Understanding Scalable Realtime Collaborative Workflows

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Research at the Lab

Fusion - Relationships between magnetic and velocity fields in a tokomak.

http://adsabs.harvard.edu/abs/2012APS..DPPYP8009S
Research at the Lab

Nuclear Energy - Modeling a Nuclear Power Plant from pellet to plant

Research at the Lab

Understanding Biological, Chemical, and Material Properties

Research at the Lab

Ocean Modeling (Visualizing Oil Dispersion) - Deep Water Horizon Oil Spill in Gulf of Mexico

Study of currents in Gulf of Mexico

Distributed Finite-Time Lyapunov Exponent Computation

Research at the Lab

Extreme Climate Event Detection - Hurricane, Tropical Cyclone, Atmospheric Rivers Detection, etc…

Big Data Challenges

• Cataloging the universe & determining the fundamental constants of cosmology
• Characterizing extreme weather events in a changing climate
• Extracting knowledge from scientific literature
• Investigating cortical mechanisms for speech production
• Google Maps for Bio-Imaging
• Perform extreme scale genome assembly
• Precision toxicology
• Seeking designer materials
• Determining the fundamental constituents of matter

What do many large DOE Projects have in common.

- Multi institutional (just a few)
  - Labs: LBNL, LLNL, PNNL, LANL
  - Facilities: ALS, BNL, SLAC (SSRL & LCLS), NSLS2
  - Sites: Hanford (Washington), F-Area (Savannah River)
  - Resources: NERSC, ORNL, SDSC, TACC

- Expertise from several domains working together.
  - Domain Scientists, Physicists, Mathematicians, Statisticians, Engineers
  - Research Focused (Fair amount of software development)
  - Complex workflow – Highly specialized hardware and custom software.

The rest of the Talk will delve into two specific projects
Science Use Case #1: Environmental Management (Macro)

- Understand Cleanup efforts at the Hanford & F-Area Savannah River Sites.
  - Hanford - the first full-scale plutonium production reactor in the world.
  - F-Area (Savannah River) – Site for refinement of nuclear materials

- Create a process combining strengths of observed data, modeling, analysis, and simulation to gain insight.
Java Eclipse application al
Provides Model-Setup, Inverse Parameter Estimation, UQ, Remote Job Launching & Monitoring of Simulations, and Visualization.
VisIt visualization framework
VisIt visualization framework

Parallel Cluster

VisIt Engine

Data Plugin

Data

Data

Data

Data Flow Network

Filter

Filter

Filter

Remote Clients

VisIt Viewer

Local Components

VisIt GUI

VisIt CLI

Python Clients

Java Clients

network connection

network connection

network connection

network connection
VisIt: Customizable Interfaces

Embedded

Lightweight, Collaboration

Tailored Vis
VisIt: Collaborative Capabilities

Custom UI

Domain Processing

Collaborators
Visualization Services

ASCEM Data Browser

3D visualization

Provenance
Data Storage

Visualization Service

2D visualization

2D Visualization (F-Area)

ASCEM Data Browser
- Google Map Overlay
- Query by: Aquifer Zone, Analyte, and Year
- Contours of concentration levels
- Time-varying data

3D Visualization (F-Area)

Evolution of Tritium Concentration from 1990-2009

Time Sliders
Depositional Environment
All Aquifer Layers
Context: Overlay, Well Sites, Legend,
Concentration Levels, Contours/IsoSurfaces
3D Visualization (Hanford Site)

Ground Penetrating Radar

Observation vs Simulation
Domain Centric Collaborative Visualization
2D Visualization

- Google Map API
  - Intuitive, Easy to use, Familiar, Powerful

- Delaunay Triangulation Overlay (VisIt-backend)
  - Shows concentration levels
  - API allows for Custom Color-maps and Concentration levels
  - Temporal view provides powerful and intuitive understanding of concentration levels over time. (Impact of proposed mitigation solutions)
3D Visualization

- Interactive – Supports visualization of multiple layers
- Visually coherence
  - Sensors, Injection + Logging Sites, Well Bores, Image Overlays
- Provides easy to use spatial + temporal visualization
- Visual Comparisons:
  - Same information different sources.
  - Observed and simulated data.
Observations

Simulations

Analysis
Project Summary

• Challenge: Provide a diverse team of scientists together to understand and mitigate a major environmental issue.

• 2D + 3D Visualizations (Provide a complete picture)
  ◦ GIS information, Sensor data, Well Site location, Depositional Environments, Spatial + Temporal information, Comparative visualization

• Domain Centric Collaborative visualization.
  ◦ Allows tools to address needs of complex and diverse team.

