Scientific Applications and Heterogeneous Architectures – Data Analytics and the Intersection of HPC and Edge Computing

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Sponsors:
Trends in Next-Generation Systems: IO Gap and Ensembles

Widening IO Gap

Rising Importance of Ensembles

Source: Lucy Nowell (DOE)

Source: https://wci.llnl.gov/simulation/computer-codes/uncertainty-quantification
Trends in Workflows: Compute + Analytics + Data

Laser Interferometer Gravitational-Wave Observatory (LIGO)
Extending HPC to Connect to the “Edge”

<table>
<thead>
<tr>
<th>Simulations</th>
<th>Data Analytics</th>
<th>Real System with Sensors</th>
</tr>
</thead>
</table>

Two Use Cases

• Extending HPC to integrate data analytics
  ▪ Next generation MD workflows
  ▪ Molecular structures
  ▪ **Data transformation** – *i.e.*, capturing information
  ▪ **Dataflow modeling** – *i.e.*, lost information

• Extending HPC to connect to the “Edge”
  ▪ Next generation precision farming
  ▪ Soil moisture data
  ▪ **Data prediction** – *i.e.*, from coarse- to fine-grained information
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Classical Molecular Dynamics Simulations

- A MD simulation comprises of hundreds of thousands of MD job
- Each job performs hundreds of thousands of MD steps
Classical Molecular Dynamics Simulations

- MD step computes **forces** on single atoms (e.g., bond, dihedrals, nonbond)
- Forces are added to compute **acceleration**
- Acceleration is used to update **velocities**
- Velocities are used to update the **atom positions**
- Every \( n \) steps (Stride) → **Store 3D snapshot or frame**

- Forces on single atoms ➔ Acceleration ➔ Velocity ➔ Position ➔ Store 3D snapshot or frame
Building a Closed-loop Workflow

Run n-Stride simulation steps

MD code
(e.g., GROMACS)

Data Generation
Building a Closed-loop Workflow

Run n-Stride simulation steps

Dataflow

MD code (e.g., GROMACS)

Plumed

Ingestor

Data Generation

Data Storage

Parallel File System

Burst Buffer

In-memory Staging Area

DataSpaces

11
Building a Closed-loop Workflow

Data Generation
- MD code (e.g., GROMACS)
  - Plumied
- Dataflow

Data Storage
- Parallel File System
- Burst Buffer
- In-memory Staging Area DataSpaces

Data Analytics
- ML-inferred algorithms
  - Collective variables
- Dataflow
- Retriever
- Analytics representations + algorithms
Building a Closed-loop Workflow

Data Feedback

ML-inferred algorithms
Collective variables

Analytics representations + algorithms

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Data Analytics
Extending HPC to Integrate Data Analytics
Augmenting HPC with In Situ and In Transit Analytics

Example of tools:
- DataSpaces (Rutgers U.)
- DataStager (GeorgiaTech)
**In Situ and In Transit Analytics for MD Simulations**

Frames (or snapshots) of an MD trajectory with a stride of 5 steps:

- We want to capture what is going on in each frame **without**:
  - Disrupting the simulation (e.g., stealing CPU and memory on the node)
  - Moving all the frames to a central file system and analyzing them once the simulation is over
  - Comparing each frame with past frames of the same job
  - Comparing each frame with frames of other jobs
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Proteins with Similar Functions

Key principle: proteins with similar structures have similar functions

- Measure millions of protein variants expressed from yeast or bacteria
- Structure proteins to produce desired properties (protein engineering)
Protein Representations

3D Cartesian representation

Multi-fold representation

Surface representation


From Multi-fold Representation to Image Encoding

1. Ramachandran Plot
2. Distance Matrix
3. Channel Encoding
4. Final Encoding

Every channel encodes information associated with particular secondary structures and their spatial relationship.
From Multi-fold Representation to Image Encoding


Graphic Encoding of Proteins for Efficient High-Throughput Analysis. ICPP 2018.
From Multi-fold Representation to Image Encoding
High-Throughput Protein Analysis

- Eight biological processes from biological process taxonomy in RCSB-PDB
- 62,991 proteins from the PDB

Normalized Confusion Matrix - Accuracy 80.66%
Capturing Changes in Folding with Transfer Learning

Protein: Opsin

Frame 50

Frame 1500

Frame 1950

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  ▪ Data prediction – *i.e.*, from coarse- to fine-grained information
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- **Data Feedback**
  - Analytics feedback
Modeling Lost Frames

