SurrogateTrain: Drastically Improving Performance of Data Loading for Training Scientific Surrogate Models

Background & Motivation

Pytorch Imaging

APS-U
High-flux X-Ray Beams Experiments

Data Scale
Hundreds of Petabytes

Surrogate Models

PtychoNN
Predicts the 2D amplitude and phase images.

AutoPhaseNN
Predicts the amplitude and phase patterns.

BraggNN
Predicts the positions of diffraction peaks.

- Ptychography imaging techniques aim to increase the resolution of images beyond x-ray optics.
- Traditional iterative algorithms are computationally expensive.
- Advanced Photon Source Upgrade (APS-U) will provide immense data.
- Surrogate models are designed to achieve the task more efficiently.

From Single Device to Distributed Training

The Architecture of DGX-A100 Nodes

- To train surrogates on large datasets:
  - Utilize supercomputers like ThetaGPU
  - Utilize data parallelism in distributed training.
- Data loading takes >80% of training time!

Proposed Design

Part I: Offline Scheduling

- (a & b) Epoch order optimization.
- (c) Data locality optimization + Load balancing scheduling

Part II: Runtime Buffering

1. Idle time while waiting for data loading.
2. Load imbalance incurred.
3. Overall time reduced from balancing the load.

Reference


Acknowledgment

This research was supported by the U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research (ASCR), under contract No. DE-AC02-06CH11357 and by the National Science Foundation through Award OAC-2003709 and. We gratefully acknowledge the computing resources provided on Theta/ThetaGPU supercomputer operated by the Argonne Leadership Computing Facility.

Evaluation

Setup

- Environment: ThetaGPU supercomputer
- Baseline: PtychoNN using Pytorch DataLoader.
- Dataset: In-house dataset from ANL APS. 262,896 images

Number of Data Loaded From PFS

<table>
<thead>
<tr>
<th>Dataset</th>
<th>V1 Rank Avg.</th>
<th>V2 Rank Avg.</th>
<th>V3 Rank Avg.</th>
</tr>
</thead>
<tbody>
<tr>
<td>In-house dataset from ANL APS</td>
<td>52.5 67.9 58.2</td>
<td>67.9 58.2 67.9</td>
<td>67.9 58.2 67.9</td>
</tr>
</tbody>
</table>

Performance on Each Optimization Step

- The baseline method loads 512 images on each rank in each step.
- Compared to PtychoNN, our reduced data loading, reducing data loading by 6.7x.

Optimization Speedup

- V1: data access order optimization.
- V2: load balancing optimization.
- V3: chunked loading optimization.

<table>
<thead>
<tr>
<th>Optimization Step</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>V1</td>
<td>2.45x</td>
</tr>
<tr>
<td>V2</td>
<td>4.60x</td>
</tr>
<tr>
<td>V3</td>
<td>7.40x</td>
</tr>
</tbody>
</table>