• ASCEM-Akuna Software Toolkit (Open Source)
  ◦ Provides Model-Setup, Inverse Parameter Estimation, UQ, Remote Job Launching & Monitoring of Simulations, and Visualization.

https://akuna.labworks.org/download.html
Science Use Case #2: X-ray Light Sources (Micro/Nano)

- Image reconstruction images from multiple lower resolution diffraction patterns (Ptychography).

- A high throughput realtime data analysis pipeline.

https://arxiv.org/abs/1609.02831 (Streaming Ptychography)
X-ray microscopes, spectrometers, and scattering instruments

- Characterization of structure and properties of materials for example:
  - New drug synthesis
  - Dust particles from space
  - New super conductors
  - Battery research on nanoscale internal structures to understand reactivity
  - Carbon sequestration by porous rock at nanometer scale

- New generation of 3D microscopes
  - brighter x-ray light sources
  - fast parallel detectors

Improvements in image resolution enables this work
Ptychography

**Fundamental idea: combine:**
- High precision scanning microscope with
- High resolution diffraction measurements.
- Replace single detector with 2D CCD array.
- Measure intensity distribution at many scattering angles

**Each recorded diffraction pattern:**
- contains short-spatial Fourier frequency information
- only intensity is measured: need phase for reconstruction.
- phase retrieval comes from recording multiple diffraction patterns from same region of object.

**Ptychography:**
- uses a small step size relative to illumination geometry to scan sample.
- diffraction measurements from neighboring regions related through this geometry
- Thus, phase-less information is replaced with a redundant set of measurements.

Several ptychographic equipment/codes throughout DOE, universities, worldwide
ALS beamline
Nanosurveyor chamber
ALS beamline
Nanosurveyor chamber
FastCC D detector

200x1024x1024 pixels/s
ALS beamline
Nanosurveyor chamber
FastCCD detector
200x1024x1024 pixels/s
ALS beamline
Nanosurveyor chamber
GPU cluster

FastCC D detector
200x1024x1024 pixels/s

LBLne
Phasis

10 Gbps
ALS beamline User Display

Nanosurveyor chamber

GPU cluster

FastCC D detector

200x1024x1024 pixels/s

10 Gbps

LBLne

Phasis

Thermal survey, K-side
Ptychography is similar to Scanning Microscope but trades greater complexity for higher resolution.

Scanning Microscopes are the most oversubscribed instruments at ALS and other Synchrotrons.
Ptychography is similar to Scanning Microscope but trades greater complexity for higher resolution.

Scanning Microscopes are the most oversubscribed instruments at ALS and other Synchrotrons.
Ptychography is similar to Scanning x-ray microscope but trades greater complexity for higher resolution.

2D Diffraction measurements

\[ I = |F(P_i \cdot O)|^2 \]

- **I** = Recorded intensities
- **\( P_i \)** = Illumination probe of frame \( i \)
- **F** = Fourier transform
- **O** = Sample Object
Only a few kernels are necessary to implement basic ptychographic reconstruction on a GPU.

Split kernel

Start with a random image

Merge kernel
Only a few kernels are necessary to implement basic ptychographic reconstruction on a GPU.

Split kernel

Start with a random image

Merge kernel
Only a few kernels are necessary to implement basic ptychographic reconstruction on a GPU.

Multiply Object with Probes

Start with a random image

Merge kernel
Only a few kernels are necessary to implement basic ptychographic reconstruction on a GPU.

Start with a random image

Split kernel
Multiply Object with Probes

FFT frames

Merge kernel
Only a few kernels are necessary to implement basic ptychographic reconstruction on a GPU.

Split kernel

Multiply Object with Probes

Start with a random image

Merge kernel

For each pixel replace magnitude with experimental value
Only a few kernels are necessary to implement basic ptychographic reconstruction on a GPU.

Start with a random image

Multiply Object with Probes

Split kernel

FFT frames

CUFFT

For each pixel replace magnitude with experimental value

IFFT frames

CUFFT

Merge kernel
Only a few kernels are necessary to implement basic ptychographic reconstruction on a GPU.

Split kernel

Multiply Object with Probes

Split kernel

FFT frames

CUFFT

Overlap kernel

Overlap and average frames.

IFFT frames

CUFFT

For each pixel replace magnitude with experimental value

Merge kernel
Higher level parallelization

• To be able to process data in real time (200Hz) we need to use multiple GPUs.
Higher level parallelization

• Split without overlap
• Synchronize every iteration

• Split with overlap
• Synchronize every iteration

• Split without overlap
• Do not synchronize every iteration

• Split with overlap
• Do not synchronize every iteration
Strong scaling tests on an experimental dataset show the code is scalable.

