WSE (Wafer Scale Engine) Applications for CCS (Carbon Capture and Storage)

Hyoungkeun Kim[1,2], Alex Sun[1,2], Chung Yan Shih[2]

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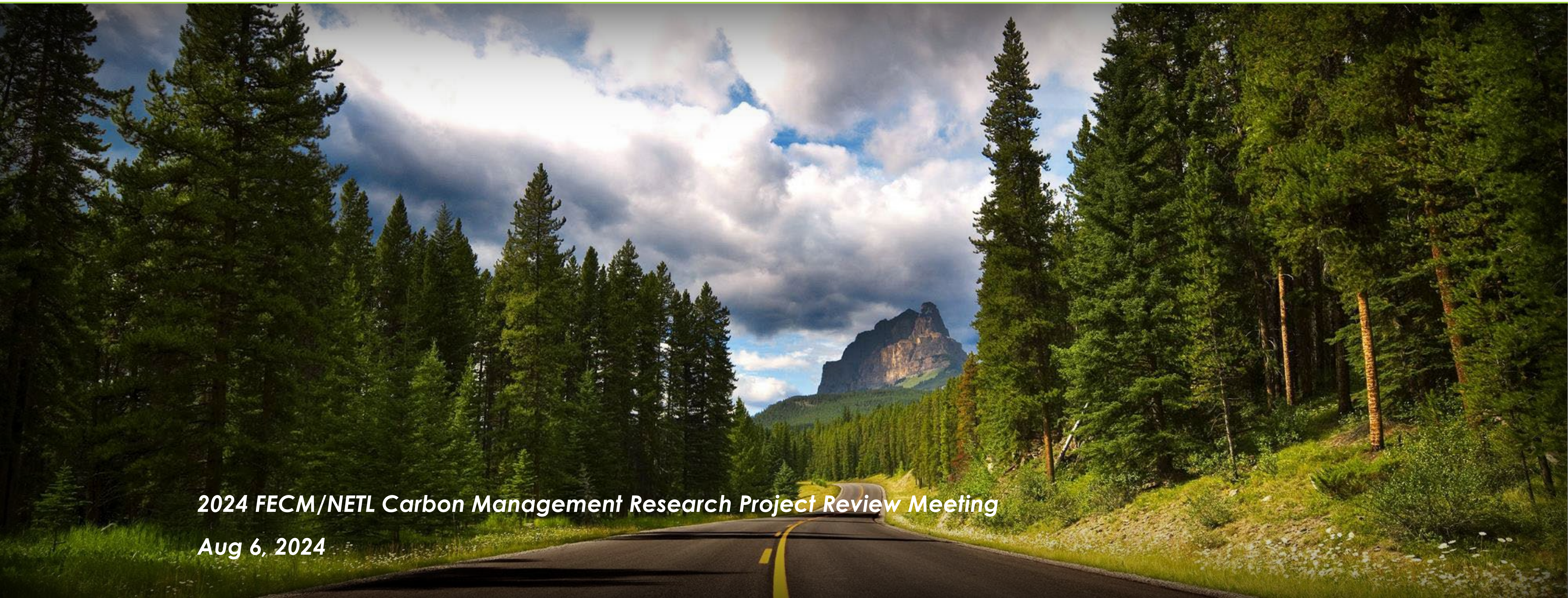

2024 FECM/NETL Carbon Management Research Project Review Meeting

Aug 6, 2024

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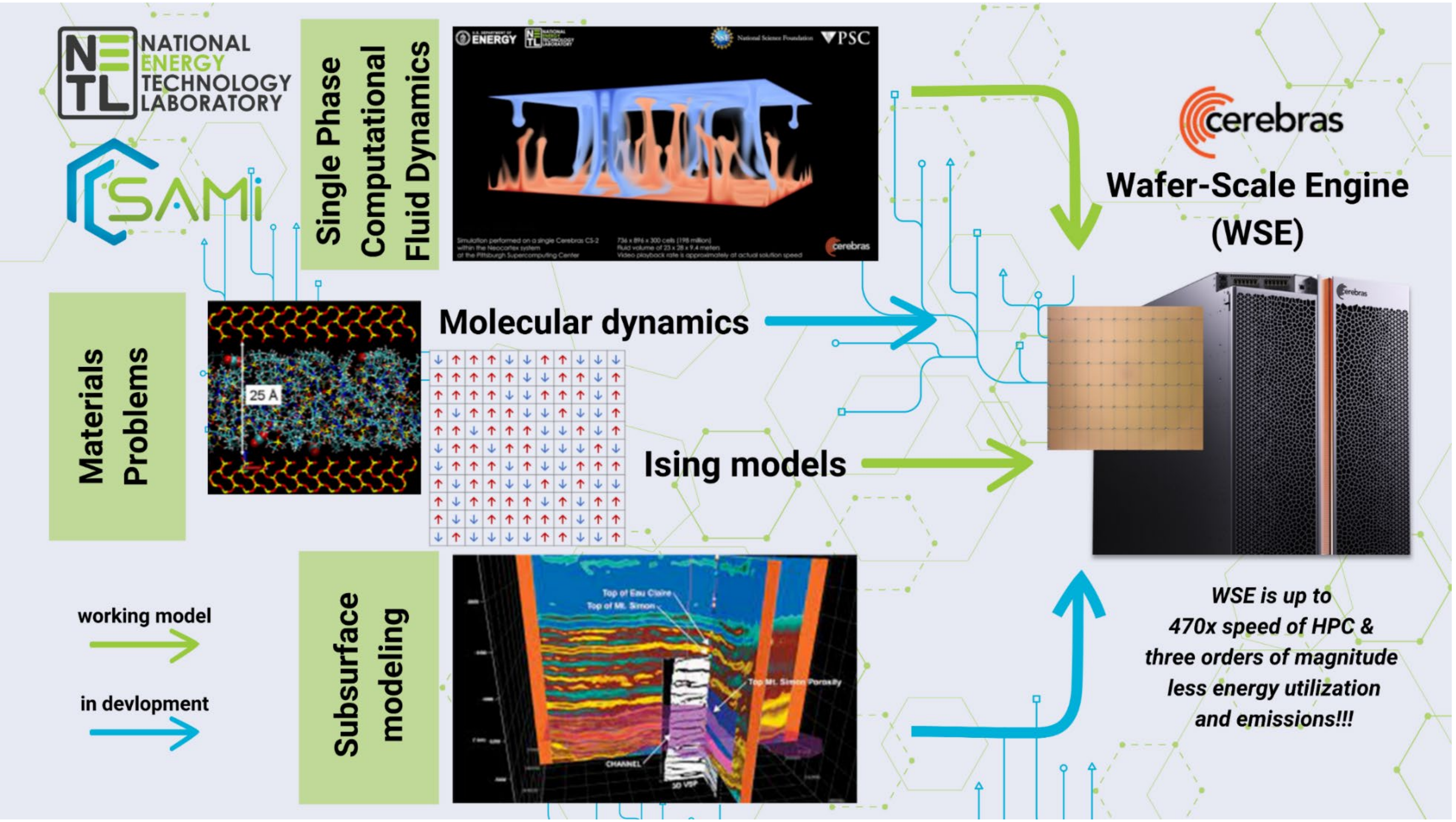
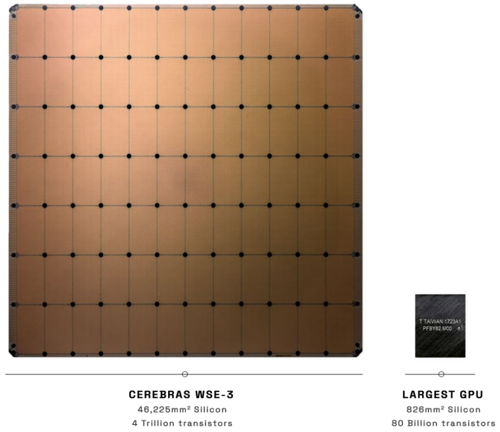
Objectives

