### Welcome!

Thank you for joining us today! As we wait for everyone to get settled, we'd like to bring a few things to your attention:

- 1. This webinar is being recorded. The recording will be available via the Neocortex webinar webpage. Slides will also be made available online.
- 2. There will be 50 minutes of presentations followed by Q&A. To maintain a quality experience for everyone, please mute your microphone during the presentations.
- 3. We hope you will participate in this interactive webinar by:
  - Asking questions to our team via the Q&A Zoom feature.
  - These questions will seed the Q&A session in the final 10 minutes.
- 4. This webinar abides to the Neocortex code of conduct.



### *Neocortex* Code of Conduct

*Neocortex* has an external code of conduct which represents our commitment to providing an inclusive and harassment-free environment in all interactions regardless of race, age, ethnicity, national origin, language, gender, gender identity, sexual orientation, disability, physical appearance, political views, military service, health status, or religion. The code of conduct extends to all *Neocortex*-related events, services, and interactions.

**Code of Conduct:** <u>www.cmu.edu/psc/aibd/neocortex/neocortex-code-of-conduct</u>

#### **Contact:**

Neocortex ombudspersons:

- Paola A. Buitrago, PSC, Carnegie Mellon University (paola@psc.edu)
- Sergiu Sanielevici, PSC, Carnegie Mellon University (<u>sergiu@psc.edu</u>)

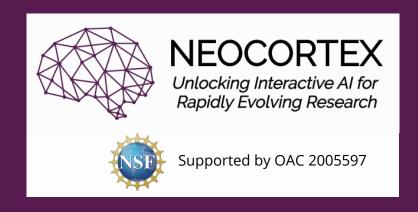


# Neocortex Overview and Spring 2023 Call for Proposals

#### Paola A. Buitrago

Principal Investigator & Project Director, Neocortex Director, Al and Big Data, Pittsburgh Supercomputing Center Carnegie Mellon University University of Pittsburgh

February 28, 2023



### Questions We are Addressing Today

- 1. What is the Neocortex program and what are its goals?
- 2. What is the innovative hardware a researcher can get access through Neocortex?
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  - What can I expect as Neocortex researcher?
- 5. How to get additional information or support from the Neocortex team?



### Speakers









### Dirk T. VanEssendelft

SDK researcher, Neocortex HPC, Al, and Data Scientist, NETL

#### **Leighton Wilson**

SDK support collaborator, Neocortex HPC Solutions Engineer, Cerebras

#### **Claire Zhang**

ML support collaborator, Neocortex ML Solutions Engineer, Cerebras

#### Paola A. Buitrago

Principal Investigator, Neocortex Director of AI and Big Data, PSC



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### The Neocortex Program





#### Context – NSF Solicitation



#### NSF Solicitation – 19-587

## Advanced Computing Systems and Services: Adapting to the Rapid Evolution of Science and Engineering Research

"The intent of this solicitation is to request proposals from organizations to serve as service providers ... to provide advance cyberinfrastructure (CI) capabilities and/or services ... to support the full range of computational-and data-intensive research across all science and engineering (S&E)."

#### Two categories:

- Category I, Capacity Systems: production computational resources.
- Category II, Innovative Prototypes/Testbeds: innovative forward-looking capabilities deploying novel technologies, architectures, usage modes, etc., and exploring new target applications, methods, and paradigms for S&E discoveries.



#### Context – NSF Award



Acquisition and operation of *Bridges, Bridges-AI*, *Bridges-2*, and *Neocortex* are made possible by the National Science Foundation:

NSF Award OAC-2005597 (\$12.25M awarded to date): Category II: Unlocking Interactive AI Development for Rapidly Evolving Research





Cerebras and HPE delivered *Neocortex* 



### Context – Project Goals



## **Neocortex**, Unlocking Interactive AI Development for Rapidly Evolving Research

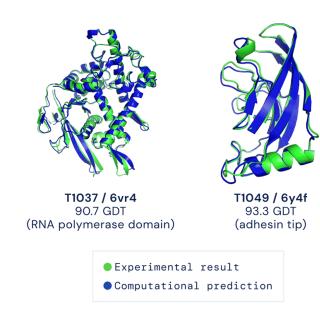
A new NSF funded advanced computing project with the following goals:

- Deploy Neocortex and offer the national open science community revolutionary hardware technology to accelerate AI training at unprecedented levels.
- Explore, support and operate Neocortex for 5 years.
- Engage a wide audience and foster adoption of innovative technologies.



### **Driving Use-Cases**

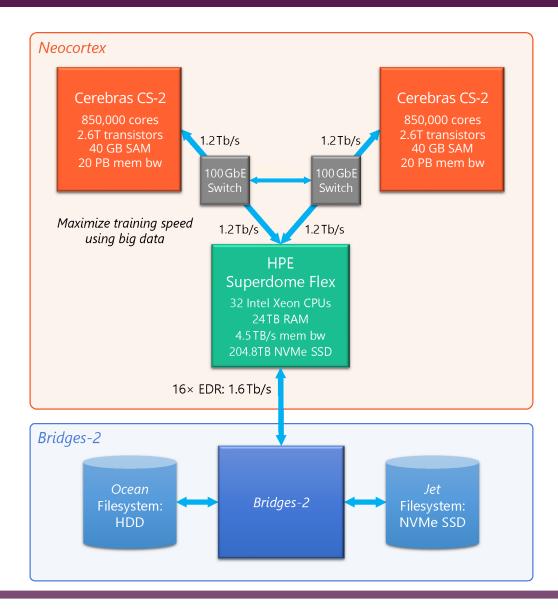
- Transform and accelerate Al-enabled research
- Development of new and more efficient AI algorithms and graph analytics
- Foster greater integration of artificial deep learning with scientific workflows
- Democratize access to game changing compute power
- Explore the potential of a groundbreaking new hardware architecture
- Support research needing large-scale memory (genomics, brain imaging, simulation modeling)
- Augmenting traditional computational science with rapidlyevolving methodologies and technologies
- User-centric and interactive computing modalities



Animation from https://deepmind.com/blog/article/alphafold-a-solution-to-a-50-year-old-grand-challenge-in-biology. Retrieved on August 2021.

