# ERLANGEN REGIONAL COMPUTING CENTER



# Single Instruction Multiple Data (SIMD) processing



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# **SIMD terminology**

### A word on terminology

- SIMD == "one instruction → several operations"
- "SIMD width" == number of operands that fit into a register
- No statement about parallelism among those operations
- Original vector computers: long registers, pipelined execution, but no parallelism (within the instruction)
   R0
   R1

### Today

- x86: most SIMD instructions fully parallel
  - "Short Vector SIMD"
  - Some exceptions on some archs (e.g., vdivpd)
- NEC Tsubasa: 32-way parallelism but SIMD width = 256 (DP)



# **Scalar execution units**

```
for (int j=0; j<size; j++){
    A[j] = B[j] + C[j];
}</pre>
```

# **Register widths**

- 1 operand
- 2 operands (SSE)
- 4 operands (AVX)
- 8 operands (AVX512)

### **Scalar execution**



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# Data-parallel execution units (short vector SIMD)

Single Instruction Multiple Data (SIMD)

```
for (int j=0; j<size; j++){
    A[j] = B[j] + C[j];
}</pre>
```

# **Register widths**

- 1 operand
- 2 operands (SSE)
- 4 operands (AVX)
- 8 operands (AVX512)

# **SIMD** execution



SIMD

# Example: Data types in 32-byte SIMD registers (AVX[2])

Supported data types depend on actual SIMD instruction set

				-				
double		double		double		double		
	_			_	_			
float	float	float	float	float	float	float fl	oat	
			_		-			
int	int	int	int	int	int	int i	nt	
_							_	





Scalar slot





# Von Neumann bottleneck reloaded: "DRAM gap"

DP peak performance and peak main memory bandwidth for a single Intel processor (chip) – without SIMD and FMA





### **SIMD processing – Basics**

Steps (done by the compiler) for "SIMD processing"



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SIMD

### SIMD processing: roadblocks

No SIMD vectorization for loops with data dependencies:

"Pointer aliasing" may prevent SIMDfication

```
void f(double *A, double *B, double *C, int n) {
    for(int i=0; i<n; ++i)
        C[i] = A[i] + B[i];
}</pre>
```

C/C++ allows that  $A \rightarrow \&C[-1]$  and  $B \rightarrow \&C[-2]$  $\rightarrow C[i] = C[i-1] + C[i-2]$ : dependency  $\rightarrow No SIMD$ 

If "pointer aliasing" is not used, tell the compiler:

```
-fno-alias (Intel), -Msafeptr (PGI), -fargument-noalias (gcc) restrict keyword (C only!):
```

void f(double \*restrict A, double \*restrict B, double \*restrict C, int n) {...}



# How to leverage SIMD: your options

**Options:** 

- The compiler does it for you (but: aliasing, alignment, language, abstractions)
- Compiler directives (pragmas)
- Alternative programming models for compute kernels (OpenCL, ispc)
- Intrinsics (restricted to C/C++)
- Implement directly in assembler

### To use intrinsics the following headers are available:

- xmmintrin.h (SSE)
- pmmintrin.h (SSE2)
- immintrin.h (AVX)
- x86intrin.h (all extensions)

SIMD

# **Vectorization compiler options (Intel)**

- The compiler will vectorize starting with –02.
- To enable specific SIMD extensions use the –x option:
  - -xSSE2 vectorize for SSE2 capable machines
     Available SIMD extensions:

```
SSE2, SSE3, SSSE3, SSE4.1, SSE4.2, AVX, ...
```

- -xAVX on Sandy/Ivy Bridge processors
- -xCORE-AVX2
   on Haswell/Broadwell
  - -xCORE-AVX512 on Skylake (certain models)
- -xMIC-AVX512 on Xeon Phi Knights Landing

### Recommended option:

- -xHost will optimize for the architecture you compile on (Caveat: do not use on standalone KNL, use MIC-AVX512)
- To really enable 512-bit SIMD with current Intel compilers you need to set:
   -qopt-zmm-usage=high

