Atlanta, GA | more than hpc.

SC20 vSCC Reproducibility Challenge

8/6/2020

Welcome and Announcements

Webinar Schedule

https://sc20.supercomputing.org/program/studentssc/studentssc-webinars/

Speakers





Stephen Lien Harrell - SC20 Reproducibility Challenge Chair
Michela Taufer - Founder of Reproducibility Effort at SC
Beth Plale - SC20 Transparency & Reproducibility Chair
Verónica Melesse Vergara - SC20 vSCC Co-chair
Scott Michael - SC20 vSCC Co-chair
Mert Hidayetoglu - Author of reproducibility challenge paper
Tekin Bicer - Co-author of reproducibility challenge paper


Reproducibility in HPC and Our Everyday Lives

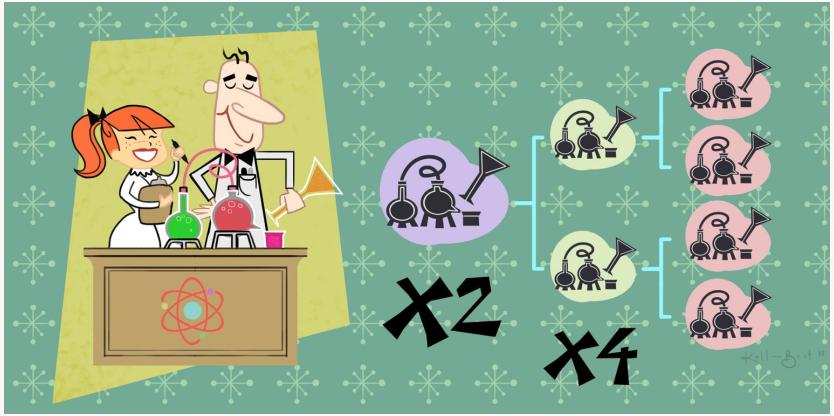

Illustration by Kallum Best

"Do we trust the experimental results published in, e.g., the Nature journal? "
Yes, because …

- **The experiment was reproduced multiple times converting to the same scientific conclusions**

Image sources:
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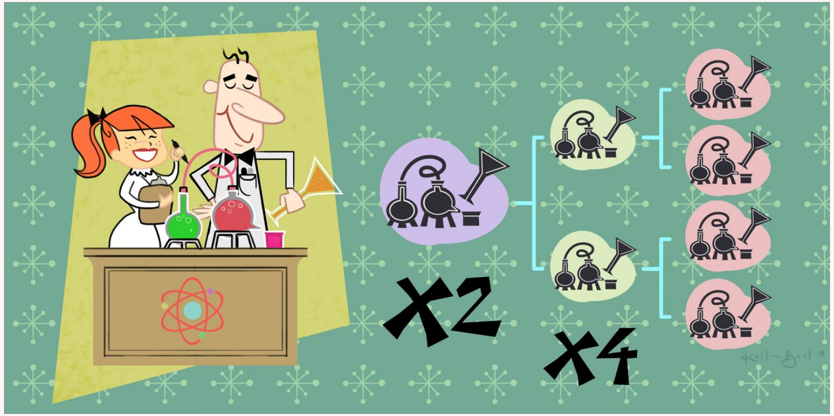

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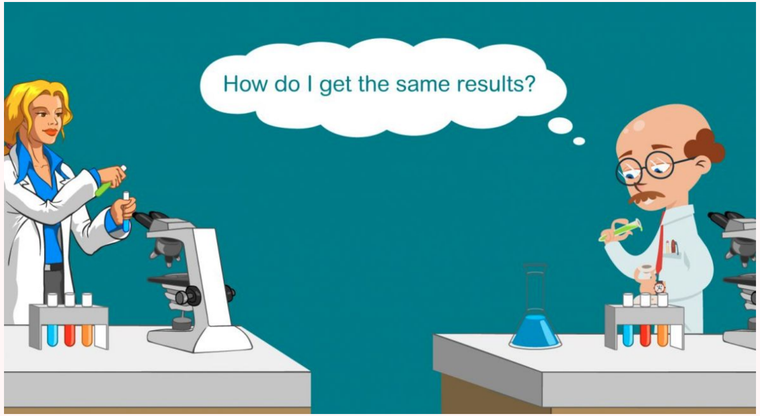

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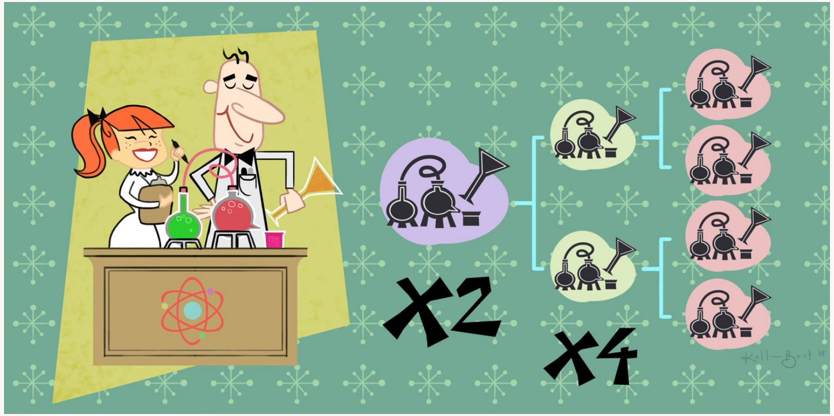

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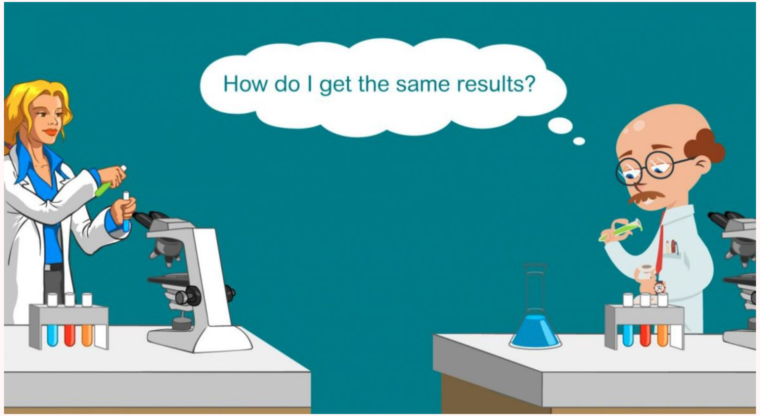

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"What is one of the advantages of a reproducible and well documented experiment?"

- **Everyone can reproduce the experiment**
- **Anyone can build new science by leveraging the reproduced results**

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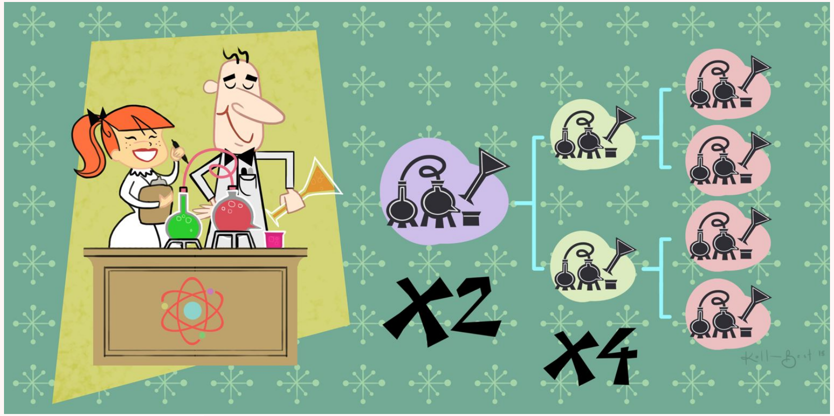

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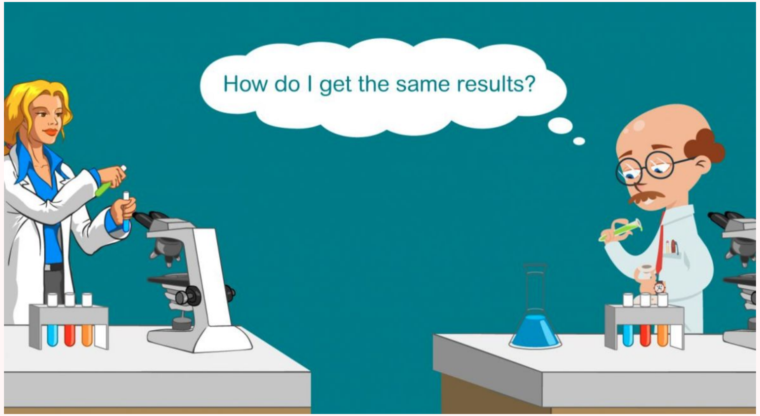

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What if we replace "*experimental results*" with "computational results"?

