**Towards an Understanding of Facets and Exemplars of Big Data Applications**

*Geoffrey C.Fox1, Shantenu Jha2, Judy Qiu1, Andre Luckow2*

*(1) School of Informatics and Computing, Indiana University, Bloomington, IN 47408, USA*

*(2) RADICAL, Rutgers University, Piscataway, NJ 08854, USA*

**Abstract**

We study many Big Data applications from a variety of research and commercial areas and suggest a set of characteristic features and possible kernel benchmarks that stress those features for data analytics. We draw conclusions for the hardware and software architectures that are suggested by this analysis.

**1. Introduction**

With the proliferation of data intensive applications, there is a critical and timely need to understand these properties and the relationship between different applications. The aim of our work is to capture the essential and fundamental Big Data properties, and then to understand applications with those properties.

There are many different types of Big Data applications, and we cover them broadly including both research and commercial cases. However our focus is on Science and Engineering research of data-intensive applications. We compare and contrast some general properties of Big Data applications with classical HPC simulation applications. Pulling together these observations, we identify six key system architectures and note different emphases of commercial and research use cases. Furthermore we point out that combining ideas from HPC and commercial Big Data systems leads to an attractive and powerful Big Data software model.

Section 2 describes the sources of information for our study and their properties. It also details lessons from related studies of parallel computing. Section 3 showcases the features of Big Data use cases and the facets into which we group them, and introduce Ogres to designate broad groupings of applications that exhibit facets. We describe some generic kernels (mini-applications), or instances of Ogres, in the data analytics area. In section 4, we present implications for needed hardware and software while conclusions are in section 5.

**2. Sources of Information**

**2.1. Data Intensive Use Cases**

In discussing the structure of Big Data applications, let us first discuss the inevitably incomplete input that we used to do our analysis. We have gained quite a bit of experience from our research over many years, but 3 explicit sources that we used were a recent use case survey by NIST from Fall 2013[1]; an important NRC report [2], a survey of data intensive research applications by Jha et al. [3, 4]; in addition we conducted a study of members of data analytics libraries including R[5], Mahout [6] and MLLib [7]. We start with a summary of the first two sources.

The NIST Big Data Public Working Group (NBD-PWG) was launched in June 2013 with a set of working groups covering Big Data Definitions, Taxonomies, Requirements, Security and Privacy Requirements, Reference Architectures White Paper Survey, Reference Architectures, Security and Privacy Reference Architectures and Big Data Technology Roadmap. The Requirements working group gathered 51 use cases from a public call and then analyzed them in terms of requirements of a reference architecture [8]. Here we will look at them in an alternate fashion to identify common patterns and characteristics, which can be used to guide and evaluate Big Data hardware and software. The 51 use cases are organized into nine broad areas, with the number of associated use cases in parentheses: Government Operation (4), Commercial (8), Defense (3), Healthcare and Life Sciences (10), Deep Learning and Social Media (6), The Ecosystem for Research (4), Astronomy and Physics (5); Earth, Environmental and Polar Science (10) and Energy (1).

Note that the majority of use cases come from research applications, but commercial, defense and government operations have some coverage. A template was prepared by the requirements working group, which allowed experts to categorize each use case by 26 features including those listed below.

*Use case Actors/Stakeholders and their roles and responsibilities; use case goals and description. Specification of current analysis covering compute system, storage, networking and software. Characteristics of use case Big Data with Data Source (distributed/centralized), Volume (size), Velocity (e.g. real time), Variety (multiple datasets, mashup), Variability (rate of change). The so-called Big Data Science (collection, curation, analysis) with Veracity (Robustness Issues, semantics), Visualization, Data Quality (syntax), Data Types and Data Analytics. These detailed specifications were complemented by broad comments including Big Data Specific Challenges (Gaps), Mobility issues, Security & Privacy Requirements and identification of issues for generalizing this use case.*

The complete set of 51 responses, in addition to a summary from the working group of applications, current status and futures (as well as extracted requirements), can be found in [8]. They are summarized in the Appendix which also gives 20 other use cases coming from the NBD-PWG which do not have the detailed 26 feature template recorded. These 20 cover enterprise data applications and security & privacy.

The impressive NRC report [2] is a rich source of information. It has several relevant examples in chapter 2; most of these are also present in the NIST study, but NRC does have an interesting discussion of Big Data in Networking and Telecommunication that is omitted from the NIST compilation. We will return to the important “Giants” in chapter 10, which are related to different facets of our Ogres.

For the case of distributed applications there are at least two existing attempts to survey and analyze them. In Jha et al [4], the authors examine at a high-level approximately 20 distinct scientific applications that have either been distributed by design or were distributed “by nature”. They reduce the number of carefully examined applications to six representative selections. These applications range from the ubiquitous “@home” class of distributed applications, to Montage – an image reconstruction application which is now emblematic of loosely coupled workflows – to highly specialized and performance oriented applications such as NEKTAR.

Building upon [4], Jha et al [3] seek to understand distributed, dynamic and data-intensive applications (D3 Science) investigating the programming models and abstractions, the runtime and middleware services, and the computational infrastructure. The survey includes the following applications: NGS Analytics, CMB, Fusion, Industrial Incident Notification and Response, MODIS Data Processing, Distributed Network Intrusion Detection, ATLAS/WLCG, LSST, SOA Astronomy, Sensor Network Application, Climate, Interactive Exploration of Environmental Data, and Power Grids.

**2.2 Lessons from Parallel Computing**

Before we get to discussing features and patterns of Big Data applications, it is instructive to consider the better understood parallel computing situation. Here the application requirements have been captured in many ways:

1. **Benchmark Sets.** These vary from full applications [9] to kernels or mini-applications such as the NAS Parallel Benchmarks [10, 11] or Parkbench [12], with the Top500 [13] pacing application Linpack (HPL) being particularly well-known [14]. The new sparse HPCG conjugate gradient benchmark is worthy of mention [14]. Note benchmarks can be specified via explicit code and/or by a “pencil and paper specification” that can be optimized in any way for a particular platform.
2. **Patterns or Templates.** These can be similar to benchmarks but have different goals, such as providing a generic framework that can be modified by users with details of their application as in Template book [15, 16]. Alternatively they can be aimed at illustrating different applications as in the original Berkeley Dwarfs [17].

