## Code Synthesis for Automatic Tuning

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## Automatic Performance Tuning

- Motivation: replace hand tuning of computational kernels
- Tedious and difficult
- Too hard to keep up with new architectures, compilers, kernels
- Sometimes tuning must be done at runtime
- Automatic performance tuning:
- Approach
- Generate "space" of candidate algorithms
- Search space for best one
- Examples
- ATLAS - adopted by Matlab and elsewhere
- PHiPAC - ATLAS predecessor
- FFTW - 1999 Wilkinson Prize for Numerical Software
- Spiral - signal processing
- Sparsity/OSKI - sparse matrix-vector multiply


## Dense Matrix-Matrix Multiplication



Finding the best block size is like finding a needle in a haystack!

## Most Implementations are Not Good



## Phillip Colella’s "Seven dwarfs"

## 7 numerical methods domain scientific computing

1. Structured Grids (including adaptive)
2. Unstructured Grids
3. Spectral methods (Fast Fourier Transform)
4. Dense Linear Algebra ↔ Atlas
5. Sparse Linear Algebra
6. Particle Methods
7. Monte Carlo

Slide from "Defining Software
Requirements for Scientific
Computing", Phillip Colella, 2004

## Stencil on Grid $\rightarrow$ Matrix Vector Multiply on Matrix

- Shown for the 2D case, the matrix $T$ is now
- Grid points numbered left to right, top row to bottom row


Graph and "stencil"


- Similar to "adjacency matrix" for arbitrary graph


## Conversion between a mesh and matrix



Matrix A , in natural order


Hidden slide: shown in earlier lecture on sources of parallelism

## Project Proposal: Stencil Generator

- Stencil operations on regular meshes are very common and have many variations
- Dimension: 1D (e.g. 3pt), 2D (5pt or 9pt), 3D (7pt or 27pt)
- Shape: 1D (e.g. 3pt), 2D (5pt or 9pt), 3D (7pt or 27pt), they need not be regular
- Band: just your immediate neighbors (band=1), or their neighbor (band=2), or...
- Balanced or unbalanced in various directions (isotropic, anisotropic)
- coefficients (NAS MG)
- constant, 1 point and all others
- constant, 1 point and distance-based coefficients
- variable, relative to each position
- Update in place vs. $2^{\text {nd }}$ grid
- Colored algorithms (red-black in 2D)



## Optimizing Stencils

- Stencil operations have simple structure
- Loop nest with single assignment in the simple case
- Real applications use these and more complicated cases
- Low floating point rate:
- Typically ~1 FLOP per load
- Good spatial locality, but little temporal locality (re-use)
- Run at small fraction of peak (<15\%)!
- Optimizations:
- Improve reuse within a sweep through the grid
- Tile to improve chance that previous plane (or row) is still in cache when the neighboring one is processes


## Tiling Stencil Computations

- Several papers on tiling stencil computations
- E.g., Rivera and Tseng SC2002, ...
- Old Conventional Wisdom
- Cache misses are the most important factor


Cache misses in blocked/unblocked


Time for unblocked/blocked

## Stencil Probe Cache Blocking Revisited

New Conventional Wisdom: Prefetching is as important as caching

- Little’s Law (Bailey ‘97): need data in-flight = latency * bandwidth Cache blocking is useful for

1. large grid sizes: 3 planes do not fit in cache for 3D problem
2. do not cut/block the unit-stride dimension


## Blocking Over Time / Iterations

- Can we do better than this?
- Code is still severely limited by memory bandwidth
- For some computations, you can merge across $k$ sweeps over the grid
- Re-use data $k$ times (as well as re-use within a plane)
- Dependencies produce pyramid patterns

Frigo \& Strumpen, ICS05.


## The Algorithm - Base Case

If the height is 1 (ie t1-t0=1) then we simply have a line of points $(\mathrm{t} 0, \mathrm{x})$ where $\mathrm{x} 0<=\mathrm{x}<=\mathrm{x}$. Do the kernel on this set of points. Order does not matter (no interdependencies).


## The Algorithm - Space Cut

- If the width <= 2*height, then cut with slope=-1 through the center.

- Do T1, then T2. No point in T1 depends on values from T2.


## The Algorithm - Time Cut

- Otherwise, cut trapezoid in half in the time dimension.

- Do T1, then T2. No point in T1 depends on values of T2.


## Initial Results - Itanium2

Itanium2 Naive vs. Oblivious Cycles


## Initial Results - Itanium2

Itanium2 Naive vs. Oblivious Misses


## Best Performance



Opteron Best Case Oblivious Performance


Power5 Best Case Oblivioius Performance


## Project Idea Revisited

- Cache oblivious stencils not well tested
- Only limited stencils (3D 7pt)
- Applications use many different stencils
- Requested work by apps folks
- Paper by S. Kamil, Oliker, Shalf so that many optimizations are needed to make it really work
- Recursion is useful for understanding the algorithm
- Can't use recursion all the way to the bottom
- A fixed tiling approach may work as well
- Key inside is tile shapes: Pyramids and Parallelopipeds


## General Sparse Matrix Case

- If this works for stencils, what about arbitrary matrices?
- Tuning arbitrary matrices
- Project: code generator that is more flexible, maintainable, extensible than current approach
- The time-blocked approach extended to matrices
$-A^{k}{ }^{*} x$
- Intuition: most of cost in $A^{*} x$ is reading matrix $A$
- Can we read $A$ once and do $k$ operations with it?
- Notes:
- "Time" is used loosely; this is typically iterations in a solver
- Many numerical "details" to make $A^{k}$ * x useful [Hoemmen]


## A "Familiar" Sparse Matrix



## I am a Big Repository Of useful And useless <br> Facts alike.

## Who am I?

(Hint: Not your e-mail inbox.)