S1, S2, S3: generate MD frame
W1, W2, W2: write to shared memory
R1, R2, R3: read from shared memory
A1, A3: analyze frame
Dataflow for Modeling Lost Frames

Data Generation
- **Generator of MD frames**
  - Plumed
- **Ingestor**

Data Storage
- **In-memory Staging Area**
  - *DataSpaces*

Data Analytics
- **Retriever**
- **Analytics representations**
- **Distance matrices**
  - $D = \begin{bmatrix}
  0 & 0 & 0 & \times & \times & \times \\
  0 & 0 & 0 & d & \times & \times \\
  0 & 0 & 0 & \times & \times & \times \\
  \times & d & \times & 0 & 0 & 0 \\
  \times & \times & \times & 0 & 0 & 0 \\
  \times & \times & \times & 0 & 0 & 0 
\end{bmatrix}$
- **$\lambda_{max}$ eigenvalues**

Eigenvalues: Proxy for Structural Changes

Frames (or snapshots) of an MD trajectory with a stride of 5 steps:

\[\lambda_{max55}, \lambda_{max60}, \lambda_{max65}, \lambda_{max70}, \lambda_{max75}, \lambda_{max80}\]

The distance between two max eigenvalues can serve as a proxy for distance between the two associated conformations.
Single frame at time $t$

$\text{N}_\alpha \ C_\alpha$ atoms
Single frame at time $t$

$N_\alpha C^\alpha$ atoms

Distance of two segments with segment length:

$N_\alpha/2 \times C^\alpha$ atoms

$(C^\alpha_{1} - C^\alpha_{N_\alpha/2 - 1}) (C^\alpha_{N_\alpha/2} - C^\alpha_{N_\alpha/2})$

Single $\lambda_{max}$

Single frame at time $t$  
$N_\alpha C^\alpha$ atoms

Distance of two segments with segment length: 
$N_\alpha/2 \times C^\alpha$ atoms 
$\left( C^\alpha_1 - C^\alpha_{N\alpha/2-1} \right) \left( C^\alpha_{N\alpha/2} - C^\alpha_{N\alpha/2} \right)$ 
Single $\lambda_{max}$

Distances of $N_\alpha/2$ segments with segment length: $2 \times C^\alpha$ atoms 
$\left( C^\alpha_1 - C^\alpha_2 \right) \left( C^\alpha_3 - C^\alpha_4 \right)$  
$\left( C^\alpha_5 - C^\alpha_6 \right) \left( C^\alpha_7 - C^\alpha_8 \right)$  
...  
$\left( C^\alpha_{N\alpha/2-3} - C^\alpha_{N\alpha/2-2} \right) \left( C^\alpha_{N\alpha/2-1} - C^\alpha_{N\alpha/2} \right)$

$\lambda_{max}, 1 \lambda_{max}, 2 ... \lambda_{max}, N\alpha/2$
Segment size = proxy of **number of matrices** and **matrix sizes**

Many small matrices

Few large matrices

\[
\frac{(N_{\alpha} \sqrt{\frac{m}{N_{\alpha}}} - 1)}{2}
\]

\[
(2m)^2
\]

**S. Thomas et al.** Characterization of In Situ and In Transit Analytics of Molecular Dynamics Simulations for Next-generation Supercomputers. *eScience*, 2019.
2-step Model: Fraction of Analyzed Frames

Observables: small segment lengths (i.e., 2, 4, 6, 8, 10, 12, 14, 16, and 18)

Trp cage 12,619 atoms  T cell receptor  81,092 atoms

Gltp 270,088 atoms

2-step Model: Fraction of Analyzed Frames

Observables: segment lengths (i.e., 2, 4, 6, 8, 10, 12, 14, 16, and 18)

Model: polynomial model of degree 2 obtained by least-square fitting observables

$R^2 = 0.88$
2-step Model: Fraction of Analyzed Frames

Observables

Degree 2 polynomial model

Absolute error between data and fitting model

R² = 0.88
2-step Model: Frames Distribution

- Given a trajectory, we model the proportions $p$ and $q$ of analyzed frames ($f$) with periods $k$ and $k+1$
  - Example: Gltph (27,000 atoms and TPS 318), trajectory of 1,000 frames.