**Reconstruction Walltime**

**Reconstruction Speedup**

- **Time (s)**
  - 150.0
  - 112.5
  - 75.0
  - 37.5
  - 0

- **Number of Nodes**
  - 0
  - 10
  - 20
  - 30
  - 40

- **CUDA**
- **OpenMP**

- **Speedup Ratio**
  - 30.0
  - 22.5
  - 15.0
  - 7.5
  - 0

- **Number of Nodes**
  - 0
  - 10
  - 20
  - 30
  - 40

- **CUDA**
- **OpenMP**
First experimental results show a large improvement in resolution over STXM.

Traditional STXM image.

Ptychography image using the same data.

SEM image.

Resolution of about 10 nm.
COSMIC-Nanosurveyor

- Microscope - under construction
- 100 frame / sec CCD - developed at LBNL
- High performance computing - use of NERSC infrastructure

1 MHz CCD in 3 years
Enabling Streaming Ptychography
Enabling Streaming Ptychography
Nanosurveyor
Conclusions

- Image reconstruction at nanometer scales enables to new science insight.

- New light sources, parallel detectors, and computational hardware now makes novel algorithms such as real-time Ptychography and tomography possible.

- The rate of data acquisition is also increasing and need for immediate feedback is necessary to ensure optimal use of X-ray beamline.
Final Thoughts

• Thank you!

• Acknowledgements:
  ◦ ASCEM – ASCR/DOE funded Environmental Management project
  ◦ CAMERA/ALS – ASCR/BES funded project Team members – X-ray light sources
Publications

- http://adsabs.harvard.edu/abs/2012APS..DPPYP8009S
- http://scripts.iucr.org/cgi-bin/paper?S1600576716008074
- http://scitation.aip.org/content/aip/proceeding/aipcp/10.1063/1.4952921
- https://publications.lbl.gov/islandora/object/ir%3A1005825
- http://www.tandfonline.com/doi/abs/10.1080/08940886.2015.1013413
Software

- https://wci.llnl.gov/simulation/computer-codes/visit/
- https://akuna.labworks.org/download.html
- https://github.com/eclipse/ice
- https://github.com/CameraIA/F3D
- https://bitbucket.org/lbl-camera/xi-cam
- https://github.com/UV-CDAT/uvcdat
- https://github.com/LBL-EESA/TECA
- https://github.com/visit-vis/visit_java_client
- http://www.camera.lbl.gov/software
Why is ptychography so interesting?
- Diffraction resolution
- Macroscopic field of view
- Increased contrast through phase
- In-situ optical metrology (blind ptychography)
- Turns more data into better resolution
- Extendible to spectro-ptychography, ptychotomography, near field, Fourier Ptychography, time resolved dynamics

Why not is everyone doing it (cons)
- Requires fast detectors
- Requires a bright source
- Requires mathematics
- Requires parallel code
  - Alternating Projections
  - “RAAR”,

![Ptychography and Microscopy Comparison]
an overdetermined problem in high dimensional space.

How to solve it?
Algorithms in this talk

- Projection algorithms
  - Alternating Projections
  - “RAAR”,
  - Augmented Lagrangian
  - “Difference Map”, “HIO”

- (Weighted) Least Square methods, maximum likelihood:
  - Conjugate Gradient,
  - Newton,
  - CG Newton

- Spectral methods
  - synchronization
  - Graph Laplacian

Low dimensional space

fit data

Large dimensional data

fit model

tutorial in use

acceleration noise model

large scale robust
Alternating projections

sample space

fit model

fit data

split frames

normalize

merge frames

propagate

propagate back

Replace magnitudes

measurement space
Ptychographic imaging setup

How to simulate it?

Fourier transform data

translate and illuminate

amplitude = propagation scanning illumination sample

\[ \alpha = |Fz|, \]
\[ z = Q\psi^{\dagger}, \]

“frames”

find unknown
Fracture Analysis of High-res Images

Identification of structures

**Raw data**

- Apply F3D filters to extract composite
- Apply F3D filters to improve contrast

**Prototype examples**

**Template matching with high tolerance**

**Template matching with low tolerance**

**For each slice in the stack**

**Intersection with "Base Result"**

**Union**

**Template matching approach**
Template matching

\[ \text{MSE}(x, y) = \frac{1}{n} \sum_{i,j} [p(i, j) - f(x + i, y + j)]^2 \]