## Motivation for Tuning Sparse Matrices

- Sparse matrix kernels can dominate solver time
- Sparse matrix-vector multiply (SpMV)
- SpMV: runs at < $10 \%$ of peak
- Improving SpMV's performance is hard
- Performance depends on machine, kernel, matrix
- Matrix known only at run-time
- Best data structure + implementation can be surprising
- Tuning becoming more difficult over time
- Approach: Empirical modeling and search
- Off-line benchmarking + run-time models
- Up to $4 x$ speedups and $31 \%$ of peak for SpMV
- Other kernels: 1.8 x triangular solve, $4 \mathrm{x} A^{T} A \cdot x, 2 x A^{2} \cdot x$


## OSKI: Optimized Sparse Kernel Interface

- Sparse kernels tuned for user's matrix \& machine
- Hides complexity of run-time tuning
- Low-level BLAS-style functionality
- Includes fast locality-aware kernels: $A^{T} A \cdot x, A^{k} \cdot x ~ . .$.
- Initial target: cache-based superscalar uniprocessors
- Target users: "advanced" users \& solver library writers
- Current focus on uniprocessor tuning
- Shared/distributed memory versions in progress
- Open-source (BSD) C library
- 1.0 available: bebop.cs.berkeley.edu/oski
- Recently integrated into PETSc


## Road Map

- Sparse matrix-vector multiply (SpMV) review
- Why doesn't my compiler solve the problem?
- Historical trends
- Automatic tuning in OSKI
- Future work


A
Matrix-vector multiply kernel: $y(i) \leftarrow y(i)+A(i, j) \cdot x(j)$
for each row i

$$
\begin{aligned}
& \text { for } k=p t r[i] \text { to } p \operatorname{tr}[i+1] \text { do } \\
& \quad y[i]=y[i]+\operatorname{val}[k]^{*} x[i n d[k]]
\end{aligned}
$$



Uniprocessor Sparse Matrix-Vector Multiply Performance


## Example: The Difficulty of Tuning



- $\mathrm{n}=21216$
- nnz = 1.5 M
- kernel: SpMV
- Source: NASA structural analysis problem


## Example: The Difficulty of Tuning



- $\mathrm{n}=21216$
- nnz = 1.5 M
- kernel: SpMV
- Source: NASA structural analysis problem
- 8x8 dense substructure


## What We Expect

- Assume
- $\operatorname{Cost}(S p M V)=$ time to read matrix
- 1 double-word = 2 integers
- r, c in $\{1,2,4,8\}$
- CSR: 1 int / non-zero
- BCSR( x c): 1 int / ( $r^{*} \mathrm{c}$ non-zeros)
- As $r^{*}$ c increases, speedup should
- Increase smoothly
- Approach 1.5

$$
\text { Speedup }=\frac{T_{C S R}}{T_{B C S R}(r, c)} \approx \frac{1.5}{1+\frac{1}{r c}} \xrightarrow{r, c=\infty} 1.5
$$

## What We Get (The Need for Search)

900 MHz Itanium 2, Intel C v8: ref=275 Mflop/s


333 MHz Sun Ultra 2i, Sun C v6.0: ref=35 Mflop/s


2 GHz Pentium M, Intel C v8.1: ref=308 Mflop/s


900 MHz Ultra 3, Sun CC v6: ref=54 Mflop/s

1.4 GHz Opteron, gcc 3.4.2: ref=308 Mflop/s


375 MHz Power3, IBM xIc v6: ref=145 Mflop/s


800 MHz Itanium, Intel C v7: ref=146 Mflop/s

1.3 GHz Power4, IBM xlc v6: ref=577 Mflop/s


900 MHz Itanium 2, Intel C v8: ref=275 Mflop/s


## Still More Surprises



- More complicated non-zero structure in general


## Still More Surprises



- More complicated non-zero structure in general
- Example: 3x3 blocking
- Logical grid of $3 \times 3$ cells


## Extra Work Can Improve Efficiency!



- More complicated non-zero structure in general
- Example: 3x3 blocking
- Logical grid of $3 \times 3$ cells
- Fill-in explicit zeros
- Unroll 3x3 block multiplies
- "Fill ratio" = 1.5
- On Pentium III: 1.5x speedup!


## Historical Trends: Mixed News

- Observations
++ Moore's law like behavior
---- "Untuned" is $10 \%$ peak or less, worsening
++ "Tuned" roughly $2 x$ better today, and growing
---- Tuning is complex
- LINPACK not representative of sparse apps


## Road Map

- Sparse matrix-vector multiply (SpMV) in a nutshell
- Historical trends and the need for search
- Automatic tuning in OSKI
- How does OSKI work?
- Current and future work


## How OSKI Tunes (Overview)

Library Install-Time (offline)

$\longrightarrow$ Application Run-Time


Extensibility: Advanced users may write \& dynamically add "Code variants" and "Heuristic models" to system.

## Example of a Tuning Heuristic

- Example: Selecting the rxc block size
- Off-line benchmark: characterize the machine
- Precompute Mflops(r,c) using dense matrix for each rxc
- Once per machine/architecture
- Run-time "search": characterize the matrix
- Sample A to estimate Fill(r,c) for each rxc
- Run-time heuristic model
- Choose r, c to maximize Mflops(r,c) / Fill(r,c)
- Run-time costs
- Up to ~40 SpMVs (empirical worst case)
- Dominated by conversion
- May be amortized if pattern fixed

Accuracy of the Tuning Heuristics [Itanium 2]


NOTE: "Fair" flops used (ops on explicit zeros not counted as "work")

Accuracy of the Tuning Heuristics [Itanium 2]


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## Calling OSKI: Interface Design

- Support "legacy applications"
- Gradual migration of apps to use OSKI
- Must call "tune" routine explicitly
- Exposes cost of tuning and data structure reorganization
- May provide tuning hints
- Structural: Hints about matrix
- Workload: Hints about frequency of calls, to limit tuning time
- May save/restore tuning results
- To apply on future runs with similar matrix
- Stored in "human-readable" format


## How to Call OSKI: Basic Usage

- May gradually migrate existing apps
- Step 1: "Wrap" existing data structures
- Step 2: Make BLAS-like kernel calls

```
int* ptr = ..., *ind = ...; double* val = ...; /* Matrix, in CSR format */
double* x = ..., *y = ...; /* Let x andl y be two dense vectors */
```

```
/* Compute y = \beta\cdoty + \alpha'A'x, }500\mathrm{ times */
for( i = 0; i < 500; i++ )
    my_matmult( ptr, ind, val, \alpha, x, }\beta, y )
```


