Code Performance Analysis

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Performance

- Theoretical peak performance of the ASCI machines are in the Teraflops range, but sustained performance with real applications is far from the peak
  - Salinas, one of the 2002 Gordon Bell Awards, was able to sustain 1.16 Tflops on ASCI White (less than 10% of peak)
- On the Earth Simulator, a custom engineered system with exceptional memory bandwidth, interconnect performance and vector processing capabilities
  - Global atmospheric simulation was able to achieve 65% of the 40 Tflops of peak performance

Applications

- Our main applications, CDP and TFLO, are coded in F90 and use MPI for message passing.
  - CDP: LES unstructured finite volume code for the combustor:
    - Uses a lot of advanced features of F90
  - TFLO: RANS multi-block structured finite volume code for the turbo-machinery.
    - Uses F90 features mainly for flexible data-structures (derived data type and pointer)

Objective

- Our objective is to have portable, fast and scalable codes
- Portability and performance are often conflicting requirements
- Strike a balance between codes that are easy to maintain and perform well.

- To achieve high performance, particular attention needs to be devoted to unrolling, software pipelining, etc.
- We express our intent in the code and let the compiler do the tuning:
  - Hand tuning is going to affect portability
  - The compiler usually does a better job

Example

```
do i=1,n
    A(i) = A(i) + B(i)*C
end do
```

Simple code	Unrolled 4x	Unrolled 4x, pipelined
1 ldt Ai; ldt Bi 2 3 4 5 mult Bi 6 7 8 9 addt Ai 10 11 12 13 stt Ai; bne loop	1 ldt Bi; ldt Bi+1 2 ldt Bi+2; ldt Bi+3 3 ldt Ai; ldt Ai+1 4 ldt Ai+2; ldt Ai+3 5 mult Bi 6 mult Bi+1 7 mult Bi+2 8 mult Bi+3 9 addt Ai 10 addt Ai+1 11 addt Ai+2 12 addt Ai+3 13 stt Ai 14 stt Ai+1 15 stt Ai+2 16 stt Ai+3; bne loop	1 ldt Bi ;ldt Bi+1; mult Bi-4;addt Ai-8 2 ldt Bi+2 ;ldt Bi+3; mult Bi-3;addt Ai-7 3 ldt Ai ;ldt Ai+1; mult Bi-2;addt Ai-6 4 ldt Ai+2 ;ldt Ai+3; mult Bi-1;addt Ai-5 5 stt Ai-12;stt Ai-11 6 stt Ai-10;stt Ai-9;bne loop
13 cycles per iteration	4 iteration in 16 cycles = 4 cycles per iteration	4 iteration in 6 cycles = 1.5 cycles

Alpha EV68: 4 cycles for f.p. load from cache;
f.p. add and multiply 4 cycles (pipelined)

Performance tuning

- Coding style
- Compilers
- Message passing implementation

Code style / compiler interaction

```
integer, parameter:: rfp=kind(0.d0)
  type adt_type
    real(kind=rfp), dimension(:,:,:), pointer :: Ex, Ey, Ez, Hx, Hy, Hz
  end type adt_type

real(kind=rfp), dimension(:,:,:), allocatable :: Ex, Ey, Ez, Hx, Hy, Hz
type(adt_type) :: a


call update_array(Ex,Ey,Ez,Hx,Hy,Hz,n)

call update_adt(a,n)

call update_array(a%Ex,a%Ey,a%Ez,a%Hx,a%Hy,a%Hz,n)
```

Effect of coding style

All values in MFlops	ASCI Q Compaq F90	Blue Horizon xlf	Origin 300 Mips Pro	P4 IFC 7.1	P4 PGI 4.02
Using F77 style arrays	1509	543	545	749	423
Using derived data type	665	395	382	369	47
Using components of the derived data type	1501	191	532	743	423