In this paper, our approach adheres closest to the Dwarfs framework; this is one motivation for choosing to name it the Big Data ‘Ogres’. In looking at this previous work, we note that benchmarks often cover a variety of different application aspects and are accompanied by principles or folklore that can guide the writing of parallel code or designing suitable hardware and software. For example, data locality and cost of data movement, sparseness, Amdahl’s law, communication latency, bisection bandwidth and scaled speedup are associated with substantial folklore.

The famous NAS Parallel Benchmarks (NPB) consist of: *MG: Multigrid, CG: Conjugate Gradient, FT: Fast Fourier Transform, IS: Integer sort, EP: Embarrassingly Parallel, BT: Block Tridiagonal, SP: Scalar Pentadiagonal, and LU: Lower-Upper symmetric Gauss Seidel.* All these are fairly uniform. With the exception of EP, which is an application class, the other members are typical constituents of a low level library for parallel simulations. On the other hand, the Berkeley Dwarfs are Dense Linear Algebra , Sparse Linear Algebra, Spectral Methods, N-Body Methods, Structured Grids, Unstructured Grids, MapReduce, Combinational Logic, Graph Traversal, Dynamic Programming, Backtrack and Branch-and-Bound, Graphical Models and Finite State Machines. The Dwarfs are not exact kernels, but instead describe problems from different points of view, including programming model (MapReduce), numerical method (Grids, Spectral method), kernel structure (dense or sparse linear algebra), algorithm (dynamic programming) and application class (N-body), etc. We believe it is generally accepted that both parallel computing and Big Data cannot be characterized with a single criterion, and so we introduce multiple Ogres exhibiting a set of facets in four different directions. We anticipate that there will be a correlation between the values of specific facet and application type and the needed computing architecture to support them.

**2.3 Properties of the 51 NIST use cases**

Tables 1 to 3 summarize characteristics of the 51 use cases, which we will combine with other input for the Ogres. Note that Big Data and parallel programming are intrinsically linked, as any Big Data analysis is inevitably processed in parallel. Parallel computing is almost always implemented by dividing the data between processors (data decomposition); the richness here is illustrated in Table 1, which lists the members of space that are decomposed for different use cases. Of course these sources of parallelism are broadly applicable outside the 51 use cases from which they were extracted. In Table 2, we identify 15 use case features that will be used later as facets of the Ogres. The second column of Table 2 lists our estimate of the number of use cases that illustrate this feature; note these are not exclusive, so any one use case will illustrate many features.

It is important to note that while machine learning is commonly used, there is an interesting distinction between what are termed Local Machine Learning (LML) and Global Machine Learning (GML) in Table 2. In LML, there is parallelism over items of Table 1 and machine learning is applied separately to each item; needed machine learning parallelism is limited, typified by the use of accelerators (GPU). In GML, the machine learning is applied over the full dataset with MapReduce, MPI or an equivalent. Typically GML comes from maximum likelihood or χ2 with a sum over the data items – documents, sequences, items to be sold, images, etc., and often links (point-pairs). Usually GML is a sum of positive numbers, as in least squares, and is illustrated by algorithms like PageRank, clustering/community detection, mixture models, topic determination, Multidimensional scaling, and (Deep) Learning Networks. Somewhat quixotically, GML can be termed Exascale Global Optimization or EGO.

|  |
| --- |
| Table 1: What is Parallelism Over for NIST Use Cases? |
| General Class | **Examples** |
| People | Users (see below) or Subjects of application and often both |
| Decision makers | Researchers or doctors (users of application) |
| Items | Experimental observations |
| Contents of online store |
| Images or “Electronic Information nuggets” |
| EMR: Electronic Medical Records (often similar to people parallelism) |
| Protein or Gene Sequences |
| Material properties, Manufactured Object specifications, etc., in custom dataset |
| Modelled entities | Vehicles and people |
| Sensors | Internet of Things |
| Events | Detected anomalies in telescope, credit card or atmospheric data |
| Graph Nodes | RDF databases |
| Regular Nodes | Simple nodes as in a learning network |
| Information Units | Tweets, Blogs, Documents, Web Pages, etc., and characters/words in them |
| Files or data | To be backed up, moved or assigned metadata |
| Particles/cells/ mesh points | Used in parallel simulations |

|  |
| --- |
| Table 2: Some Features of NIST Use Cases |
| Abbreviation | **#** | **Description** |
| PP | 26 | Pleasingly Parallel or Map Only |
| MR | 18 | Classic MapReduce MR (add MRStat below for full count) |
| MRStat | 7 | Simple version of MR where key computations are simple reduction as found in statistical averages, such as histograms and averages |
| MRIter | 23 | Iterative MapReduce or MPI |
| Graph | 9 | Complex graph data structure needed in analysis  |
| Fusion | 11 | Integrate diverse data to aid discovery/decision making; could involve sophisticated algorithms or just be a portal |
| Streaming | 41 |  Some data comes in incrementally and is processed this way |
| Classify | 30 | **Classification:** divide data into categories |
| S/Q | 12 | **Index**, Search and Query |
| CF | 4 | **Collaborative Filtering** for recommender engines |
| LML | 36 | **Local Machine Learning** (Independent for each parallel entity) |
| GML | 23 | **Global Machine Learning:** Deep Learning, Clustering, LDA, PLSI, MDS, Large Scale Optimizations as in Variational Bayes, MCMC, Lifted Belief Propagation, Stochastic Gradient Descent, L-BFGS, Levenberg-Marquardt. Can call EGO or Exascale Global Optimization with scalable parallel algorithm |
|  | 51 | **Workflow**: Universal, so no label |
| GIS | 16 | **Geotagged data** often displayed in ESRI, Microsoft Virtual Earth, Google Earth, GeoServer, etc. |
| HPC | 5 | Classic **large-scale simulation** of cosmos, materials, etc., generating (visualization) data |
| Agent | 2 | Simulations of models of data-defined macroscopic entities represented as **agents** |

