CASK, Cray Adaptive Sparse Kernels

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CScADS 2008, Summer Workshop 2008

Questions we are going to answer

- What architecture/platform should we target?
  - Cray's systems!
- Will self-tuned libraries always outperform compiler-generated code?
  - Yes, because we search the best combination of compiler's tuning flags and auto-generated code.
- Will simple performance models obviate the need for empirical search?
  - Simple and **good** performance models would reduce the search space a lot (since we do just for Cray).

Cray's role in libraries (in the past)

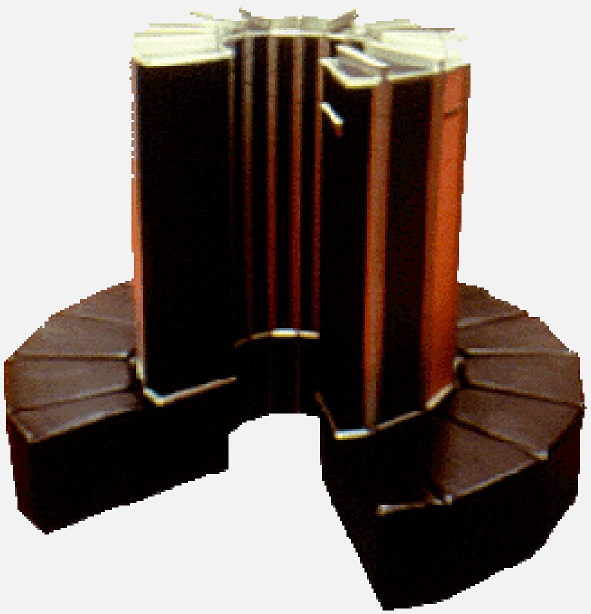
- Early Cray machines were important in the evolution of Math Software – e.g. BLAS 3

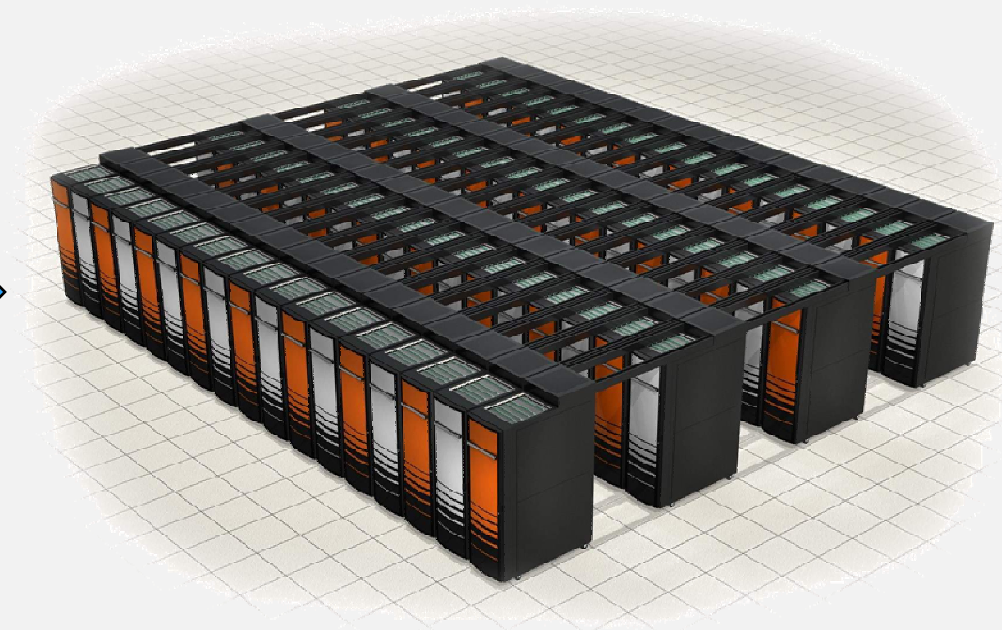
- Extensive tuning of BLAS and FFT in assembly language
  - Tuned for Cray's hardware (usually vector)

- Provide custom sparse solvers and special data structures
- Things were simple then
  - Same or similar ISA
  - Hardware complexity was at register level
  - Single processing cores and bandwidth galore
  - API's were sufficient for good performance
  - Custom solvers were attractive

Nothing was adaptive because it was not necessary

Things change…





3 main things have changed that motivate auto-tuning

Reason why we do auto-tuning

1. Hardware

2. Evolution of Linear System Solvers

3. Application Dependent Performance

#1 Hardware

- Now Cray sell mostly x86 based supercomputers
  - AMD Opteron currently
  - Intel Xeon in near future
- No longer control the ISA – it keeps changing on us!
  - Single core (AMD64)
  - Dual core (faster memory, includes SSE3 instructions)
  - Quad-core (new memory hierarchy + new instructions)
  - Very short development cycle (compared to old vector supercomputers)
  - Cray sells machines for all 3 concurrently
- Now have Multi-core chips, existing methods and API's may not allow us to overcome the memory bandwidth wall.

#2 Evolution of Linear System Solvers

- ¼ PetaFlop and 31,000 cores motivates a deep emphasis on sparse iterative solvers
  - Even more cores in our future machines!