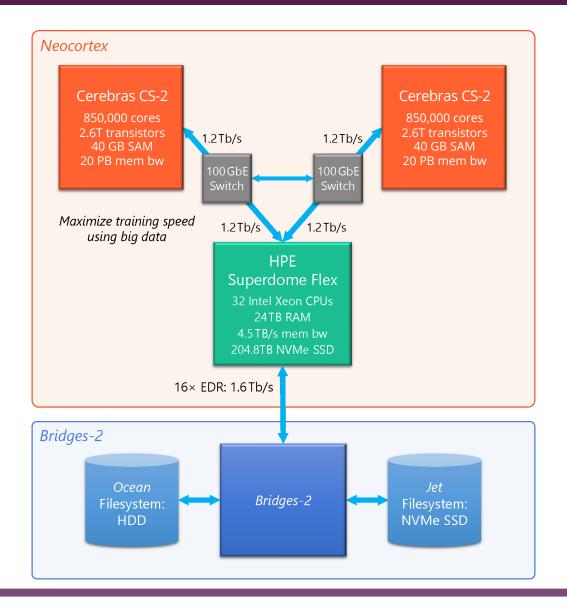


### **Neocortex System Overview**





### Neocortex System Overview



Neocortex main Al accelerator is the Cerebras WSE, an alternative to other accelerators like GPUs.



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Cerebras modelzoo ML models 2

Models similar to the Cerebras modelzoo models

3

General purpose SDK

4

WFA, WSE Fieldequation API

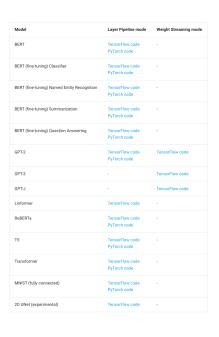








15 DL models: BERTx5 (standard, classifier, name entity recognition, summarization, question answering), GPT-2, GPT-3, GPT-J, Linformer, RoBERTa, T5, Transformer, FC-MNIST, 2D Unet.

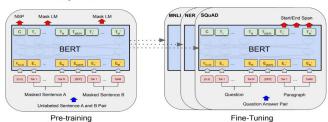


#### List of topics · Overview of the mode · Sequence of the steps to perforn Key features from CSoft platform used in this reference implementation Variable Sequence Lengt Multi-Replica data parallel training Structure of the code Before you start Dataset Preparations Download OpenWebText datase Other datasets and download links Allocate subsets for training and validation Create TFRecords Create TFRecords for 2-phase pre-training Phase 1: MSL 128 Phase 2: MSI 512 BERT input function BERT features dictionar To compile/validate, run train and eval on Cerebras System To run train and eval on GPU/CPU MLM loss scaling Configurations included for this mode References

#### Overview of the model

Bidirectional Transformers for Language Understanding (BERT) is an encoder-only transformer-based model designed for natural language understanding. This directory contains implementations of the BERT model. It uses a stack of transformer blocks with multi-head attention followed by a multi-layer perceptron feed-forward network. We support removing next-sentence-prediction (NSP) loss from BERT training processing with only masked-language-modeling (MLM) loss. The training pipeline has 2 phases. We first train with maximum sequence length of 128 and then train with maximum sequence length of 512. More details of the model can be found in the appendix

An overview of the model diagram is here:



We also support the ROBERTa model, which is very similar to BERT in terms of architectural design. In order to improve the results on BERT some changes are made with objective functions (removing NSP), batch sizes, sequence lengths and masking patterns (dynamic vs. static) Difference between dynamic and static masking is discussed here

We also support [ PubMedBERT ] model, which is pre-trained from scratch using abstracts from PubMed dataset. PubMedBERT model achieves state-of-the-art performance on several biomedical NLP tasks, as shown on the [Biomedical Language Understanding and Reasoning Benchmark

https://portal.neocortex.psc.edu/docs/models\_supported.html





Models similar to the Cerebras modelzoo models

ML models that are a **combination of the building blocks** used by modelzoo
models and/or the layers supported by
Cerebras as listed in their documentation.

https://docs.cerebras.net/en/latest/tensor flow-docs/api-rst/tf.html

**15 Modelzoo DL models**: BERTx5 (standard, classifier, name entity recognition, summarization, question answering), GPT-2, GPT-3, GPT-J, Linformer, RoBERTa, T5, Transformer, FC-MNIST, 2D Unet.

https://portal.neocortex.psc.edu/docs/models\_supported.html



- Pioneering algorithm coding from scratch.
- Analogous to CUDA for Nvidia GPUs.
- ML kernels cannot be integrated with Pytorch and/or TensorFlow.
- Requires significant commitment.
- Will learn more form Leighton in the upcoming presentation.



General purpose

**SDK** 



General

purpose!



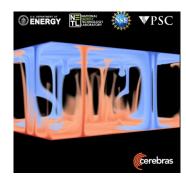
**WFA**: API recently used for advancing CFP simulations at unprecedented resolution and speed

(more info).

• Pioneering work - Beta testing of the WFA library.

- Only a few groups would be welcomed.
- Close collaboration with Dirk's team, PSC, and Cerebras.
- More details in Dirk's upcoming presentation.

Field equations, includes ML inference







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### Spring 2023 Call for Proposals

 All details available in the official webpage: <a href="https://www.cmu.edu/psc/aibd/neocortex/2023-03-cfp-spring-2023.html">https://www.cmu.edu/psc/aibd/neocortex/2023-03-cfp-spring-2023.html</a>

Neocortex Spring 2023 Allocation Submissions		
Name	Date (ET)	
Application begins	March 15, 2023	
Application ends	April 12, 2023 (Anywhere on Earth time zone)	
Response ends	May 10, 2023	
Allocation starting date	User access to start mid-May 2023 (rough estimate)	



### Spring 2023 Call for Proposals

- Open to all U.S.-based university and non-profit researchers.
- Offered at no cost for researchers advancing open-science work.
- Applications welcomed and processed through EasyChair.
- Applications welcomed for a period of 5 weeks.
- Applications will be evaluated as they come in. Apply as soon as convenient!
- Lightweight application via a short form.
- Onboarding meetings will be scheduled to confirm scope of the project and suitability.



### Spring 2023 Call for Proposals

- Users expected to be onboarded by mid May.
- Allocations to Neocortex resources and Bridges-2 will be initially granted for a year by default.
- Close collaboration and constant communication between domain projects,
   PSC, and vendors is expected. Checkpoint sessions every 3 months or so.
- Feedback and user experiences are expected to further enrich the project.
- More technical details on the Cerebras servers, the ML frameworks, SDK, WFA, and applications supported, in the second part of the webinar to be presented by Cerebras and NETL collaborators.



