

Module: Design of HPC Cluster – Ecosystem

Building blocks of HPC cluster: Case for accelerators and new paradigms

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C-DAC



500+ TF (With Accelerators)

54 TF (Without Accelerators)

Contents

- Why accelerators: Background
- What are Accelerators
- Accelerator types
 - GP-GPU
 - Xeon Phi (KNC, KNL)
 - Data Centre Accelerators
 - FPGA based accelerators
- Accelerator architecture building blocks

High Performance Computing (HPC)

- Computer Simulation +Theory & Experiments
 - Real experiments too small, large, complex, expensive, dangerous Or impossible

- Computational Sciences: Multidisciplinary field
 - Uses advanced computational capabilities to solve complex problems & understand, design
 - Protein folding/ computational biology
 - Climate, weather modelling
 - Astrophysics
 - Nano- Science

High Performance Computing (HPC) - 2

- HPC: Solving problems using
 - Supercomputers +
 - fast networks +
 - large storage +
 - visualization
- LINPACK: Bench mark for Top 500 supercomputers of the world
 - Summit@Oak Ridge National Laboratory (ORNL) USA 143.5 PF
 - Sierra@Lawrence Livermore National Laboratory (LLNL) USA 94.6 PF IBM Power9 CPUs and NVIDIA V100 GPUs.

Why use parallel Computers?

- Only way to achieve computational goals
 - Sequential system is very slow
 - ⇒ Calculation takes days, months, years
 - ✓ Use more than one processor to get faster calculation

- Sequential system is very small
 - ⇒ Data does not fit in memory
 - ✓ Parallel system to accommodate more memory

HPC Fastest Growing Sector

HPC, the massive horsepower of IT is one of the fastest growing sector in the Industry

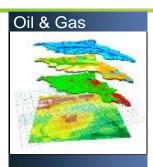
- Rapidly growing data generated in the enterprise...
 - Every industrial sector

Every one wants fast results

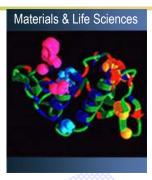
HPC Segment Application Areas



- Fin. Modeling
- Data Mining



- Seismic
- Reservoir Mod



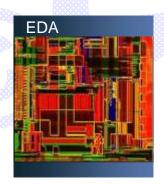
- Molecular Dyn
- Med. Imaging
- DNA / iRNA
- Material Sci



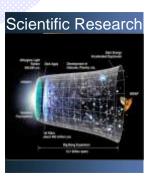
- Weather
- Crypto
- Data Mining



- Rendering
- Compositing



- Verification
- Layout



- Cosmology
- Physics
- Math



- Structures
- Fluids
- Impact

Emerging Application Areas

..sometime not evident



- Froth formation in the washing machine
- Model production/Packaging of Pringles

(potato chips)



Study Rotting (decay) of wood



HPC is everywhere !!

Ref: SC

Background: Need for Accelerators





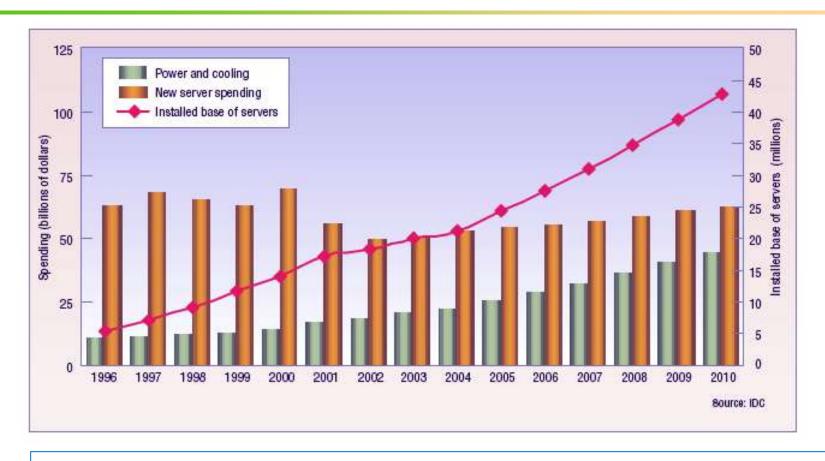


- Tackle large, complex computational problems
 - Multi-core to Many Core transition
- Large number of Computing Servers
 - Large rack Space
- High power consumption requirements



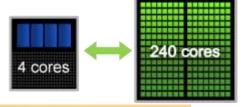
Computing cluster

Power Requirement Trends

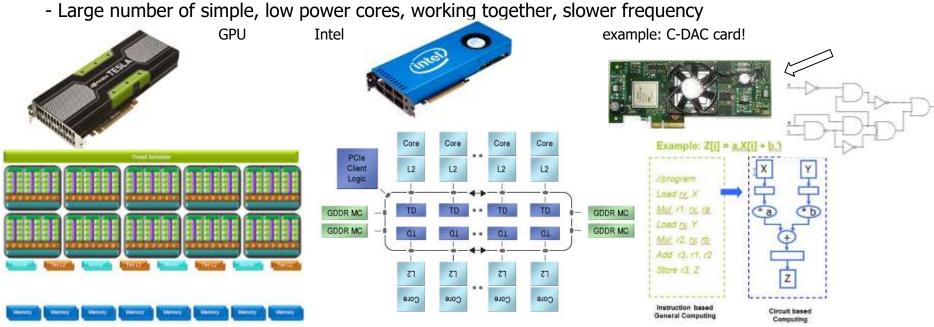


Power and cooling costs increasing faster than equipment cost

Accelerators (devices): I



- Currently best alternatives to Increase computing power at the same time energy and space efficient
- Contain a large number of processing cores, as well as internal memory
- Most often used in conjunction with the CPUs of the node to accelerate certain 'hot spots' of a computation that requires a large amount of algebraic operations
- GPU, Xeon-phi and FPGA based



Accelerators (devices): II



Historically

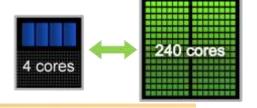
- Special hardware for accelerating computations :long tradition in HPC
 - Floating point units
 - SIMD/vector units
- Cell-chip based (chip jointly developed by Sony, Toshiba and IBM)
 - IBM RoadRunner Supercomputer
 Hybrid system- general purpose CPU (AMD Opteron)
 + cell processors (PowerPC core)