# **User-mandated vectorization (OpenMP 4)**

- Since OpenMP 4.0 SIMD features are a part of the OpenMP standard
- #pragma omp simd enforces vectorization
- Essentially a standardized "go ahead, no dependencies here!"
  - Do not lie to the compiler here!
- Prerequesites:
  - Countable loop
  - Innermost loop
  - Must conform to for-loop style of OpenMP worksharing constructs
- There are additional clauses:

```
reduction, vectorlength, private, collapse, ...
for (int j=0; j<n; j++) {
    #pragma omp simd reduction(+:b[j:1])
    for (int i=0; i<n; i++) {
        b[j] += a[j][i];
    }
</pre>
```

SIMD

## **x86 Architecture:** *SIMD and Alignment*

- Alignment issues
  - Alignment of arrays should optimally be on SIMD-width address boundaries to allow packed aligned loads (and NT stores on x86)
  - Otherwise the compiler will revert to unaligned loads/stores
  - Modern x86 CPUs have less (not zero) impact for misaligned LOAD/STORE, but Xeon Phi KNC relies heavily on it!
  - How is manual alignment accomplished?
- Stack variables: alignas keyword (C++11/C11)
- Dynamic allocation of aligned memory (align = alignment boundary)
  - C before C11 and C++ before C++17: posix\_memalign(void \*\*ptr, size\_t align, size\_t size);
  - C11 and C++17:

aligned\_alloc(size\_t align, size\_t size);





### Reading Assembly Language

### (Don't Panic)



E



### **Assembler: Why and how?**

Why check the assembly code?

- Sometimes the only way to make sure the compiler "did the right thing"
  - Example: "LOOP WAS VECTORIZED" message is printed, but Loads & Stores may still be scalar!
- Get the assembler code (Intel compiler):

icc -S -O3 -xHost triad.c -o a.out

Disassemble Executable:

objdump -d ./a.out | less

The x86 ISA is documented in:

Intel Software Development Manual (SDM) 2A and 2B AMD64 Architecture Programmer's Manual Vol. 1-5



### **Basics of the x86-64 ISA**

- Instructions have 0 to 3 operands (4 with AVX-512)
- Operands can be registers, memory references or immediates
- Opcodes (binary representation of instructions) vary from 1 to 15 (?) bytes
- There are two assembler syntax forms: Intel (left) and AT&T (right)
- Addressing Mode: BASE + INDEX \* SCALE + DISPLACEMENT
- C: A[i] equivalent to \*(A+i) (a pointer has a type: A+i\*8)

Intel syntax	AT&T syntax		
<pre>movaps [rdi + rax*8+48], xmm3 add rax, 8 js 1b</pre>	<pre>movaps %xmm3, 48(%rdi,%rax,8) addq \$8, %rax jsB1.4</pre>		
401b9f: 0f 29 5c c7 30movaps401ba4: 48 83 c0 08addq401ba8: 78 a6js	<pre>\$ %xmm3,0x30(%rdi,%rax,8) \$0x8,%rax 401b50 <triad_asm+0x4b></triad_asm+0x4b></pre>		



## **Basics of the x86-64 ISA with extensions**

```
16 general Purpose Registers (64bit):

rax, rbx, rcx, rdx, rsi, rdi, rsp, rbp, r8-r15

alias with eight 32 bit register set:

eax, ebx, ecx, edx, esi, edi, esp, ebp

8 opmask registers (16bit or 64bit, AVX512 only):

k0-k7

Floating Point SIMD Registers:

xmm0-xmm15 (xmm31) SSE (128bit) alias with 256-bit and 512-bit registers

ymm0-ymm15 (xmm31) AVX (256bit) alias with 512-bit registers
```

zmm0-zmm31 AVX-512 (512bit)

### SIMD instructions are distinguished by:

VEX/EVEX prefix:	v
Operation:	mul, add, mov
Modifier:	nontemporal (nt), unaligned (u), aligned (a), high (h)
Width:	scalar (s), packed (p)
Data type:	single (s), double (d)



### **Example for masked execution**

Masking for predication is very helpful in cases such as e.g. remainder loop handling or conditional handling.







