

Open Source Software Development

Getting ready for Knights Landing!

Intel High Performance and Throughput Computing (EMEA) Hans Pabst, March 12th 2015



Abstract

After a short introduction on what to expect from Intel's next iteration of the Many Integrated Core Architecture, the talk will portrait a selection of recent work of Intel's High Performance and Throughput Computing Team in Europe. Among the selected projects are <u>LIBXSMM</u> (library for multiplying batches of small matrices as common in quantum dynamics applications), <u>LIBXSTREAM</u> (library for stream programming), and <u>pyMIC</u> (module to offload computation in a Python program to the Intel Xeon Phi coprocessor).

The tutorial part of the talk shows how to run and debug an application in the Intel Software Development Emulator (Intel SDE). Compiling, running, and debugging an application in the Intel SDE can be a useful step to exercise the development tool chains such as the GNU Compiler Collection (GNU GCC) or the Intel Compiler. The talk closes with some tricks and hints on how to approach code modernization and further optimizations making an application ready for lots of cores and wide vectors.

Open Source Software Development – Getting ready for Knights Landing!

Open Source Software Development

"Getting ready for Knights Landing!"

- Selection of work (Intel Intel High Performance and Throughput Computing team*)
- Introduction of the Intel AVX-512 Instruction Set Extension with focus on HPC
- Practical steps to prepare software for Knights Landing

^{*} This is only focusing on our team, and cannot represent all of Intel's Open Source Software Commitment.



Intel Knights Landing?

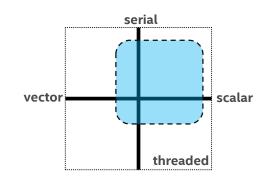
The 2nd iteration of Intel Many Integrated Core Architecture

 Available today: Intel® Xeon Phi™ Coprocessor (codenamed "Knights Corner")

What's publicly known? Just have a look:

https://software.intel.com/e
 n-us/articles/what disclosures-has-intel-made about-knights-landing

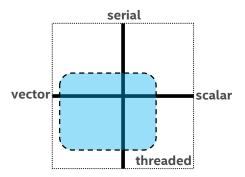




Most Commonly Used Parallel Processor*

Parallel, fast serial execution Multicore and vectors





Optimized for Highly Parallel Applications

Many cores, 512 bit vectors, and higher mem. bw. Common languages, directives, libraries and tools

There is a growing catalog of applications...

More than 100 applications are listed as available today or in flight



http://software.intel.com/XeonPhiCatalog

Agenda

Examples of our 2014 work in the Open Source domain

- LIBXSMM small matrix-matrix multiplications
- pyMIC offload computation to Xeon Phi coprocessors
- LIBXSTREAM streams, events, and offload functions

Introducing the AVX-512 Instruction Set Extension Running an application using the Intel SDE

Intel® AVX-512

Instruction Set Extension

Intel Instruction Set Extension (1998-2010)

2009 1998 1999 2004 2006 2007 2008 Intel® Intel® Intel® Intel Intel® Intel® Intel® SSE2 SSE3 SSSE3 **SSE4.1** SSE4.2 SSE AES 70 new 144 new 13 new 32 new 7 new 7 new 47 new instructions instructions instructions instructions instructions instructions instructions FP vector 4 single-2 doubleenhanced packed string (XML) 6 for calculation processing acceleration precision precision packed integer vector FP vector FP of AES integer calculation & **POP-Count** x87 integer calculation conversion algorithm scalar FP 8/16/32/64 conversion CRC32 instructions Plus carryvector better 128-bit less 64bť vectorization integer cacheability instructions integer by compiler multiply 128-bit unaligned integer load load with control & streaming thread sync. conversion memory & hint instructions power management

media extensions

Intel Instruction Set Extension (after 2010)