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```
int* ptr = ..., *ind = ...; double* val = ...; /* Matrix, in CSR format */
double* x = ..., *y = ...; /* Let x andl y be two dense vectors */
/* Step 1: Create OSKI wrappers around this data */
oski_matrix_t A_tunable = oski_CreateMatCSR(ptr, ind, val, num_rows,
    num_cols, SHARE_INPUTMAT, ...);
oski_vecview_t x_view = oski_CreateVecView(x, num_cols, UNIT_STRIDE);
oski_vecview_t y_view = oski_CreateVecView(y, num_rows, UNIT_STRIDE);
```

/* Compute $\mathbf{y}=\beta \cdot \mathbf{y}+\alpha \cdot \mathbf{A} \cdot \mathbf{x}, 500$ times */
for( i = 0; i < 500; i++ )
my_matmult( ptr, ind, val, $\alpha, \mathrm{x}, \beta, \mathrm{y}$ );

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```

/* Compute $\mathbf{y}=\beta \cdot \mathbf{y}+\alpha \cdot A \cdot x, 500$ times */
for ( i = 0; i < 500; i++ )
oski_MatMult(A_tunable, OP_NORMAL, $\alpha$, x_view, $\beta, y_{-v i e w) ; / * ~ S t e p ~}^{2}$ */

## How to Call OSKI: Tune with Explicit Hints

- User calls "tune" routine
- May provide explicit tuning hints (OPTIONAL)

```
oski_matrix_t A_tunable = oski_CreateMatCSR( ... );
    /* ... */
/* Tell OSKI we will call SpMV 500 times (workload hint) */
oski_SetHintMatMult(A_tunable, OP_NORMAL, \alpha, x_view, \beta, y_view, 500);
/* Tell OSKI we think the matrix has 8x8 blocks (structural hint) */
oski_SetHint(A_tunable, HINT_SINGLE_BLOCKSIZE, 8, 8);
oski_TuneMat(A_tunable); /* Ask OSKI to tune */
for( i = 0; i < 500; i++ )
    oski_MatMult(A_tunable, OP_NORMAL, \alpha, x_view, \beta, y_view);
```


## How the User Calls OSKI: Implicit Tuning

- Ask library to infer workload
- Library profiles all kernel calls
- May periodically re-tune

```
oski_matrix_t A_tunable = oski_CreateMatCSR( .. );
    /* ... */
for( i = 0; i < 500; i++ ) {
    oski_MatMult(A_tunable, OP_NORMAL, \alpha, x_view, }\beta,y_view)
    oski_TuneMat(A_tunable); /* Ask OSKl to tune */
}
```


## Saving and Restoring Tuning Transformations

- May selecting customized, complex transformations using embedded scripting language (OSKI-Lua)

```
/* In "my_app.c" */
fp = fopen("my_xform.txt", "rt");
fgets(buffer, BUFSIZE, fp);
oski_ApplyMatTransform(A_tunable,
    buffer);
oski_MatMult(A_tunable, ...);
```

```
# In file, "my_xform.txt"
# Compute (fast = P* A* P
    Pinar's reordering algorithm
A_fast, P =
    reorder_TSP(InputMat);
# Split Afast = A 
    block format, A in CSR
A1, A2 =
    A_fast.extract_blocks(2, 2);
return transpose(P)*(A1+A2)*P;
```


## Additional Features

- Currently 5 tunable kernels
- SpMV, triangular solve, $A \cdot x \& A^{T} \cdot w, A^{T} A \cdot x, A^{k} \cdot \boldsymbol{x}$
- Support for several scalar type combinations
- \{32-bit, 64-bit int\} $\times$ \{single, double prec. $\} \times$ \{real, complex\}
- "Plug-in" extensibility
- Very advanced users may customize library (at run-time)
- New heuristics (e.g., Buttari, et al.)
- Alternative data structures \& code variants (e.g., seg-scan for vector architectures)


## Exploiting Problem-Specific Structure

- Optimizations for SpMV
- Register blocking (up to 4x over CSR)
- Variable block splitting (2.1x over CSR, 1.8x over RB)
- Diagonals (2x over CSR)
- Reordering to create dense structure + splitting (2x over CSR)
- Symmetry (2.8x over CSR, 2.6x over RB)
- Cache blocking (2.2x over CSR)
- Multiple vectors (7x over CSR)
- And combinations...
- Sparse triangular solve
- Hybrid sparse/dense data structure (1.8x over CSR)
- Higher-level kernels
- AA ${ }^{\top} \cdot x, A^{\top} A \cdot x$ (4x over CSR, 1.8x over RB)
- $A^{2} \cdot x$ (2x over CSR, 1.5x over RB)


## Example: Variable Block Structure

12-raefsky4.rua in VBR Format: $51 \times 51$ submatrix beginning at $(715,715)$

2.1x over CSR 1.8x over RB

## Example: Row-Segmented Diagonals



2x
over CSR

## Mixed Diagonal and Block Structure



- Raefsky4 (structural problem) + SuperLU + colmmd
- $\mathrm{N}=19779, \mathrm{nnz}=12.6 \mathrm{M}$

Dense trailing triangle: dim=2268, 20\% of total nz

Can be as high as 90+\%!
1.8x over CSR

## Cache Optimizations for $A A^{T *} \chi$

- Cache-level: Interleave multiplication by $A, A^{T}$
- Sparse matrix-vector multiply (SpMV) in a nutshell
- Historical trends and the need for search
- Automatic tuning in OSKI
- Current and future work

$$
A A^{T} \cdot x=\left(\begin{array}{ll}
a_{1} \Lambda & a_{n}
\end{array}\right)\left(\begin{array}{c}
u_{1} \\
\mathrm{M} \\
a_{n}^{T}
\end{array}\right) \cdot x=\sum_{i=1}^{n} a_{\text {"axpy" }}^{\left(a_{i}^{T} x\right)}
$$

- Register-level: $a_{i}{ }^{T}$ to be $r \times c$ block row, or diag row
- Algorithmic-level transformations for $A^{2 *} x, A^{3 *} x, \ldots$


## Example applications

- T3P - Accelerator Design - Ko
- Register blocking, Symmetric Storage, Multiple vector
- 1.68x faster on Itanium 2 for one vector
- 4.4x faster for 8 vectors
- Omega3P - Accelerator Design - Ko
- Register blocking, Symmetric storage, Reordering
- 2.1x faster on Power4
- Semiconductor Industry:
- 1.9x speedup over SPOOLES in CG at design firm
- Recent integration of OSKI into PETSc


## Status and Future Work

- OSKI Release 1.0 and docs available bebop.cs.berkeley.edu/oski
- Performance bounds modeling (ongoing)
- Future OSKI work
- Release of PETSc version with OSKI
- Better "low-level" tuning, including vectors
- Automatically tuned parallel sparse kernels
- Development of a new HPC Challenge Benchmark
- Evaluate platforms based on tuned (blocked) SpMV performance
- Tuning higher level algorithms using $A^{k} x$
- Models indicate large speedups possible


## Current SPMV OSKI Code Generator