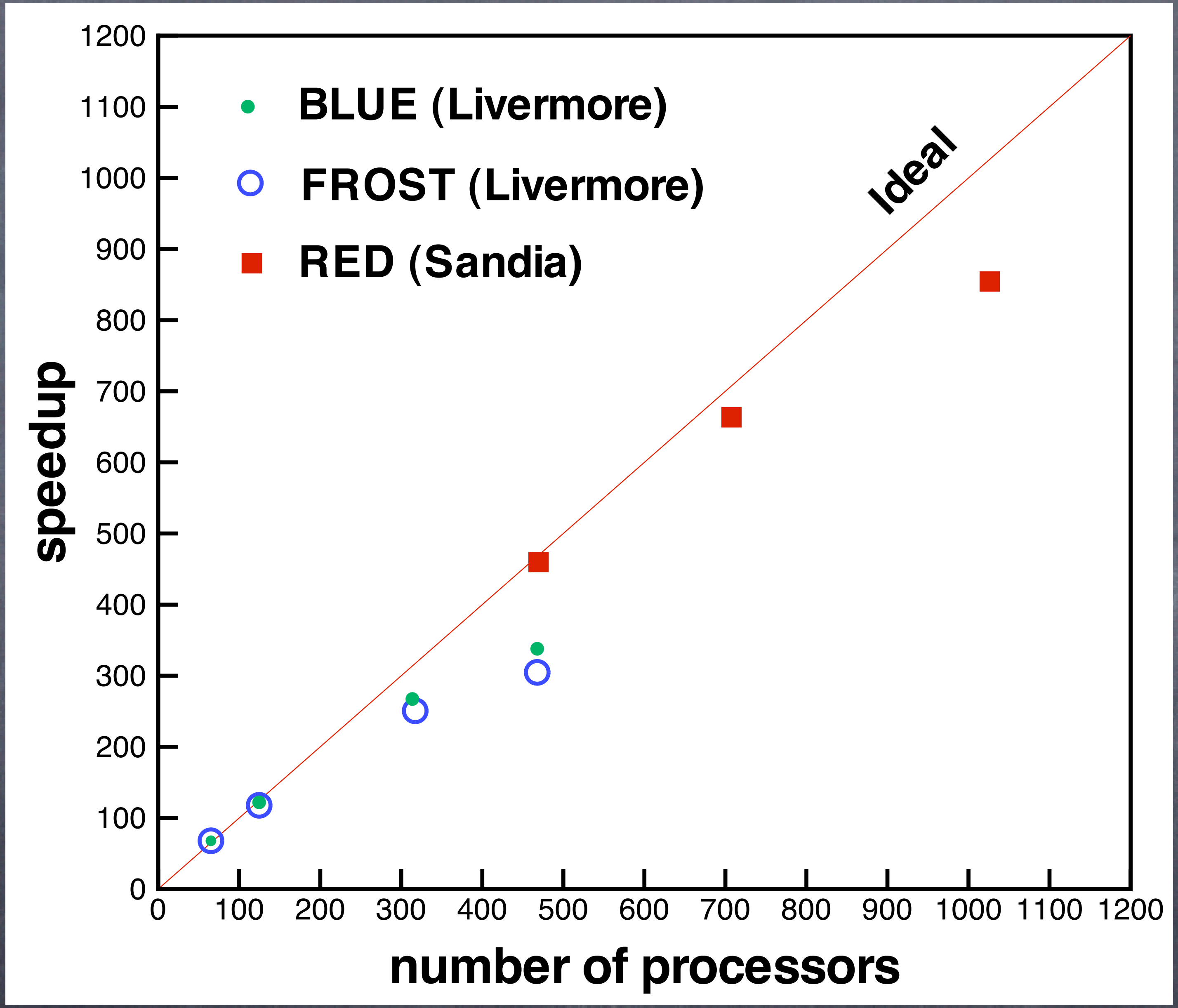
TFLO

- The current version of TFLO stores everything in 1D arrays and uses starting indices for every block and multigrid level.
- The new version of TFLO uses derived datatype and pointers
  - The new version is 10-20% slower
  - The new version is more readable and maintainable
  - Implementing new algorithms and turbulence models is much easier

