ATPESC

We resume @ 10:30am

(Argonne Training Program on Extreme-Scale Computing)

Vectorization (SIMD), and scaling (TBB and OpenMP*)

James Reinders, Intel August 4, 2014, Pheasant Run, St Charles, IL 10:30 – 11:15



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Using A Single Vector Lane Can Inhibit Performance



What Maximum Performance Can Look Like With Permission To Use All Lanes And Resources





Modernized Software Delivers Significant Performance Advantages





Following up on "data parallelism is KEY"

- dive into the topic of vectorization
- explicit vectorization in OpenMP 4.0
- consider a few other programming considerations along the way



Summary

We need to embrace *explicit* vectorization in our programming.



How many of us here today...
have ever worried about vectorization for your application?



Shouldn't we solve with better tools?

What is vectorization?

Could we just ignore it?

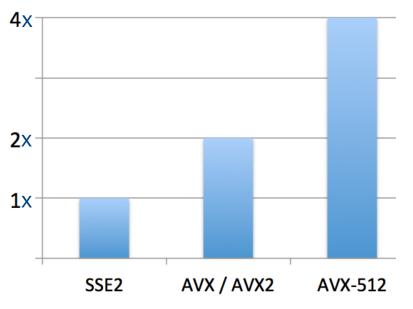


Vectors Instructions (SIMD instructions) Make things Faster

(that's the premise)

Up to 4x Performance

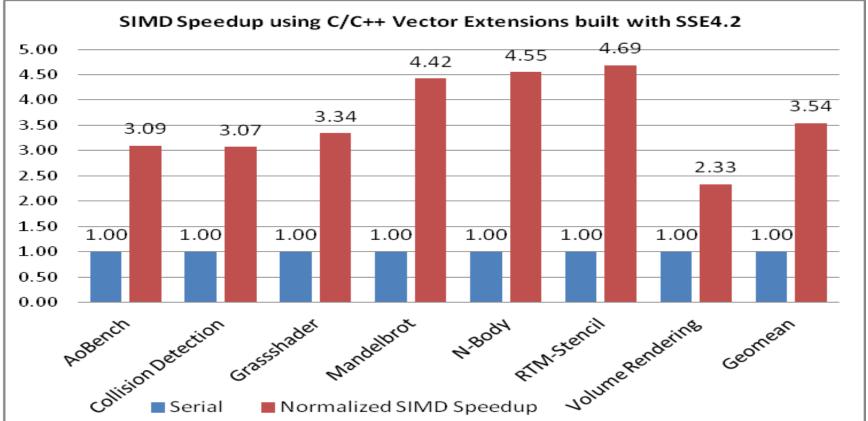
with Intel® Advanced Vector Extensions 512 (Intel® AVX-512) Support



- Significant leap to 512-bit SIMD support for processors
- Intel® Compilers and Intel® Math Kernel Library include AVX-512 support
- Strong compatibility with AVX
- Added EVEX prefix enables additional functionality
- Appears first in future Intel® Xeon Phi[™] coprocessor, code named Knights Landing

Higher performance for the most demanding computational tasks

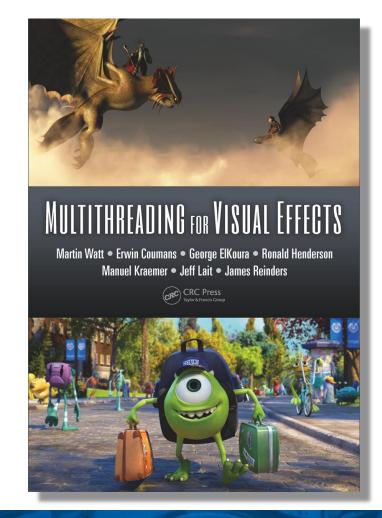
Performance with Explicit Vectorization



Configuration: Intel® Core™ i7 CPU X980 system (6 cores with Hyper-Threading On), running at 3.33GHz, with 4.0GB RAM, 12M smart cache, 64-bit Windows Server 2008 R2 Enterprise SP1. For more information go to http://www.intel.com/performance

Parallel first

Vectorize second





What is a Vector?



