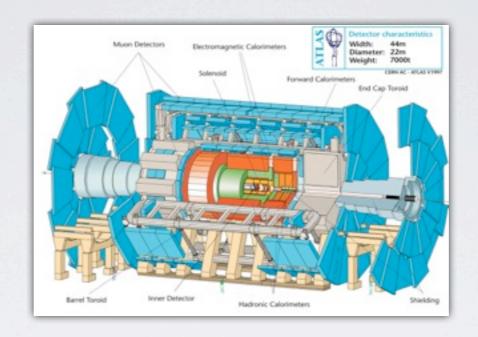
VECTORIZATION IN ATLAS

Roberto A. Vitillo (LBNL)

THE ATLAS EXPERIMENT



- ▶ ATLAS is one of the six particle physics experiment at the Large Hadron Collider (LHC)
- Proton beams interact in the center of the detector
- The ATLAS detector has been designed to provide the most complete information of the ~1000 particles that emerge from the proton collisions
- ► ATLAS acts as a huge digital camera composed of ~100 Million of channels which provide a "picture" of about 1 Mbyte defined as event
- Each event is fully analyzed to obtain the information needed for the physics analysis
- ▶ The software behind ATLAS consists of millions of LOC; a monstrosity to optimize!

DESIGN LEVELS

Architecture

Algorithms & Data Structures

Code

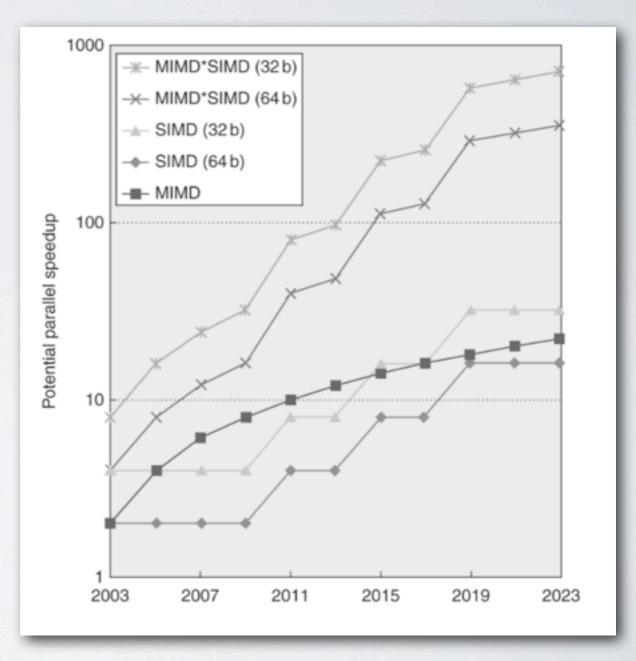
System Software

Hardware

- Independent changes on different levels causes speedups to multiply
- Clock speed free lunch is over
 - hardware parallelism is increasing
- How can parallelism be exploited at the bottom layers?

EXPLOITING SIMD

- Single Instruction, Multiple Data:
 - processor throughput is increased by handling multiple data in parallel (MMX, SSE, AVX, ...)
 - vector of data is packed in one large register and handled in one operation
 - exploiting SIMD is even more of importance for the Xeon PHI and future architectures



Source: "Computer Architecture, A Quantitative Approach"

EXPLOITING SIMD

ATLAS USE CASES

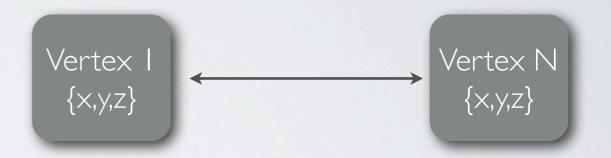
- Linear algebra operations
 - ▶ small rectangular matrices (e.g. 2x5, 3x5, 3x6, ...) for error propagation
 - ▶ small square matrices (e.g. 3x3, 4x4, 5x5, ...) for transforms in geometry calculations
 - ▶ separate use of matrices up to ~25x25 in a few places
- Hot loops that invoke transcendental functions
- · Other numerical hotspots, e.g. Kalman Filter in Tracking

EXPLOITING SIMD

APPROACHES

- I.hand-tuning numerical hotspots
- 2. vectorized linear algebra libraries
- 3.autovectorization
- 4. language extensions