- Maturity of numerical methods and software infrastructure
  - Iterative methods and preconditioning
    - Templates, SciDAC TOPs Projects, etc.
  - De facto standard software packages
    - PETSc, Trilinos, hypre

- Cray supports these software packages and tune them for our systems
  - Like how we support dense linear algebra packages
  - No change in API
  - No change in functionality

#3 Application Dependent Performance

- SpMV performance depends wildly on sparsity pattern / character
- Density (number of non-zeroes per row) and sparsity pattern govern how well the base CSR kernel performs
  - Unlike dense linear algebra
- General purpose tuned codes cannot be written for these types of problem

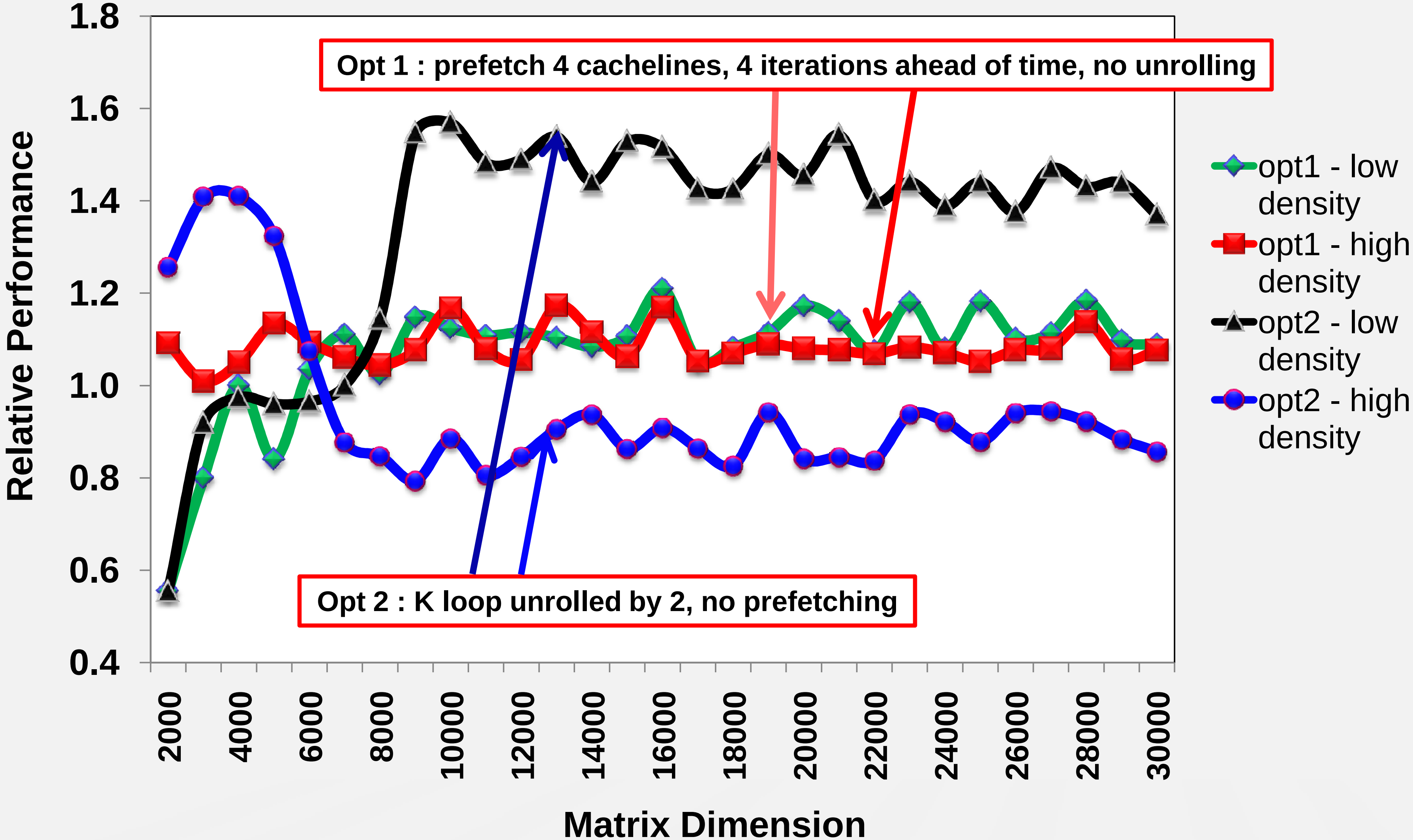
Generic CSR SpMV code (the Bedrock)

```
do q = 1, n_rhs

     next_row_begin = row_start (1)

     do i = 1, n_rows

         row_begin      = next_row_begin
         next_row_begin = row_start (i +1)
         ip             = 0.0

         do k = row_begin, next_row_begin - 1
               ip   = ip  +  values (k) * x (col_index (k), q)
         end do

         y (i, q) = ip

     end do

end do
```