Vector of numbers

 4.4
 1.1
 3.1
 -8.5
 -1.3
 1.7
 7.5
 5.6
 -3.2
 3.6
 4.8



Vector addition

	4.4	1.1	3.1	-8.5	-1.3	1.7	7.5	5.6	-3.2	3.6	4.8	
+	-0.3	-0.5	0.5	0	0.1	0.8	0.9	0.7	1	0.6	-0.5	
=	4.1	0.6	3.6	-8.5	-1.2	2.5	8.4	6.3	-2.2	4.2	4.3	



...and Vector multiplication

1.55

$$\begin{bmatrix} 4.4 & 1.1 & 3.1 & -8.5 & -1.3 & 1.7 & 7.5 & 5.6 & -3.2 & 3.6 & 4.8 \\ -0.3 & -0.5 & 0.5 & 0 & 0.1 & 0.8 & 0.9 & 0.7 & 1 & 0.6 & -0.5 \\ = \begin{bmatrix} 4.1 & 0.6 & 3.6 & -8.5 & -1.2 & 2.5 & 8.4 & 6.3 & -2.2 & 4.2 & 4.3 \\ \end{bmatrix}$$

$$\begin{bmatrix} 4.4 & 1.1 & 3.1 & -8.5 & -1.3 & 1.7 & 7.5 & 5.6 & -3.2 & 3.6 & 4.8 \\ -0.3 & -0.5 & 0.5 & 0 & 0.1 & 0.8 & 0.9 & 0.7 & 1 & 0.6 & -0.5 \\ \end{bmatrix}$$

0 -0.13 1.36 6.75 3.92



An example



Loop:

- 1. LOAD a[i] -> Ra
- 2. LOAD b[i] -> Rb
- 3. ADD Ra, Rb -> Rc
- 4. STORE Rc -> c[i]
- 5. ADD i + 1 -> i



void v add (float *c,

Loop:

- 1. LOADv4 a[i:i+3] -> Rva
- 2. LOADv4 b[i:i+3] -> Rvb
- 3. ADDv4 Rva, Rvb -> Rvc
- 4. STOREv4 Rvc -> c[i:i+3]
- 5. ADDi + 4 -> i

Loop:

- 1. LOAD a[i] -> Ra
- 2. LOAD b[i] -> Rb
- 3. ADD Ra, Rb -> Rc
- 4. STORE Rc -> c[i]
- 5. ADDi + 1 -> i

vector data operations:



void v add (float *c,

Loop:

- 1. LOADv4 a[i:i+3] -> Rva
- 2. LOADv4 b[i:i+3] -> Rvb
- 3. ADDv4 Rva, Rvb -> Rvc
- 4. STOREv4 Rvc -> c[i:i+3]
- 5. ADDi + 4 -> i

Loop:

- 1. LOAD a[i] -> Ra
- 2. LOAD b[i] -> Rb
- 3. ADD Ra, Rb -> Rc
- 4. STORE Rc -> c[i]
- 5. ADDi + 1 -> i



```
void v_add (float *c, float *a, float *b)
{
    for (int i=0; i<= MAX; i++)
        c[i]=a[i]+b[i];
}</pre>
```



```
void v_add (float *c, float *a, float *b)
{
    for (int i=0; i<= MAX; i++)
        c[i]=a[i]+b[i];
}</pre>
```

PROBLEM:

This LOOP is NOT LEGAL to (automatically) VECTORIZE in C / C++ (without more information).

Arrays *not* really in the language Pointers are, evil pointers!



Choice 1: use a compiler switch for auto-vectorization

(and hope it vectorizes)



Choice 2: give your compiler hints

(and hope it vectorizes)



C99 restrict keyword



IVDEP (ignore assumed vector dependencies)



Choice 3: code explicitly for vectors

(mandatory vectorization)



OpenMP* 4.0: #pragma omp simd

OpenMP* 4.0: #pragma omp declare simd



SIMD instruction intrinsics

```
void v add (float *c,
                                            Hard coded to 4 wide
        float *a,
        float *b)
   m128* pSrc1 = ( m128*) a;
   m128* pSrc2 = (m128*) b;
   m128* pDest = ( m128*) c;
   for (int i=0; i \le MAX/4; i++)
       *pDest++ = mm add ps(*pSrc1++, *pSrc2++);
```



array operations (Cilk™ Plus)

Challenge: long vector slices can cause cache issues; fix is to keep vector slices short.

