SCIENTIFIC COMPUTING AND WORKFLOWS AT THE EDGE (AND BEYOND)

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RESEARCH & DEVELOPMENT ACTIVITIES

- High-performance, parallel and distributed computing; scientific computing runtime systems; Application of AI/ML to X-ray
- (Large-scale) X-ray image analysis problems
  - Inverse problems
- Scientific workflows
  - Edge to Supercomputers
  - Federated facilities: Leadership Computing

<table>
<thead>
<tr>
<th>Charcoal Reconstruction (mCT)</th>
<th>Shale Reconstruction (mCT)</th>
</tr>
</thead>
<tbody>
<tr>
<td>200-250 GB</td>
<td>10-15 GB</td>
</tr>
<tr>
<td>2-3 days of processing</td>
<td></td>
</tr>
</tbody>
</table>
EXPERIMENTAL AND COMP. CHALLENGES IN MULTI-DIMENSIONAL PTYCHOGRAPHY

<table>
<thead>
<tr>
<th>Experimental Configuration</th>
<th>Experiment Time</th>
<th>Dataset Size</th>
<th>Analysis Times*</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D</td>
<td>2 mins</td>
<td>5 GB</td>
<td>~2 mins</td>
</tr>
<tr>
<td>Single View</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3D</td>
<td>12 hours (360 Views)</td>
<td>1.8 TB</td>
<td>12 hours</td>
</tr>
<tr>
<td>Mult. Views (MV)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4D</td>
<td>25 days (+ 50 E.)</td>
<td>90 TB</td>
<td>1 month</td>
</tr>
<tr>
<td>MV + Mult.E. (ME)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5D</td>
<td>1250 days (50 Time)</td>
<td>4.5 PB</td>
<td>3.5 years</td>
</tr>
<tr>
<td>MV + ME + Time</td>
<td></td>
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</tbody>
</table>

* (estimation) based on 10 GPUs
(IRREGULAR) DATA ACCESS PATTERN

Optimization with Hilbert Ordering
COMMUNICATION PATTERN IN 3D RECONS.

Multi-level Hierarchical Communication

• 3-level of communication and reduction
• Overlapping communication
• Mixed-precision implementation
• 24K GPUs, >65PFLOPS; <3 mins.

Supercomputer
WORKFLOW SYSTEM FOR IMAGE DATA ANALYSIS

- System components
  - Globus Automate
  - FuncX
  - Globus Transfer
  - Globus Auth

Tekin Bicer et al., “High-Performance Ptychographic Reconstruction with Federated Facilities,” Smokey Mountain Conference 2021
REINVENTING COHERENT IMAGING DATA INVERSION

PtychoNN is >100X faster
Requires 25X less data

Requires >PFLOPs of on-demand to keep up with experiments

AI@EDGE FOR PTYCHOGRAPHY

Sample chamber
X-ray detector
NVIDIA Jetson
Al-Accelerated Ptychography Workflows

Train Al @ ALCF, deploy Al @ beamline

- Real-time imaging: >100X faster than phase retrieval
  - Live inference at 100 Hz on 512x512 detector images (1 Gb/s)
- Lower-dose imaging: 25X less data than phase retrieval
- Future work: other techniques, closed-loop experimental steering

Anakha V. Babu, Tao Zhou, Saugat Kandel, Yi Jiang, Yudong Yao, Sinisa Veselli, Zhengchun Liu, Tekin Bicer, Francesco deCarlo, Ekaterina Sirazitdinova, Geetika Gupta, Martin V. Holt, Antonino Miceli and Mathew J. Cherukara, “Real-time nanoscale ptychographic X-ray imaging using deep learning at the edge”

TAKE-AWAY MESSAGES

- Collaboration opportunities
  - HPC for large-scale data analysis
  - Runtime and workflow systems
  - AI/ML accelerated data analysis
  - Experimentation steering
- Focus on synchrotron radiation (X-ray) imaging problems
- Very diverse set of collaborators
  - Computer, computational, beamline scientists and experts

- APS: Anakha V. Babu, Tao Zhou, Saugat Kandel, Yi Jiang, Yudong Yao, Junjing Deng, Daniel Ching, Jeff Klug, Doga Gursoy, Sinisa Veselli, Francesco de Carlo, Martin V. Holt, Antonino Miceli, Nicholas Schwarz, Stefan Vogt and Mathew J. Cherukara
- DSL: Zhengchu Liu, Joaquin Chung, Xiaodong Yu, Rajkumar Kettimuthu, Ian T. Foster
- Mert Hidayetoglu (UIUC), Wen-mei W. Hwu (UIUC), Bin Ren (W&M), Simon Garcia de Gonzalo (BSC)
- Argonne Leadership Computing Facility
- and many others!