

Accelerating Scientific Machine Learning with AI Accelerators

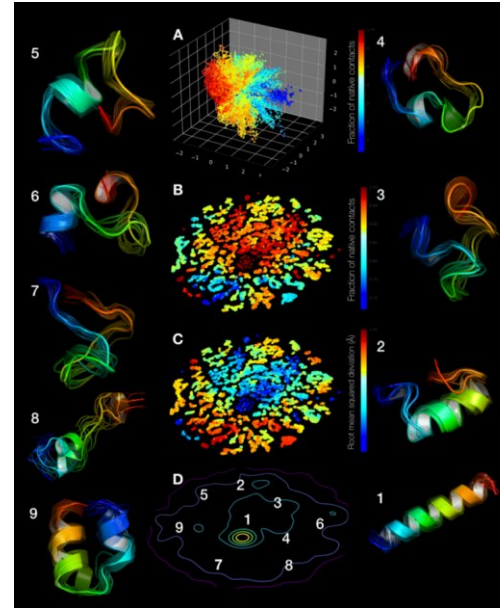
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ARGONNE TRAINING PROGRAM ON EXTREME-SCALE COMPUTING (ATPESC)
July 31, 2023

Surge of Scientific Machine Learning

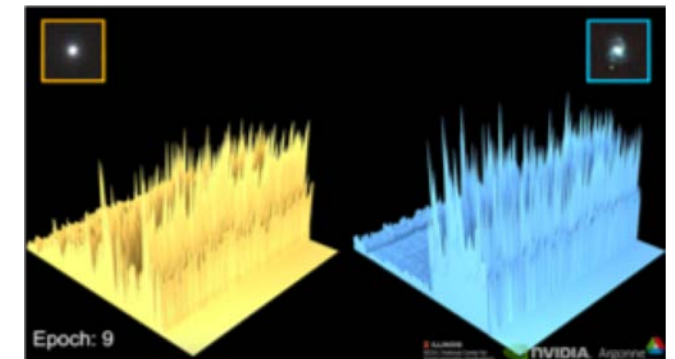
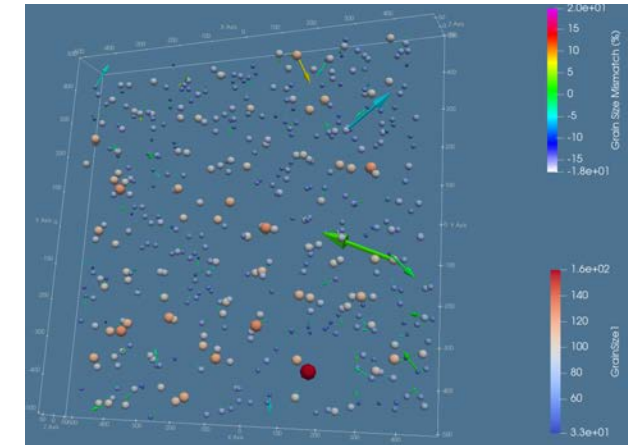
- Simulations/ surrogate models
 - Replace, in part, or guide simulations with AI-driven surrogate models
- Data-driven models
 - Use data to build models without simulations
- Co-design of experiments
 - AI-driven experiments

Design infrastructure to facilitate and accelerate AI for Science (AI4S) applications



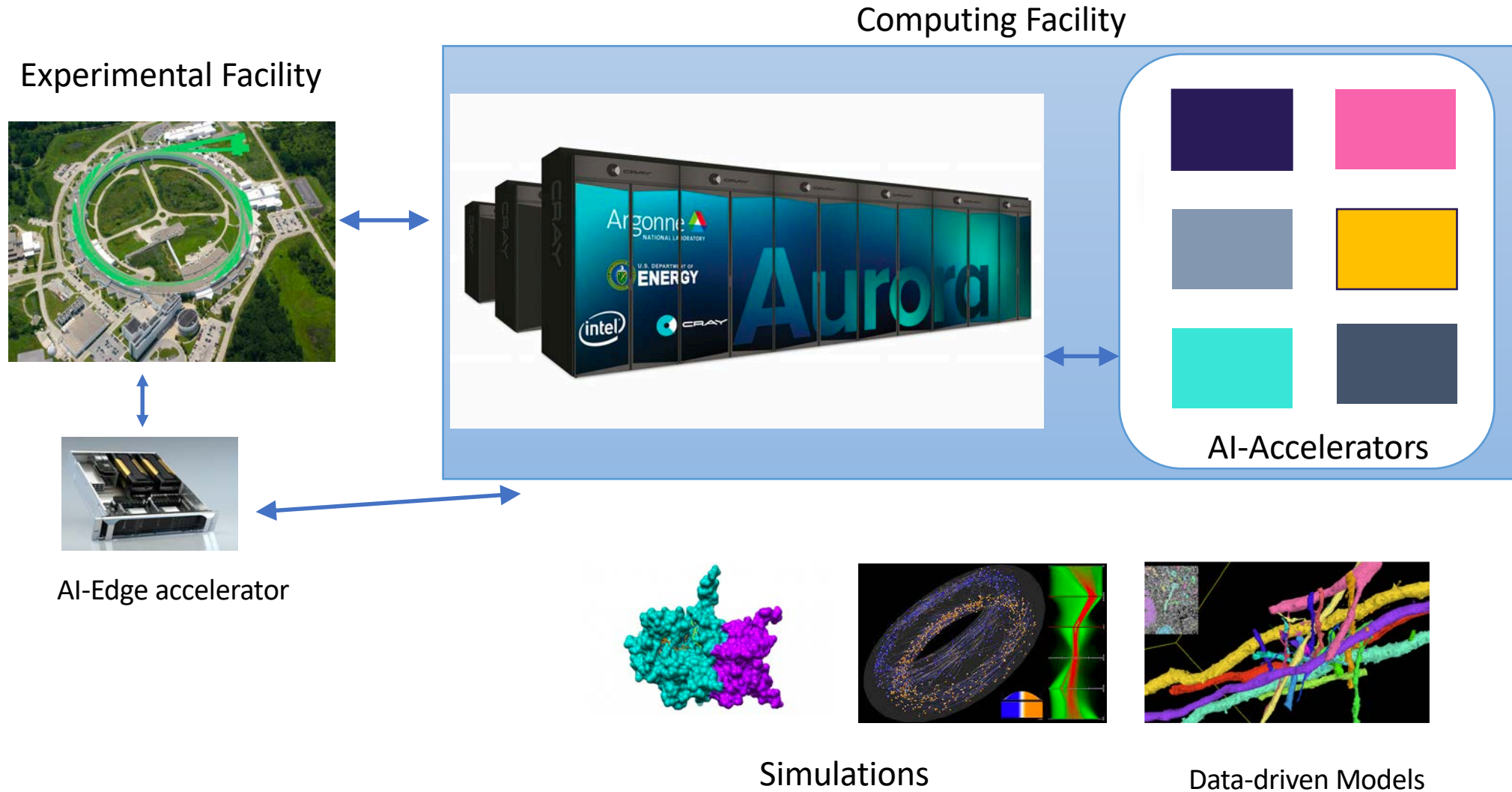
Protein-folding

Braggs Peak



Galaxy Classification

Integrating AI Systems in Facilities



ALCF AI Testbed

<https://www.alcf.anl.gov/alcf-ai-testbed>



Cerebras CS-2



SambaNova DataScale
SN30



Graphcore
Bow Pod64



Habana
Gaudi1



GroqRack

- Infrastructure of next-generation machines with AI hardware accelerators
- Provide a platform to evaluate usability and performance of AI4S applications
- Understand how to integrate AI systems with supercomputers to accelerate science

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GroqRack

- Cerebras: 2 CS-2 nodes, each with 850,000 Cores, compute-intensive models
- SambaNova: DataScale SN30 8 nodes (8 SN30 RDUs per node) - 1TB mem per device, models with large memory footprint
- Graphcore: Bow Pod64 4 nodes (16 IPU's per node) - MIMD, irregular workloads such as graph neural networks
- GroqRack: 8 nodes, 8 GroqNodes per node - inference at batch 1
- Habana Gaudi1: 2 nodes, 8 cards per node - On-chip integration of RDMA over Converged Ethernet (RoCE2), scale-out efficiency

Getting Started on ALCF AI Testbed:

Apply for a Director's Discretionary (DD) Allocation Award

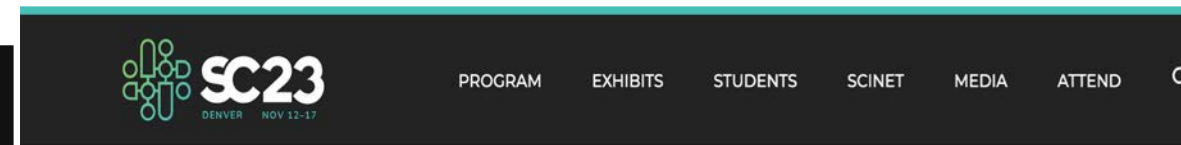
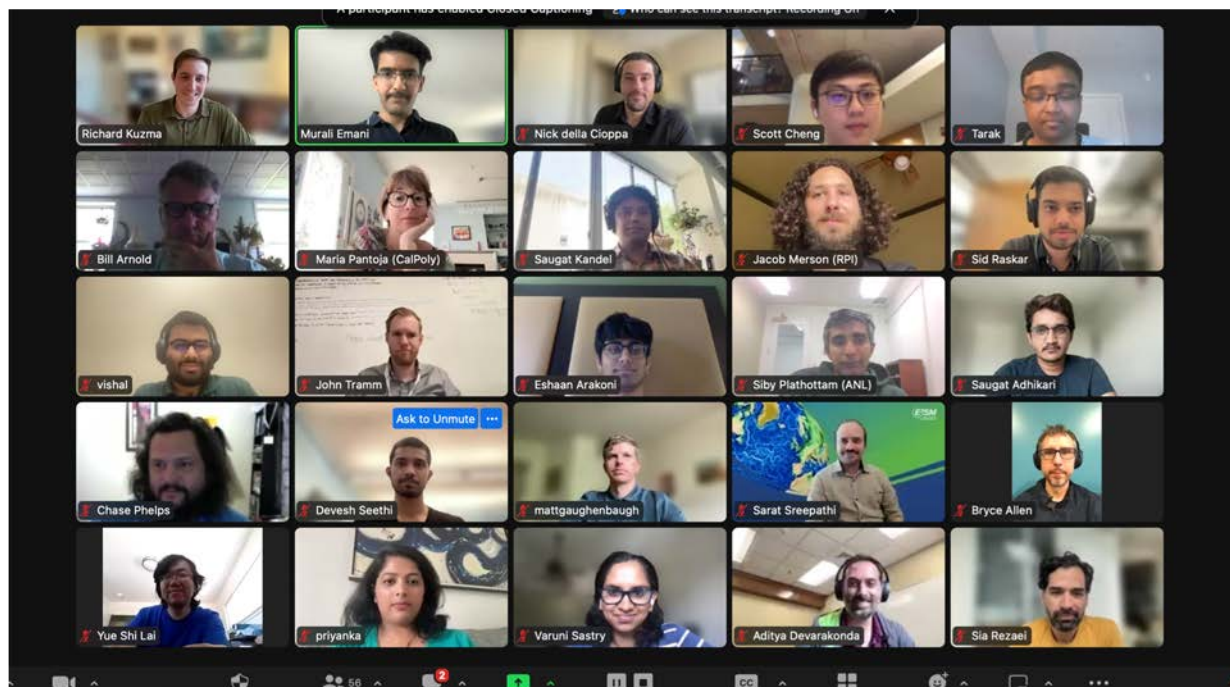
Director's Discretionary (DD) awards support various project objectives from scaling code to preparing for future computing competition to production scientific computing in support of strategic partnerships.

Cerebras CS-2, SambaNova Datascale SN30 and Graphcore Bow Pod64 are available for allocations

[Allocation Request Form](#)

[AI Testbed User Guide](#)

AI Testbed Community Engagement



Presentation

Programming Novel AI Accelerators for Scientific Computing

Scientific applications are increasingly adopting Artificial Intelligence (AI) techniques to advance science. There are specialized hardware accelerators designed and built to run AI applications efficiently. With a wide diversity in the hardware architectures and software stacks of these systems, it is challenging to understand the differences between these accelerators, their capabilities, programming approaches, and how they perform, particularly for scientific applications. In this tutorial, we will cover an overview of the AI accelerators landscape with a focus on SambaNova, Cerebras, Graphcore, Groq, and Habana systems along with architectural features and details of their software stacks. We will have hands-on exercises that will help attendees understand how to program these systems by learning how to refactor codes written in standard AI framework implementations and compile and run the models on these systems. The tutorial will enable the attendees with an understanding of the key capabilities of emerging AI accelerators and their performance implications for scientific applications.

Tutorial

Sunday, 12 November 2023
8:30am - 12pm MST

Location: 203

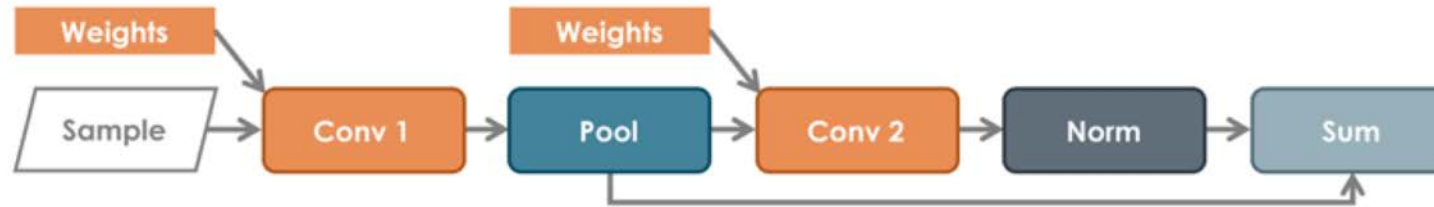
NEXT PRESENTATION > STARTS IN 106:07:40

Energy-Efficient GPU Computing

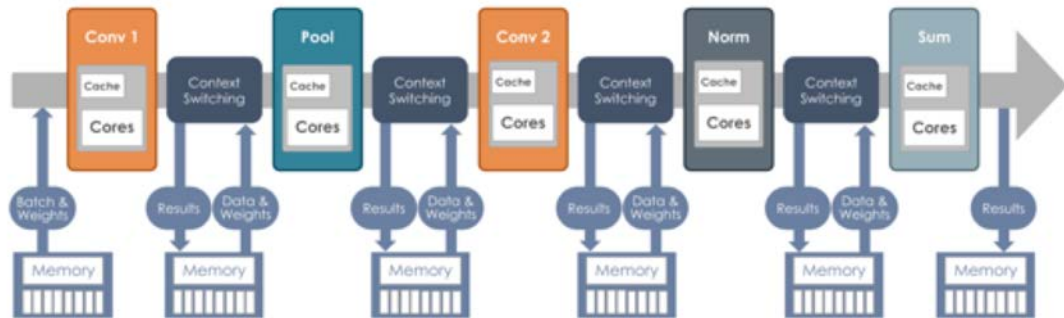
- AI training workshops
 - Cerebras: <https://events.cels.anl.gov/event/420/>
 - SambaNova: <https://events.cels.anl.gov/event/421/>
 - Graphcore: <https://events.cels.anl.gov/event/422/>