2011 2011 **TBD** 2012 2013 2014 Intel® Initial Intel® Intel® Broadwell Intel® Many Core "AVX-1.5" New In-AVX AVX-2 AVX-512 structions Instructions Promotion of Hundreds of Promotion of Some 5 new 7 new Promotion of new 512 bit instructions 128 bit FP integer instruction to vector vector vector instruction to enhance instructions 16 bit FP 256 bit instructions instructions support for to 512 bits support to 256 bit only available random and a lot - FMA for MIC number more **RDRAND** architecture generation, - Gather prefetching not supported by - TSX/RTM and multiand not precision compatible to arithmetic x86 architecture

Intel® AVX

256-bit AVX 16 SP / 8 DP Flops/Cycle



256-bit AVX2 32 SP / 16 DP Flops/Cycle (FMA)



512-bit AVX-512 64 SP / 32 DP Flops/Cycle (FMA)

(LINV)

AVX

256-bit basic FP 16 registers NDS (and AVX128) Improved blend MASKMOV Implicit unaligned

SNB 2011

AVX2

Float16 (IVB 2012) 256-bit FP FMA 256-bit integer PERMD Gather

HSW 2013

AVX-512

512-bit FP/Integer32 registers8 mask registersEmbedded roundingEmbedded broadcast

Scalar/SSE/AVX "promotions"

HPC additions

Transcendental support

Gather/Scatter

AVX-512: More and Larger Registers

AVX / AVX-2: VADDPS YMM0, YMM3, [mem]

- Up to 16 AVX registers
 - 8 in 32-bit mode
- 256-bit width
 - 8 x FP32
 - 4 x FP64

AVX-512: VADDPS ZMM0, ZMM24, [mem]

- Up to 32 AVX registers
 - 8 in 32-bit mode
- 512-bit width
 - 16 x FP32
 - 8 x FP64

There is a lot more (instructions) needed in order to effectively use the new real estate...

```
float32 A[N], B[N];
for(i=0; i<8; i++)
   A[i] = A[i] + B[i];
float32 A[N], B[N];
for(i=0; i<16; i++)
   A[i] = A[i] + B[i];
```

AVX-512: Mask Registers

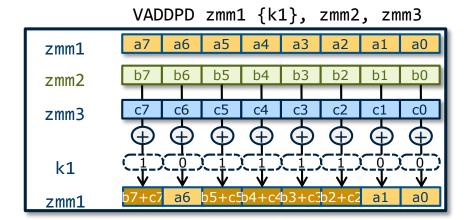
8 Mask registers of size 64-bits

- k1-k7 can be used for predication

 - k0 can be used as a destination or source for mask manipulation operations

4 different mask granularities. For instance, at 512b:

- Packed Integer Byte use mask bits [63:0]
 - VPADDB zmm1 {k1}, zmm2, zmm3
- Packed Integer Word use mask bits [31:0]
 - VPADDW zmm1 {k1}, zmm2, zmm3
- Packed IEEE FP32 and Integer Dword use mask bits [15:0]
 - VADDPS zmm1 {k1}, zmm2, zmm3
- Packed IEEE FP64 and Integer Qword use mask bits [7:0]
 - VADDPD zmm1 {k1}, zmm2, zmm3



Why Separate Mask Registers?

- Avoids using registers as vector of Booleans
- Separate control flow and data flow
- Boolean operations on logical predicates consume less energy (separate functional unit)
- Tight encoding allows orthogonal operand
- All instructions support an extra mask operand

AVX-512: Masking

VADDPS ZMM0 {k1}, ZMM3, [mem]

Mask bits are used to:

- 1. Suppress reading individual elements as well as signaling memory faults for masked elements
- Avoid signaling individual FP faults per instruction
- 3. Avoid updating individual destination elements or force to zero (zeroing)

```
for (I in vector length)
   if (no masking or mask[I]) {
      dest[I] = OP(src2, src3)
   } else {
      if (zeroing masking)
         dest[I] = 0
      else
         // dest[I] is preserved
}
```

Caveat: vector shuffles do no suppress memory fault exceptions since the mask refers to the "output" not to the "input".