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### To Learn More and Participate

Watch the Neocortex website for updates!	https://www.cmu.edu/psc/aibd/neocortex/
Join the neocortex-updates list	https://www.cmu.edu/psc/aibd/neocortex/newsletter-sign-up.html
Apply to upcoming CFP	https://www.cmu.edu/psc/aibd/neocortex/2 023-03-cfp-spring-2023.html
Contact us with additional questions, input, or requests	neocortex@psc.edu



### To Learn More and Participate

Watch the Neocortex website for updates!	https://www.cmu.edu/psc/aibd/neocortex/
Join the neocortex-updates list	https://www.cmu.edu/psc/aibd/neocortex/newsletter-sign-up.html
Apply to upcoming CFP	https://www.cmu.edu/psc/aibd/neocortex/2 023-03-cfp-spring-2023.html
Contact us with additional questions, input, or requests	neocortex@psc.edu



### **Thank you** to all those contributing to *Neocortex*!

























































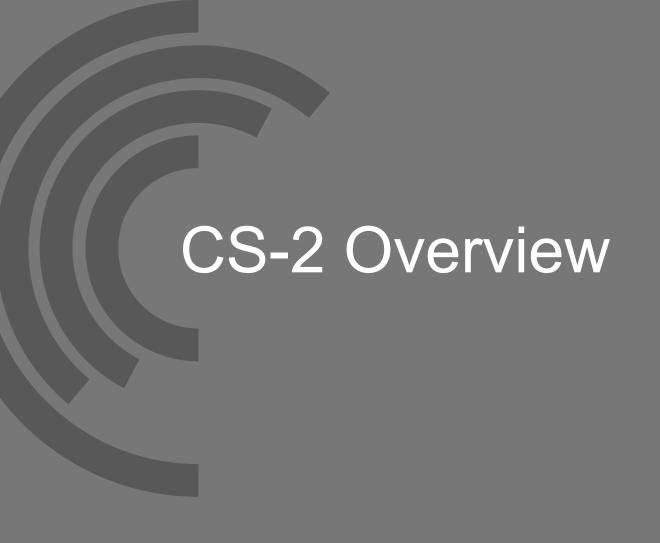
# Cerebras CS-2: the AI Compute Engine for Neocortex

**February 28, 2023** 

### **Outline**

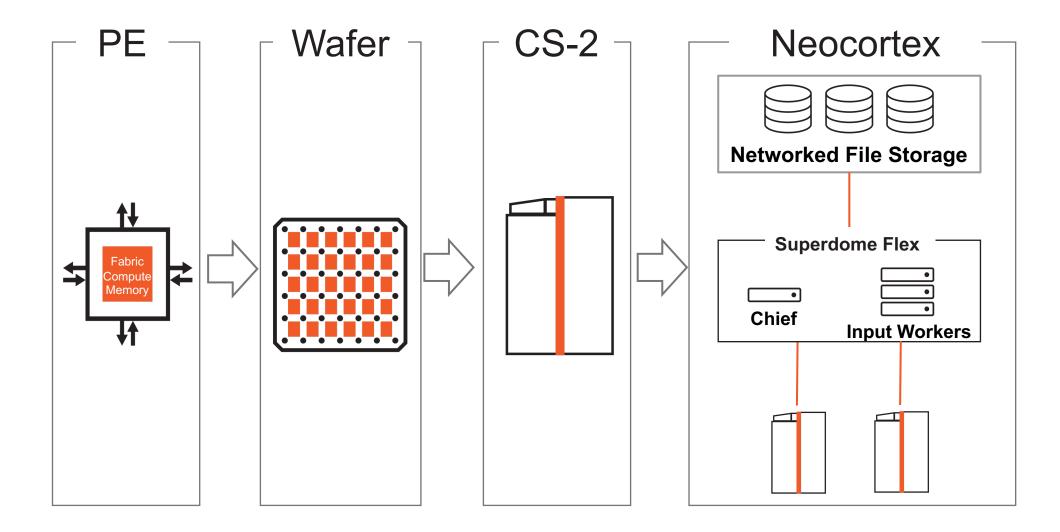
- CS-2 Overview
- CS-2 for Deep Learning
  - PyTorch and TensorFlow integration
  - Reference implementations, docs, supported layers
  - DL projects of interest with examples
- CS-2 for HPC using the SDK
  - Programming with the Software Development Kit (SDK) and Cerebras Software Language (CSL)
  - Examples of successful HPC projects
  - HPC topics of interest







### System Hierarchy







# Cerebras Wafer Scale Engine (WSE-2)

#### The Most Powerful Processor for Al & HPC

**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

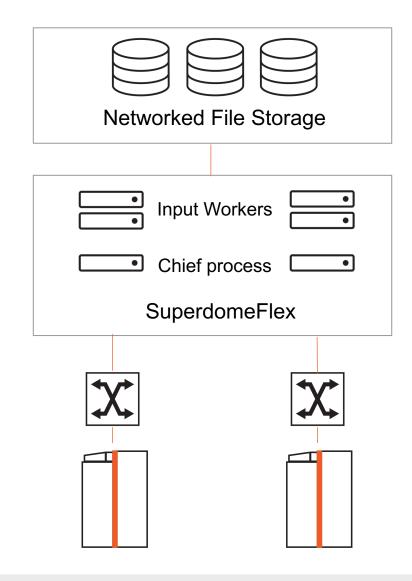
**7nm** process technology

### Cluster-scale performance in a single chip



### Deployment and job execution within Neocortex

- CS-2 is a network-attached accelerator
- Cerebras software runs on CS-2 and on the SuperdomeFlex
  - Chief compiles the code and manages CS-2
  - Input workers read data, run the input pipeline, and stream data to CS-2
- Loss output, summaries, checkpoints are streamed from CS-2 to SuperdomeFlex
- Jobs are managed by slurm

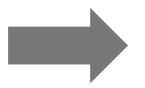




### Developer Resources

\*please refer to the <u>Original Cerebras Installation</u> version/sections for both the Model Zoo repository and Software Documentation

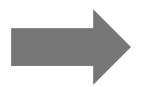
For ML developers



#### Cerebras Model Zoo repository

(<a href="https://github.com/Cerebras/modelzoo/tree/original-cerebras-installation">https://github.com/Cerebras/modelzoo/tree/original-cerebras-installation</a>)



