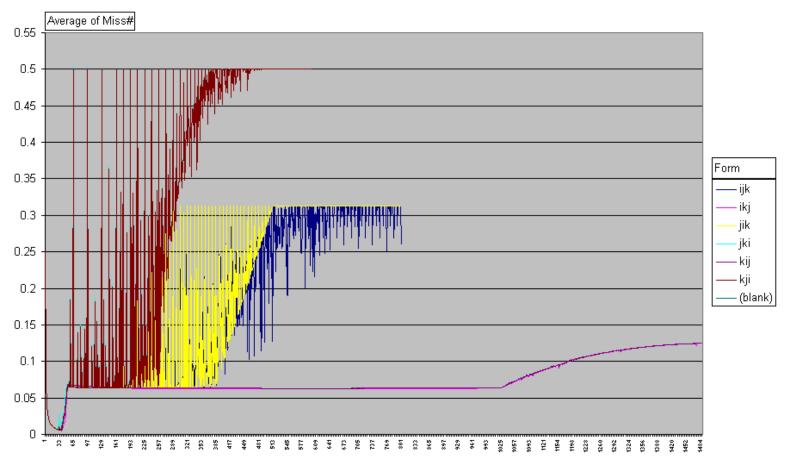
Optimizing MMM & ATLAS Library Generator

Recall: MMM miss ratios

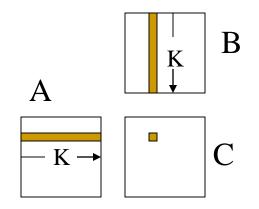
L1 Cache Miss Ratio for Intel Pentium III

- MMM with N = 1...1300
- 16KB 32B/Block 4-way 8-byte elements



IJK version (large cache)

DO I = 1, N//row-major storage DO J = 1, N DO K = 1, N C(I,J) = C(I,J) + A(I,K)*B(K,J)



Large cache scenario:

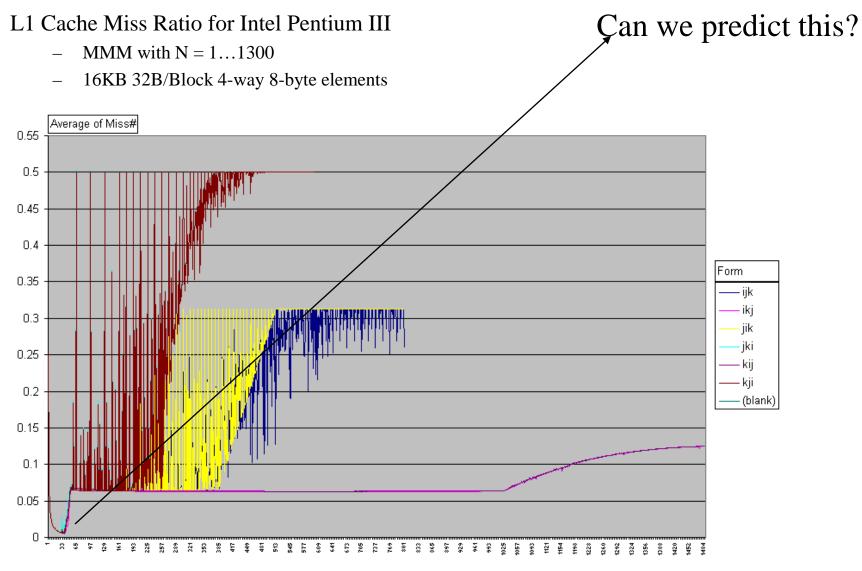
- Matrices are small enough to fit into cache
- Only cold misses, no capacity misses
- Miss ratio:
 - Data size = 3 N²
 - Each miss brings in b floating-point numbers
 - Miss ratio = 3 N²/b*4N³ = 0.75/bN = 0.019 (b = 4,N=10)

IJK version (small cache)

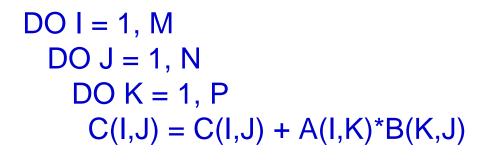
DO I = 1, N DO J = 1, N DO K = 1, N C(I,J) = C(I,J) + A(I,K)*B(K,J)