- Develop data loader and foundational algorithms towards a two-phase compressible CO_2-brine solver for running on WSE
- Demonstrate numerical accuracy and scalability of the wafer scale engine (WSE)-based solver on synthetic problems
- Demonstrate the WSE-based solver on well data from the Illinois Basin - Decatur Project (IBDP)

WSE/WFA(Wafer Field Application)





WSE

- Colovore
  (https://www.colovore.com/cerebras-systems-a-global-leader-in-ai-hardware-deploys-their-most-powerful-supercomputers-at-colovore/)
- Neocortex
  (https://www.cmu.edu/psc/aibd/neocortex/)

WFA

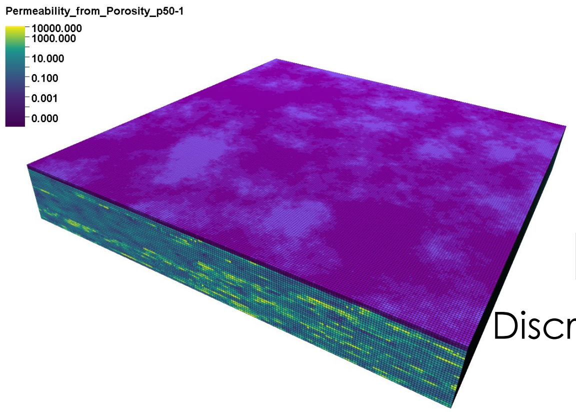
- General CFD
- Material Problems
- Subsurface modeling

WSE/WFA Software

1. Scientific physical approach for high-fidelity results
2. Faster speed than traditional simulations comparable to AI/ML (Artificial Intelligence/ Machine Learning)

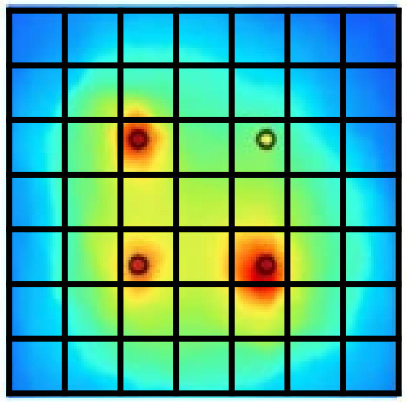
Approximation Through Discretization

Quantities and behaviors affected mostly by local values and immediate neighbor values



Discretize

Carbon Storage Problem in 3D/4D



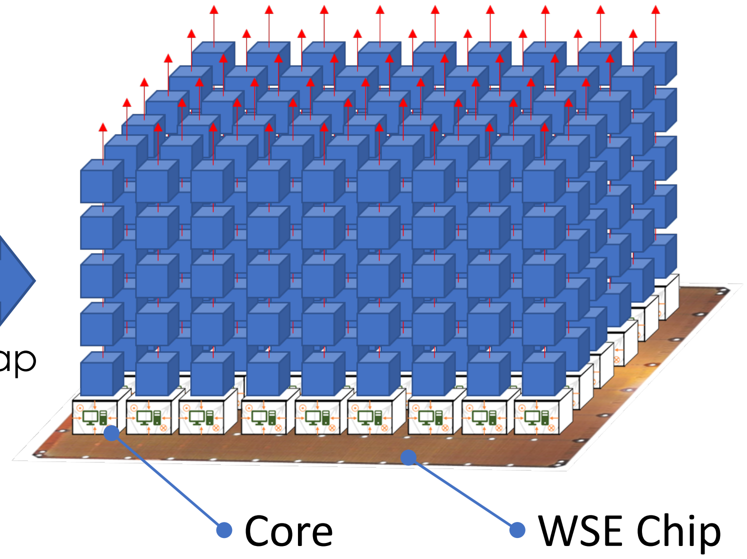
Discretization of the Problem in 3D/4D

Formulate Problem

WFA Connection

Mapping to WSE

Map



850,000 Cores -> 84 Dies -> 1 WSE Chip

Numerical Model – Governing Equations

Two-Phase Model

- The two-phase model for fluid flow in porous media is developed based on the water and gas equations. The model accounts for the PVT (pressure – volume - temperature) properties and the relative permeability calculations. The gas solubility in the liquid phase and the gravity effect are considered in the model.