Tutorial at SC23 on Programming Novel AI accelerators for Scientific Computing *in collaboration with Cerebras, Intel Habana, Graphcore, Groq and SambaNova*

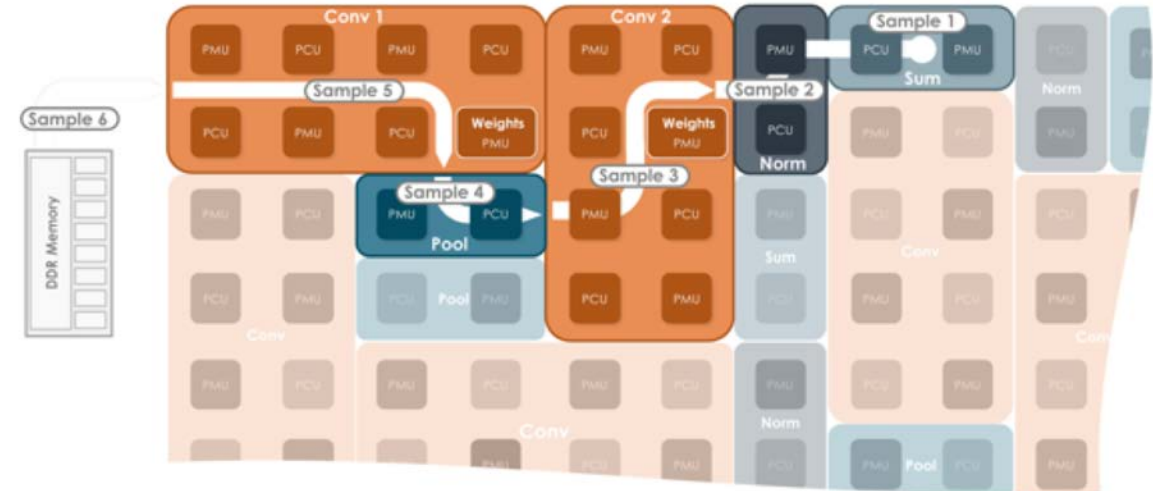
Dataflow Architectures



Simple Convolution Graph



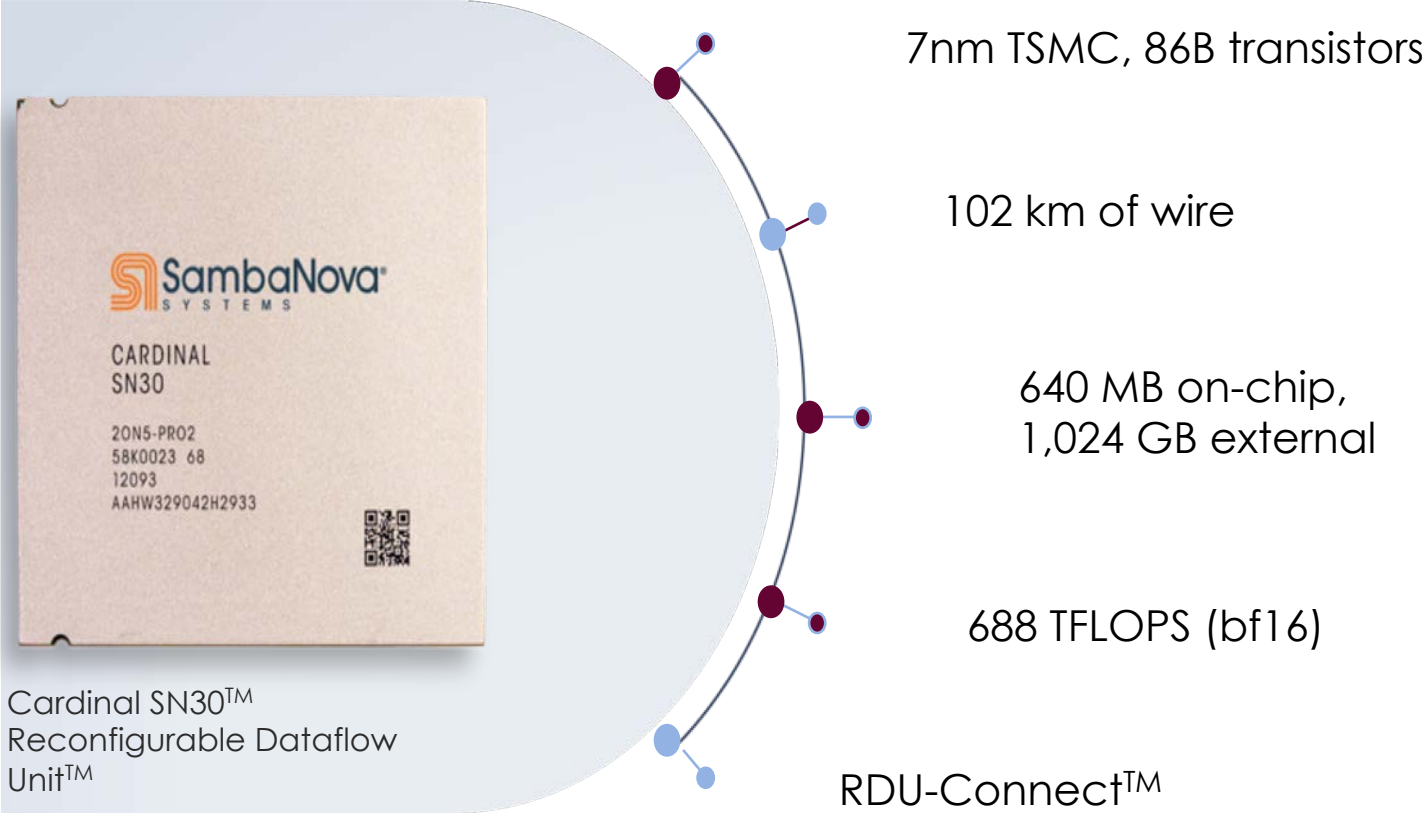
The old way: kernel-by-kernel
Bottlenecked by memory bandwidth
and host overhead



The Dataflow way: Spatial
Eliminates memory traffic and overhead

Image Courtesy: SambaNova

SambaNova Cardinal SN30 RDU



as-a-SERVICE
Pre-trained
Foundation Models

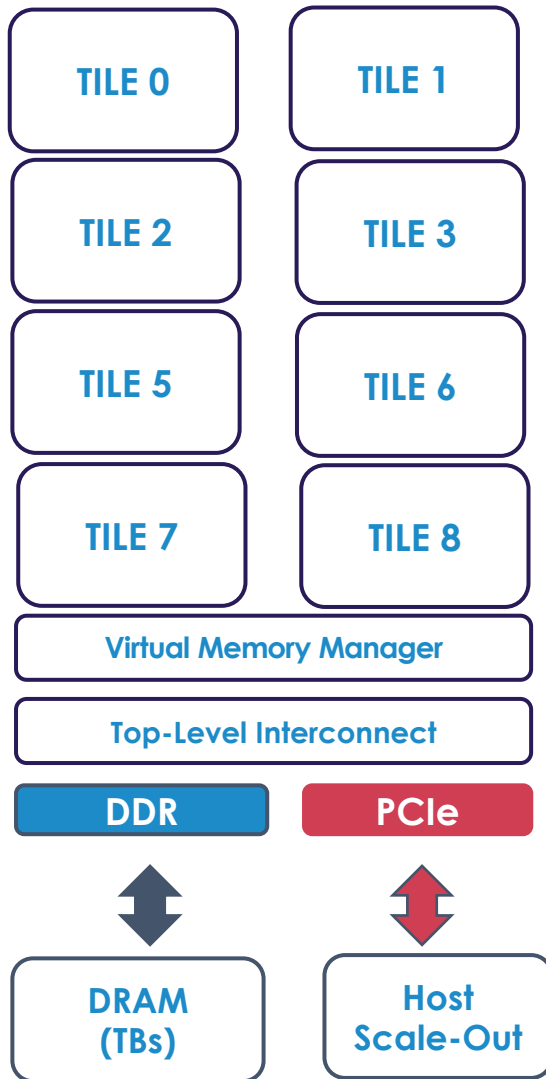
SYSTEMS
DataScale®

SOFTWARE
SambaFlow™

SILICON
RDU

Image Courtesy: SambaNova

Cardinal SN30: Chip and Architecture Overview



- RDU broken up into 8-tiles
 - 160 PMU and PCUs per tile
 - Additional sub-components like coalescing units (CU) for connectivity to other tiles and off-chip components, switches to set up communication between PMU, PCUs, and CU
- Tile resource management: Combined or independent mode
 - Combined: Combine adjacent to form a larger logical tile for one application
 - Independent: Each tile controlled independently, allows running different applications on separate tiles concurrently.
- Direct access to TBs of DDR4 off-chip memory
- Memory-mapped access to host memory
- Scale-out communication support

Image Courtesy: SambaNova

Cardinal SN30: Tile

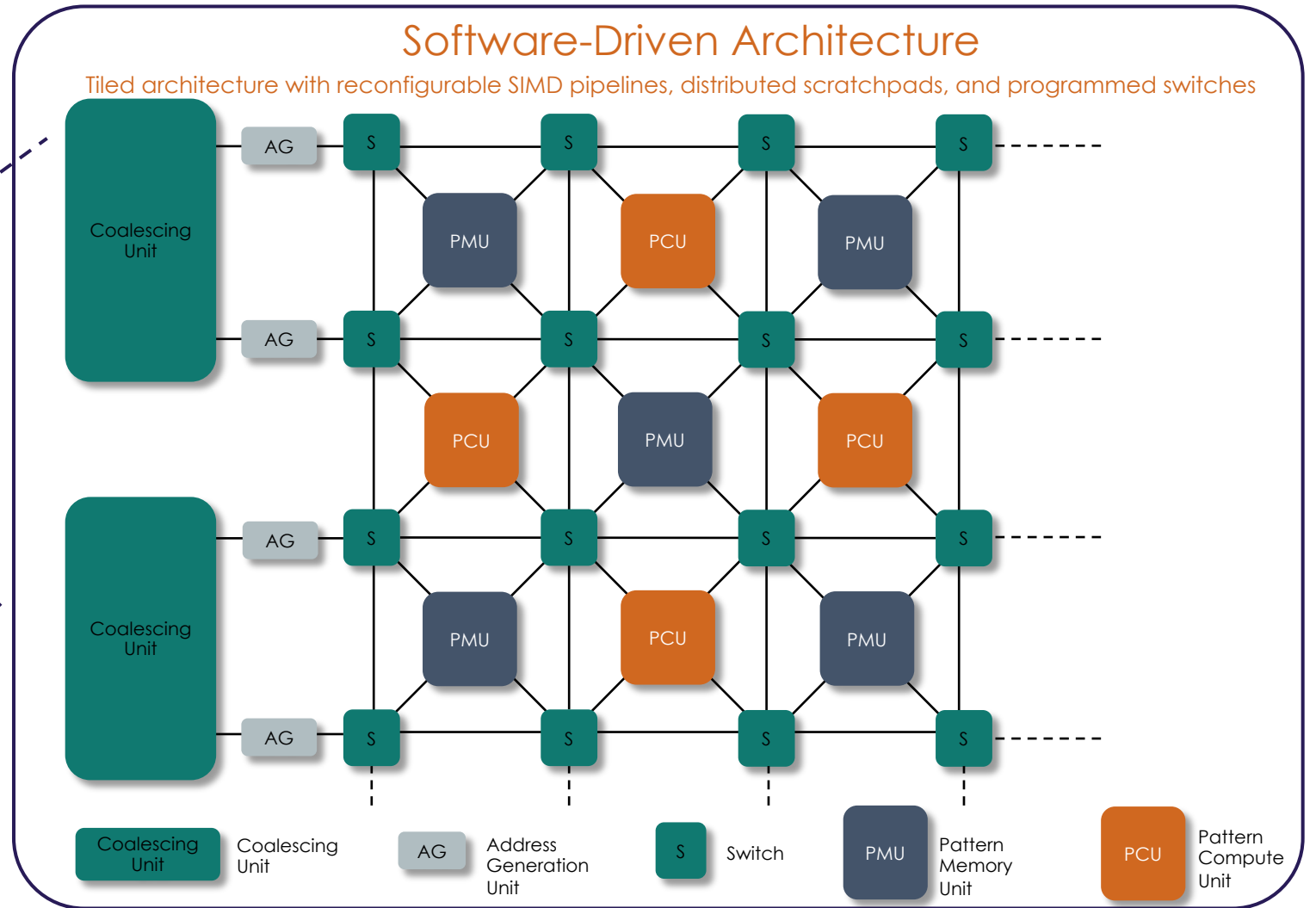
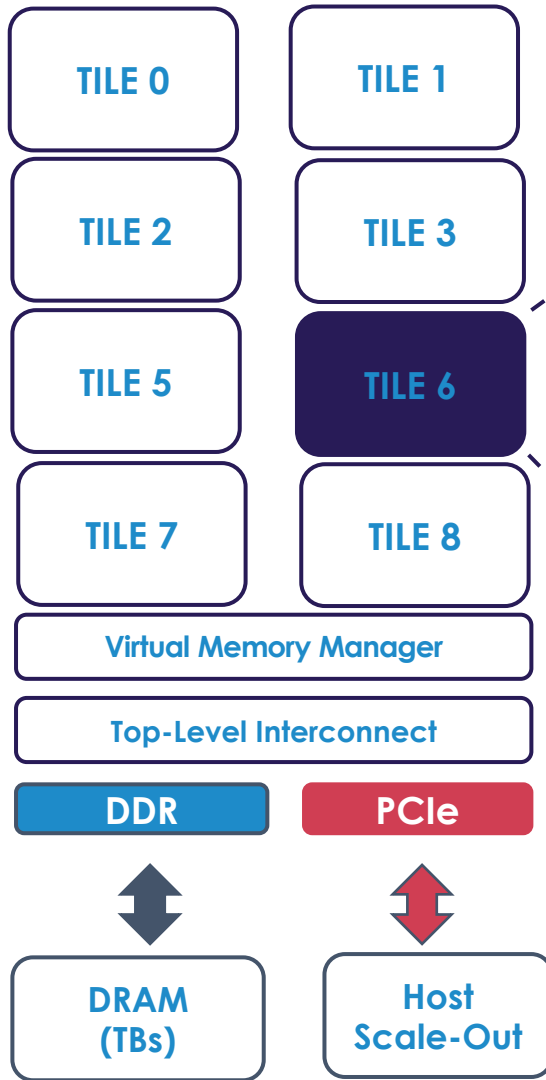