Case Study: 1BDD Protein Conformations

Frame 1330  Frame 1360  Frame 1390

S. Thomas et al. Characterization of In Situ and In Transit Analytics of Molecular Dynamics Simulations for Next-generation Supercomputers. *eScience*, 2019. *(Submitted)*
Case Study: 1BDD Protein Conformations

Frame 1330

Frame 1360

Frame 1390

Helix 1-2: $\lambda_{\text{max}}$  

Helix 1-3: $\lambda_{\text{max}}$  

Helix 2-3: $\lambda_{\text{max}}$  

S. Thomas et al. Characterization of In Situ and In Transit Analytics of Molecular Dynamics Simulations for Next-generation Supercomputers. *eScience*, 2019. *(Submitted)*
Case Study: 1BDD Protein Conformations

Frame 1330  Frame 1360  Frame 1390

Helix 1-2: $\lambda_{\text{max}}$  Helix 1-3: $\lambda_{\text{max}}$  Helix 2-3: $\lambda_{\text{max}}$
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Soil Moisture Data for Precision Farming

- Satellites collect raster data across the surface of the Earth
Soil Moisture: Incomplete Data

Image source: Ricardo Llamas, University of Delaware
Data source: ESA-CCI soil moisture database (http://www.esa-soilmoisture-cci.org/)

Soil moisture \((m^2/m^2)\)

High: 0.86247

Low: 0

December 2000 Averages
Soil Moisture: Incomplete Data

Causes of missing data:
- dense vegetation
- snow/ice cover
- frozen surface
- extremely dry surface

Image source: Ricardo Llamas, University of Delaware
Data source: ESA-CCI soil moisture database (http://www.esa-soilmoisture-cci.org/)
Soil Moisture: Coarse-grained Data

Original Resolution
27 km × 27 km

Desired Resolution
1 km × 1 km

Building a Closed-loop Workflow

Data Generation

- Satellite and sensors data
- Course-grained, incomplete data

- Weather Data NOAA
- Landscape Surface DSM
- Soil Moisture ESA-CCI
Building a Closed-loop Workflow

- Analytics representations + algorithms
- Data predictions
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A4MD analytics representations + algorithms
Building a Closed-loop Workflow

Soil moisture integrated in FDS for:
- Controlled combustion;
- Wildfire propagation

Compute

Fire Dynamics Simulator

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Fine-grained, complete data

Shifter and Docker

Singularity

Kubernetes

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Singularity
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Fire Dynamics Simulator
Augmenting HPC with the Cloud

Source: https://www.nextplatform.com/2018/02/26/adaptive-approach-bursting-hpc-cloud/
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Fine-grained, complete data

Course-grained, incomplete data

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Global versus Local Data Modeling

Data (observations)

Parameter

Dependent Variable

Data (observations)
Global versus Local Data Modeling

Global modeling

Local modeling
SBM vs. k-NN

Observations
- Piecewise linear data
- Surrogate-based model
- 2-Nearest Neighbor Model

SBM vs. k-NN

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Hybrid Piecewise Polynomial Modeling (HYPPO)

k Nearest Neighbors
• Use local data
• Compute the average
  (many simple local models)

Surrogate-Based Modeling
• Use all sampled data
• Construct one polynomial
  (single complex global model)

Hybrid Piecewise Polynomial Modeling (HYPPO)

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Hybrid modeling $\rightarrow$ HYPPO
• Use **local** data
• Construct many **polynomials**
  (*many complex local models*)

Observations

Surrogate-based Model

Hybrid Piecewise Polynomial Model (HYPPO)

Observations

k Nearest Neighbors Model

Case Study: Fine-grained Modeling of Mid-Atlantic Region

Challenges and Opportunities (I)

- Two trends in HPC are impacting scientific applications:
  - Convergence of simulations and data analytics
  - Emergence of edge computing
- Applications in precision medicine and precision farming are leveraging these trends
- There is the need to further integrate these trends in HPC
  - New challenges and opportunities for the HPC community
Challenges and Opportunities (II)

- **Efficiency**: Optimize performance and power usage associated to data generation, movement, and analytics
- **Non-invasive**: Capture knowledge from data without rewriting simulations’ legacy codes or simulations’ scripts
- **Generality**: Build workflows that support different types of analytics across different applications and different data
- **Portability**: Execute combined compute and analytics across different systems, including the edge, and with heterogenous resources
- **Scalability**: Design methods for knowledge discovery at scale (e.g., scalable ML algorithms) for “compute + analytics + data” workflows