- Water flow equation:

$$\frac{\partial\,(\varphi\,\rho_w\,S_w)}{\partial t} = \nabla.\,(\frac{\rho_w}{\mu_w}\;k\,k_{rw}\,(\nabla \mathrm{p_w} + \gamma_w \nabla \mathrm{z})) + q_w$$

- Gas flow equation:

$$\frac{\partial\,(\varphi\,(\rho_g\,S_g + \,\rho_w\,S_w R_{sw}))}{\partial t} = -\nabla.\,((\frac{\rho_g}{\mu_g} k\,k_{rg} + \frac{\rho_w}{\mu_w} k\,k_{rw} R_{sw})\,(\nabla \mathrm{p_g} + \gamma_g \nabla \mathrm{z})) + q_g$$

where, φ is porosity. ρ_w, μ_w, γ_w , and S_w are density, viscosity, specific gravity, and saturation (for water). k and k_{rw} are permeability and relative permeability. $\nabla \mathrm{p_w}$ and $\nabla \mathrm{z}$ are pressure and elevation. q_w is injection/production rate. R_{sw} is gas solubility in water.

Numerical Model - Materials

PVT Properties and Relative Permeability

- The model used for the calculations of PVT properties is the Peng-Robinson Equation of State. The properties calculated for CO_2 as a function of pressure at 100 °C are given in Figure 1.
- Relative permeability is estimated using Corey's model, as given in Figure 2.

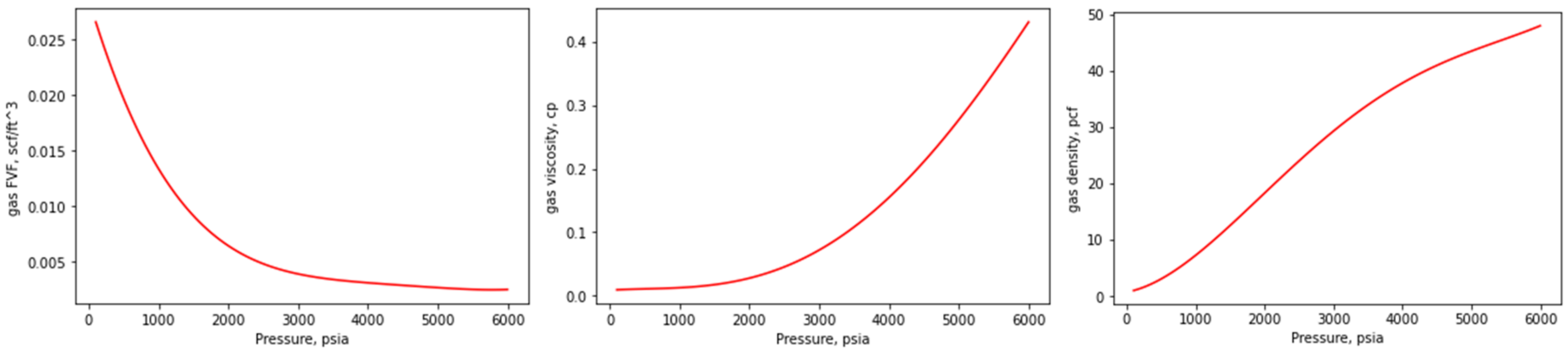


Figure 1: CO_2 PVT properties estimated using Peng-Robinson model.

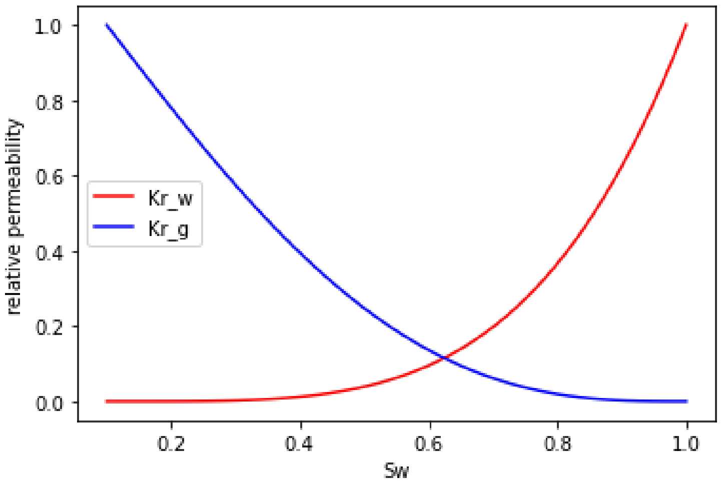


Figure 2: Relative permeability calculations.