AVX-512: More Features...

- Embedded Broadcasts and Masking
- Conflict Detection Instructions
- Embedded Rounding Control
- Suppress All Exceptions (SAE)
- Compressed Displacement
- Bit Manipulation
- Shuffles
- ...

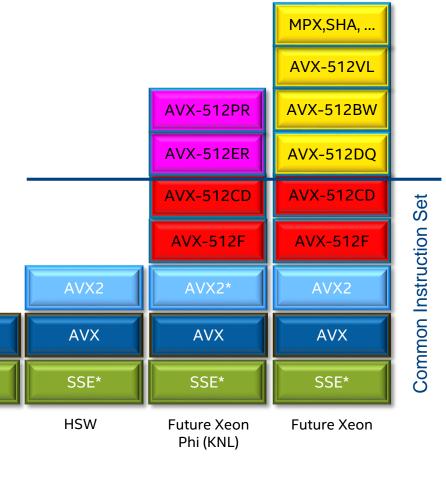
Intel AVX-512: Hardware Support

AVX

SSE*

SNB

- Future Intel® MIC architecture (codenamed KNL) and future Xeon architecture share a large set of instructions
- Subsets are represented by individual feature flags (CPUID)



SSE*

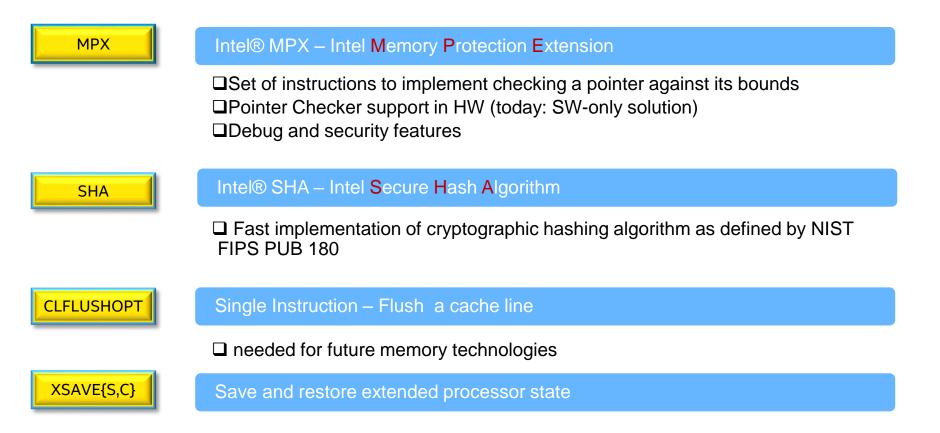
NHM

AVX-512: Instruction Subsets

AVX-512F AVX-512 F: 512-bit Foundation instructions common between MIC and Xeon ☐ Comprehensive vector extension for HPC and enterprise ☐ All the key AVX-512 features: masking, broadcast... ☐ 32-bit and 64-bit integer and floating-point instructions ☐ Promotion of many AVX and AVX2 instructions to AVX-512 ☐ Many new instructions added to accelerate HPC workloads AVX-512CD AVX-512 CD (Conflict Detection instructions) ☐ Allow vectorization of loops with possible address conflict AVX-512ER AVX-512 extensions for exponential and prefetch operations ☐ fast (28 bit) FP instr. for exponential, reciprocal and Transcendentals (incl. RSQRT) AVX-512PR

□ New prefetch instructions: gather/scatter prefetches and PREFETCHWT1

AVX-512: Other New Instructions



Optimization Notice

AVX-512: Summary (F, CD, ER, PR)

AVX-512 F: new 512-bit vector ISA extension

Common between Xeon and Xeon Phi (KNL)

AVX-512 CD Conflict detection instructions

- Will be available both for Xeon and Xeon Phi (KNL)
- Improves auto-vectorization

AVX-512 ER & PR

- 28-bit Transcendentals and new prefetch instructions
- On Xeon Phi (KNL) only

Optimization Notice

AVX-512: How to use?