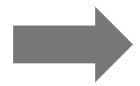


Cerebras ML Software Documentation (Original Cerebras Installation sections of

https://docs.cerebras.net/en/latest/index.html



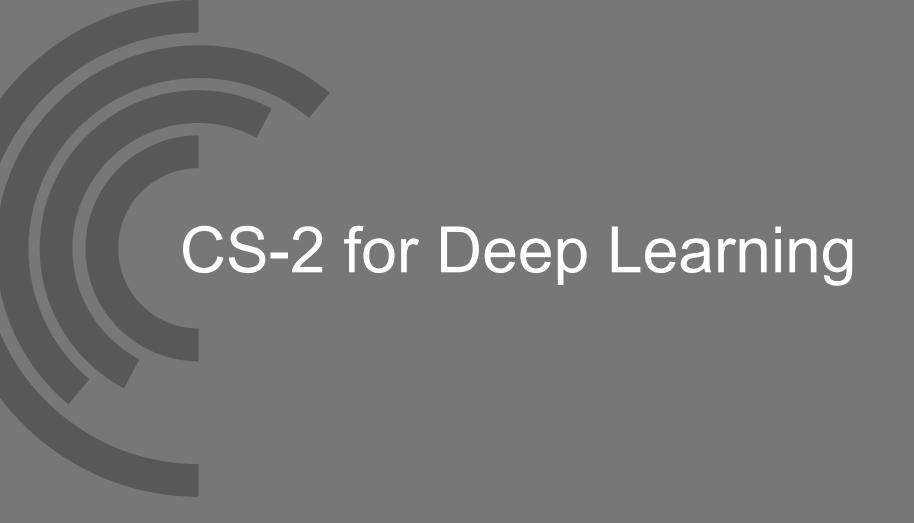
For HPC developers



Cerebras SDK









# Frameworks supported



### **TensorFlow**

#### Class:

#### CerebrasEstimator

- Based on TF Estimator, takes over executions after XLA compilation
- TensorFlow 2.2



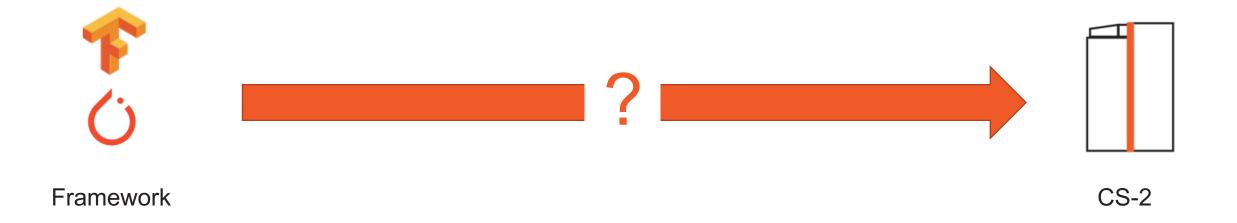
### **Python Module:**

#### cerebras.framework.torch

- Based on PyTorch XLA
- Wrappers for Dataloader, Module, Session
- PyTorch 1.11

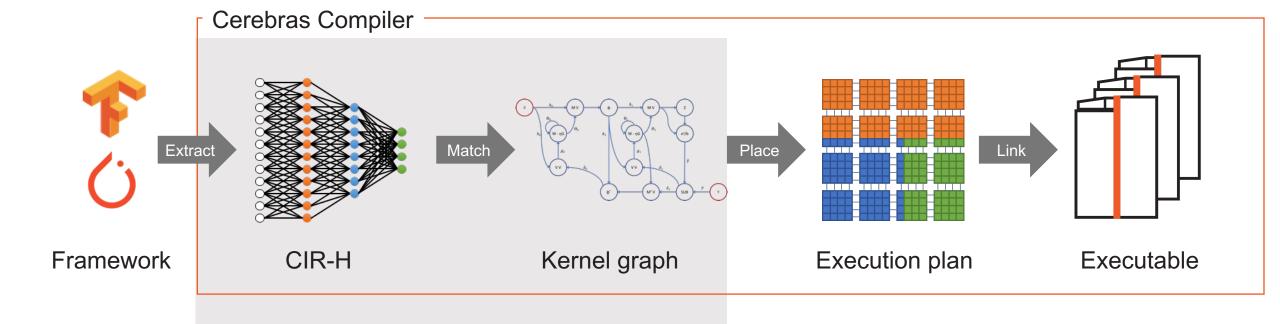


### How do we translate a model into a CS executable?





### The Cerebras Software Platform

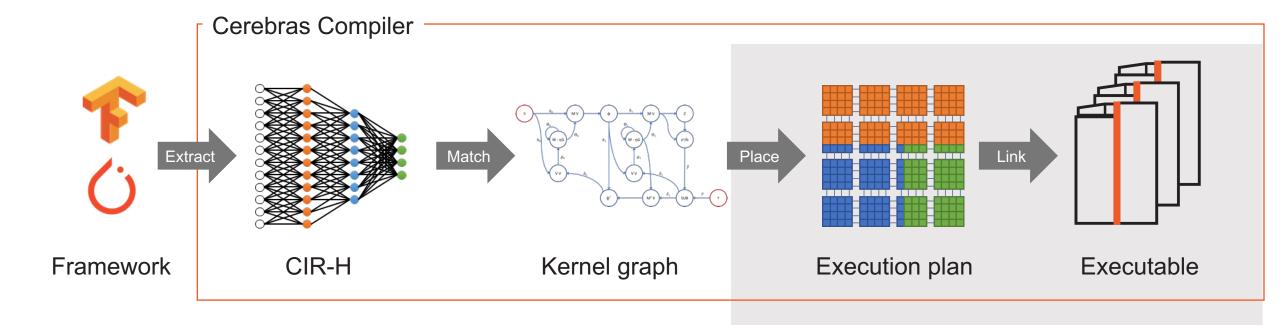


### Feature Support

Extract **graph representation** of model from framework and match operations with **kernel library** 



### The Cerebras Software Platform

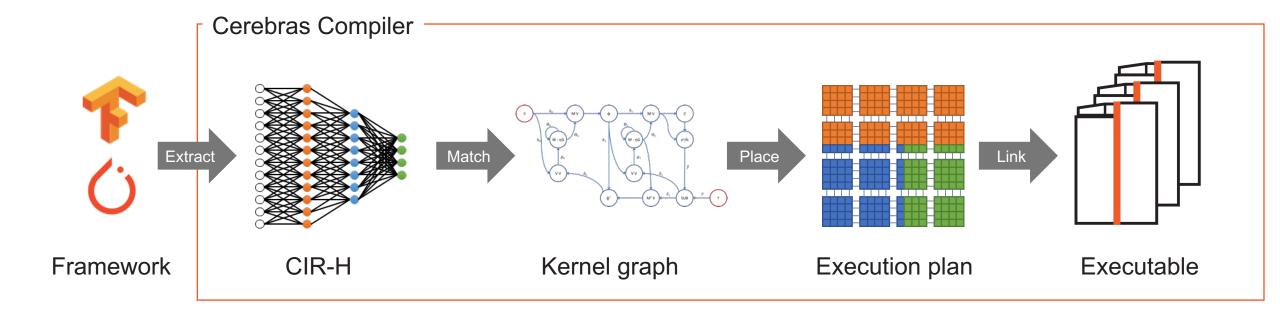


#### **Hardware Placement**

Assign kernels to **regions of fabric** and create **executable** to be run by CS-2.