Code performance

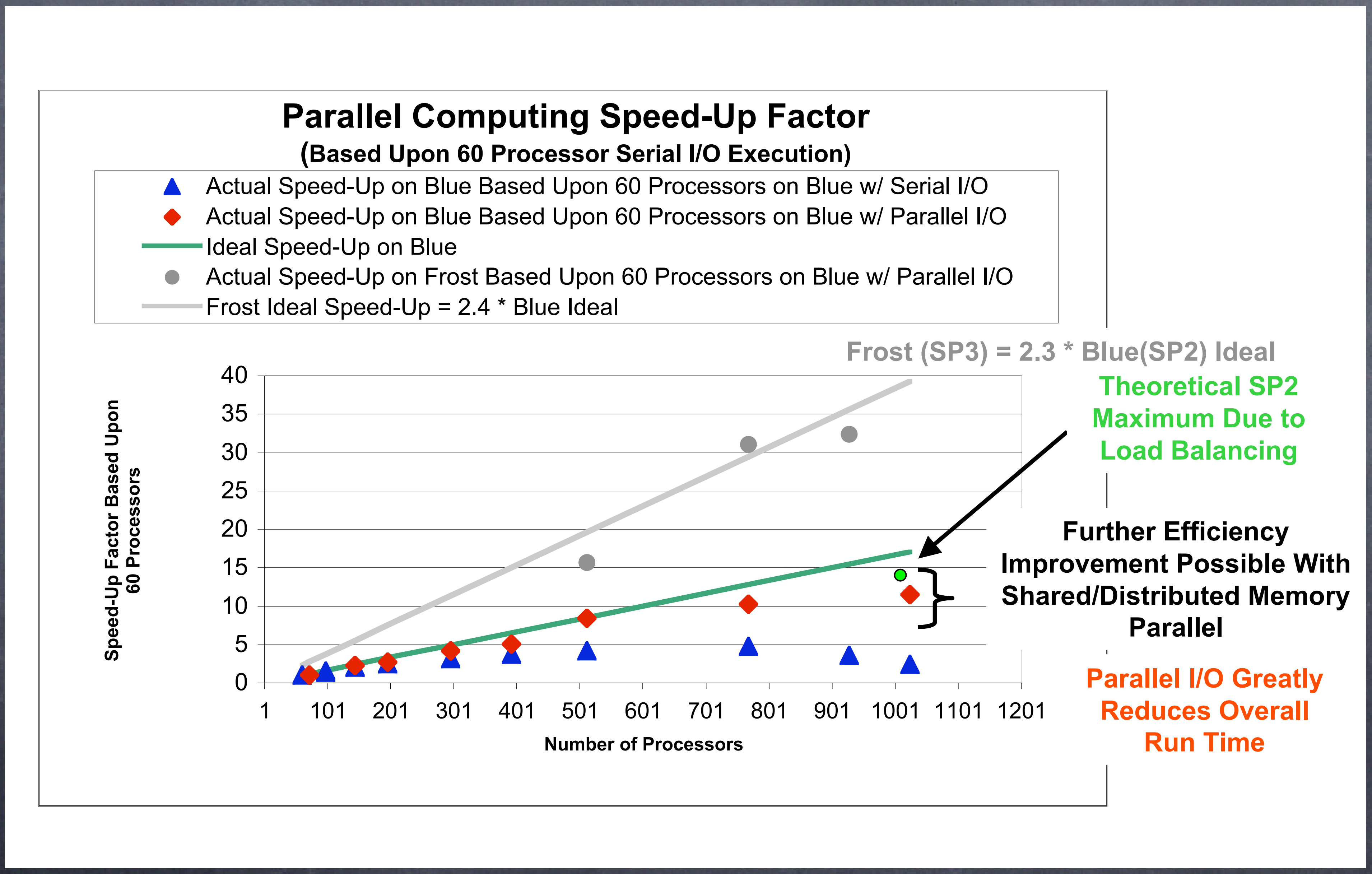
- Machine: FROST (IBM SP3, Power3 at 375 Mhz) Peak rate 1500 Mflops
  - CDP: LES of a reacting flow in a coaxial combustor
    GRID 2.5 million control volumes 64 proc total memory 3GB or 1.22 GB/million CV's
    Performance measured with hpmcount: 87 MFlops
  - TFLO: 210 Mflops

CDP scalability test



16 million control volumes

TFLO scalability test



Queue systems

The interaction with the queue system is an important factor in the choice of the number of nodes for a run:

- Lower bound: memory needed by the code
- Upper bound: number of CPUs available
- Frequency of high node count availability is very low

Performance metric

- What is really important, it is the Time to Solution
  - I/O can account for a large portion of the runtime
  - Improving the pre/post processing steps
- The real gain usually comes from algorithm improvement

Future work

- We are going to devote more efforts to performance analysis once the code implementation is complete:
  - improve the single node performance
  - improve the network performance