#1 system in June 2008 Top 500 list

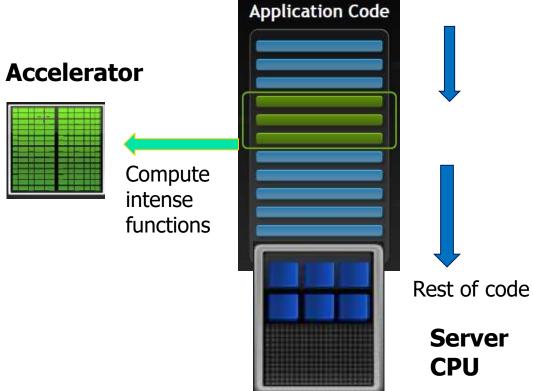
1st Supercomputer to run PetaFlop speeds



Accelerators (devices): III



 Most often used in conjunction with the CPUs of the node to accelerate certain 'hot spots' of a computation that requires a large amount of algebraic operations



Part of the code runs on CPUs of Servers

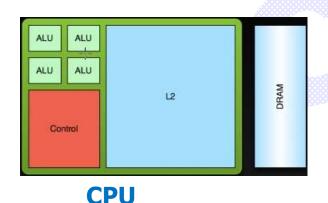
Compute intense functions also called kernel run on accelerators



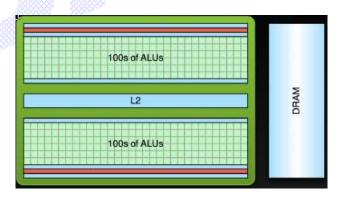
Mainly popularized by NVIDIA & AMD for HPC ~2007

What is GPU Accelerated computing?

- Using Graphics Processing Unit along with CPU to accelerate applications
 - Highly parallel many-core systems, processing large blocks of data in parallel



Optimized for low latency access

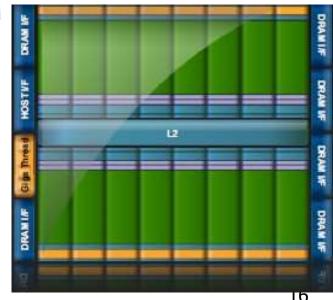


GPU *Optimized for data parallel, high throughput*

GPU Architecture

Two main components

- Streaming Multiprocessors (SM)
 - perform computations
 - Control unit, execution pipeline, caches,...
- Global Memory
 - Analogous to RAM in server
 - Accessible to GPU & CPU



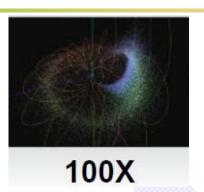
What kind of codes benefit ?

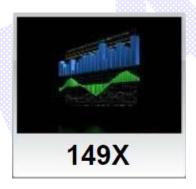
- Codes that spend lot of time in a task
 - If the task can be divided into hundreds of parallel sub-tasks
- Double precision performance for (√ accuracy)
 - Aerodynamics, Reservoir simulation, ...
- Single precision performance for (√ speed)
 - Image rendering,

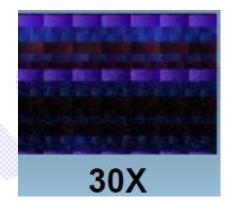
GPU Accelerated Applications

- Astrophysics
- Gene sequencing
- Financial analysis
- Visualization
- AI/Deep learning

...



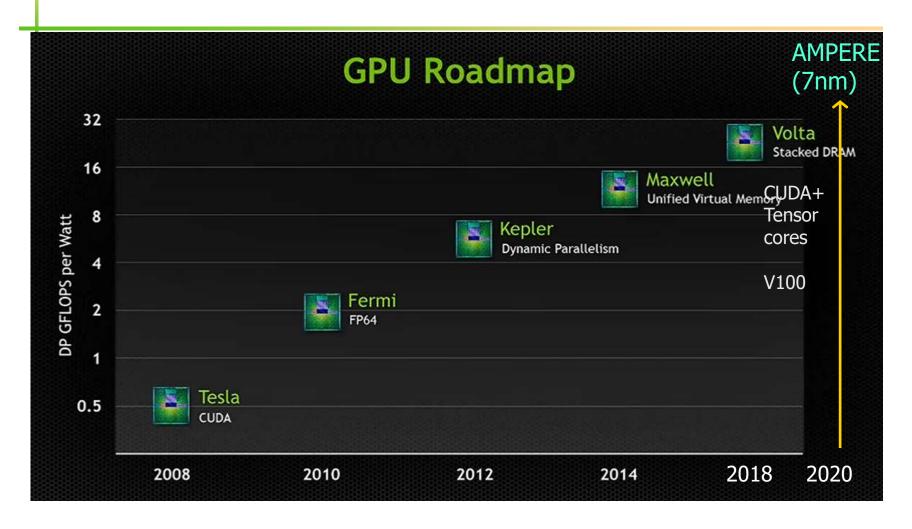






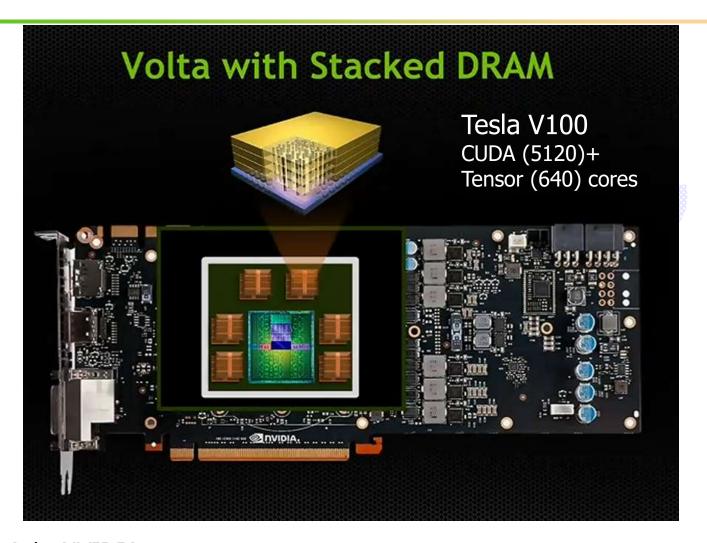
Ref: NVIDIA website

GPU roadmap (NVIDIA): 1



Ack: NVIDIA

GPU roadmap (NVIDIA): 2



Ack: NVIDIA

Accelerators – GPU (AMD) Specifications

- FirePro S9170 (for servers)
 - 2.62 TFLOPS (Peak) Double Precision
 - 5.24 TFLOPS (Peak) Single Precision

Memory

- Ultra fast, large 32 GB GDDR5 memory
 - Help to accelerate memory intensive applications,
 & computational complex workflows
- Error Correcting Code (ECC) Memory