The difference between LML and GML is illustrated in Table 3, which contrasts 9 of the 51 NIST use cases that involve image-based data. For example, use case 18 with light source data is largely independent machine learning on each image from the source, i.e. LML. In contrast, deep learning in use case 26 works by constructing a learning network integrating all the images.

|  |
| --- |
| Table 3: 9 Image-based NIST Use Cases |
| Use Case | **Title** | **Application** | **Features** |
| 17 | Pathology Imaging/ Digital Pathology | Moving to terabyte size 3D images, Global Classification | PP, LML, MR for search |
| 18 | Light sources | Biology and Materials | PP, LML |
| 26  | Large-scale Deep Learning | Stanford ran 10 million images and 11 billion parameters on a 64 GPU HPC; vision (drive car), speech, and Natural Language Processing | GML |
| 27 | Organizing large-scale, unstructured collections of photos | Fit position and camera direction to assemble 3D photo ensemble | GML |
| 36 | Catalina Real-Time Transient Synoptic Sky Survey (CRTS) | Processing of individual images for events based on classification of image structure (GML) | PP, LML, GML |
| 43 | Radar Data Analysis for CReSIS Remote Sensing of Ice Sheets | Identify glacier beds and snow layers.See GML when one addresses full ice sheet | PP, LML moving to GML  |
| 44  | UAVSAR Data Processing | Find and display slippage from radar images. Includes Data Product Delivery, and Data Services | PP |
| 45, 46 | Analysis of Simulation visualizations | Find paths, classify orbits, classify patterns that signal earthquakes, instabilities, climate, turbulence | PP, LML, GML |

**2.4 Properties of Distributed Use Cases**

In the process of reduction and classification, the authors of [3, 4] analyze the structure of applications and find commonalities; they introduce the term “vectors” to capture four essentially orthogonal but critical properties that determine both the development and the execution of the application. These vectors are: execution unit, communication, coordination and an execution environment. The first three are internal properties of a distributed application, whereas the last is essentially an external property. Based upon recurring values of vectors, the authors propose a set of common patterns that help elucidate the structure of the distributed applications. It is worth noting that vectors and patterns for distributed applications do not provide insight into performance aspects of the applications.

In [3], the authors propose a framework for describing applications, distributed and dynamic data and infrastructure. Figure 1 shows the data lifecycle model used for the analysis capturing both applications using sensors and computationally generated data.



*Figure 1. Application Stages*

The authors call out the Big Data aspects, the dynamic aspects and the distributed aspects of a large set of applications, and introduce quantitative estimates for various performance related properties.

Table 4 below (from [4]) shows the specific values of the “DPA vectors” for the set of six distinct applications investigated. It is interesting to note that the categorization did not lead to a well-defined and non-overlapping classification of application, as the complexity of considering the end-to-end aspects and the diverse ways in which applications are utilized resulted in classes that had overlapping characteristics.

|  |
| --- |
| Table 4: Characteristics of 6 Distributed Applications |
| Application Example | **Execution Unit** | **Communication** | **Coordination**  | **Execution Environment** |
| Montage | Multiple sequential and parallel executable | Files | Dataflow (DAG) | Dynamic process creation, execution |
| NEKTAR | Multiple concurrent parallel executables | Stream based | Dataflow | Co-scheduling, data streaming, async. I/O  |
| Replica-Exchange | Multiple seq. and parallel executables | Pub/sub | Dataflow and events | Decoupled coordination and messaging |
| Climate Prediction (generation) | Multiple seq. & parallel executables | Files and messages | Master-Worker, events | @Home (BOINC) |
| Climate Prediction(analysis) |  Multiple seq. & parallel executables |  Files and messages | Dataflow  | Dynamics process creation, workflow execution |
| SCOOP |  Multiple Executable | Files and messages | Dataflow | Preemptive scheduling, reservations |
| Coupled Fusion  |  Multiple executable | Stream-based | Dataflow | Co-scheduling, data streaming, async I/O |

|  |
| --- |
| Table 5: 7 Computational Giants of Massive Data Analysis [2] |
| G1 | Basic Statistics |
| G2 | Generalized N-Body Problems |
| G3 | Graph-Theoretic Computations |
| G4 | Linear Algebraic Computations |
| G5 | Optimizations |
| G6 | Integration |
| G7 | Alignment Problems |

**3. The Big Data Ogres and their Four Facets**

Synthesizing lessons learned from HPC, distributed applications and the NIST use case given above, we argue that there is a need to construct classes of mini-applications that facilitate the understanding and characterization of the Big Data properties of these applications. We further introduce facets or features in 4 classification dimensions or views to categorize Big Data applications. These are the Problem architecture, Execution features, Data Source or Style, and Processing views. There are of course other ways of looking at the Ogres and our work should be treated as an initial suggestion for further discussion. These views and their facets build on earlier discussions, especially Table 2. Note that a given application can be made up of components with different facets in Ogre classification. We will reference the 7 computational giants G1-G7 from the NRC report recorded in Table 5. These are important Big Data patterns, although the Ogres go into more detail. The final subsection discusses a selection of kernels focusing on analytics which are instances of Ogres. We intend to follow up with other Ogre “mini-app” or “kernel” instances covering a broader set of facets, including those from database benchmarking [18].

