

Preparing for Post-Exascale Computing

Jeffrey S. Vetter

With many contributions from ACSR Section and Colleagues

The 30th Anniversary Symposium of the Center for Computational Sciences University of Tsukuba 13 Oct 2022

ORNL is managed by UT-Battelle, LLC for the US Department of Energy



tions and the same



https://www.ornl.gov/section/advanced-computing-systems-research (https://j.mp/acsrs)

vetter@computer.org

Highlights

- 15 years to go from Exascale ideation to deployment
 - Reports and predictions
- Current status
 - Systems (Frontier)
 - Exascale Computing Project
- Exascale: What did we get right, get wrong, overlook?
- Post Exascale?
 - Heterogeneous systems enabled by Heterogeneous integration and Chiplets
 - Codesign becomes even more important
- Abikso: Microelectronics codesign project



Exascale Reports (and predictions) from 2007 to 2014

Modeling and Simulation at the Exascale for Energy and the Environment

	Simulatio	Report on the Advanced Town Ha on and Modeling at the Exa	ExaScale Computing Study: Technology Challenges in	TRUDGING THE GAL				
		and Glob	Achieving Exascale Systems					
7	Co-Chairs:	Lawrence Berkeley Natior Oak Ridge National Labor Argonne National Labora	Peter Kogge, Editor & Study Lead Keren Bergman	SCIENTIFIC GRAND CHALLENG TECHNOLOGIES FOR COMPUTI				
	Office of Advanced		Shekhar Borkar					
	Scientific Computing Research Contact:	Michael Strayer	Dan Campbell William Carlson	Report from the Workshop Held	February 2-4, 2010			
	Special Assistance Technical:	Lawrence Berkeley Natior Deb Agarwal, David Bailey,	William Dally Monty Denneau	Sponsored by the U.S. Department of Energy, O Research, Office of Science; and the Office of A National Nuclear Security Administration	ASCAC Subcommittee for the Top Te	n Exascale Research Challenges		
		William Collins, Nikos Kyrpi Peter Nugent, Leonid Olike		National Nuclear Security Administration	Subcommittee Chair		The International Journal of High	
1		Lin-Wang Wang, Michael W	Kerry Hill	Chair, David L. Brown	Robert Lucas (University of Southern California	The International Exascale Softwar	Performance Computing Applications	
		Oak Ridge National Labor	r řen	Lawrence Livermore National Laboratory			© The Author(s) 2011	
		Eduardo D'Azevedo, David				Project roadmap	Reprints and permission: sagepub.co.uk/journalsPermissions.nav	
		James Hack, Victor Hazlew Bronson Messer, Anthony N	Stephen Keckler	Chair, Paul Messina			DOI: 10.1177/1094342010391989 hpc.sagepub.com	
		B. (Rad) Radhakrishnan, N	Dean Klein	Argonne National Laboratory	Subcommittee Members		(\$)SAGE	
		Jeffrey Vetter, Gilbert Weiga		Theme I: Domain Science and System Architecture	James Ang (Sandia National Laboratories)	Jack Dongarra, Pete Beckman, Terry Moore, Patrick	Aerts,	
		Argonne National Laborat	Mark Richards	,,	Keren Bergman (Columbia University)	Giovanni Aloisio, Jean-Claude Andre, David Barkai,		
		Raymond Bair, Pete Beckm		Principal Lead, David Keyes	Shekhar Borkar (Intel)	Jean-Yves Berthou, Taisuke Boku, Bertrand Braunsch		
		Ed Frank, Ian Foster, Willia Robert Jacob, Kenneth Ker		King Abdullah University of Science and Technology a	William Carlson (Institute for Defense Analyses)	Franck Cappello, Barbara Chapman, Xuebin Chi, Alok		
		Jorge Moré, Lois McInnes,	Thomas Starling	Co. / and John Marrison	Laura Carrington (UC, San Diego)	Thom Dunning, Sandro Fiore, Al Geist, Bill Gropp, Ro		
		Michael Papka, Robert Ros	Thomas Sterling R. Stanley Williams	Co-Lead, John Morrison Los Alamos National Laboratory	George Chiu (IBM)	Michael Heroux, Adolfy Hoisie, Koh Hotta, Zhong Jin, Sanjay Kale, Richard Kenway, David Keyes, Bill Kramer	· •	
	Administrative:	Lawrence Berkeley Nation		Los Alamos National Laboratory	Robert Colwell (DARPA)	Thomas Lippert, Bob Lucas, Barney Maccabe, Satoshi		
		Oak Ridge National Labor		Co-Lead, Robert Lucas	William Dally (NVIDIA)	Peter Michielse, Bernd Mohr, Matthias S. Mueller, Wolf		
		Argonne National Laborat	September 28, 2008	University of Southern California	Jack Dongarra (U. Tennessee)	Michael E Papka, Dan Reed, Mitsuhisa Sato, Ed Seidel,		
	Publication:	Oak Ridge National Labor			Al Geist (ORNL)	Marc Snir, Thomas Sterling, Rick Stevens, Fred Streit	z, Bob Sugar, Shinji Sumimoto,	
		Argonne National Laborat	This work was sponsored by DARPA IPTO i	Co-Lead, John Shalf	Gary Grider (LANL)	William Tang, John Taylor, Rajeev Thakur, Anne Tref		
	Editorial:	Oak Ridge National Labor		Lawrence Berkeley National Laboratory	Rud Haring (IBM)	Aad van der Steen, Jeffrey Vetter, Peg Williams, Robe	ert Wisniewski and Kathy Yelick	
		Argonne National Laborat		Theme II: System Software	Jeffrey Hittinger (LLNL)			
			Government's approval or disapproval of its i		Adolfy Hoisie (PNLL)			
	This report is available	on the web at http://www.sc.c	N	Principal Lead, Pete Beckman	Dean Klein (Micron)	Abstract		
- L			1	Argonne National Laboratory	Peter Kogge (U. Notre Dame)	Over the last 20 years, the open-source community has provided more a performance computing systems depend for performance and producti		
			Using Government drawings, specifications,	Co-Lead, Ron Brightwell	Richard Lethin (Reservoir Labs)	dollars and years of effort to build key components. However, although t		
			purpose other than Government procurement	Sandia National Laboratories	Vivek Sarkar (Rice U.)	ments have been tremendously valuable, a great deal of productivity has		
			The fact that the Government formulated or s		Robert Schreiber (Hewlett Packard)	coordination, and key integration of technologies necessary to make then within individual petascale systems and between different systems. It see		
			does not license the holder or any other perso	Co-Lead, Al Geist	John Shalf (LBNL)	development model will not provide the software needed to support the		
			manufacture, use, or sell any patented inventi	Oak Ridge National Laboratory	Thomas Sterling (Indiana U.)	exascale computation on millions of cores, or the flexibility required to ex-	xploit new hardware models and features, such	1
			APPROVED FOR PUBLIC RELEASE, DIS	Theme III: Programming Models and Environment	Rick Stevens (ANL)	as transactional memory, speculative execution, and graphics processing community to prepare for the challenges of exascale computing, ultimatel national Exascale Software Project.		
				Principal Lead, Jeffrey Vetter Oak Ridge National Laboratory and Georgia Institute o	fTechnology	Keywords		
					i rechnology	exascale computing, high-performance computing, software stack		
						Table of Contents		GF