Cilk[™] Plus is supported in Intel compilers, and gcc (4.9).



vectorization solutions

- auto-vectorization (use a compiler switch and hope it vectorizes)
 - sequential languages and practices gets in the way
- 2. give your compiler hints and hope it vectorizes
 - C99 restrict (implied in FORTRAN since 1956)
 - #pragma ivdep
- 3. code explicitly
 - OpenMP 4.0 #pragma omp simd
 - Cilk™ Plus array notations
 - SIMD instruction intrinsics
 - Kernels: OpenMP 4.0 #pragma omp declare simd; OpenCL; CUDA kernel functions



vectorization solutions

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Best at being Reliable, predictable and portable



Explicit parallelism



parallelization

Try auto-parallel capability 1

- -parallel (Linux* or OS X*)
- -Qparallel (Windows*)

```
1  PROGRAM TEST
2  PARAMETER (N=10000000)
3  REAL A, C(N)
4  DO I = 1, N
5  A = 2 * I - 1
6  C(I) = SQRT(A)
7  ENDDO
8  PRINT*, N, C(1), C(N)
9  END
```

Or explicitly use...

Fortran directive (!DIR\$ PARALLEL)

C pragma (#pragma parallel)
Intel® Threading Building Blocks (TBB)



parallelization

Try auto-parallel capability:

- -parallel (Linux or OS X*)
- -Qparallel (Windows)

Best at being Reliable, predictable and portable

Or explicitly use...

OpenMP

Intel® Threading Building Blocks (

```
c$OMP PARALLEL DO

DO I=1,N B(I) = (A(I) + A(I-1)) / 2.0

END DO

c$OMP END PARALLEL DO
```

OpenMP 4.0

Based on a proposal from Intel based on customer success with the Intel® Cilk™ Plus features in Intel compilers.

simd construct

Summary

The **simd** construct can be applied to a loop to indicate that the loop can be transformed into a SIMD loop (that is, multiple iterations of the loop can be executed concurrently using SIMD instructions).

OpenMP 4.0

Based on a proposal from Intel based on customer success with the Intel® Cilk™ Plus features in Intel compilers.

simd construct

```
#pragma omp simd reduction(+:val) reduction(+:val2)
for(int pos = 0; pos < RAND_N; pos++) {
    float callValue=
        expectedCall(Sval,Xval,MuByT,VBySqrtT,I_Random[pos]);
    val += callValue;
    val2 += callValue * callValue;
}</pre>
```

simd construct

(OpenMP 4.0)

YES - VECTORIZE THIS !!!



Summary

The simd construct can be applied to a loop to indicate that the loop can be transformed into a SIMD loop (that is, multiple iterations of the loop can be executed concurrently using SIMD instructions).

C/C++

#pragma omp simd [clause[[,] clause] ...] new-line
 for-loops

where clause is one of the following:

safelen (length)
linear (list[:linear-step])
aligned (list[:alignment])
private (list)
lastprivate (list)
reduction (reduction-identifier:list)
collapse(n)

The **simd** directive places restrictions on the structure of the associated *for-loops*. Specifically, all associated *for-loops* must have *canonical loop form* (Section 2.6 on page 51).

C/C++

```
Fortran
```

```
!$omp simd [clause[[,] clause ...]
    do-loops
[!$omp end simd]
```

where clause is one of the following:

```
safelen(length)
linear(list[:linear-step])
aligned(list[:alignment])
private(list)
lastprivate(list)
reduction(reduction-identifier:list)
collapse(n)
```

If an end simd directive is not specified, an end simd directive is assumed at the end of the do-loops.

All associated *do-loops* must be *do-constructs* as defined by the Fortran standard. If an **end simd** directive follows a *do-construct* in which several loop statements share a DO termination statement, then the directive can only be specified for the outermost of these DONSTATEMENT OPEN STANDARD, the "for-loop" must have canonical loop form.

