
- Aggressively optimized: copies minimized, communication aggregated and overlapped, caches and registers reused, memory chunks preallocated, inspector-executor model for repetitive tasks (e.g., gather/scatter)
- Supports a wide variety of sparse matrix formats, including user-defined.
- Extensible with user-defined preconditioners, iterative methods, etc.

Parallel Fun3d

- Uses PETSc for parallelism
  - Almost no MPI in Fun3d itself
  - MPI used only for initialization from data files
- OpenMP
  - Used only for flux evaluation
- Where did programmer time go?
  - Uniprocessor performance tuning
  - Primarily *locality* management
- (Parallel programming is easy compared to performance programming)
- Why was OpenMP only used for the flux evaluation?

Competing for the Available Memory Bandwidth

- The processors on a node compete for the available memory bandwidth
- The computational phases that are memory-bandwidth limited will not scale
  - They may even run slower because of the extra synchronizations

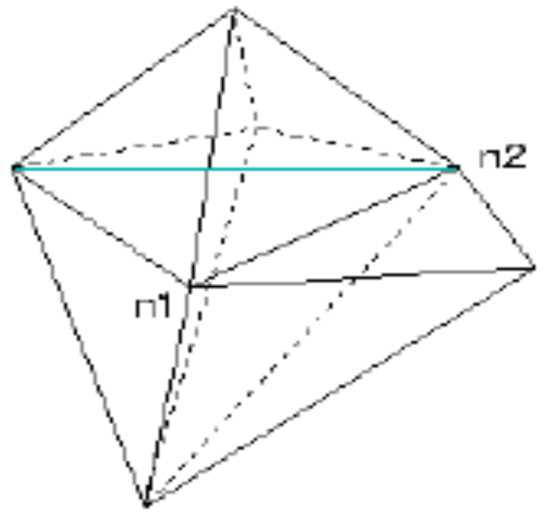
Stream Benchmark on ASCI Red MB/s for the Triad Operation

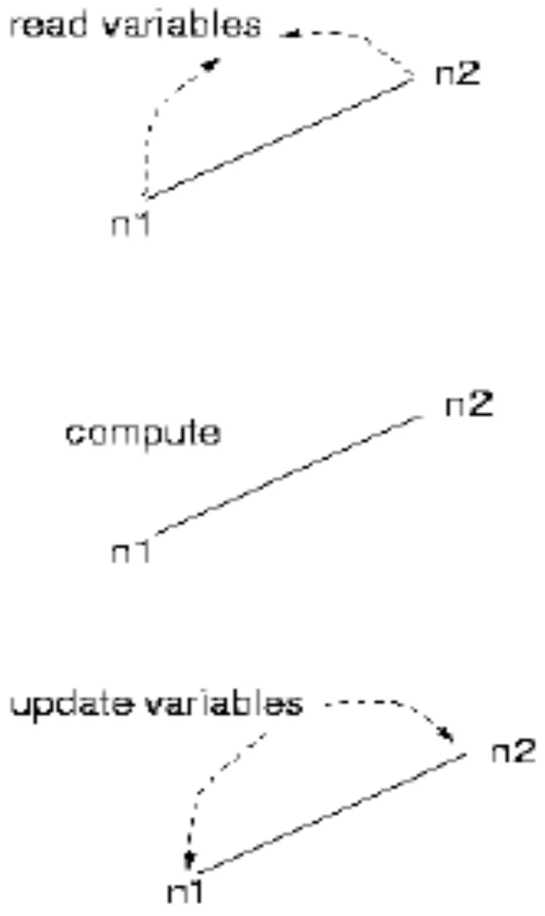
Vector Size	1 Thread	2 Threads
10^4	666	1296
5×10^4	137	238
10^5	140	144
10^6	145	141
10^7	157	152

Redundant Storage and Work

- To manage memory updates efficiently, we might need to create extra private work arrays
- These work arrays need to be copied into a shared array at the end of the parallel region
    - A memory-bandwidth limited sequential phase
- The vector reduction in OpenMP v.2 may help

Flux Evaluation in PETSc-FUN3D





Variables at each node:
density,
momentum (*x,y,z*),
energy,
pressure

Variables at edge:
identity of nodes,
orientation(*x,y,z*)

Apply the “Owner Computes” Rule for OpenMP

- Create the disjoint working sets to eliminate the redundant private arrays (e.g. by coloring the edges and nodes)
- Alternatively, use OpenMP over subdomains
  - each MPI process will repartition its domain
  - each thread will work on its assigned subdomain
- Brings in the complexity of programming as the user is taking care of the memory updates

MPI/OpenMP in PETSc-FUN3D

- Only in the flux evaluation phase as it is not memory-bandwidth bound
- Gives the best execution time as the number of nodes increases because the subdomains are chunkier as compared to pure MPI case