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Life Cycle of Reproducibility at SC

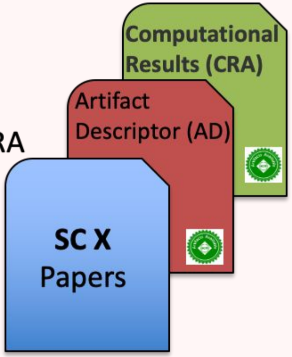
Technical Program @ SC X

Select BP/BSP candidates

Assign badge

Check AD or CRA

Review papers



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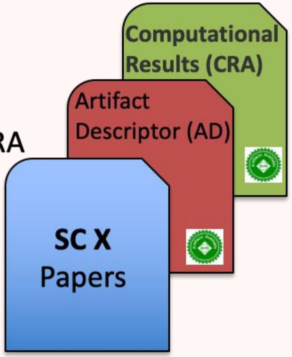

Select one (1) **SC X** paper for **SC X+1** SCC

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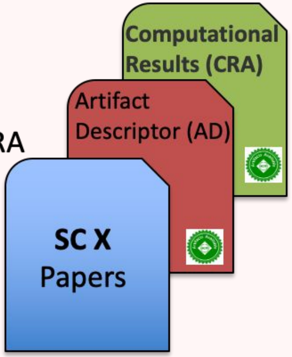

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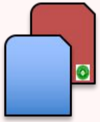

Generate replication benchmark for diverse set of HPC platforms

Life Cycle of Reproducibility at SC

Technical Program @ SC X

Select BP/BSP candidates

Assign badge

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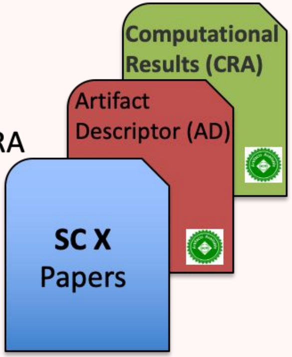
Review papers



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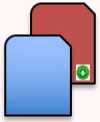

Generate replication benchmark for diverse set of HPC platforms

Student Cluster Competition @ SC X+1

Partner with vendors

Build a cluster

Test performance benchmarks

Replicate **SC X** Paper

Generate replication reports

Life Cycle of Reproducibility at SC

Technical Program @ SC X

Select BP/BSP candidates

Assign badge

Check AD or CRA

Review papers

Computational Results (CRA)

Artifact Descriptor (AD)

SC X
Papers

Select one (1) **SC X** paper for **SC X+1** SCC

Technical Program @ SC X+1

Assign badge to SC X paper

Give SIGHPC certificate to SC X paper authors

Present Journal SI with SCC reports from SCC @ SC X-1

Generate replication benchmark for diverse set of HPC platforms

Student Cluster Competition @ SC X+1

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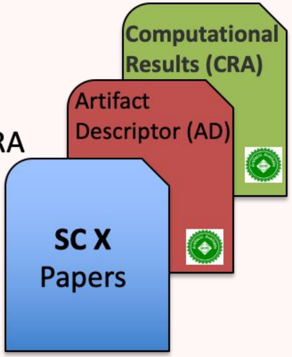


Technical Program @ SC X+2

Review IEEE TPDS paper with SCC reports from SCC @ SC X+1

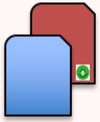
Select one (1) **SC X** paper for **SC X+1** SCC

Technical Program @ SC X+1

Assign badge to SC X paper

Give SIGHPC certificate to SC X paper authors

Present Journal SI with SCC reports from SCC @ SC X-1



Generate replication benchmark for diverse set of HPC platforms

Student Cluster Competition @ SC X+1

Partner with vendors

Build a cluster

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Replicate **SC X** Paper

Generate replication reports

Student Cluster Competition

Overview

- Four applications plus benchmarks -- GROMACS, CESM, **MemXCT**, Mystery application
- Reproducibility application scoring is unique; based on report

Recommendations

- Start your reports early; you already know a lot about your infrastructure and can plan your experiment in advance
- Plan for contingencies; have a target number of runs but also know what is the minimum you need
- Reproduction is not required for a good score, however, a good explanation of why the experiment was reproduced or not is required for a good score.

Beginning: Summer Internship at Argonne

Argonne National Laboratory

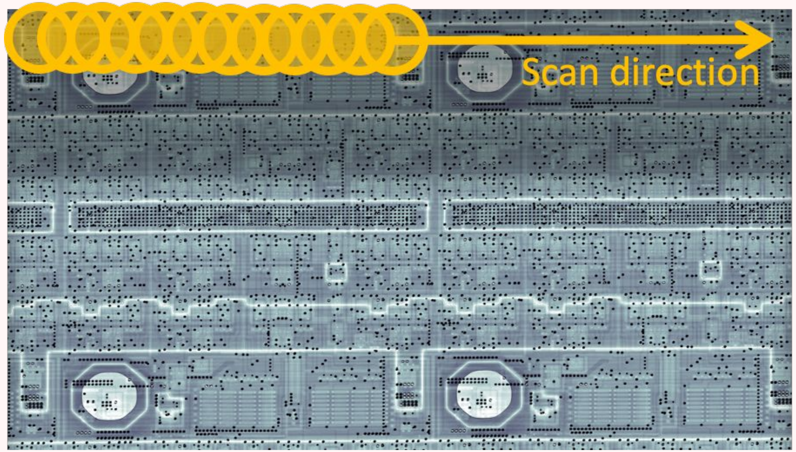
Advanced Photon Source

- Hosts 5,300 researchers each year
- High-energy, high-brightness, highly penetrating, x-ray beams
  - 1,000,000,000 times brighter than dentist X-rays
- Helps answer the big questions about materials, superconductors, disease, battery electrodes, etc.

Argonne Leadership Computing Facility

- Theta supercomputer
  - Intel KNL, 11 petaflops
- 1,240+ users in 2019, 8.7B core-hours, 413 active projects, 275+ publications
- Aurora: Next exascale computer
  - Intel and Cray, 2021

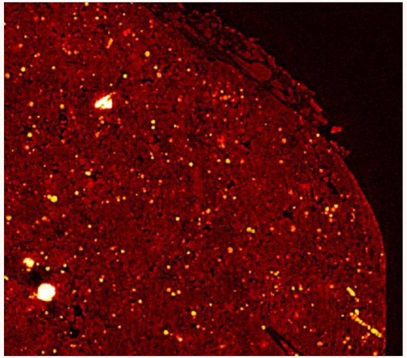
Applications of MemXCT



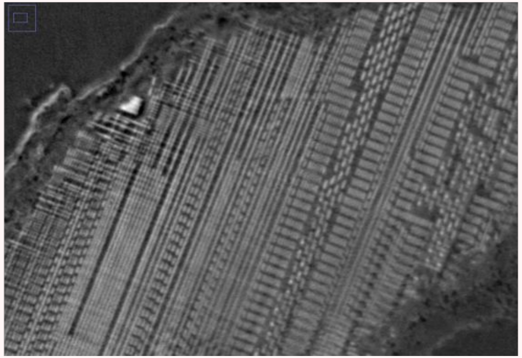
X-Ray Ptychographic Imaging

- Reconstruction of a Integrated Circuit
- 25000 Hz pixel sampling
- 1cm^2 area - 41 nm pixels – 10GB/s
- 1 month of data collection