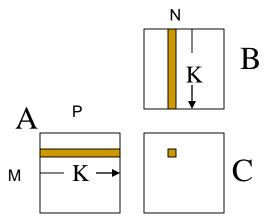
- Small cache scenario:
 - Matrices are large compared to cache
 - reuse distance is not O(1) => miss
 - Cold and capacity misses
 - Miss ratio:
 - C: N²/b misses (good temporal locality)
 - A: N³/b misses (good spatial locality)
 - B: N³ misses (poor temporal and spatial locality)
 - Miss ratio \rightarrow 0.25 (b+1)/b = 0.3125 (for b = 4)

MMM experiments



How large can matrices be and still not suffer capacity misses?





- How large can these matrices be without suffering capacity misses?
 - Each iteration of outermost loop walks over entire B matrix, so all of B must be in cache
 - We walk over rows of A and successive iterations of middle loop touch same row of A, so one row of A must be in cache
 - □ We walk over elements of C one at a time.
 - So inequality is NP + P + 1 <= C</p>

Check with experiment

- For our machine, capacity of L1 cache is 16KB/8 doubles = 2¹¹ doubles
- If matrices are square, we must solve

 $N^2 + N + 1 = 2^{11}$

which gives us N = 45

This agrees well with experiment.

High-level picture of high-performance MMM code

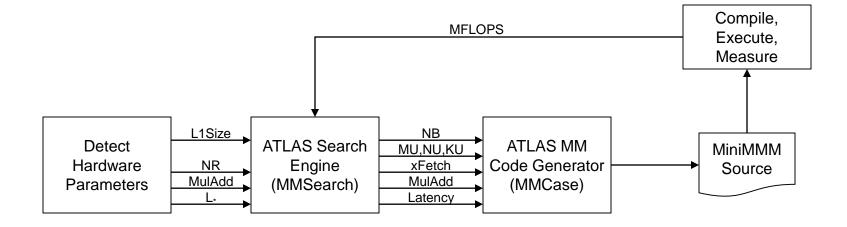
- Block the code for each level of memory hierarchy
 - Registers
 - L1 cache
 -
- Choose block sizes at each level using the theory described previously
 - Useful optimization: choose block size at level
 L+1 to be multiple of the block size at level L

ATLAS

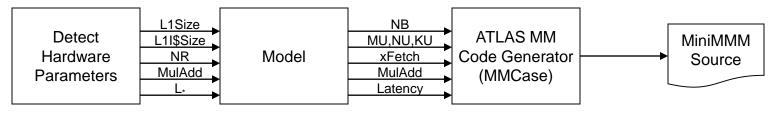
- Library generator for MMM and other BLAS
- Blocks only for registers and L1 cache
- Uses search to determine block sizes, rather than the analytical formulas we used
 - Search takes more time, but we do it once when library is produced
- Let us study structure of ATLAS in little more detail

Our approach

Original ATLAS Infrastructure



Model-Based ATLAS Infrastructure



BLAS

Let us focus on MMM:

```
for (int i = 0; i < M; i++)
for (int j = 0; j < N; j++)
for (int k = 0; k < K; k++)
C[i][j] += A[i][k]*B[k][j]</pre>
```

Properties

- □ Very good reuse: O(N²) data, O(N³) computation
- Many optimization opportunities
 - Few "real" dependencies
- Will run poorly on modern machines
 - Poor use of cache and registers
 - Poor use of processor pipelines

Optimizations

Cache-level blocking (tiling)

- Atlas blocks only for L1 cache
- NB: L1 cache time size

Register-level blocking

- Important to hold array values in registers
- MU,NU: register tile size
- Filling the processor pipeline
 - Unroll and schedule operations
 - Latency, xFetch: scheduling parameters

Versioning

- Dynamically decide which way to compute
- Back-end compiler optimizations
 - Scalar Optimizations
 - Instruction Scheduling

Cache-level blocking (tiling)