# **ISA support on Intel chips**

The current Skylake architecture supports all legacy ISA extensions: MMX, SSE, AVX, AVX2

### Furthermore **KNL** supports:

- AVX-512 Foundation (F), KNL and Skylake
- AVX-512 Conflict Detection Instructions (CD), KNL and Skylake
- AVX-512 Exponential and Reciprocal Instructions (ER), KNL
- AVX-512 Prefetch Instructions (PF), KNL

### AVX-512 extensions only supported on **Skylake**:

- AVX-512 Byte and Word Instructions (BW)
- AVX-512 Doubleword and Quadword Instructions (DQ)
- AVX-512 Vector Length Extensions (VL)

### **ISA Documentation**:

Intel Architecture Instruction Set Extensions Programming Reference

# **Case Study: Sum reduction (double precision)**

```
double sum = 0.0;
for (int i=0; i<size; i++){
    sum += data[i];
}
```

To get object code use objdump -d on object file or executable or compile with -s

Assembly code w/ -O1 (Intel syntax, Intel compiler):

```
.label:
    addsd xmm0,[rdi + rax * 8]
    inc rax
    cmp rax, rsi
    jl .label
    AT&T syntax:
    addsd 0(%rdi,%rax,8),%xmm0
```



### Sum reduction (double precision) – AVX512 version

Assembly code w/ -O3 -xCORE-AVX512 -qopt-zmm-usage=high:

.label	:	
	vaddpd	zmm1, zmm1, [rdi+rcx*8]
	vaddpd	zmm4, zmm4, [64+rdi+rcx*8]
	vaddpd	zmm3, zmm3, [128+rdi+rcx*8] Bulk loop code
	vaddpd	zmn2, $zmn2$ , [192+rdi+rcx*8] (8x4-way uprolled)
	add	rcx, 32
	cmp	rcx, rdx
	jb	.label
;		
	vaddpd	zmm1, zmm1, zmm4
	vaddpd	zmm2, zmm3, zmm2
	vaddpd	zmm1, zmm1, zmm2
; [ SI	NIP]	Remainder omitted
	vshuff32x	zmm2, zmm1, zmm1, 238 Sum up 32
	vaddpd	$z_{mm1}, z_{mm2}, z_{mm1}$ > partial sums into
	vpermpd	zmm3, zmm1, 78 xmm0.0
	vaddpd	zmm4, zmm1, zmm3
	vpermpd	zmm5, zmm4, 177
	vaddpd	zmm6, zmm4, zmm5
	vaddsd	xmm0, xmm6, xmm0



### Sum reduction (double precision) – sequential performance



SIMD is an in-core performance feature! If the bottleneck is data transfer, its benefit is limited.



# **SIMD** with masking

```
double sum = 0.0;
 for (int i=0; i<size; i++){</pre>
       if(data[i]>0.0)
          sum += data[i];
 }
                        .label:
                                        (%r12,%rsi,8), %zmm5
                               vmovups
                                        64(%r12,%rsi,8), %zmm6
                               vmovups
                                        128(%r12,%rsi,8), %zmm7
                               vmovups
                                        192(%r12,%rsi,8), %zmm8
                               vmovups
                               vcmpgtpd %zmm4, %zmm5, %k1
                                                                        SIMD mask
                               vcmpgtpd %zmm4, %zmm6, %k2
   Bulk loop code
                               vcmpgtpd %zmm4, %zmm7, %k3
                                                                        generation
                               vcmpgtpd
                                        %zmm4, %zmm8, %k4
(8x4-way unrolled)
                               vaddpd
                                        %zmm5, %zmm0, %zmm0{%k1}
                                                                        masked SIMD
                               vaddpd
                                        %zmm6, %zmm3, %zmm3{%k2}
                                                                        ADDs
                                        %zmm7, %zmm2, %zmm2{%k3}
                               vaddpd
                                                                        (accumulates)
                                        %zmm8, %zmm1, %zmm1{%k4}
                               vaddpd
                               addq
                                        $32, %rsi
                                        %rdx, %rsi
                               cmpq
                                         .label
                               ib
```



