Accelerating Data-driven Science using the Cyberinfrastructure Continuum

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• Facilities-based, data-driven since: Opportunities & challenges

• The Virtual Data Collaboratory (VDC) project: Leveraging the computing continuum for facilities-based science
  Data discovery, *data access*, data integration

• Conclusion and next steps
Science and Engineering in 21st Century

- New paradigms and practices in science and engineering
- Inherently multi-disciplinary
- Extreme scales, data-driven, data and compute-intensive
- Collaborative (university, national, global)

- Nearly every field discovery is transitioning from “data poor” to “data rich”
- The scientific process has evolved to include computation & data
Large, Shared-use Facilities can Transform S&E Research
Credit: John Delaney, University of Washington
Credit: John Delaney, University of Washington

7 Arrays
57 Stable Platforms
   Moorings, Profilers, Nodes
31 Mobile Assets
   Gliders, AUVs
1227 Instruments (~850 deployed)
>2500 Science Data Products
>100K Science/Engineering Data Products

ooinet.oceanobservatories.org
Types of Data

Telemetered

Recovered

Cabled

Data Product Types

- Fixed Timeseries: 1,680
- Profiler Timeseries: 472
- Trajectory Timeseries: 238
- Other: 241

approximate counts based on design
Types of Data

Telemetered

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Product Types
approximate counts based on design

Fixed
Timeseries
1,680
Data Download Statistics (Jun’16 – Jun’17)

<table>
<thead>
<tr>
<th>OOINet (UI Portal)</th>
<th>THREDDS Server</th>
<th>Raw Data Server</th>
</tr>
</thead>
<tbody>
<tr>
<td>Visits</td>
<td>28,341</td>
<td>3,681</td>
</tr>
<tr>
<td>Distinct countries</td>
<td>104</td>
<td>36</td>
</tr>
<tr>
<td>Direct entries</td>
<td>22,446 (79%)</td>
<td>3,324 (90%)</td>
</tr>
<tr>
<td>Search engines</td>
<td>227 (1%)</td>
<td>51 (1%)</td>
</tr>
<tr>
<td>From websites</td>
<td>3,228 (26%)</td>
<td>306 (8%)</td>
</tr>
<tr>
<td>Distinct websites</td>
<td>131 (540 distinct URLs)</td>
<td>17 (92 distinct URLs)</td>
</tr>
<tr>
<td>Data transferred</td>
<td>75.31 GB</td>
<td>923.3 GB</td>
</tr>
</tbody>
</table>

**OOINet**

- **United States**: 22,029 visits
- **China**: 1,942 visits
- **Unknown**: 1,937 visits
- **Brazil**: 965 visits
- **France**: 659 visits
- **Unknown**: 426 visits
- **United Kingdom**: 297 visits

**Raw Data**

- **United States**: 16,989 visits
- **Unknown**: 929 visits
- **Germany**: 215 visits
- **Canada**: 104 visits
- **China**: 116 visits
- **Israel**: 84 visits

**Country visits**

- **Europe**: 17,191 visits
- **Asia**: 17,021 visits
- **Unknown**: 11,372 visits
- **South America**: 4,092 visits
- **Others**: 4,324 visits

**Data transferred**

- **United States**: 16,989 GB
- **Unknown**: 929 GB
- **Germany**: 215 GB
- **Canada**: 127 GB
- **China**: 116 GB
- **Israel**: 84 GB

**Languages**

- **English**: 90%
- **French**: 5%
- **Spanish**: 2%
- **Other**: 3%
Large, Shared-use Facilities can Transform S&E Research

LIGO: Gravitational wave

EHT: Black hole

Observatory data repository

Search data

Gather data

Process data

Scientific discovery


[LIGO image] https://www.ligo.caltech.edu/system/media_files/binaries/266/original/162571main_GPB_circling_earth3_516.jpg?1446243770
Virtual Data Collaboratory: Enabling The Large Facilities Science

- Data and services provided by large-scale instruments and observatories have become **important enablers** of scientific discoveries.

- The VDC project explores how the emerging cyberinfrastructures continuum can improve the performance, usability and science impact of data and services provided by facilities.