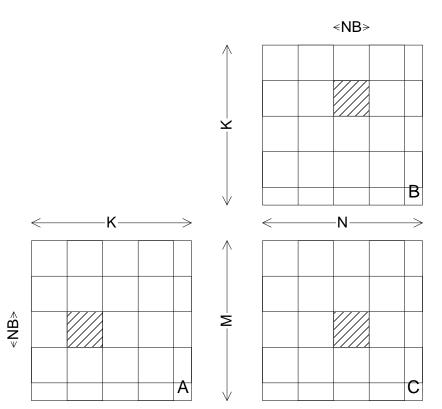
Tiling in ATLAS

- Only square tiles (NBxNBxNB)
- Working set of tile fits in L1
- Tiles are usually copied to continuous storage
- Special "clean-up" code generated for boundaries

Mini-MMM

```
for (int j = 0; j < NB; j++)
for (int i = 0; i < NB; i++)
for (int k = 0; k < NB; k++)
C[i][j] += A[i][k] * B[k][j]</pre>
```

NB: Optimization parameter



Register-level blocking

Micro-MMM

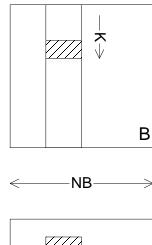
- A: MUx1
- B: 1xNU
- C: MUXNU
- MUxNU+MU+NU registers
- Unroll loops by MU, NU, and KU
- Mini-MMM with Micro-MMM inside

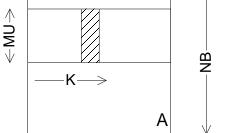
```
for (int j = 0; j < NB; j += NU)
for (int i = 0; i < NB; i += MU)
load C[i..i+MU-1, j..j+NU-1] into registers
for (int k = 0; k < NB; k++)

KU times
{
load A[i..i+MU-1,k] into registers
load B[k,j..j+NU-1] into registers
multiply A's and B's and add to C's
store C[i..i+MU-1, j..j+NU-1]
}</pre>
```

- Special clean-up code required if NB is not a multiple of MU,NU,KU
- MU, NU, KU: optimization parameters

<NU>

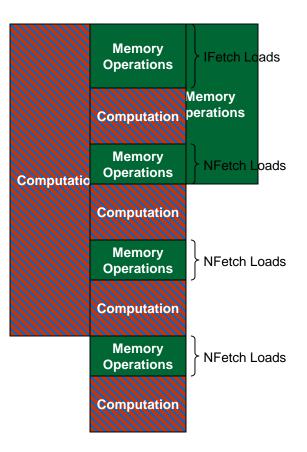






Scheduling

- FMA Present?
- Schedule Computation
 - Using Latency
- Schedule Memory Operations
 - Using IFetch, NFetch, FFetch



. . .

Latency, xFetch: optimization parameters

Search Strategy

Multi-dimensional optimization problem:

- Independent parameters: NB,MU,NU,KU,...
- Dependent variable: MFlops
- Function from parameters to variables is given implicitly; can be evaluated repeatedly
- One optimization strategy: orthogonal line search
 - Optimize along one dimension at a time, using reference values for parameters not yet optimized
 - □ Not guaranteed to find optimal point, but might come close

Find Best NB

Search in following range

□ 16 <= NB <= 80

 \square NB² <= L1Size

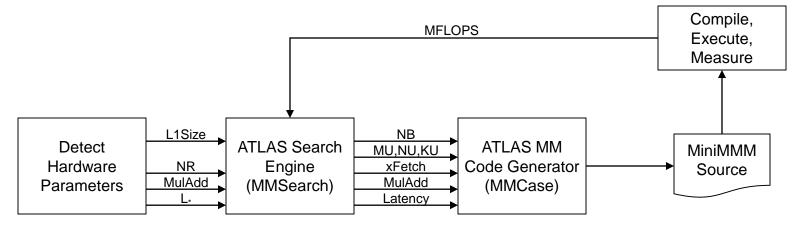
In this search, use simple estimates for other parameters

□ (eg) KU: Test each candidate for

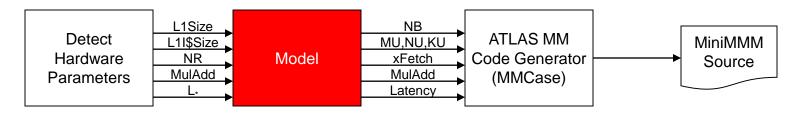
- Full K unrolling (KU = NB)
- No K unrolling (KU = 1)