Image Courtesy: SambaNova

Dataflow Architecture for Terabyte Sized Models

Dataflow Efficiency

+

Compute Capability

+

Large Memory Capacity



DataScale SN30-8R

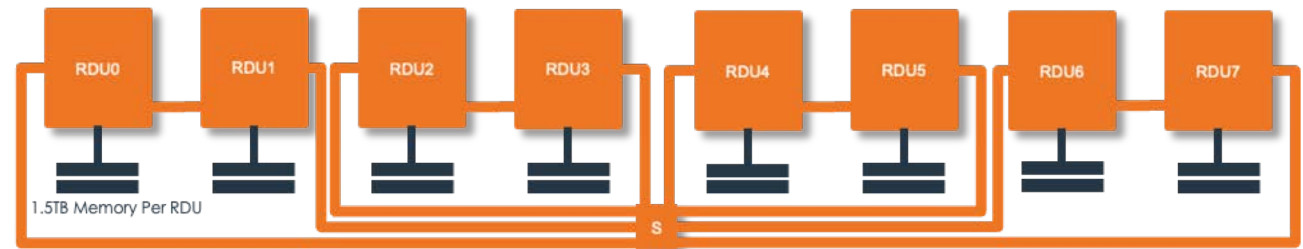
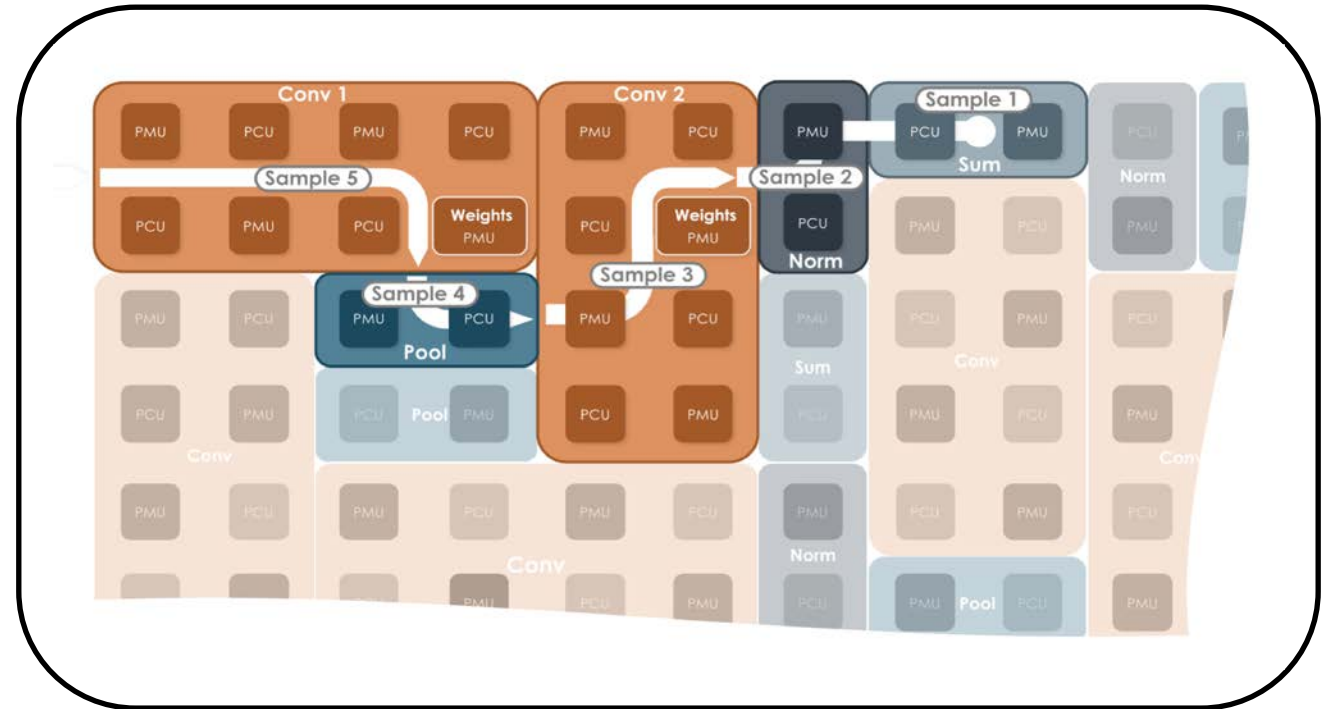


Image Courtesy: SambaNova

SambaNova DataScale SN30-8 System



- 8 x Cardinal SN30 Reconfigurable Dataflow Unit
- 8 TB total memory (using 64 x 128 GB DDR4 DIMMs)
- 6 x 3.8 TB NVMe (22.8 TB total)
- PCIe Gen4 x16
- Host module

Image Courtesy: SambaNova

SambaNova Datascale SN30

<https://www.alcf.anl.gov/alcf-ai-testbed>



SambaNova Datascale SN30

- 4 Racks
- 8 nodes of SN30
- 8 RDUs or 4 XRDU's per node
- 8 Tiles per RDU
- Group of 4 tiles



SambaFlow Architecture

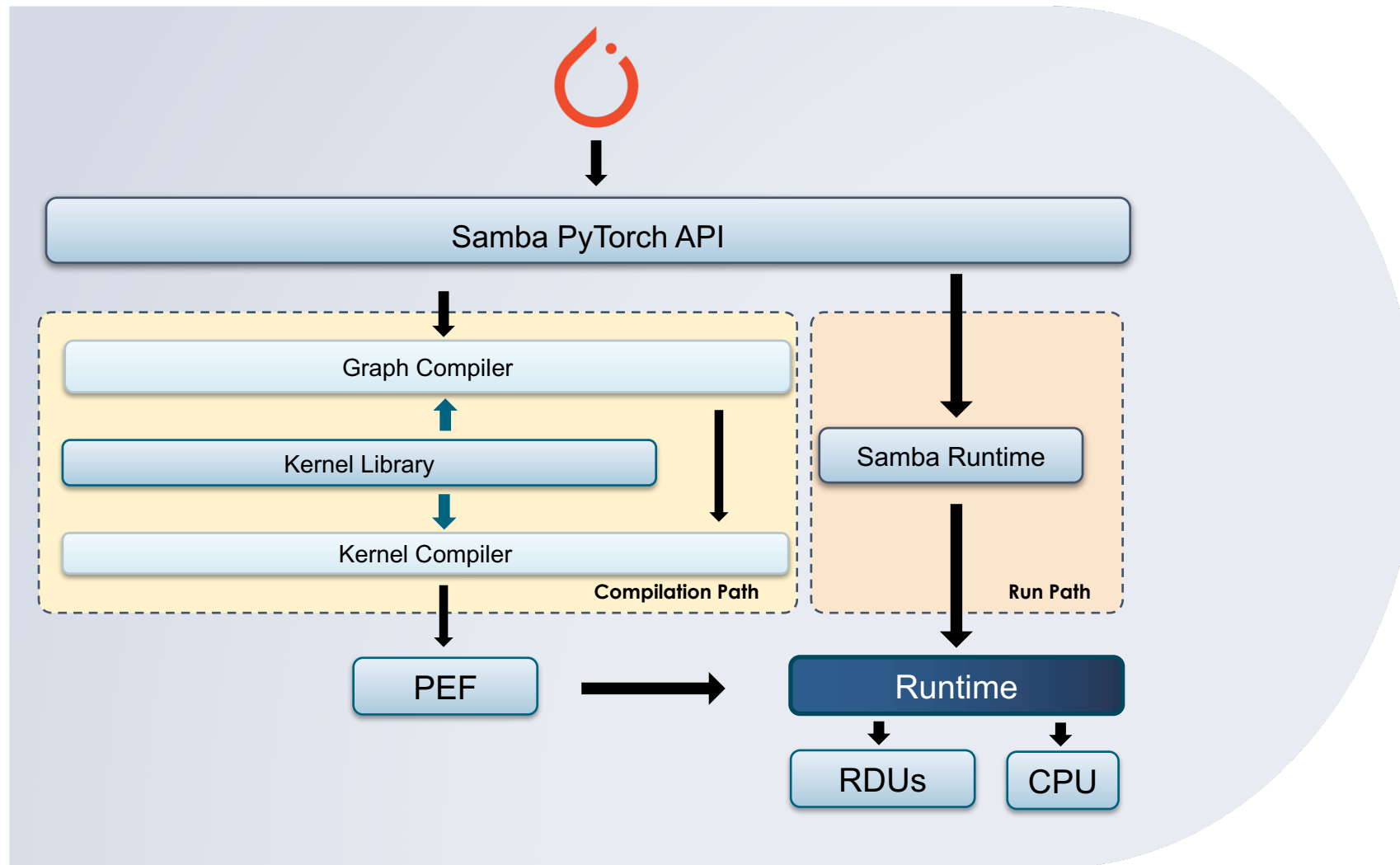


Image Courtesy: SambaNova

Cerebras Wafer-Scale Engine (WSE-2)

850,000 cores optimized for sparse linear algebra

46,225 mm² silicon

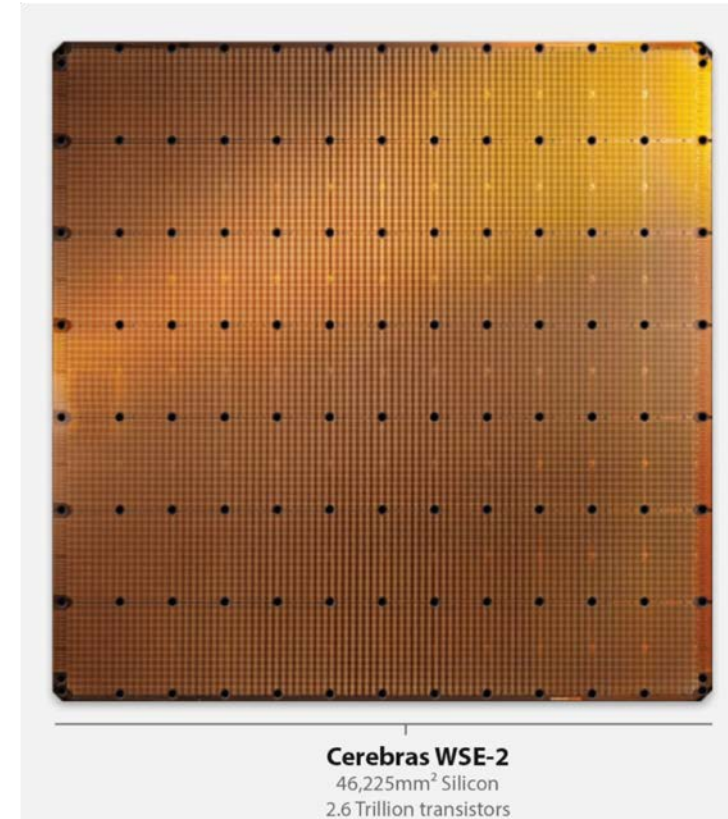
2.6 trillion transistors

40 gigabytes of on-chip memory

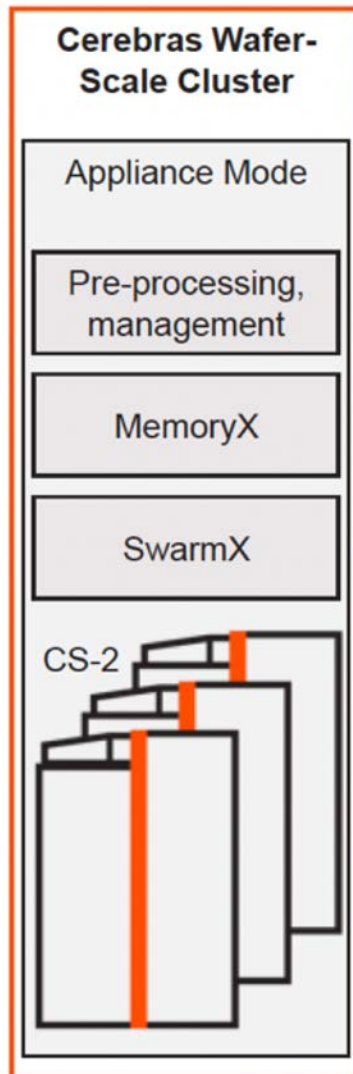
20 PByte/s memory bandwidth

220 Pbit/s fabric bandwidth

7nm process technology



Wafer-Scale Cluster



Input preprocessing servers stream training data

MemoryX - Stores and streams model's weights

SwarmX – weight broadcasts and gradient across multiple CS2s

Compilation (maps graph to kernels) Execution (training)