Benchmark Test with t-Navigator

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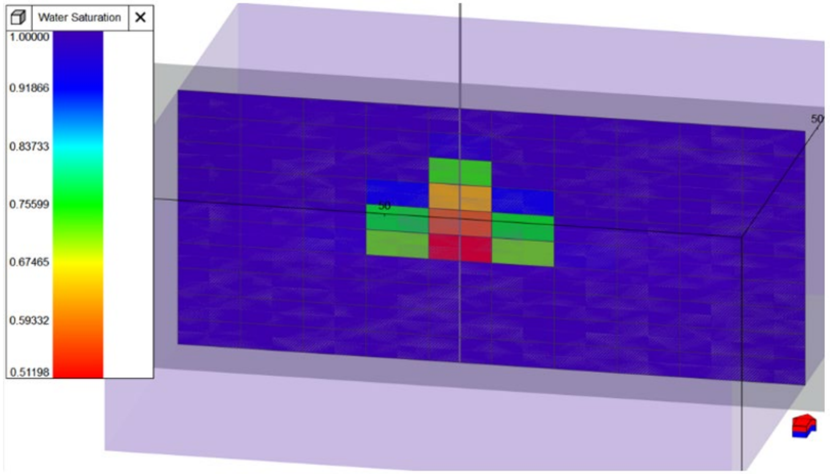
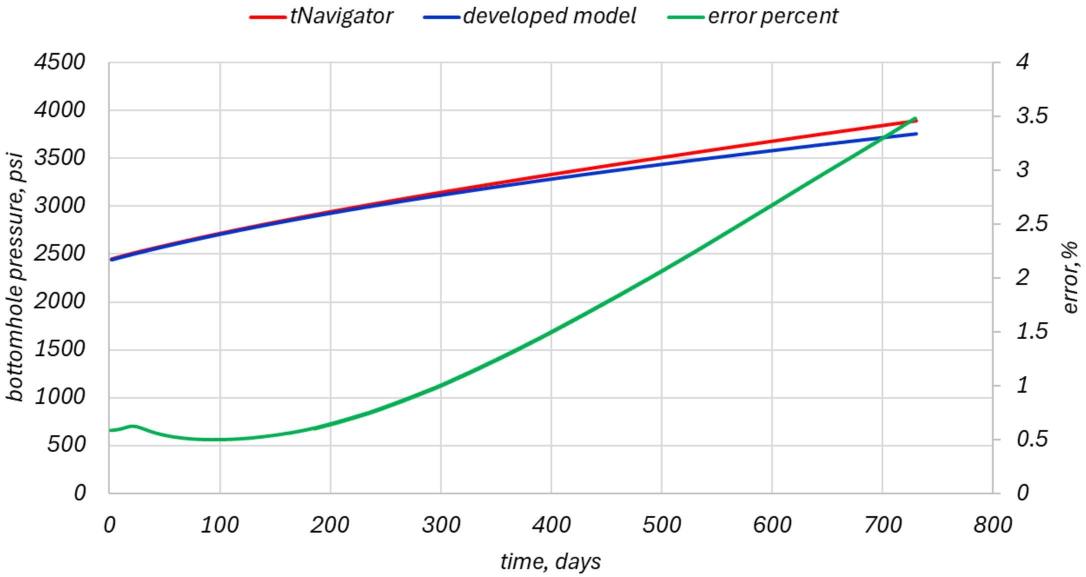
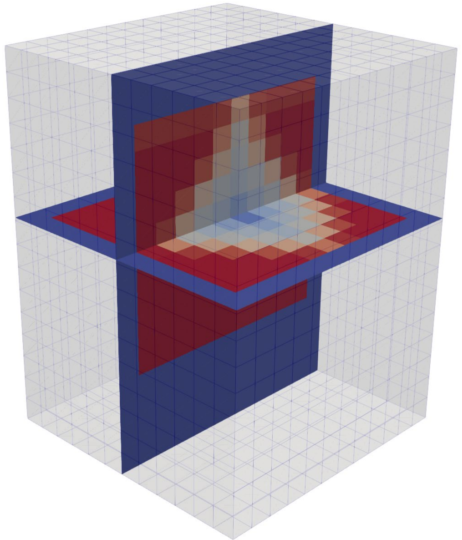


t-Navigator Mesh Size of (10 x 10 x 10)



WSE/WFA Mesh Size of (10 x 10 x 10)

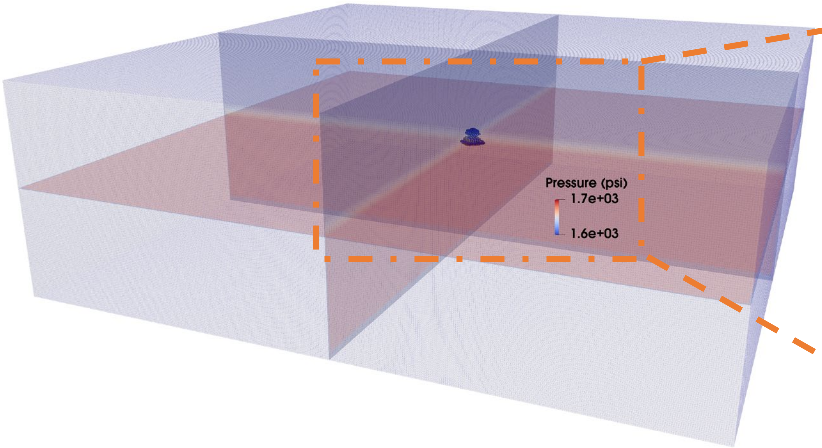


Consistent simulation setup on t-Navigator and WSE/WFA code

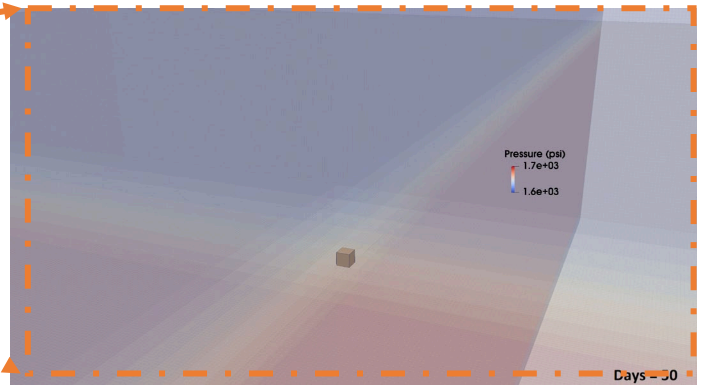
- dx = dy = dz = 30 ft
- Q_gas = 10,000 scf/day
- T_res = 100 °C
- Permeability = 100 md
- Phi = 0.2 (porosity)
- Sw_if = 0.1 (minimum water saturation)
- Sw_if = 0 (minimum gas saturation)