```
#!/bin/bash
#!/b
# This script uses some bash extensions.
#
mattype=BCSR
if test x"$1" = x ; then
    echo ""
    echo "usage: $0 {full, source, makestub}"
    echo ""
    exit 1
fi
GENSOURCE="
GENMAKE='
case $1 in
[fF]*) GENSOURCE=yes ; GENMAKE=yes ;
[sS]*) GENSOURCE=yes; GENMAKE=no ;;
[mM]*) GENSOURCE=no ; GENMAKE=yes ;;
*) echo "*** Unknown option, '$1' ***" ; exit 1;;
esac
CreateOutfile() {
#---------------------------
## a
R=$1
C=$2
outfile=$3
echo "/**
* \\file ${mattype}_${R}\times${C}.c
* IVbrief \$\{mattype\} \(\$\{R\} \times \$\{C\}\) SpMV implementation, for all transpose options.
* Ilingroup MATTYPE_\$\{mattype\}
* Automatically generated by \$0 on `date`.
```

if test ${GENMAKE} = yes ; then
    makestub=Make.${mattype}
echo "\#

# Automatically generated by \$USER@`hostname

# on `date`, running \$0

# 

" > ${makestub}
fi
for R in 12 345678; do # row block size
for C in 12 345678; do # column block size
        echo "${MATTYPE} ${R}x${C}..."
outfile=${R}x${C}.c
if test \${GENSOURCE} = yes ; then
CreateOutfile \${R} \${C} \${outfile}
for OP in normal trans conj herm ; do \# transpose option
for S in 1 general ; do \# stride
WriteKernel \${R} \${C} \${OP} \${S} \${outfile}
done \# S
WriteShell_v1 \${OP} \${outfile}
WriteShell \${OP} \${R} \${C} \${outfile}
done \# OP
WriteMatReprMult \${R} \${C} \${outfile}
WriteFooter \${outfile
fi
if test \${GENMAKE} = yes ; then
WriteMakeStub \${R} \${C} \${makestub}

## Project: Improved Code Generation

- Consider common kernels:
- Matrix-vector multiply, triangular solve, etc.
- Different emphasis than Bernoulli
- These are simpler kernels than they were interested in
- Generate code for many formats, not fixed by programmer
- Select between them using
- Performance models
- Search
- Approach may still apply
- Use high level language (Matlab?) to "specify" kernels
- Separate language to specify matrix format


## Project Idea: Inter Iteration Tiling

- $\mathrm{A}^{2}$ * x is done in Rich Vuduc's PhD thesis
- General case in Michelle Strout's thesis
- Code generation technology would be useful


## Inter-Iteration Sparse Tiling (1/3)



- Let A be $6 \times 6$ tridiagonal
- Consider $y=A^{2} x$
$-t=A x, y=A t$
- Nodes: vector elements
- Edges: matrix elements $\mathrm{a}_{\mathrm{ij}}$


## Inter-Iteration Sparse Tiling (2/3)



- Let A be 6x6 tridiagonal
- Consider $y=A^{2} x$
- t=Ax, $y=A t$
- Nodes: vector elements
- Edges: matrix elements $\mathrm{a}_{\mathrm{ij}}$
- Orange = everything needed to compute $y_{1}$
- Reuse $\mathrm{a}_{11}, \mathrm{a}_{12}$


## Inter-Iteration Sparse Tiling (3/3)



- Let A be 6x6 tridiagonal
- Consider $y=A^{2} x$

$$
-\mathrm{t}=\mathrm{Ax}, \mathrm{y}=\mathrm{At}
$$

- Nodes: vector elements
- Edges: matrix elements $\mathrm{a}_{\mathrm{ij}}$
- Orange = everything needed to compute $y_{1}$
- Reuse $\mathrm{a}_{11}, \mathrm{a}_{12}$
- Grey $=y_{2}, y_{3}$
- Reuse $a_{23}, a_{33}, a_{43}$

Extra slides

## Creating Locality: TSP Reordering (Before)


(Pinar '97;
Moon, et al ‘04)

## Creating Locality: TSP Reordering (After)


(Pinar '97;
Moon, et al ‘04)

## Up to 2x speedups

over CSR

## Road Map

- Sparse matrix-vector multiply (SpMV) in a nutshell
- Historical trends and the need for search
- Automatic tuning in OSKI
- Current and future work

- Tile sizes (colored regions) grow with no. of iterations and increasing out-degree
- G likely to have a few nodes with high out-degree (e.g., Yahoo)
- Mathematical tricks to limit tile size?
- Judicious dropping of edges [ Ng '01]


## Splitting for Variable Blocks and Diagonals

- Decompose $A=A_{1}+A_{2}+\ldots A_{t}$
- Detect "canonical" structures (sampling)
- Split
- Tune each $A_{i}$
- Improve performance and save storage
- New data structures
- Unaligned block CSR
- Relax alignment in rows \& columns
- Row-segmented diagonals


## Historical Trends in SpMV Performance

- The Data
- Uniprocessor SpMV performance since 1987
- "Untuned" and "Tuned" implementations
- Cache-based superscalar micros; some vectors
- LINPACK
- Dense LU factorization
- Top 500 List


## Features

- Explicit Hints
- Can suggest particular tuning technique
- Implicit Tuning: Ask library to infer workload
- Library profiles all kernel calls
- May periodically re-tune
- Scripting language for selecting customized transformations
- Mechanism to save/restore transformations
- "Plug-in" extensibility
- Very advanced users may customize library (at run-time)


## Summary of High-Level Themes

- "Kernel-centric" optimization
- Vs. basic block, trace, path optimization, for instance
- Aggressive use of domain-specific knowledge
- Performance bounds modeling
- Evaluating software quality
- Architectural characterizations and consequences
- Empirical search
- Hybrid off-line/run-time models
- Statistical performance models
- Exploit information from sampling, measuring


## Related Work

- My bibliography: 337 entries so far
- Sample area 1: Code generation
- Generative \& generic programming
- Sparse compilers
