Computational Science and new perspectives for the analysis of massive data sets

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Summary

- The data tsunami
- Virtual Organizations
- A new scientific paradigm
- Bottlenecks: moving programs not data
- Knowledge discovery in databases
- Conclusions
The forerunner: LHC

ATLAS detector event

Data Stream: 330 TB/week

LHC Computing Model

Computationally demanding but still a relatively simple (embarassingly parallel) KDD task

Pruning of uninteresting events and detection of specific ones either known from simulations or outliers
• Huge data sets (ca. Pbyte)
• Thousands of different problems
• Many, many thousands of users
Jim Gray

“One of the greatest challenges for 21st-century science is how we respond to this new era of data intensive science.

This is recognized as a new paradigm beyond experimental and theoretical research and computer simulations of natural phenomena—one that requires new tools, techniques, and ways of working.”
1. **Experiment** (ca. 3000 years)

2. **Theory** (few hundreds years)
   mathematical description, theoretical models, analytical laws (e.g. Newton, Maxwell, etc.)

3. **Simulations** (few tens of years)
   Complex phenomena

4. **Data-Intensive science** (now!!)

http://research.microsoft.com/fourthparadigm/
An Outline of Basic Ideas

Three centuries ago science was transformed by the dramatic new idea that rules based on mathematical equations could be used to describe the natural world. My purpose in this book is to initiate another such transformation, and to introduce a new kind of science that is based on the much more general types of rules that can be embodied in simple computer programs.

It has taken me the better part of twenty years to build the intellectual structure that is needed, but I have been amazed by its results. For what I have found is that with the new kind of science I have developed it suddenly becomes possible to make progress on a remarkable range of fundamental issues that have never successfully been addressed by any of the existing sciences before.

If theoretical science is to be possible at all, then at some level the systems it studies must follow definite rules. Yet in the past throughout the exact sciences it has usually been assumed that these rules must be ones based on traditional mathematics. But the crucial realization that led me to develop the new kind of science in this book is that there is in fact no reason to think that systems like those we see in nature should follow only such traditional mathematical rules.
The fourth paradigm relies upon....

1. Most data will never be seen by human

2. Complex correlations (precursors of physical laws) cannot be visualized and recognized by the human brain

Most if not all empirical correlations depend on three parameters only: ...
Simple universe or rather human bias?
First hint about the need for complex visualization

Astronomy

Oceanography

Petrology
3. Real world physics is too complex. Validation of models requires *accurate simulations, tools to compare simulations and data*, and better ways to deal with complex & massive data sets.

Need to increase computational and algorithmic capabilities beyond current and expected technological trends.
Data Intensive Science

Data Gathering (e.g., from sensor networks, telescopes...)

Data Farming:
- Storage/Archiving
- Indexing, Searchability
- Data Fusion, Interoperability, ontologies, etc.

Data Mining (or Knowledge Discovery in Databases):
- Pattern or correlation search
- Clustering analysis, automated classification
- Outlier / anomaly searches
- Hyperdimensional visualization

Data understanding
- Computer aided understanding
  - KDD
  - Etc.

New Knowledge
Distributed data sets and virtual organizations

The International Virtual Observatory Alliance
<table>
<thead>
<tr>
<th></th>
<th>TB</th>
<th>Total</th>
<th>epochs</th>
<th>parameters</th>
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<td>0.15 TB/day</td>
<td>100 TB</td>
<td>tens</td>
<td>&gt;100</td>
</tr>
<tr>
<td>HST</td>
<td></td>
<td>120 TB</td>
<td>few</td>
<td>&gt;100</td>
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<tr>
<td>PANSTARRS</td>
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<td>600 TB</td>
<td>Few-many</td>
<td>&gt;&gt;100</td>
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<td></td>
<td>1 PB</td>
<td>many</td>
<td>&gt;&gt;100</td>
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<tr>
<td>SKA</td>
<td>1.5 PB/day</td>
<td></td>
<td>&gt;&gt; 10^2</td>
<td>hundreds</td>
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<td>US-Meteo</td>
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<td>460 TB/yr</td>
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<td>Hundreds heterogeneous</td>
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<tr>
<td>You Tube</td>
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<td>530 TB</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Google</td>
<td>1 Pbyte/min</td>
<td></td>
<td></td>
<td>heterogeneous</td>
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</table>
The measurable parameter space of KDD

Each datum is defined by $n$ measured parameters.