Energy efficient

- 275 W Power consumption (max)
- Open CL 2.0 support

Specifications: Cooling/Power/Form Factor

- Bus Interface: PCIe x16
- Slots: Two
- Form Factor: Full height/ Full length
- Cooling: Passive heat sink

Specifications: System Requirements

- 20 CFM airflow cooling at 45° C maximum inlet temperature
- Available PCI Express® x16 (dual slot) 3.0 for optimal performance
- Power supply plus one 2x4 (8-pin) and one 2x3 (6-pin) AUX power connectors
- 2GB system memory
- Supported OS

There are four main ways:

Applications

Accelerator enabled libraries

Directives /Pragma Explicit
Programming
languages

Accelerator enabled Applications

There are four main ways:

Applications

Accelerator enabled libraries

Only requires use of libraries (already written & available)



Ack: NVIDIA

There are four main ways:

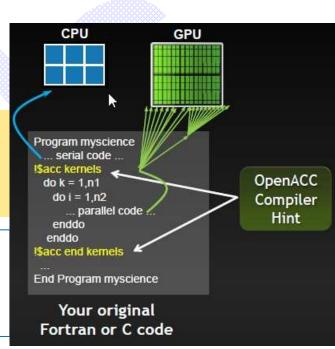
Applications

Accelerator enabled libraries

Directives /Pragma

Explicit
Programming
languages

Accelerator code directly generated from source code by compiler (by adding hints)



There are four main ways:

Applications

Accelerator enabled libraries

Directives /Pragma Explicit
Programming
languages

Accelerator enabled Applications

Programmer writes instructions specific to accelerator for - Executing algorithm

Transfer of data

Standard C Code

Parallel C Code

CUDA C

CUDA (Compute Unified Device Architecture)

// Perform SAXPY on 1M elements

saxpy_serial(4096*256, 2.0, x, y);

Programmer writes instructions specific to accelerator for - Executing algorithm

Transfer of data

GPGPU Programming: Low-level

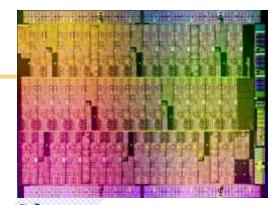
- Proprietary programming languages or extensions
 - NVIDIA: CUDA (C/C++ based)
 - AMD: StreamSDK or Brooks+ (C/C++ based)
- Open Computing Language (OpenCL)
 - Open standard for portable, parallel programming of heterogeneous parallel computing
 - CPUs, GPUs, and other processors
- Major rewriting of the code required, not portable
- Best performance, usually only needed for Important kernels, Libraries

GPGPU Programming: High-level

- Compilation systems with (OpenMP-like) directives for GPU programming
 - User tells compiler which part of code to accelerate
 - Portland Group Fortran and C compilers
 - http://www.pgroup.com/resources/accel.htm
 - CAPS HMPP (Fortran, C)
 - http://www.caps-enterprise.com/hmpp.html
 - AMD: StreamSDK or Brooks+ (C/C++ based)
- OpenACC joint-venture by:
 - NVIDIA
 - Portland Group
 - CRAY
 - CAPS

Intel Xeon Phi – 1st generation

Intel 5110P (B1) or



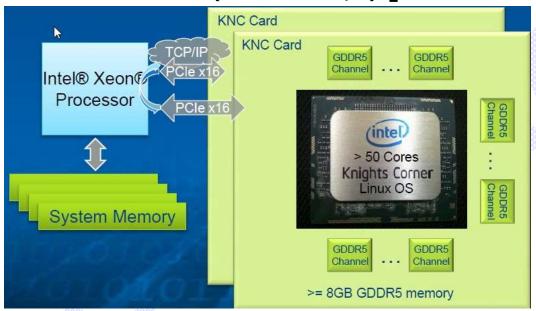
Many Integrated Core (MIC)
or

Knights Corner (KNC)



Xeon Phi Coprocessor

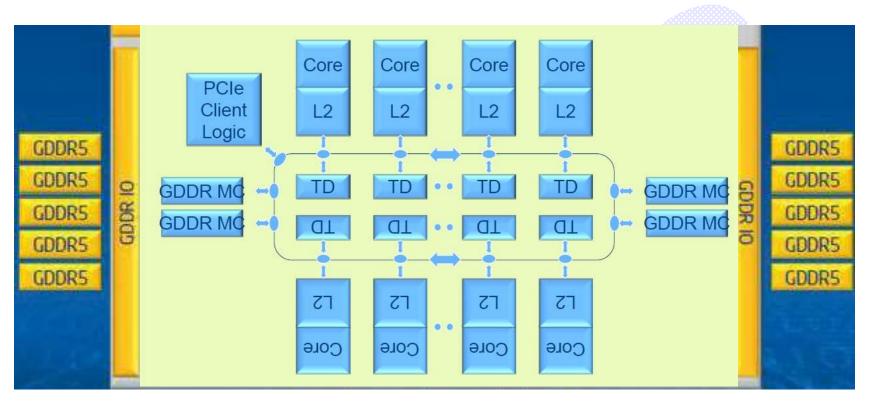
- Many core initiative from Intel
 - Available Cores (57/ 60/ 61,..) [based on 1st gen Pentium]



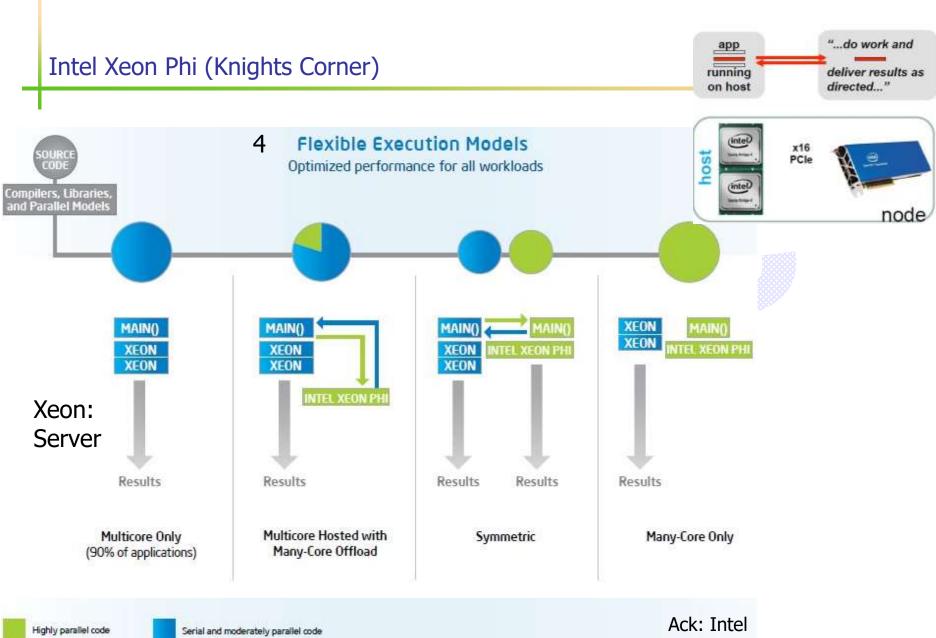
- ~ 1 TF Peak; Clock Speed (1053/1100/1238 MHz)
- Memory size (6 / 8/ 16 GB)
- PCI express card