I. Introduction

3.1 Technology Trends

2. Destination of the IESP Roadmap

3. Technology Trends and their Impact on Exascale

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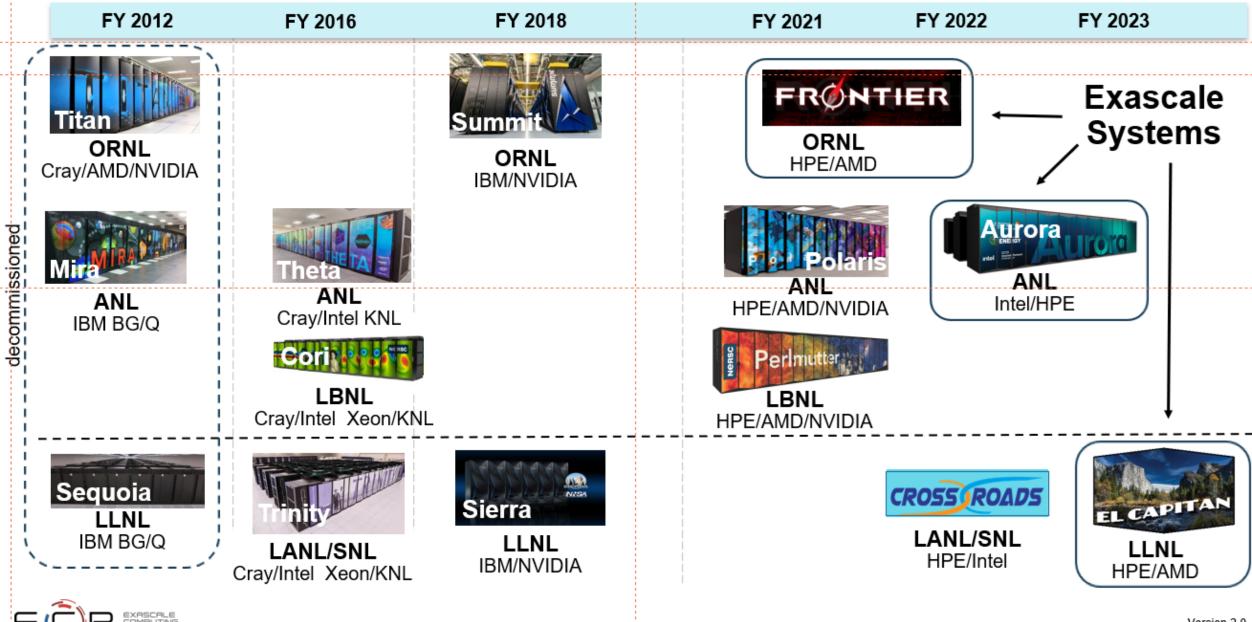
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My first trip to Tsukuba!

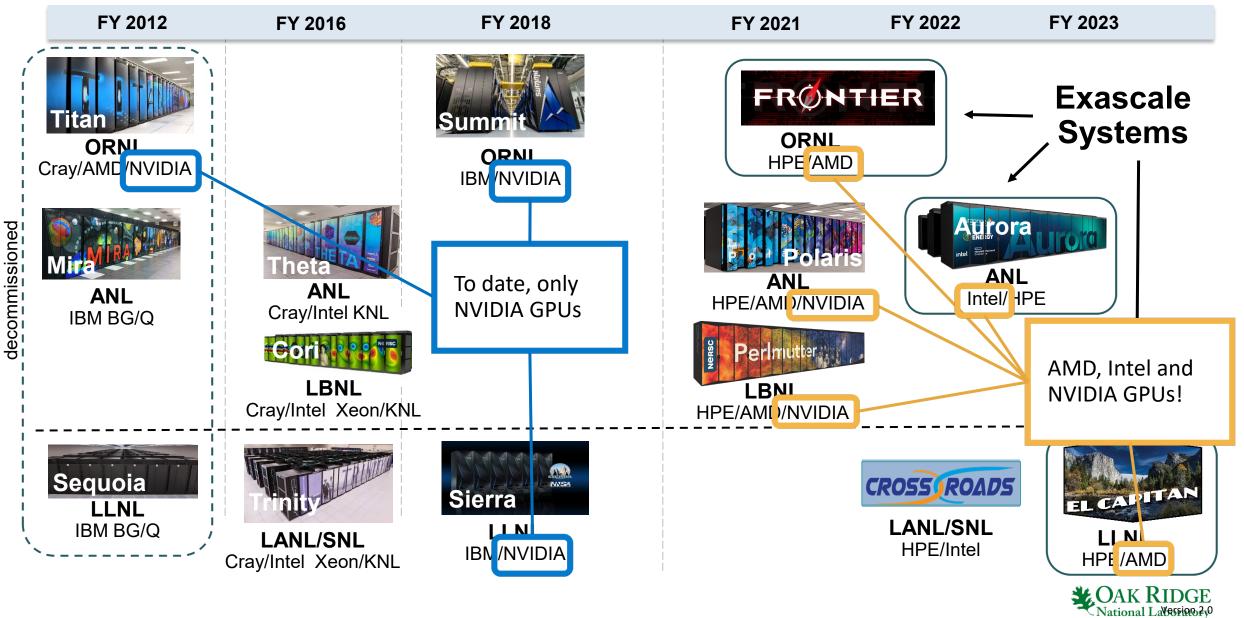
- International Exascale Software Project
- Meeting 3: Tsukuba, Japan Oct. 18-20, 2009



DOE HPC Roadmap to Exascale Systems



DOE HPC Roadmap to Exascale Systems



Frontier System

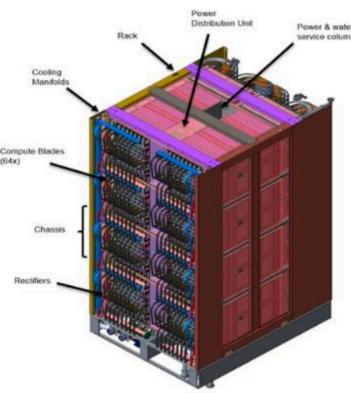
System

- 74 compute racks
- 29 MW Power Consumption
- 9,408 nodes
- 9.2 PB memory (4.6 PB HBM, 4.6 PB DDR4)
- Cray Slingshot network with dragonfly topology
- 37 PB Node Local Storage
- 716 PB Center-wide storage
- 4000 ft^2 foot print