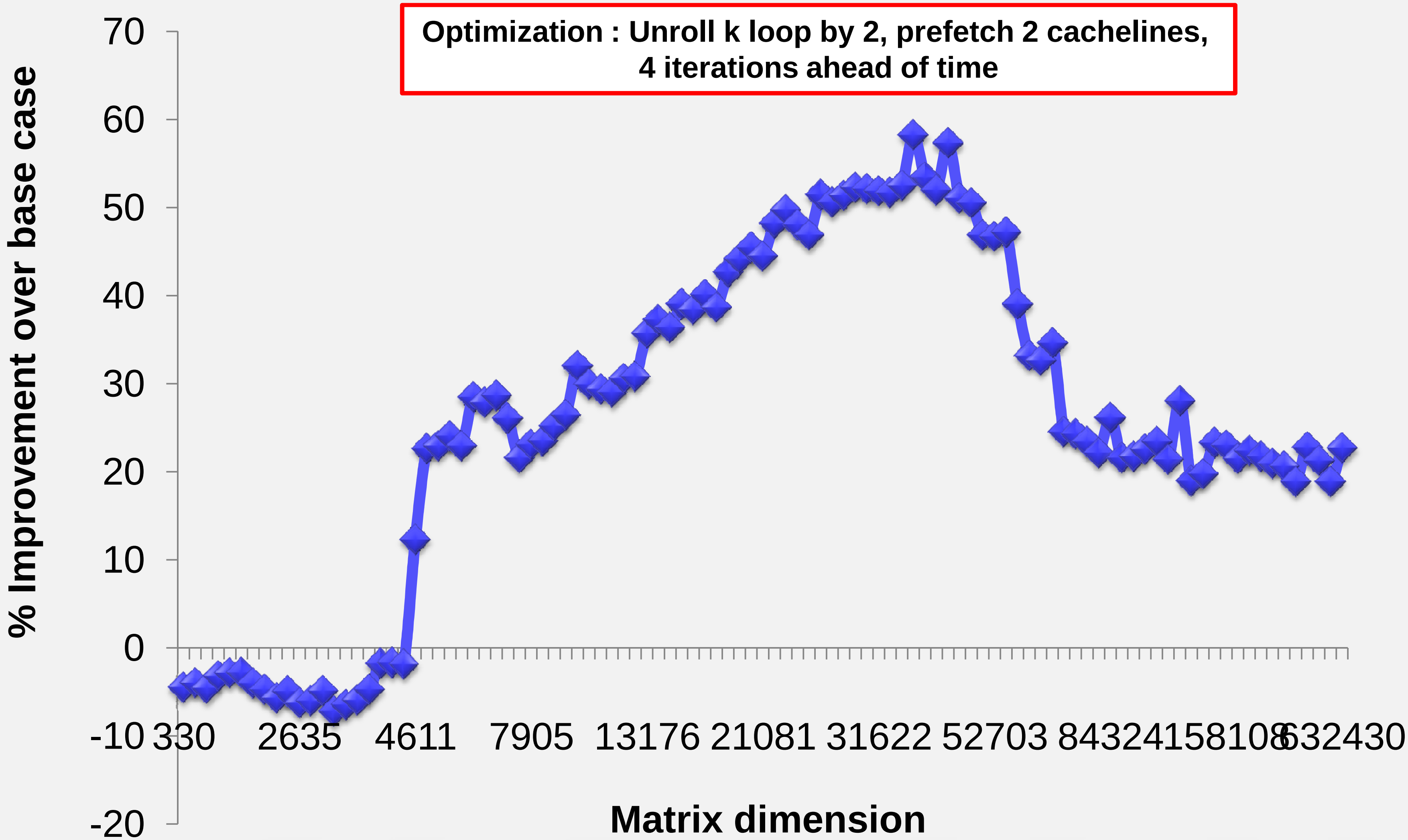
Irregular memory access on values
Irregular access on col_index
Very little re-use of col_index and values
Code is memory bandwidth bound

Vendors have not been ‘doing their part’ here

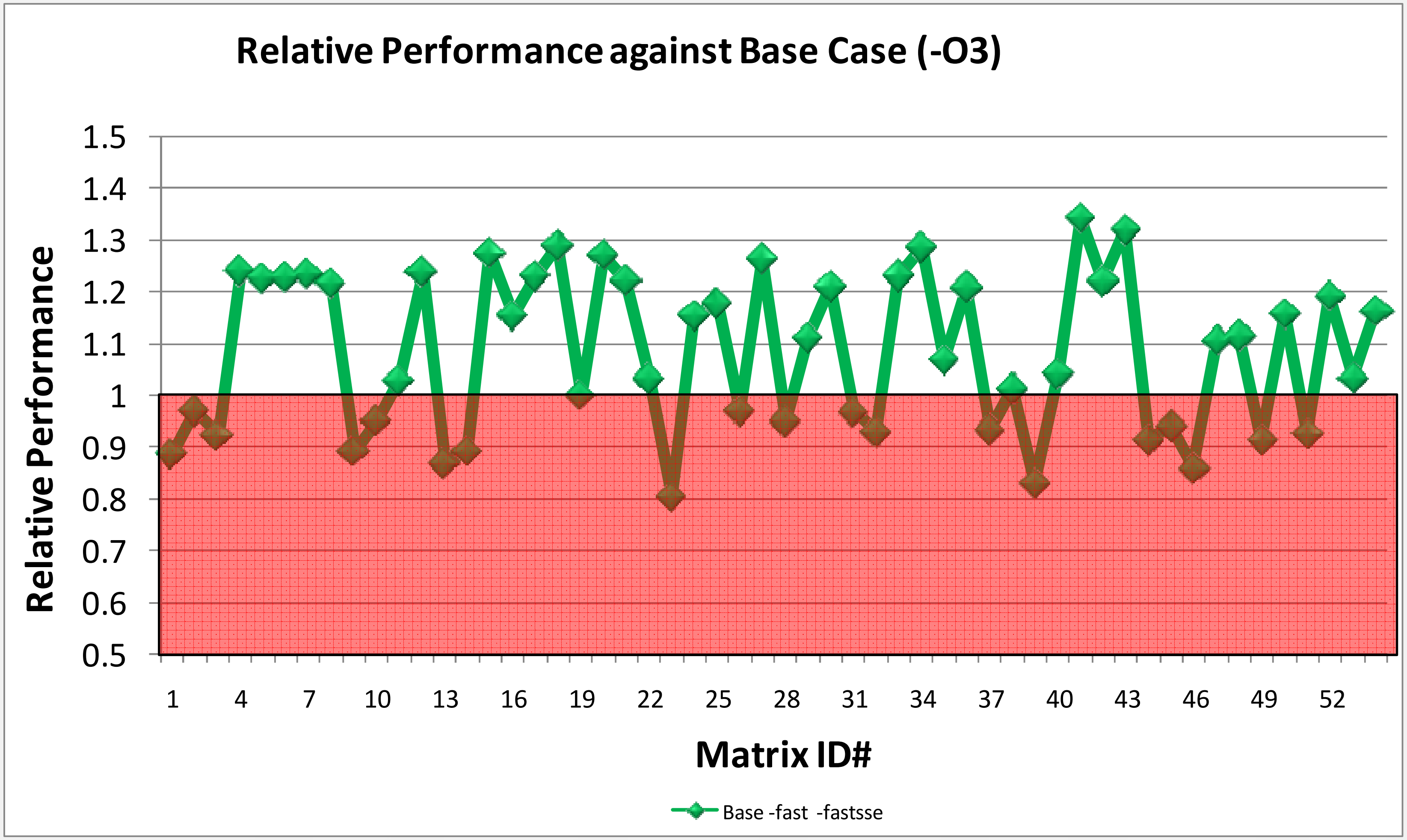
Performance of 2 tuned SpMV kernels relative to BASE case