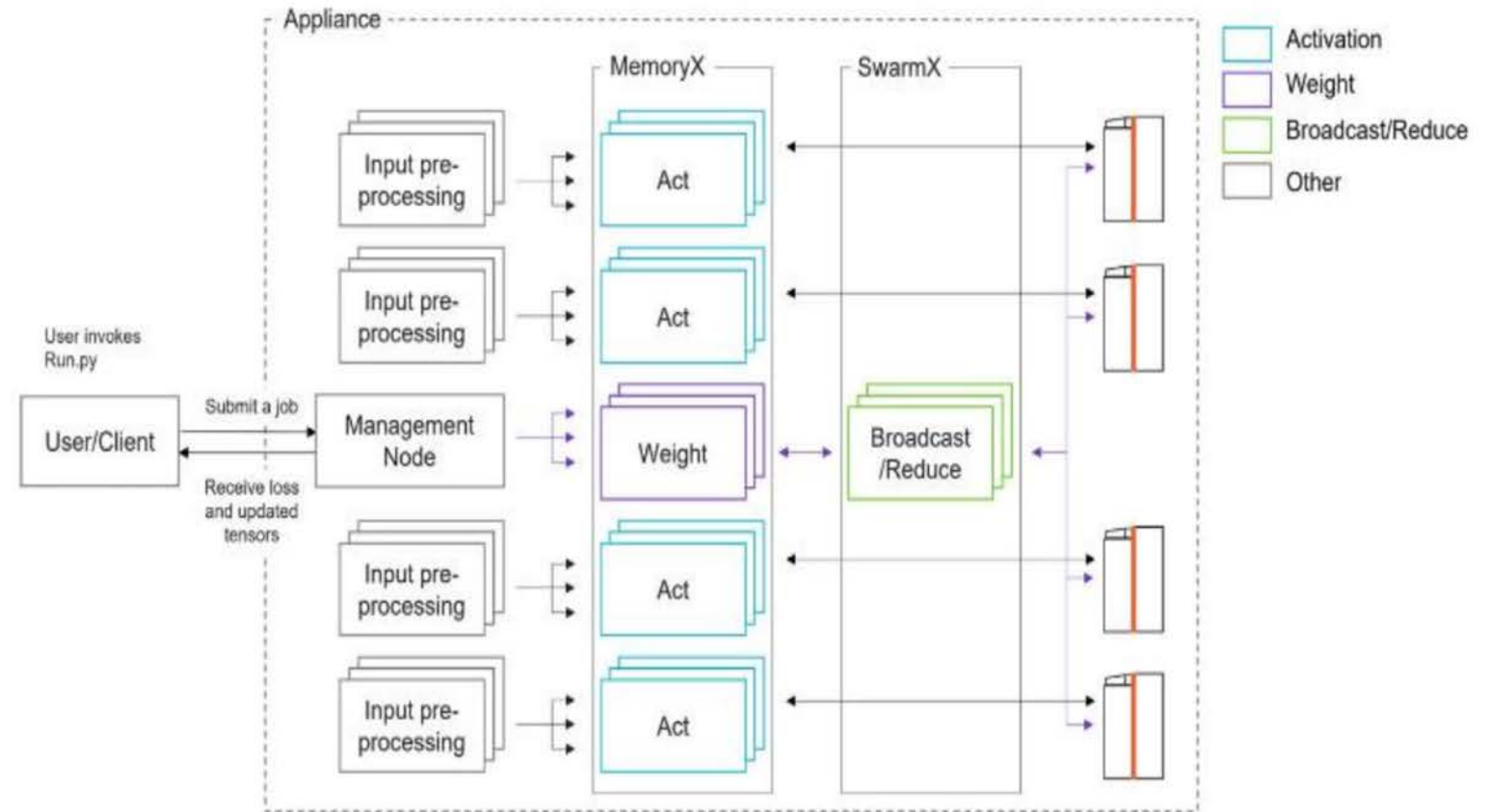
Image Courtesy: Cerebras

Cerebras CS-2 Cluster

<https://www.alcf.anl.gov/alcf-ai-testbed>

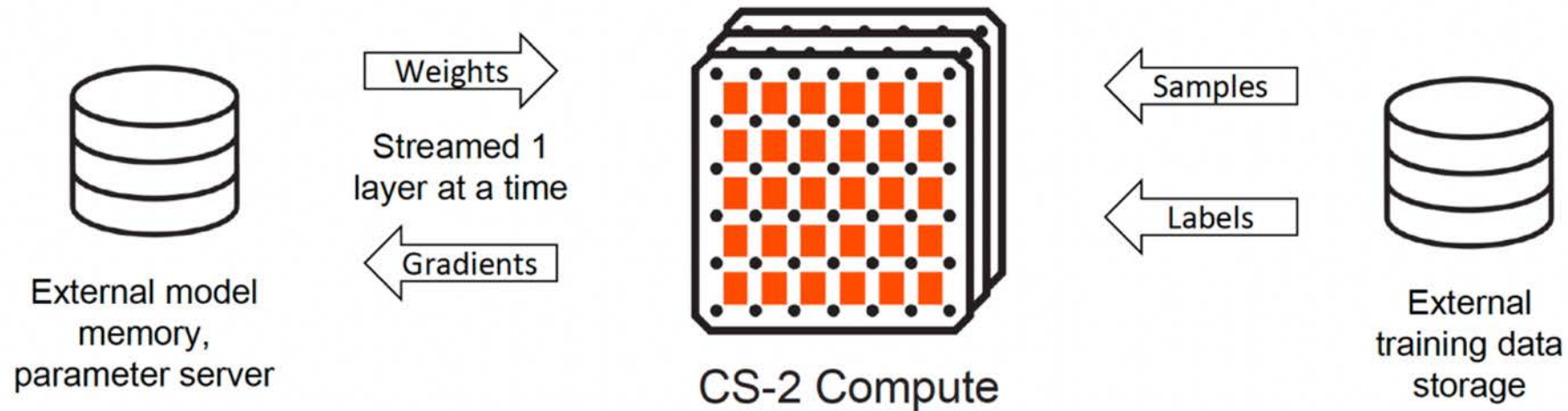
ALCF's CS-2 Cluster

- 2 CS-2 Appliances (each chip 46225 mm²)
- 1 Management node
- 16 Worker nodes
- 24 MemoryX nodes
- 6 SwarmX nodes
- 3 user login nodes



Topology of a Cerebras Wafer-Scale cluster

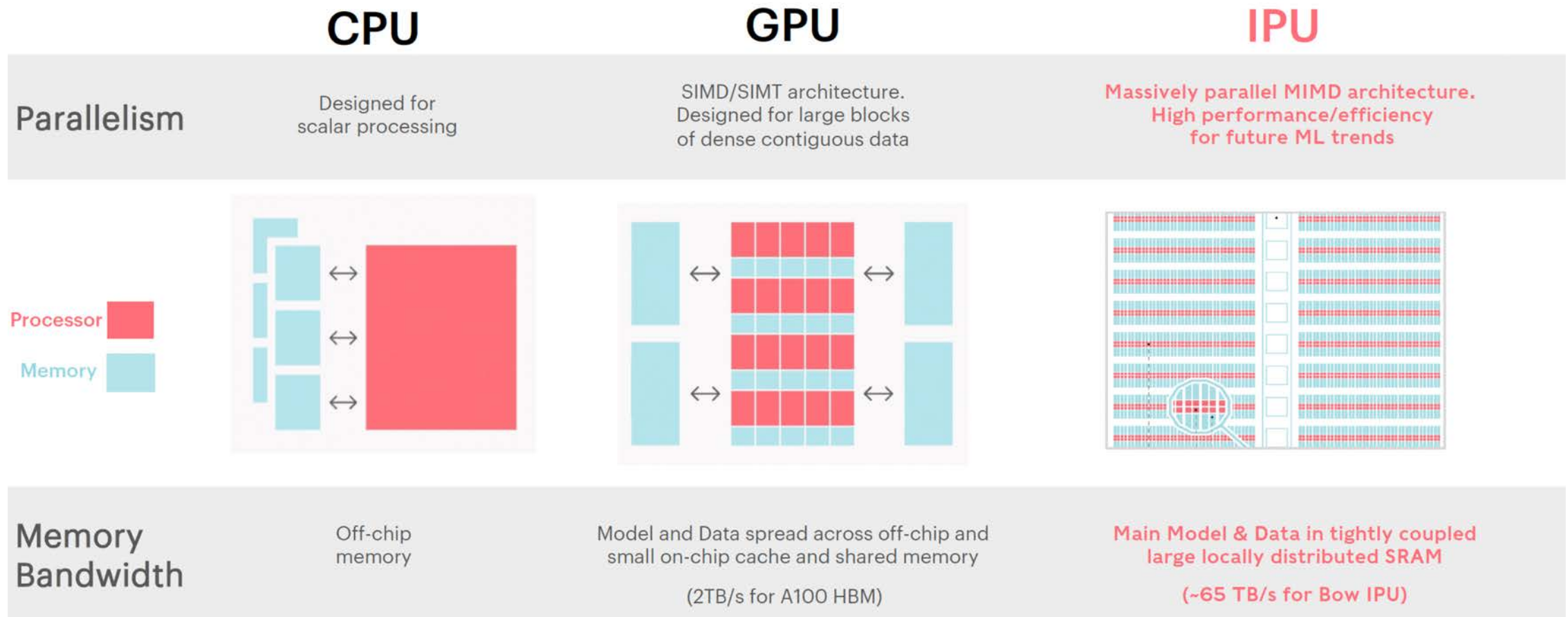
Cerebras Weight Streaming Technology



Disaggregate storage and compute
Enable scaling model size

Image Courtesy: Cerebras

Graphcore Intelligence Processing Unit (IPU)



Slide Courtesy: Graphcore

BOW IPU

IPU-Tiles™

1472 independent IPU-Tiles™ each with an IPU-Core™ and In-Processor-Memory™

IPU-Core™

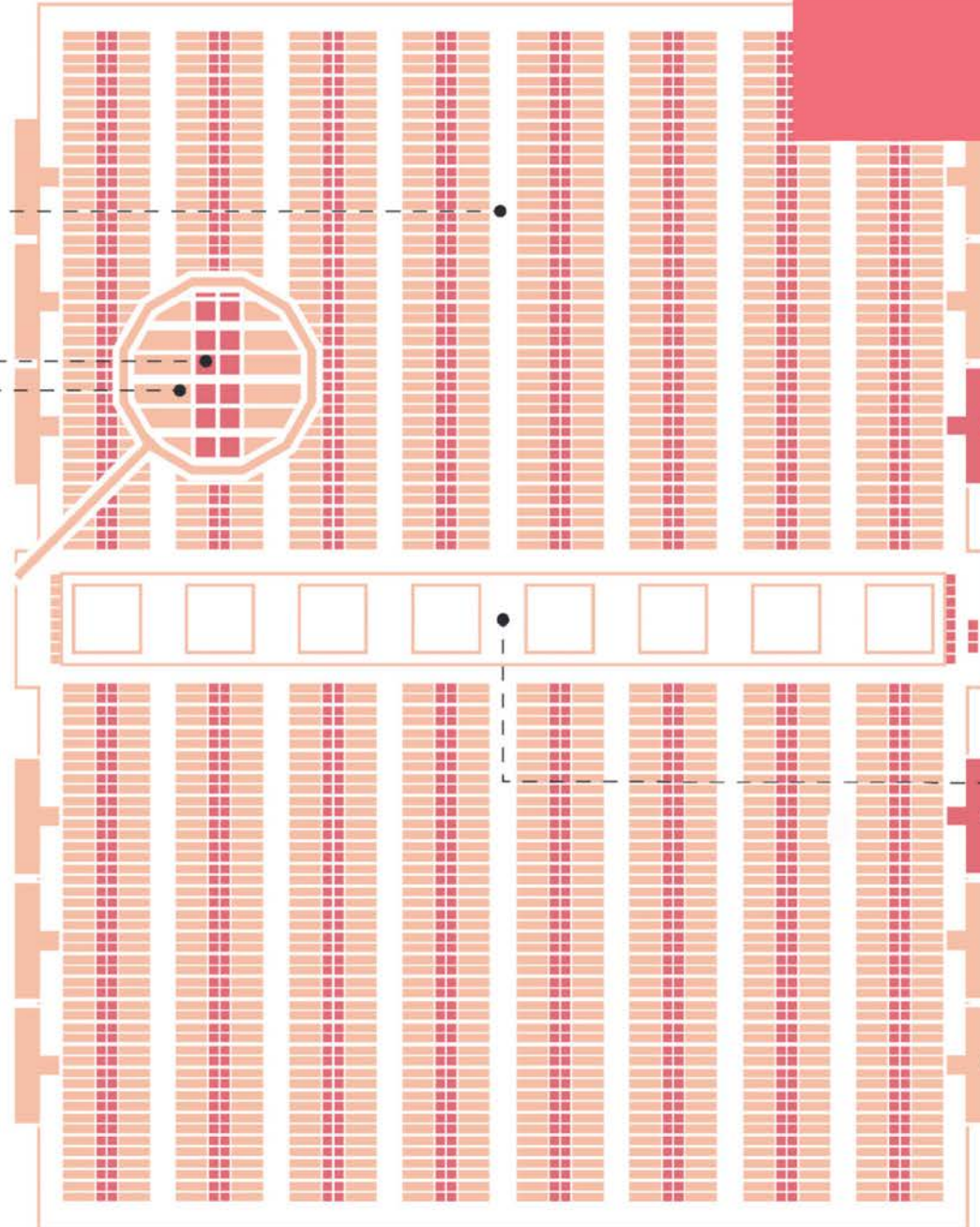
1472 independent IPU-Core™

8832 independent program threads executing in parallel

In-Processor-Memory™

900MB In-Processor-Memory™ per IPU

65TB/s memory bandwidth per IPU



IPU-Exchange™

11 TB/s all to all IPU-Exchange™
Non-blocking, any communication pattern

PCIe

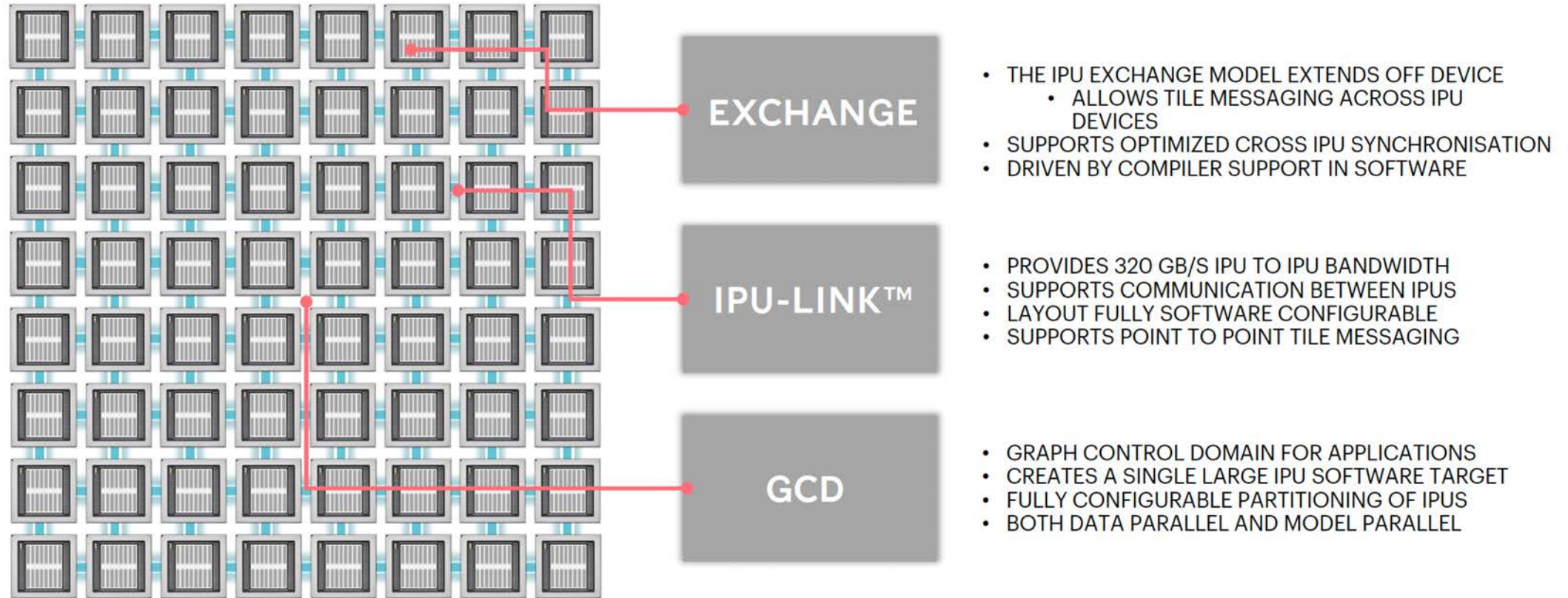
PCI Gen4 x16
64 GB/s bidirectional bandwidth to host