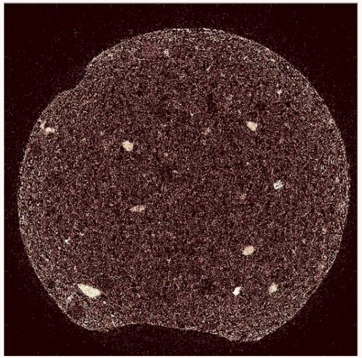
Shale Rock



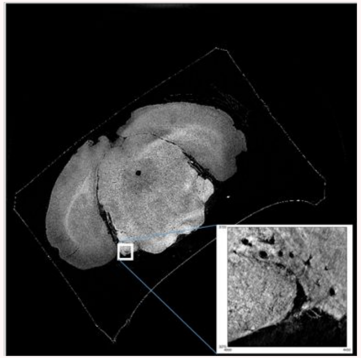
IC Chip



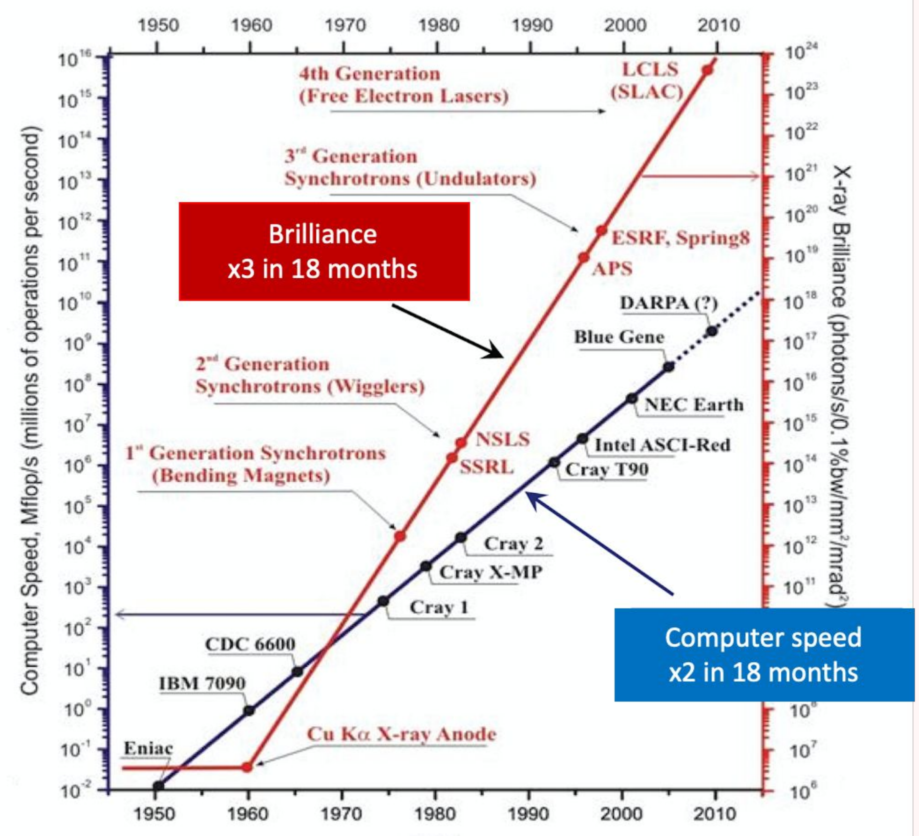
Activated Charcoal

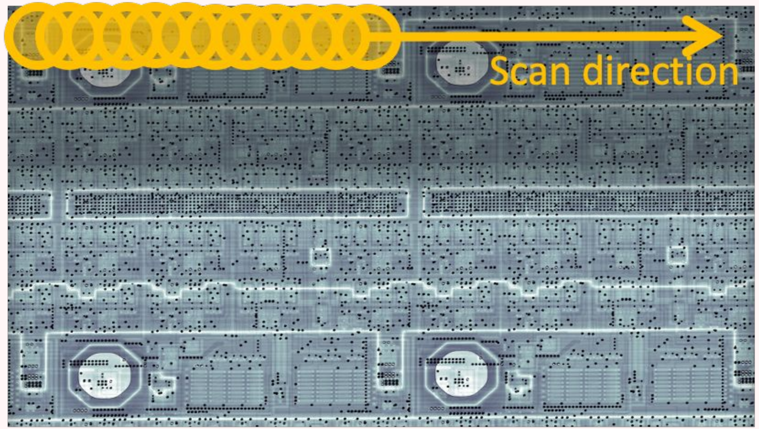


Mouse Brain



Motivation: Advancement Trends





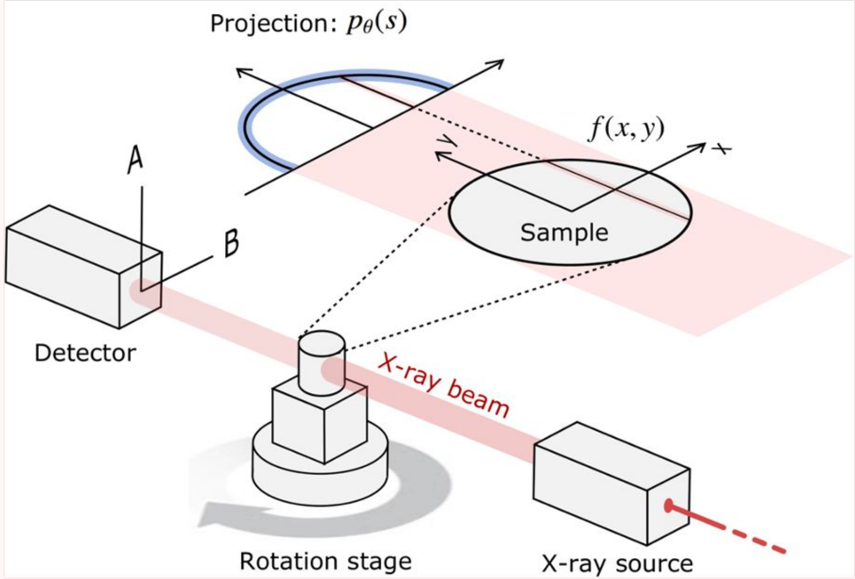
X-Ray Ptychographic Imaging

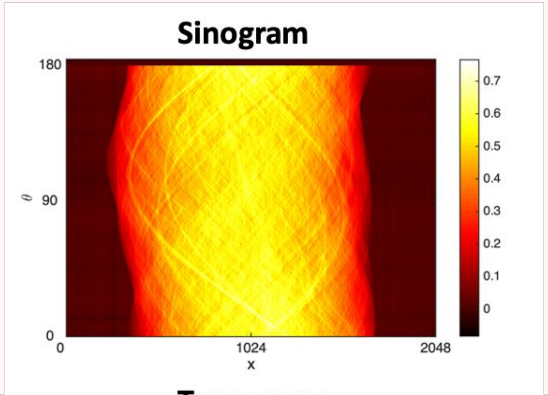
- Reconstruction of a Integrated Circuit
- 25000 Hz pixel sampling
- $1cm^2$ area - 41 nm pixels – 10GB/s
- 1 month of data collection