Instructions are accessible using Intrinsics (built-in functions)

- No need to supply any additional compiler flags
- Supported since Intel Compiler 14 and GCC 4.8

Compiler code generation

Intel C/C++ and Fortran Compiler (Version 15 and newer)

- KNL via "MIC-AVX512" (-xMIC-AVX512)
- Future Xeon via "CORE-AVX512" (-xCORE-AVX512)

GNU Compiler Collection (GCC 4.9)

- Subset support, all Intrinsics, and basic auto-vectorization via -mavx512f, -mavx512pf, -mavx512er, and -mavx512cd
- Example for KNL: supply all flags from above (F/PF/ER/CD)

LLVM Compiler

Full support (patch: https://groups.google.com/forum/)

AVX-512: References

Reference manual for Intel® AVX-512 instructions

• http://software.intel.com/en-us/intel-isa-extensions

Other references

http://software.intel.com/en-us/blogs/2013/avx-512-instructions

Discussion and critics

- http://software.intel.com/en-us/forums/topic/477541
- See <u>www.agner.org</u>

Intel® SDE and use cases (examples)

Intel® Software Development Emulator

Overview

Run an application using an instruction set extension which is not (yet) available in hardware.

- Correctness testing (exercising the compiler's code generation)
- Prepare the build system (compiler flags)
- Debugging

Technology background

- Runs an application roughly an order of magnitude slower (compared to the host system which is running the SDE)
- Not a performance tool (profiler) as it uses binary translation to the host's instruction set

\$\$ /path/to/sde/sde64 -knl -- /path/to/application

Example: LIBINT Version 1.1.5

Prerequisites

- Intel Cluster Studio XE (e.g., composer_xe_2015.1.133 or newer)
- Intel SDE (sde-external-7.15.0-2015-01-11-lin)

Notes

- Unfortunately the configure script attempts to run a program;
 cross-compilation complicates the configure/build process
- Therefore the SDE must be used during configuration (and initial steps of make; make can be interrupted and continued without the SDE)

Example: LIBINT (cont.)

Configuration

```
$ make realclean
$ env AR=xiar \
    FC=ifort F77=ifort F90=ifort CXX=icpc CC=icc \
    FCFLAGS="-02 -xMIC-AVX512 -ipo" \
    CFLAGS="-02 -xMIC-AVX512 -ipo" \
    CXXFLAGS="-02 -xMIC-AVX512 -ipo" \
    CXXFLAGS="-02 -xMIC-AVX512 -ipo" \
    --with-cc-optflags="-02 -xMIC-AVX512 -ipo" \
    --with-cxx-optflags="-02 -xMIC-AVX512 -ipo" \
    --with-libint-max-am=5 --with-libderiv-max-am1=4 \
    --prefix=$HOME/libint
```

Building LIBINT

```
$ make -j (initially: ~/sde/sde64 -knl -- make)
```

Optimization Notice

Example: LIBXC Version 2.2.2

Configuration

```
$ make clean (note: there is no "realclean")
$ env AR=xiar \
    FC=ifort F77=ifort F90=ifort CC=icc \
    FCFLAGS="-02 -xMIC-AVX512 -ipo" \
    CFLAGS="-02 -xMIC-AVX512 -ipo" \
    ~/sde/sde64 -knl -- ./configure \
    --prefix=$HOME/libint
```

Building LIBXC

```
$ make -j
$ make install
```

CP2K

Prerequisites

- Intel Cluster Studio XE (composer_xe_2015.1.133, impi-5.0.2.044)
- Intel SDE (sde-external-7.15.0-2015-01-11-lin)
- LIBINT (Version 1.1.5) and LIBXC (Version 2.2.2)

Source code

- git clone https://github.com/cp2k/cp2k.git
- git checkout intel

Edit arch file

• arch/Linux-x86-64-intel-mic.psmp: -xHost → -xMIC-AVX512 -g

CP2K (cont.)