Frontier Cabinet

Olympus rack

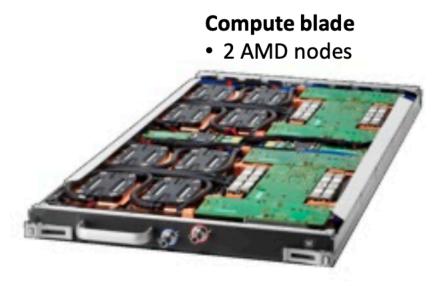
- 128 AMD nodes
- 8,000 lbs
- Supports 400 KW



Frontier Node

AMD extraordinary engineering

- 1 AMD "Trento" CPU (optimized Milan)
- 4 AMD MI250X GPUs
- 512 GiB DDR4 memory on CPU
- 512 GiB HBM2e total per node
- 4 Cassini NICs connected to the 4 GPUs



All water cooled, even DIMMS and NICs



OAK RIDGE NATIONAL LABORATORY'S FRONTIER SUPERCOMPUTER



- 74 HPE Cray EX cabinets
- 9,408 AMD EPYC CPUs, 37,632 AMD GPUs
- 700 petabytes of storage capacity, peak write speeds of 5 terabytes per second using Cray Clusterstor Storage System
- 90 miles of HPE Slingshot networking cables



1.1 exaflops of performance on the May 2022 Top500.





62.04 gigaflops/watt power efficiency on a single cabinet. 52.23 gigaflops/watt power efficiency on the full system.

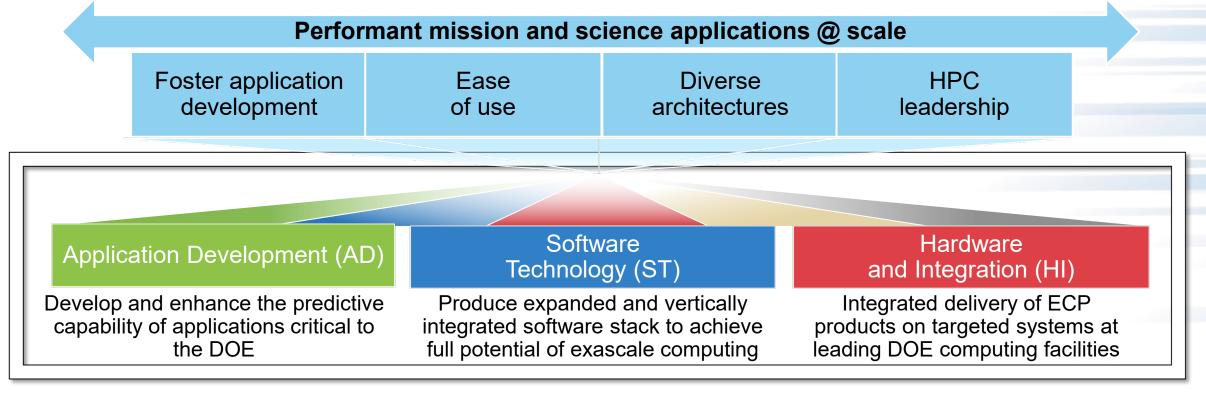


6.88 exaflops on the HPL-AI benchmark.



Sources: May

Exascale Computing Project has three technical areas to meet national goals



25 applications ranging from national security, to energy, earth systems, economic security, materials, and data 80+ unique software products spanning programming models and run times, math libraries, data and visualization 6 vendors supported by PathForward focused on memory, node, connectivity advancements; deployment to facilities

EXASCALE COMPUTING PROJECT

https://www.exascaleproject.org/

Application Development KPP-1 and KPP-2 Readiness Overview

КРР-1 Арр	Aurora EAS (Intel Proprietary)	Frontier TDS			
LatticeQCD	Verified	Improving Perf.			
NWChemEx	Full Build/Test	Initial Build/Test			
EXAALT	Verified	Improving Perf.Improving Perf.Improving Perf.Improving Perf.Improving Perf.Improving Perf.Improving Perf.			
QMCPACK	Initial Build/Test				
ExaSMR	Improving Perf.				
WDMApp	Improving Perf.				
WarpX	Verified				
ExaSky	Improving Perf.				
EQSIM	Initial Build/Test	Improving Perf.			
E3SM-MMF	Improving Perf.	Improving Perf.			
CANDLE	Ready	Improving Perf.			

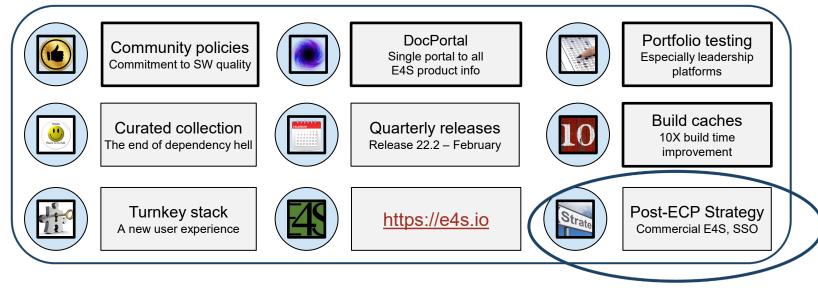
КРР-2 Арр	Aurora EAS (Intel Proprietary)	Frontier TDS				
GAMESS	Improving Perf.	Improving Perf.				
ExaAM	Initial Build/Test	Improving Perf. Improving Perf. Improving Perf. Improving Perf.				
ExaWind	Verified					
Combustion-PELE	Initial Build/Test					
MFIX-Exa	Verified					
ExaStar	Full Build/Test	Improving Perf.				
Subsurface	Stretch	Improving Perf.				
ExaSGD	Stretch	Improving Perf.				
ExaBiome	Stretch	Improving Perf.				
ExaFEL	Full Build/Test	Blocked (ROCm)				

ExaFel (Blocked ROCm) – The project team noticed during a recent work around to compiler bugs preventing compilation of Spinifel relies on an upstream compiler built locally by the OLCF team. Integration into a formal ROCm release is still pending, so we have chosen to mark this as formally blocked even though the team can currently make progress with the unofficial compiler build.