Model-based optimization

Original ATLAS Infrastructure



Model-Based ATLAS Infrastructure



Modeling for Optimization Parameters

Optimization parameters

NB

- Hierarchy of Models (later)
- MU, NU

• $MU * NU + MU + NU + Latency \le NR$ • KU

maximize subject to L1 Instruction Cache

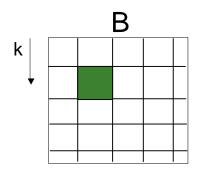
Latency

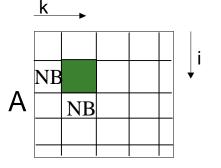
■ 「(L_{*} + 1)/2]

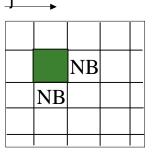
- MulAdd
 - hardware parameter
- xFetch
 - set to 2

Largest NB for no capacity/conflict misses

 If tiles are copied into contiguous memory, condition for only cold misses:
 3*NB² <= L1Size







Largest NB for no capacity misses

MMM:

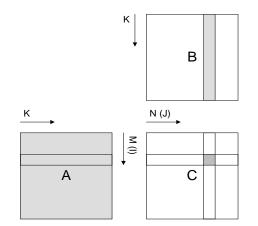
```
for (int j = 0; i < N; i++)
for (int i = 0; j < N; j++)
for (int k = 0; k < N; k++)
c[i][j] += a[i][k] * b[k][j]</pre>
```

• Cache model:

- Fully associative
- Line size 1 Word
- Optimal Replacement
- Bottom line:

NB²+NB+1<C

- One full matrix
- One row / column
- One element



Summary: Modeling for Tile Size (NB)

^∧NB⇒

- Models of increasing complexity
 - $\Box \quad 3^* NB^2 \le C$
 - Whole work-set fits in L1
 - $\Box \quad NB^2 + NB + 1 \le C$
 - Fully Associative
 - Optimal Replacement
 - Line Size: 1 word

$$\square \left[\frac{NB^2}{B}\right] + \left[\frac{NB}{B}\right] + 1 \le \frac{C}{B} \text{ or } \left[\frac{NB^2}{B}\right] + NB + 1 \le \frac{C}{B}$$

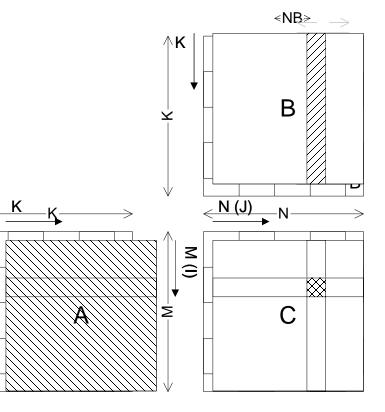
• Line Size > 1 word

$$\square \left[\frac{NB^2}{B}\right] + 2\left[\frac{NB}{B}\right] + \left(\left[\frac{NB}{B}\right] + 1\right) \le \frac{C}{B} \text{ or}$$