Xeon Phi

- Each core L1 cache 64KB, L2 cache 512KB
 - Cores interconnected by a ring bus



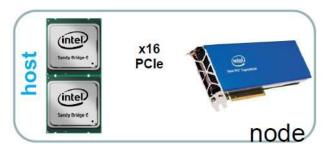
GDDR MC → memory controller; GDDR5 – Graphic double data rate – type 5 synchronous memory



Offload directive Xeon Phi: sample

snapshop





offloads



```
F90
program main
  use omp lib
                                      offload directive
  integer :: nprocs
   !dir$ offload target(mic)
  nprocs = omp get num procs() ← runs on MIC
  print*, "procs: ", nprocs
                                      runs on host
end program
#include <stdio.h>
                                C/C++
#include <omp.h>
int main ( void ) {
 int totalProcs;
 #pragma offload target(mic)
 totalProcs = omp get num procs();
 printf( "procs: %d\n", totalProcs );
 return 0;
```

Ack: Intel

Xeon Phi Programming

- Based on "standard" programming models MPI, OpenMP, or MPI/OpenMP
 - On a set of MIC nodes
 - On a set of Cluster and MIC nodes
- Using offload directives
 - MPI program on Cluster nodes
 - Offloading (OpenMP) kernels to MIC nodes
- Various Intel proprietary programming models
 - Cilk Plus
 - TBB
 - OpenCL

Sample Xeon Phi Applications/performance

- Deep learning image classification training
- High performance ray tracing visualization
- Financial risk modelling

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Ref: https://newsroom.intel.com/newsroom/wp-content/uploads/sites/11/2016/06/intel-xeon-phi-product-family-performance-fact-sheet.pdf

Sample Application: WRF

Weather Research & Forcast (WRF)



Ref: https://software.intel.com/en-us/articles/weather-research-and-forecasting-model-optimized-for-knights-landing http://www.intel.com/performance/datacenter.

Accelerators: Many Core (Xeon-Phi)

- "PARAM Yuva-II", C-DAC : 500+ TF
- Green500

44th rank, Level 3 measurement



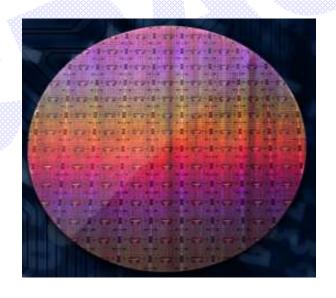


Greenest HPC System of India

Launched: June 2016

Knights Landing (KNL)

KNL wafer (typically size of a wafer is that of a dinner plate! ~ 12 inch diameter)

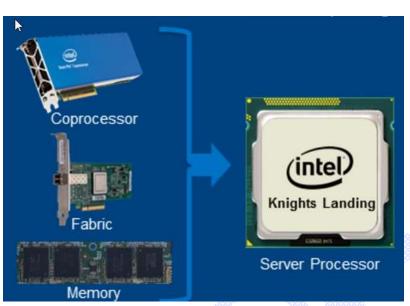


14 nm Process Technology

Motivation behind KNL ??

- Memory bandwidth, one of the bottleneck in computational Application performance
 - BLAS Level 1 & 2 (Basic Linear Algebra Subprograms) such as vector dot-product, matrix-vector multiplications...
 - Fast Fourier Transform (FFT),...
 - Memory latency also addressed
 - Bringing near CPU
 - Bootable host Chip
 - No PCIe bottleneck (limitation in the data send back and forth from the host CPU to the accelerator or coprocessor)

Intel Xeon Phi – 2nd generation Knights Landing (KNL)



3+ TeraFlops Double Preci

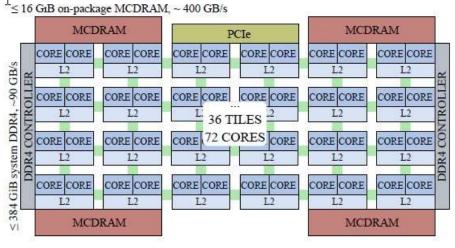
72 cores, 1.5 GHz

~ 245 Watt power Power efficient (25%) 5x Memory bandwidth (DDR5)



Xeon Phi 2nd generation - KNL

- 72 cores (new Atom based)
- Tile structure (36)
 - 2 cores
 - L2 cache shared 2 cores
- Improved cache organization
 - => complexity in chip HW



- High Bandwidth Memory (HBM)
 - MCDRAM (multi-Channel DRAM)

What applications run best on KNL? 1

- Having high degree of parallelism & wellbehaved communication with memory.
 Specifically,
- If memory traffic is negligible compared to the processing of arithmetic, the application is computebound
 - may run well on KNL due to its high arithmetic peak performance

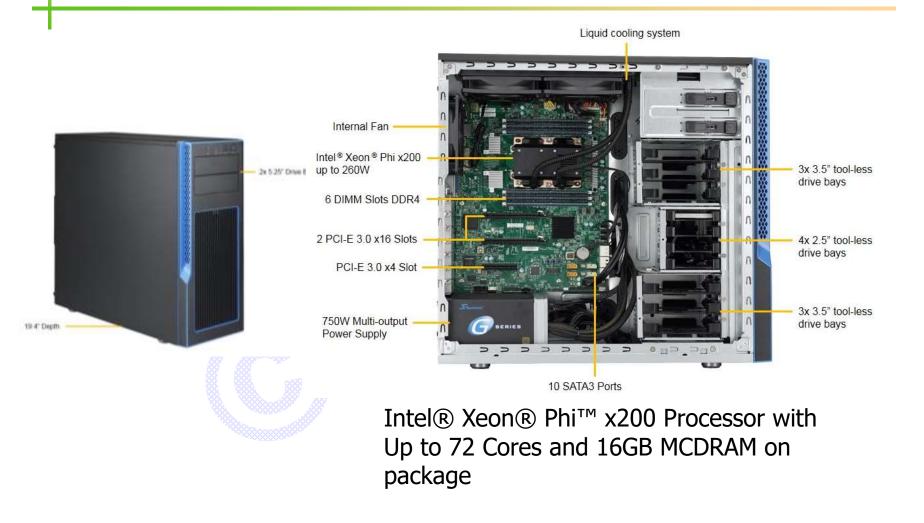
What applications run best on KNL? 2

- If memory access has predictable, sequential pattern, the application is bandwidth-bound
 - run well on KNL due to its high-bandwidth memory (HBM)