 **3.1 Problem Architecture View of Ogres**

The Problem Architecture view has facets that describe the overall structure of the application, which determines the overall software and is an important driver of the software and hardware architecture discussed later.

|  |  |
| --- | --- |
|  | Table 6: Problem Architecture View Facets of Ogres (Meta or Macro Pattern) |
| Pleasingly Parallel | Seen in BLAST, Protein docking, some (bio-) imagery including Local Analytics or Local Machine Learning with pleasingly parallel filtering |
| Classic MapReduce | Search, Index and Query and Classification algorithms like collaborative filtering (G1 for MRStat in Table 2, G7) |
| Map Collective | Seen in machine learning – especially with linear algebra kernels |
| Map P2P | Point to Point Communication seen in parallel simulation and graph algorithms |
| Map Streaming | Combination of (parallel) long running maps accepting streamed data |
| Shared Memory | As opposed to distributed data (memory). Corresponds to problem where shared memory implementations are important. Tend to be dynamic asynchronous |
| SPMD | Single Program Multiple Data, well-known parallel computing style |
| BSP | Bulk Synchronous Processing: well-defined compute-communication phases |
| Fusion  | Knowledge discovery often involves fusion of multiple methods or sources |
| Dataflow | Composite structure with multiple components linked by exchanged data |
| Agents | As used in epidemiology, discrete event simulations, etc. Swarm approaches |
| Workflow | Many applications often involve orchestration (workflow) of multiple components |

**3.2 Execution Features View of Ogres**

|  |
| --- |
| Table 7: Execution Features View Facets of Ogres |
| Performance metrics  | As measured in benchmarks |
| Flops per byte | Important for performance |
| Execution Environment | Cloud or HPC; are Core libraries needed such as matrix-matrix/vector algebra, conjugate gradient, reduction, broadcast … (G4) |
| Volume | Data size |
| Velocity | Measures Streaming |
| Variety | Multiple data sources are often mixed. See Fusion facet |
| Veracity | Accuracy of data affecting pre-processing needed and reliability of answer |
| Communication Structure  | Interconnect structure? Is communication Synchronous or Asynchronous? In latter case shared memory may be attractive; |
| Static or Dynamic? | Does application (graph) change during execution? |
| Regularity | Most applications consist of a set of interconnected entities; is this regular as a set of pixels or is it a complicated irregular graph? |
| Iterative or not? | Important algorithm characteristic |
| Data Abstraction | Key-value, pixel, graph, vector, HDF5, Bag of words, etc. |
| Data Space? | Are data points in metric or non-metric spaces (G2)? |
| Complexity | Is algorithm O(N2) or O(N) (up to logs) for N points per iteration (G2)? |

This facet contains application characteristics that are familiar from the simulation domain as well as the famous V’s of Big Data. The data abstraction layer is a key facet that we highlight in the software architecture rather than burying it as is done now in particular packages like Hadoop (key-value) and Giraph (graph). Simulations are often set up in well-defined physical spaces, however data is generally more abstract and the algorithms are typically quite different for metric and non-metric spaces. In contrast to the problem architecture facet, the computational features facet has a direct handle/relevance to performance. Note non-metric space algorithms are often O(N2). As discussed in the NRC report, there is a great deal of opportunity to incorporate sophisticated new algorithms to reduce O(N2) to O(N and logs). This is commonly used in search and sort algorithms but not yet applied in computation despite promising initial work [2, 19, 20].

**3.3 Data Source and Data Style View of Ogres**

|  |
| --- |
| Table 8: Data Source and Style View Facets of Ogres |
| SQL, NoSQL or NewSQL | NoSQL includes Document, Column, Key-value, Graph, Triple store |
| Enterprise data systems  | 10 examples from NIST [1] integrate SQL/NoSQL |
| Files or Objects | Files as managed in iRODS and extremely common in scientific research. Objects most common in ABDS |
| HDFS/Lustre/GPFS | Are data and compute collocated? |
| Archive/Batched/Streaming  | Streaming is Incremental update of datasets with new algorithms to achieve real-time response (G7) |
| Storage system styles | Styles include Shared, Dedicated, Permanent, and Transient |
| Metadata/Provenance | Define overall features of data and processing |
| Internet of Things | 24 [21] to 50 (Cisco [22, 23]) billion devices on the Internet by 2020 |
| HPC generated data | Simulations generate visualization output that often needs to be mined |
| GIS | Geographical Information Systems provide access to geospatial data |

The facets of Table 8 cover the acquisition, storage, management and access to the data. The mantra of bringing computing to the data is an important principle, especially for the Internet of Things when it is often not practical since backend (clouds) are needed to provide adequate computing. It is interesting that the HPC approach of large shared file systems uses technologies like Lustre, which is rather different from commercial systems that use databases or HDFS. Before the data gets to the compute system, there is often an initial data gathering phase which is characterized by a block size and timing. Block size varies from month (Remote Sensing, Seismic) to day (genomic) to seconds or lower (Real time control, streaming). This is measured by Archived/Batched/Streaming facets. Figure 1 stresses that an important source of data is the output of other programs, as data is streamed through a workflow. Other characteristics are needed for permanent auxiliary/comparison datasets which could be interdisciplinary, implying nontrivial data movement/replication. This is covered by the Variety facet in the Execution view.

**3.4 Processing or Run-time View of Ogres**

|  |
| --- |
| Table 9: Processing or Run-time View Facets of Ogres |
| Micro Benchmarks | A simple kernel or mini-app used to measure core system performance |
| LML | Local Analytics or Local machine Learning |
| GML | Global Analytics or Machine Learning requiring iterative runtime (G5, G6) |
| Base Statistics | Simple statistics seen in Table 2 as MRStat  |
| Recommendations | Collaborative Filtering and other recommender analytics |
| Search/Query/Index | Rich set of technologies used in Search, Query and Indexing data |
| Classification | Technologies to label data (SVM, Bayes, deep learning, clustering) |
| Learning | Training algorithms |
| Optimization Methodology | Machine Learning, Nonlinear Optimization, Least Squares, Linear/Quadratic Programming, Combinatorial Optimization, expectation maximization, Monte Carlo, Variational Bayes, Global Inference |
| Streaming | Growing class of fast online O(N) algorithms  |
| Alignment | Variant of Search seen in sequence comparison as in BLAST |
| Linear Algebra | Many machine learning algorithms build on linear algebra kernels |
| Graph | Problem set up as a graph as opposed to vector, grid, etc. (G3) |
| Visualization | Important component of many analysis pipelines |

We have already stressed the importance and distinction between Local and Global Machine Learning. These are often associated with Expectation Maximization and Steepest descent methods.