IPU-Links™

10 x IPU-Links,
320GB/s chip to chip bandwidth

Slide Courtesy: Graphcore

SCALING ACROSS DEVICES

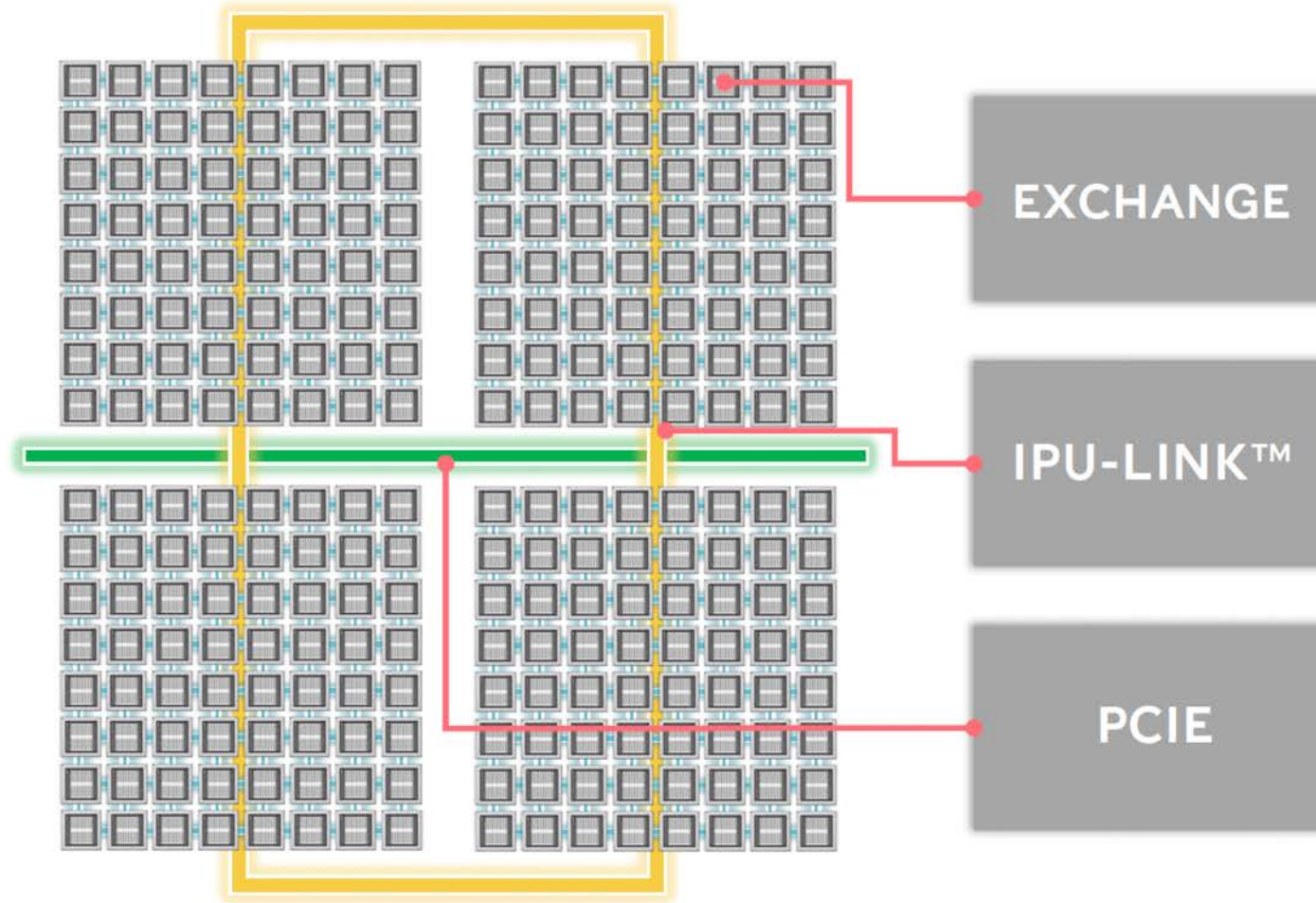


UP TO 64 IPU DEVICES USABLE AS A SINGLE LARGE IPU FROM APPLICATIONS

565248 FULLY INDEPENDENT WORKERS, 57.6GB IN-PROCESSOR MEMORY™, LEVERAGING OVER 3.8 TRILLION TRANSISTORS

Slide Courtesy: Graphcore

SCALING ACROSS SYSTEMS



- IPU EXCHANGE SUPPORT ACROSS DOMAINS
 - DRIVEN BY COMPILER SUPPORT IN SOFTWARE
- ENABLES APPLICATION COLLECTIVES SUPPORT
- ALLOWS SCALING UP TO 64000 IPU DEVICES

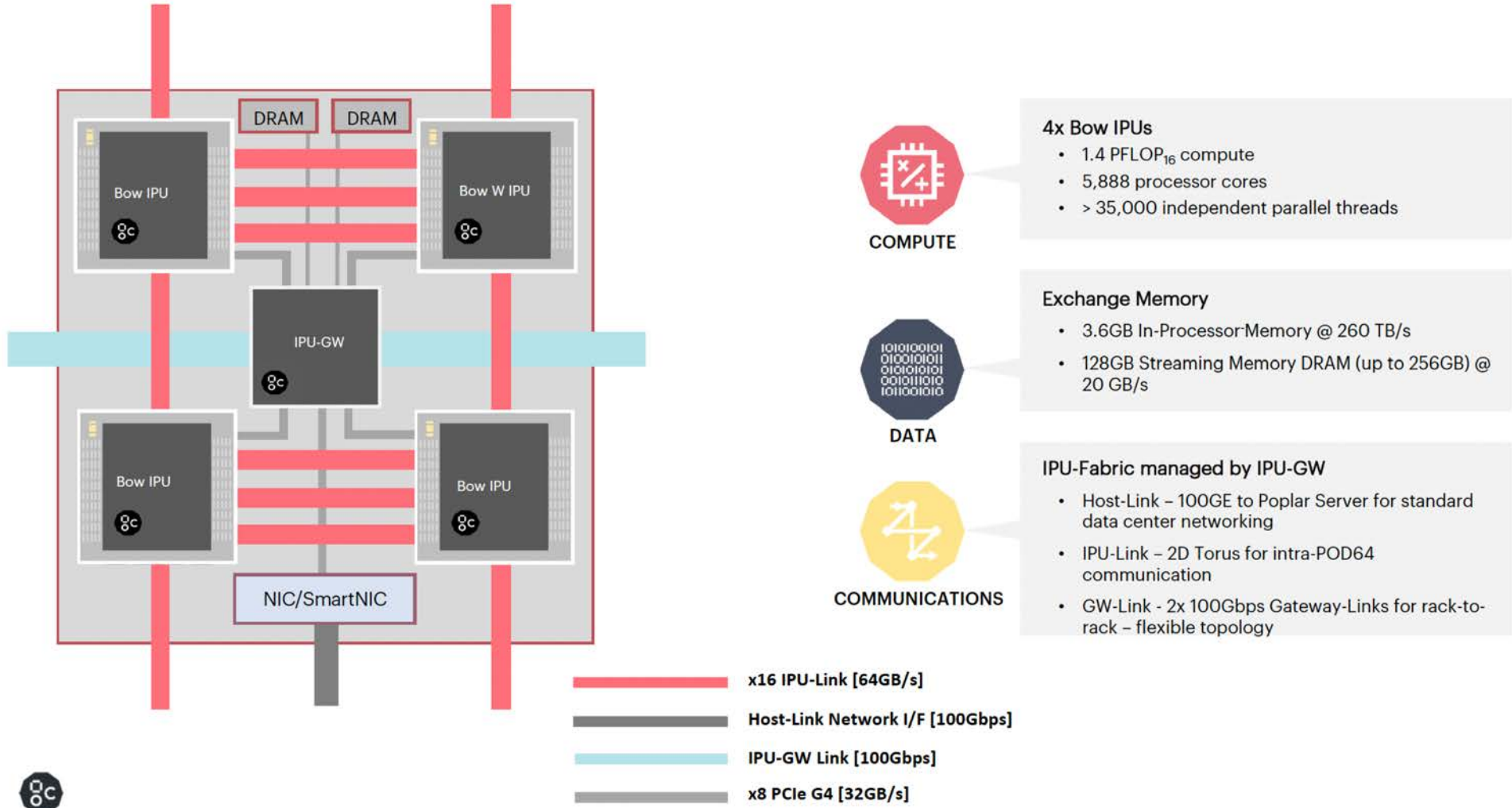
- IPU LINK™ CAN BE EXTENDED ACROSS DOMAINS
- SUPPORTS OPTIMIZED IPU LINK™ COLLECTIVES
- ALLOWS REPLICATION ACROSS SYSTEMS
- SUPPORTS A STANDARD IPU SOFTWARE MODEL

- IPUS CAN ACCESS MEMORY AND DEVICES OVER PCIE
- ALLOWS INTERFACING WITH HOST BASED SOFTWARE
- APPLICATIONS CAN BUILD ON HOST NETWORKING
- ALLOWS SCALING IN STANDARD SERVER PLATFORMS

256 IPU APPLICATION TARGET BUILT FROM INTERCONNECTED 64 IPU DOMAINS

Slide Courtesy: Graphcore

BOW-2000: THE BUILDING BLOCK OF LARGE PODS



Slide Courtesy: Graphcore

Graphcore POD-64

<https://www.alcf.anl.gov/alcf-ai-testbed>



POD64

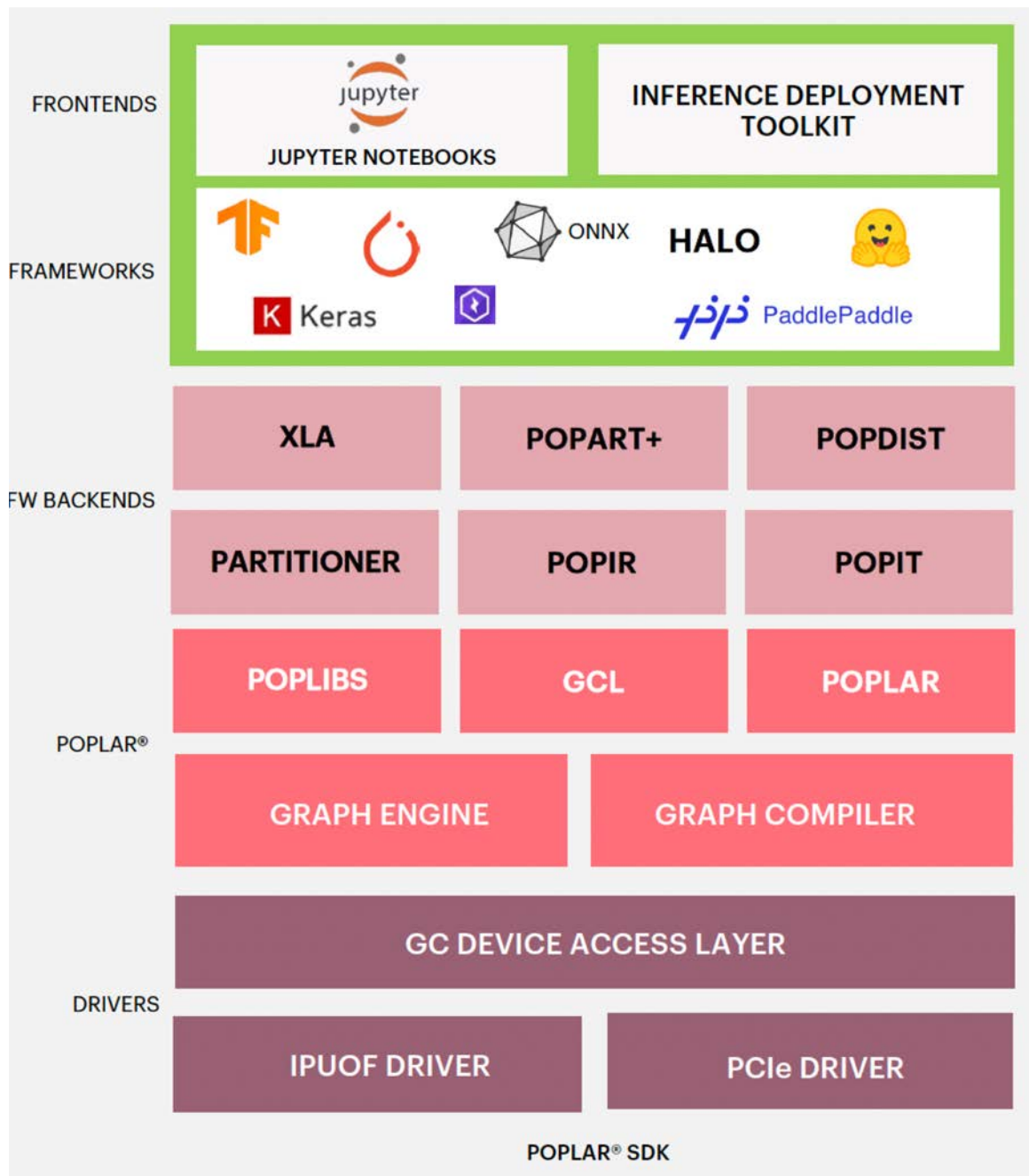
- 4 Nodes
- 64 IPUs

gc-
poplar-01

gc-
poplar-02

gc-
poplar-03

gc-
poplar-04



Slide Courtesy: Graphcore

| | Cerebras CS2 | SambaNova Cardinal SN30 | Groq GroqRack | GraphCore GC200 IPU | Habana Gaudi1 | NVIDIA A100 |
|---|--|--------------------------------|-----------------------------|-----------------------------|------------------------------------|--------------------------|
| Compute Units | 850,000 Cores | 640 PCUs | 5120 vector ALUs | 1472 IPUs | 8 TPC + GEMM engine | 6912 Cuda Cores |
| On-Chip Memory | 40 GB L1, 1TB+ MemoryX | >300MB L1 1TB | 230MB L1 | 900MB L1 | 24 MB L1 32GB | 192KB L1 40MB L2 40-80GB |
| Process | 7nm | 7nm | 7 nm | 7nm | 7nm | 7nm |
| System Size | 2 Nodes including Memory-X and Swarm-X | 8 nodes (8 cards per node) | 9 nodes (8 cards per node) | 4 nodes (16 cards per node) | 2 nodes (8 cards per node) | Several systems |
| Estimated Performance of a card (TFlops) | >5780 (FP16) | >660 (BF16) | >250 (FP16) >1000 (INT8) | >250 (FP16) | >150 (FP16) | 312 (FP16), 156 (FP32) |
| Software Stack Support | Tensorflow, Pytorch | SambaFlow, Pytorch | GroqAPI, ONNX | Tensorflow, Pytorch, PopArt | Synapse AI, TensorFlow and PyTorch | Tensorflow, Pytorch, etc |
| Interconnect | Ethernet-based | Ethernet-based | RealScale™ | IPU Link | Ethernet-based | NVLink |

Challenges

- Understand how these systems perform for different workloads given diverse hardware and software characteristics
- What are the unique capabilities of each evaluated system
- Opportunities and potential for integrating AI accelerators with HPC computing facilities

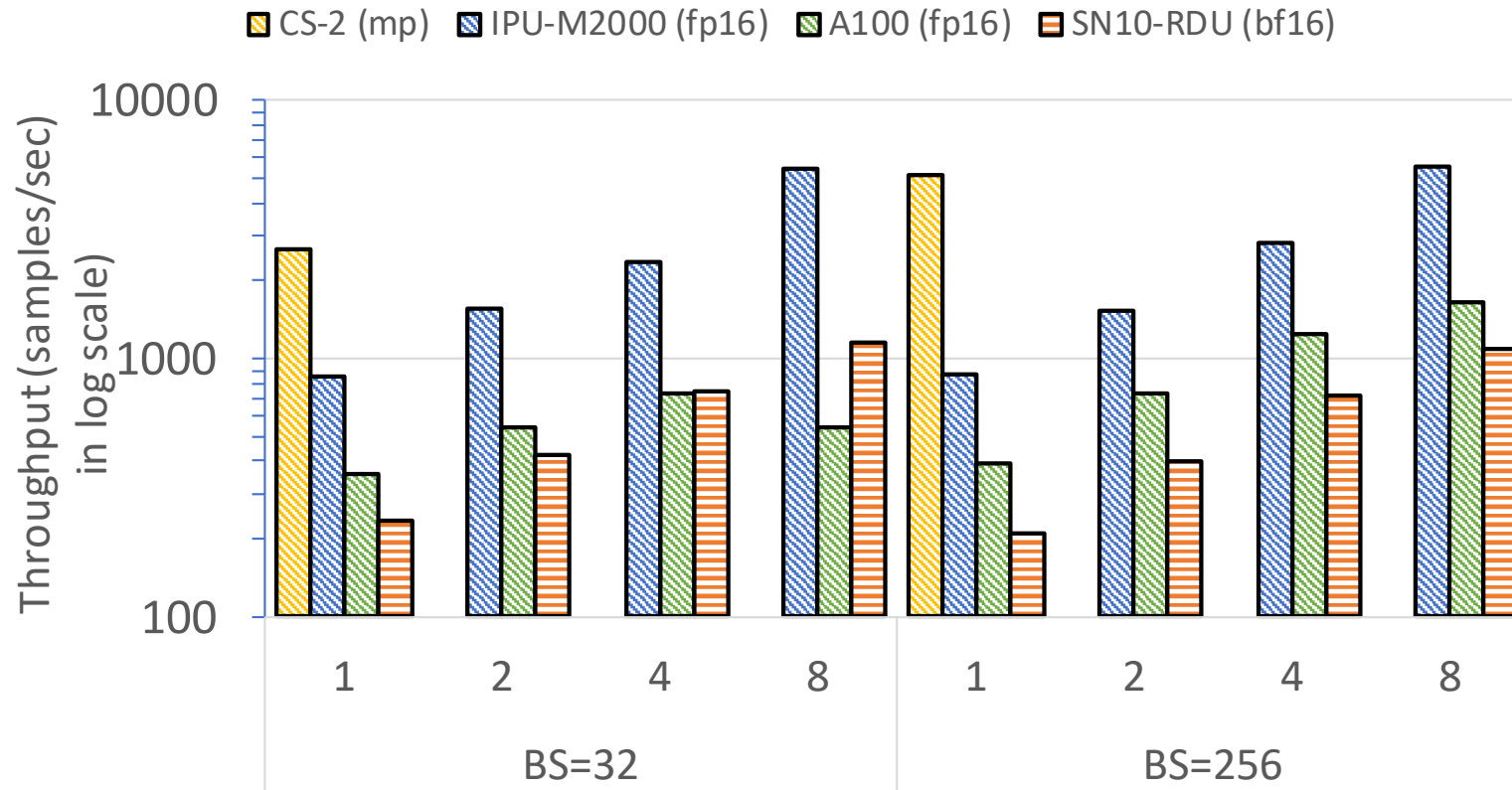
Approach

- Perform a comprehensive evaluation with a diverse set of Deep Learning (DL) models:
 - *DL primitives*: GEMM, Conv2D, ReLU, and RNN
 - *Benchmarks*: U-Net, BERT-Large, ResNet-50
 - *AI4S applications*: BraggNN and Uno
 - Scalability and Collective communications
- Evaluated SambaNova, Cerebras, Graphcore, Groq systems and Nvidia A100 as a baseline*

Emani et al. “A Comprehensive Evaluation of Novel AI Accelerators for Deep Learning Workloads”,
13th IEEE International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS) at SC 2022.