# **Rules and guidelines for vectorizable loops**

- 1. Inner loop
- 2. Countable (loop length can be determined at loop entry)
- 3. Single entry and single exit
- 4. Straight line code (no conditionals) unless masks can be used
- 5. No (unresolvable) read-after-write data dependencies
- 6. No function calls (exception intrinsic math functions)

### Better performance with:

- 1. Simple inner loops with unit stride (contiguous data access)
- 2. Minimize indirect addressing
- 3. Align data structures to SIMD width boundary (minor impact)

In C use the **restrict** keyword and/or **const** qualifiers and/or compiler options to rule out array/pointer aliasing





# Efficient parallel programming on ccNUMA nodes

Performance characteristics of ccNUMA nodes First touch placement policy "The other affinity" to care about

### ccNUMA:

- Whole memory is transparently accessible by all processors
- but physically distributed across multiple locality domains (LDs)
- with varying bandwidth and latency
- and potential contention (shared memory paths)
- How do we make sure that memory access is always as "local" and "distributed" as possible?



### How much bandwidth does nonlocal access cost?



Example: AMD "Epyc" 2-socket system (8 chips, 2 sockets, 48 cores): *STREAM Triad bandwidth measurements* [Gbyte/s]

CPU nod	le 0	1	2	3	4	5	6	7
MEM node								
0	32.4	21.4	21.8	21.9	10.6	10.6	10.7	10.8
1	21.5	32.4	21.9	21.9	10.6	10.5	10.7	10.6
2	21.8	21.9	32.4	21.5	10.6	10.6	10.8	10.7
3	21.9	21.9	21.5	32.4	10.6	10.6	10.6	10.7
4	10.6	10.7	10.6	10.6	32.4	21.4	21.9	21.9
5	10.6	10.6	10.6	10.6	21.4	32.4	21.9	21.9
6	10.6	10.7	10.6	10.6	21.9	21.9	32.3	21.4
7	10.7	10.6	10.6	10.6	21.9	21.9	21.4	32.5



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### numactl as a simple ccNUMA locality tool : How do we enforce some locality of access?



numactl can influence the way a binary maps its memory pages:

```
numactl --membind=<nodes> a.out  # map pages only on <nodes>
    --preferred=<node> a.out  # map pages on <node>
    # and others if <node> is full
    --interleave=<nodes> a.out  # map pages round robin across
    # all <nodes>
```

### Examples:

```
for m in `seq 0 7`; do ccNUMA map scan
for c in `seq 0 7`; do for EPYC system
    env OMP_NUM_THREADS=6 \
    numactl --membind=$m likwid-pin -c M${c}:0-5 ./stream
    done
done
```

numactl --interleave=0-7 likwid-pin -c E:N:8:1:12 ./stream

But what is the default without numactl?



Golden Rule" of ccNUMA:

# A memory page gets mapped into the local memory of the processor that first touches it!

- Except if there is not enough local memory available
- This might be a problem, see later
- Caveat: "to touch" means "to write", not "to allocate"
- Example:

Memory not mapped here yet

double \*huge = (double\*)malloc(N\*sizeof(double));

```
for(i=0; i<N; i++) // or i+=PAGE_SIZE/sizeof(double)
huge[i] = 0.0;
Mapping takes
place here</pre>
```

It is sufficient to touch a single item to map the entire page

# **Coding for ccNUMA data locality**



### Most simple case: explicit initialization

```
integer, parameter :: N=1000000
                                   integer, parameter :: N=1000000
                                  double precision A(N), B(N)
double precision A(N), B(N)
                                   !$OMP parallel
                                   !$OMP do schedule(static)
                                  do i = 1, N
                                    A(i) = 0.00
A=0.d0
                                  end do
                                   !$OMP end do
                                   . . .
                                   !$OMP do schedule(static)
!$OMP parallel do
                                  do i = 1, N
do i = 1, N
                                    B(i) = function (A(i))
 B(i) = function (A(i))
                                  end do
end do
                                   !$OMP end do
!$OMP end parallel do
                                   !$OMP end parallel
```