Can't just throw a great optimization at SpMV



Same problem with aggressive tuning by compiler (PGI using -fast –fastsse)

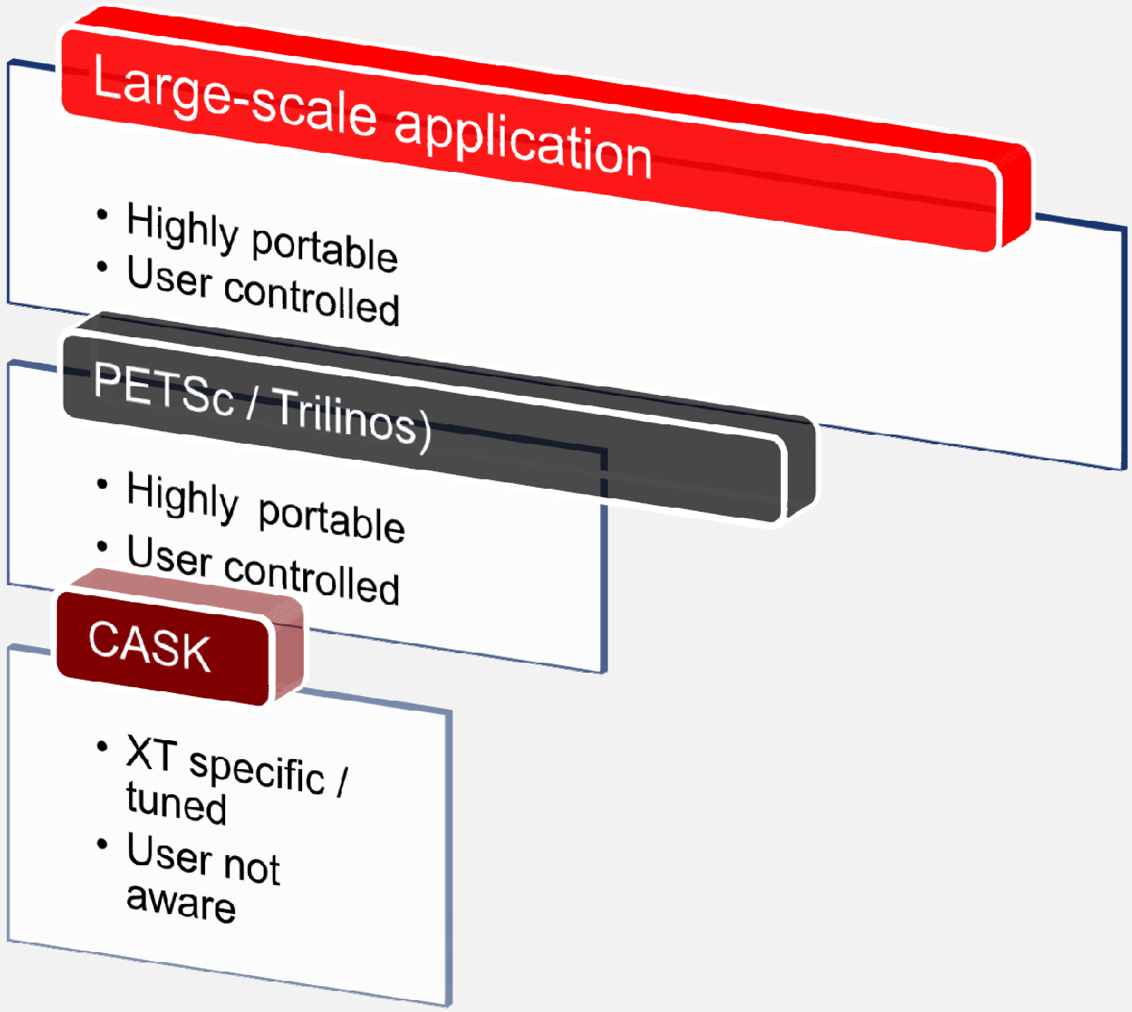


SpMV summary

- Linear solve results in many serial SpMV operations
- These are the most expensive part of a linear solve
- Code is memory bandwidth bound
- Performance of SpMV changes with respect to matrix characteristics
- Applicability of an optimization applies only to a certain problem or set of problems

There is no “General Purpose” SpMV Code

Cray Adaptive Sparse Kernels



Consider this reasonable optimization space

Unroll k loop from 1, up to 8	8 variants	8 implementations
Unroll q loop, from 1 to 4	4 variants	32 implementations
Prefetch 1 to 5 cache lines before loop	5 variants	160 implementations
Prefetch before loop 1 to 10 rows in advance	10 variants	1600 implementations
Prefetch 1 cacheline with inner loop, 1 to 30 iterations ahead of time	30 variants	48000 implementations