**3.5 Analytics Algorithm/Kernels as Ogre Instances**

|  |
| --- |
| Table 10: Ogre Instances covering important Analytics |
| Pleasingly Parallel (Map Only) or Local Machine Learning: ~any algorithm |
| Map-Reduce |
| Search, Query, Index: Dominant commercial use and important in Science with fewer users |
| Recommender Systems including Collaborative filtering: Major commercial use, little use in Science |
| Summarizing statistics (MRStat) as in LHC Data analysis (histograms) (G1) |
| Linear Classifiers: Bayes, Random Forests |
| Alignment and Streaming (G7) |
| Genomic Alignment, Incremental Classifiers |
| Global Analytics – Nonlinear Solvers (Structure depends on Objective Function) (G5, G6) |
| Stochastic Gradient Descent SGD |
| (L-)BFGS approximation to Newton’s Method |
| Levenberg-Marquardt solver |
| Global Analytics – Map-Collective (See Mahout, MLlib) (G2, G4, G6) |
| Outlier Detection |
| Clustering (many methods) related to community identification in networks |
| Mixture Models, LDA (Latent Dirichlet Allocation), PLSI (Probabilistic Latent Semantic Indexing) |
| SVM and Logistic Regression |
| PageRank (find leading eigenvector of sparse matrix) |
| SVD (Singular Value Decomposition) |
| MDS (Multidimensional Scaling) |
| Learning Neural Networks (Deep Learning) |
| Hidden Markov Models |
| Global Analytics – Map-Communication (targets for Giraph) (G3) |
| Graph Structure (Communities, subgraphs/motifs, diameter, maximal cliques, connected components) |
| Network Dynamics - Graph simulation Algorithms (epidemiology) |
| Global Analytics – Asynchronous Shared Memory (may be distributed algorithms) |
| Graph Structure (Betweenness centrality, shortest path) (G3) |
| Linear/Quadratic Programming, Combinatorial Optimization, Branch and Bound (G5) |

Table 10 records particular data analysis algorithms that play the same role as the members of the NAS parallel benchmarks. They form instances of Ogres covering a range of facets already introduced. These are deliberately kernels and further work is needed to specify more precise mechanisms. For example, there are many very different outlier and clustering algorithms corresponding to different scenarios (such as metric or non-metric spaces) and goals (such as tradeoff between performance and quality). Working with colleagues, we are developing benchmarks in the areas identified in Table 9. One should also introduce Ogre instances corresponding to full applications and workflows. These are important but not discussed here. We intend to investigate further work to introduce mini-apps as Ogre instances with broad coverage of the different facets in the 4 views.

**4. Hardware and Software Architecture Issues**

**4.1 Six Important Architectures**

|  |
| --- |
| Table 11: Distinctive Software/Hardware Architectures for Data Analytics |
| 1 | Pleasingly Parallel (Map Only) | Includes local machine learning (LML) as in parallel decomposition over items and apply data processing to each item. Hadoop could be used but also other High Throughput Computing or Many Task tools |
| 2 | Classic MapReduce | Includes MRStat, search applications and those using collaborative filtering and motif finding implemented using classic MapReduce (Hadoop) |
| 3 | Iterative Map-Collective | Iterative MapReduce using Collective Communication as needed in clustering – Hadoop with Harp, Spark, etc. |
| 4 | Iterative Map- (Point to Point) Communication | Iterative MapReduce such as Giraph with point-to-point communication; includes most graph algorithms such as maximum clique, connected component, finding diameter, community detection. Vary in difficulty of finding partitioning (classic parallel load balancing) |
| 5 | Map-Streaming | Architecture such as that of Apache Storm that supports streaming data. [24] A set of brokers holding data as it streams, supplying a set of long running tasks that filter and accumulate data. |
| 6 | Shared (Large) Memory | Thread-based (event driven) graph algorithms such as shortest path and Betweenness centrality. Large memory applications |

In Table 11, we present 6 problem architectures that map into 6 distinct system architectures which seem to cover the Ogres and their facets discussed in previous sections. Category 11.6 is the shared memory architecture needed for some graph algorithms that perform better here as well as for some large memory applications. The central batch architectures are 11.1 to 11.4 which correspond exactly to the four forms of MapReduce we have presented previously [25] summarized in Figures 2a) and Figure 2b), which introduces the Map-Streaming architecture. Note these six architectures only describe some of the facets in Tables 6-9. There are many other issues that need to be addressed including support of workflow and the data systems captured in the facets of Table 8.



*Figure 2. Six Distinctive Software/Hardware Architectures for Data Analytics*

Note that we separate Map-Collective [26, 27] and Map-(Point to Point) Communication following the Apache projects Hadoop, Spark and Giraph which focus on these cases. These programming models or runtimes differ in communication style (bandwidth versus latency), application abstraction (key-value versus graph), possible scheduling or load-balancing. HPC with MPI suggests that one could integrate categories 11.3 and 11.4 into a single environment. This approach is illustrated by the Harp plug-in for Hadoop which supports both models [28]. We recently added the map-streaming architecture of Table 11.5 and Fig. 2b); recall that Table 2 listed 41 streaming applications in the 51 use cases.

**4.2 Comparison between Data Intensive and Simulation Problems**

We can use the Ogre facet analysis and the data analytics architectures to compare data intensive and simulation applications. Looking back at Table 6, there are some clear similarities between them, with “Pleasingly parallel” (11.1), BSP and SPMD being common in both arenas. However the Classic MapReduce architecture (11.2) is a major Big Data paradigm though much less common in simulations. One example is the execution of multiple simulations (as in Quantum Monte Carlo) followed by a reduce operation to collect the results of different simulations. The Iterative Map-Collective architecture (category 11.3) is common in Big Data analytics such as clustering where there is no local graph structure and the parallel algorithms involve large-scale collectives but no point-to-point communication. The same structure is seen in N-body (long range force) or other “all-pairs” simulations without the locality typical from discretizing differential operators.