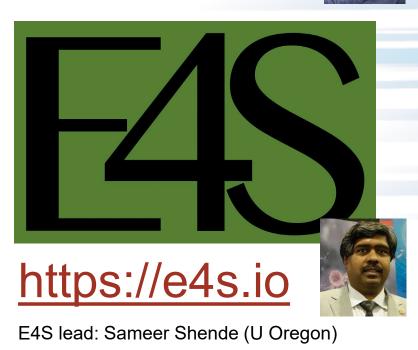


Extreme-scale Scientific Software Stack (E4S)

- <u>E4S</u>: HPC software ecosystem a curated software portfolio
- A **Spack-based** distribution of software tested for interoperability and portability to multiple architectures
- Available from **source**, **containers**, **cloud**, **binary caches**
- Leverages and enhances SDK interoperability thrust
- Not a commercial product an open resource for all
- Growing functionality: May 2022: E4S 22.05 100+ full release products







Also includes other products, e.g., AI: PyTorch, TensorFlow, Horovod Co-Design: AMReX, Cabana, MFEM



ECP is Improving the LLVM Compiler Ecosystem



COMPILER INFRASIRUCIUR												
LLVM		+ SOLLVE		+ PROTEAS-TUNE		+ FLANG		+ HPCToolkit		+ NNSA		Vendors
•Very popular open- source compiler infrastructure		•Enhancing the implementation of OpenMP in LLVM		•Core optimization improvements to LLVM		•Developing an open- source, production Fortran frontend		•Improvements to OpenMP profiling interface OMPT		Enhancing LLVM to optimize template expansion for FlexCSI, Kokkos,		 Increasing dependence on LLVM
•Permissive license •Modular, well- defined IR allows use by a lot of different languages		•Unified memory •Prototype OMP		•OpenMP offload •OpenACC capability for LLVM		•Upstream to LLVM public release		•OMPT specification improvements		Flang testing and evaluation		 Many vendors import and redistribute LLVM
different languages, ML frameworks, etc. •Backend infrastructure		features for LLVMOMP Optimizations		•Clacc •Flacc •Autotuning for		 Support for OpenMP and OpenACC Recently approved 		•Refine HPCT for OMPT improvements		Kitsune and Tapir		•Contributions and collaborations with many vendors
allowing the efficient creation of backends for new (heterogeneous)		•OMP test suite •Tracking OMP		OpenACC and OpenMP in LLVM		•Initial implementation						through LLVM •AMD •ARM
hardware. •A state-of-the-art C++ frontend, CUDA support,		implementation quality		Integration with Tau performance tools		of serial F77 compiler for CPUs under review						•Cray •HPE •IBM •Intel
scalable LTO, sanitizers and other debugging		•Training		 SYCL characterizing and benchmarking Leading LLVM-DOE 								•NVIDIA
Capabilities, and more. The LLVM Compiler Infrastructure LVM Overview The ULVM Compiler Infrastructure LVM Overview The ULVM Compiler Infrastructure LVM Overview The ULVM Compiler Infrastructure LVM Overview The ULVM Compiler Infrastructure			•Training						2255			
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Active involvement with broad LLVM community: LLVM Dev, EuroLLVM ECP personnel had 10+ presentations at the 2020 Dev Meeting



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So how did we do?



Reflections from ECP Panel at ECP AHM in May 2022

Panel Overview

- As we enter the era of Exascale, it is time to reflect
 - What did we get right?
 - What did we miss?
 - What did we omit?
- Many of you participated in these workshops and reports
 - Comments and questions welcome!
 - Please use ZOOM Q&A window

enable scientists within control technologies possible significant dynamic power runtime ta algorithms important 🚺 modeling simulations issues process USE EXAS processes components computational large time one major Computing include management technology hardware provide scale requirements understanding address approaches codes current storage different 🌭 challenges scientific code techniques however hpc simulation development computation new energy capabilities develop example complex software need critical require tools used appli research analysis needed climate future support required 10rV across performance community programming problems methods approach parallel architectures optimization high expected environment uncertainty co-design security based

> Jeffrey Vetter (ORNL), Moderator Pete Beckman (ANL) Jack Dongarra (UTK, ORNL) Bob Lucas (Ansys) Kathy Yelick (UCB)

National Laboratory

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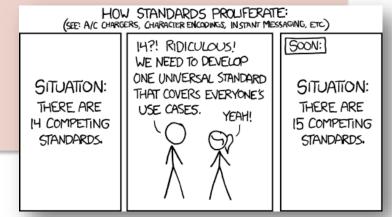
15 years is an eternity in computing - How did our predictions do?

Hits

- System power came in at O(20MW) not O(1GW)
- Few major software rewrites / evolution
 - So far, FORTRAN -> C++ is the main conversion
- ECP included applications, software, and hardware
 - ~70 teams, ~1000 researchers
 - IESP
- Concurrency (1B-way parallelism)
- Open-source software

Misses

- Systems deployed 4 years later than expected (of 2018)
- Programming systems are multiplying and immature/incomplete
- Hardware diversity
- Demise of vendor interest in HPC
- Fault tolerance



Overlooked

- Productive programming models (ala AI/ML): Python, Jupyter, Julia
- Cost of ECP + NRE + Procurements approaches \$3.6B USD
- AI/ML is not predicted (or even mentioned)
- Cloud deployment models
- Green/sustainable computing





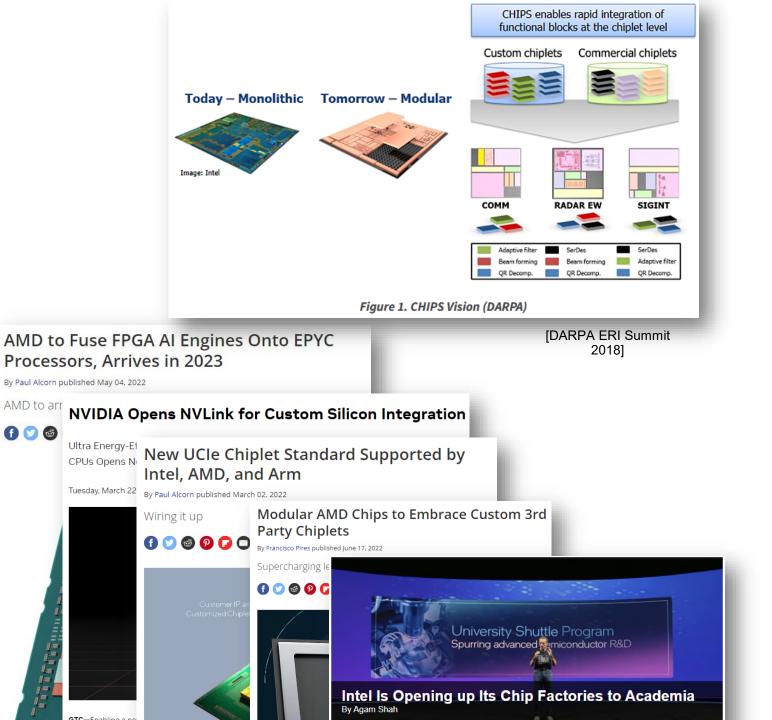
Pondering Post-Exascale Computing

• Thinking about the next 10 years



Important Architectural Trends

- Heterogeneous integration
- Chiplets
- Ecosystems and Standards
 - CXL, UCIe, BoW, ...
- Open-source Tools and IP
 - RISC-V, OpenLane, Silicon Compiler, etc
- Open foundries
- Codesign will be more important than ever