### The Cerebras Software Platform



Program a cluster-scale resource with the ease of a single node



# ML Software Key Features

#### **Network Architectures**

- Transformers (TF and PyT)
  - E.g., BERT, RoBERTa, AIAYN, T5, GPT
- Multi-layer Perceptrons (MLP) (TF and PyT)
- Experimental (TF only)
  - UNet limited functionality

#### **General features**

- Supports Train, Eval
- Trained weights in standard TF and PyT formats
- Monitor your runs with TensorBoard
- Multi-replica support for smaller models
- \* Please refer to the Original Cerebras Installation Model Zoo repository for architectures we support.
- \* We recommend starting from the Model Zoo implementations to build your models.



## Topics of interest for ML applications

- Neocortex is best suited for running Transformer style models such as BERT, GPT, Transformer, T5, and ViT.
- Transformer style models cover a wide range of data modeling tasks such as:
  - Sequence classification sentiment analysis, molecule properties
  - Sequence annotation extractive summarization, protein binding site identification
  - Sequence generation abstractive summarization, candidate drug generation
  - Sequence to sequence mapping Natural language translation, code translation
  - Representation learning for biological sequences (genome, epigenome, protein)
- Many data modeling task that historically used other architectures can and have been reframed to leverage the transformer architecture. Some examples are:
  - Image classification: CNN → BERT(ViT)
  - Autoregressive sequence/time-series modeling: RNN → GPT
  - Graph modeling: GNN → BERT with adjacency attention mask



## Example Projects/ Models

- GSK: new sequence modeling for genetic medicine
  - "Epigenomic language models powered by Cerebras" Trotter, 2021
- PubMedBERT
  - "Domain-specific language model pretraining for biomedical NLP" Gu, 2021
- AntiBERTa
  - "Deciphering the language of antibodies using self-supervised learning" Leem, 2021
- TAPE
  - "Evaluating protein transfer learning with TAPE" Rao, 2019
- SMILES-BERT
  - SMILES-BERT: Large Scale Unsupervised Pre-Training for Molecular Property Prediction" Wang, 2019.



### Resources

#### Documentation: docs.cerebras.net



Software Documentation

Q Search the docs ...

Software Release Notes

Documentation Updates

#### **CEREBRAS BASICS**

How Cerebras Works

The Cerebras ML Workflow

#### **GETTING STARTED**

Checklist Before You Start

TensorFlow Quickstart

PyTorch Quickstart

#### MODEL ZOO

Model Support Matrix

#### DEVELOP WITH

Develop Wilde Terroreller

DEVELOP WITH PYTORCH

#### **Explore the Documentation**

This documentation will help you program for the CS system. It covers both basic and advanced topics. Use these docs to accelerate your machine learning training and inference applications on the CS system. Here you will find getting started guides, quickstarts, tutorials, code examples, release notes. and more.

#### Learn Cerebras basics

#### Big picture view of a CS system

#### How Cerebras works

Start with this big picture before you dive into your ML development with Cerebras system.

#### Programming model and the compiler

Get to know how Cerebras separates compile vs execution, and the compiler flow from framework to the executable.

#### The Cerebras CPU cluster

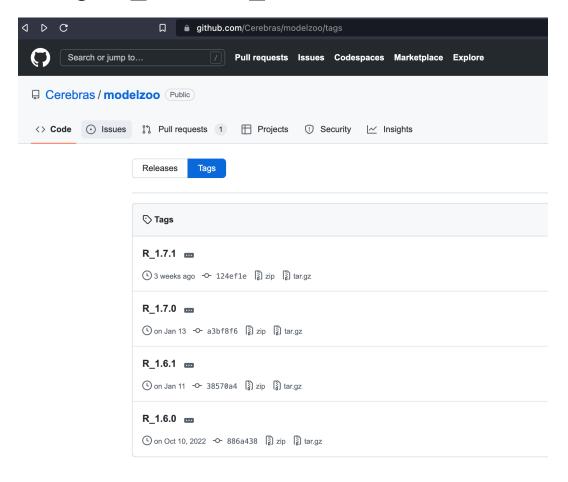
How a Cerebras multi-worker configuration differs from a GPU multi-worker configuration.

#### MI workflow on Carebras

Cerebras ML workflow

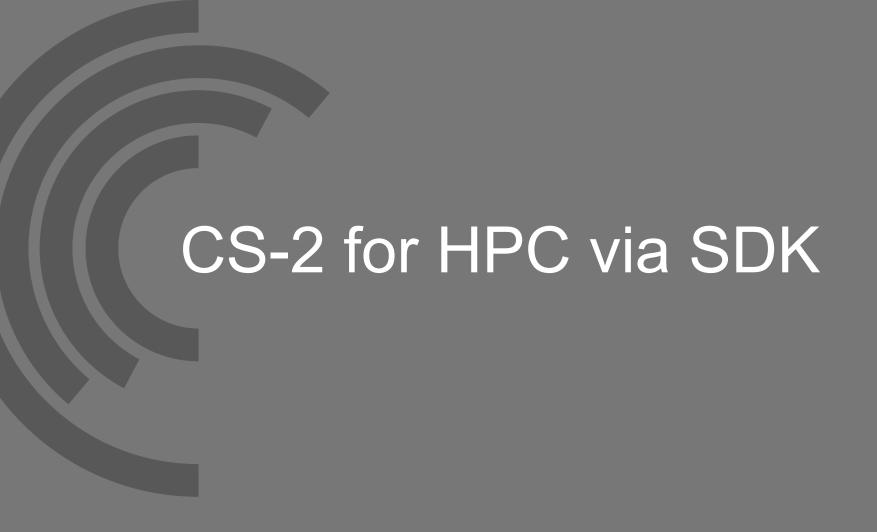
Cerebras Model Zoo:

github.com/Cerebras/modelzoo/tree/ original\_cerebras\_installation



Please check out the **Original Cerebras Installation** version/sections.