Horizontal Vectorization



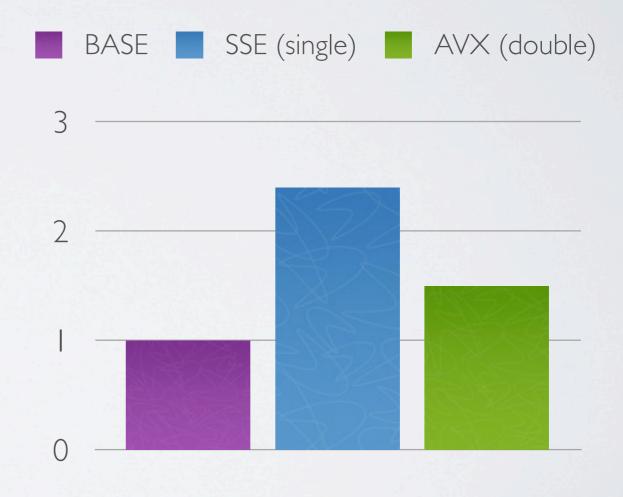
HAND TUNING NUMERICAL HOTSPOTS

- GOoDA told us that most cycles are spent in RungeKuttaPropagator::rungeKuttaStep
- Most nested loop accounts for ~50% of its cycles
 - contains lots of floating point operations
- Good candidate for vectorization
 - autovectorization failed

```
for(int i=0; i<42; i+=7) {</pre>
    double* dR = &P[i];
    double* dA
                = &P[i+3];
   double dA0
                = H0[2]*dA[1]-H0[1]*dA[2];
    double dB0
                = H0[0]*dA[2]-H0[2]*dA[0];
    double dC0 = H0[1]*dA[0]-H0[0]*dA[1];
    if(i==35) \{dA0+=A0; dB0+=B0; dC0+=C0;\}
   double dA2
                = dA0+dA[0];
   double dB2
                = dB0+dA[1];
   double dC2
                = dC0+dA[2];
                = dA[0]+dB2*H1[2]-dC2*H1[1];
    double dA3
    double dB3 = dA[1]+dC2*H1[0]-dA2*H1[2];
   double dC3 = dA[2]+dA2*H1[1]-dB2*H1[0];
    if(i==35) {dA3+=A3-A00; dB3+=B3-A11; dC3+=C3-A22;}
   double dA4 = dA[0]+dB3*H1[2]-dC3*H1[1];
                = dA[1]+dC3*H1[0]-dA3*H1[2];
   double dB4
   double dC4 = dA[2]+dA3*H1[1]-dB3*H1[0];
    if(i==35) {dA4+=A4-A00; dB4+=B4-A11; dC4+=C4-A22;}
                = dA4+dA4-dA[0];
   double dA5
   double dB5
                = dB4+dB4-dA[1];
   double dC5
                = dC4+dC4-dA[2];
   double dA6
                = dB5*H2[2]-dC5*H2[1];
   double dB6
                = dC5*H2[0]-dA5*H2[2];
   double dC6
               = dA5*H2[1]-dB5*H2[0];
   if(i==35) \{dA6+=A6; dB6+=B6; dC6+=C6;\}
   dR[0] += (dA2+dA3+dA4)*S3; dA[0] = (dA0+dA3+dA3+dA5+dA6)*.33333333;
   dR[1] += (dB2+dB3+dB4)*S3; dA[1] = (dB0+dB3+dB5+dB6)*.33333333;
   dR[2] += (dC2+dC3+dC4)*S3; dA[2] = (dC0+dC3+dC3+dC5+dC6)*.33333333;
```

```
for(int i = 0; i < 42; i+=7){
    _{m256d} dR = _{mm256_loadu_pd(\&P[i]);}
    _{m256d} dA = _{mm256_loadu_pd(&P[i + 3]);}
   _{m256d} dA_{201} = CROSS_SHUFFLE_{201}(dA);
    _{m256d} dA_{120} = CROSS_{SHUFFLE}120(dA);
    _{\rm m256d} d0 = _{\rm mm256}_{\rm sub_pd}(_{\rm mm256_mul_pd}(H0_201, dA_120), _{\rm mm256_mul_pd}(H0_120, dA_201));
   if(i==35){
        d0 = _mm256_add_pd(d0, V0_012);
    _{m256d} d2 = _{mm256} add_{pd}(d0, dA);
    __m256d d2_201 = CROSS_SHUFFLE_201(d2);
    _{m256d} d2_{120} = CROSS_SHUFFLE_{120}(d2);
    _{\rm m256d} d3 = _{\rm mm256\_sub\_pd(_mm256\_add\_pd(dA, _mm256\_mul\_pd(d2_120, H1_201)), _mm256_mul\_pd(d2_201, H1_120));
   _{m256d} d3_{201} = CROSS_{SHUFFLE}20\overline{1}(d3);
   __m256d d3_120 = CROSS_SHUFFLE_120(d3);
   if(i==35){
        d3 = _mm256_add_pd(d3, _mm256_sub_pd(V3_012, A_012));
    __m256d d4 = _mm256_sub_pd(_mm256_add_pd(dA, _mm256_mul_pd(d3_120, H1_201)), _mm256_mul_pd(d3_201, H1_120));
   if(i==35){
        d4 = _mm256_add_pd(d4, _mm256_sub_pd(V4_012, A_012));
     _m256d d5 = _mm256_sub_pd(_mm256_add_pd(d4, d4), dA);
    _{m256d} d5_{201} = CROSS_SHUFFLE_{201}(d5);
    _{m256d} d5_{120} = CROSS_SHUFFLE_{120}(d5);
    _{m256d} d6 = _{mm256\_sub\_pd(_{mm256\_mul\_pd(d5\_120, H2\_201), _{mm256\_mul\_pd(d5\_201, H2\_120))};
   if(i==35){
        d6 = _mm256_add_pd(d6, V6_012);
    _mm256_storeu_pd(&P[i], _mm256_add_pd(dR, _mm256_mul_pd(_mm256_add_pd(d2, _mm256_add_pd(d3, d4)), S3_012)));
    _mm256_storeu_pd(&P[i + 3], _mm256_mul_pd(C_012, _mm256_add_pd(d0, _mm256_add_pd(d3, _mm256_add_pd(d3, _mm256_add_pd(d5, d6))
```