Scalability Study on Neocortex sdf WSE

Mesh Size of (400 x 400 x 124)



CO_2 Plume evolution animation (50~1000 days)



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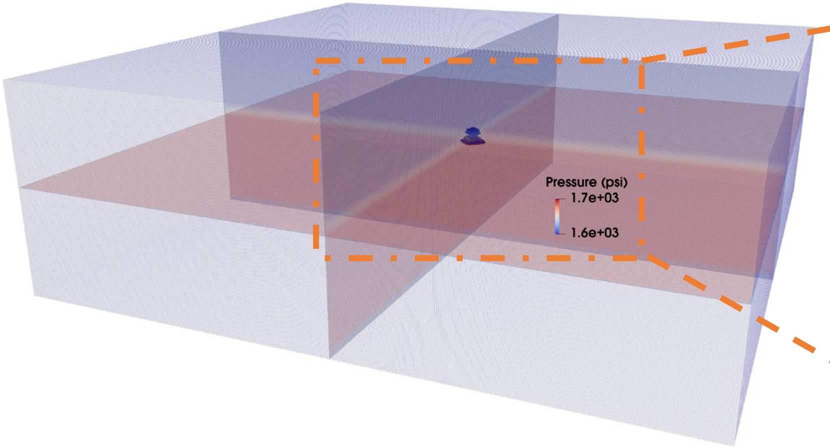
- Sw_if = 0.1 (minimum water saturation)
- Sw_if = 0 (minimum gas saturation)
- (nx,ny,nz) = (100,100,124), (200, 200,124), (300,300,124), (400,400,124)

Nx	Ny	Nz	Total # cells	cs-2 time
100	100	124	1.24 M	~ 1.38 sec
200	200	124	4.96 M	~ 1.54 sec
300	300	124	~ 11.2 M	~ 1.65 sec
400	400	124	~ 19.8 M	~ 1.79 sec

Scalability Study on Neocortex sdf WSE

Mesh Size of (400 x 400 x 124)



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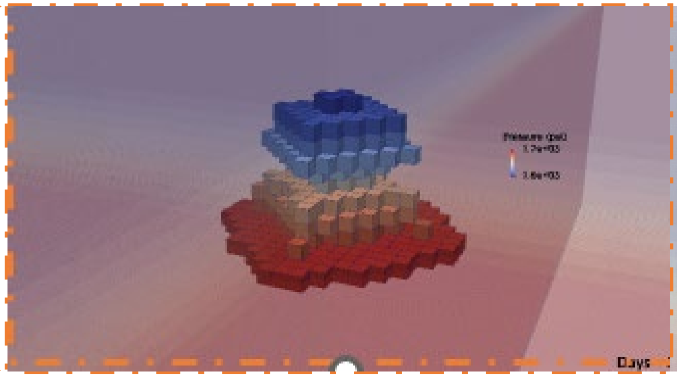

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Comparison Study with IBDP Experiment

Preliminary Result Using Stand-Alone Code Toward WSE/WFA Implementation

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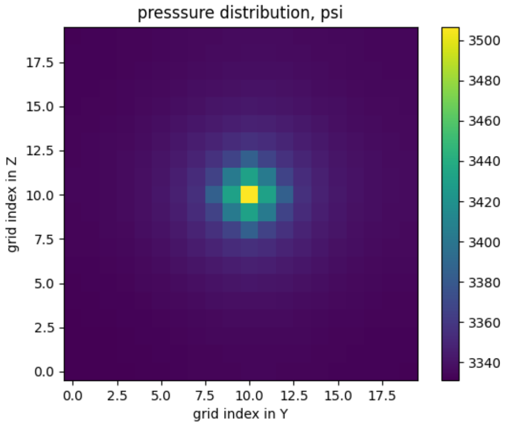