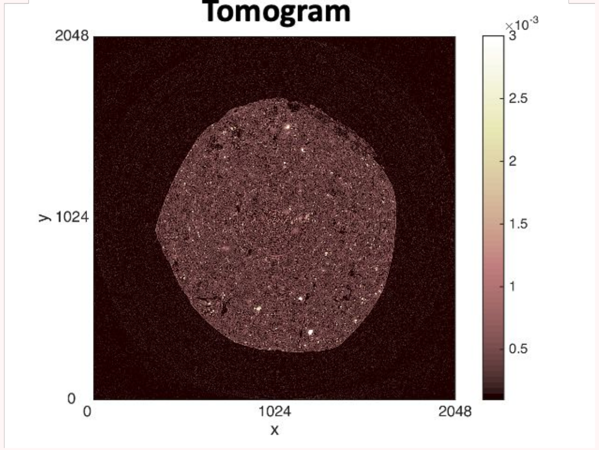
Data Acquisition

Ax=b

A^TA=A^Tb

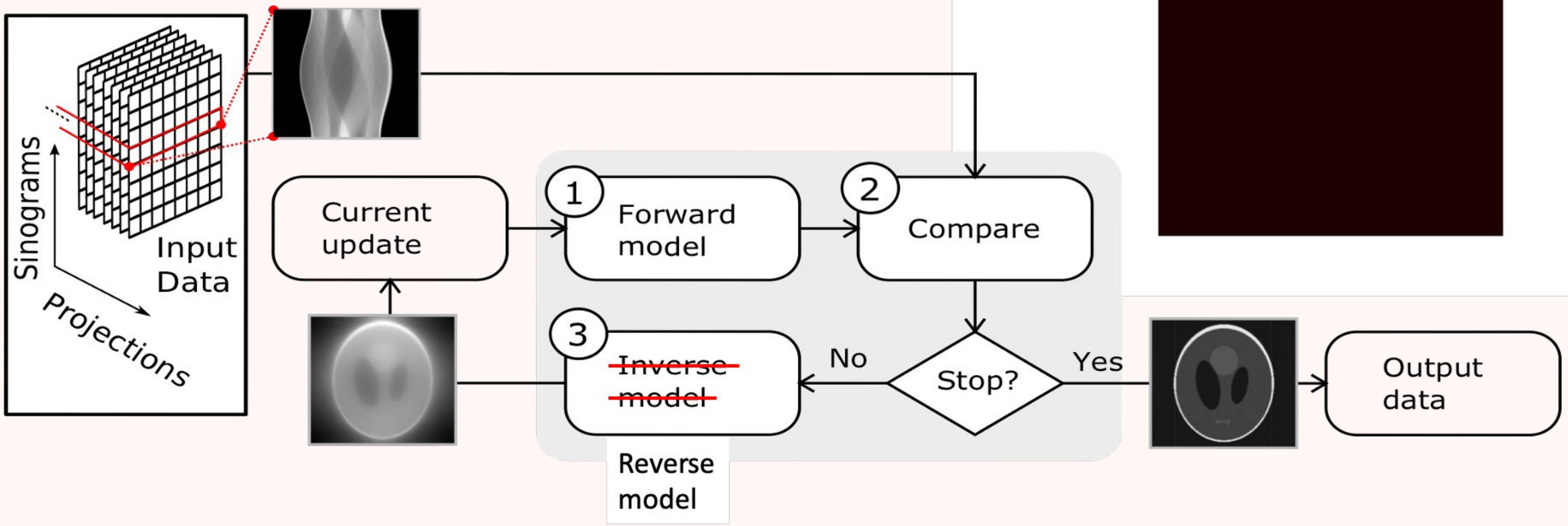




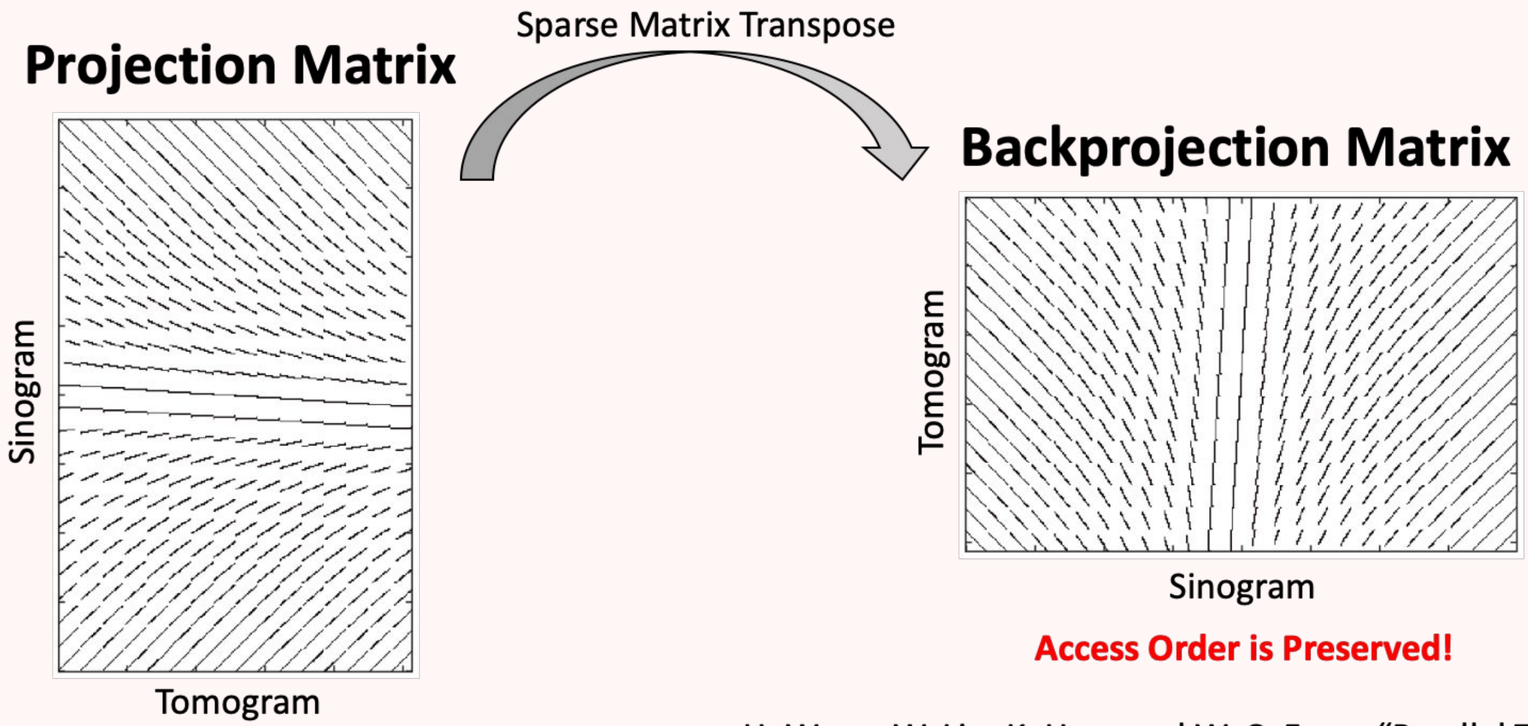


Iterative Image Reconstruction

$$Ax=b$$



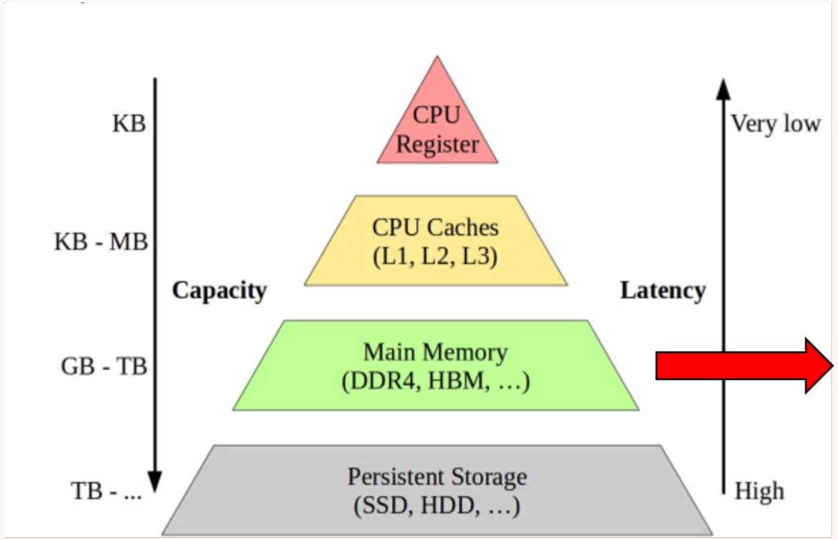
Memory-Centric Approach

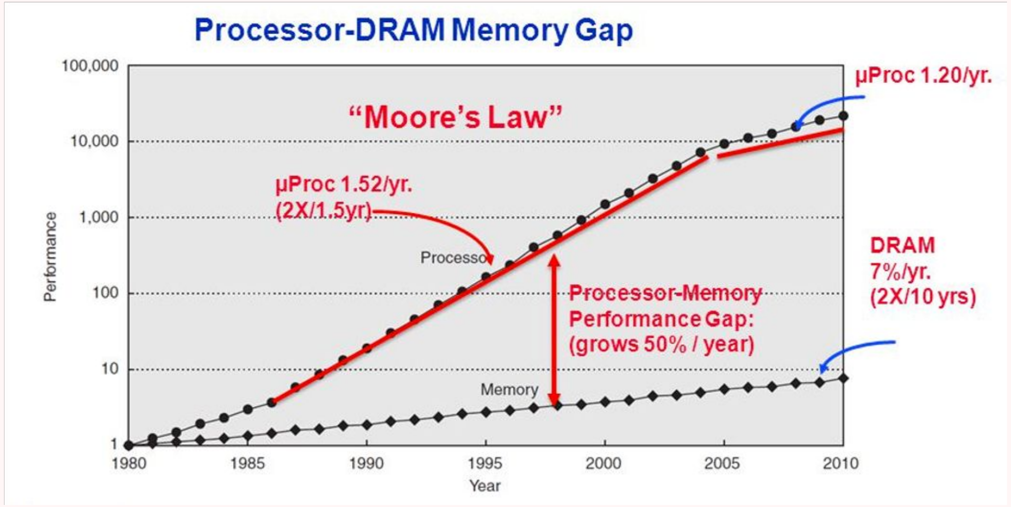


Access Order is Preserved!

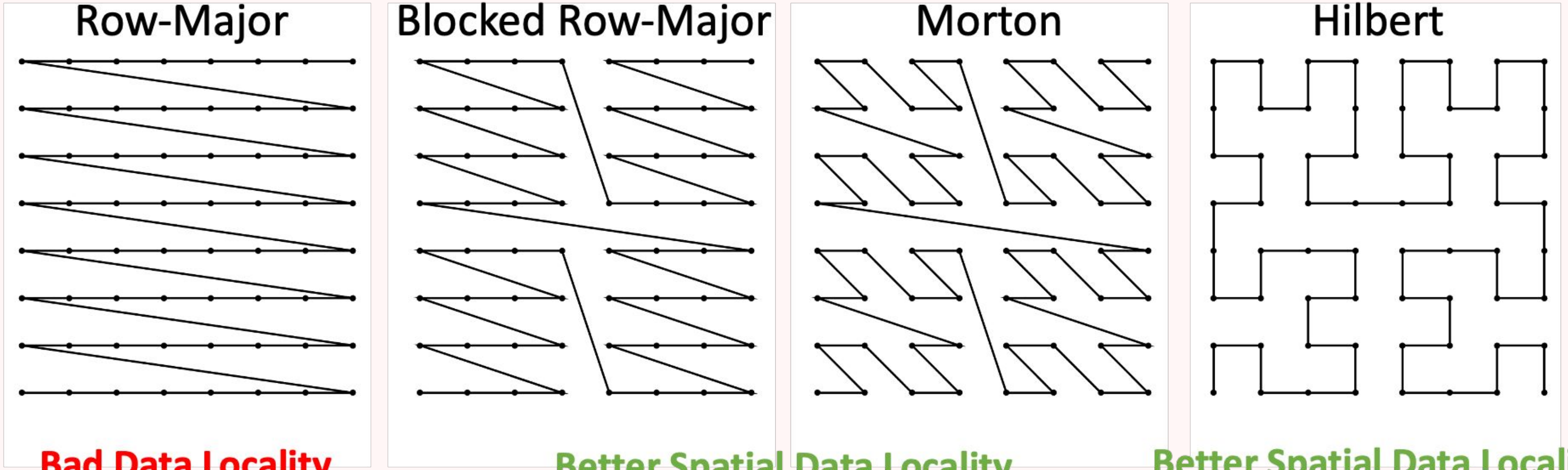
H. Wang, W. Liu, K. Hou, and W.-C. Feng, “Parallel Transposition of Sparse Data Structures,” ICS16, Istanbul, Turkey.

Memory Wall Problem





How to Store 2-D Data?

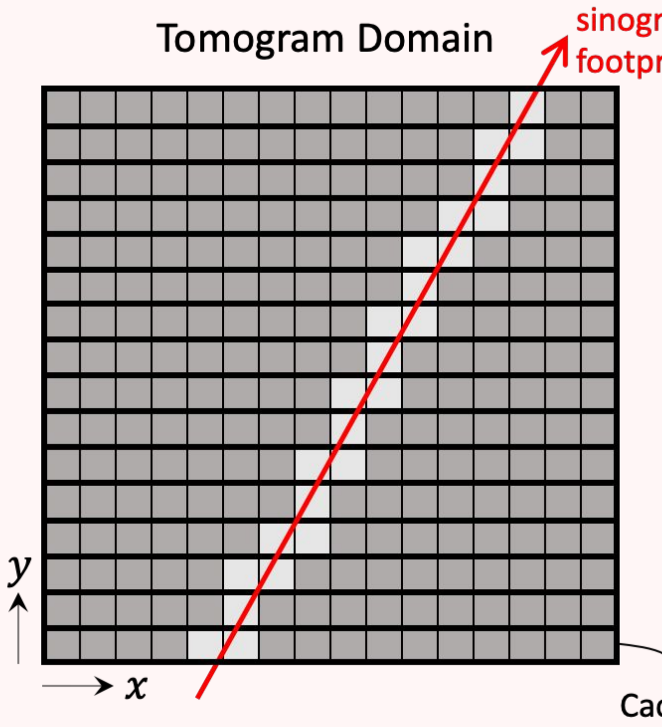


Bad Data Locality
Most Intuitive Storage

Better Spatial Data Locality
Does Not Provide Connectivity

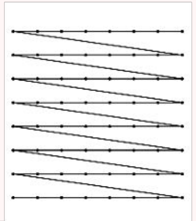
Better Spatial Data Locality
Provides Connectivity

Access Pattern to Tomogram Data

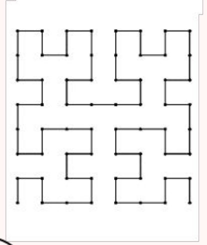


Single Level - Single Line

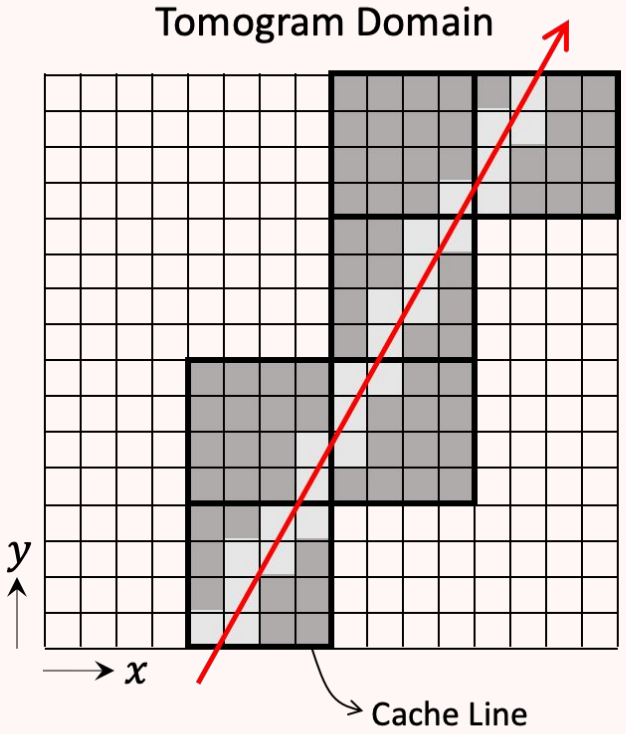
Capacity: 64 bytes (16 floats)