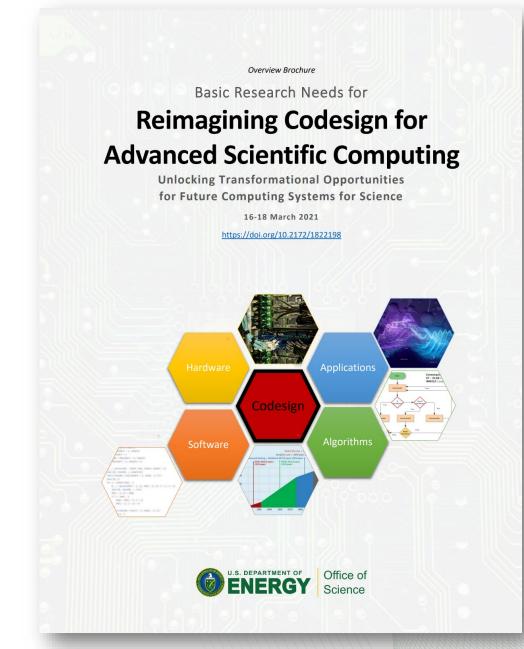


Reimagining Codesign

2021 Workshop

Four priority research directions

- Drive Breakthrough Computing Capabilities with Targeted Heterogeneity and Rapid Design
- Software and Applications that Embrace Radical Architecture Diversity
- Engineered Security and Integrity from Transistors to Applications
- Design with Data-Rich Processes
- We must make codesign agile, more accurate, and use real workloads



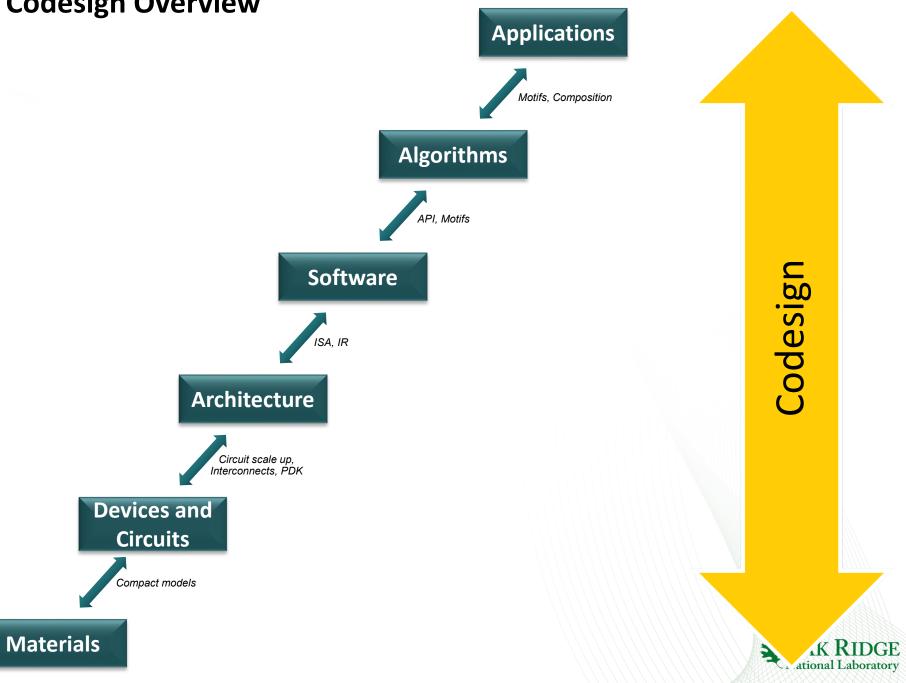
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Abisko: Microelectronics Codesign



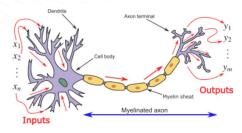
Abisko Microelectronics Codesign Overview



Abisko Microelectronics Codesign Overview



- 1. Develop better techniques for codesign from algorithms to devices and materials
- 2. Design Spiking Neural Network chiplet that can be integrated with contemporary computer architectures
- 3. Explore new devices and materials for the SNN chiplet (neuron, synapse, plasticity, etc.)
- 4. Design language abstractions and runtime support for SNN chiplet



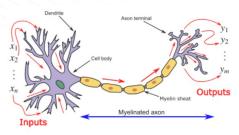
Source: Wikipedia



Abisko Microelectronics Codesign Overview



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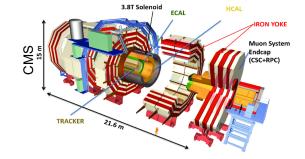
Source: Wikipedia