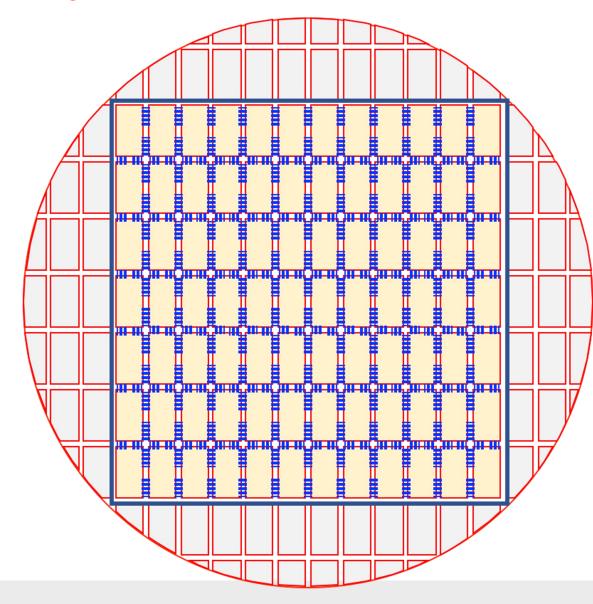


# Does your application scale poorly across nodes?

**Examples:** FFT-based solvers, particle simulators, non-linear problems with iterative solvers

#### The Cerebras solution:

- The WSE-2 has a fabric that is high bandwidth and low-latency, allowing for excellent parallel efficiency for non-linear and highly communicative codes
- The CS-2 system has **850k cores** and can fit problems on an individual chip that take tens to hundreds of traditional small compute nodes.
  - Each core is individually programmable





# Is your application constrained by data access?



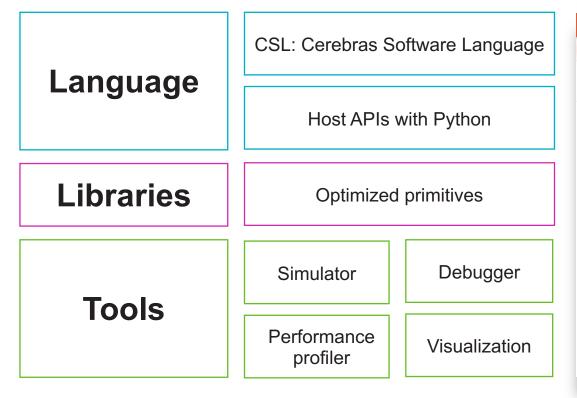
**Examples:** Stencil based PDE solvers, linear algebra solvers, signal processing, sparse tensor math, big data analysis

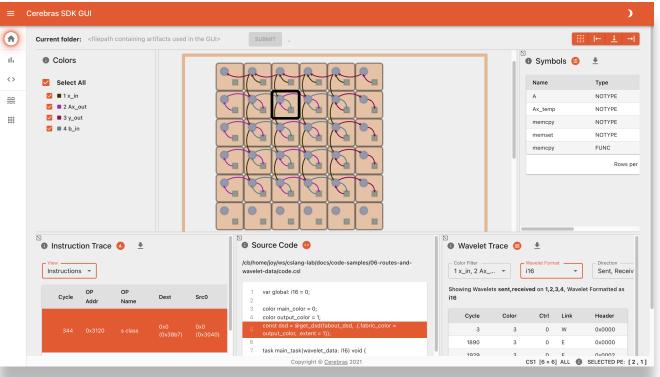
#### The Cerebras solution:

- The CS-2 system has 40 GB of SRAM uniformly distributed across the wafer that is 1 cycle away from the processing element
  - Speeds up memory access by orders of magnitude
- The CS-2 system is capable of 1.2 Tb/s bandwidth onto the chip
  - Stream data onto the chip as required



### Cerebras SDK

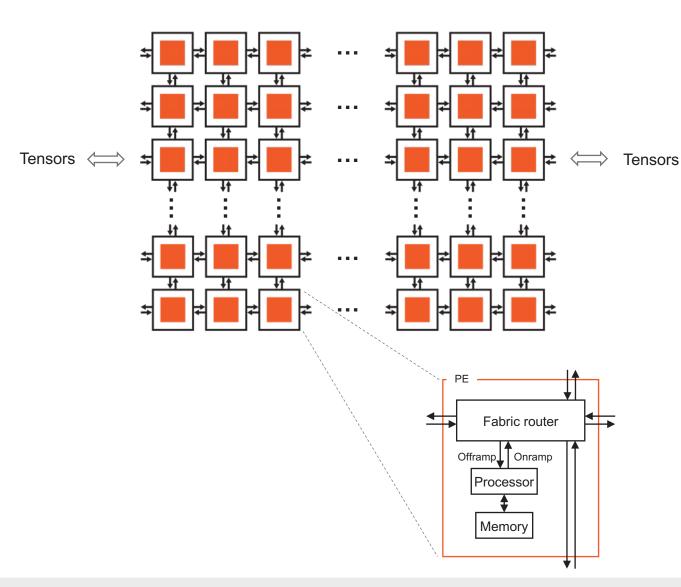




A general-purpose parallel-computing platform and API allowing software developers to write custom programs ("kernels") for Cerebras systems.



# **CS-2 Dataflow Programming**



To the programmer, the CS-2 appears as a logical 2D array of 850k individually programmable Processing Elements (PEs)

#### Flexible compute

- General purpose CPU
- 16- and 32-bit native FP and integer data types
- Tasks triggered by the arrival of data packets

#### Flexible communication

- Programmable router
- Static or dynamic routes (aka colors)
- Data packets (aka wavelets) passed between PEs
- 1 cycle for PE-to-PE communication

#### **Fast memory**

- 40GB on-chip SRAM
- Data and instructions
- 1 cycle read/write



# From a Programmer's Perspective

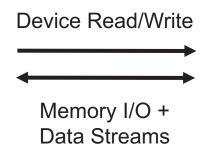
### **Host CPU(s): Python**

- Loads program onto simulator or CS-2 system
- Streams in/out data from one or more workers
- Reads/writes device memory

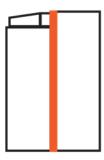
### **Device: CSL**

- Target software simulator or CS-2
- CSL programs run on groups of cores on the WSE, specified by programmer
- Executes dataflow programs











# **CSL: Language Basics**

- Types
- Functions
- Control structures
- Structs/Unions/Enums
- Comptime
- Builtins
- Module system
- Params
- Tasks
- Data Structure Descriptors
- Layout specification

Straight from C (via Zig)