Many simulation problems have the Map-Communication (category 11.4) architecture with many smallish point-to-point messages coming from local interactions between points defining systems to be simulated. The importance of sparse data structures and algorithms is well understood in simulations and is seen in some Big Data problems such as PageRank, which calculates the leading eigenvector of the sparse matrix formed by internet site links. Other Big Data sparse data structures are seen in user-item ratings and bags of words problems (although these have feature that suggest sparseness corresponds to missing information and not to zero values). Most items are rated by only a few users and many documents contain a small fraction of the word vocabulary. However important data analytics involve full matrix algorithms. For example, recent papers [28-30] on a new Multidimensional Scaling method use conjugate gradient solvers with full matrices as opposed to the new sparse conjugate gradient benchmark HPCG being developed for supercomputer (Top500) evaluations [31].

Note that there are similarities between some Big Data graph problems and particle simulations with an unusual potential defined by the graph node connectivity. Both use the Map-Communication architecture, and the links in a Big Data graph are equivalent to strength of force between the graph nodes considered as particles. In this analogy, many Big Data problems are “long range force” corresponding to a graph where all nodes are linked to each other. As in simulation cases, these O(N2) problems are typically very compute intense but straightforward to parallelize efficiently. It is interesting to consider the analogue of the “fast multi-pole” methods for the fully connected Big Data problems, which can dramatically improve the performance to O(N) or O(NlogN) as discussed in Sec. 3.3. Finally note the network connections used in deep learning are indeed sparse, but in recent image interpretation studies [32], the network weights are block sparse (corresponding to links to pixel blocks) and can be formulated as full matrix operations with GPUs and MPI running efficiently with these blocks.

The map-streaming architecture (11.5) is seen in problems such as Twitter analysis and data assimilation where large-scale simulations are updated by streaming data. The final architecture of category11.6 (Shared Memory) is important in some applications but not heavily used in either simulations or Big Data, although large memory systems are used extensively in gene assembly applications.

The above discussion focuses on a qualitative comparison of Big Data applications with traditional simulation (HPC) applications, namely comparing the structure. As is evident, there are similarities as well as points of distinction. It is likely, however, that there will be significant differences in values of facets of the “execution features” view for the two application classes; for instance the distribution of the values of different ratios (e.g., ratio of computing to I/O, ratio of memory to I/O, etc.) characterizing the computational feature will be different. We will investigate both quantitative and qualitative differences in future work.

**4.3 A Big Data Software Environment**

We have previously described [33-35] how we propose to implement Big Data applications exploiting the HPBDS architecture sketched in Table 12 [36]. This combines the best practice commercial Big Data software with an emphasis on Apache projects with HPC subsystems. Table 12 illustrates by green shading those layers where HPC adds significant value to the Apache stack ABDS. Note that high performance communication is known to be critical for simulations but is also essential for many scientific Big Data applications. Commercial applications have large “search” (10.2) components corresponding to the huge number of users accessing commercial Big Data systems. In science, this step is necessary – especially for good data management – but is a much lower fraction of system use as the number of scientists accessing data is far lower than the number of users of commercial Big Data.

**5 Discussion and Conclusion**

This is only an initial discussion about our objectives, scope and methodology, and is by no means a complete or comprehensive body of work. It is motivated by the fact that there are several existing efforts at describing and highlighting Big Data applications, yet many are domain or usage specific. We move beyond any specific set of applications, and focus on Big Data applications and analytics kernels that are generally considered to be of relevance/importance to science and engineering using a context that includes a limited set of commercial problems. Using this broad range of Big Data applications as our working set, this paper is an attempt at distilling the Big Data properties (facets divided into 4 views) and organizing the plethora of disparate Big Data applications using these properties. Although we validate using analytics kernels, this classification/organization will in turn shed light on and help provide better understanding of both the structure of science and engineering Big Data applications, as well as determinants of their performance. In Section 4, we show how a deeper appreciation of the Ogre facets will help design and implement better hardware and software systems.

**Acknowledgements**

This work was partially supported by NSF CAREER grant OCI-1149432 for Qiu, NSF XPS RaPyDLI project 1439007, and NSF Datanet Dibbs SPIDAL 1443054.

**Appendix: 71 NIST Use Cases**

|  |
| --- |
| The 71 NIST Use Cases with number in each broad area |
| Government Operation(4): National Archives and Records Administration, Census Bureau |
| Commercial(8): Finance in Cloud, Cloud Backup, Mendeley (Citations), Netflix, Web Search, Digital Materials, Cargo shipping (as in UPS) |
| Defense(3): Sensors, Image surveillance, Situation Assessment |
| Healthcare and Life Sciences(10): Medical records, Graph and Probabilistic analysis, Pathology, Bioimaging, Genomics, Epidemiology, People Activity models, Biodiversity |
| Deep Learning and Social Media(6): Driving Car, Geolocate images/cameras, Twitter, Crowd Sourcing, Network Science, NIST benchmark datasets |
| The Ecosystem for Research(4): Metadata, Collaboration, Language Translation, Light source experiments |
| Astronomy and Physics(5): Sky Surveys including comparison to simulation, Large Hadron Collider at CERN, Belle Accelerator II in Japan |
| Earth, Environmental and Polar Science(10): Radar Scattering in Atmosphere, Earthquake, Ocean, Earth Observation, Ice sheet Radar scattering, Earth radar mapping, Climate simulation datasets, Atmospheric turbulence identification, Subsurface Biogeochemistry (microbes to watersheds), AmeriFlux and FLUXNET gas sensors |
| Energy(1): Smart grid |
| Enterprise Data Systems(10): Multiple users performing interactive queries and updates on a database with basic availability and eventual consistency (BASE); Perform real time analytics on data source streams and notify users when specified events occur; Move data from external data sources into a highly horizontally scalable data store, transform it using highly horizontally scalable processing (e.g. Map-Reduce), and return it to the horizontally scalable data store (ELT); Perform batch analytics on the data in a highly horizontally scalable data store using highly horizontally scalable processing (e.g. MapReduce) with a user-friendly interface (e.g. SQL); Perform interactive analytics on data in analytics-optimized database; Visualize data extracted from horizontally scalable Big Data store; Move data from a highly horizontally scalable data store into a traditional Enterprise Data Warehouse; Extract, process, and move data from data stores to archives; Combine data from Cloud databases and on premise data stores for analytics, data mining, and/or machine learning; Orchestrate multiple sequential and parallel data transformations and/or analytic processing using a workflow manager |
| Security & Privacy(10): Consumer Digital Media Usage; Nielsen Homescan; Web Traffic Analytics; Health Information Exchange; Personal Genetic Privacy; Pharma Clinic Trial Data Sharing; Cyber-security; Aviation Industry; Military - Unmanned Vehicle sensor data; Education - “Common Core” Student Performance Reporting |