Motivation

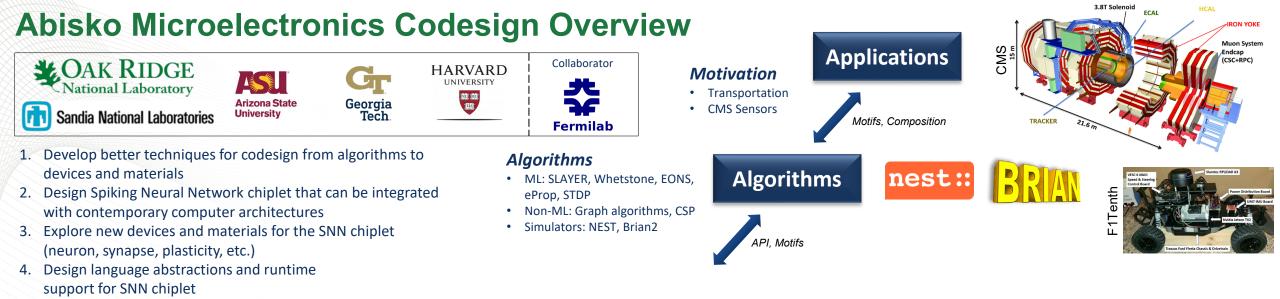
TransportationCMS Sensors

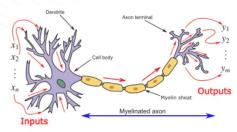
Motifs, Composition

Applications

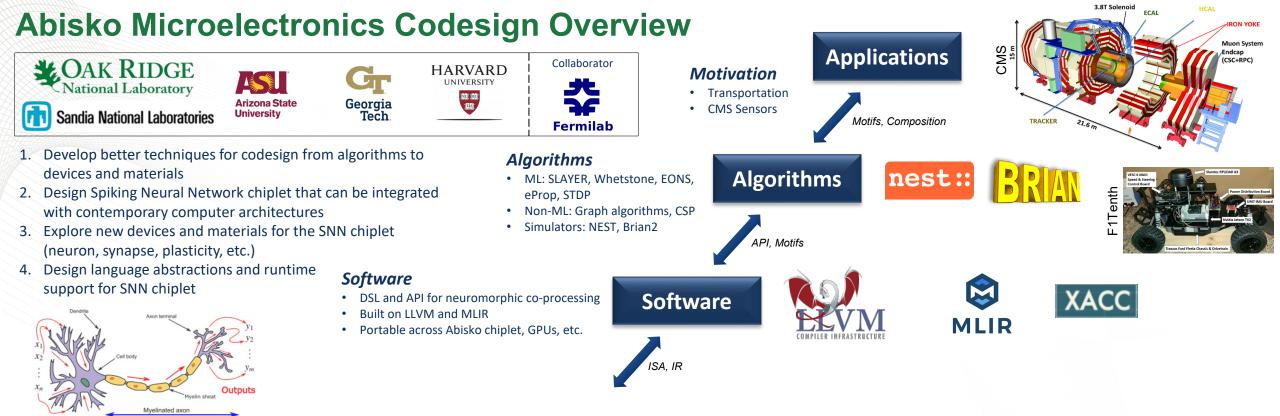




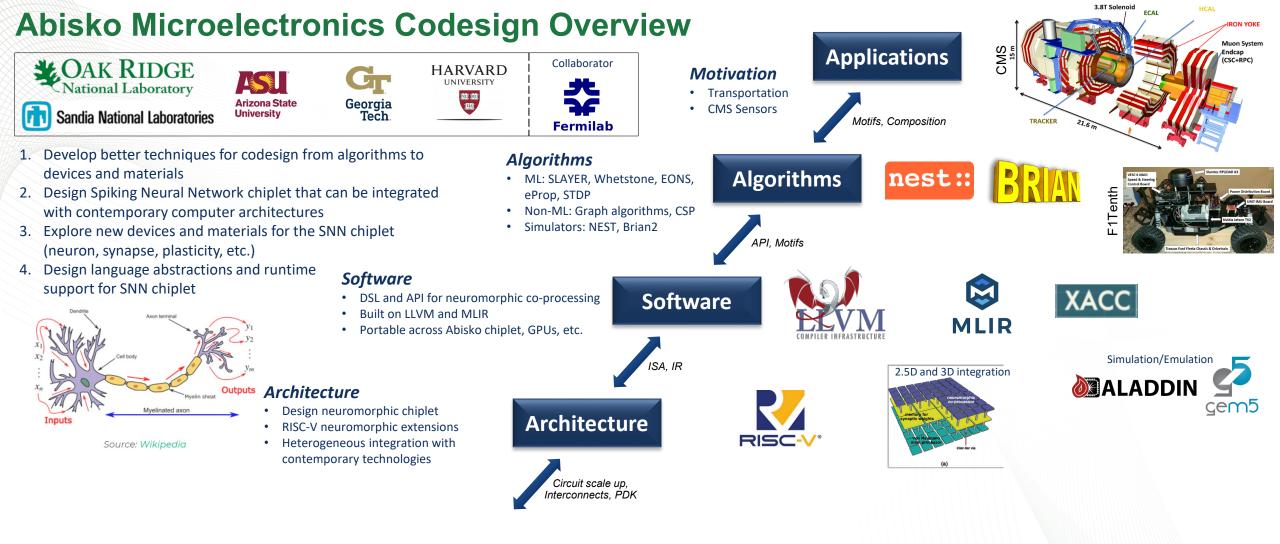




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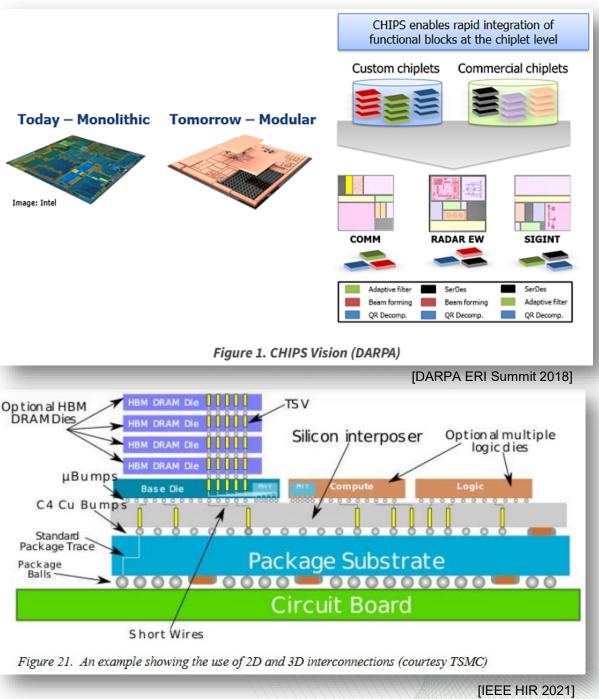
Chiplet Architectures

- Design an (analog) SNN chiplet that can be easily integrated with contemporary technologies
 - Heterogeneous integration with mixed processes
 - Compatible with existing processes
- Extensive advances in chiplets, packaging, and heterogeneous integration recently
 - Open Domain-Specific Architecture
 - UCIe, BoW, TSMC SoIC-CoW, Intel Foveros
- Using open toolchain and architecture to explore chiplet designs: RISC-V, OpenLane

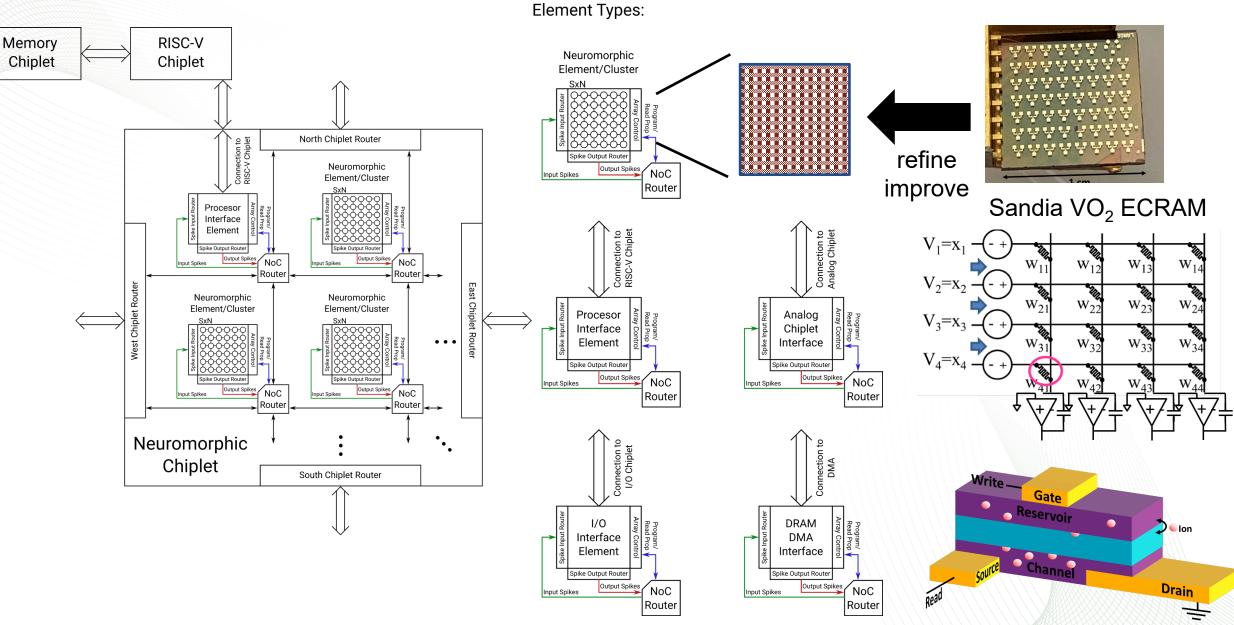




Abisko



Evaluation of 2.5D Chiplet for Neuromorphic Computing



7 Sep 2022

ASIC Flow for Digital NN (baseline)

- Investigate the performance of fully customized ASIC design for ultra-fast NN inference
 - ORNL: HLS and RTL
 - Geogia Tech: ASIC Synthesis and PD
- Model details:
 - Fixed NN architecture with quantized weights
 - Experimented with 2bit or 3bit of inputs (limited by FermiLab implementation)
- Flow:

3.