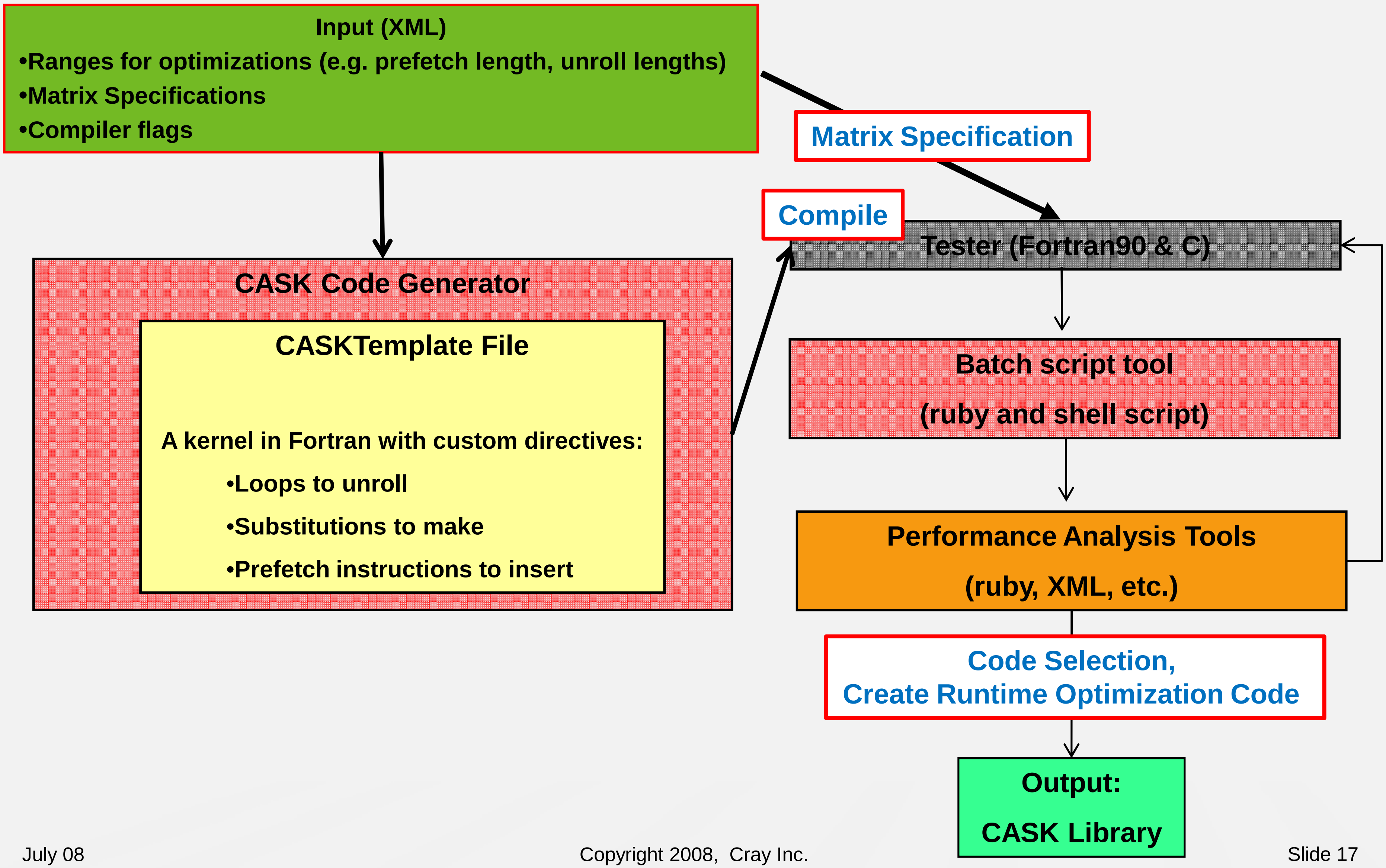
= work for 250 summer internships

CASK design / philosophy

- Using limited analysis and without the involvement of the user

1. Analyze matrix at minimal cost
2. Categorize matrix against internal classes
3. Based on offline experience, find best CASK code for particular matrix class
4. Previously assign “best” compiler flags to CASK code
5. Assign best CASK kernel and perform Ax