What applications run best on KNL? 3

- Application, neither compute-bound, nor bandwidth-bound because it has significant irregular memory access pattern, it belongs to the class of latencybound applications
 - 1st generation Xeon PhiKnights Corner (KNC), performed poorly compared to Intel Xeon
 - KNL, improvements in cache organization reduce the impact of latency-bound operations

Workstation with KNL



Super Workstation SYS-5038K-I with KNL

How many GPU/ Xeon Phi can be put in a server?

- PCIe slots available on the server ?
- Power supply rating ?
- Power connectors provided by the power supply
- Server must provide enough physical clearance for the cards and the power connectors









Server nodes with multiple GPU & Xeon-Phi

SuperServer 1028GQ-TRT with 4 GPU cards





- Dual 10-core Intel[®] Xeon[®] E5-2600 v2 Series Processors
- Up to 512GB of DDR3 Memory
- Supports up to 8 Intel® Xeon Phi® coprocessors or 8 GPGPU cards utilizing proprietary PCIe switch



Features at a Glance

- Dual Intel® Xeon® Processor E5-2600 v3 Product Family
- Supports 8 GPU Graphics Cards in Dedicated PCle x16 Gen 3 slots
- Up to 1TB of DDR4 Memory
- Up to 8TB of SATA Storage
- Maximum 96 GPUs per BladeRack*

Each node
contains 16 GPU
cards in one 3U
enclosure cabled
to a server
through a PCIe
Gen3 X16
Connection

Active versus Passive cooling

Example: GPU



Passive

- No fan to take power
- No fan to get dusty
- No fan that can fail and destroy the card
- Quiet



- Active cooling gpu card are more powerful
- Better Performance than passive ones
- Runs continuously longer than the passive

Data Center Accelerators:



Optimizing Workloads

Intel Xeon Scalable Processors

for Visual Cloud

Visual Compute Accelerator (VCA): VCA2 from Intel

Graphics rendering & Media transcode

PCIe Gen3 add-in card, 235W TDP. 3 x Intel Xeon processors E3-1585L v5 Intel Iris Pro-graphics P580



Deep Learning/AI Accelerator: Intel Nervana platform with Neural Network processor

Network optimization

5G and other workloads



FPGA Based HW Accelerators



Approaches for Faster Solutions

- Large clusters
- Application tuning
- Latest processors Frequencies/Cores/Architectures...
- Change Algorithm to suite the FIXED hardware

....Reconfigurable Computing, a Novel Approach

for Speeding-up applications having

FLEXIBLE hardware

Reconfigurable Computing System

 Systems that dynamically modify their hardware for accelerating applications - Mainly based on FPGAs

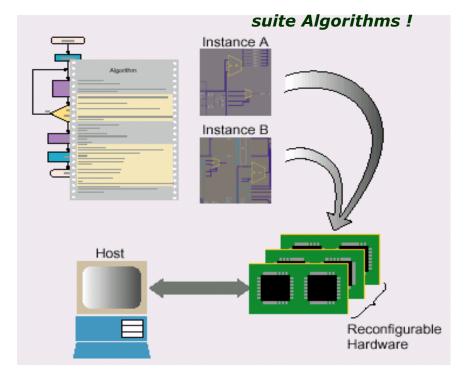
(Field Programmable Gate Array)

Fixed Instructions

Configurable

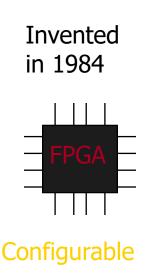
Fixed function

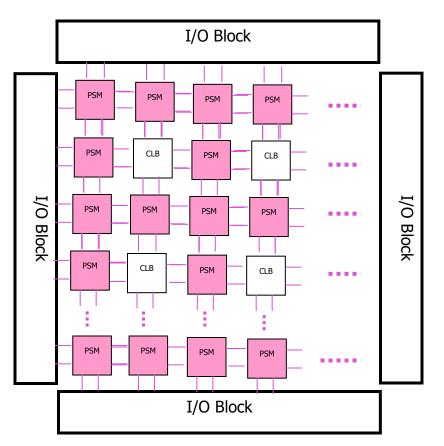




Field Programmable Gate Array (FPGA)

- A chip that can be configured by a user to implement different digital logic circuits
- Configurable Logic Blocks and interconnects

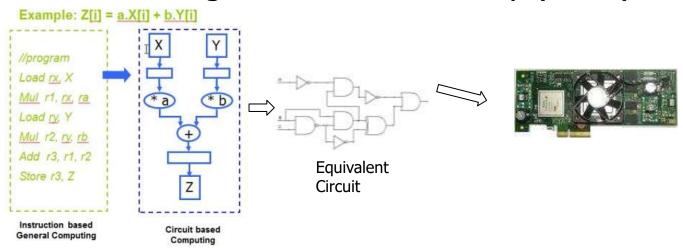




Reconfigurable Computing (RC): What is it?

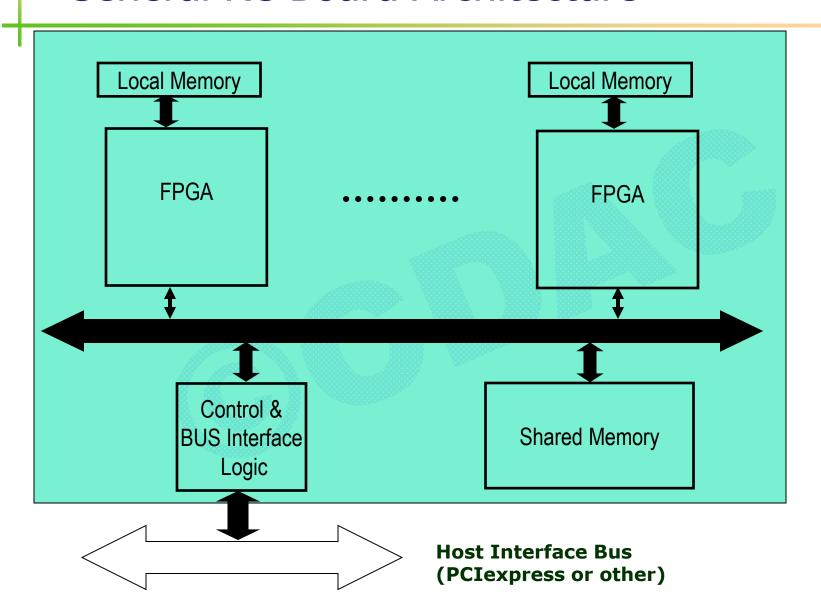
Highly Energy Efficient

- Implements Circuit corresponding to algorithm/ compute portion of application rather than executing instructions.
- Uses Field Programmable Gate Array (FPGA)