- Domain-specific generators
- Sample area 2: Empirical search-based tuning
- Kernel-centric
- linear algebra, signal processing, sorting, MPI, ...
- Compiler-centric
- profiling + FDO, iterative compilation, superoptimizers, selftuning compilers, continuous program optimization


## Next Steps

## - BeBOP Current Work

- Public software release
- Impact on library designs: Sparse BLAS, Trilinos, PETSc, ...
- Integration in large-scale applications
- Accelerator design, plasma physics (DOE)
- Geophysical simulation based on Block Lanczos ( $A^{T} A^{*} X$; LBL)
- Systematic heuristics for data structure selection?
- Evaluation of emerging architectures
- Revisiting vector micros
- Other sparse kernels
- Matrix triple products, $A^{k *} x$
- Parallelism


## Future Directions (A Bag of Flaky Ideas)

- Composable code generators and search spaces
- New application domains
- PageRank: multilevel block algorithms for topic-sensitive search?
- New kernels: cryptokernels
- rich mathematical structure germane to performance; lots of hardware
- New tuning environments
- Parallel, Grid, "whole systems"
- Statistical models of application performance
- Statistical learning of concise parametric models from traces for architectural evaluation

Compiler/automatic derivation of parametric models


- Super-advisors: Jim and Kathy
- Undergraduate R.A.s: Attila, Ben, Jen, Jin, Michael, Rajesh, Shoaib, Sriram, Tuyet-Linh
- See pages xvi-xvii of dissertation.


## Road Map

- Sparse matrix-vector multiply (SpMV) in a nutshell
- Historical trends and the need for search
- Automatic tuning techniques
- Upper bounds on performance
- SC'02
- Statistical models of performance


## Motivation for Upper Bounds Model

- Questions
- Speedups are good, but what is the speed limit?
- Independent of instruction scheduling, selection
- What machines are "good" for SpMV?


## Upper Bounds on Performance: Blocked SpMV

- $\mathrm{P}=$ (flops) / (time)
- Flops = 2 * nnz(A)
- Lower bound on time: Two main assumptions
- 1. Count memory ops only (streaming)
- 2. Count only compulsory, capacity misses: ignore conflicts
- Account for line sizes
- Account for matrix size and nnz
- Charge min access "latency" $\alpha_{i}$ at $\mathrm{L}_{i}$ cache $\& \alpha_{\text {mem }}$
- e.g., Saavedra-Barrera and PMaC MAPS benchmarks

Time $\geq \sum_{i=1}^{\kappa} \alpha_{i} \cdot$ Hits $_{i}+\alpha_{\text {mem }} \cdot$ Hits $_{\text {mem }}$
$=\alpha_{1} \cdot$ Loads $+\sum_{i=1}^{\kappa}\left(\alpha_{i+1}-\alpha_{i}\right) \cdot$ Misses $_{i}+\left(\alpha_{\text {mem }}-\alpha_{\kappa}\right) \cdot$ Misses $_{\kappa}$

Performance Bounds on Register Blocked SpMV [Itanium 2]


Performance Bounds on Register Blocked SpMV [Itanium 2]


Performance Bounds on Register Blocked SpMV [Itanium 2]


Fraction of Upper Bound Achieved


## Achieved Performance and Machine Balance

- Machine balance [Callahan '88; McCalpin '95]
- Balance = Peak Flop Rate / Bandwidth (flops / double)
- Ideal balance for mat-vec: $\leq 2$ flops / double
- For SpMV, even less

Time $\geq \alpha_{1} \cdot$ Loads $+\sum_{i}\left(\alpha_{i+1}-\alpha_{i}\right) \cdot$ Misses $_{i}+\left(\alpha_{\text {mem }}-\alpha_{\kappa}\right) \cdot$ Misses $_{\kappa}$

- SpMV ~ streaming
- 1 / (avg load time to stream 1 array) ~ (bandwidth)
- "Sustained" balance = peak flops / model bandwidth



## Where Does the Time Go?

$$
\text { Time } \geq \sum_{i=1}^{K} \alpha_{i} \cdot \text { Hits }_{i}+\alpha_{\mathrm{mem}} \cdot \text { Hits }_{\mathrm{mem}}
$$

- Most time assigned to memory
- Caches "disappear" when line sizes are equal
- Strictly increasing line sizes

Where Does the Time Go? Other/LP 18-44 [Analytic Model]


Maximum Speedup for $1 \times 1$ SpMV as Line Size Increases


## Summary: Performance Upper Bounds

- What is the best we can do for SpMV?
- Limits to low-level tuning of blocked implementations
- Refinements?
- What machines are good for SpMV?
- Partial answer: balance characterization
- Architectural consequences?
- Example: Strictly increasing line sizes


## Road Map

- Sparse matrix-vector multiply (SpMV) in a nutshell
- Historical trends and the need for search
- Automatic tuning techniques
- Upper bounds on performance
- Tuning other sparse kernels
- Statistical models of performance
- FDO '00; IJHPCA '04a


## Statistical Models for Automatic Tuning

- Idea 1: Statistical criterion for stopping a search
- A general search model
- Generate implementation
- Measure performance
- Repeat
- Stop when probability of being within $\varepsilon$ of optimal falls below threshold
- Can estimate distribution on-line
- Idea 2: Statistical performance models
- Problem: Choose 1 among m implementations at run-time
- Sample performance off-line, build statistical model


## Example: Select a Matmul Implementation



## Example: Support Vector Classification




Distribution of Non-zeros: rma10.pua


## Register Profile: Itanium 2

SpMV BCSR Profile [ref=294.5 Mflop/s; 900 MHz Itanium 2, Intel C v7.0]