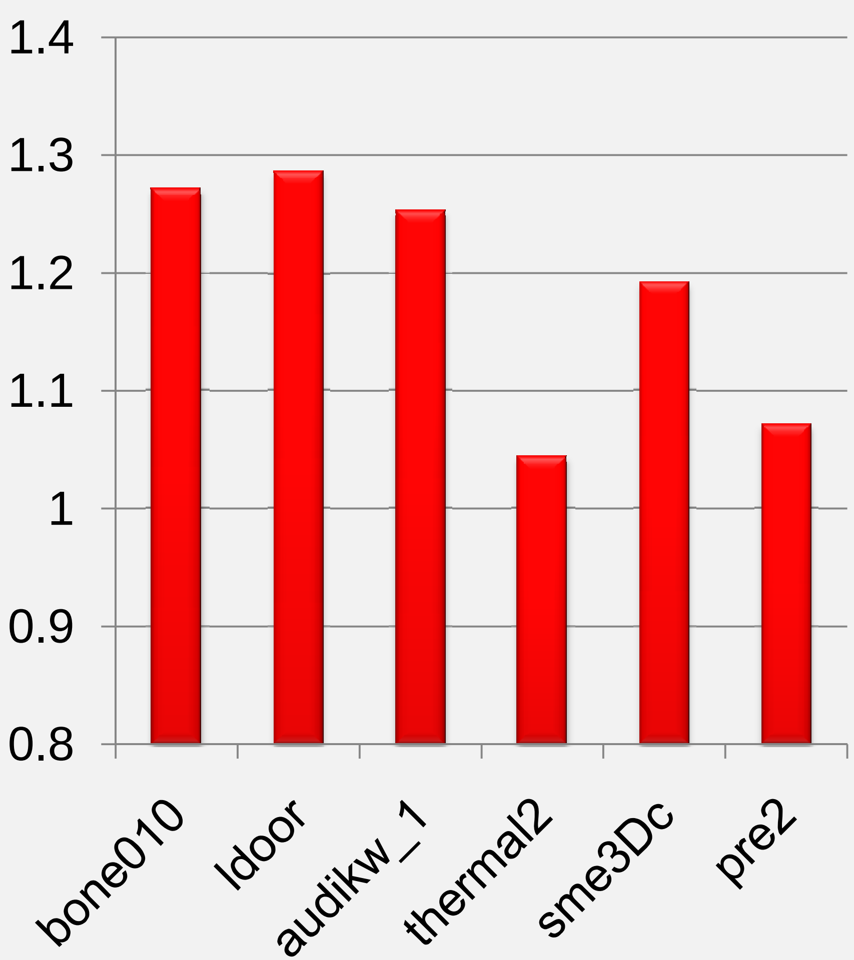
Auto-tuning Framework

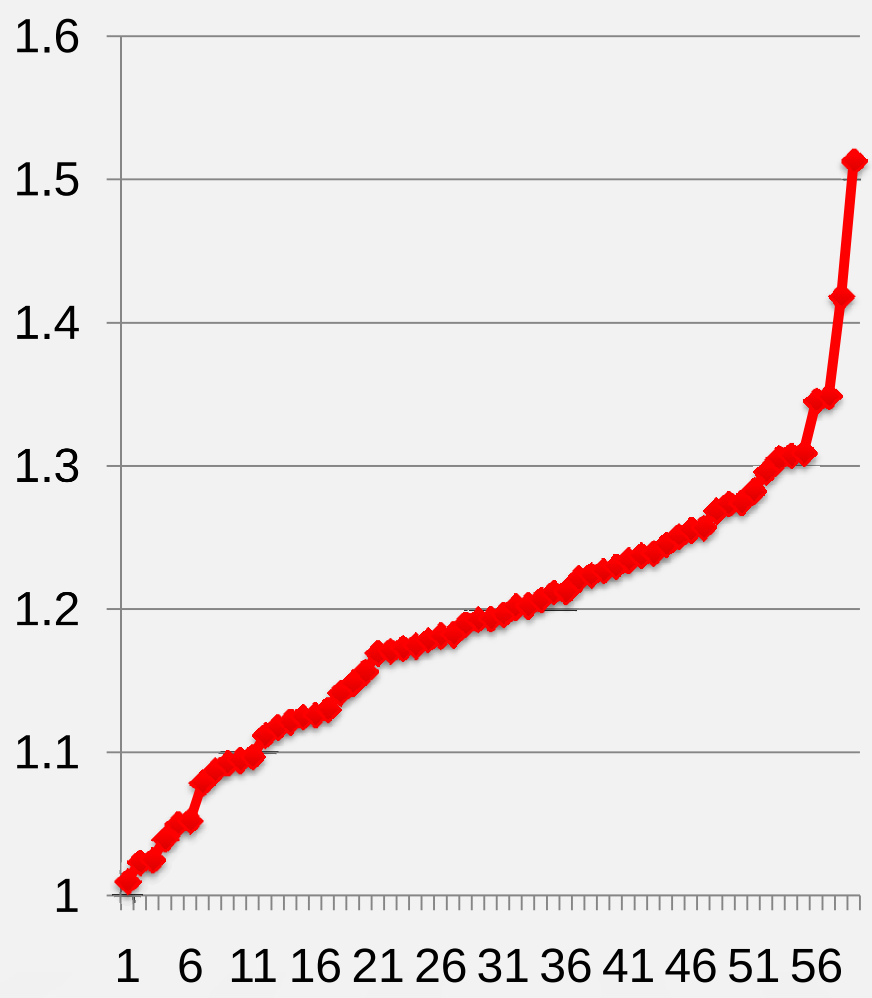


Auto-tuning Framework (Continued)

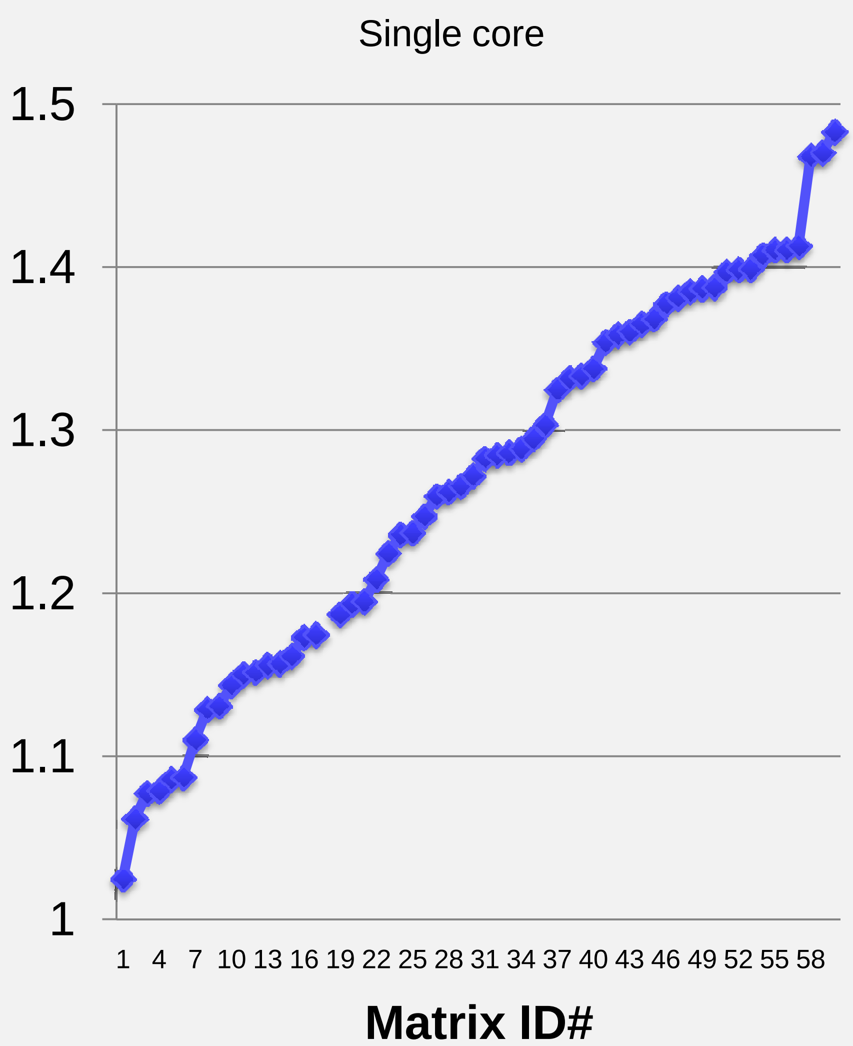
- Implemented with Ruby and XML
  - Ruby orchestrates the tuning process
  - XML defines the target range of tuning parameters and test sparse matrix
- Code generator
- Tester program contains a random matrix generator
  - Takes 10+ parameters
  - Can generate blocked and banded sparse matrices
  - Also imports HB format sparse matrix files
- Performance analysis tool integrated with CrayPat
  - Allows off-line tuning as well as establishing a scheme for on-line tuning with a negligible runtime overhead.