**References**

1. NIST. *Big Data Working Group Reports from V1*. 2013 [accessed 2014 March 26]; Report at <http://bigdatawg.nist.gov/V1_output_docs.php> Available from: <http://bigdatawg.nist.gov/home.php>.

2. Committee on the Analysis of Massive Data; Committee on Applied and Theoretical Statistics; Board on Mathematical Sciences and Their Applications; Division on Engineering and Physical Sciences; National Research Council, *Frontiers in Massive Data Analysis*. 2013: National Academies Press. <http://www.nap.edu/catalog.php?record_id=18374>

3. Shantenu Jha, Neil Chue Hong, Simon Dobson, Daniel S. Katz, Andre Luckow, Omer Rana, and Yogesh Simmhan, *Introducing Distributed Dynamic Data-intensive (D3) Science: Understanding Applications and Infrastructure*. 2014. <https://dl.dropboxusercontent.com/u/52814242/3dpas-draft.v0.1.pdf>.

4. S. Jha, M. Cole, D. Katz, O. Rana, M. Parashar, and J. Weissman, *Distributed Computing Practice for Large-Scale Science & Engineering Applications.* Concurrency and Computation: Practice and Experience, 2013. 25(11): p. 1559-1585. DOI:<http://dx.doi.org/10.1002/cpe.2897>

5. *R open source statistical library*. [accessed 2012 December 8]; Available from: <http://www.r-project.org/>.

6. *Apache Mahout Scalable machine learning and data mining* [accessed 2012 August 22]; Available from: <http://mahout.apache.org/>.

7. *Machine Learning Library (MLlib)*. [accessed 2014 April 1]; Available from: <http://spark.apache.org/docs/0.9.0/mllib-guide.html>.

8. NIST, *NIST Big Data Public Working Group (NBD-PWG) Use Cases and Requirements.* 2013. <http://bigdatawg.nist.gov/usecases.php>

9. Berry, M., D. Chen, P. Koss, D. Kuck, S. Lo, Y. Pang, L. Pointer, R. Roloff, A. Sameh, E. Clementi, S. Chin, D. Schneider, G. Fox, P. Messina, D. Walker, C. Hsiung, J. Schwarzmeier, K. Lue, S. Orszag, F. Seidl, O. Johnson, R. Goodrum, and J. Martin, *The Perfect Club Benchmarks: Effective Performance Evaluation of Supercomputers.* International Journal of High Performance Computing Applications, September 1, 1989, 1989. 3(3): p. 5-40. DOI:10.1177/109434208900300302. <http://hpc.sagepub.com/content/3/3/5.abstract>

10. NASA Advanced Supercomputing Division. *NAS Parallel Benchmarks*. 1991 [accessed 2014 March 28]; Available from: <https://www.nas.nasa.gov/publications/npb.html>.

11. Rob F. Van der Wijngaart, Srinivas Sridharan, and Victor W. Lee, *Extending the BT NAS parallel benchmark to exascale computing*, in *Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis*. 2012, IEEE Computer Society Press. Salt Lake City, Utah. pages. 1-9.

12. *PARKBENCH (PARallel Kernels and BENCHmarks)*. 1996 [accessed 2014 July 19]; Available from: <http://www.netlib.org/parkbench/>.

13. Jack Dongarra, Erich Strohmaier, and Michael Resch. *Top 500 Supercomputer Sites*. 2014 [accessed 2014 July 19]; Available from: <http://www.top500.org/>.

14. A. Petitet, R. C. Whaley, J. Dongarra, and A. Cleary. *HPL - A Portable Implementation of the High-Performance Linpack Benchmark for Distributed-Memory Computers*. 2008 September 10 [accessed 2014 July 19,]; Available from: <http://www.netlib.org/benchmark/hpl/>.

15. R. Barrett, M. Berry, T. F. Chan, J. Demmel, J. Donato, J. Dongarra, V. Eijkhout, R. Pozo, C. Romine, and H. Van der Vorst, *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods, 2nd Edition*. 1994, Philadelphia, PA: SIAM. <http://www.netlib.org/linalg/html_templates/Templates.html>

16. Timothy G. Mattson, Beverly A. Sanders, and Berna L. Massingill, *Patterns for Parallel Programming*. 2013: Addison-Wesley Professional. ISBN:0321940784

17. Asanovic, K., R. Bodik, B.C. Catanzaro, J.J. Gebis, P. Husbands, K. Keutzer, D.A. Patterson, W.L. Plishker, J. Shalf, S.W. Williams, and K.A. Yelick. *The Landscape of Parallel Computing Research: A View from Berkeley*. 2006 December 18 [accessed 2009 December]; Available from: <http://www.eecs.berkeley.edu/Pubs/TechRpts/2006/EECS-2006-183.html>.

18. Chaitan Baru and Tilmann Rabl. *Tutorial 4 " Big Data Benchmarking" at 2014 IEEE International Conference on Big Data*. 2014 [accessed 2015 January 2 ]; Available from: <http://cci.drexel.edu/bigdata/bigdata2014/tutorial.htm>.

19. P. Ram, D. Lee, W. March, and A.G. Gray. *Linear-time algorithms for pairwise statistical problems*. in *Advances in Neural Information Processing Systems. NIPS* 2009. Vancouver, BC.