Building CP2K

\$ make ARCH=Linux-x86-64-intel-host VERSION=sopt \
LIBINTROOT=~/libint LIBXCROOT=~/libxc

Running CP2K

\$ ~/sde/sde64 -knl -- exe/Linux-x86-64-intelhost/cp2k.sopt tests/LIBTEST/dbcsr_blocks_04.inp

Debugging

\$ ~/sde/sde64 -knl -debug -- exe/Linux-x86-64-intelhost/cp2k.sopt tests/LIBTEST/dbcsr blocks 04.inp

Steps for Debugging

- 1. Run application with SDE's "-debug" option; starts gdb-server and prints command on how to connect using the gdb client
- Open gdb (or try "gdb-ia" if Intel compiler suite is source'd) but supply the /path/to/executable on command line (ensures that debug symbols are loaded)
- 3. Paste command shown by SDE on how to connect to the gdb-server (port), and continue (c) execution

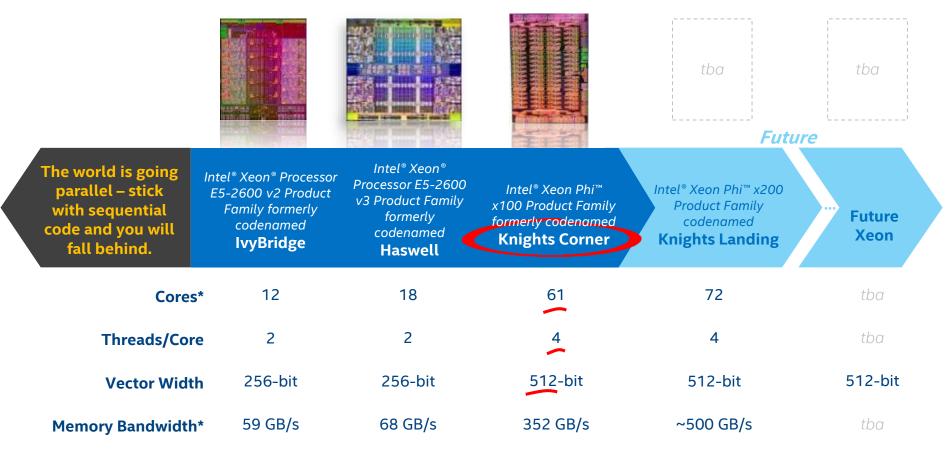
Reference

https://software.intel.com/en-us/articles/debugging-applications-with-intel-sde

What else?

Code Modernization

Code Modernization using Intel® Xeon Phi™ coprocessor(s)



Code Modernization: Getting Started

- Preparing the build system (compiler flags) and linking Intel Math Kernel Library (Intel MKL)
 - Potentially low-hanging fruits with using industry-standard interfaces such as (Sca-)LAPACK/BLAS and FFTW3
- Evaluating parallel scalability (MPI and OpenMP) using higher core-count systems (Xeon Phi, Xeon E5, and Xeon E7)
 Initially this does not even ask for advanced profiling, just a wall clock...
- Generating and reviewing compiler vectorization reports
 Intel Compiler Version 15 reports are much more readable/correlated
 Hint: try upcoming version of Intel Advisor (vector reports, and more)

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Notice revision #20110804



Backup **AVX-512**

Why True Masking?

Memory fault suppression

- Vectorize code without touching memory that the correspondent scalar code would not touch
 - Typical examples are if-conditional statements or loop remainders
 - AVX is forced to use VMASKMOV* (risc)