- Vitis HLS to generate RTL
- Catapult logic synthesis

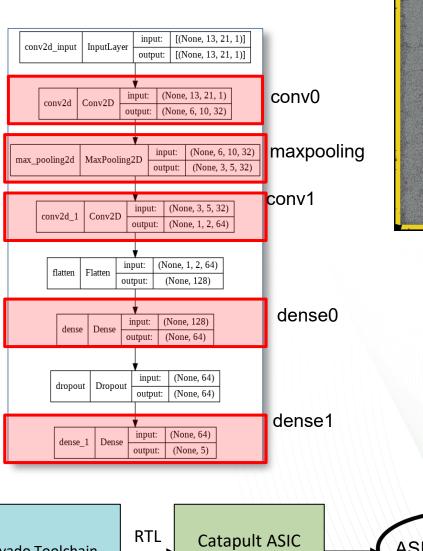
Layer Parameters

Bus width of Interface

Fixed / Loadable Weights

Bitwidth of features and weights

- Customized backend layout tool (incl. tech mapping, placement and routing)
- Achieved clock frequency of 1~ 2GHz in a 28nm technology





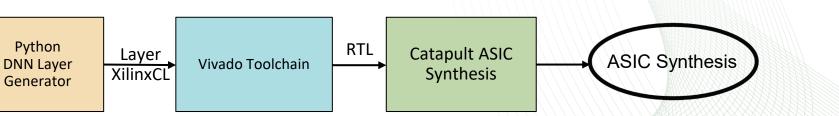
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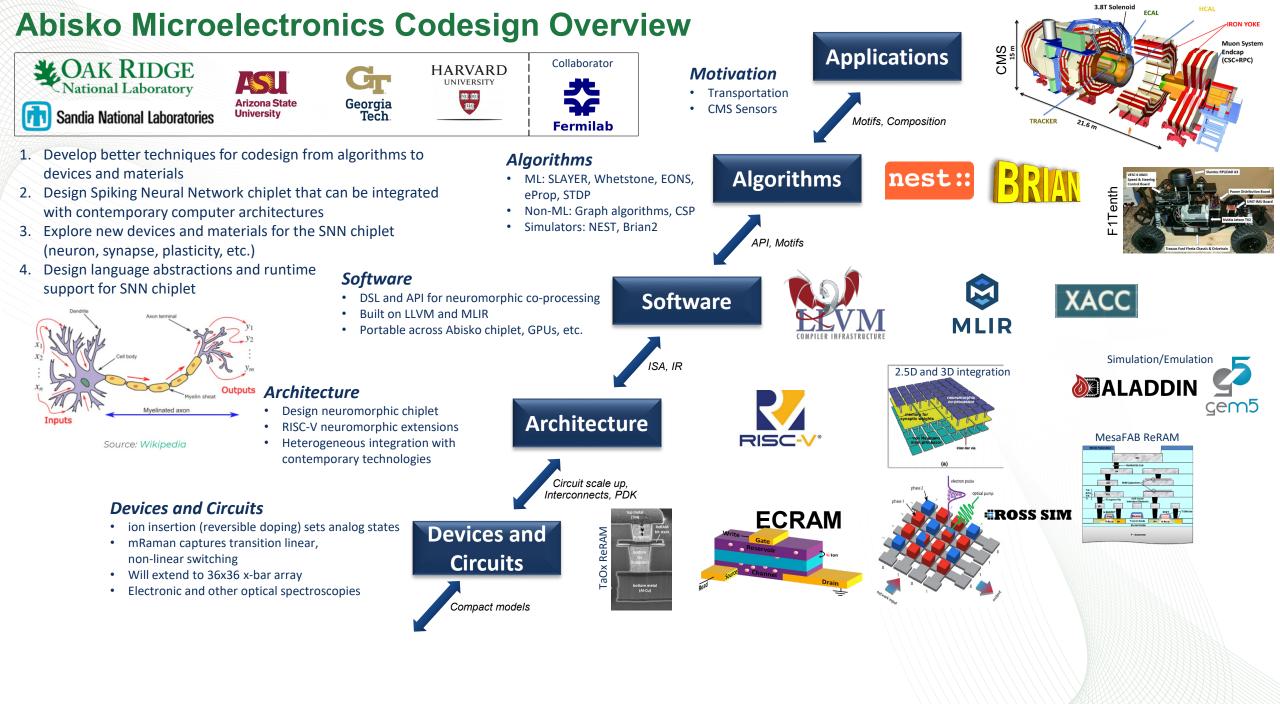