* run out-of-box.

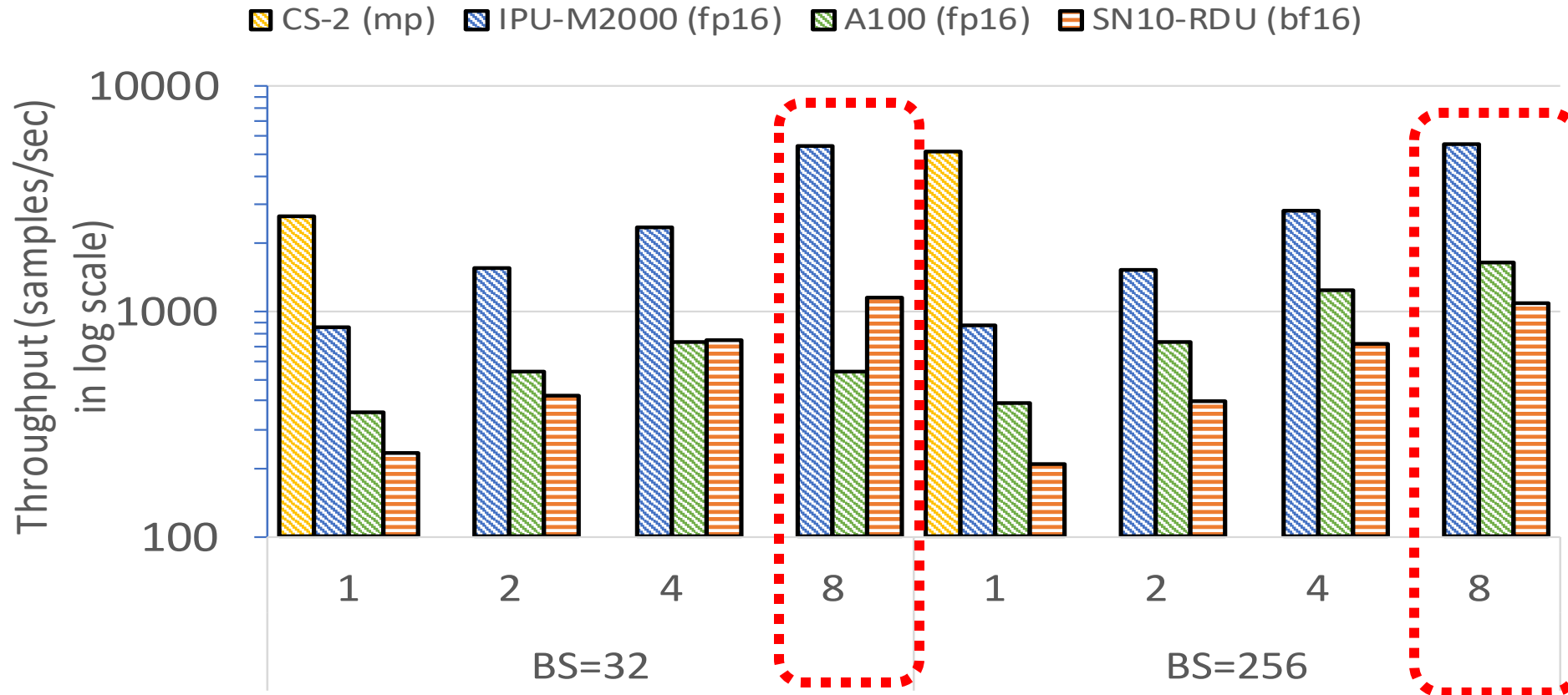
Scaling UNet-2D Training



Scale across 1, 2, 4, and 8 devices with two batch sizes (BS)
GraphCore uses data-prefetching optimization, CS-2 uses 1 wafer-scale engine

- 256x256 BMRI dataset
- A100, SN10 – Pytorch
Graphcore – Tensorflow
CS2 -- TF estimator
- Accelerators capable of handling much larger image sizes.

Scaling UNet-2D Training



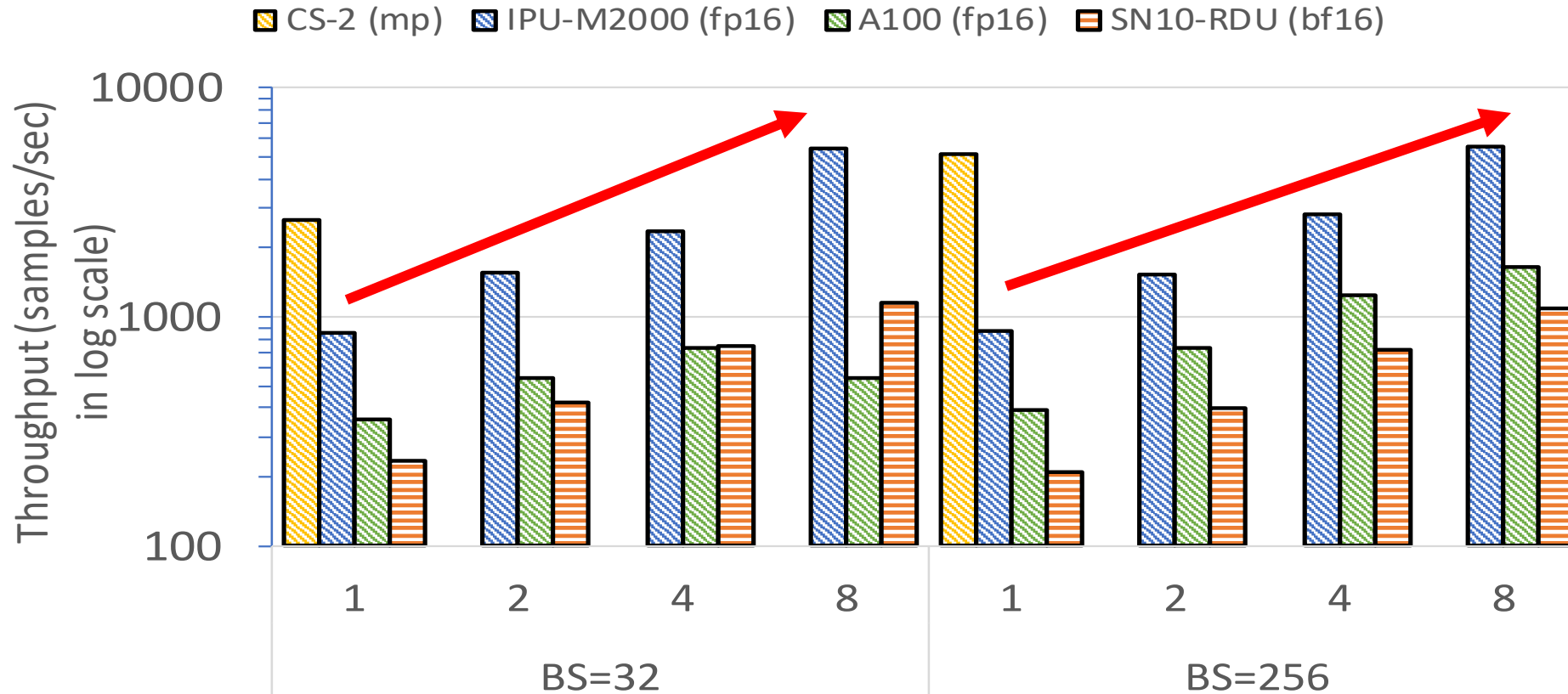
Scale across 1, 2, 4, and 8 devices with two batch sizes (BS)
 GraphCore uses data-prefetching optimization, CS-2 uses 1 wafer-scale engine

Increased Throughput over 8 A100s

| Batch Size | 8 SN10 - RDUs | 1 CS2 | 8 GC 200 IPU |
|------------|---------------|-------|--------------|
| 32 | 2.1x | 4.9x | 10x |

*2x increase in latest sw release

Scaling UNet-2D Training



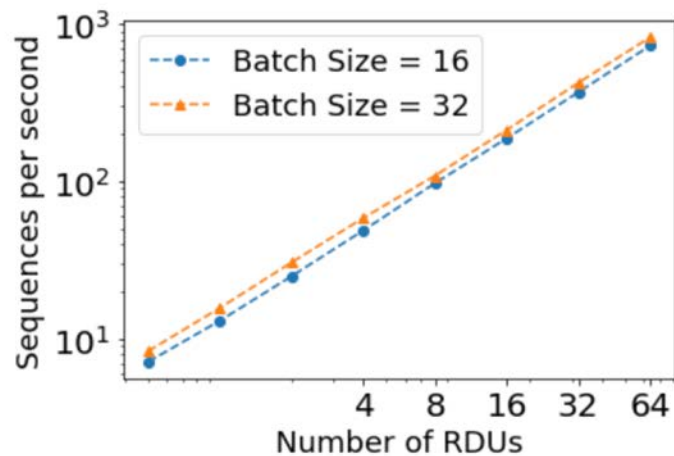
Scale across 1, 2, 4, and 8 devices with two batch sizes (BS)
 GraphCore uses data-prefetching optimization, CS-2 uses 1 wafer-scale engine

Scaling efficiency

| Batch Size | A100 | SN10 | GC |
|------------|-------|------|-------|
| 32 | 18.8% | 42% | 79.5% |
| 256 | 52% | 28% | 79.6% |

GPT Small (1.5B / 2B / xl)

SN30

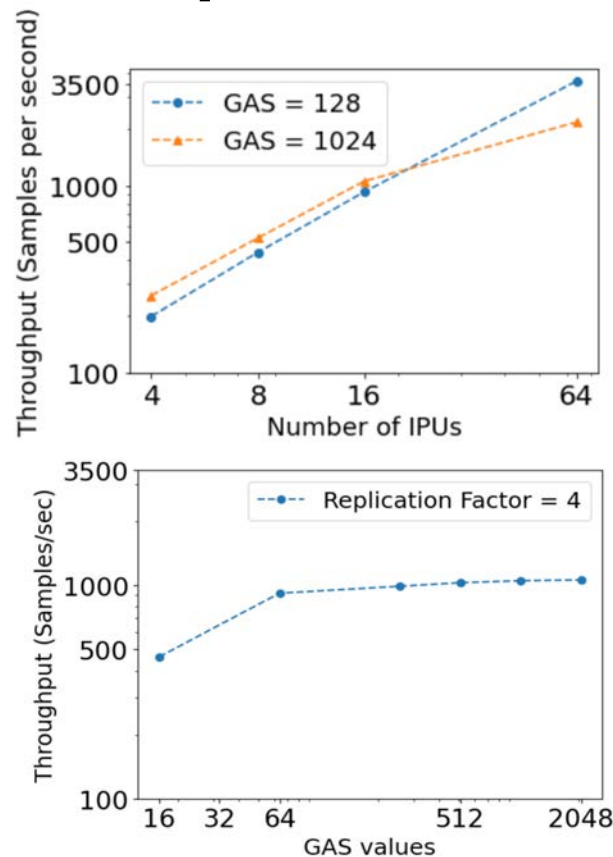


Sequence length = 1024, fits on 4 tiles.

Maximum of 128 instances run on 8 SN30 nodes.

~ 2x speed up observed over the nodes.

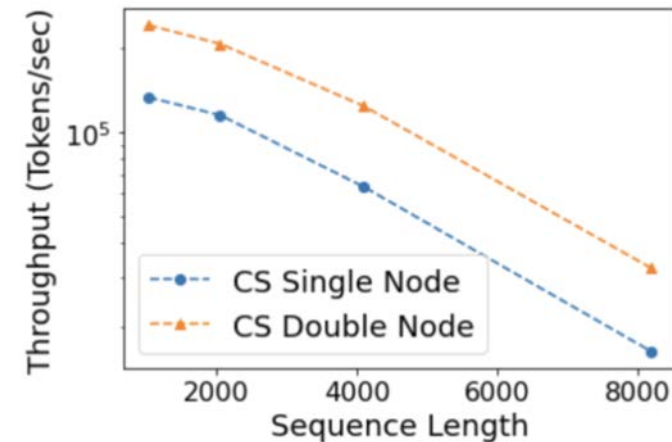
Graphcore



Scaling over replication factor better for smaller GAS values.

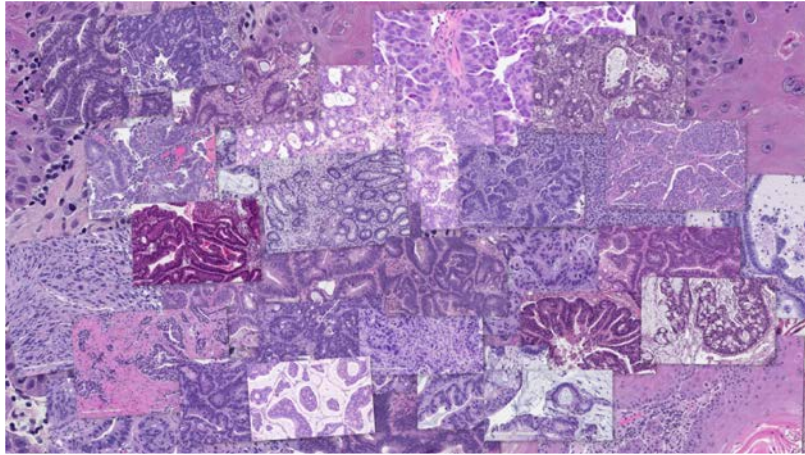
poprun for improved scaling efficiency.