MXCSR flag updates and fault handlers

Avoid spurious floating-point exceptions without having to inject neutral data

Zeroing/merging

- {z} bit syntax to EVEX z-bit implies 'zeroing' - default is 'merging'
- Use zeroing to avoid false dependencies in OOO architecture
- Use merging to avoid extra blends in if-thenelse clauses (predication) for great code density

```
float32 A[N], B[N], C[N];

for(i=0; i<16; i++)
{
    if(B[i] != 0) {
        A[i] = A[i] / B[i];
    else {
        A[i] = A[i] / C[i];
    }
}</pre>
```

```
VMOVUPS zmm2, A
VCMPPS k1, zmm0, B
VDIVPS zmm1 {k1}{z}, zmm2, B
KNOT k2, k1
VDIVPS zmm1 {k2}, zmm2, C
VMOVUPS A, zmm1
```

Embedded Broadcasts and Masking

VFMADD231PS zmm1, zmm2, C {1to16}

- Scalars from memory are first class citizens
 - Broadcast one scalar from memory into all vector elements before operation
- Memory fault suppression avoids fetching the scalar if no mask bit is set to 1

Other "tuples" supported

- Memory only touched if at least one consumer lane needs the data
- For instance, when broadcast a tuple of 4 elements, the semantics check for every element being really used
 - e.g.: element 1 checks for mask bits 1, 5, 9, 13, ...

```
float32 A[N], B[N], C;
for(i=0; i<8; i++)
   if ( A[i]!=0.0 )
      A[i] = A[i] + C*B[i];
```

```
VBROADCASTSS zmm1 {k1}, [rax]
VBROADCASTF64X2 zmm2 {k1}, [rax]
VBROADCASTF32X4 zmm3 {k1}, [rax]
VBROADCASTF32X8 zmm4, {k1}, [rax]
```

Optimization Notice

AVX-512: Embedded Rounding Control and Suppress All Exceptions (SAE)

Embedded Rounding Control:

- MXCSR.RC can be overridden on all FP instructions
 - VADDPS ZMM1 {k1}, ZMM2, [mem] {1→16} {rne-sae}
- "Suspend All Exceptions"
 - · Always implied by using embedded RC
 - NO MXCSR updates / exception reporting for any lane
 - Changes to RC without SAE via LDMXCSR
 - Not needed for most common case (truncating FP convert to int)
 - Only available for reg-reg mode and 512b operands

Main application:

- Saving, modifying and restoring MXCSR is usually slow and cumbersome
- Being able to avoid suppressions and set the rounding-mode on a per instruction basis simplifies development of high performance math software sequences (math libs)
 - E.g.: avoid spurious overflow/underflow reporting in intermediate computations
 - E.g: make sure that RM=rne regardless of the contents of MXCSR

AVX-512: Compressed Displacement

VADDPS zmm1, zmm2, [rax+256]

- Observation is that displacement in generated vector code is a multiple of the actual operand size
 - An obvious side effect of unrolling
- Unfortunately, regular IA 8-bit displacement format have limited scope for 512-bit vector sizes (unrolling look-ahead of +/-2 at most)
 - So we would end up using 32-bit displacement formats too often

AVX-512 disp8*N compressed displacement

- AVX-512 implicitly encodes a 8-bit displacement as a multiple of the actual size of the memory operand
 - VADDPD zmm1 {k1}, zmm2, [rax] memory size operand is 512bits
 - VADDPD xmm1 {k1}, xmm2, [rax] memory size operand is 128bits
 - VADDPD zmm1 {k1}, xmm2, [rax] {1toN} memory size operand is 64 bits
- Assembler/compiler reverts to 32-bit displacement when the real displacement is not a multiple

Motivation for Conflict Detection

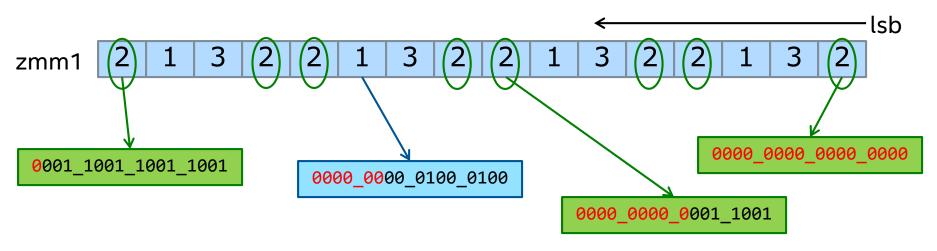
Sparse computations are common in HPC, but hard to vectorize due to race conditions