Fortran

declare simd construct (OpenMP 4.0)

Make VECTOR versions of this function.



Summary

The declare simd construct can be applied to a function (C, C++ and Fortran) or a subroutine (Fortran) to enable the creation of one or more versions that can process multiple arguments using SIMD instructions from a single invocation from a SIMD loop. The declare simd directive is a declarative directive. There may be multiple declare simd directives for a function (C, C++, Fortran) or subroutine (Fortran).

```
Fortran
                                     C/C++
                                                                                       !$omp declare simd(proc-name) [clause[[,] clause] ...]
  #pragma omp declare simd[clause[[,] clause] ...] new-line
  [#pragma omp declare simd[clause[[,] clause] ...] new-line]
      function definition or declaration
                                                                                     where clause is one of the following::
where clause is one of the following:
                                                                                               simdlen (length)
          simdlen (length)
                                                                                               linear (argument-list[:constant-linear-step])
          linear (argument-list[:constant-linear-step])
                                                                                               aligned(argument-list[:alignment])
          aligned(argument-list[:alignment])
                                                                                               uniform (argument-list)
          uniform(argument-list)
                                                                                               inbranch
          inbranch
                                                                                               notinbranch
          notinbranch
```

Fortran -

Parallelize and Vectorize.

Loop SIMD construct

7

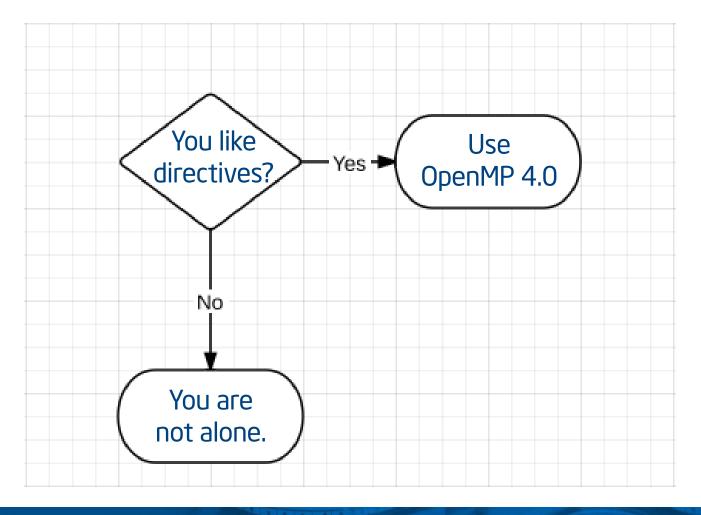
(OpenMP 4.0)

Summary

The loop SIMD construct specifies a loop that can be executed concurrently using SIMD instructions and that those iterations will also be executed in parallel by threads in the team.

icani.		
Syntax C/C++	Fortran —	
C/CTT -	Tottali	
<pre>#pragma omp for simd[clause[[,] clause]] new-line for-loops</pre>	<pre>!\$omp do simd[clause[[,] clause]] do-loops [!\$omp end do simd [nowait]]</pre>	
where <i>clause</i> can be any of the clauses accepted by the for or simd directives with identical meanings and restrictions. C/C++	where <i>clause</i> can be any of the clauses accepted by the simd or do directives, with identical meanings and restrictions.	
	If an end do simd directive is not specified, an end do simd directive is assumed at the end of the do-loop.	
	A Fortran	







for your consideration: Intel 15.0 Compilers (in beta now) support keywords as an alternative

Keyword versions of SIMD pragmas added:

```
_Simd, _Safelen, _Reduction
```

• __intel_simd_lane() intrinsic for SIMD enabled functions

Keywords / library interfaces being discussed for SIMD constructs in C and C++ standards



History of Intel vector instructions



Intel Instruction Set Vector Extensions from 1997-2008

1997 Intel® MMX™ technology 1998 Intel® 1999 Intel® SSE2 2004 Intel® SSE3

Intel® SSSE3

2006

Intel® SSE4.1

2007

2008 Intel® SSE4.2

57 new instructions

64 bits

Overload FP stack

Integer only

media extensions 70 new instructions

128 bits

4 singleprecision vector FP

scalar FP instructions

cacheability instructions

control & conversion instructions

media extensions 144 new instructions

128 bits

2 doubleprecision vector FP

8/16/32/64 vector integer

128-bit integer

memory & power management

13 new instructions

128 hits

FP vector calculation

x87 integer conversion

128-bit integer unaligned load thread sync.