### **Coding for ccNUMA data locality**



Sometimes initialization is not so obvious: I/O cannot be easily parallelized, so "localize" arrays before I/O

```
integer, parameter :: N=1000000
                                  integer, parameter :: N=1000000
double precision A(N), B(N)
                                  double precision A(N), B(N)
                                   !$OMP parallel
                                   !$OMP do schedule(static)
                                  do i = 1, N
                                    A(i) = 0.d0
                                  end do
READ(1000) A
                                   !$OMP end do
                                   !$OMP single
                                  READ(1000) A
                                   !$OMP end single
!$OMP parallel do
                                   !$OMP do schedule(static)
do i = 1, N
                                  do i = 1, N
 B(i) = function (A(i))
                                    B(i) = function (A(i))
end do
                                  end do
!$OMP end parallel do
                                   !$OMP end do
                                   !$OMP end parallel
```

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#### ccNUMA

# **Coding for Data Locality**

- Required condition: OpenMP loop schedule of initialization must be the same as in all computational loops
  - Only choice: static! Specify explicitly on all NUMA-sensitive loops, just to be sure...
  - Imposes some constraints on possible optimizations (e.g. load balancing)
  - Presupposes that all worksharing loops with the same loop length have the same thread-chunk mapping
  - If dynamic scheduling/tasking is unavoidable, the problem cannot be solved completely if a team of threads spans more than one LD
    - Static parallel first touch is still a good idea
    - OpenMP 5.0 will have rudimentary memory affinity functionality
- How about global objects?
  - If communication vs. computation is favorable, might consider properly placed copies of global data
- C++: Arrays of objects and std::vector<> are by default initialized sequentially
  - STL allocators provide an elegant solution



- If your code is cache bound, you might not notice any locality problems
- Otherwise, bad locality limits scalability (whenever a ccNUMA node boundary is crossed)
  - Just an indication, not a proof yet
- Running with numactl --interleave might give you a hint
   See later
- Consider using performance counters
  - LIKWID-perfctr can be used to measure nonlocal memory accesses
  - Example for Intel dual-socket system (IvyBridge, 2x10-core):

likwid-perfctr -g NUMA -C M0:0-4@M1:0-4 ./a.out

# Using performance counters for diagnosing bad ccNUMA access locality



 Intel Ivy Bridge EP node (running 2x5 threads): measure NUMA traffic per core

likwid-perfctr -g NUMA -C M0:0-4@M1:0-4 ./a.out

### Summary output:

·				
Metric	Sum	Min	Max	Avg
Runtime (RDTSC) [s] STAT	4.050483	0.4050483	0.4050483	0.4050483
Runtime unhalted [s] STAT	3.03537	0.3026072	0.3043367	0.303537
Clock [MHz] STAT	32996.94	3299.692	3299.696	3299.694
CPI STAT	40.3212	3.702072	4.244213	4.03212
Local DRAM data volume [GByte] STAT	7.752933632	0.735579264	0.823551488	0.7752933632
Local DRAM bandwidth [MByte/s] STAT	19140.761	1816.028	2033.218	1914.0761
Remote DRAM data volume [GByte] STAT	9.16628352	0.86682464	0.957811776	0.916628352
Remote DRAM bandwidth [MByte/s] STAT	22630.098	2140.052	2364.685	2263.0098
Memory data volume [GByte] STAT	16.919217152	1.690376128	1.69339104	1.6919217152
Memory bandwidth [MByte/s] STAT	41770.861	4173.27	4180.714	4177.0861

 Caveat: NUMA metrics vary strongly between CPU models About half of the overall memory traffic is caused by remote domain!

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### A weird observation

- Experiment: memory-bound Jacobi solver with sequential data initialization
  - No parallel data placement at all!
  - Expect no scaling across LDs
- Convergence threshold  $\delta$  determines the runtime
  - The smaller  $\delta$ , the longer the run
- Observation
  - No scaling across LDs for large δ (runtime 0.5 s)
  - Scaling gets better with smaller δ up to almost perfect efficiency ε (runtime 91 s)
- Conclusion
  - Something seems to "heal" the bad
     access locality on a time scale of tens of seconds







Linux kernel supports automatic page migration

```
$ cat /proc/sys/kernel/numa_balancing
0
```