Nodes	MPI/OpenMP		MPI	
	1 Thr	2 Thr	1 Proc	2 Proc
256	483s	261s	456s	258s
2560	76s	39s	72s	45s
3072	66s	33s	62s	40s

For the Fun3d Application:

- The 1-thread/process case shows loop overhead costs in OpenMP implementation
- OpenMP allows the *easy* implementation of a *better* algorithm
- Vector reduction should improve the OpenMP advantage

The Good

- Effective Incremental Parallelism
  - ♦ Important contributor to ASCI Red results (not exactly OpenMP, but same philosophy)
- Good SMP and SMP-cluster match
  - ♦ Larger domain decomposition blocks
  - ♦ Encourages more dynamic code

The Not so Good

- Performance
  - In apples-to-apples comparison with MPI
  - Data placement important
  - Cache blocking etc. mismatch with OpenMP loop scheduling
- Restrictions on atomic update/reduce
  - No vector reduce (p 29) (but see OpenMP 2.0)
  - Complexity *for user* comes from exceptions and limitations

The Bad

- Program correctness
  - It is too easy to write incorrect programs
- Software Modularity
  - At best 2-level modularity
  - Many modern algorithms built out of components; how will OpenMP support them?
  - E.g., each component uses limited parallelism to fit problem into local caches; application uses task parallelism to perform intelligent (not exhaustive parameter-space search) design optimization.

Program Correctness

- It is much too easy to write incorrect programs
- Updates to variables
  - Should be atomic unless specifically requested (see p 21)
  - Principle: user *omission* of a directive shouldn't *create* incorrect code
  - Current model is like Fortran implicit typing—convenient if you never make a mistake
- Volatile?
  - Even better, shared non-volatile (read-only shared)
- Consistency model
  - What is the model?
    - Not sequential consistency (see atomic, flush)
- Example: Using flags instead of locks
  - Requires FLUSH (maybe not so bad, but the documentation is not sufficient for users to understand the need for this operation)

Software Modularity

- Libraries must either
  - Use OpenMP at “leaves” (e.g., the loop-level), or
  - Take complete control (user program has no OpenMP parallelism when library is called).
  - But some libraries call other library routines …
    - E.g., should BLAS use OpenMP? LAPACK? What if user uses OpenMP for task parallelism for a routine that calls an LAPACK routine?
- Using OpenMP at loop-level incurs startup costs
  - Some vendors suggest

    -
      ```
      Program Main
      !omp parallel
      …
      !omp end parallel
      stop
      end
      ```
- OpenMP language bindings poorly chosen for mixed-language programming
  - I.e., programs that use libraries …

Language Bindings for Mixed Language Programming

- Libraries used by Fortran may be written in C (and vice versa)
  - OpenMP naming convention can make this (nearly) impossible
- C names should *always* be distinguishable from Fortran names
  - Unless bindings are *identical*
  - Using mixed case for C (as in MPI) is an easy way to do this
- Consider (from SGI)
  - f77 –noappend –c –mp s1.f
  - cc –mp –o s2 s2.c s1.o

Simple Mixed-Language Program

-
  ```
  subroutine setnthreads(req)
  integer req
  call omp_set_num_threads(req)
  end
  ```

-
  ```
  #include <stdio.h>
  #include <omp.h>
  int main(int argc, char *argv[] )
  {
      int n_c, n_f, req=4;
      setnthreads(&req);
  #pragma omp parallel
  {
      n_f = omp_get_num_threads();
  }
      omp_set_num_threads( req );
  #pragma omp parallel
  {
      n_c = omp_get_num_threads();
  }
      printf( "n_c=%d n_f=%d\n", n_c, n_f );
  }
  ```

What is printed out?