- Tested on a Sandy Bridge-EP CPU
- SSE version with single precision intrinsics is 2.4x faster
- AVX version with double precision intrinsics is 1.5x faster
 - slower than SSE in this particular example because of costly cross lane permutations
 - not as mature as SSE
 - ► AVX2 (Haswell) will change that



- Hand-vectorizing may be suitable for vertical vectorization or when maximum speed-up is required and/or other approaches fail
- · Using compiler intrinsics or inline assembly is not ideal
- Options:
 - ► C++ Vector Class Library

 http://www.agner.org/optimize/vectorclass.zip
 - VC Library (recommended) http://code.compeng.uni-frankfurt.de/projects/vc

VC LIBRARY

- Implements vector classes that abstract the SIMD registers
 - vector register size is not directly exposed
 - memory abstraction allows to handle uniformly arrays of any size
 - masked ops syntax
- Transcendental functions are implemented within the library
- Vectors implemented with SSE2, SSE3, SSSE3, SSE4.1, SSE4.2, AVX
- Implementation is chosen at compile-time

```
void testVc(){
    Vc::Memory<double_v, SIZE> x;
    Vc::Memory<double_v, SIZE> y;

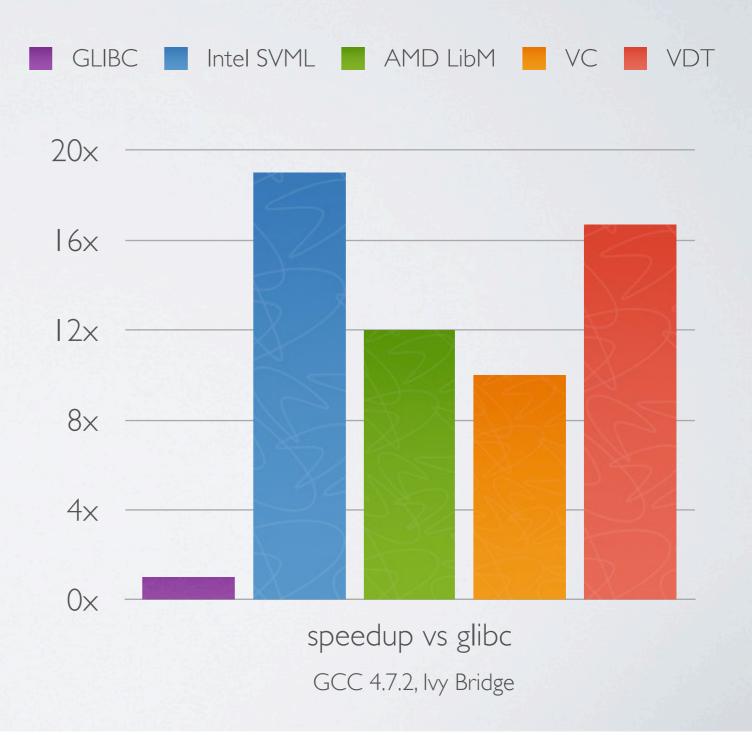
    for(int i = 0; i < x.vectorsCount(); i++){
        y.vector(i) = cos(x.vector(i) * 3);
    }
}</pre>
```

TRANSCENDENTAL FUNCTIONS

VECTOR PERFORMANCE

Accuracy				
GLIBC 2.17	SVML 11.0.1	AMD LibM 3	VC 0.6.7- dev	VDT 0.2.3
2 ulp	2-4 ulp	l ulp	1160 ulp	2 ulp

- Test performed applying cos() on an array of 100 doubles
- GLIBC
 - repeatedly calls scalar function on vector
- AMD LibM
 - supports only SSE2 for non-AMD processors
- VDT
 - accuracy comparable to SVML, see: http:// indico.cern.ch/contributionDisplay.py? contribld=48sessionId=98confld=202688



VECTORIZED LINEAR ALGEBRA LIBRARIES

(FOR SMALL MATRICES)

- Showcasing vertical vectorization
- Simplest possible example: 4x4 double precision matrix multiplication
 - matrix fits in two cache lines
 - AVX supports vectors of 4 doubles
- OptimizedMult vectorized without horizontal sums
- Speedup of 3 vs nonvectorized BasicMult