32 new instructions

128 bits

enhanced packed integer calculation 47 new instructions

128 bits

packed integer calculation & conversion

better vectorization by compiler

load with streaming hint

7 new instructions

128 bits

string (XML) processing

POP-Count

CRC32



Intel Instruction Set Vector Extensions since 2011

2011

Intel® AVX

Promotion of 128 bit FP vector instructions to 256 bit 2011

Co-processor only 512

Coprocessor predecessor to AVX-512. New 512 bit vector instructions for MIC architecture, binary compt. not supported by processors – mostly source compatible with AVX-512

2012

"AVX-1.5"

7 new instructions

16 bit FP support RDRAND

...

2013

Intel® AVX-2

Promotion of integer instruction to 256 bit

- FMA
- Gather
 - TSX/RTM

TBD

Intel® AVX-512

Promotion of vector instructions to 512 bits

Xeon Phi: Fl, CDI, ERI, PFI

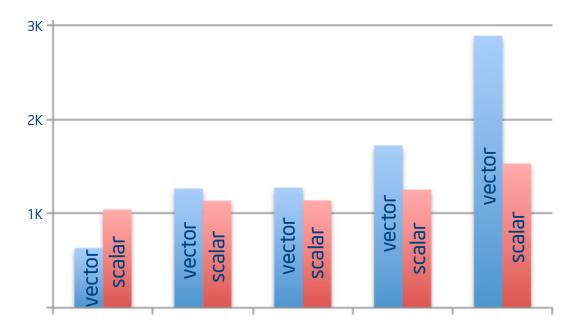
Xeon: FI, CDI, BWI, DQI, VLE

Reinders blogs announced – July 2013, and June 2014.

		width	Int.	SP	DP
1997	MMX	64	~		
1999	SSE	128	~	✓ (x4)	
2001	SSE2	128	~	✓	√ (x2)
2004	SSE3	128	~	✓	✓
2006	SSSE 3	128	~	✓	✓
2006	SSE 4.1	128	~	✓	✓
2008	SSE 4.2	128	~	~	✓
2011	AVX	256	~	✓ (x8	B) ~ (x4)
2013	AVX2	256	~	~	V
future	AVX-512	512	~	✓ (x ²	16) ~ (x8)



Growth is in vector instructions



Disclaimer: Counting/attributing instructions is in inexact science. The exact numbers are easily debated, the trend is quite real regardless.



Motivation for AVX-512 Conflict Detection

Sparse computations are common in HPC, but hard to vectorize due to race conditions

```
for(i=0; i<16; i++) { A[B[i]]++; }
```

Consider the "histogram" problem:



Motivation for AVX-512 Conflict Detection

Sparse computations are common in HPC, but hard to vectorize due to race conditions

- Code above is wrong if any values within B[i] are duplicated
 - Only one update from the repeated index would be registered!
- A solution to the problem would be to avoid executing the sequence gather-op-scatter with vector of indexes that contain conflicts



Conflict Detection Instructions in AVX-512 improve vectorization!

VPCONFLICT instruction detects elements with previous conflicts in a vector of indexes

- Allows to generate a mask with a subset of elements that are guaranteed to be conflict free
- CDI instr.

 VPCONFLICT{D,Q} zmm1{k1}, zmm2/mem

 VPBROADCASTM{W2D,B2Q} zmm1, k2

 VPTESTNM{D,Q} k2{k1}, zmm2, zmm3/mem

 VPLZCNT{D,Q} zmm1 {k1}, zmm2/mem
- The computation loop can be re-executed with the remaining elements until all the indexes have been operated upon

```
index = vload &B[i]
pending_elem = 0xFFFF;

do {
   curr_elem = get_conflict_free_subset(index, pending_elem)
   old_val = vgather {curr_elem} A, index
   new_val = vadd old_val, +1.0
   vscatter A {curr_elem}, index, new_val
   pending_elem = pending_elem ^ curr_elem
} while (pending_elem)
// Load 16 B[i]
// all still remaining
// Grab A[B[i]]
// Compute new values
// Update A[B[i]]
// remove done idx
// while (pending_elem)
```

for illustration: this not even the fastest version



-vec-report

"Dear compiler, did you vectorize my loop?" We heard your feedback.....