$$\left[NB^2\right] = C$$

$$\left|\frac{NB^2}{B}\right| + 3NB + 1 \le \frac{C}{B}$$

LRU Replacement

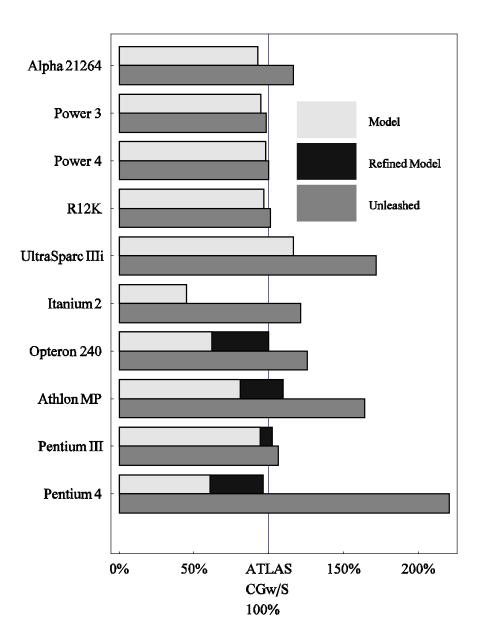


Summary of model

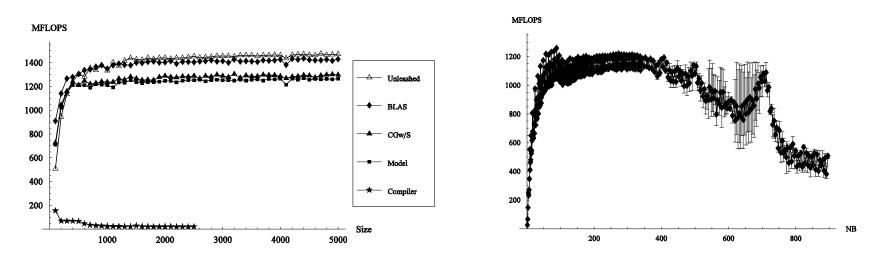
• Estimating FMA: Use the machine parameter FMA • Estimating L_s: $L_s = \left\lceil \frac{L_* \times |ALU_{FP}| + 1}{2} \right\rceil$ • Estimating M_U and N_U : $M_{U} \times N_{U} + N_{U} + M_{U} + L_{s} \leq N_{R}$ 1) $M_U, N_U \leftarrow u$. Solve constraint for u. 3) $M_U \leftarrow \max(u, 1)$. 4) Solve constraint for NU. 5) $N_U \leftarrow \max(N_U, 1)$. 6) If $M_U < N_U$ then swap M_U and N_U . • Estimating N_B: $\left\lceil \frac{N_B^2}{B_1} \right\rceil + 3 \left\lceil \frac{N_B \times N_U}{B_1} \right\rceil + \left\lceil \frac{M_U}{B_1} \right\rceil \times N_U \leq \frac{C_1}{B_1}$ Trim N_B , to make it a multiple of M_U , N_U , and 2. • Estimating K_U : Choose K_U as the maximum value for which mini-MMM fits in the L1 instruction cache. Trim K_U to make it divide N_B evenly. • Estimating F_F , I_F , and N_F : $F_F = 0, I_F = 2, N_F = 2$

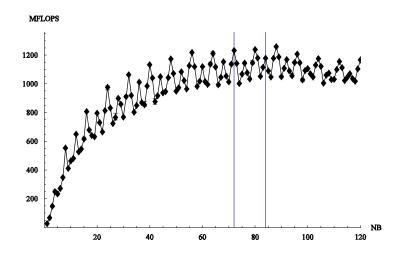
Experiments

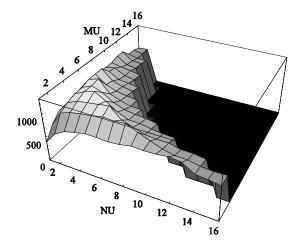
- Ten modern architectures
- Model did well on
 RISC architectures
 - •UltraSparc: did better
- Model did not do as well on
 - •Itanium
 - CISC architectures
- Substantial gap between ATLAS CGw/S and ATLAS Unleashed on some architectures



Some sensitivity graphs for Alpha 21264







Eliminating performance gaps

- Think globally, search locally
- Gap between model-based optimization and empirical optimization can be eliminated by

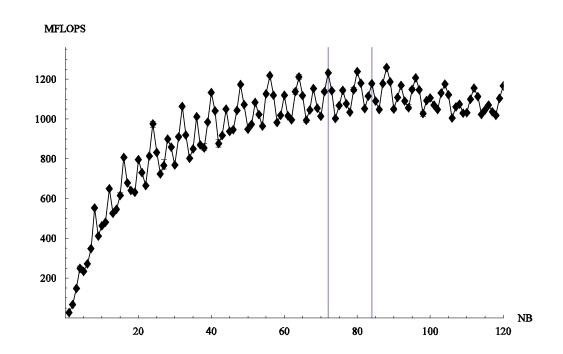
Local search:

- for small performance gaps
- in neighborhood of model-predicted values
- Model refinement:
 - for large performance gaps
 - must be done manually
 - (future) machine learning: learn new models automatically