<table>
<thead>
<tr>
<th>SYSTEM PLANE</th>
<th>Physical infrastructure (compute, storage, network, FIONAS), operating system and networking. Virtual infrastructure management: VMs, containers, etc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>DATA PLANE</td>
<td>Cross-repository data indexing and discovery, provenance records and other data-related services.</td>
</tr>
<tr>
<td>KNOWLEDGE PLANE</td>
<td>Data analytics, cross-repository data fusion, in-transit processing.</td>
</tr>
<tr>
<td>USER PLANE</td>
<td>Productivity tools, streaming-based interfaces, advanced caching and prefetching strategies.</td>
</tr>
</tbody>
</table>

Collaborative data services to enable facilities’ data to be **discovered, accessed, integrated** and **analyzed** in a timely manner
Leveraging the Computing Continuum

Emerging computing landscape

- **Cloud**
  - Hosted in data centers at the core
  - Relatively inexpensive; seemingly infinite
  - Far from data; data access expensive

- **Fog/Edge**
  - Computation/storage limited and expensive
  - Closer to the data; lower latencies
  - Limited and unreliable connectivity

- **In-Transit**
  - Distributed along the data path
  - Limited, but can be effective
  - Intermediate latency
  - Fewer guarantees
Leveraging the Computing Continuum

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Computing across the Continuum

- Leverage resources and services at the logical extreme of the network and along the data path to increase the value of the data while potentially reducing costs
- Exploit the rich ecosystem of data and computation resources at the edge so that data is not moved
Driving Use-case: Tsunami Early Warning

Increase precision and timeliness of tsunami warning by analyzing multiple geo-graphically-distributed data sources simultaneously,

- **Tsunami Early Warnings** require earthquakes to first be characterized (magnitude, location, speed of displacement, etc.).
  - A **single data source** doesn’t able to cover a whole spectrum of events. **Seismometers** are good for the smaller earthquakes (< 6.5), **high-precision GPS** are good for larger earthquakes.
- **Centralized data processing** does not support real-time and high volume of data constraints of such system.
- Goal: Combine multiple data sources to cover the whole spectrum of events.
- **Decentralized Early Earthquake Magnitude (DEEM):** A new two-step ensemble ML algorithm leveraging the two types of data for magnitude prediction using in-network resources.

<table>
<thead>
<tr>
<th># 60s MTS</th>
<th>GPS (# Events)</th>
<th>Seismic (# Events)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Magnitude &lt; 5</td>
<td>7,718 (170)</td>
<td>1,038 (349)</td>
</tr>
<tr>
<td>5 ≤ Magnitude &lt; 6</td>
<td>3,859 (85)</td>
<td>None</td>
</tr>
<tr>
<td>6 ≤ Magnitude &lt; 7</td>
<td>991 (4)</td>
<td>266 (4)</td>
</tr>
<tr>
<td>7 ≤ Magnitude &lt; 8</td>
<td>432 (6)</td>
<td>249 (6)</td>
</tr>
<tr>
<td>Magnitude &gt; 8</td>
<td>265 (4)</td>
<td>133 (4)</td>
</tr>
<tr>
<td>Total</td>
<td>13,265 (269)</td>
<td>1,686 (363)</td>
</tr>
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</table>

![Data sources (sensor networks)](image1)

![Observatories](image2)

![Virtual Data Collaboratory](image3)

![Centralized Data Collaboratory](image4)

![Event triggering (analytics, Machine Learning)](image5)

![Underwater Seismometers](image6)

![High-precision GPS stations](image7)

![Underwater Pressure Sensors](image8)

![USGS](image9)

![UNAVCO](image10)

![GPS](image11)

![Seismic](image12)
Driving Use-case: Tsunami Early Warning

Increase precision and timeliness of tsunami warning by analyzing multiple geo-graphically-distributed data sources simultaneously,

- Tsunami Early Warnings require:
  - A single data source can’t cover a whole spectrum of events.
  - Centralized data processing doesn’t support real-time and high volume of data constraints of such system.
- Goal: Combine multiple data sources to cover the whole spectrum of events.

Key requirements/challenges
- Data discovery
- Data access
- Data integration

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Facilities-based, Data-driven S&E: Data Access Challenge

Large volume, high data-rate, geographically distributed datasets

- Ocean Observatory Initiative
  - 1,227 instruments (~850 deployed)
  - 25,000 science data sets
  - 100,000 scientific data products

- LIGO: Generate TBs data per day, during ‘observing’ mode

- SKA: Estimate to generate an EB a day of raw data, which could be compressed to around 10 PB

- LSST: Produce 20 TB data per night

Large number of geographically distributed user communities with overlapping interests

Network bandwidth: 100Mbps, 1Gbps, 10Gbps
Objective: A *push-based* data delivery framework that leverages user access patterns and locality to accelerate the data delivery performance

**Approach:**
- Establish a distributed cache network using in-network DTNs
- Develop a hybrid prefetching model
  - Association-based model
  - Historical record-based model