Row-Major Ordering:
16 Cache Miss
1024 Bytes



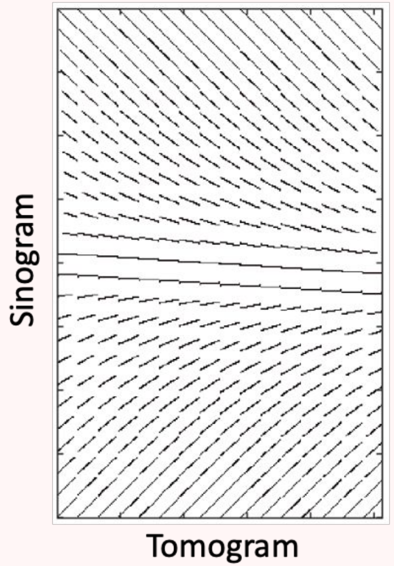
Hilbert Ordering:
6 Cache Misses
384 Bytes



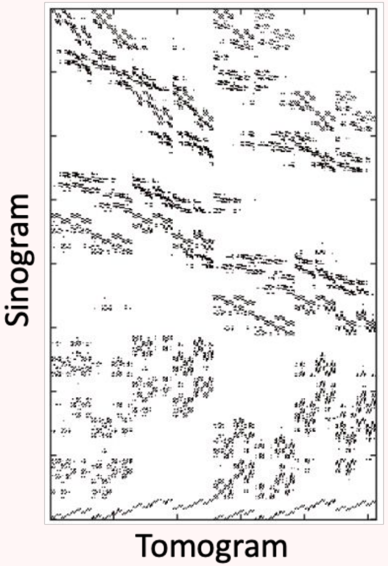
Sparsity Patterns

Projection Matrix

Row-Major Ordering



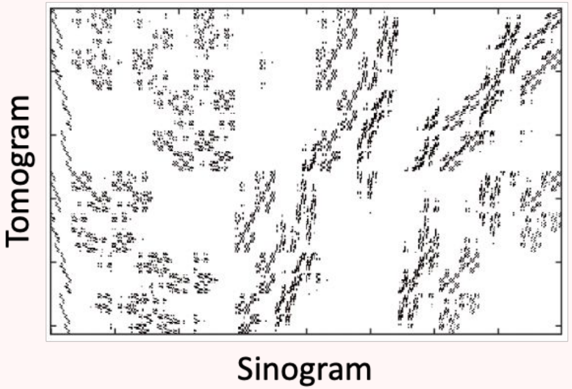
Hilbert Ordering



Sparse Matrix Transpose

Backprojection Matrix

Hilbert Ordering



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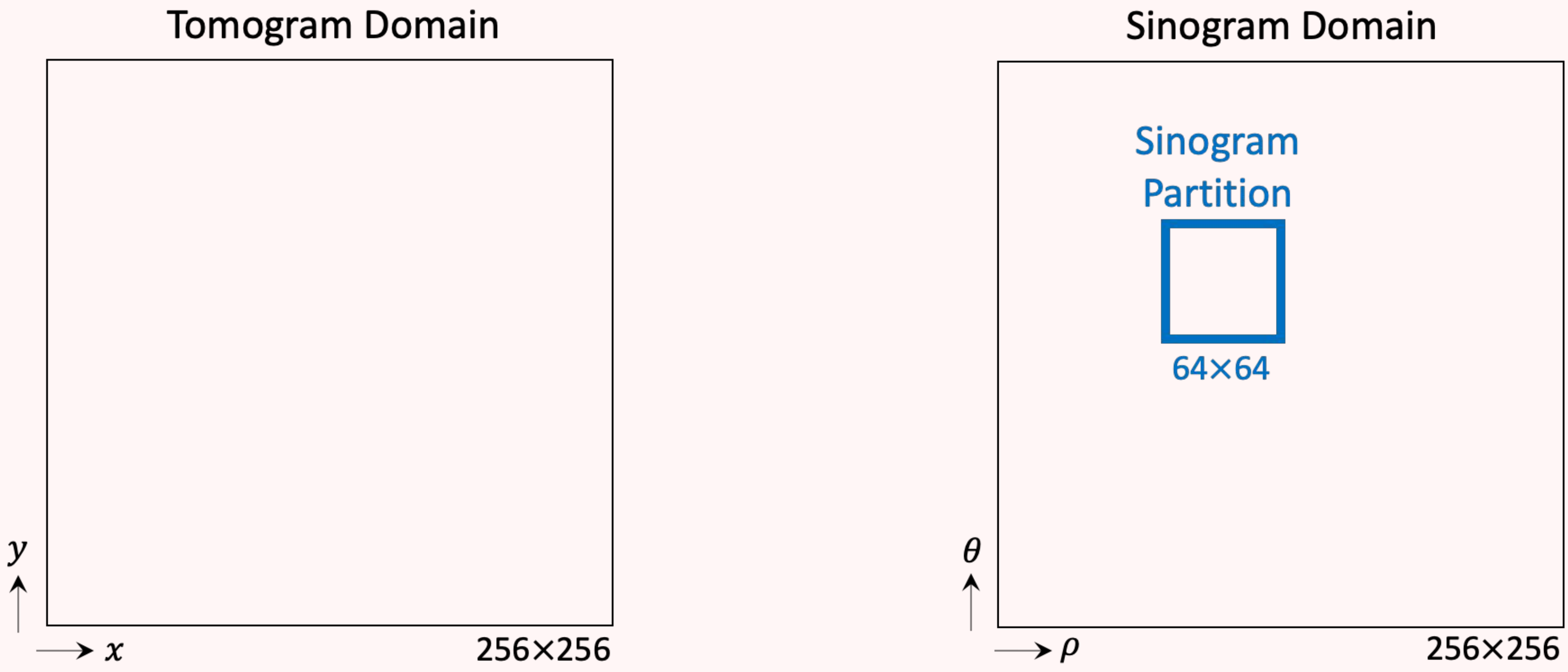
Multi-Stage Buffering



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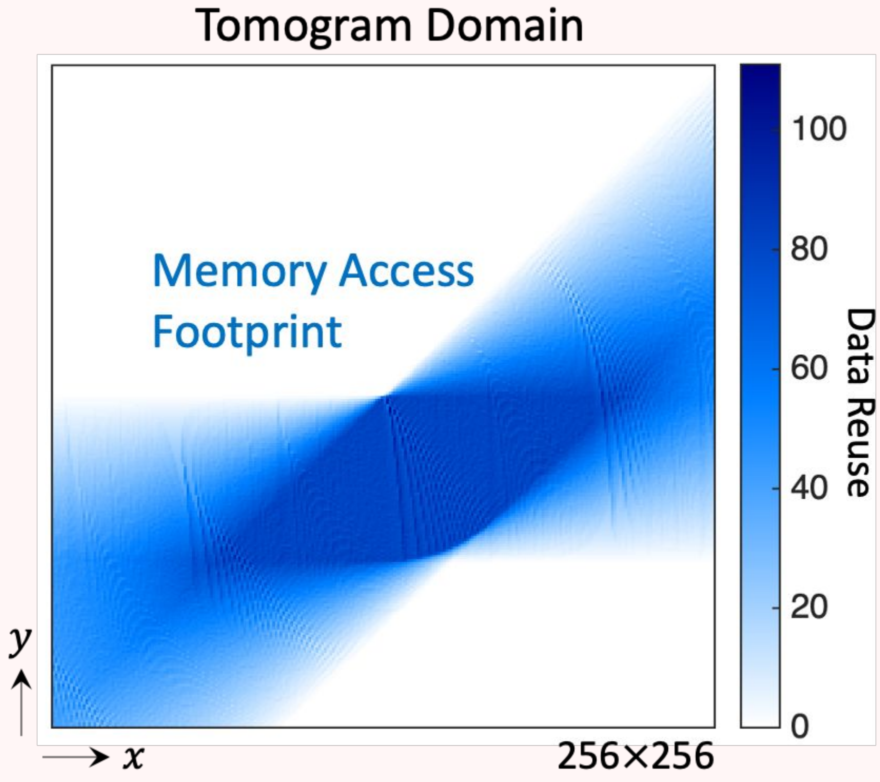
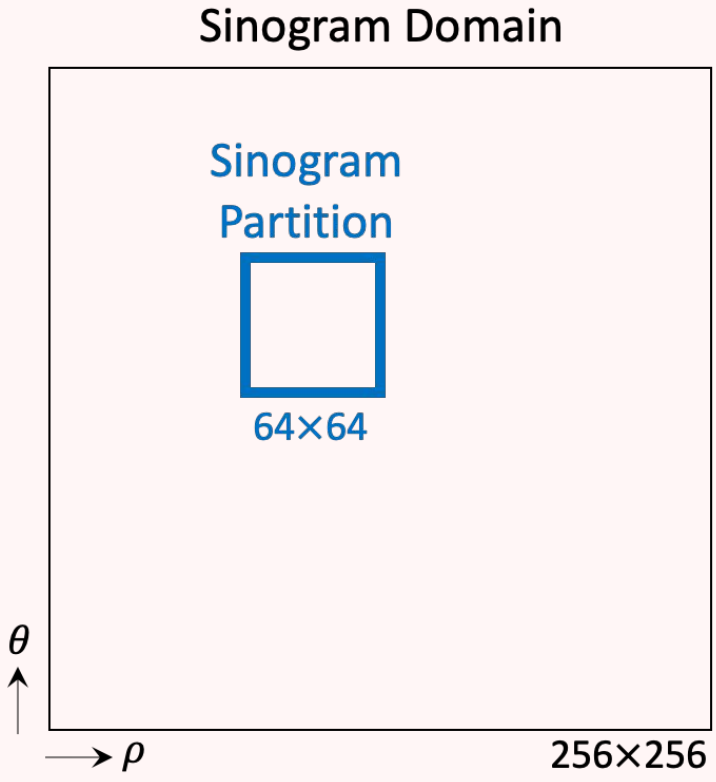
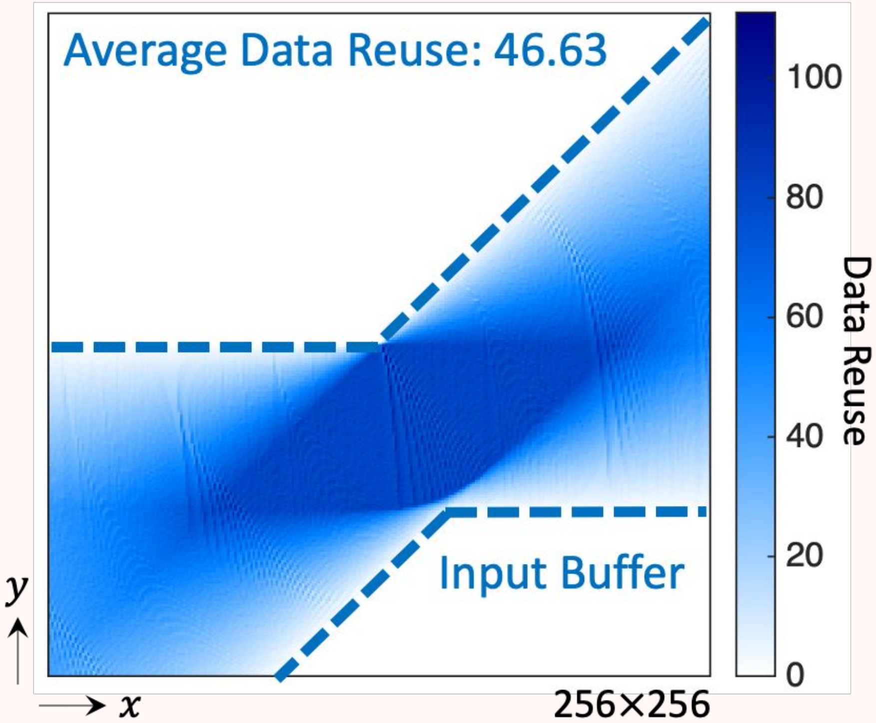