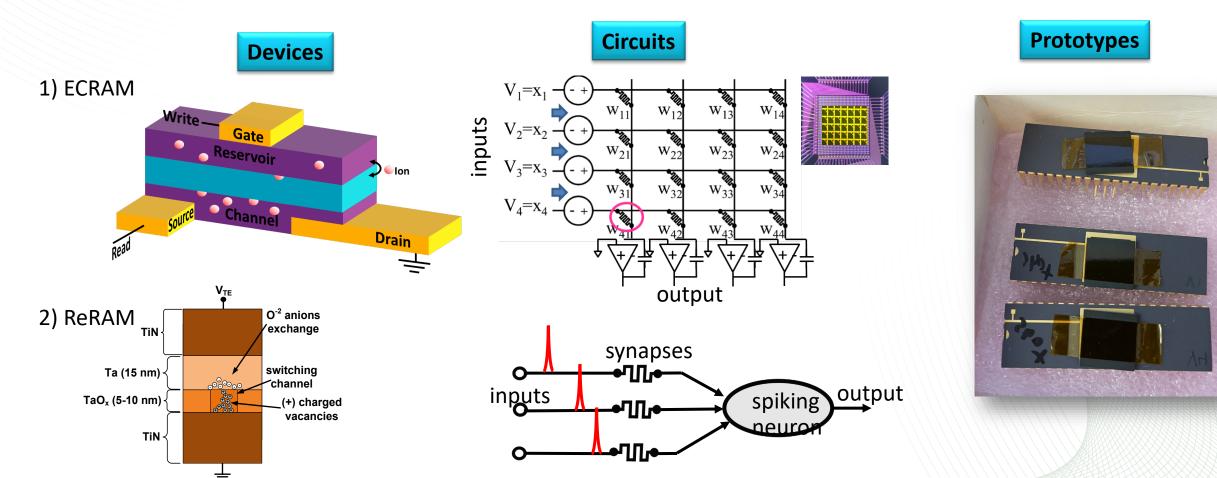
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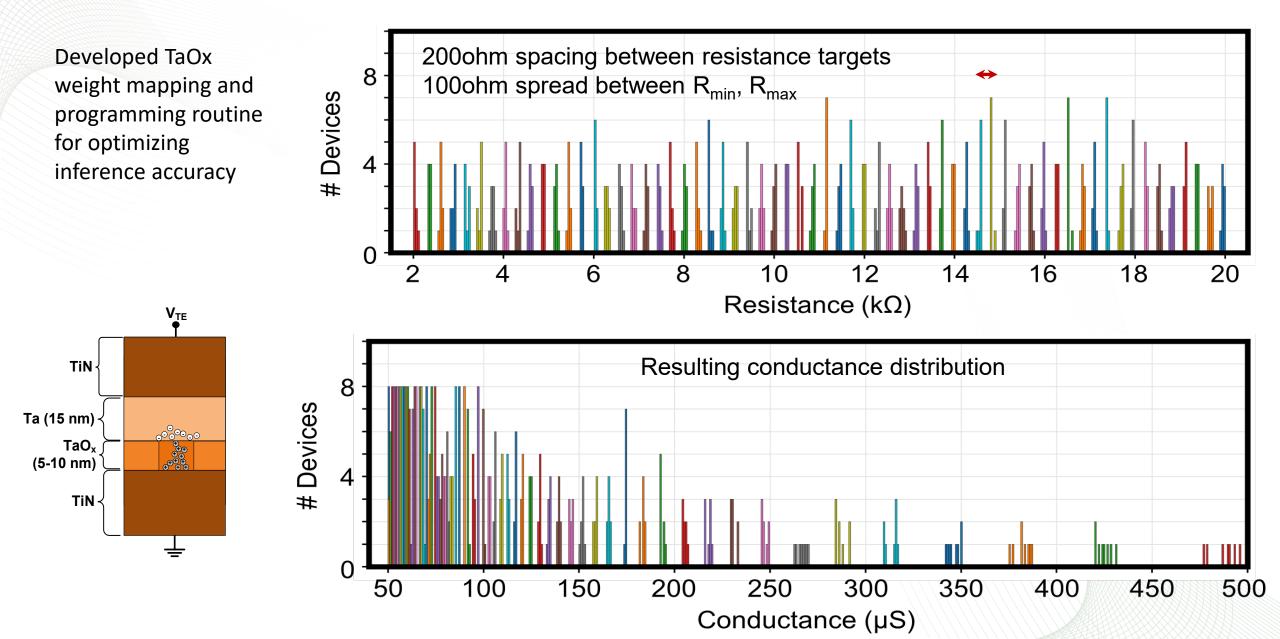


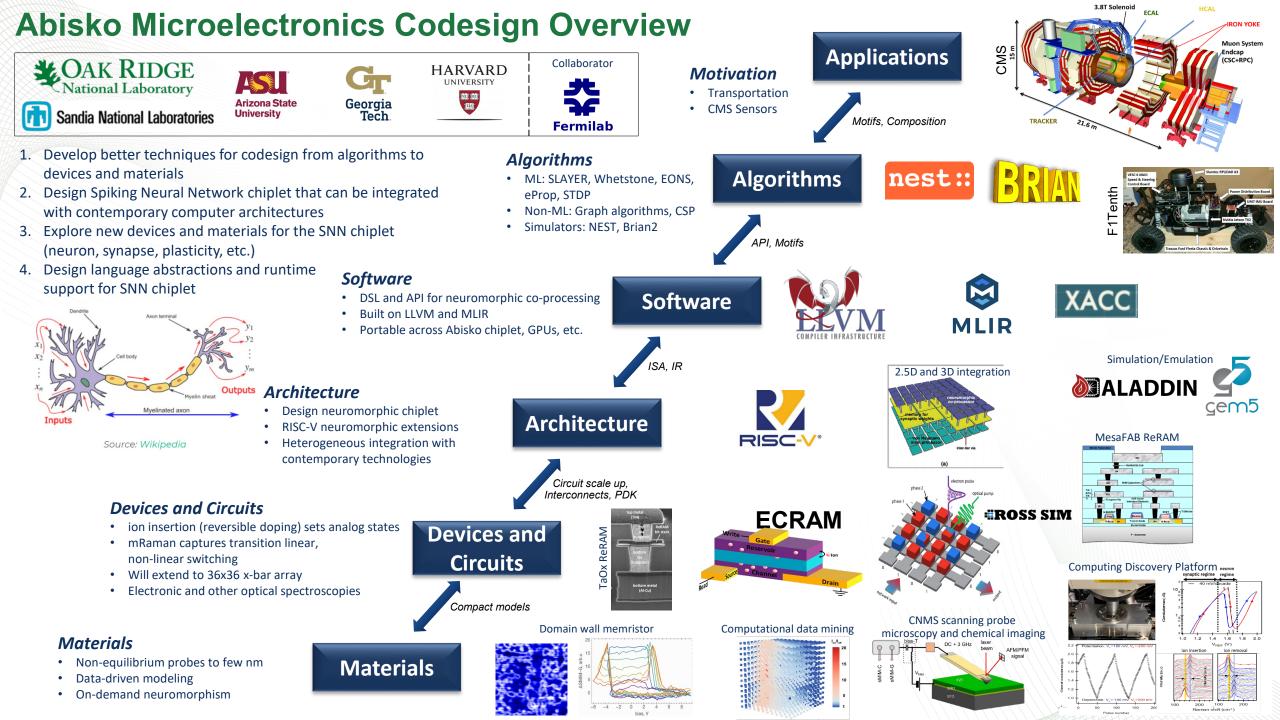
Devices and Circuits

- Goals
 - Harness the interplay between mobile defects (ions and vacancies) and electronic properties to realize functional elements for spiking and non-spiking analog neuromorphic networks
 - Create and validate small network models; generate device and network data for co-design
 - Understand and mitigate radiation induced degradation mechanisms at the device and circuit level



Experimental TaOx ReRAM Conductance Distributions







Conclusions



Recap

• Exascale is here!

- Our predictions were reasonably accurate, but we completely missed some
 - AI/ML
 - Programming systems remain major challenge
- Post-exascale
 - Heterogeneous integration and Chiplet architectures are vastly diversifying the architectural landscape
 - Post exascale will be accelerated by recent major semiconductor investments
- Abisko microelectronics codesign project developing a chiplet for analog SNN
- Start building your own chiplets today!

- Visit us (post COVID ©)
 - We host interns and other visitors year round
 - Faculty, grad, undergrad, high school, industry
- Jobs at ORNL
 - Visit <u>https://jobs.ornl.gov</u>
- Contact me <u>vetter@ornl.gov</u>
- Experimental Computing Lab
 - Lots of emerging archs
 - https://excl.ornl.gov