2) Determine the best matches:

\[ \text{NCCC}(x, y) = \frac{\sum p(i, j) - \bar{p}(i, j) \sum f(i, j) - \bar{f}(i, j)}{\left[ (\sum p(i, j) - \bar{p}(i, j) \sum f(i, j) - \bar{f}(i, j))^2 \right]^{1/2}} \]
Alternating projections
- project onto sample space
  \[ P_Q = Q(Q^*Q)^{-1}Q^* \]
- project onto measurement space
  \[ P_{\mathcal{Z}} = F^* \frac{F \mathcal{Z}}{|F \mathcal{Z}|} a \]
- repeat

Q sample space

split frames

(Q*Q)^{-1} normalize

merge frames

propagate

Q*

propagate back

Replace magnitudes

measurement space
Least square methods

These methods are equivalent

\[
\begin{align*}
    \min_{\psi} & \|a - FQ\psi\| \\
    \min_{z} & \|a - Fz\| \quad \text{s.t. } z = P_{FQ}z
\end{align*}
\]

minimize discrepancy with data

These iterative methods are equivalent

<table>
<thead>
<tr>
<th>“Alternating projections”</th>
<th>“Error Reduction”</th>
<th>“projected steepest descent”</th>
</tr>
</thead>
<tbody>
<tr>
<td>[z^{\ell+1} = P_Q P_a z^\ell = z - P_Q \nabla \epsilon^2(z^\ell)]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

How to speed up?

- Relaxed “Douglas-Rachford” (RAAR) (SHARP release) \(O(5x \text{ speedup})\)
- Conjugate directions acceleration \(O(10x \text{ speedup})\)
  - gradient from fast projections kernels
  - line search using Newton step from implicit Hessian
- Synchronization-Conjugate directions-line search \(O(20x \text{ speedup})\)
Nearest Neighbor Overlap Enables Robust Convergence

Numerical experiments show linear convergence rate, however…
The problem with size

Long range interactions among frames decay exponentially with distance

- at each iteration a frame only talks to neighbors
- how to achieve long range scaling?
Phase synchronization

2 frames

\( z(1) = \xi z(2) \)
\( |\xi| = 1 \)

How to find common phase?

best fit

\[
\min_{|\xi|=1} ||z(1) - \xi z(2)||^2
\]

\[
||z(1)||^2 + ||z(2)||^2 - 2Re\left( \frac{z^*(2)z(1)}{(z^*_1 z(2))} \right) \xi^*
\]

maximize product

Align phases:

\[
\xi = \frac{(z^*_1 z(2))}{(z^*_1 z(2))} \quad \text{Normalize dot product}
\]
what if many frames are out of phase?

\[ |\xi| = 1 \]

minimize all the differences

\[
\min_{|\xi|=1} \sum_{i,j} \|z_{(i)}\| + \|z_{(j)}\| - 2\xi_{(i)} (\mathcal{H})_{(i,j)} \xi_{(j)}
\]

Dot product between frames

\[
(\mathcal{H})_{(i,j)} = (z_{(i)}^* z_{(j)})
\]

Simplify

\[
\max_{\xi} \xi^* (\mathcal{H}) \xi
\]

Phase synchronization

Any meaning? Yes! Spectral method
Synchronize phases by spectral methods
to align the phases, find: \( \max_{\xi} \xi^* (\mathcal{H}) \xi \)

Which is equivalent to finding* largest eigenvector
*quick, scalable (e.g. by ARPACK)

what does it mean?
\( H \) is the “graph laplacian” of a network

\[
\mathcal{H} = R^* \begin{pmatrix} \lambda_0 & & \\ & \lambda_1 & \\ & & \ddots \end{pmatrix} R
\]
accelerate and build a better starting guess:

(1) View every pixel of every frame as a dimension. Each data point lives on a torus (complex plane)

(2) Build “relationship network RN: a graph (V,E) that relates each frame to its neighbors.

(3) Construct Graph Laplacian of RN: defined as difference between the degree matrix D and the adjacency matrix A: \( GL = D - A \)

(4) The largest eigenvector of the Connection graph provides the most aligned phases encoding the (approximate) data topology.

This provides a strong starting guess.
•RAAR

•synchro-RAAR

**Fast multiscale approach:**

(1) Above approach can be augmented by alternating long range/short range (framewise/pointwise) relaxations of the connection graph Laplacian. Additionally, use implicit Hessian for fast line search.

(2) This achieves accelerated convergence for large scale phase retrieval problems spanning multiple length-scales. We also show that

(3) This approach also recovers experimental fluctuations over a large range of time-scales.

(4) Brand-new: Framewise rank-1 accelerated illumination recovery by transparency estimation.