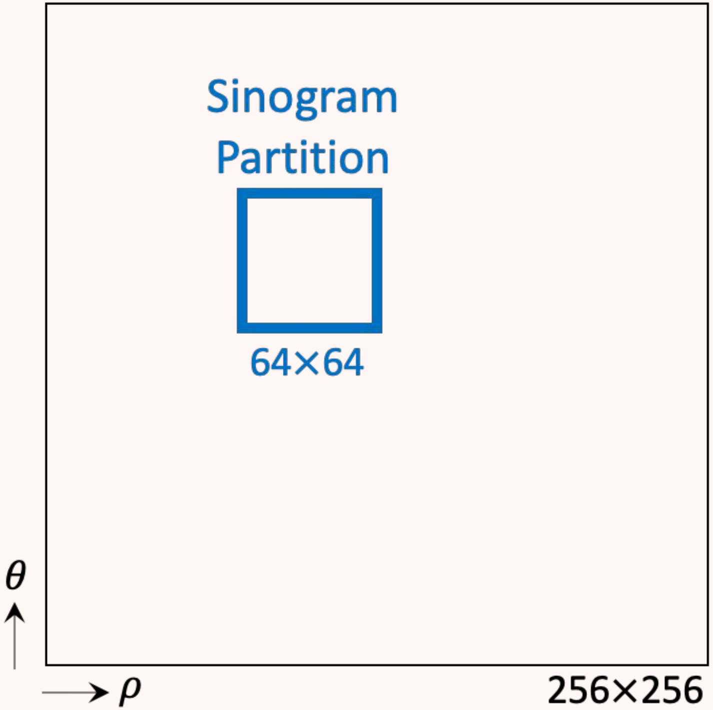


Multi-Stage Buffering

Tomogram Domain



Sinogram Domain



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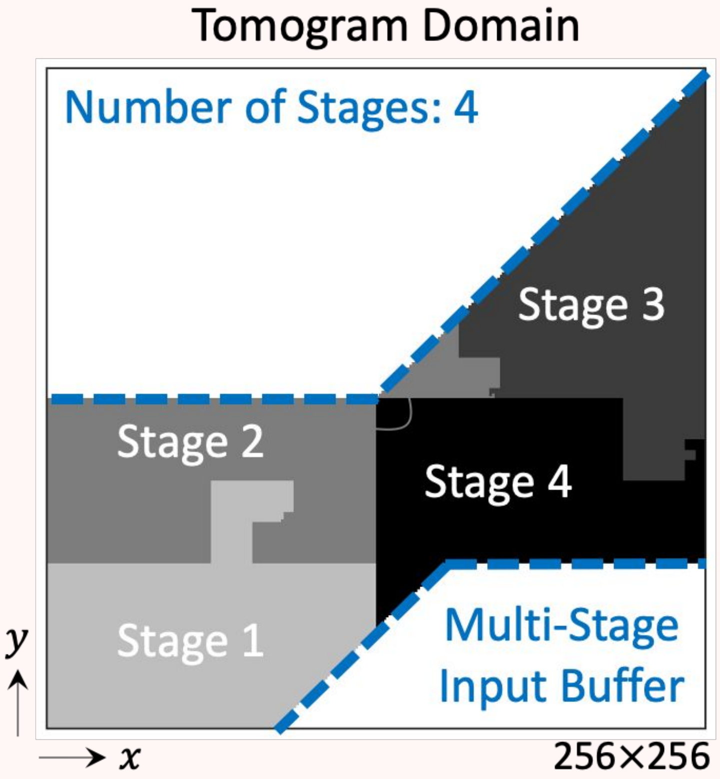
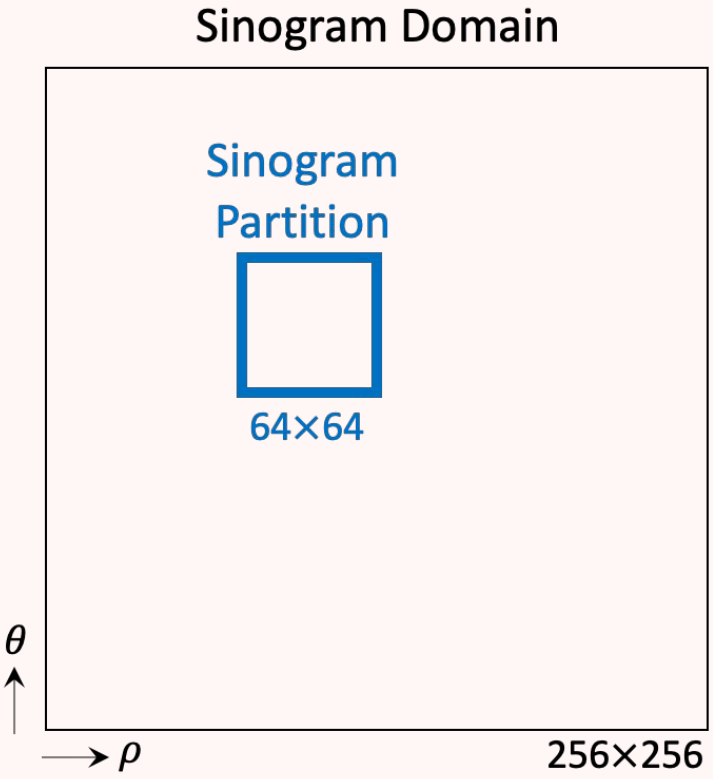




Leadership Class Supercomputers

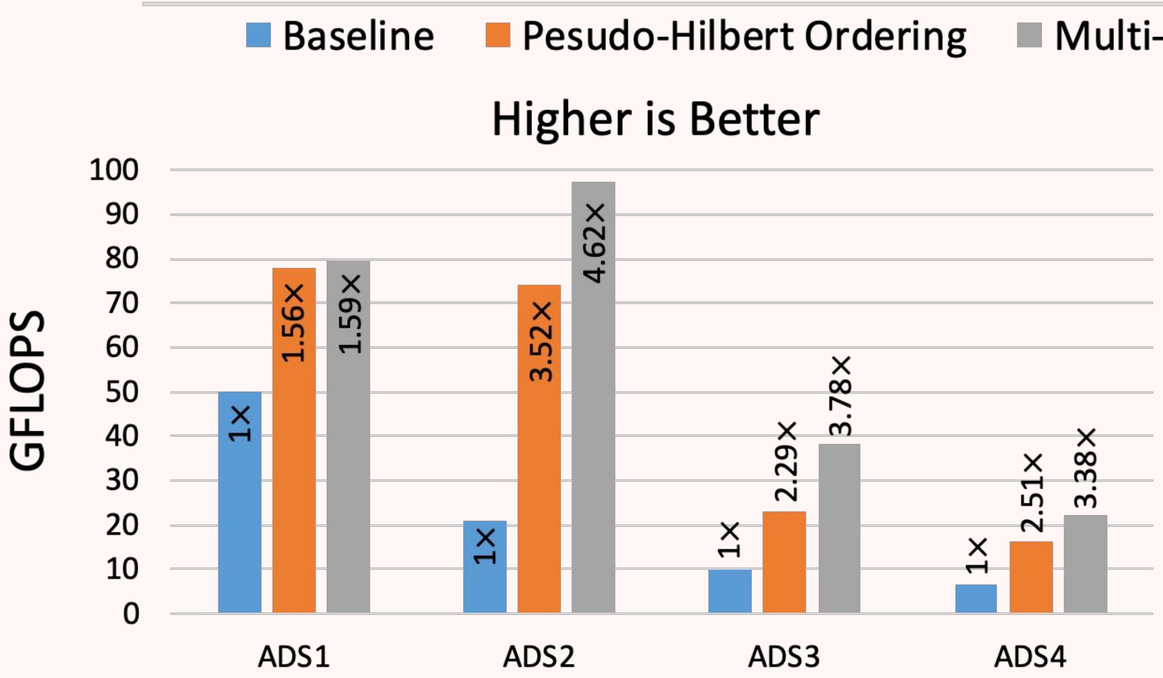
Theta @ Argonne National Lab. (2016)