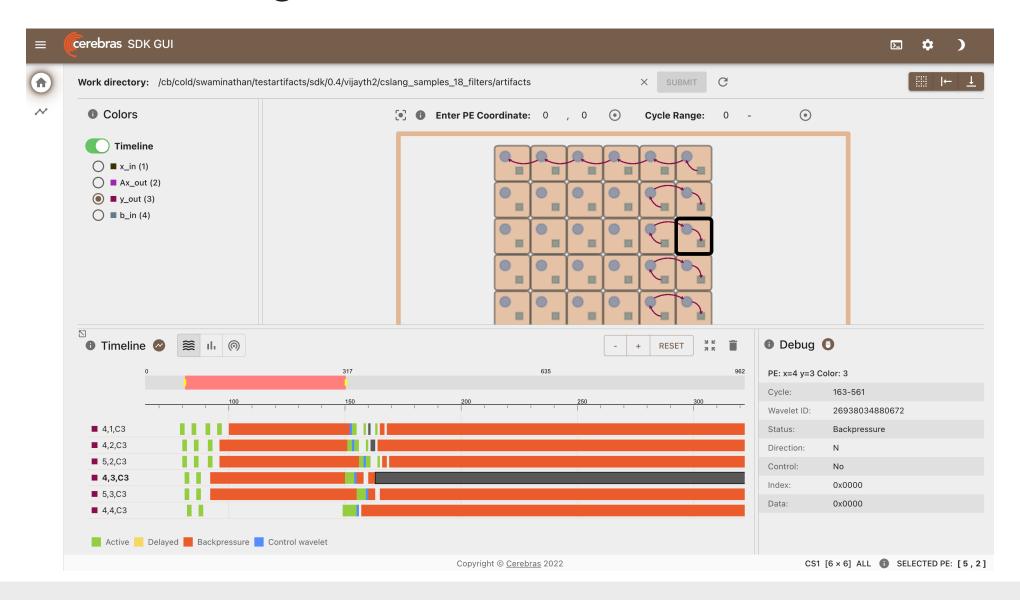
CSL specific

# Used for writing device kernel code

Familiar to C/C++/HPC programmers

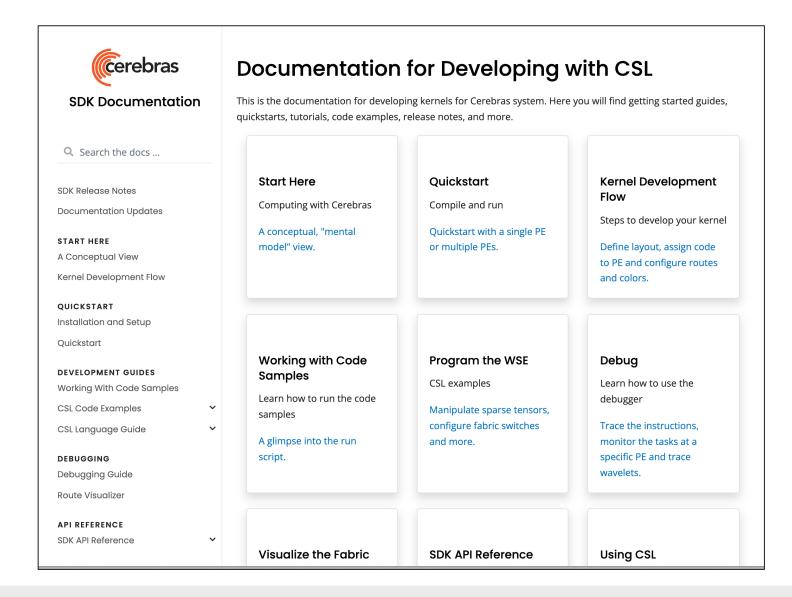


# Simulation Debug Tools





### Private Documentation: sdk.cerebras.net





# Examples Included in the SDK

- Basic tasks and colors
- Multiple source files
- Multi-PE kernel
- Basic parameters
- Wavelet-triggered Tasks
- Arrays and Pointers
- Sparse Tensors
- Memory DSDs
- Fabric DSDs
- Reduction

- Basic Branches
- Initializers
- Modules
- Loops
- Kernel Parameterization
- Fabric Switches
- GEMV
- FFT
- Stencil (Finite Differences)
- Shift-Add Multiply



# Accelerated energy research at TotalEnergies



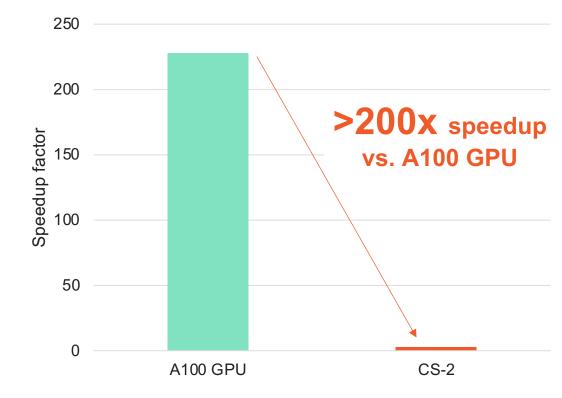
**Objective:** Enable order-of-magnitude speedups on a wide range of simulations: batteries, biofuels, wind flows, drillings, and CO2 storage



**Challenge:** Participate in Total study to evaluate hardware architectures, using finite difference seismic modelling code as a benchmark



**Outcome:** Cerebras CS-2 system outperformed a A100 AI GPU by >200X using code written in the Cerebras Software Language (CSL). System now installed and running at customer facility in Houston, TX





"We count on the CS-2 system to boost our multi-energy research and give our research 'athletes' that extra competitive advantage."

Dr. Vincent Saubestre, CEO and President, TotalEnergies Research & Technology USA



Mathias Jacquelin, Mauricio <u>Araya-Polo</u>, <u>Jie Meng</u>, "<u>Mass</u>ively Scalable Stencil Algorithm" Presented at SC22, <a href="https://arxiv.org/abs/2204.03775">https://arxiv.org/abs/2204.03775</a>



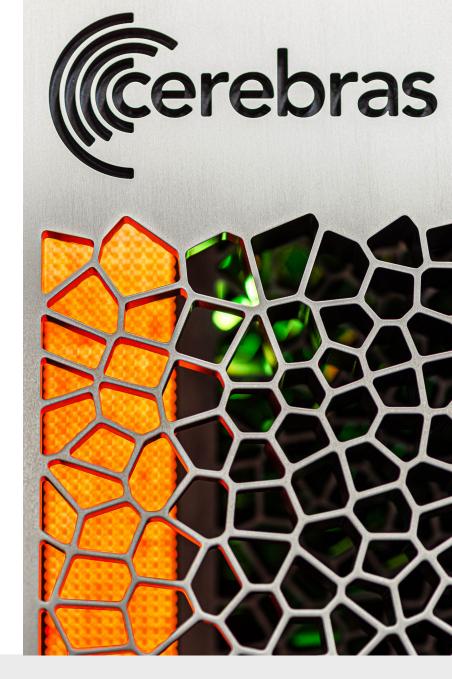
# Topics of interest for HPC applications