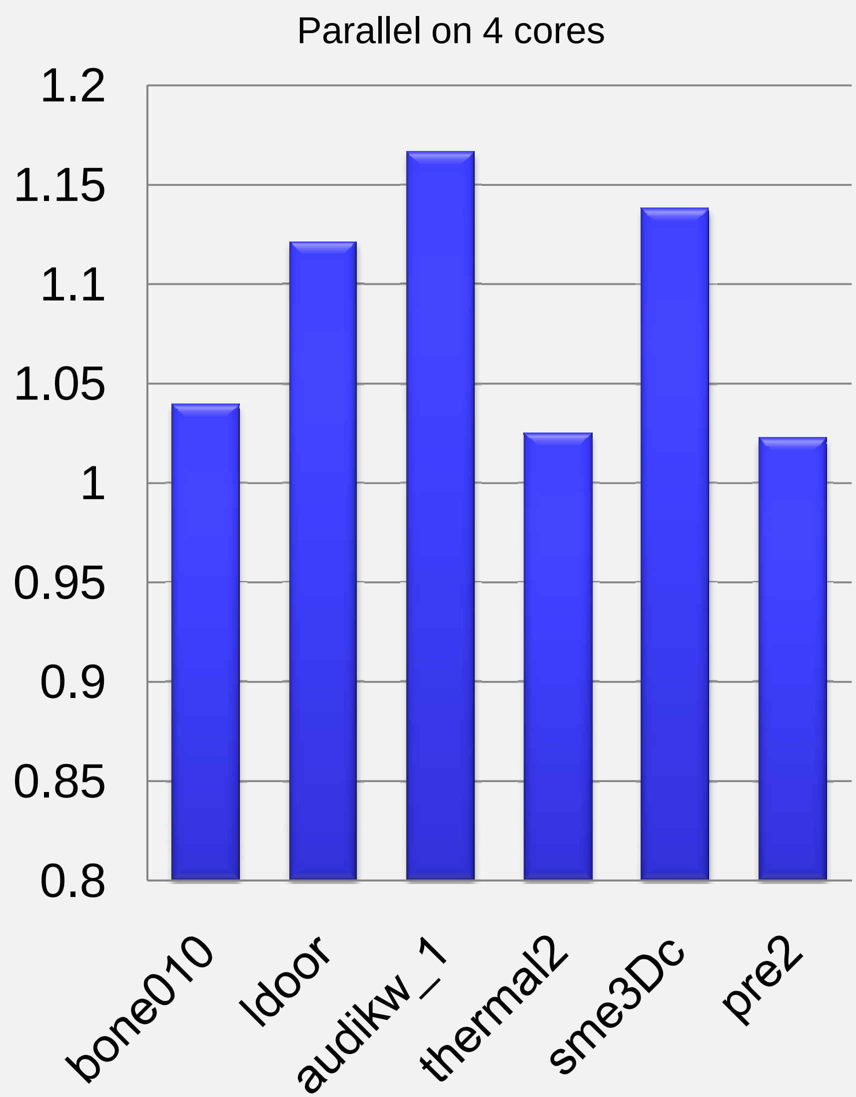
CASK and PETSc, single core



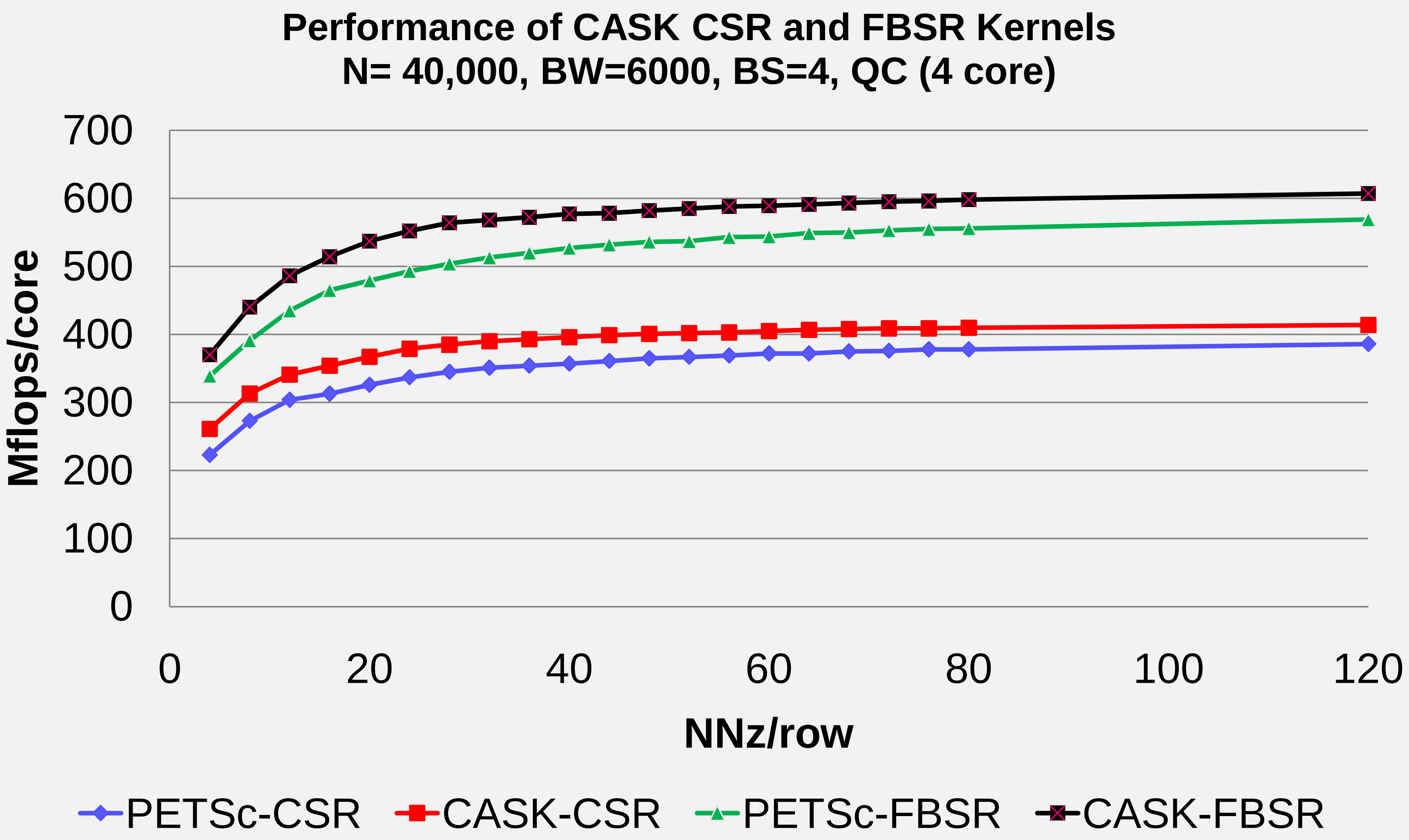


CASK and PETSc – quad core





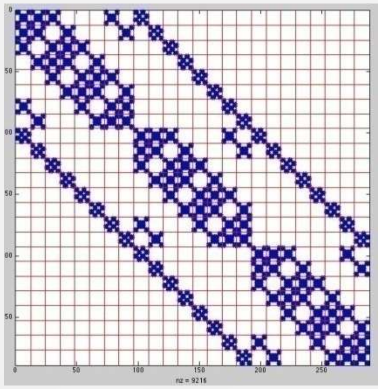
FBSR and CSR Comparison



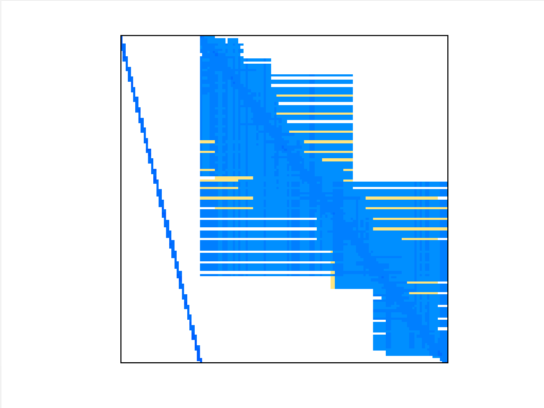
Auto-tuning Experience

- Good performance model is required to enable good auto-tuning
  - We incrementally refined our performance model!
  - Often the auto-tuning results pointed out what we were missing.

- Good matrix generator is required
  - Even for random matrices, it is possible reproduce real-application-like matrices in terms of performance behavior
  - Care must be taken when using matrices in the public repositories (NIST, U of Florida)



Common



Very rare

Auto-tuning Experience (Continued)

- Ruby and XML provides a great flexibility of tool development
  - Easy to add a new tuning feature
  - XML is used to control the tuning, parameter search space, and log-keeping, etc.

- The size of the search space for parameters seems to be big at the beginning, but it can be reduced.
  - Supervised search using our knowledge in compiler flags and sparse matrix computation
  - Every auto-tuning results tell us what to trim
  - How to automate this trimming process?

- Works as a good regression test tool!

Further Auto-tuning Work in LibSci

- CASK 1.0 released in August 2008
  - Runs with PETSc
  - CSR and FBSR SpMV
  - Version 2.0 will support Trilinos, VBR and Transpose SpMV, Triangular Solution and more.
- CRAFFT Version 1.0 will be released in July 2008
  - Very simple API
  - FFTW, ACML support
  - Less runtime tuning overhead
- Working with Spiral team for CRAFFT Version 2
- Parallel FFTs
- Auto-tuning in Dense Linear Algebra? (GEMM, eigensolvers, ScaLAPACK)

Special Thanks

- CASK Team
  - Adrian Tate
  - John Lewis