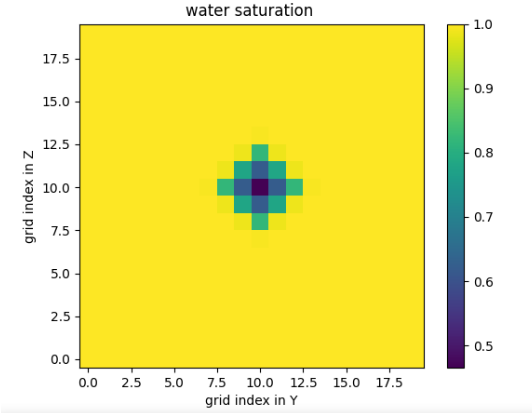

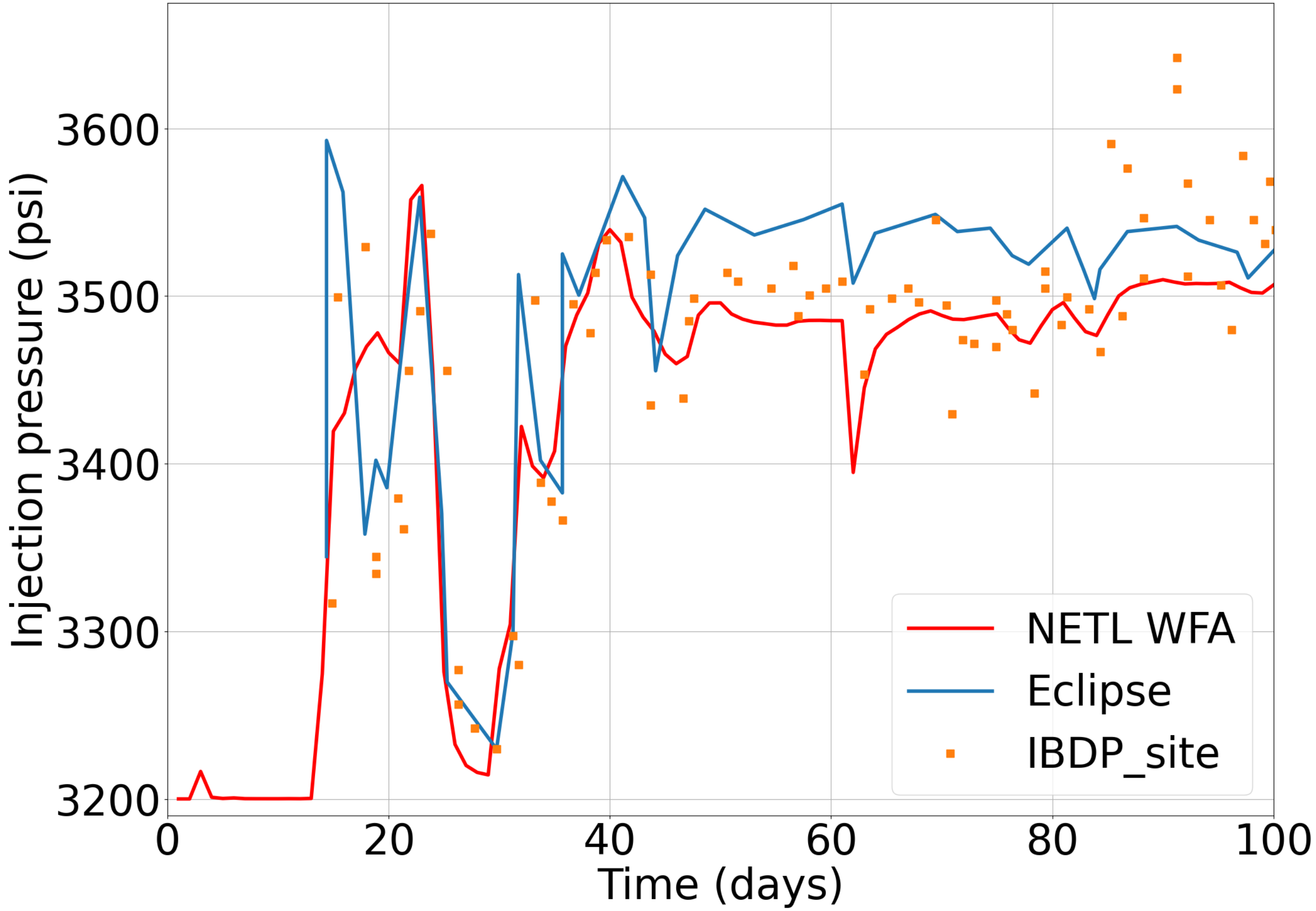

- 100 days CO_2 injection data
- Uniform permeability and porosity
- Converting stand-alone version into WSE/WFA

WSE/WFA IBDP Data Loading

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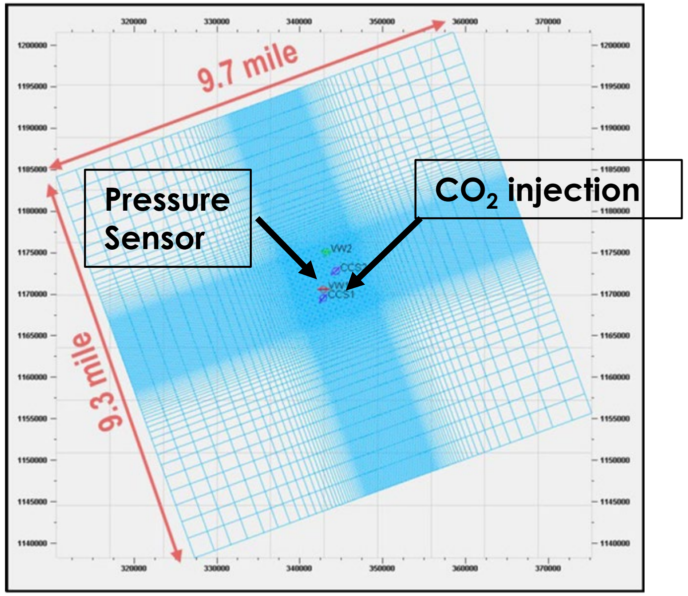
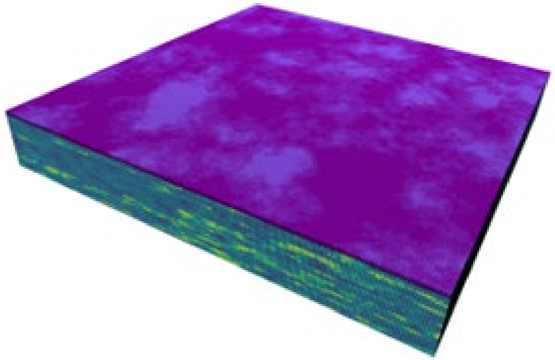
Goal: IBDP Real Reservoir