BasicMult

OptimizedMult

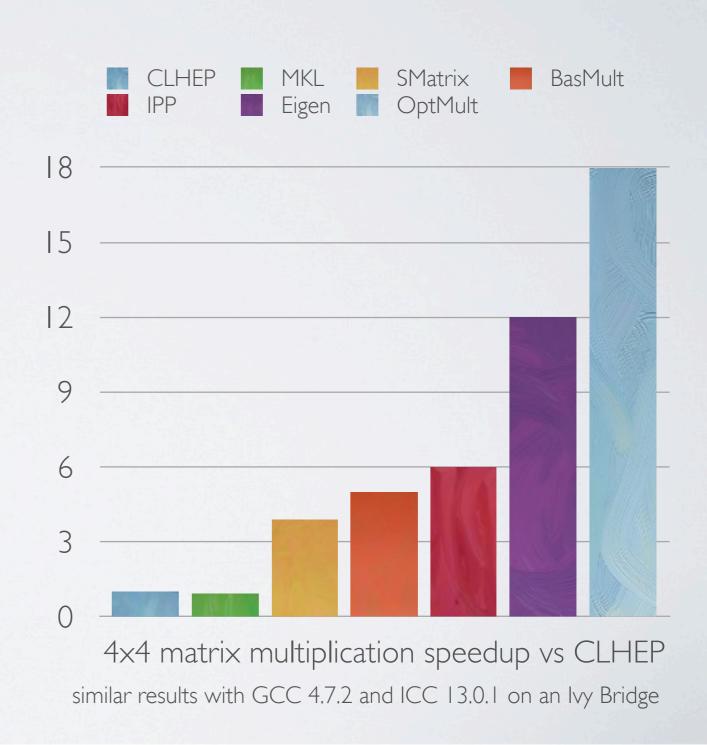
```
for(int i = 0; i < 16; i+=4){
    Vec4d r1 = Vec4d(x[i]) * Vec4d(y);

    for(int j = 1; j < 4; j++){
        r1 += Vec4d(x[i+j]) * Vec4d(&y[j*4]);
    }

    r1.store(&z[i]);
}</pre>
```

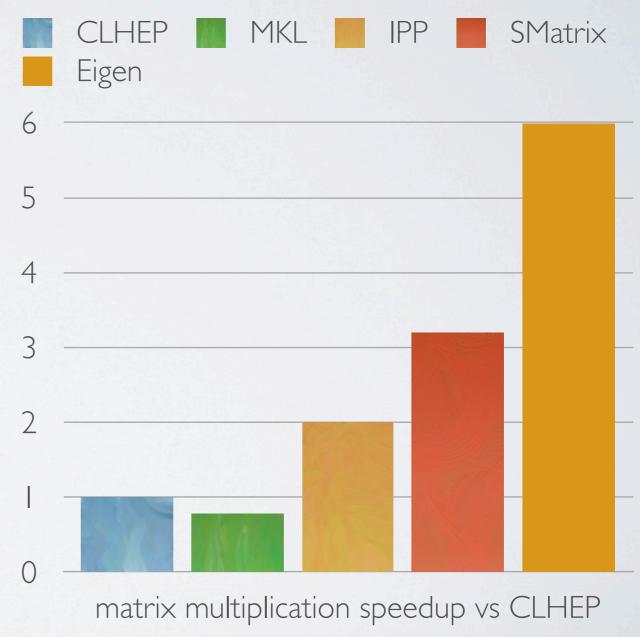
SQUARE MATRICES

- Eigen3 doesn't support yet AVX
- CLHEP provides a generic interface for any-dimension matrix
- MKL is optimized for large matrices and BLAS operations: $C = \alpha AB + \beta C$
- SMatrix operations are not vectorized
- Benefits of template expressions are not shown in this simple example
- OptMult represents the maximum speedup that can be achieved



RECTANGULAR MATRICES

- Evaluating $A_{5\times3} \times B_{3\times5}$
- None of the libraries is using vectorized code!
 - vectorization is not trivial in this case
 - alternative: horizontal vectorization



APPROACH 3 AUTOVECTORIZATION

AUTOVECTORIZATION CAVEATS

```
void foo(double *a, double *b)
   for(int i = 0; i < SIZE; i++)</pre>
         a[i] += b[i];
```

what we would like:



```
vmovapd ymm0,YMMWORD PTR [rdi+rax*1]
1a8:
       vaddpd ymm0,ymm0,YMMWORD PTR [rsi+rax*1]
1ad:
1b2:
       vmovapd YMMWORD PTR [rdi+rax*1],ymm0
1b7:
              rax,0x20
       add
1bb:
              rax, 0xc3500
       cmp
              1a8 <foo2+0x8>
1c1:
       jne
```

- Alignment of arrays unknown to the compiler
- GCC has to check if the arrays overlap but doesn't check if the arrays are aligned!
- If they do, scalar addition is performed
 - otherwise loop is only partially vectorized

what we actually get:



79: ine

```
0: lea
            rax, [rsi+0x20]
4: cmp
            rdi, rax
7: jb
            4b < f00 + 0 \times 4b >
9: xor
            eax,eax
            DWORD PTR [rax+rax*1+0x0]
b: nop
10: vmovupd xmm0, XMMWORD PTR [rsi+rax*1]
15: vmovupd xmm1, XMMWORD PTR [rdi+rax*1]
1a: vinsertf128 ymm0,ymm0,XMMWORD PTR [rsi+rax*1+0x10],0x1
22: vinsertf128 ymm1, ymm1, XMMWORD PTR [rdi+rax*1+0x10], 0x1
2a: vaddpd ymm0,ymm1,ymm0
2e: vmovupd XMMWORD PTR [rdi+rax*1],xmm0
33: vextractf128 XMMWORD PTR [rdi+rax*1+0x10],ymm0,0x1
3b: add
            rax,0x20
3f: cmp
            rax, 0xc3500
45: jne
            10 < f00 + 0 \times 10 >
47: vzeroupper
4a: ret
4b: lea
            rax, [rdi+0x20]
4f: cmp
            rsi, rax
            9 < f00 + 0 \times 9 >
52: jae
54: xor
            eax,eax
            WORD PTR cs:[rax+rax*1+0x0]
56: nop
60: vmovsd xmm0,QWORD PTR [rdi+rax*1]
65: vaddsd xmm0,xmm0,QWORD PTR [rsi+rax*1]
6a: vmovsd QWORD PTR [rdi+rax*1],xmm0
            rax, 0x8
6f: add
73: cmp
            rax, 0xc3500
            60 < f00 + 0 \times 60 >
```

AUTOVECTORIZATION CAVEATS

```
void foo(double * restrict a, double * restrict b)
{
   for(int i = 0; i < SIZE; i++)
        {
        a[i] += b[i];
    }
}</pre>
```



- GCC knows now that the arrays do not overlap but...
- It doesn't know if the arrays are aligned and doesn't check for it
 - loop only partially vectorized

```
r9,rdi
r9d,0x1f
                 rbp,rsp
        push
                 r9,0x3
        push
                 edx,r9d
                 rsp,0xffffffffffffe0
                 rsp,0x20
                 edx,0x3
185 <foo1+0x105>
                 eax.eax
        nop DWORD PTR [rax+0x0]
vmovsd xmm0,QWORD PTR [rdi+rax*8]
                 r10d.eax
                r11d,[rax+0x1]
        vaddsd xmm0,xmm0,QWORD PTR [rsi+rax*8]
vmovsd QWORD PTR [rdi+rax*8],xmm0
                 rax,0x1
                edx,eax
b8 <foo1+0x38>
                 r12d.0x186a0
                 r12d,edx
                 r8d,0x3
edx,r12d
                 edx,0x2
                 ebx,[rdx*4+0x0]
                ebx,ebx
140 <foo1+0xc0>
        je
shl
                 r8,0x3
                 eax,eax
                ecx,ecx
r9,[rdi+r8*1]
                DWORD PTR [rax+0x0]
        vmovupd xmm0,XMMWORD PTR [r8+rax*1]
        vinsertf128 ymm0,ymm0,XMMWORD PTR [r8+rax*1+0x10],0x1
        vaddpd ymm0,ymm0,YMMWORD PTR [r9+rax*1]
vmovapd YMMWORD PTR [r9+rax*1],ymm0
                rax,0x20
        cmp
jb
add
                ecx,edx
110 <foo1+0x90>
133:
                 r11d,ebx
                 r12d,ebx
179 <foo1+0xf9>
        movsxd r11,r11d
                r10d.0x1
                rdx,[r11*8+0x0]
                 r11.r10
                 rcx,[rdi+r11*8+0x8]
                 rdx,rsi
        xchq
                ax,ax
         vmovsd xmm0,QWORD PTR [rax]
        vaddsd xmm0,xmm0,QWORD PTR [rdx]
                 rdx,0x8
        vmovsd QWORD PTR [rax],xmm0
                rax,0x8
                 rax, rcx
                 160 <foo1+0xe0>
179:
17d:
                 rsp,[rbp-0x10]
                 rbp
        vzeroupper
                 r10d,0x186a0
                 r11d, r11d
        data32 data32 data32 nop WORD PTR cs:[rax+rax*1+0x0]
```

AUTOVECTORIZATION CAVEATS

```
void foo(double * restrict a, double * restrict b)
{
   double *x = __builtin_assume_aligned(a, 16);
   double *y = __builtin_assume_aligned(b, 16);
   for(int i = 0; i < SIZE; i++)
   {
        x[i] += y[i];
   }
}</pre>
1a8: vmovapd y
1b2: vmovapd Y
1b7: add ra
1bb: cmp ra
1bb: cmp ra
1c1: jne 1a
```

```
1a8: vmovapd ymm0, YMMWORD PTR [rdi+rax*1]
1ad: vaddpd ymm0, ymm0, YMMWORD PTR [rsi+rax*1]
1b2: vmovapd YMMWORD PTR [rdi+rax*1], ymm0
1b7: add rax,0x20
1bb: cmp rax,0xc3500
1c1: jne 1a8 <foo2+0x8>
```

- GCC finally generates optimal code
- Don't assume that the compiler generates efficient vector code
- For ICC see: http://software.intel.com/sites/default/files/m/4/8/8/2/a/31848-CompilerAutovectorizationGuide.pdf

LAR CALIBRATION

- Input for test: Barrel-presampler calibration run
- According to VTune, the hottest hotspot in this job is the wave convolution method
 - called from inside a fit method (many million times)
- Autovectorizing the inner loop of the convolution
 - requires -fassociative-math, -fno-signed-zeros and -fno-trapping-math
 - ▶ CPU time 121 -> 76 seconds (~ 40% faster)
 - result is not identical; relative diff about 1e-7

