#### October 10-12, 2023



# ALCF Hands-on HPC Workshop



## **ALCF AI Testbed**

Murali Emani, Argonne Leadership Computing Facility memani@anl.gov

## **Surge of Scientific Machine Learning**

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



Protein-folding





**Galaxy Classification** 



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

## **Integrating AI Systems in Facilities**



Simulations

Data-driven Models





## **ALCF AI Testbed**

#### https://www.alcf.anl.gov/alcf-ai-testbed





## **ALCF AI Testbed**

#### https://www.alcf.anl.gov/alcf-ai-testbed



- 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 IPUs per node) - MIMD, irregular workloads such as graph neural networks
- GrogRack: 8 nodes, 8 GrogNodes 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



Gaudi1



## Agenda

#### https://github.com/argonne-lcf/ALCF\_Hands\_on\_HPC\_Workshop/tree/master/aiTestbeds

- Time: October 11, 2023.
  - 11-12 PM : ALCF AI Testbeds (Talk)
  - 2.30 5.00 PM : Hands-On Session
- Location: Room 1416
- Slack Channel: #ai-test-beds : Use to post questions,

#### Agenda 2

Time(CST)	Торіс
2.30 - 3.00	Sambanova
3.00 - 3.15	Break
3.15 - 3.45	Graphcore
3.45 - 4.15	Cerebras
4.15 - 5.00	Hands on, Q&A, Debugging



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.



#### **Getting Started on ALCF AI Testbed:**

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

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**





#### PROGRAM EXHIBITS STUDENTS SCINET MEDIA

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#### 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.



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

Location: 203



ATTEND

Energy-Efficient GPU Computing

• Al training workshops

Cerebras: <u>https://events.cels.anl.gov/event/420/</u> SambaNova: <u>https://events.cels.anl.gov/event/421/</u> Graphcore: <u>https://events.cels.anl.gov/event/422/</u> **Tutorial at SC23** on Programming Novel AI accelerators for Scientific Computing *in collaboration with Cerebras, Intel Habana, Graphcore, Groq and SambaNova* 



### **Dataflow Architectures**





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

The Dataflow way: Spatial Eliminates memory traffic and overhead



## SambaNova Cardinal SN30 RDU





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## **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



## **Cardinal SN30: Tile**





Image Courtesy: SambaNova





## **Dataflow Architecture for Terabyte Sized Models**





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)
- PCle Gen4 x16
- Host module



## SambaFlow Architecture





## SambaNova Datascale SN30

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







## Cerebras Wafer-Scale Engine (WSE-2)

850,000 cores optimized for sparse linear algebra
46,225 mm<sup>2</sup> 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**

Cerebras Wafer-Scale Cluster Appliance Mode Pre-processing, management MemoryX SwarmX CS-2

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)



## **Cerebras CS-2 Cluster**

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

ALCF's CS-2 Cluster

- 2 CS-2 Appliances (each chip 46225 mm<sup>2</sup>)
- 1 Management node
- 16 Worker nodes
- 24 MemoryX nodes
- 6 SwarmX nodes



Topology of a Cerebras Wafer-Scale cluster

NATIONAL LABORATOR

3 user login nodes

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#### **Cerebras Weight Streaming Technology**



Disaggregate storage and compute Enable scaling model size



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## **Graphcore Intelligence Processing Unit (IPU)**





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#### IPU-Tiles™

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

#### IPU-Core<sup>™</sup>

1472 independent IPU-Core™

8832 independent program threads executing in parallel

#### In-Processor-Memory<sup>™</sup>

900MB In-Processor-Memory™ per IPU

65TB/s memory bandwidth per IPU



#### 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<sup>TM</sup>, LEVERAGING OVER 3.8 TRILLION TRANSISTORS

Slide Courtesy: Graphcore



#### SCALING ACROSS SYSTEMS



256 IPU APPLICATION TARGET BUILT FROM INTERCONNECTED 64 IPU DOMAINS

Slide Courtesy: Graphcore



#### **BOW-2000: THE BUILDING BLOCK OF LARGE PODS**





## **Graphcore POD-64**

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









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	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 <sup>™</sup>	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, Uno
  - Scalability and Collective communications
- Evaluation of Large Language Models

   —Transformer block micro-benchmark, GPT-2, and GenSLM

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



#### **Scaling UNet-2D Training**

SCS-2 (mp) SIPU-M2000 (fp16) A100 (fp16) SN10-RDU (bf16)



#### Increased Throughput over 8 A100s

Batch Size	8 SN10 - RDUs	1 CS2	8 GC 200 IPUs	*2x increase in latest sw release
32	2.1x	4.9x	10x	

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#### **Scaling UNet-2D Training**

SCS-2 (mp) SIPU-M2000 (fp16) A100 (fp16) SN10-RDU (bf16)



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%



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🖾 CS-2 (mp) 🛽

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#### **GPT Model Performance**



Used GPT-2 XL 1.5B parameter model

- same sequence length, tuned batch sizes
- 16 SN30 RDUs, 2 CS-2s, and 16 IPUs outperformed the runs on 64 A100s
- Scaling efficiencies range from 78% to 104%

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System (model Size)	Seq Length	Devices	Throughput (tokens/s)
A100 (1.5B)	1024	4	134,144
	2048	4	124,928
CS-2 (1.5B)	1024	1	133,069
	2048	1	114,811
	4096	1	63,488
	8192	1	16,302
CS-2 (13B)	1024	1	20,685
	2048	1	20,173
	4096	1	17,531
	8192	1	15,237
	16384	1	11,796
	32768	1	7537
	51200	1	5120
SN30 (13B)	1024	8	22,135
	2048	8	21,684
	4096	8	17,000
	8192	8	10,581
	16384	8	4936
	32768	8	5021
	65536	8	1880

TABLE III: Impact of Sequence length on model throughput



## **AI FOR SCIENCE APPLICATIONS**



#### Cancer drug response prediction



Imaging Sciences-Braggs Peak



#### Tokomak Fusion Reactor operations



#### Protein-folding(Image: NCI)

#### and more..



## 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  $\frac{1}{2}$  day

Number of de	vices				
	GenSLI	M 123M	GenSl	M 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**



GenSLM 13B Model Training Performance with 1024 length

- 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
- Limited capability to support low-level HPC kernels
  - Work in progress to improve coverage



#### **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 Har dy, Tom Burnley, Lei Huang, John McCalpin, Murali Emani, Hyenseung Yoo, Junqi Yin, Aristeidis Tsaris, Vishal Subbiah, Tanveer Raza, J essica 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 Al 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-inthe-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.

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

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## Thank You

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- Venkatram Vishwanath, Michael Papka, William Arnold, Varuni Sastry, Sid Raskar, Zhen Xie, Rajeev Thakur, Bruce Wilson, Anthony Avarca, Arvind Ramanathan, Alex Brace, Zhengchun Liu, Hyunseung (Harry) Yoo, Corey Adams, Ryan Aydelott, Kyle Felker, Craig Stacey, Tom Brettin, Rick Stevens, and many others have contributed to this material.
- Our current AI testbed system vendors Cerebras, Graphcore, Groq, Intel Habana and SambaNova. There are ongoing engagements with other vendors.

Please reach out for further details Venkat Vishwanath, <u>Venkat@anl.gov</u> Murali Emani, memani@anl.gov



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