n_c=4 n_f=8

8 is the default maximum number of threads

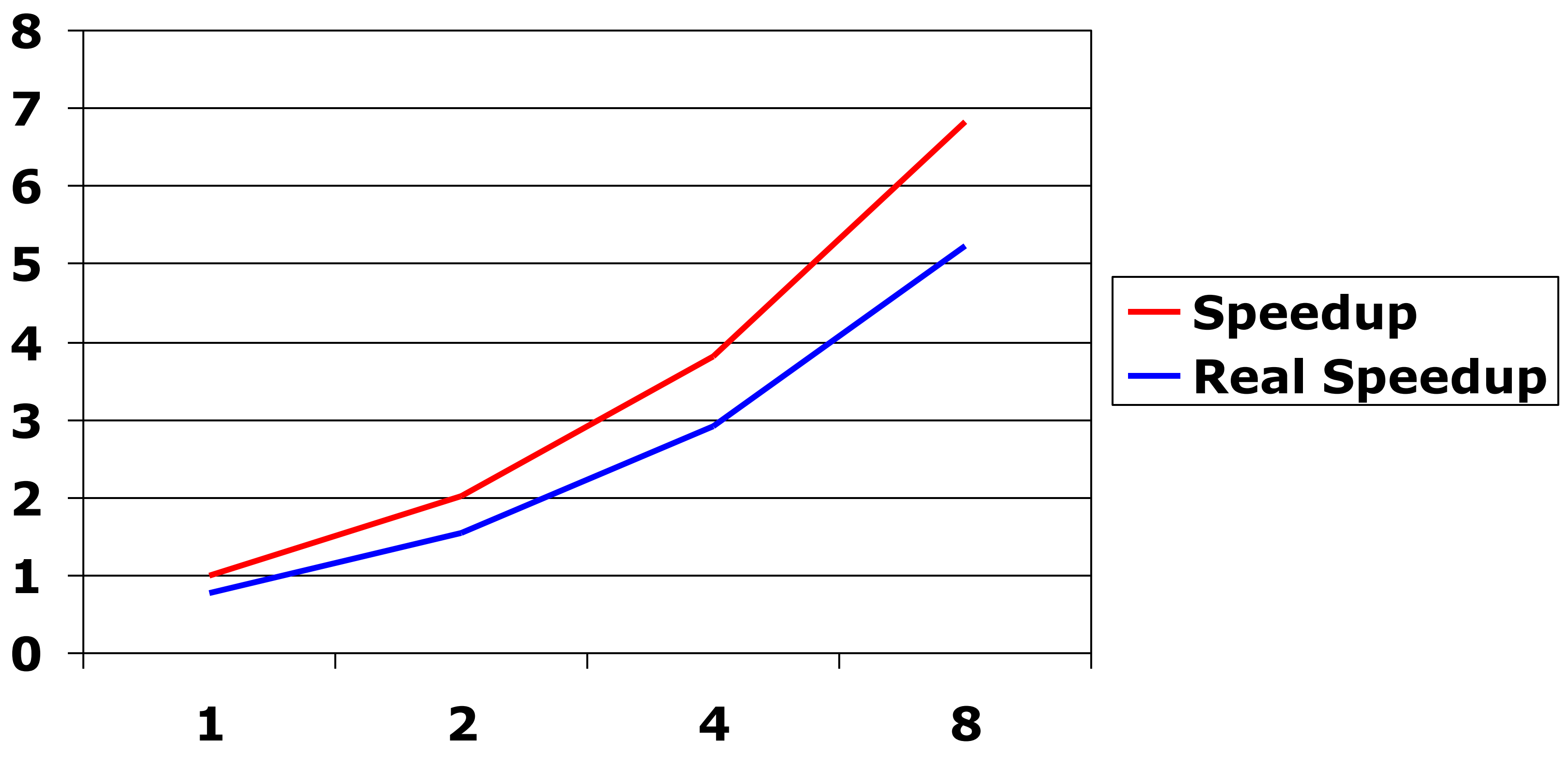
Performance

- Data distribution matters for performance
  - There are *no* UMA machines
    - (cache, vector registers, even if all main memory is uniformly far away)
- C mallocs (all shared; scalability?)
  - Task parallel applications; data is primarily private
  - Ok for SMP platforms, but what about DSM?
- No way to get the compiler to compute good dynamic blocking (default chunk = 1)
  - OpenMP directives tell the compiler to do something specific
  - Does not match user model
    - E.g., -O often includes "unroll by a good amount"
    - Does not mean that user-control is not valuable, just that some decisions are system dependent

The Ugly
(E.g. Implementation Problems)

- David Bailey's rule #8 (roughly)
  - ♦ Base the operation count on the parallel implementation, not the best sequential implementation
- Early tests with Fun3D showed base OpenMP case (1 thread/process) took longer than reference MPI case.
- Consider the performance of the jacobi.f example from www.openmp.org :

Scaling of an OpenMP Example



Data Placement

- Performance often depends on managing memory motion
- First touch is inadequate
  - ♦ Requires code just for OpenMP version
  - ♦ Conflicts with incremental parallelism
    - Requires parallelization of initialization
  - ♦ Conflicts with libraries that may share data
- Dependent on page/cache line size
  - ♦ Architecture-dependent information
  - ♦ The compiler (often) has this information: let OpenMP use it

Conclusions

- OpenMP provides good support for incremental parallelism; integrates well with other tools
- Needs attention to
  - ♦ Modularity
    - Good support for single-level and two-level codes
    - Thread groups or something else needed for libraries
  - ♦ Software engineering
    - Incorrect programs are too easy to write
    - Mixed-language programming needs to be fixed
  - ♦ Performance
    - Data motion expensive
- Backward-compatible improvements can be made