- Structured grid based PDE and ODE solvers
- Dense linear algebra
- Sparse linear algebra
- Particle methods with regular communication
- Monte Carlo type problems that can fill the wafer
- Towards development of HPL, HPCG type benchmarks
- Custom ML kernels



## Recap

- CS-2 is a dense and powerful single system, powered by 1 enormous chip
  - Cluster-scale compute on a single device => good fit for large DL models
  - 40GB SRAM with massive memory bandwidth => good fit for sparse problems
- CS-2 for Deep Learning
  - Leveraging TensorFlow and PyTorch frontends
  - No low-level programming required
  - Cerebras Software takes care of distributing computations across 850,000 cores
- CS-2 for HPC via SDK
  - Use CSL language for low-level programming on the wafer
  - Users decide how to distribute the computations
  - Cannot be integrated with TensorFlow/ PyTorch workloads
- Next: CS-2 for field equations via NETL's WFA







# Thank you!

https://cerebras.net/

Using the WFA for Scientific Computing on the WSE

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Neocortex Spring 2023 CFP February 28, 2023



### What is the WFA

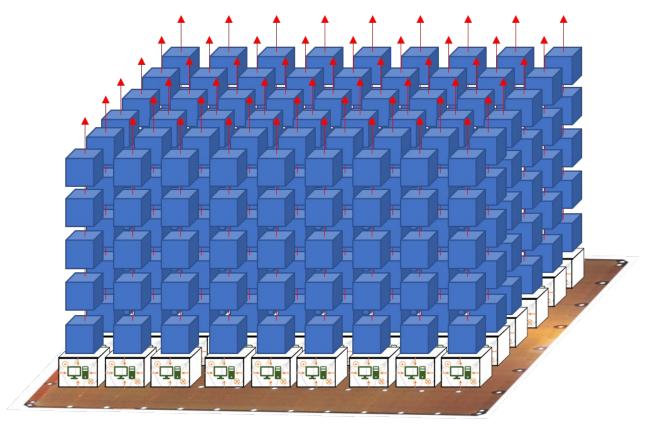
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### DSL for Solving Spatial-Temporal Problems on Structured Grids

Simple Python Front End (like Numpy)

Simple Pencil Memory Layout

```
from WSE FE.WSE Interface import WSE Interface
from WSE FE.WSE Array import WSE Array
from WSE FE.WSE Loops import WSE For Loop
import numpy as np
# Instantiate the WSE Interface
wse = WSE Interface()
# defince constants
c = 0.1
center = 1.0 - 6.0 * c
# Create the initial temperature field and BC's
T init = np.ones((102, 102, 102))*500.0
T init[1:-1, 1:-1, 0] = 300.0
T init[1:-1, 1:-1, -1] = 400.0
# Instantiate the WSE Array objects needed
T n = WSE Array(name='T n', initData=T init)
# Loop over time
with WSE For Loop('time loop', 400000):
    T n[1:-1, 0, 0] = center * T n[1:-1, 0, 0]
        + c * (T_n[2:, 0, 0] + T_n[:-2, 0, 0]
               + T n[1:-1, 1, 0] + T n[1:-1, 0, -1]
               + T n[1:-1, -1, 0] + T n[1:-1, 0, 1])
wse.make WSE(answer=T n)
```



https://dirk-netl.github.io/WSE\_FE/

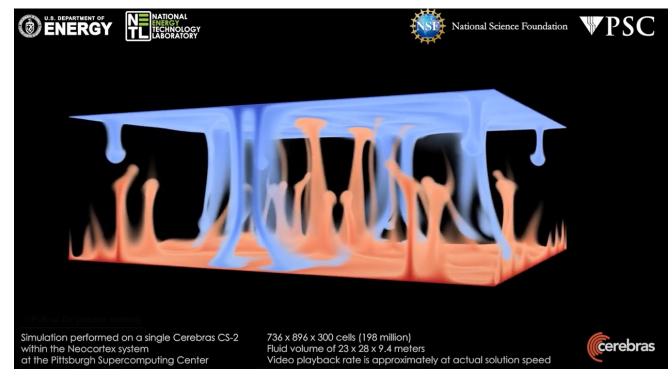


# Near Real Time Scientific Modeling

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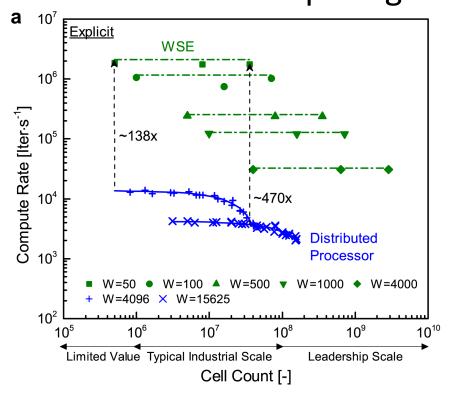
### **Exceptionally Fast PDE Solutions On Wafer Scale Engine**

CFD Demonstration Completely on WSE



https://www.youtube.com/watch?v=5ad9f70ORvQ

# Several Hundred Times Faster Than Distributed Computing



https://arxiv.org/abs/2209.13768



## Seeking Beta Testers for Scientific Computing

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### **Project Guidelines**

- Problem Requirements
  - Must lay out on a Hex grid (3d or many 2d parallel)
  - Should involve Spatial Locality
  - Should be Data Intense
  - Single Precision, <40GB</li>
- Problem Examples
  - Computational Fluid Dynamics (FVM, FDM, FEM, LBM)
  - Structural Mechanics
  - Geomechanics
  - Weather/Climate
  - Materials Ising Model, Density Functional Theory
  - CNN/RNN inference
- Project Requirements
  - Build a Python class that imports the WFA and contains a "Library" to solve your scientific problem
  - Post on a public github
- What to expect
  - Development at the high-level Python interface that is similar to Numpy
  - A container (provided by Cerebras) to compile and generate binaries and run on the WSE
  - An unpolished product (Beta level) that will require some hand holding from our team on slack
    - Be prepared for bugs and unpolished documentation
  - Exceptional speed if successful, strong scaling that can't be matched elsewhere