-vec-report output was hard to understand;

Messages were too cryptic to understand;

Information about one loop showing up at many places of report;

Was easy to be confused about multiple versions of one loop created

by the compiler

We couldn't do everything you asked, but here are the improvements made for 15.0 compiler.

Expect more changes to come, during beta and in future versions.



Optimization Report Redesign

- Old functionality implemented under -opt-report, -vec-report, -openmp-report, -par-report replaced by unified -opt-report compiler options
 - [vec,openmp,par]-report options deprecated and map to equivalent opt-report-phase
- Can still select phase with -opt-report-phase option. For example, to only get vectorization reports, use -opt-report-phase=vec
- Output now defaults to a <name>.optrpt file where <name> corresponds to the output object name. This can be changed with -opt-report-file=[<name>|stdout|stderr]
- Windows*: /Qopt-report, /Qopt-report-phase=<phase> etc.
 - Optimization report integration with Microsoft* Visual Studio planned to appear in beta update 1



Summary

We need to embrace explicit vectorization in our programming.

Vectorization today uses

"Not your father's vectorizer"





Vectorization solved in 1978?

Communications of the ACM
The CRAY-1 computer system
By Richard M. Russell
Cray Research, Inc., Minneapolis, MN
Communications of the ACM,
January 1978 (Vol. 21 No. 1), Pages 63-72



The CRAY-1's Fortran compiler (CFT) is designed to give the scientific user immediate access to the benefits of the CRAY-1's vector processing architecture. An optimizing compiler, CFT, "vectorizes" innermost DO loops. Compatible with the ANSI 1966 Fortran Standard and with many commonly supported Fortran extensions, CFT does not require any source program modifications or the use of additional nonstandard Fortran statements to achieve vectorization. Thus the user's investment of hundreds of man months of effort to develop Fortran programs for other contemporary computers is protected.

Vectorization solved in 1978?



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The CRAY-1's Fortran compiler (CFT) is designed to give the scientific user immediate access to the

Communications of the ACM October 1978 (Vol. 21, No. 10), Pages 806-820

Fortran 77

There is a new standard Fortran. The official title is "American National Standard Programming Language Fortran, X3.9-1978," but it is more commonly referred to as "Fortran 77," since its development was completed in 1977. It ...

Walt Brainerd

programs for other contemporary computers is protected.



Livermore loop #1

Vector code generation straightforward Emphasis on analysis and disambiguation



It's messy today

Vectorization yesterday

```
DO 1 k = 1,n
1 A(k) = B(k) + C(k)
```

K=1 K=2

Ld C(1) Ld C(2)

Ld B(1) Ld B(2)

Add

St A(1) St A(2)

Scalar code

K=1..2

Ld C(1) Ld C(2)

Ld B(1) Ld B(2)

Add Add

St A(1) St A(2)

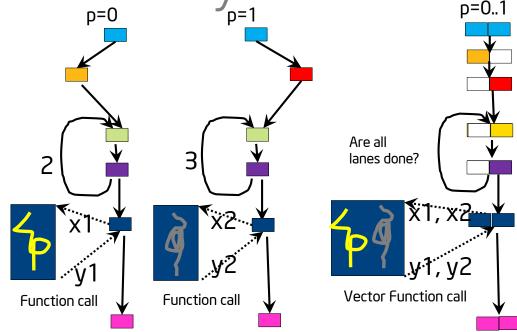
Vector code

Vector code generation was straightforward Emphasis on analysis and disambiguation Vectorization today
#pragma omp simd reduction(+:....)
for(p=0; p<N; p++) {

p=0
p=1
p=1

```
// Blue work
   // Green work
} else {
  // Red work
while(...) {
  // Gold work
  // Purple work
y = foo(x);
Pink work
```