## 1190 Mflop/s

Ultra 2i-11\% ofile [ref= $35.8 \mathrm{Mflop} / \mathrm{s}$; 333 MHz Sun Ultra 2i, Sun C v6.0]


## Pentium III-21\%



72 Mflop/ s


108 Mflop/ s $\longrightarrow 107.1$
102.2
97.2
92.2
87.2
$-82.2$
77.2
$-72.2$
$-67.2$
$-62.2$
$-57.2$
52.2
47.2

42 Mflop/ s

Ultra 3-5\% Profile [ref $50.3 \mathrm{Mfilop} /$; ; 900 MHz Sun Ultra 3 , Sun C ve.0]


Pentium III-M - 15\%


90 Mflop/ s
$\begin{array}{r}\hline 88.7 \\ -86.4 \\ -84.4 \\ -82.4 \\ \hline-80.4 \\ \hline-78.4 \\ \hline-76.4 \\ \hline-74.4 \\ \hline-72.4 \\ \hline-70.4 \\ \hline 68.4 \\ \hline 66.4 \\ \hline-64.4 \\ \hline-62.4 \\ \hline 60.4 \\ \hline 58.4 \\ 56.4 \\ \hline 54.4 \\ \hline 52.4 \\ 50.4 \\ \hline \mathbf{5 0 ~ M f l o p / ~ s ~}\end{array}$
122 Mflop/ s


Power3 - 17\% 'rofile [ref= $163.9 \mathrm{Mflop} / \mathrm{s}$; 375 MHz Power3, $\mathrm{IBM} \times 1 \mathrm{c}$ v5]


## Itanium 1-8\%

252 Mflop/ s


247 Mflop/ s


Power4 - 16\% - file [ref=594.9 Mflop/s; 1.3 GHz Power4, IBM xlc v6]


Itanium 2-33\%


820 Mflop/ s

1.2 Gflop/ s


## Accurate and Efficient Adaptive Fill Estimation

- Idea: Sample matrix
- Fraction of matrix to sample: $s \in[0,1]$
- Cost ~ O(s * nnz)
- Control cost by controlling s
- Search at run-time: the constant matters!
- Control s automatically by computing statistical confidence intervals
- Idea: Monitor variance
- Cost of tuning
- Lower bound: convert matrix in 5 to 40 unblocked SpMVs
- Heuristic: 1 to 11 SpMVs


## Sparse/Dense Partitioning for SpTS

- Partition $L$ into sparse $\left(L_{1}, L_{2}\right)$ and dense $L_{D}$ :

$$
\left(\begin{array}{ll}
L_{1} & \\
L_{2} & L_{D}
\end{array}\right)\binom{x_{1}}{x_{2}}=\binom{b_{1}}{b_{2}}
$$

- Perform SpTS in three steps:
(1) $L_{1} x_{1}=b_{1}$
(2) $\hat{b}_{2}=b_{2}-L_{2} x_{1}$
(3) $L_{D} x_{2}=\hat{b}_{2}$
- Sparsity optimizations for (1)—(2); DTRSV for (3)
- Tuning parameters: block size, size of dense triangle


## SpTS Performance: Power3



A $^{\top}$ Ax Performance [power3-aix]


## Summary of SpTS and $A A^{T *} x$ Results

- SpTS — Similar to SpMV
- 1.8x speedups; limited benefit from low-level tuning
- $A A^{T} X, A^{T} A X$
- Cache interleaving only: up to 1.6x speedups
- Reg + cache: up to 4x speedups
- 1.8x speedup over register only
- Similar heuristic; same accuracy (~ 10\% optimal)
- Further from upper bounds: 60-80\%
- Opportunity for better low-level tuning a la PHiPAC/ATLAS
- Matrix triple products? $A^{k *} x$ ?
- Preliminary work

Speedup of Register Blocked SpMV


Performance of Register Blocked SpMV


Fraction of Machine Peak Achieved by Register Blocked SpMV


Fill Ratio Estimate: Matrix \#2-raefsky3, 3×4









- Even dense matrix multiply can be notoriously difficult to tune

Needle in a Haystack $\left[k_{0}=1\right.$; Sun Ultra 2i/333]


Dense matrix multiply: surprising performance as register tile size varies.


Sparsity Register Blocking Performance [Itanium 2-900, Intel C v7.0]


Sparse Matrix Multiple-Vector Multiply [itanium2-linux-ecc7]


Cache Blocking Performance: Intel Itanium $2(900 \mathrm{MHz})$


## What about the Google Matrix?

- Google approach
- Approx. once a month: rank all pages using connectivity structure
- Find dominant eigenvector of a matrix
- At query-time: return list of pages ordered by rank
- Matrix: $A=\alpha G+(1-\alpha)(1 / n) u u^{\top}$
- Markov model: Surfer follows link with probability $\alpha$, jumps to a random page with probability 1- $\alpha$
- G is $\mathrm{n} \times \mathrm{n}$ connectivity matrix [ $\mathrm{n} \approx 3$ billion]
- $g_{i j}$ is non-zero if page $i$ links to page $j$
- Normalized so each column sums to 1
- Very sparse: about 7-8 non-zeros per row (power law dist.)
- $u$ is a vector of all 1 values
- Steady-state probability $x_{i}$ of landing on page $i$ is solution to $x=A x$
- Approximate $x$ by power method: $x=A^{k} x_{0}$
- In practice, $\mathrm{k} \approx 25$





Performance Summary [pentium3-linux-icc]


Performance Summary [pentium3-linux-icc]


Performance Summary [pentium3-linux-icc]


Where Does the Time Go? Other/LP 18-44 [PAPI]


Sparsity Register Blocking Performance [Itanium 2-900, Intel C v7.0]


## Tuning Sparse Triangular Solve (SpTS)

- Compute $x=L^{-1 *} b$ where $L$ sparse lower triangular, $x$ \& $b$ dense
- L from sparse LU has rich dense substructure
- Dense trailing triangle can account for 20-90\% of matrix non-zeros
- SpTS optimizations
- Split into sparse trapezoid and dense trailing triangle
- Use tuned dense BLAS (DTRSV) on dense triangle
- Use Sparsity register blocking on sparse part
- Tuning parameters
- Size of dense trailing triangle
- Register block size


## Sparse Kernels and Optimizations

- Kernels
- Sparse matrix-vector multiply (SpMV): $y=A^{*} x$
- Sparse triangular solve (SpTS): $x=T^{-1 *} b$
- $y=A A^{T *} x, y=A^{\top} A^{*} x$
- Powers ( $y=A^{k *} x$ ), sparse triple-product ( $R^{*} A^{*} R^{\top}$ ), $\ldots$
- Optimization techniques (implementation space)
- Register blocking
- Cache blocking