Consider the "histogram" problem:

- 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-opscatter with vector of indexes that contain conflicts

VPCONFLICT{D,Q}

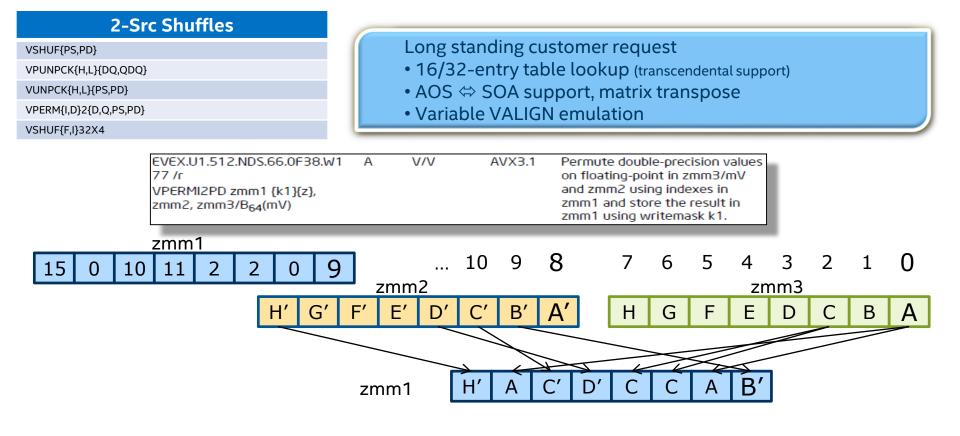
- VPCONFLICT{D,Q} zmm1{k1}{z}, zmm2/B(mV)
 - For every element in ZMM2, compare it against everybody and generate a mask identifying the matches (but ignoring elements to the 'left' of the current one –i.e. "newer")
 - Store every mask in every element destination in ZMM1



Optimized Algorithm

```
Obtain recurrence
   for each 16 scalar iterations {
                                                                      indices
      indices = vload &index array[i]
        vpconflictd comparisons, indices
       vplzcntd tmp lzcnt, comparisons
       vpsubd perm idx, all 31s, tmp lzcnt
       temp values - do first iteration(); // gather + compute
       vptestmd to do {k0}, comparisons, all ones // anything left?
       while (to do) {
         vpbroadcastmd tmp, to do
         vptestnmd mask {to do}, comparisons, tmp
         vpermd tmp values {mask}, perm idx
          tmp values = do work(mask); // just compute!
Store
          to do ^= mask;
                                                                     Re-do conflicting
results
         while(to do):
                                                                      indices reusing
        vscatter indices. A two values
                                                                    results directly from
                                                                        the vector
```

New 2-Source Shuffles



Expand & Compress

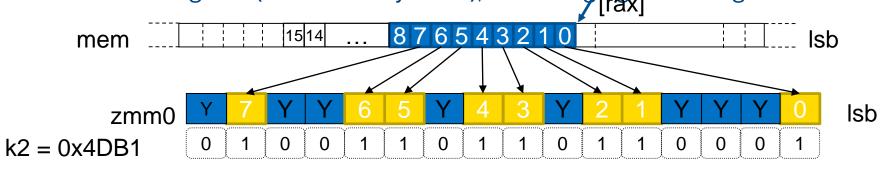
Allows vectorization of conditional loops

- Opposite operation (compress) not in AVX-512F
- Similar to FORTRAN pack/unpack intrinsics
- Provides mem fault suppression
- Faster than alternative gather/scatter

for(j=0, i=0; i<N; i++) { if(C[i] != 0.0) B[i] = A[i] * C[j++]; }</pre>

VEXPANDPS zmm0 {k2}, [rax]