APPROACH 4 LANGUAGE EXTENSIONS

CILK PLUS

- Introduces
 - array notations, data parallelism for arrays or sections of arrays
 - SIMD pragma, specifies that a loop is to be vectorized
 - elemental functions, i.e. functions that can be vectorized when called from within an array notation or a #pragma simd loop
- Supported by recent ICC releases and a GCC branch
- Offers other features not related to vectorization, see: http://software.intel.com/en-us/intel-cilk-plus

```
// Copies x[i..i+n-1] to z[i..i+n-1]
z[i:n] = x[i:n];

// Sets z[i..i+n-1] to twice the
// corresponding elements in x[i+1..i+n]
z[i:n] = 2*x[i+1:n];
```

```
_declspec (vector)
float v_add(float x, float y){
    return x+y;
}

void foo(){
#pragma simd
    for(int j = 0; j < N; ++j){
        r[j] = v_add(a[j],b[j]);
    }
}</pre>
```

OPENMP 4

- Based on the SIMD directives of Cilk Plus
- Provides data sharing clauses
- Vectorizes functions by promoting scalar parameters to vectors and replicates control flow using elemental functions
- Up to 4x speedup vs autovectorization http://iwomp-2012.caspur.it/sites/iwomp-2012.caspur.it/files/ Klemm_SIMD.pdf
- OpenMP 4.0 specification was released recently

http://openmp.org/wp/openmp-specifications/

MEET ISPC

- Intel SPMD Program Compiler (ISPC) extends a C-based language with "single program, multiple data" (SPMD) constructs
- An ISPC program describes the behavior of a single program instance
 - even though a "gang" of them is in reality being executed
 - pang size is usually no more than 2-4x the native SIMD width of the machine
- For CUDA affectionados
 - ISPC Program is similar to a CUDA thread
 - An ISPC gang is similar to a CUDA warp

SPMD PARADIGM

Execution of a SPMD program with a gang size of 4

DEBUGGING SUPPORT

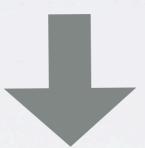
BEYOND GDB

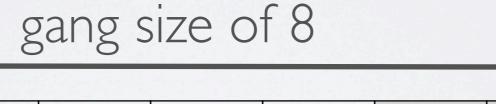
```
foreach(k = 0 ... 6){
   int i = k * 7;

   print("%\n", i);

   double* dR = &P[i];
   double* dA = &P[i+3];
}
```

Prints [0, 7, 14, 21, 28, 35, ((42)), ((49))]





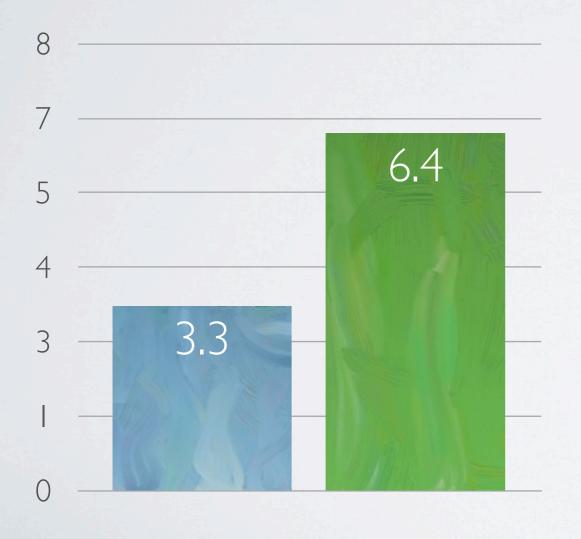
0 7 14 21 28 35 (42) (49)



Inactive Program Instances

EXPLOITING HORIZONTAL VECTORIZATION WITH SMALL MATRICES



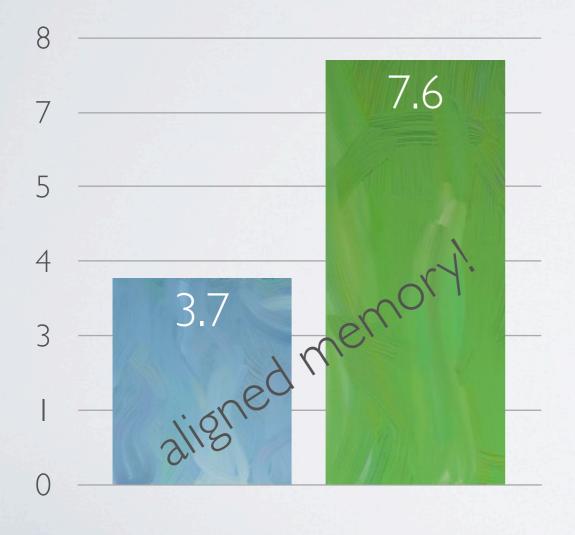


```
inline void mxm(uniform scalar_t * uniform A,
                 uniform scalar_t * uniform B,
                 uniform scalar_t * uniform C,
                 uniform int M,
                 uniform int N,
                 uniform int K,
                 uniform int nmat,
                 int idx)
    for(uniform int i = 0; i < M; i++){
        for(uniform int j = 0; j < N; j++){
            scalar_t sum = 0;
            for(uniform int k = 0; k < K; k++){
                sum += A[i*K*nmat + k*nmat + idx] * B[k*N*nmat + j*nmat + idx];
            C[i*N*nmat + j*nmat + idx] = sum;
export void gemm(uniform scalar_t * uniform A,
                 uniform scalar_t * uniform B,
                 uniform scalar_t * uniform C,
                 uniform int M,
                 uniform int N,
                 uniform int K,
                 uniform int nmat)
   foreach(i = 0 \dots nmat)
       mxm(A, B, C, M, N, K, nmat, i);
```