- Multiple dense vectors (x)
- A has special structure (e.g., symmetric, banded, ...)
- Hybrid data structures (e.g., splitting, switch-to-dense, ...)
- Matrix reordering
- How and when do we search?
- Off-line: Benchmark implementations
- Run-time: Estimate matrix properties, evaluate performance models based on benchmark data


## Cache Blocked SpMV on LSI Matrix: Ultra $2 i$



## A

10k $\times 255 \mathrm{k}$
3.7M non-zeros

Baseline:
16 Mflop/s
Best block size \& performance:
16k x 64k
28 Mflop/s

## Cache Blocking on LSI Matrix: Pentium 4



## A

10k x 255k
3.7M non-zeros

Baseline:
44 Mflop/s
Best block size \& performance: 16k x 16k 210 Mflop/s

## Cache Blocked SpMV on LSI Matrix: Itanium



## A

10k x 255k
3.7M non-zeros

Baseline: 25 Mflop/s

Best block size \& performance: 16k x 32k
72 Mflop/s

## Cache Blocked SpMV on LSI Matrix: Itanium



A
10k x 255k
3.7M non-zeros

## Baseline:

170 Mflop/s
Best block size \& performance: 16k x 65k 275 Mflop/s

## Summary and Questions

- Need to understand matrix structure and machine
- BeBOP: suite of techniques to deal with different sparse structures and architectures
- Google matrix problem
- Established techniques within an iteration
- Ideas for inter-iteration optimizations
- Mathematical structure of problem may help
- Questions
- Structure of G?
- What are the computational bottlenecks?
- Enabling future computations?
- E.g., topic-sensitive PageRank $\rightarrow$ multiple vector version [Haveliwala '02]
- See www.cs.berkeley.edu/~richie/bebop/intel/google for more info, including more complete Itanium 2 results.


## Exploiting Matrix Structure

- Symmetry (numerical or structural)
- Reuse matrix entries
- Can combine with register blocking, multiple vectors, ...
- Matrix splitting
- Split the matrix, e.g., into rxc and $1 \times 1$
- No fill overhead
- Large matrices with random structure
- E.g., Latent Semantic Indexing (LSI) matrices
- Technique: cache blocking
- Store matrix as $2^{i} \times 2^{j}$ sparse submatrices
- Effective when $x$ vector is large
- Currently, search to find fastest size


## Symmetric SpMV Performance: Pentium 4



## SpMV with Split Matrices: Ultra $2 i$



## Cache Blocking on Random Matrices: Itanium

Speedup on four banded random matrices.


$Z=1.000000$; ref $=43.5 \mathrm{MFLOPS}$


## Sparse Kernels and Optimizations

- Kernels
- Sparse matrix-vector multiply (SpMV): $y=A^{*} x$
- Sparse triangular solve (SpTS): $x=T^{-1 *} b$
- $y=A A^{T *} x, y=A^{\top} A^{*} x$
- Powers ( $y=A^{k *} x$ ), sparse triple-product ( $R^{*} A^{*} R^{\top}$ ), $\ldots$
- Optimization techniques (implementation space)
- Register blocking
- Cache blocking
- Multiple dense vectors (x)
- A has special structure (e.g., symmetric, banded, ...)
- Hybrid data structures (e.g., splitting, switch-to-dense, ...)
- Matrix reordering
- How and when do we search?
- Off-line: Benchmark implementations
- Run-time: Estimate matrix properties, evaluate performance models based on benchmark data

Performance Summary [pentium3-linux-icc]


Performance Summary [ultra-solaris]


Performance Summary [power3-aix]


Performance Summary [itanium-linux-ecc]


## Possible Optimization Techniques

- Within an iteration, i.e., computing (G+uu $\left.{ }^{\top}\right)^{*} x$ once
- Cache block G*x
- On linear programming matrices and matrices with random structure (e.g., LSI), 1.5-4x speedups
- Best block size is matrix and machine dependent
- Reordering and/or splitting of G to separate dense structure (rows, columns, blocks)
- Between iterations, e.g., $\left(G+u u^{\top}\right)^{2} x$
$-\left(G+u u^{\top}\right)^{2} x=G^{2} x+(G u) u^{\top} x+u\left(u^{\top} G\right) x+u\left(u^{\top} u\right) u^{\top} x$
- Compute $\mathrm{Gu}, \mathrm{u}^{\top} \mathrm{G}, \mathrm{u}^{\top} u$ once for all iterations
- $\mathrm{G}^{2} \mathrm{x}$ : Inter-iteration tiling to read G only once


## Multiple Vector Performance: Itanium



## Sparse Kernels and Optimizations

- Kernels
- Sparse matrix-vector multiply (SpMV): $y=A^{*} x$
- Sparse triangular solve (SpTS): $x=T^{-1 *} b$
- $y=A A^{T *} x, y=A^{\top} A^{*} x$
- Powers $\left(y=A^{k *} x\right)$, sparse triple-product $\left(R^{*} A^{*} R^{\top}\right), \ldots$
- Optimization techniques (implementation space)
- Register blocking
- Cache blocking
- Multiple dense vectors (x)
- A has special structure (e.g., symmetric, banded, ...)
- Hybrid data structures (e.g., splitting, switch-to-dense, ...)
- Matrix reordering
- How and when do we search?
- Off-line: Benchmark implementations
- Run-time: Estimate matrix properties, evaluate performance models based on benchmark data


## SpTS Performance: Itanium


(See POHLL '02 workshop paper, at ICS '02.)

## Sparse Kernels and Optimizations

- Kernels
- Sparse matrix-vector multiply (SpMV): $y=A^{*} x$
- Sparse triangular solve (SpTS): $x=T^{-1 *} b$
- $y=A A^{T *} x, y=A^{T} A^{*} x$
- Powers $\left(y=A^{k *} x\right)$, sparse triple-product $\left(R^{*} A^{*} R^{\top}\right), \ldots$