 Model-based optimization and empirical optimization are not in conflict

Small performance gap: Alpha 21264

ATLAS CGw/S: mini-MMM: 1300 MFlops NB = 72 (MU,NU) = (4,4)ATLAS Model mini-MMM: 1200 MFlops NB = 84 (MU,NU) = (4,4)



Local search

•Around model-predicted NB

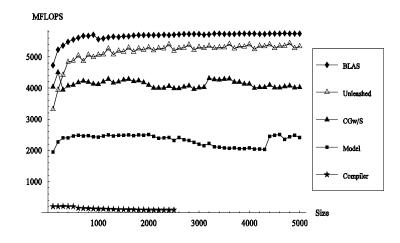
•Hill-climbing not useful

Search interval:[NB-lcm(MU,NU),NB+lcm(MU,NU)]

Local search for MU,NU

•Hill-climbing OK

Large performance gap: Itanium



MMM Performance

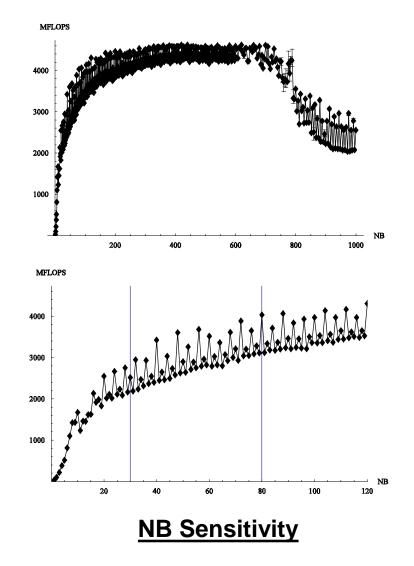
Performance of mini-MMM

- ATLAS CGw/S: 4000 MFlops
- ATLAS Model: 1800 MFlops

Problem with NB value

ATLAS Model: 30 ATLAS CGw/S: 80 (search space max)

Local search will not solve problem.



Itanium diagnosis and solution

Memory hierarchy

- L1 data cache: 16 KB
- L2 cache: 256 KB
- L3 cache: 3 MB

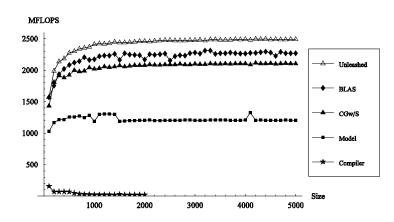
Diagnosis:

- Model tiles for L1 cache
- On Itanium, FP values not cached in L1 cache!
- Performance gap goes away if we model for L2 cache (NB = 105)
- Obtain even better performance if we model for L3 cache (NB = 360, 4.6 GFlops)

Problem:

- □ Tiling for L2 or L3 may be better than tiling for L1
- How do we determine which cache level to tile for??
- Our solution: model refinement + a little search
 - Determine tile sizes for all cache levels
 - Choose between them empirically

Large performance gap: Opteron



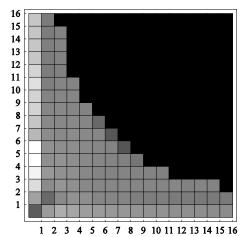
MMM Performance

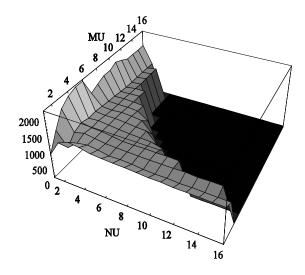
Performance of mini-MMM

- ATLAS CGw/S: 2072 MFlops
- ATLAS Model: 1282 MFlops

Key differences in parameter values:MU/NU

- ATLAS CGw/S: (6,1)
- ATLAS Model: (2,1)





MU,NU Sensitivity

Opteron diagnosis and solution

Opteron characteristics

- Small number of logical registers
- Out-of-order issue
- Register renaming
- For such processors, it is better to
 - let hardware take care of scheduling dependent instructions,
 - use logical registers to implement a bigger register tile.
- x86 has 8 logical registers
 - □ → register tiles must be of the form (x,1) or (1,x)