**Data sets:**
- Ocean Observatory Initiative
  - Nov. 2018
  - 17.9 million records
- UNAVCO
  - One year of 2018
  - 77.8 million records
Addressing Data Access: Studying User Access Patterns

User access classification:
- Interactive access: users manually download data
- Program access: scripts automatically download data

Observations:
- Interactive users are the major users (~90%)
- Programs are the major data consumers (~90%)

Program access classification:
- Regular data download: at regular intervals; no overlap
- Overlapping access: at regular intervals; large overlap with previous access
- Real-time access: high frequency access (e.g. every 5 sec); no overlap

Data usage pattern:
- Duplicated data transfer volume
  - OOI: 60.8%
  - UNAVCO: 17.2%

Summary:
- Focus on the program access: ~90% of total data transfer
- Add a cache layer to alleviate redundant data transfers
- Implement prefetching: program accesses are predictable (~90%)
Addressing Data Access: Prefetching

A hybrid prefetching model:
- Association-based prediction model
  - Spatial correlation
- Historical record-based prediction model
  - Temporal correlation

Example: OOI Instruments distributed across 7 platforms

Spatial locality:
- User requests target specific locations
- Multiple users request the same data

Temporal locality:
Prefetching Approach

Modeling the request sequence

- Request: \( R = \langle TS_n, D_n, I_n, TR_n \rangle \)
- Timestamp: \( TS_n = \langle ts_1, ts_2, ..., ts_n \rangle \)
- Data stream ID: \( D_n = \langle d_1, d_2, ..., d_n \rangle \)
- Instrument ID: \( I_n = \langle i_1, i_2, ..., i_n \rangle \)
- Time range: \( TR_n = \langle tr_1, tr_2, ..., tr_n \rangle \)

Association-based prediction model

- Exploit spatiotemporal correlation
- Use the Frequent Pattern growth algorithm (FP-growth) to predict next request
  - Construct the frequent-pattern tree (FP-tree)
  - Prefetch the data with confidence \( \emptyset_j > \text{threshold} \)
    - \((d_1, d_2, ..., d_{i+m-1}) \rightarrow \langle d_{i+m}, \emptyset_j \rangle, \emptyset_j \) is confidence value

Historical record-based prediction model

- Identifying program-based access (PA)
  - Maintain a detection time window (e.g. 2 weeks)
  - Check repetition patterns for a user’s request \( R \)
- Once PA is identified
  - Determine \( \langle D_n, I_n, TR_n \rangle \)
- Use ARIMA to predict \( TS_n \)

System Architecture

Science & Education Use Cases

Data Service Layer
Cataloging, curating, querying, discovery, federation, etc

Network Service Layer
Data DMZ

Virtual Data Collaboratory

Cache server

Data Management Engine

Data Prefetching Engine

Cache client

Data Repository

DTN cache
Users

Command Flow

Data Flow
Experimental Evaluation

- System setup emulated:
  - 8 DTNs based on parameters obtained from the PRP Dashboard (Feb. 13, 2019 at 15:39:00)
  - Cache sizes: 128GB, 256GB, 512GB, 1TB, 2TB; LRU cache eviction

- Data source: OOI access log from November 2018 (17 Million records)

- Four scenarios:
  - W/O Cache
  - Simple Cache (LRU)
  - Simple Cache W/ Virtual Group
  - Smart Cache (including prefetch)

The Smart Cache enables users get more than 56% data from their local DTN cache
Facilities-based Data-driven S&E: Challenges

#1 Data access

- Users typically manually explore data via a web portal

#2 Data discovery

- Manually searching for data/data products is not efficient (feasible)

Remember, OOI has:
- 1,227 instruments (~850 deployed)
- > 25,000 science data sets
- > 100,000 scientific data products
Facilities-based Data-driven S&E: Challenges

#1 Data access

#2 Data discovery

- Users have to manually explore data from the observatory data web portal
- Gets even more tedious when exploring data across multiple repositories
Facilities-based Data-driven S&E: Challenges

#1 Data access

#2 Data discovery

#3 Data integration

Enable data from multiple data sources to be dynamically (opportunistically) integrated as part of support data-driven workflows

Example: Tsunami early warning system

- Integrate three data sources:
  - GPS (UNAVCO)
  - Seismograph (USGS)
  - Underwater pressure (OOI)

Data-driven science and engineering research enabled by large-scale, shared-use experimental and observational facilities presents new opportunities for discovery.

Data distribution, size, heterogeneity presents discovery, access, integration, processing challenges
- Large scale, heterogeneous in nature and geographic location
- Data needs to be processed by complex application workflows in a timely manner

The VDC project aims to provide data services that can leverage the computing continuum to address the needs for facilities-based data-driven science.
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