- Optimization techniques (implementation space)
- Register blocking
- Cache blocking
- Multiple dense vectors (x)
- A has special structure (e.g., symmetric, banded, ...)
- Hybrid data structures (e.g., splitting, switch-to-dense, ...)
- Matrix reordering
- How and when do we search?
- Off-line: Benchmark implementations
- Run-time: Estimate matrix properties, evaluate performance models based on benchmark data


## Optimizing $A A^{T *} X$

- Kernel: $y=A A^{T *} x$, where $A$ is sparse, $x$ \& $y$ dense
- Arises in linear programming, computation of SVD
- Conventional implementation: compute $z=A^{T *} x, y=A * z$
- Elements of $A$ can be reused:

$$
y=\left(\begin{array}{ll}
a_{1} \Lambda & a_{n}
\end{array}\right)\left(\begin{array}{c}
a_{1}^{T} \\
\mathrm{M} \\
a_{n}^{T}
\end{array}\right) x=\sum_{k=1}^{n} a_{k}\left(a_{k}^{T} x\right)
$$

- When $a_{k}$ represent blocks of columns, can apply register blocking.


## Optimized $A A^{T *} x$ Performance: Pentium III



## Current Directions

- Applying new optimizations
- Other split data structures (variable block, diagonal, ...)
- Matrix reordering to create block structure
- Structural symmetry
- New kernels (triple product $R A R^{T}$, powers $A^{k}, \ldots$ )
- Tuning parameter selection
- Building an automatically tuned sparse matrix library
- Extending the Sparse BLAS
- Leverage existing sparse compilers as code generation infrastructure
- More thoughts on this topic tomorrow


## Related Work

- Automatic performance tuning systems
- PHiPAC [Bilmes, et al., '97], ATLAS [Whaley \& Dongarra '98]
- FFTW [Frigo \& Johnson '98], SPIRAL [Pueschel, et al., '00], UHFFT [Mirkovic and Johnsson '00]
- MPI collective operations [Vadhiyar \& Dongarra '01]
- Code generation
- FLAME [Gunnels \& van de Geijn, '01]
- Sparse compilers: [Bik '99], Bernoulli [Pingali, et al., '97]
- Generic programming: Blitz++ [Veldhuizen '98], MTL [Siek \& Lumsdaine '98], GMCL [Czarnecki, et al. '98], ...
- Sparse performance modeling
- [Temam \& Jalby '92], [White \& Saddayappan '97], [Navarro, et al., '96], [Heras, et al., '99], [Fraguela, et al., '99], ...


## More Related Work

- Compiler analysis, models
- CROPS [Carter, Ferrante, et al.]; Serial sparse tiling [Strout '01]
- TUNE [Chatterjee, et al.]
- Iterative compilation [O'Boyle, et al., '98]
- Broadway compiler [Guyer \& Lin, '99]
- [Brewer '95], ADAPT [Voss '00]
- Sparse BLAS interfaces
- BLAST Forum (Chapter 3)
- NIST Sparse BLAS [Remington \& Pozo '94]; SparseLib++
- SPARSKIT [Saad '94]
- Parallel Sparse BLAS [Fillipone, et al. '96]


## Context: Creating High-Performance Libraries

- Application performance dominated by a few computational kernels
- Today: Kernels hand-tuned by vendor or user
- Performance tuning challenges
- Performance is a complicated function of kernel, architecture, compiler, and workload
- Tedious and time-consuming
- Successful automated approaches
- Dense linear algebra: ATLAS/PHiPAC
- Signal processing: FFTW/SPIRAL/UHFFT


## Cache Blocked SpMV on LSI Matrix: Itanium

Speedup of Cache Blocking: LSI ( $10 \mathrm{~K} \times 255 \mathrm{~K}$ ); naive $=25 \mathrm{Mflop} / \mathrm{s}$ [itanium-ecc]


## Sustainable Memory Bandwidth



## Multiple Vector Performance: Pentium 4



## Multiple Vector Performance: Itanium



## Multiple Vector Performance: Pentium 4



## Optimized $A A^{T *} x$ Performance: Ultra 2 i



## Optimized $A A^{T *} x$ Performance: Pentium 4



## Tuning Pays Off-PHiPAC




## Tuning pays off - ATLAS

$500 \times 500$ Double Precision Matrix-Matrix Multiply Across Multiple Architectures



## Register Tile Sizes (Dense Matrix Multiply)



333 MHz Sun Ultra 2i

2-D slice of 3-D space; implementations colorcoded by performance in Mflopls

16 registers, but 2-by-3 tile size fastest

## High Precision GEMV (XBLAS)



## High Precision Algorithms (XBLAS)

- Double-double (High precision word represented as pair of doubles)
- Many variations on these algorithms; we currently use Bailey's
- Exploiting Extra-wide Registers
- Suppose s(1) , ... , s(n) have f-bit fractions, SUM has F>f bit fraction
- Consider following algorithm for $S=\Sigma_{i=1, n} s(i)$
- Sort so that $|s(1)| \geq|s(2)| \geq \cdots \geq|s(n)|$
- $\operatorname{SUM}=0$, for $\mathrm{i}=1$ to n SUM $=$ SUM + s(i), end for, sum = SUM
- Theorem (D., Hida) Suppose F<2f (less than double precision)
- If $\mathrm{n} \leq 2^{\mathrm{F}-\mathrm{f}}+1$, then error $\leq 1.5$ ulps
- If $\mathrm{n}=2^{\mathrm{F}-\mathrm{f}}+2$, then error $\leq 2^{2 \mathrm{f}-\mathrm{F}}$ ulps (can be $\gg 1$ )
- If $n \geq 2^{F-f}+3$, then error can be arbitrary $(S \neq 0$ but sum $=0)$
- Examples
- $s(i)$ double ( $f=53$ ), SUM double extended ( $F=64$ )
- accurate if $\mathrm{n} \leq \mathbf{2}^{\mathbf{1 1}}+1=2049$
- Dot product of single precision $x(i)$ and $y(i)$
$-\mathrm{s}(\mathrm{i})=x(\mathrm{i})^{*} y(\mathrm{i}) \quad(\mathrm{f}=2 * 24=48)$, SUM double extended $(\mathrm{F}=64) \Rightarrow$
- accurate if $n \leq 2^{16}+1=65537$