CS2

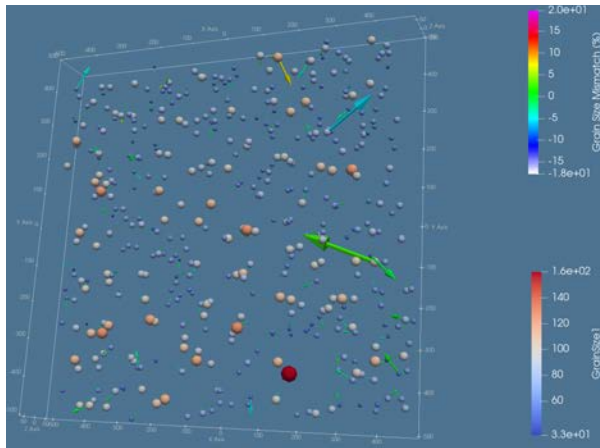


Work in progress for higher sequence length and wider models.

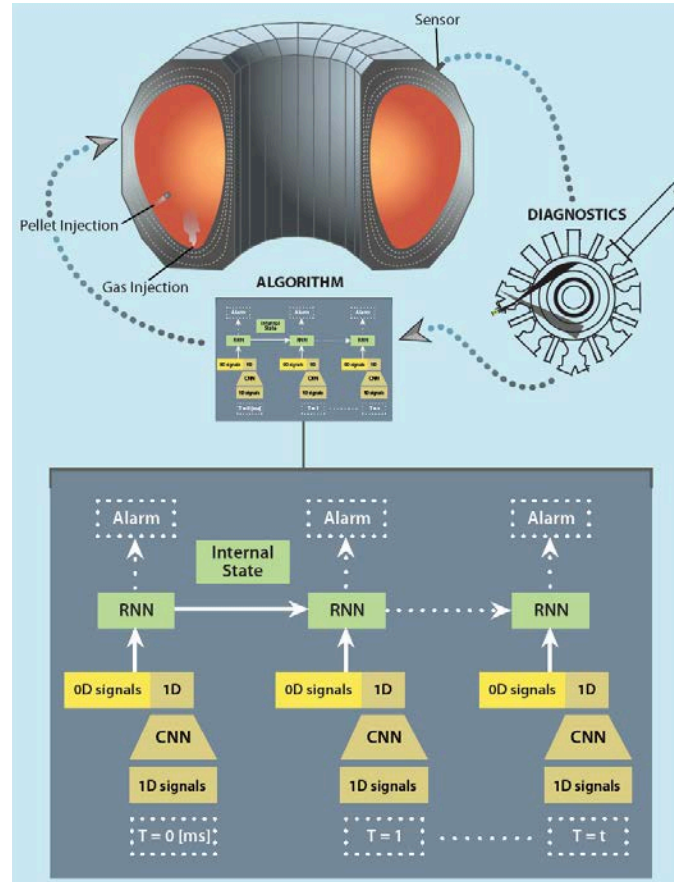
AI FOR SCIENCE APPLICATIONS



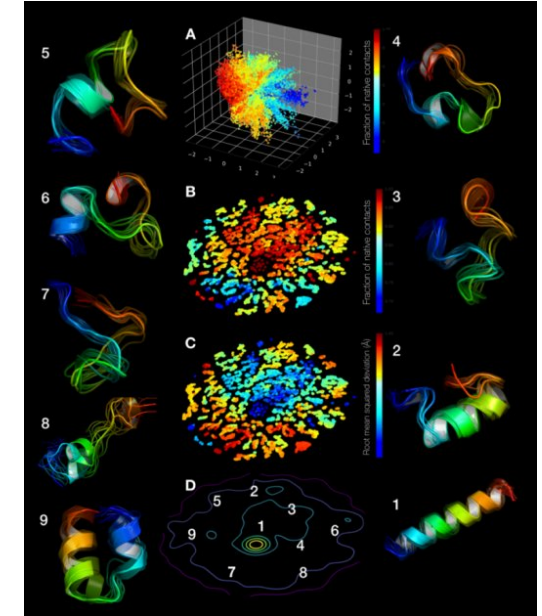
Cancer drug response prediction



Imaging Sciences-Braggs Peak



Tokamak Fusion Reactor operations



Protein-folding(Image: NCI)

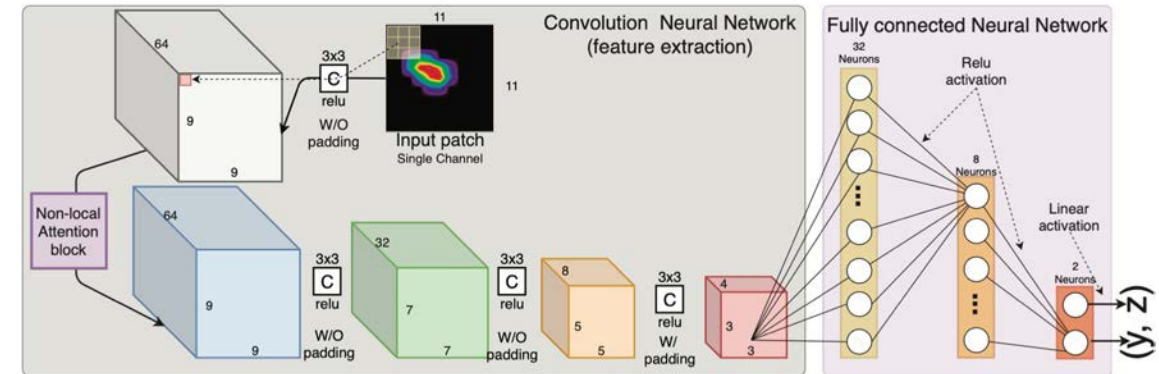
and more..

Fast X-Ray Bragg Peak Analysis

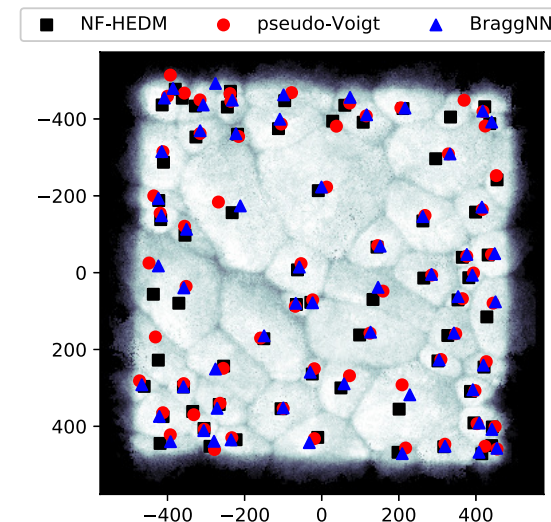
Goal: Enable rapid analysis and real-time feedback during an in-situ experiment with complex detector technologies

Proposed Approach: Deep learning-based method, BraggNN, for massive extraction of precise Bragg peak locations from far-field high energy diffraction microscopy data. BraggNN has achieved 200X improvement over conventional pseudo-Voigt profiling

Challenges: Model training capability is limited by the hardware



Application of the BraggNN deep neural network to an input patch yields a peak center position (y, z) . All convolutions are 2D of size 3×3 , with rectifier as activation function. Each fully connected layer, except for the output layer, also has a rectifier activation function.



A comparison of BraggNN, pseudo-Voigt FF-HEDM and NF-HEDM. (a) Grain positions from NF-HEDM (black squares), pseudo-Voigt FF-HEDM (red circles) and BraggNN FF-HEDM (blue triangles) overlaid on NF-HEDM confidence map

Courtesy: Z. Liu et al. [BraggNN: Fast X-ray Bragg Peak Analysis Using Deep Learning](#). International Union of Crystallography (IUCrJ), Vol. 9, No. 1, 2022

Fast X-Ray Bragg Peak Analysis

End-to-End Execution time (lower is better)

Fixed Time (compile, I/O and pre-processing)
 Training Time

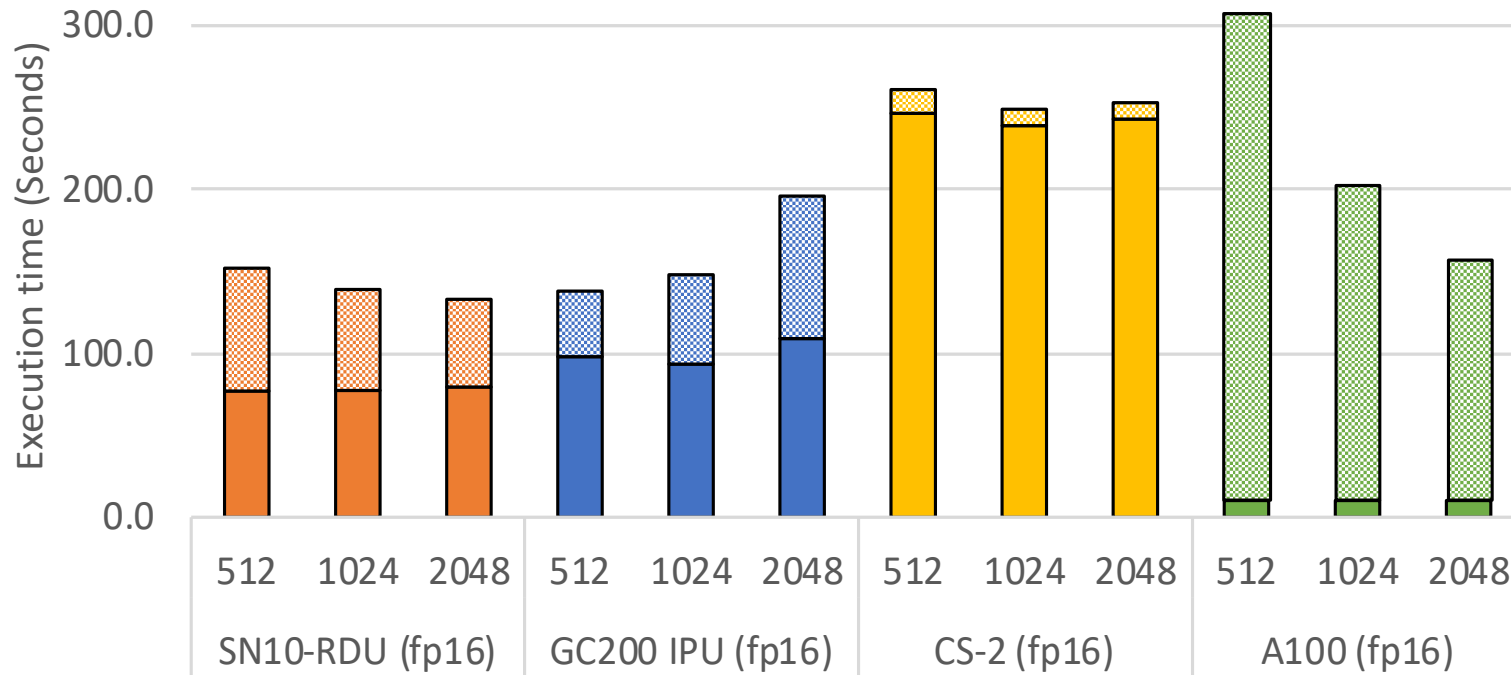


TABLE II: BraggNN Throughput (in order of 1k samples/sec) with various batch sizes (BS)

| System | BS=512 | BS=1024 | BS=2048 |
|------------------|--------|---------|---------|
| CS-2 (FP16) | 1365.4 | 2463 | 2787.9 |
| GC200 IPU (FP16) | 478.0 | 350.6 | 219.9 |
| SN10 RDU (BF16) | 369.7 | 449.8 | 518 |
| A100 (FP16) | 53.9 | 65.5 | 73.7 |

- SambaNova and Graphcore achieve lowest time to solution and achieve up to 1.55x and 1.46x speedup in comparison to Nvidia A100 respectively.
- Cerebras achieves up to 37.8x throughput improvement over A100.

Genome-scale Language Models (GenSLMs)

Goal:

- How new and emergent variants of pandemic causing viruses, (specifically SARS-CoV-2) can be identified and classified.
- Identify mutations that are VOC (increased severity and transmissibility)
- Extendable to gene or protein synthesis.

Approach

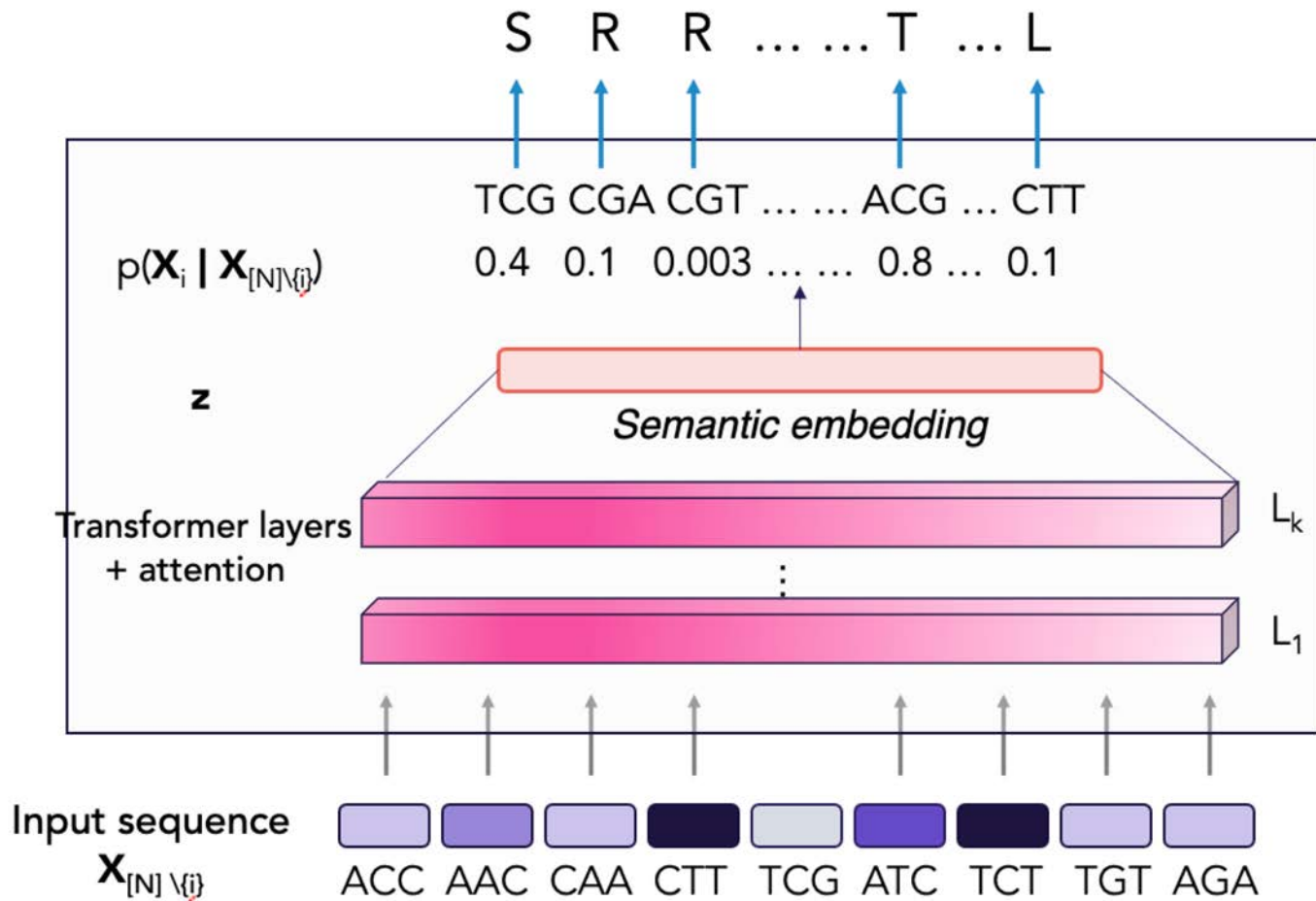
- Adapt Large Language Models (LLMs) to learn the evolution.
- Pretrain 25M – 25B models on raw nucleotides with large sequence lengths.
- Scale on GPUs, CS2s, SN30.