Two fundamental problems
Data divergence
Control divergence



Vector code generation has become a more difficult problem Increasing need for user guided explicit vectorization Explicit vectorization maps threaded execution to simd hardware



Loops

#pragma omp simd

```
for (x = 0; x < w; x++) {
   for (v = 0; v < nsubsamples; v++) {
       for (u = 0; u < nsubsamples; u++) {
       float px = (x + (u / (float)nsubsamples) - (w / 2.0f)) / (w / 2.0f);
       Ray ray; Isect isect;
          ray.dir.x = px;
              vnormalize(&(ray.dir));
              ray_sphere_intersect(&isect, &ray, &spheres[0]);
              ray_plane_intersect (&isect, &ray, &plane);
              if (isect.hit) {
                 vec col;
                 ambient_occlusion_simd(&col, &isect);
                 fimq[3 * (v * w + x) + 0] += col.x;
```

Function calls

Conditionals

Conditional Function calls

Motivational Example

```
//foo.c
float in vals[];
for(int \bar{x} = 0; \bar{x} < Width; ++x) {
    count[x] = lednam(in_vals[x]);
            //bar.c
            int lednam(float c)
              // Compute n >= 0 such that c^n > LIMIT
                float z = 1.0f;
                int iters = 0;
                while (z < LIMIT) {
                    z = z * c; iters++;
                return iters;
```

What are the simplest changes required for the program to utilize today's multicore and simd hardware?

```
float in vals[];
for(int x = 0; x < Width; ++x) {
    count[x] = lednam(in vals[x]);
     #pragma omp declare simd
      int lednam(float c)
          // Compute n >= 0 such that c^n > LIMIT
          float z = 1.0f; int iters = 0;
          while (z < LIMIT) {
               z = z * c; iters++;
          return iters;
       x = 0
                                             x = 2
                                                                x = 3
                          x = 1
     z = z * c

z = z * c
                                          z = z * c
                                          z = z^* c
                                          .......
                                                                  .......
     iters = 2
                       iters = 23
                                          iters = 255
                                                               iters = 37
```

Mandelbrot

```
#pragma omp parallel for
for (int y = 0; y < ImageHeight; ++y) {</pre>
    #pragma omp simd
for (int x = 0; x < ImageWidth; ++x) {
    count[y][x] = mandel(in_vals[y][x]);</pre>
        #pragma omp declare simd
int mandel(fcomplex c)
{ // Computes number of iterations for c to escape
             fcomplex z = c;
             for (int iters=0; (cabsf(z) < 2.0f) && (iters < LIMIT); iters++) {
                     z = z * z + c:
             return iters;
                                                                                                                                  2067.91
                             Mandelbrot Normalized Speedup with OpenMP* on Intel® Xeon Phi™ Coprocessor
                                                                                                                1580.03
                          OpenMP PAR
                                                 OpenMP SIMD
                                                                           OpenMP PAR+SIMD
            Serial
                                                                                              989.56
                                                                            510.88
          1.00 0.99 16.02 15.02
                            1.00 7.78 16.01
              1 Thread
                                8 Threads
                                                                                                        122 Threads
                                                                                                                          244 Threads
```



Summary

We need to embrace explicit vectorization in our programming.

But, generally use parallelism first (tasks, threads, MPI, etc.)





james.r.reinders@intel.com





James Reinders. Parallel Programming Evangelist. Intel.

James is involved in multiple engineering, research and educational efforts to increase use of parallel programming throughout the industry. He joined Intel Corporation in 1989, and has contributed to numerous projects including the world's first TeraFLOP/s supercomputer (ASCI Red) and the world's first TeraFLOP/s microprocessor (Intel® Xeon Phi™ coprocessor). James been an author on numerous technical books, including VTune[™] Performance Analyzer Essentials (Intel Press, 2005), Intel[®] Threading Building Blocks (O'Reilly Media, 2007), Structured Parallel Programming (Morgan Kaufmann, 2012), Intel® Xeon Phi™ Coprocessor High Performance Programming (Morgan Kaufmann, 2013), and Multithreading for Visual Effects (A K Peters/CRC Press, 2014). James is working on a project to publish a book of programming examples featuring Intel Xeon Phi programming scheduled to be published in late 2014.



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