Moves compressed (consecutive) elements in register or memory to sparse elements in register (controlled by mask), with merging or zeroing



Bit Manipulation

Basic bit manipulation operations on mask and vector operands

- Useful to manipulate mask registers
- Have uses in cryptography algorithms

Instruction	Description
KUNPCKBW k1, k2, k3	Interleave bytes in k2 and k3
KSHIFT{L,R}W k1, k2, imm8	Shift bits left/right using imm8
<pre>VPROR{D,Q} zmm1 {k1}, zmm2, imm8</pre>	Rotate bits right using imm8
<pre>VPROL{D,Q} zmm1 {k1}, zmm2, imm8</pre>	Rotate bits left using imm8
<pre>VPRORV{D,Q} zmm1 {k1}, zmm2, zmm3/mem</pre>	Rotate bits right w/ variable ctrl
<pre>VPROLV{D,Q} zmm1 {k1}, zmm2, zmm3/mem</pre>	Rotate bits left w/ variable ctrl

Sample: VPTERNLOG – Ternary Logic Instruction

Mimics a FPGA cell

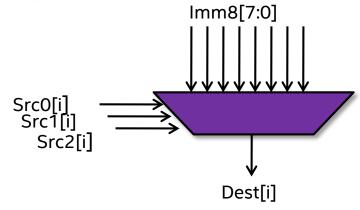
- Take every bit of three sources to obtain a 3-bit index N
 - Obtain Nth bit from imm8

VPTERNLOGD zmm0 {k2}, zmm15, zmm3/[rax], imm8

Any arbitrary truth table of 3 values can be implemented andor, andxor, vote, parity, bitwise-cmov, etc each column in the right table corresponds to imm8

S1	S2	S 3
0	0	0
0	0	1
0	1	0
0	1	1
1	0	0
1	0	1
1	1	0
1	1	1

ANDOR	VOTE	(S1)?S3:S2	
0	0	0	
1	0	1	
0	0	0	
1	1	1	
0	0	0	
1	1	0	
1	1	1	
1	1	1	



Math Support

Instruction

30

Package to aid with Math library writing

- Good value upside in financial applications
- Available in PS, PD, SS and SD data types
- Great in combination with embedded RC

$VGETXEXP_{PS,PD,SS,SD}$	zmm1 {k1}, zmm2	Obtain exponent in FP format
$VGETMANT_{\{PS,PD,SS,SD\}}$	zmm1 {k1}, zmm2	Obtain normalized mantissa
$VRNDSCALE_{\{PS,PD,SS,SD\}}$	zmm1 {k1}, zmm2, imm8	Round to scaled integral number
VSCALEF {PS,PD,SS,SD}	zmm1 {k1}, zmm2, zmm3	$X*2^{y_1}X \le getmant, Y \le getexp$
$VFIXUPIMM_{\{PS,PD,SS,SD\}}$	zmm1, zmm2, zmm3, imm8	Patch output numbers based on inputs
$VRCP14_{\{PS,PD,SS,SD\}}$	zmm1 {k1}, zmm2	Approx. reciprocal() with rel. error 2 ⁻¹⁴
VRSQRT14 _{PS,PD,SS,SD}	zmm1 {k1}, zmm2	Approx. rsqrt() with rel. error 2 ⁻¹⁴
$VDIV_{\{PS,PD,SS,SD\}}$	zmm1 {k1}, zmm2, zmm3	IEEE division
$VSQRT_{PS,PD,SS,SD}$	zmm1 {k1}, zmm2	IEEE square root

AVX-512 ER & AVX-512 PR

Set of segment-specific instruction extensions

- Will be supported in all future Intel® MIC processors
- First appear on KNL (some have similarities in KNC)

Address two HPC customer requests

- Ability to maximize memory bandwidth
 - Hardware prefetching is too restrictive
 - Conventional software prefetching results in instructions overhead
- Flexible support for transcendental operations accuracy versus speed
 - Mostly division and square root
 - Differentiating factor in HPC/TPT