- $x, y, t$
- Flux
- Polarization
- Wavelength
- Etc..

New sensor technologies:

$p \in \mathbb{R}^N \quad N >> 100$

A better exploration and sampling of an ever increasing parameter space of data intensive science.
An astronomical example

The astronomical parameter space is of high dimensionality, still sparsely covered and poorly sampled:

every time you improve either coverage or sampling you make new discoveries

Malin 1

a new type of low surface brightness galaxies (Malin, 1991)
MASSIVE, COMPLEX DATA SETS with:
\[ N > 10^9, \ D >> 100, \ K > 10 \]

\[ N = \text{no. of data vectors}, \]
\[ D = \text{no. of data dimensions} \]
\[ K = \text{no. of clusters chosen}, \]
\[ K_{\text{max}} = \text{max no. of clusters tried} \]
\[ I = \text{no. of iterations}, \ M = \text{no. of Monte Carlo trials/partitions} \]

K-means: \[ K \times N \times I \times D \]
Expectation Maximisation: \[ K \times N \times I \times D^2 \]
Monte Carlo Cross-Validation: \[ M \times K_{\text{max}}^2 \times N \times I \times D^2 \]
Correlations \( \sim N \log N \) or \( N^2 \), \( \sim D^k \) \( (k \geq 1) \)
Likelihood, Bayesian \( \sim N^m \) \( (m \geq 3) \), \( \sim D^k \) \( (k \geq 1) \)
SVM > \( \sim (NxD)^3 \)
Scalability: 1-st bottle neck

Exaflop (are needed for simulations, metereology, data fusion, data mining, etc.)

Exaflop = $100 \times$ present capability

Exascale $\neq$ Exaflops but
Exascale at the data center size
Exascale at the “rack” size embedded => Teraflops in a cube

To reach exaflops required 14 yrs

But...

We should be happy if:

- 1.000.000 CPU’s
- power supply of a nuclear plant
- Minimum changes in software

Adapted from Kogge– Astroinformatics 2010
... GPU technology?

The Graphical Processing Unit is specialized for compute-intensive, highly parallel computation (exactly what graphics rendering is about). So, more transistors can be devoted to data processing rather than data caching and flow control.

« GPU have evolved to the point where many real world apps are easily implemented on them and run significantly faster than on multi-core systems. Future computing architectures will be hybrid systems with parallel-core GPUs working in tandem with multi-core CPUs »

DAME - GAME

Genetic Algorithm Mining Experiment

GAME is a pure genetic algorithm developed in order to solve supervised problems of regression or classification, able to work on Massive Data Sets (MDS).

It is intrinsically parallel and it is now under GPU+CUDA implementation.
DAME Program is a joint effort between University Federico II, Caltech and INAF-OACN, aimed at implementing (as web 2.0 apps and services) a scientific gateway for data exploration on top of a virtualized distributed computing environment.

**Web App REsource**

- Specialized web apps for:
  - text mining (VOGCLUSTERS)
  - Transient classification (STraDiWA)
  - EUCLID Mission Data Quality

**Extensions**

- DAME-KNIME
- ML Model plugin

**Web Services**

- SDSS mirror
- WFXT Time Calculator
- GAME (GPU+CUDA ML model)

**DAME Program Website**

http://dame.dsf.unina.it/

Science and management Documents
Science cases
Newsletters

http://www.youtube.com/user/DAMEmedia
DAMEWARE Web Application media channel
DAME Main Project: DAMEWARE

DAta Mining Web Application REsource

web-based app for massive data mining based on a suite of machine learning methods on top of a virtualized hybrid computing infrastructure

http://dame.dsf.unina.it/beta_info.html

Multi Layer Perceptron trained by:
• Back Propagation
• Quasi Newton
• Genetic Algorithm

Support Vector Machines
Genetic Algorithms
Self Organizing Feature Maps
K-Means
Multi-layer Clustering
Principal Probabilistic Surfaces

Bayesian Networks
Random Decision Forest
MLP with Levenberg-Marquardt
Classification
Regression
Clustering
Feature Extraction

next …
DAMEWARE fundamentals

Based on the X-Informatics paradigm, it is multi-disciplinary platform (until now X = Astro)

End users can remotely exploit high computing and storage power to process massive datasets (in principle they can do data mining on their smartphone…)