- \$ echo 1 > /proc/sys/kernel/numa\_balancing # activate
- Active on all current Linux distributions
- Parameters control aggressiveness

```
$ ll /proc/sys/kernel/numa*
-rw-r--r-- 1 root root 0 Jun 26 09:16 numa_balancing
-rw-r--r-- 1 root root 0 Jun 26 09:16 numa_balancing_scan_delay_ms
-rw-r--r-- 1 root root 0 Jun 26 09:16 numa_balancing_scan_period_max_ms
-rw-r--r-- 1 root root 0 Jun 26 09:16 numa_balancing_scan_period_min_ms
-rw-r--r-- 1 root root 0 Jun 26 09:16 numa_balancing_scan_size_mb
```

- Deafult behavior is "take it slow"
- Do not rely on it! Parallel first touch is still a good idea!

### The curse and blessing of interleaved placement: OpenMP STREAM triad on a dual AMD Epyc 7451 (6 cores per LD)



- Parallel init: Correct parallel initialization
- LD0: Force data into LD0 via numactl -m 0
- Interleaved: numactl --interleave <LD range>



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# rr@=

### Identify the problem

- Is ccNUMA an issue in your code?
- Simple test: run with numactl --interleave

### Apply first-touch placement

- Look at initialization loops
- Consider loop lengths and static scheduling
- C++ and global/static objects may require special care

### NUMA balancing is active on many Linux systems today

- Automatic page migration
- Slow process, may take many seconds (configurable)
- Not a silver bullet
- Still a good idea to do parallel first touch

### If dynamic scheduling cannot be avoided

- Consider round-robin placement as a quick (but non-ideal) fix
- OpenMP 5.0 will have some data affinity support



## Simultaneous multithreading (SMT)

Principles and performance impact SMT vs. independent instruction streams Facts and fiction SMT Makes a single physical core appear as two or more "logical" cores → multiple threads/processes run concurrently



SMT principle (2-way example):



# **SMT** impact

- SMT is primarily suited for increasing processor throughput
  - With multiple threads/processes running concurrently
- Scientific codes tend to utilize chip resources quite well
  - Standard optimizations (loop fusion, blocking, ...)
  - High data and instruction-level parallelism
  - Exceptions do exist
- SMT is an important topology issue
  - SMT threads share almost all core resources
    - Pipelines, caches, data paths
  - Affinity matters!
  - If SMT is not needed
    - pin threads to physical cores
    - or switch it off via BIOS etc.



# SMT impactCaveat: SMT threads share all caches!

- Possible benefit: Better pipeline throughput
  - Filling otherwise unused pipelines
  - Filling pipeline bubbles with other thread's executing instructions:





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### The ideal workload for SMT

Simple loop-carried dependency benchmark A(i) = s\*A(i-1)

- Bottleneck: MULT pipeline latency
  - Haswell CPU: 5 cy/it best case
- Running 2 threads via SMT: expect 2.5 cy/it if no other bottlenecks turn up
- Further improvement?
  - Multiple independent streams of instructions per thread
- What about the data transfer?







### Simple loop-carried dependency benchmark A(i) = s\*A(i-1)



# **SMT** myths: Facts and fiction (1)



Myth: "If the code is compute-bound, then the functional units should be saturated and SMT should show no improvement."

### Truth

- A compute-bound loop does not necessarily saturate the pipelines; dependencies can cause a lot of bubbles, which may be filled by SMT threads.
- 2. If a pipeline is already full, SMT will not improve its utilization



### **SMT** myths: Facts and fiction (2)

Myth: "If the code is memory-bound, SMT should help because it can fill the bubbles left by waiting for data from memory."

Truth:

SMT

2. If the relevant bottleneck is not exhausted, SMT may help since it can fill bubbles in the LOAD pipeline.

This applies also to other "relevant bottlenecks!"





# **SMT** myths: Facts and fiction (3)

Myth: "SMT can help bridge the latency to memory (more outstanding references)."

### Truth:

Outstanding references may or may not be bound to SMT threads; they may be a resource of the memory interface and shared by all threads. The benefit of SMT with memory-bound code is usually due to better utilization of the pipelines so that less time gets "wasted" in the cache hierarchy.

See also the "ECM Performance Model" later on.