Summit @ Oak Ridge National Lab. (2019)

Blue Waters @ U. of. Illinois (2013)

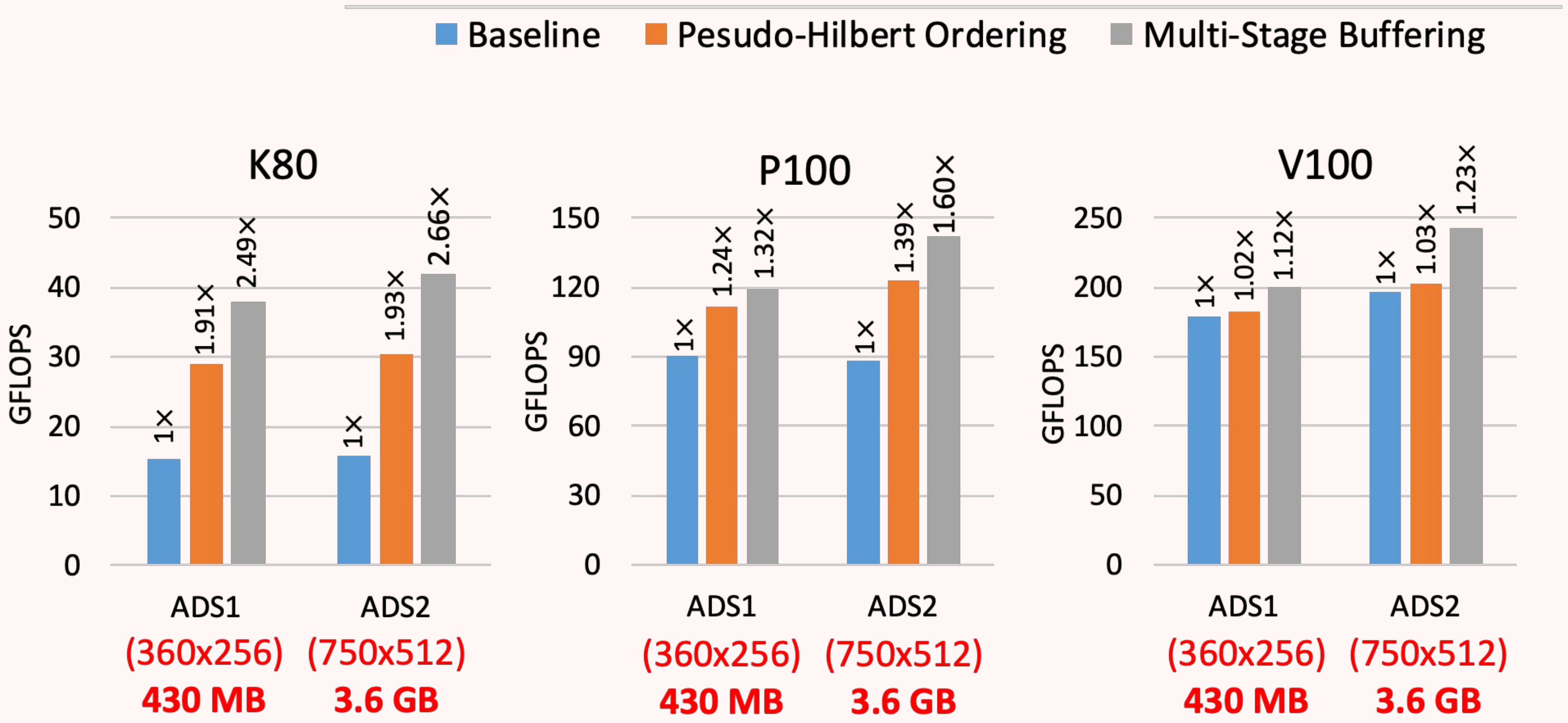
Aurora @ Argonne National Lab. (2021)

Performance Optimizations on KNL



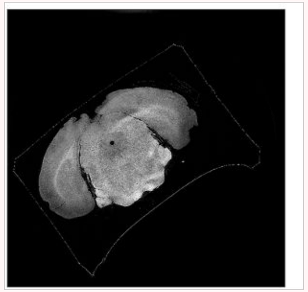
Sinogram Size:	(360x256) **430 MB**	(750x512) **3.6 GB**	(1500x1024) **28 GB**	(2400x2048) **180 GB**

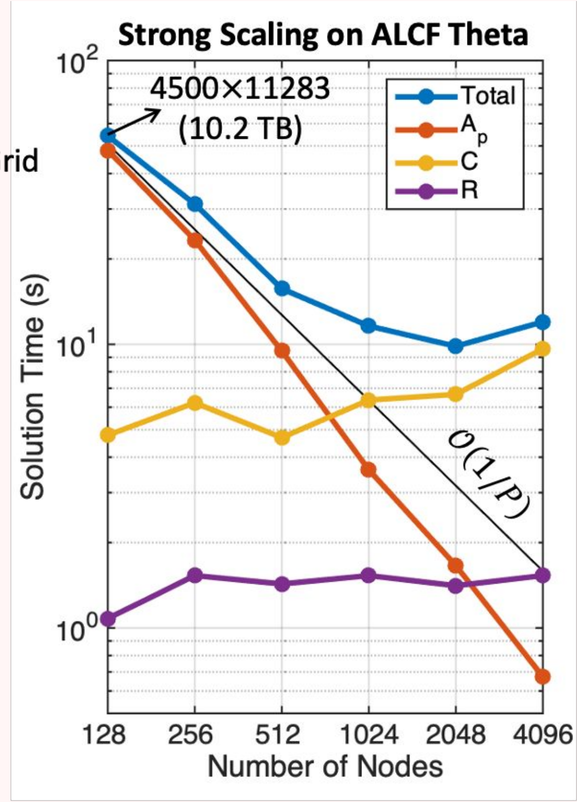
Performance Optimizations on GPU

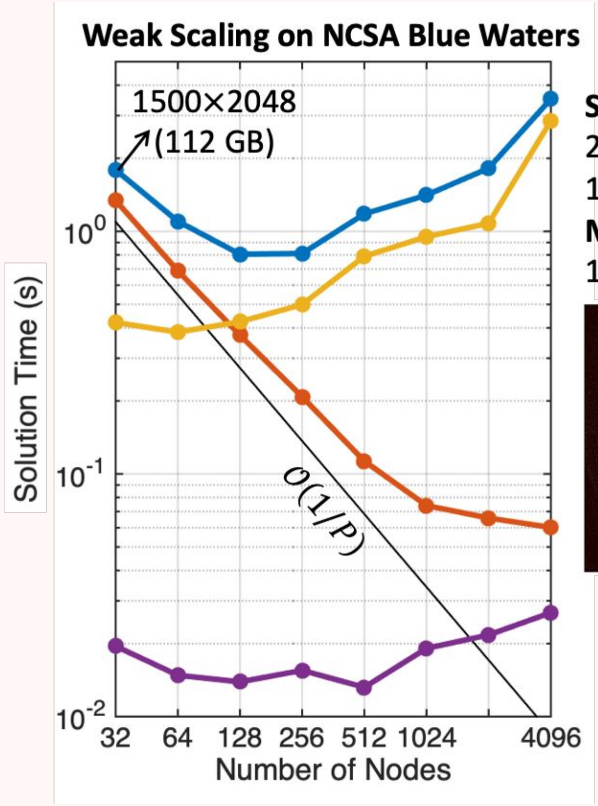


Strong Scaling

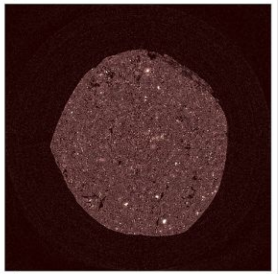
Brain Sample
11283x11283x11283 Grid
4500 Projections
Memory Footprint
10.2 TB





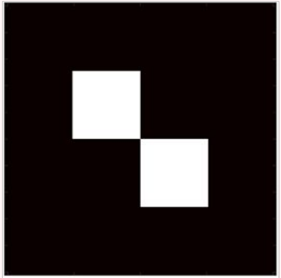


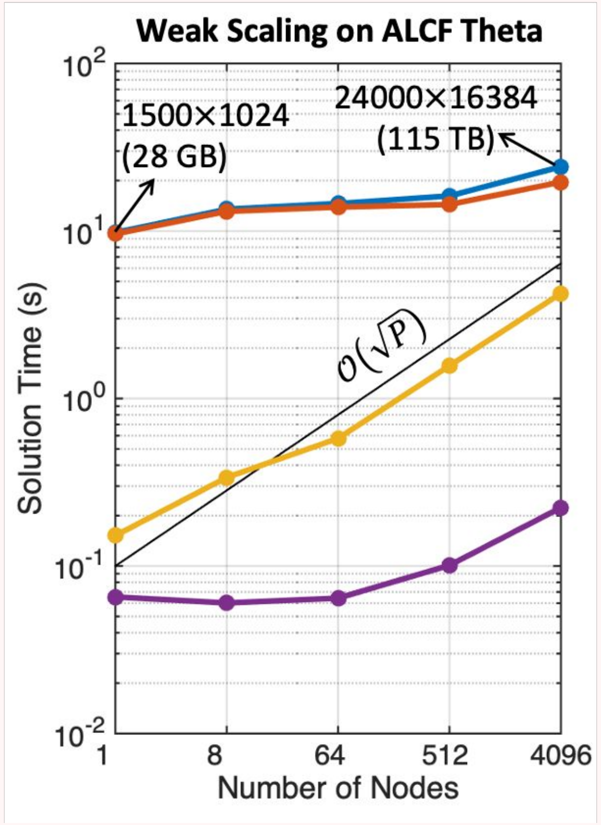
Shale Sample
2048x2048x2048 Grid
1500 Projections
Memory Footprint
112 GB