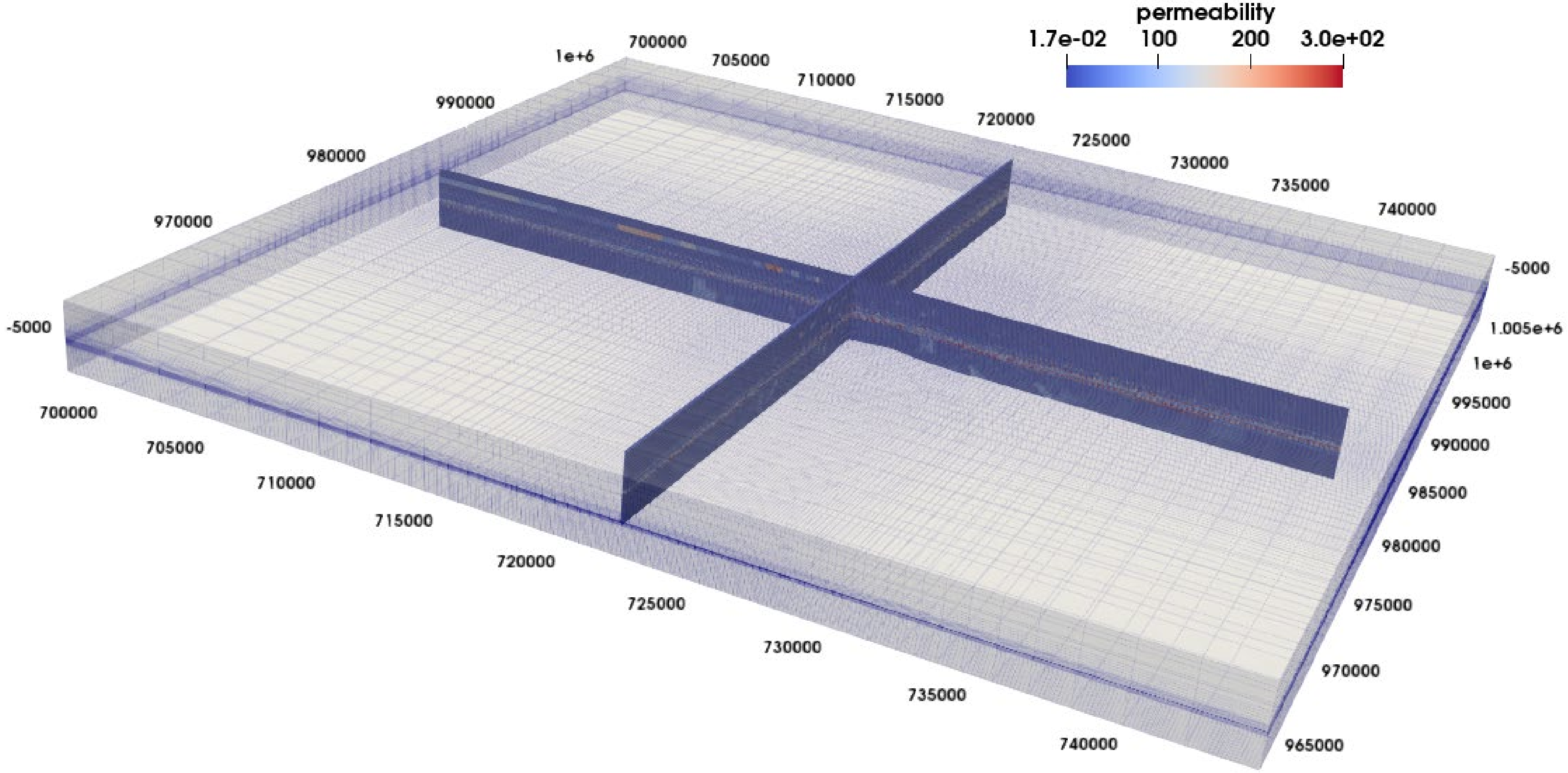


Eclipse Simulator – Mesh & Permeability

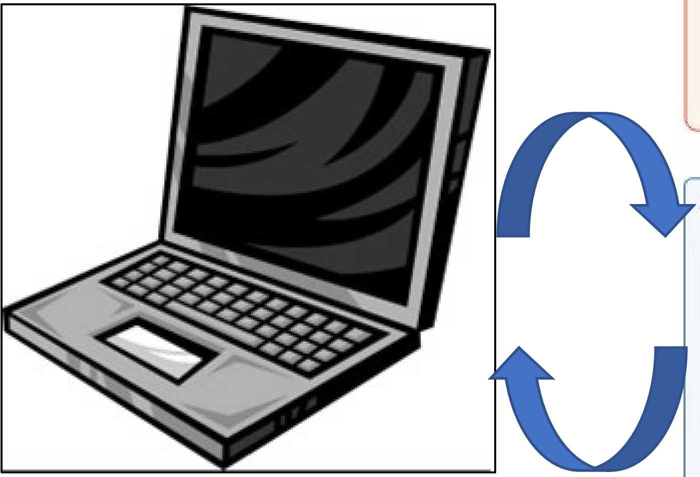


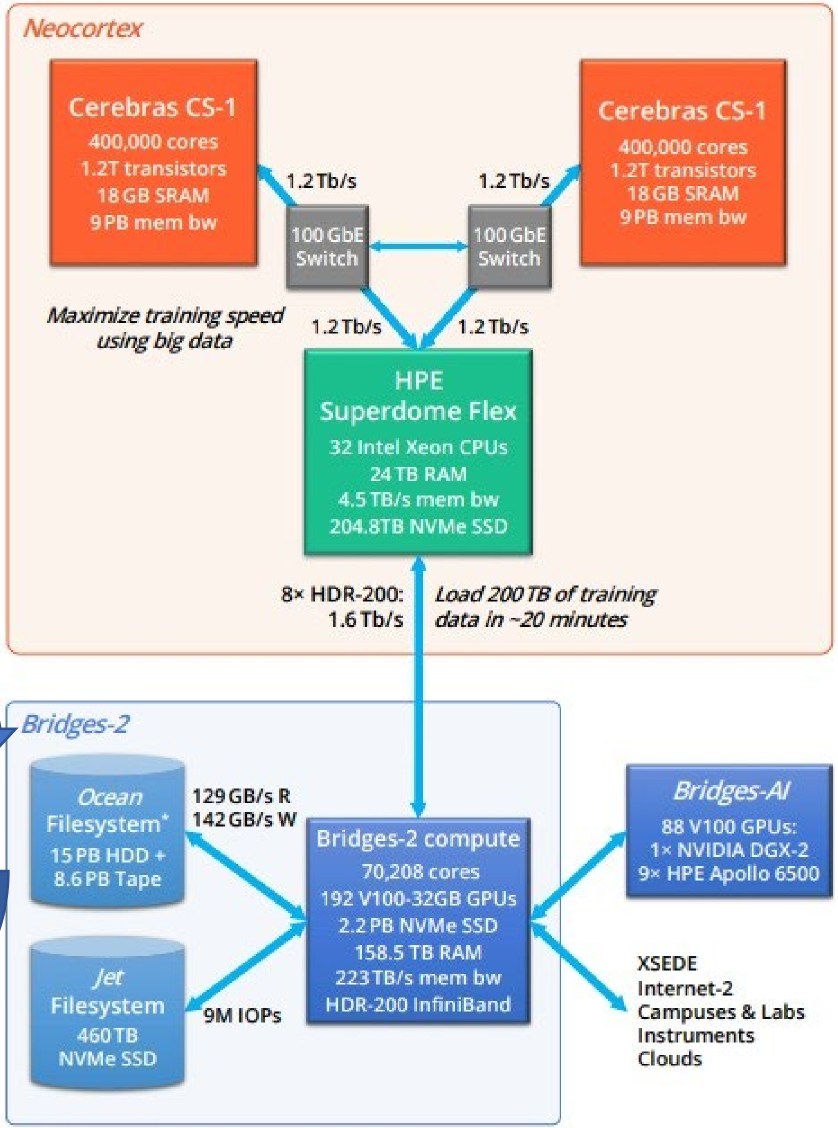
Simulation setup on WSE platform from Eclipse simulator cases of IBDP

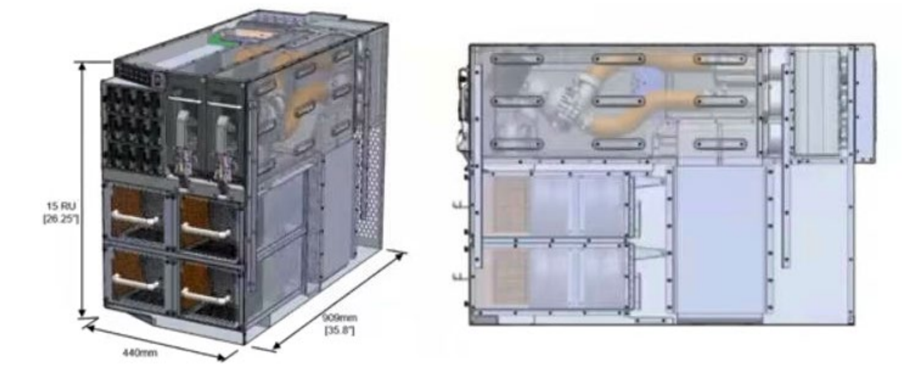
- Mesh construction of IBDP site
- 100 cases of (permeability and porosity)



Data load/download to local computer







Interior view of the Cerebras CS-1

Wafer Scale Engine (WSE) Processor

https://www.nextplatform.com/2022/04/14/psc-upgrades-neocortex-ai-supercomputer-with-new-cerebras-engines/
https://www.youtube.com/watch?v=OxA-23skBG4

Summary & Next Work

- Preliminary result
  1. Developed proof-of-concept WFA code of two-phase CO_2 and brine model
  2. Benchmarked results against t-Navigator outcomes
  3. Tested scalability on Neocortex sdf wafer engine
  4. Tested preliminary case based on IBDP CO_2 storage dataset

- Next work
  1. Development of pre-conditioner for linear solver on WSE/WFA
  2. Benchmark study using t-Navigator on Joule3 CPUs/GPUs
  3. Validation study based on IBDP experiment/eclipse simulation