20. Judy Qiu, Jaliya Ekanayake, Thilina Gunarathne, Jong Youl Choi, Seung-Hee Bae, Yang Ruan, Saliya Ekanayake, Stephen Wu, Scott Beason, Geoffrey Fox, Mina Rho, and Haixu Tang, *Data Intensive Computing for Bioinformatics*, Chapter in *Data Intensive Distributed Computing*, Tevik Kosar, Editor. 2011, IGI Publishers. <http://grids.ucs.indiana.edu/ptliupages/publications/DataIntensiveComputing_BookChapter.pdf>.

21. Om Malik. *Internet of things will have 24 billion devices by 2020 from GSMA, the global mobile industry trade group*. 2011 [accessed 2014 July 19]; Available from: <http://gigaom.com/2011/10/13/internet-of-things-will-have-24-billion-devices-by-2020/>.

22. Cisco. *Visual Networking Index: Forecast and Methodology, 2012–2017*. 2013 May 29 [accessed 2013 August 14]; Available from: <http://www.cisco.com/en/US/solutions/collateral/ns341/ns525/ns537/ns705/ns827/white_paper_c11-481360_ns827_Networking_Solutions_White_Paper.html>.

23. Cisco Internet Business Solutions Group (IBSG) (Dave Evans). *The Internet of Things: How the Next Evolution of the Internet Is Changing Everything*. 2011 April [accessed 2013 August 14]; Available from: <http://www.cisco.com/web/about/ac79/docs/innov/IoT_IBSG_0411FINAL.pdf>.

24. Supun Kamburugamuve, Leif Christiansen, and Geoffrey Fox, *A Framework for Real-Time Processing of Sensor Data in the Cloud*. November 7, 2014. <http://grids.ucs.indiana.edu/ptliupages/publications/iotcloud_hindavi_two_column_final_2.pdf>.

25. Jaliya Ekanayake, Thilina Gunarathne, Judy Qiu, Geoffrey Fox, Scott Beason, Jong Youl Choi, Yang Ruan, Seung-Hee Bae, and Hui Li, *Applicability of DryadLINQ to Scientific Applications*. January 30, 2010, Community Grids Laboratory, Indiana University. <http://grids.ucs.indiana.edu/ptliupages/publications/DryadReport.pdf>.

26. J.Ekanayake, H.Li, B.Zhang, T.Gunarathne, S.Bae, J.Qiu, and G.Fox, *Twister: A Runtime for iterative MapReduce*, in *Proceedings of the First International Workshop on MapReduce and its Applications of ACM HPDC 2010 conference June 20-25, 2010*. 2010, ACM. Chicago, Illinois. <http://grids.ucs.indiana.edu/ptliupages/publications/hpdc-camera-ready-submission.pdf>.

27. Bingjing Zhang, Yang Ruan, Tak-Lon Wu, Judy Qiu, Adam Hughes, and Geoffrey Fox, *Applying Twister to Scientific Applications*, in *CloudCom 2010*. November 30-December 3, 2010. IUPUI Conference Center Indianapolis. <http://grids.ucs.indiana.edu/ptliupages/publications/PID1510523.pdf>.

28. Bingjing Zhang, Yang Ruan, and Judy Qiu, *Harp: Collective Communication on Hadoop*, in *IEEE International Conference on Cloud Engineering (IC2E) conference* October 10, 2014. <http://grids.ucs.indiana.edu/ptliupages/publications/HarpQiuZhang.pdf>.

29. Yang Ruan and Geoffrey Fox, *A Robust and Scalable Solution for Interpolative Multidimensional Scaling with Weighting*, in *9th International conference on e-Science*. October 22-25, 2013. Beijing. DOI: <http://dx.doi.org/10.1109/eScience.2013.30>.

30. Yang Ruan, Geoffrey L. House, Saliya Ekanayake, Ursel Schütte, James D. Bever, Haixu Tang, and Geoffrey Fox, *Integration of Clustering and Multidimensional Scaling to Determine Phylogenetic Trees as Spherical Phylograms Visualized in 3 Dimensions*, in *FIRST INTERNATIONAL WORKSHOP ON CLOUD FOR BIO (C4Bio 2014)*. May 26-29, 2014. IEEE/ACM CCGrid 2014 Chicago. pages. 26-29. <http://grids.ucs.indiana.edu/ptliupages/publications/PhylogeneticTreeDisplayWithClustering.pdf>.

31. Jack Dongarra and Michael A. Heroux. *Toward a New Metric for Ranking High Performance Computing Systems*. 2013 June [accessed 2014 July 19,]; SANDIA REPORT SAND2013-4744 (Defines HPCG) Available from: <http://www.sandia.gov/~maherou/docs/HPCG-Benchmark.pdf>.

32. Adam Coates, Brody Huval, Tao Wang, David Wu, Bryan Catanzaro, and Andrew Ng. *Deep learning with COTS HPC systems*. in *Proceedings of the 30th International Conference on Machine Learning (ICML-13)* 2013.

33. Wo Chang. *ISO/IEC JTC 1 Study Group on Big Data* in *1st Big Data Interoperability Framework Workshop: Building Robust Big Data Ecosystem*. March 18-21 2014. SDSC, San Diego CA: NIST.

34. Geoffrey Fox, Judy Qiu, and Shantenu Jha, *High Performance High Functionality Big Data Software Stack*, in *Big Data and Extreme-scale Computing (BDEC)*. 2014. Fukuoka, Japan. <http://www.exascale.org/bdec/sites/www.exascale.org.bdec/files/whitepapers/fox.pdf>.

35. Shantenu Jha, Judy Qiu, Andre Luckow, Pradeep Mantha, and Geoffrey C. Fox, *A Tale of Two Data-Intensive Approaches: Applications, Architectures and Infrastructure*, in *3rd International IEEE Congress on Big Data Application and Experience Track*. June 27- July 2, 2014. Anchorage, Alaska. <http://arxiv.org/abs/1403.1528>.

36. *HPC-ABDS Kaleidoscope of over 270 Apache Big Data Stack and HPC Tecnologies*. [accessed 2014 April 8]; Available from: <http://hpc-abds.org/kaleidoscope/>.