xGEMM 5x5 speedup over 1000 matrices (GCC 4.8 -O3)

EXPLOITING HORIZONTAL VECTORIZATION WITH SMALL MATRICES

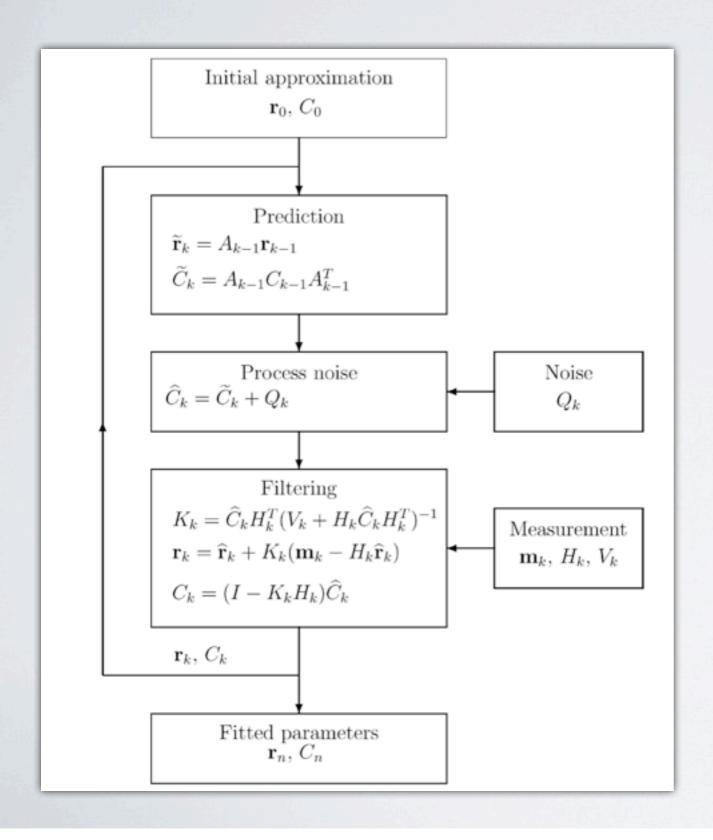




```
inline void mxm(uniform scalar_t * uniform A,
                 uniform scalar_t * uniform B,
                 uniform scalar_t * uniform C,
                 uniform int M,
                 uniform int N,
                 uniform int K,
                 uniform int nmat,
                 int idx)
   for (uniform int i = 0; i < M; i++) {
        for(uniform int j = 0; j < N; j++){
            scalar_t sum = 0;
            for(uniform int k = 0; k < K; k++){
                sum += A[i*K*nmat + k*nmat + idx] * B[k*N*nmat + j*nmat + idx];
            C[i*N*nmat + j*nmat + idx] = sum;
export void gemm(uniform scalar_t * uniform A,
                 uniform scalar_t * uniform B,
                 uniform scalar_t * uniform C,
                 uniform int M,
                 uniform int N,
                 uniform int K,
                 uniform int nmat)
   foreach(i = 0 ... nmat){
       mxm(A, B, C, M, N, K, nmat, i);
```

xGEMM 5x5 speedup over 1000 matrices (GCC 4.8 -O3)