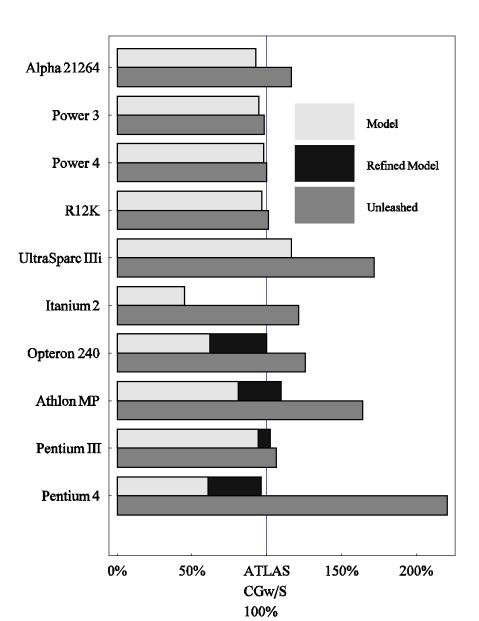
Refined model

• Estimating FMA: Use the machine parameter FMA • Estimating L_s: $L_s = \left\lceil rac{L_* imes |ALU_{FP}| + 1}{2}
ight
ceil$ • Estimating M_U and N_U : $M_U \times N_U + N_U + M_U + L_s \leq N_R$ 1) $M_U, N_U \leftarrow u$. Solve constraint for u. 3) $M_U \leftarrow \max(u, 1)$. Solve constraint for N_U. 5) $N_U \leftarrow \max(N_U, 1)$. 6) If $M_U < N_U$ then swap M_U and N_U . 7) Refined Model: If $N_U = 1$ then $-M_U \leftarrow N_R - 2$ $-N_U \leftarrow 1$ $-FMA \leftarrow 1$ Estimating N_B: $\left\lceil \frac{N_B^2}{B_1} \right\rceil + 3 \left\lceil \frac{N_B \times N_U}{B_1} \right\rceil + \left\lceil \frac{M_U}{B_1} \right\rceil \times N_U \leq \frac{C_1}{B_1}$ Trim N_B , to make it a multiple of M_U , N_U , and 2. • Estimating K_U : Choose K_U as the maximum value for which mini-MMM fits in the L1 instruction cache. Trim K_U to make it divide N_B evenly. • Estimating F_F , I_F , and N_F :

$$F_F = 0, I_F = 2, N_F = 2$$

Bottom line

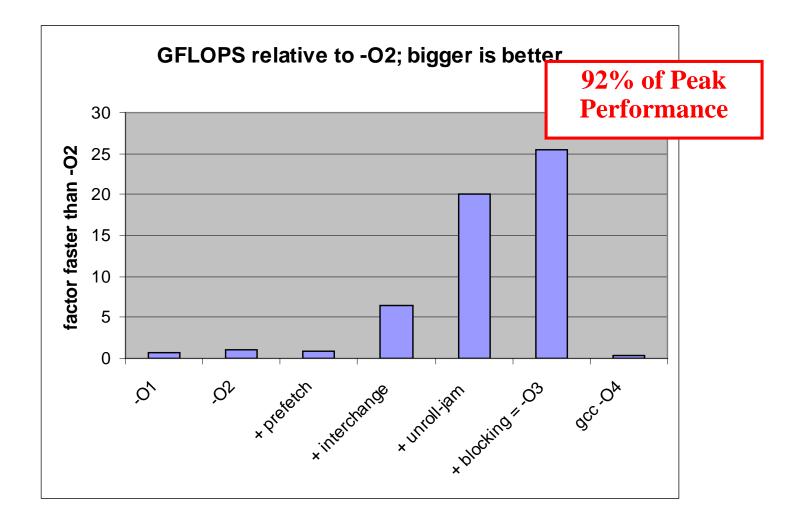
- Refined model is not complex.
- Refined model by itself eliminates most performance gaps.
- Local search eliminates all performance gaps.



Future Directions

- Repeat study with FFTW/SPIRAL
 - Uses search to choose between algorithms
- Feed insights back into compilers
 - Build a linear algebra compiler for generating highperformance code for dense linear algebra codes
 - Start from high-level algorithmic descriptions
 - Use restructuring compiler technology
 - Generalize to other problem domains

Performance of MMM code produced by Intel's Itanium compiler (-O3)



Goto BLAS obtains close to 99% of peak, so compiler is pretty good!