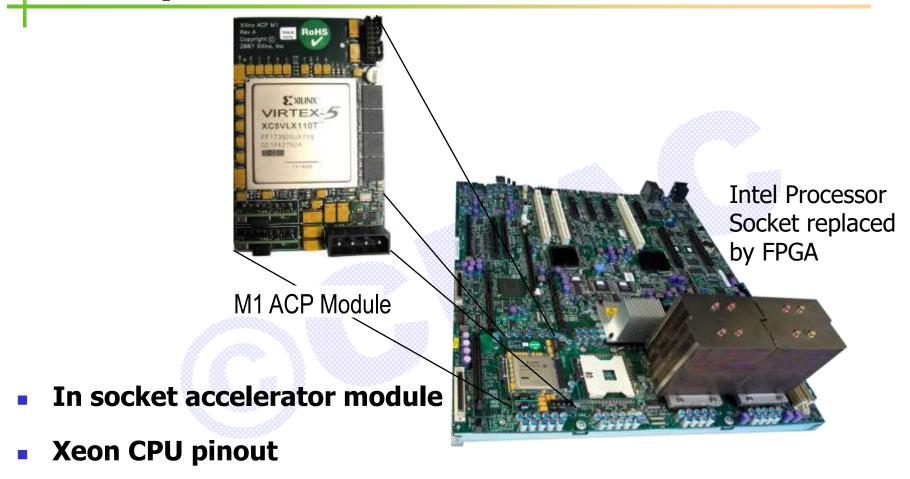


 It doesn't work on fixed data widths/ boundaries as the processors, rather the widths are *customized* as per the function, saving lot of power

General RC Board Architecture



FPGA on (intel) Server Socket: Example 1



Intel FSB bus interface (soft logic) inside FPGA

Acknowledgement: Xilinx

FPGA socket for AMD Opteron HT: Example 2



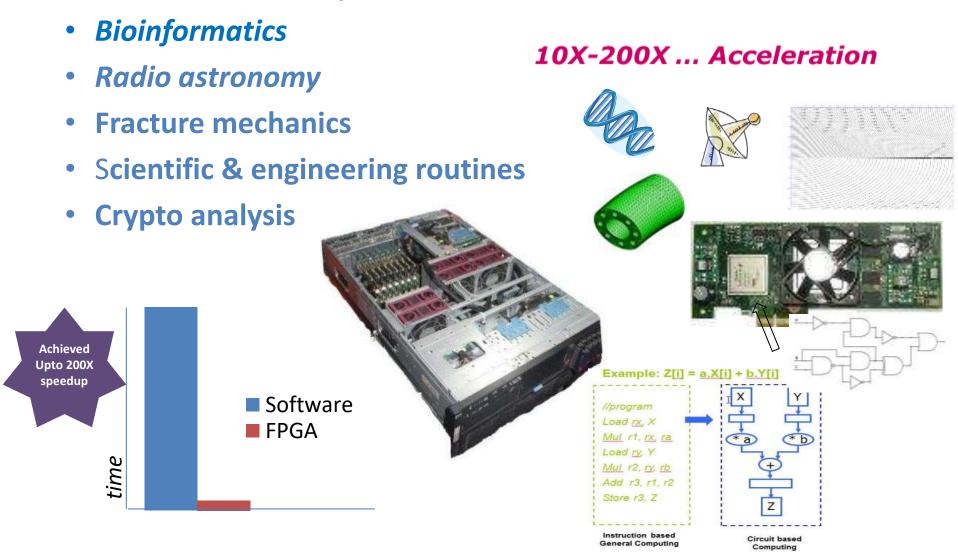
AMD Processor Socket Replaced by FPGA

- In socket FPGA based accelerator modules
- HyperTransport (HT) Socket interface
- Fits in AMD processor sockets

Acknowledgement: DRC

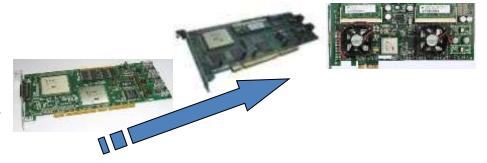
C-DAC FPGA based Reconfigurable HW Accelerators

Accelerated solution provided in various areas like

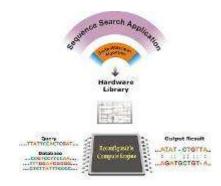


Design & Development of RC Solution Building Blocks

- RC hardware
 - -With state of the art FPGAs



- HW routines/libraries ('Avatars')
 - Application functions



- System Software ('VARADA')
 - APIs, Kernel Agent
 - Linux, Win 7 support



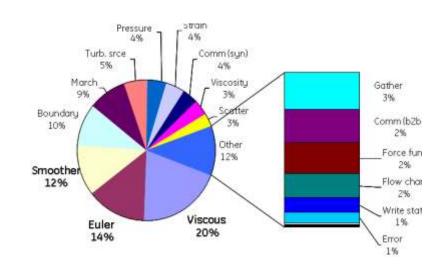
How FPGA gives Application Acceleration

Selecting suitable application

- Application/ Kernel profiling
 - Compute intensive functions
 - Inner loops run many times
- Analyze required precision
- SW/HW Partitioning



- Pipelined & Parallel
 - Hiding Computation & Communication latency
 - Many parallel blocks allows to overcome frequency limitation
- Analyze required HW resources
- High degree of Instruction efficiency