KALMAN FILTER

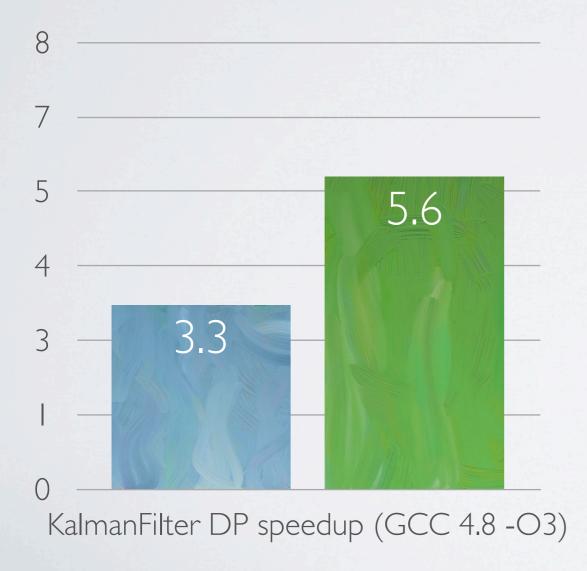


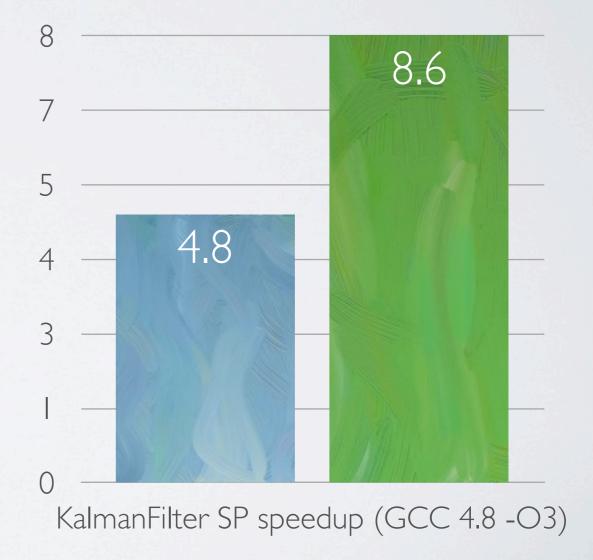
- The Kalman filter method is intended for finding the optimum estimation r of an unknown vector \mathbf{r}^t according to the measurements m_k , k=1...n, of the vector \mathbf{r}^t .
- Plenty of linear algebra operations so it's a good use case for vectorization.

KALMAN FILTER

100 EVENTS, ~100 TRACKS WITH ~10 HITS EACH

- ISPC vs GCC with AoS to SoA conversion
- ISPC vs GCC assuming data is preconverted





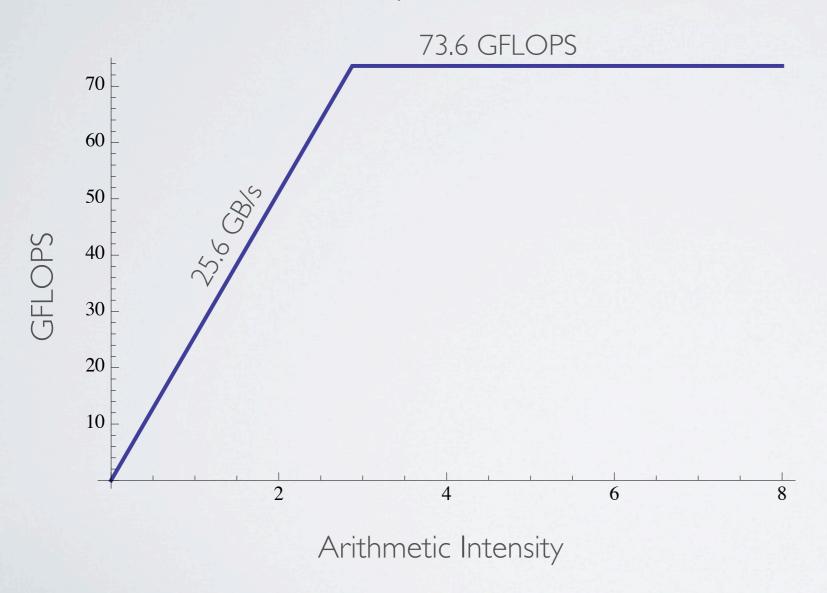
ISPC: FINALTHOUGHTS

THE VECTORIZATION FINAL SOLUTION?

- ISPC is by far the best option I have seen to exploit vectorization
 - it gives the programmer an abstract machine model to reason about
 - it warns about inefficient memory accesses (aka gathers and scatters)
- In other words, it's not going to get much easier than that
 - ▶ full C++ support would be a welcome addition
- ISPC is stable, extremely well documented, open source and has a beta support for the Xeon PHI
- I don't have yet a comparison with OpenCL

WHICH PROBLEMS LEND THEMSELVES WELL TO VECTORIZATION?

Roofline model for my machine: i7-3610QM



- The roofline model sets an upper bound on the performance of a numerical kernel
- Performance is either bandwidth or computationally limited
- Only Kernels with an arithmetic intensity greater or equal ~3 can achieve the maximum performance

MEMORY MATTERS

- Addressing modes
 - SSEx and AVXI do not support strided accesses pattern and gather-scatter accesses which force the compiler to generate scalar instructions
 - ▶ Even when "fancy" access patterns are supported (e.g. IMCI and AVX2) a penalty is paid
 - Convert your arrays of structures to structures of arrays
- Memory alignment
 - Unaligned memory access may generate scalar instructions for otherwise vectorizable code
 - Vectorized loads from unaligned memory suffer from a penalty
 - Align data in memory to the width of the SIMD unit

CONCLUSIONS

- · Use ISPC or an equivalent tool whenever possible
 - It provides the right abstraction to exploit horizontal vectorization
- Use Eigen3 for small Matrix and Geometry calculations
 - is a complete linear algebra library
 - > significant speedups can be achieved through vectorization and template expressions
- Use a SIMD vector wrapper library to hand tune numerical hotspots which lend themselves only to vertical vectorization
- What about autovectorization?
 - not trivial to exploit: generally you need to know what you are doing to get some speedup
 - > small changes in the code might silently break carefully optimized code
 - avoid whenever you want to achieve maximum performances