  4. Relevant to ML/AI CCS carbon capture storage SMART

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- Redlich, Otto; Kwong, J. N. S. (1949). "On The Thermodynamics of Solutions". Chem. Rev. 44 (1): 233–244. doi:10.1021/cr60137a013. PMID 18125401.
- Kamil Rocki, Dirk Van Essendelfty, Ilya Sharapov, Robert Schreiber, Michael Morrison, Vladimir Kibardin, Andrey Portnoy, Jean Francois Dietikeryz, Madhava Syamlaly and Michael James: Fast Stencil-Code Computation on a Wafer-Scale Processor. arXiv:2010.03660v1 [cs.DC] 7 Oct 2020
- Area of Review and Corrective Action Plan for ADM CCS #2 Oct2016, IL-115-6A-0001, Attachment B

Running on Neocortex sdf WSE

1. compile the code
   python ../build_and_test.py -st 1; python -m WFA.tests.TwoPhasePythonSolver_GasWater_Mina23May24_v4_WFA_v4 -hin hardware_test -mg bench.img -ts32 1

2. submit job to Neocortex sdf-1
   sbatch --nodelist=sdf-1 neocortex_slurm_script_bash -c hardware_test -o Pn_array_wse,Sw_array_wse

3. security copy for post-processing
   scp hkimd@bridges2.psc.edu:/jet/home/hkimd/hardware_test_ckpt_Sw_array_wse .
4. Schematic figure for data flow between neocortex and local workstation