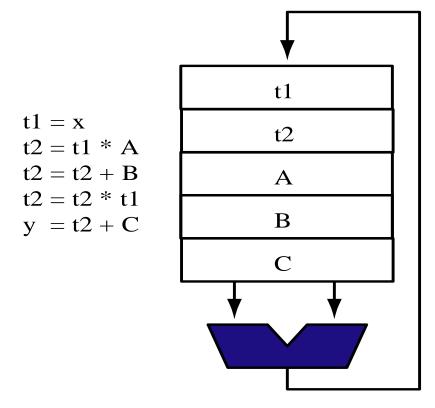
Spatial vs. Temporal Computation

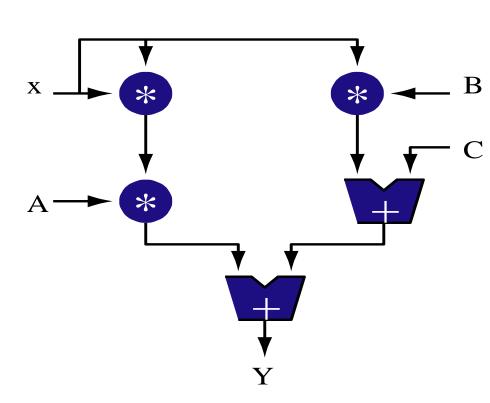
Processors divide computation across time, dedicated logic divides across space

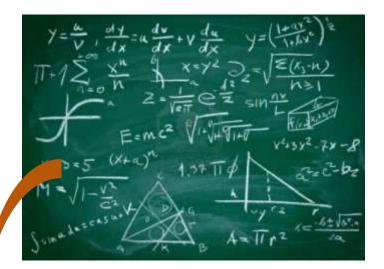
$$y = Ax^2 + Bx + C$$

Temporal Computation

Spatial Computation





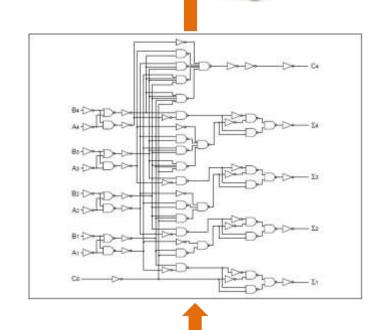


```
entity Test Counter VHDL is
   Port ( Clk xxxHz :
                               in std logic;
          Step Clk :
                               in std logic;
          Select Clk :
                               in std logic;
          Clr, Count Enable : in std logic;
          Bcd0,Bcd1,Bcd2,Bcd3 : out std logic vector(3 downto 0));
end Test_Counter_VHDL;
    itecture Behavioral of Test Counter VHDL is
     gnal Q: std_logic_vector( 15 downto 0);
      pal Clk: std logic;
   -- 2x1bit multiplexer: Clk_xxx or Step_Clk = [Btn0]
  Clk <= Clk xxxHz when Select Clk='1' else
         Step Clk;
                    ware....
        if Count_Enable='1' then

Q <= Q+1;

ENSTE
   Bcd3 <= Q(15 downto 12);
end Behavioral;
```

Design Flow

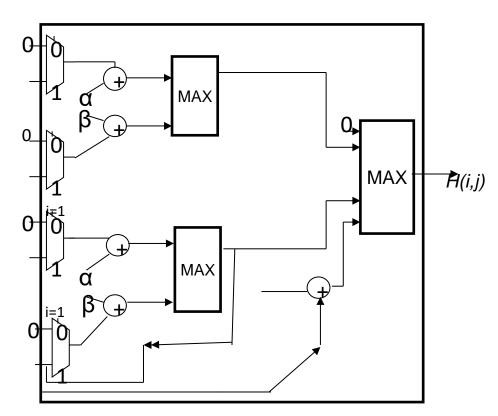


•	■ Wave :=====										77777	:====
	Messages											
	→ /test_adder/clk	0										
I	→ /test_adder/inA	01	00	, 01		05		02		03		01
Ш	→ /test_adder/inB	08	00	,01		06		02				08
l	→ /test_adder/out	09			-00		02		(Ob		04	
l	→ /test_adder/isOdd	1					Н					
l												
l												
ı												

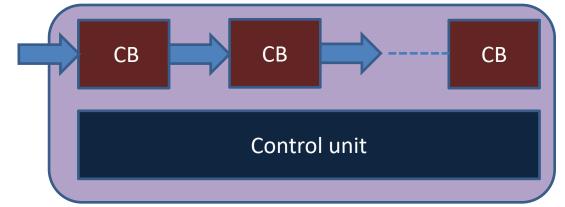
Example flow

$$H(i,j) = \max \begin{cases} 0 \\ H(i-1,j-1) + s(a_i,b_j) & \text{Match/Mismatch} \\ \max_{k \ge 1} \{H(i-k,j) + W_k\} & \text{Deletion} \\ \max_{l \ge 1} \{H(i,j-l) + W_l\} & \text{Insertion} \end{cases},$$

Equations



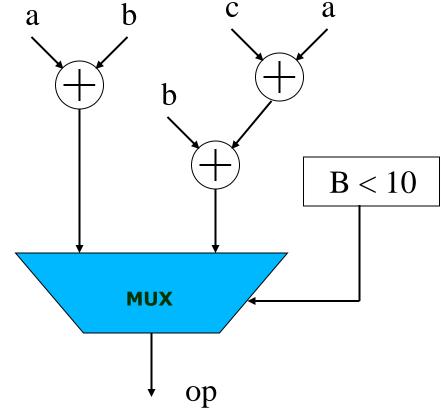
Compute Block (CB)



compute Block Array

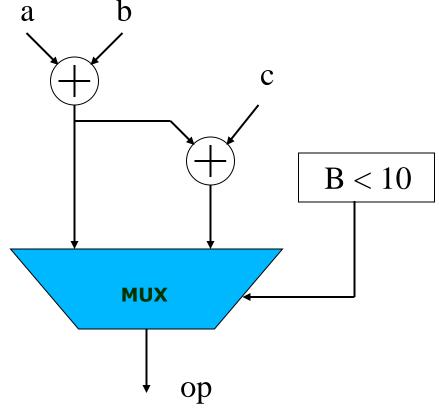
Coding Style Impact: Hardware Inference

```
entity test is
port (
  a, b, c : in std_logic_vector(5 downto 0);
     op : out std_logic_vector(5 downto 0)
end entity test;
architecture test_a of test is
begin
    if(b < "001010")then
       op <= a + b;
    else
       op \le c + a + b
    end if:
end architecture test a:
```