GenSLMs: Genome-scale language models reveal SARS-CoV-2 evolutionary dynamics

Winner of the ACM Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research, 2022,

DOI: <https://doi.org/10.1101/2022.10.10.511571>

Genome-scale Language Models (GenSLMs)



| Model | Seq. length | #Parameters | Dataset |
|-------------------|-------------|----------------------|---------|
| GenSLM-Foundation | 2048 | 25M, 250M, 2.5B, 25B | 110M |
| GenSLM | 10240 | 25M, 250M, 2.5B, 25B | 1.5M |
| GenSLM-Diffusion | 10240 | 2.5B | 1.5M |

Challenges

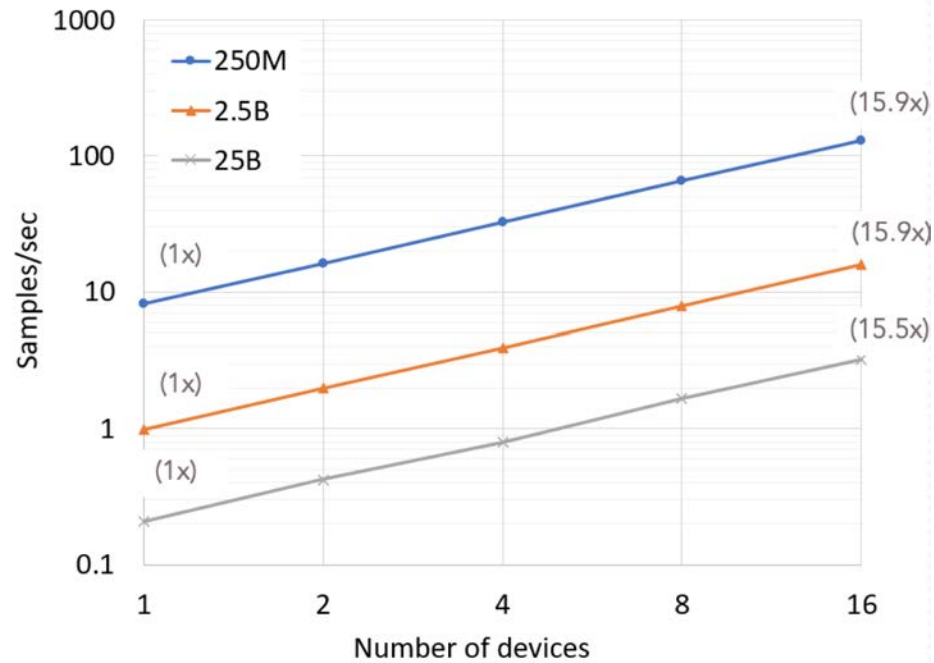
Scaling LLMs with 25B parameters:

- $O(L^2)$ complexity in the attention computation
- Overcome communication overheads
- Sharding and the training time available on GPUs imposing limitations

Solution

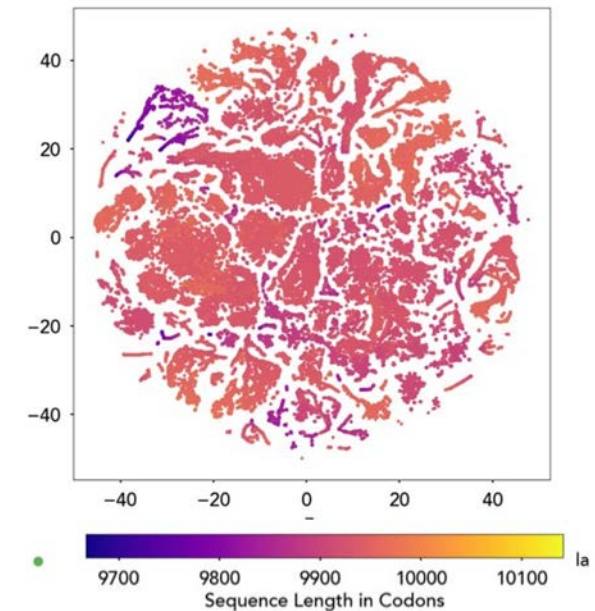
Cerebras CS-2 wafer-scale cluster and Sambanova SN30 enables pre-training and finetuning.

GenSLMs on CS2

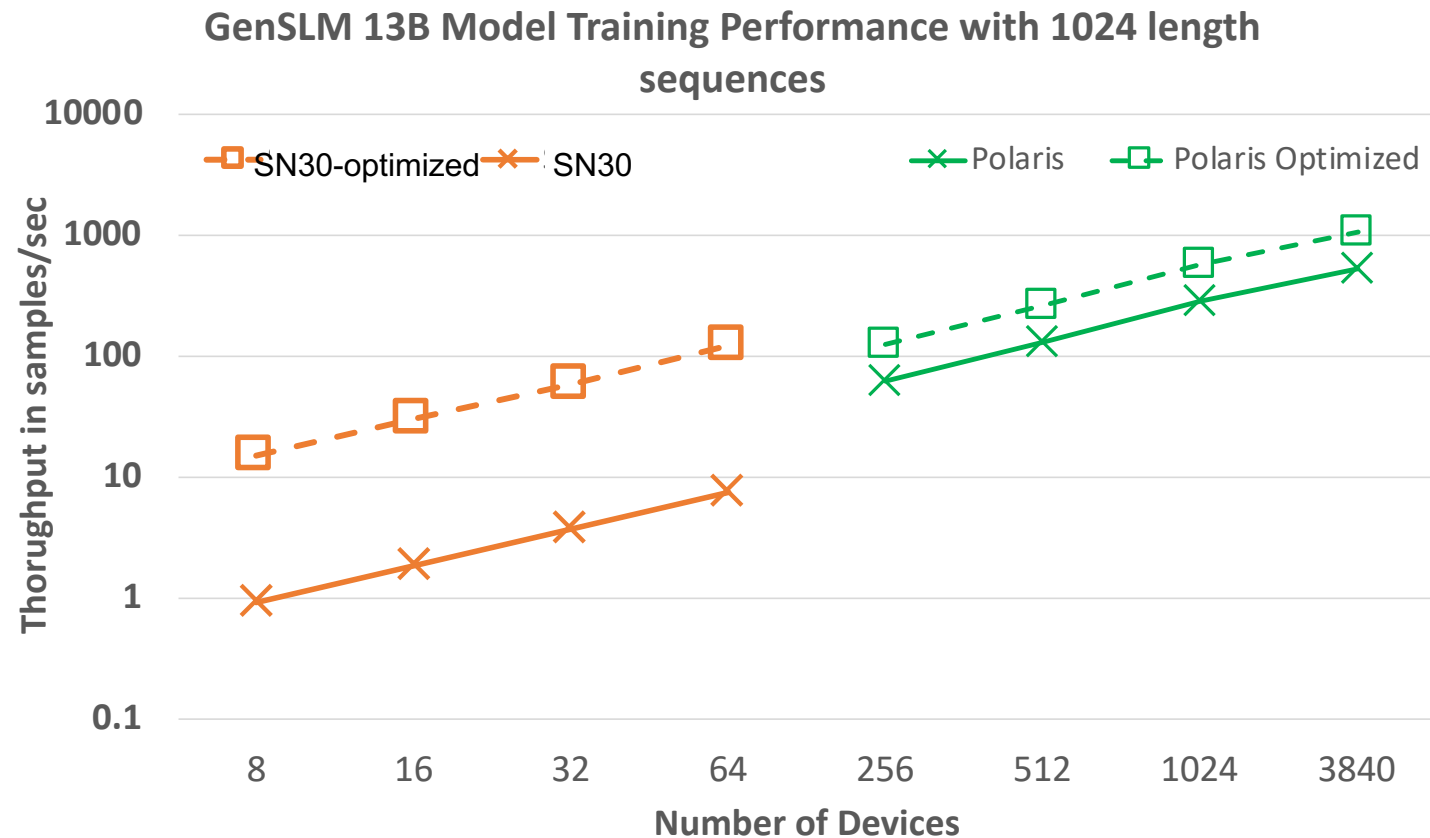


- Sequence Length = 10,240
- Trainable upto GPT3-13b model.
- Training with 4CS2, less than ½ day

| | GenSLM 123M | | GenSLM 1.3B | |
|--------------------------|-------------|------------|-------------|-------------|
| | 1 CS-2 | 4 CS-2 | 1 CS-2 | 4CS-2 |
| Training steps | 5,000 | 3,000 | 4,500 | 3,000 |
| Training samples | 165,000 | 396,000 | 49,500 | 132,000 |
| Time to train (h) | 4.1 | 2.4 | 15.6 | 10.4 |
| Validation accuracy | 0.9615 | 0.9625 | 0.9622 | 0.9947 |
| Validation perplexity | 1.031 | 1.029 | 1.031 | 1.025 |



GenSLMs on SN30



- Sequence Length = 1024
- Model Size 13B
- Achieves linear scaling across nodes.
- SN30 performance similar to 4 A100 on 1.17 release.
- Optimized on 1.18 to get 10x speed-up.
- Pretraining and FineTuning on larger sequence lengths.

Observations, Challenges and Insights

- Significant speedup achieved for a wide-gamut of scientific ML applications
 - Easier to deal with larger resolution data and to scale to multi-chip systems
- Room for improvement exists
 - Porting efforts and compilation times
 - Coverage of DL frameworks, support for performance analysis tools, debuggers

Observations, Challenges and Insights

- Good progress made in integration of AI accelerators, in production, at a national user facility and significant more work is needed for effective coupling
- Training and Outreach is critical to educate users to effectively use AI systems
- Close collaboration with vendors is necessary to realize the vision of AI for science

Ongoing Efforts

- Evaluate new AI accelerators offerings and incorporate promising solutions as part of the testbed
- Integrate AI testbed systems with the PBSPro scheduler to facilitate effective job scheduling across the accelerators
- Evaluate traditional HPC on AI Accelerators
- Understand how to integrate AI accelerators with ALCF's existing and upcoming supercomputers to accelerate science insights

Recent Publications

- **GenSLMs: Genome-scale language models reveal SARS-CoV-2 evolutionary dynamics**
Maxim Zvyagin, Alexander Brace, Kyle Hippe, Yuntian Deng, Bin Zhang, Cindy Orozco Bohorquez, Austin Clyde, Bharat Kale, Danilo Perez Rivera, Heng Ma, Carla M. Mann, Michael Irvin, J. Gregory Pauloski, Logan Ward, Valerie Hayot, Murali Emani, Sam Foreman, Zhen Xie, Diangen Lin, Maulik Shukla, Weili Nie, Josh Romero, Christian Dallago, Arash Vahdat, Chaowei Xiao, Thomas Gibbs, Ian Foster, James J. Davis, Michael E. Papka, Thomas Brettin, Rick Stevens, Anima Anandkumar, Venkatram Vishwanath, Arvind Ramanathan
** *Winner of the ACM Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research, 2022*,
DOI: <https://doi.org/10.1101/2022.10.10.511571>
- **A Comprehensive Evaluation of Novel AI Accelerators for Deep Learning Workloads**
Murali Emani, Zhen Xie, Sid Raskar, Varuni Sastry, William Arnold, Bruce Wilson, Rajeev Thakur, Venkatram Vishwanath, Michael E Papka, Cindy Orozco Bohorquez, Rick Weisner, Karen Li, Yongning Sheng, Yun Du, Jian Zhang, Alexander Tsyplikhin, Gurdaman Khaira, Jeremy Fowers, Ramakrishnan Sivakumar, Victoria Godsoe, Adrian Macias, Chetan Tekur, Matthew Boyd, *13th IEEE International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS) at SC 2022*
- **Enabling real-time adaptation of machine learning models at x-ray Free Electron Laser facilities with high-speed training optimized computational hardware**
Petro Junior Milan, Hongqian Rong, Craig Michaud, Naoufal Layad, Zhengchun Liu, Ryan Coffee, *Frontiers in Physics*
DOI: <https://doi.org/10.3389/fphy.2022.958120>

Recent Publications

- **Intelligent Resolution: Integrating Cryo-EM with AI-driven Multi-resolution Simulations to Observe the SARS-CoV-2 Replication-Transcription Machinery in Action***
Anda Trifan, Defne Gorgun, Zongyi Li, Alexander Brace, Maxim Zvyagin, Heng Ma, Austin Clyde, David Clark, Michael Salim, David Hardy, Tom Burnley, Lei Huang, John McCalpin, Murali Emani, Hyenseung Yoo, Junqi Yin, Aristeidis Tsaris, Vishal Subbiah, Tanveer Raza, Jessica Liu, Noah Trebesch, Geoffrey Wells, Venkatesh Mysore, Thomas Gibbs, James Phillips, S.Chakra Chennubhotla, Ian Foster, Rick Stevens, Anima Anandkumar, Venkatram Vishwanath, John E. Stone, Emad Tajkhorshid, Sarah A. Harris, Arvind Ramanathan, International Journal of High-Performance Computing (IJHPC'22) DOI: <https://doi.org/10.1101/2021.10.09.463779>
- **Stream-AI-MD: Streaming AI-driven Adaptive Molecular Simulations for Heterogeneous Computing Platforms**
Alexander Brace, Michael Salim, Vishal Subbiah, Heng Ma, Murali Emani, Anda Trifa, Austin R. Clyde, Corey Adams, Thomas Uram, Hyunseung Yoo, Andrew Hock, Jessica Liu, Venkatram Vishwanath, and Arvind Ramanathan. 2021 Proceedings of the Platform for Advanced Scientific Computing Conference (PASC'21). DOI: <https://doi.org/10.1145/3468267.3470578>
- **Bridging Data Center AI Systems with Edge Computing for Actionable Information Retrieval**
Zhengchun Liu, Ahsan Ali, Peter Kenesei, Antonino Miceli, Hemant Sharma, Nicholas Schwarz, Dennis Trujillo, Hyunseung Yoo, Ryan Coffee, Naoufal Layad, Jana Thayer, Ryan Herbst, Chunhong Yoon, and Ian Foster, 3rd Annual workshop on Extreme-scale Event-in-the-loop computing (XLOOP), 2021
- **Accelerating Scientific Applications With SambaNova Reconfigurable Dataflow Architecture**
Murali Emani, Venkatram Vishwanath, Corey Adams, Michael E. Papka, Rick Stevens, Laura Florescu, Sumti Jairath, William Liu, Tejas Nama, Arvind Sujeeth, IEEE Computing in Science & Engineering 2021 DOI: [10.1109/MCSE.2021.3057203](https://doi.org/10.1109/MCSE.2021.3057203).

* Finalist in the ACM Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research, 2021

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