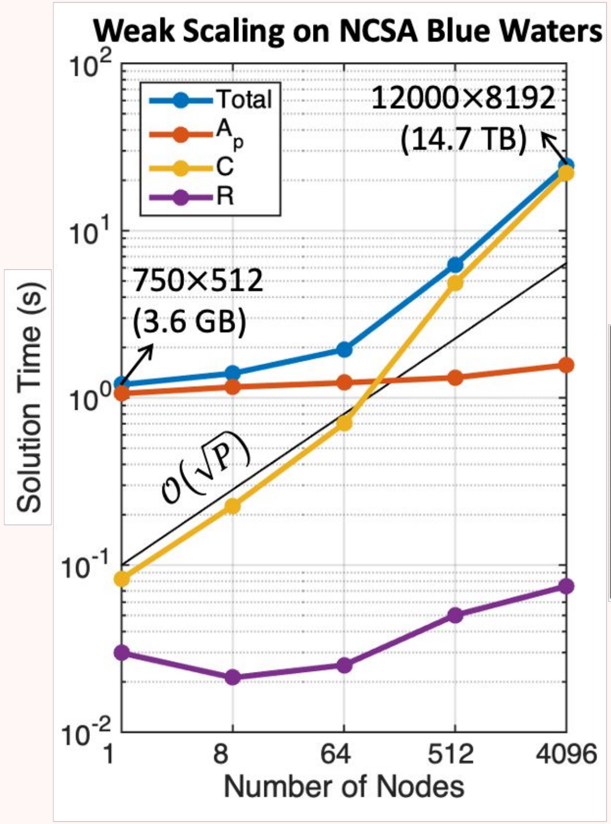


Weak Scaling

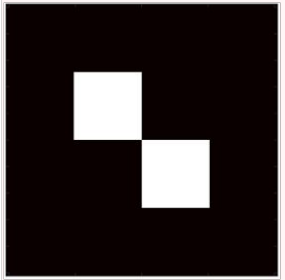
Artificial Dataset



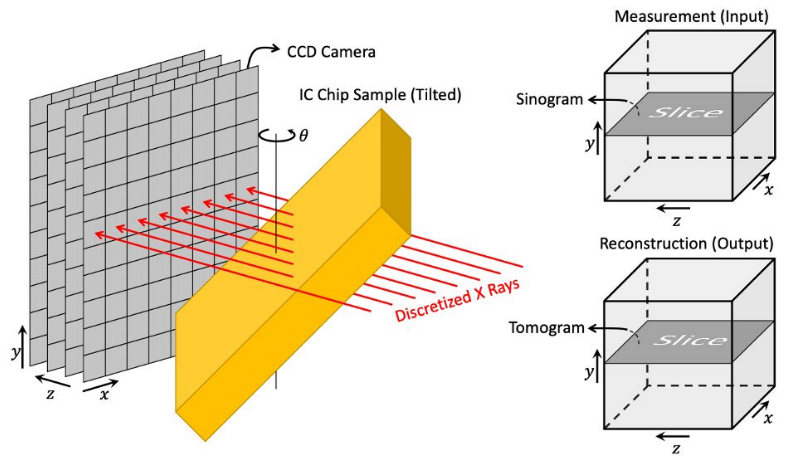




Artificial Dataset

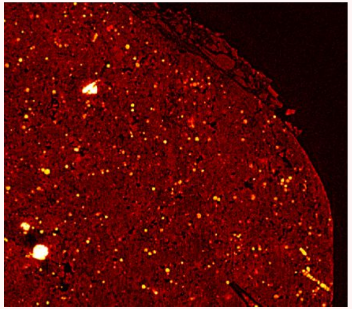


3-D Extension: SC20 Follow-up Paper

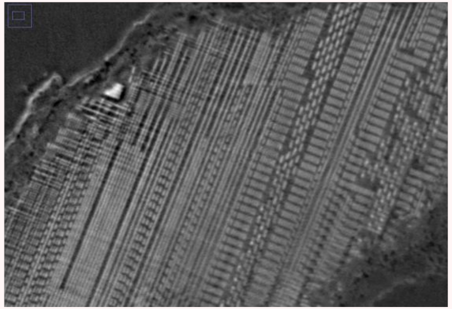


Sample	Measurement Data Cube ($K \times M \times N$)	I/O Data Footprint	Memory Footprint
Shale Rock	$1501 \times 1792 \times 2048$	52.1 GB	120 GB
IC Chip	$1210 \times 1024 \times 2448$	36.7 GB	139 GB
Activated Charcoal	$4500 \times 4198 \times 6613$	1.23 TB	2.82 TB
Mouse Brain	$4501 \times 9209 \times 11\,283$	6.56 TB	10.9 TB

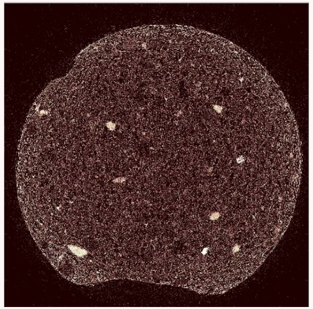
Shale Rock



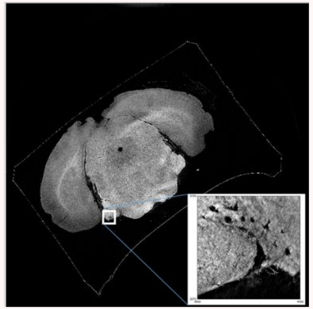
IC Chip



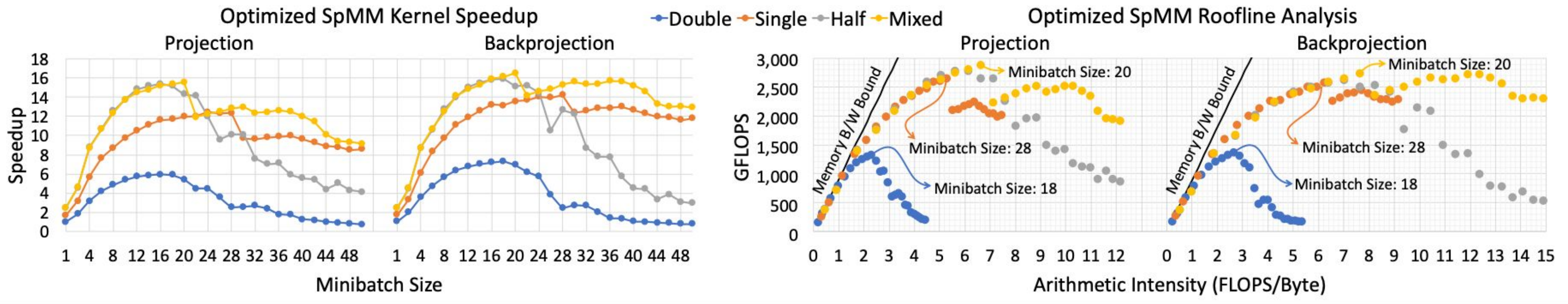
Activated Charcoal

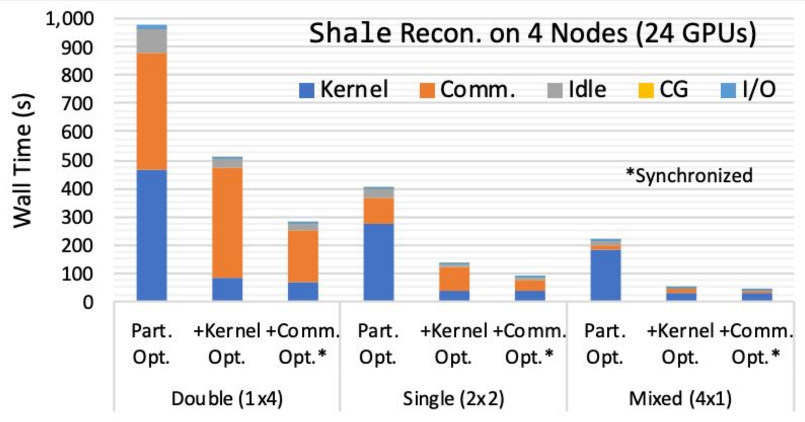


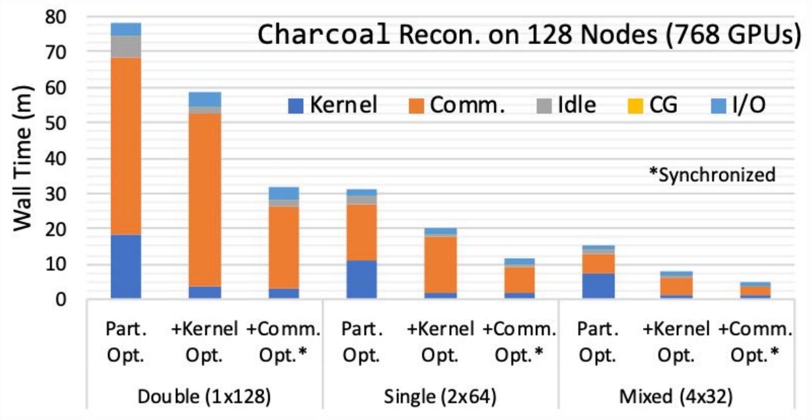
Mouse Brain



3-D Extension: SC20 Follow-up Paper







SC20

Reproducibility Reports

What to Expect

- Describe your architecture, hardware and software
- Describe your experimental setup
- Describe the design of your experiment (amount of runs, implementation details, etc)
- Describe (and plot) the outcomes of your experiment
- Visualize the output data
- Describe the differences between the paper’s results and your experiment's results

Suggestions for Preparation

- Take a look at past year’s reports (will send these out to the SCC Google Group next week)
- Write any part that you can write before the competition (architecture, experiment setup, etc)
- Think and ask about (before the competition) what could cause any differences that you may see between your results and the results of the paper.
    - Some hints on where to look: architecture, scale, software stack, interconnect, etc
- Make sure you understand weak and strong scaling

Questions or Comments?