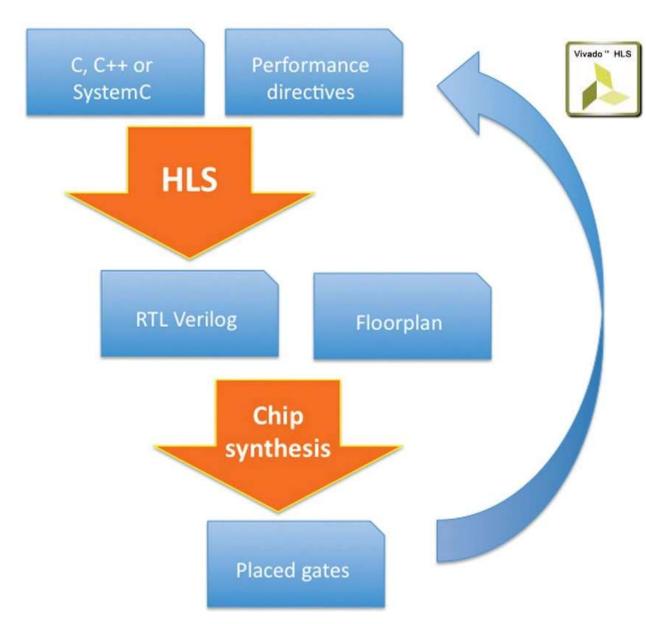
Coding Style Impact: Hardware Inference

```
entity test is
port (
  a, b, c : in std_logic_vector(5 downto 0);
     op : out std_logic_vector(5 downto 0)
end entity test;
architecture test_a of test is
begin
    if(b < "001010")then
       op <= a + b;
    else
       op \le c + (a + b);
    end if:
end architecture test a;
```



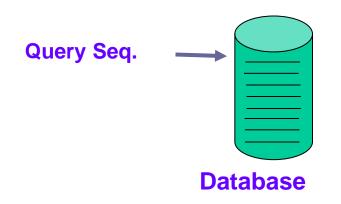
High Level Synthesis (HLS)





Application: Sequence Similarity Search

 Comparing a query sequence against a database of known sequences - "a routine work for advancement in medical science".



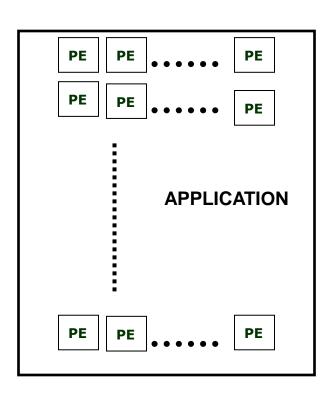
 Searching queries over large databases takes hours to days and requires high-end servers or clusters.

Sequence Search on FPGA

Multiple Parallel

Execution units in

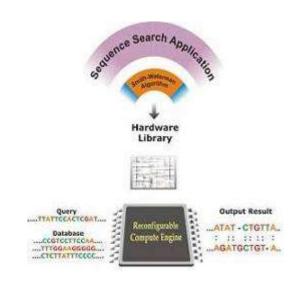
FPGA for performance



Performance

Example: RC for Accelerating Sequence search

Bioinformatics Sequence search taking <u>528 days</u> using pure software solution was completed in just <u>12 days</u> by C-DAC's RC!



[what one of our customer has to say...]

"C-DAC's Reconfigurable Hardware Accelerator has helped us to achieve high scalability and reliability in our Microarray probe, Primer design business...

Thanks C-DAC for being a great partner in our endeavour to become world number one in genomic outsourcing."

...90x acceleration

C-DAC Reconfigurable Computing Accelerator in Clustered Environment

- RC further increasing the compute power of supercomputing Clusters
- Accelerating MPI based applications
- 88% saving of power





Highly space efficient

1 RC card just 25W

Advantages of FPGA Accelerator



Customized logic, allows to execute implemented operations in parallel



No fixed data widths/ boundaries as present in processors, rather the widths are customized as per the function, saving lot of power



Space Efficient

Compact in Size
Cooling infrastructure
not required due to
low power
consumption

PCIe based cards from Xilinx





Ack: Xilinx
ALVEO U280 Data Center
accelerator card

Useful for Data Analytics, High Frequency Trading, ML Inference applications

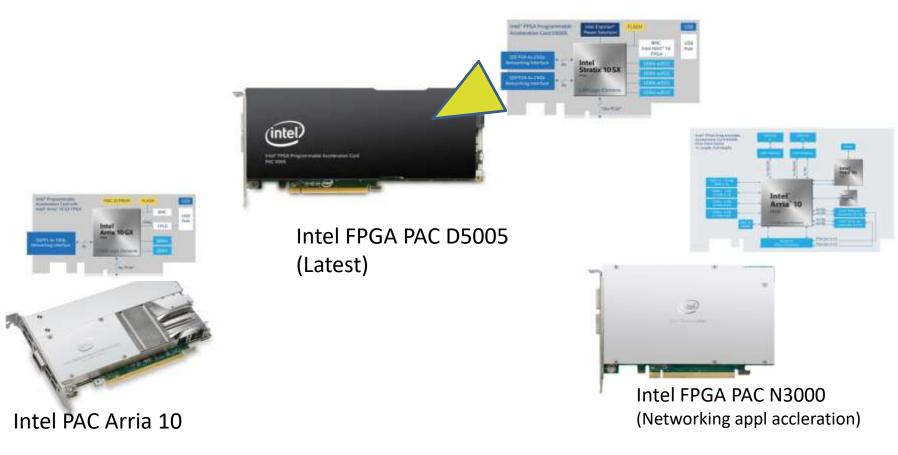
Full height, dual slot, ¾ length (passive cooling) or full length (active cooling) form factor.

PCI Express® Gen3 x16 or Gen4 x8, 8 GB High-Bandwidth Memory (HBM2), 16 GB DDR4 @ 2400 MT/s,

Two QSFP Ethernet ports capable of 100 Gb/s each. 225W

Accelerate memory-bound, compute-intensive applications

Intel FPGA Accelerators



Big data analytics, artificial intelligence, genomics, video transcoding, cybersecurity, and financial trading.

Ack: Intel

Intel SoC FPGAs



F-Series

- Increased DSP capabilities
- Quad-core integration option
- Upto 58 Gbps transceiver

I-Series

- Optimized for High performance Processor Interface
- PCleGen5; 112 Gbps transceiver

Memory appls Memory appls

- Optimized for Compute &
- DDR5 controller...

Useful for Data Center, Networking, Edge

Ack: Intel

- Applications with massive interface bandwidth & High performance
- Data-intensive applications- Massive memory + high bandwidth

Summary

- Accelerators are an important ingredient of HPC, providing performance, energy efficiency and small rack-space.
- KNL designed to take care of many drawbacks of earlier Xeon Phi (KNC)
 Discontinued by Intel June'18
- FPGA based reconfigurable accelerators are most energy efficient compared to other accelerator technologies.

Thank You

"....paving the path for building such systems to tackle

additional, unsolved important scientific problems"