User can automatically plug-in his own algorithm and launch experiments through the Suite via a simple web browser
DAME - The existing infrastructure

**DAME Grid (SCOPE)**
- DR Storage
- DR Execution

**GRID SE**
- User & Data Archives (300 TB dedicated)

**GRID UI**
- Production & WFXT service
- DAMeware web application GUI
- SDSS mirror & services
- SVN code archive

**GRID CE**
- DAMeware web app Mirror @oacn.inaf.it

**DAME Cloud**
- VOGCLUSTERS web app
- Development
- DAME website

**Domain grisu.unina.it**
- http://dame.dsf.unina.it

**Domain dsf.unina.it**
- DAMEWARE web app Mirror @oacn.inaf.it

**Domain oacn.inaf.it**
- DAMEWARE web app Mirror @oacn.inaf.it

**Incoming DAMeware mirroring at Caltech**

**Cloud facilities**
- 16 TB
- 15 processors
Moving programs not data: the true bottle neck

Data Mining + Data Warehouse = Mining of Warehouse Data

- For organizational learning to take place, data from must be gathered together and organized in a consistent and useful way – hence, Data Warehousing (DW);
- DW allows an organization to remember what it has noticed about its data;
- Data Mining apps should be interoperable with data organized and shared between DW.

**Interoperability scenarios**

<table>
<thead>
<tr>
<th>DA1</th>
<th>Data+apps Exchange</th>
<th>DA2</th>
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<tbody>
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Full interoperability between DA (Desktop Applications)
Local user desktop fully involved (requires computing power)

<table>
<thead>
<tr>
<th>DA</th>
<th>Data+apps Exchange</th>
<th>WA</th>
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<tbody>
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</table>

Full WA → DA interoperability
Partial DA → WA interoperability (such as remote file storing)
MDS must be moved between local and remote apps
user desktop partially involved (requires minor computing and storage power)

<table>
<thead>
<tr>
<th>WA</th>
<th>Data+apps Exchange</th>
<th>WA</th>
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<tbody>
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</table>

Except from URI exchange, no interoperability and different accounting policy
MDS must be moved between remote apps (but larger bandwidth)
No local computing power required
The new vision for KDD

All DAs must become WAs
Unique accounting policy (google/Microsoft like)
To overcome MDS flow, apps must be plug & play
(e.g. any WAx feature should be pluggable in WAy on demand)

No local computing power required. Also smartphones can run DM apps

Requirements

• Standard accounting system;
• No more MDS moving on the web, but just moving Apps, structured as plugin repositories and execution environments;
• Standard modeling of WA and components to obtain the maximum level of granularity;
• Evolution of SAMP architecture to extend web interoperability (in particular for the migration of the plugins);

The Lernaean Hydra DAME KDD (plugin granularity)

1. WAy asks for Px-3 from WAx
2. WAx sends Px-3 to WAy
3. WAy executes Px-3

This scheme could be iterated and extended involving all standardized web apps
The scenario will become:

No different WAs, but simply one WA with several sites (eventually with different GUIs and computing environments)

All WA sites can become a mirror site of all the others

The synchronization of plugin releases between WAs is performed at request time

Minimization of data exchange flow (just few plugins in case of synchronization between mirrors)
## Third bottle neck: lack of reliable a priori information

<table>
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<th>Longo et al. 2003</th>
<th>Ball &amp; Brunner 2009</th>
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<tbody>
<tr>
<td>S/G separation</td>
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<tr>
<td>In its various implementations</td>
<td>In its various implementations</td>
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<tr>
<td>Morphological classification of galaxies <em>(shapes, spectra)</em></td>
<td>Morphological classification of galaxies <em>(shapes, spectra)</em></td>
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<tr>
<td>Spectral classification of stars</td>
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<tr>
<td>Image segmentation</td>
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<td>Noise removal <em>(grav. waves, pixel lensing, images)</em></td>
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<td>Interstellar magnetic fields</td>
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<tr>
<td>Stellar evolution models</td>
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Citizen Science

Reproduces human biases on a higher scale
Last and most serious problem: Need for a new generation of scientists

*NSF panel for interdisciplinary computing*

- Domain experts (scientists) do not want and must not become computer scientists
- The exploitation of MDS requires a much deeper understanding of computing infrastructures and of ITC technologies than what is currently done
  - Large, crossdisciplinary teams?
  - New university curricula?
  - More user friendly SW and HW infrastructures?
...THE END