HPC, CSE, Big Data, AI, ML, where are we now?

Alvaro Coutinho
alvaro@nacad.ufrj.br

High Performance Computing Center
COPPE/Federal University of Rio de Janeiro
www.nacad.ufrj.br
Contents

- Computational Science and Engineering
- High Performance Computing
- Predictive Computational Science, the new paradigm
- Challenges in Scientific Data Analysis
- Data Science and Machine Learning
- Conclusions and Discussion
COMPUTATIONAL SCIENCE AND ENGINEERING
Computational science and engineering (CSE) is a multidisciplinary field of research and education lying at the intersection of applied mathematics, computer science, and core disciplines of science and engineering. CSE encompasses methods of high-performance computing (HPC) and it is central in data sciences.

- CSE encompasses methods of HPC and it is central in Data Sciences.

CSE Pipeline\textsuperscript{1}

\textsuperscript{1}Future Directions in CSE Education and Research, http://wiki.siam.org/siag-cse/index.php/Main_Page
HIGH PERFORMANCE COMPUTING
High Performance Computers or Supercomputers

Supercomputers are the fastest and most powerful general purpose scientific computing systems available at any given time.


Turing’s Bombe, UK, 1941

Sunway TaihuLight, Sunway SW26010
260C 1.45GHz, cores: 10.6M
Capacity: 93 PFlop/s
Power: 15.37 MW
Memory: 1,3PB
Historical Trends TOP500 List

Performance Development

LINPACK Benchmark:
solves a dense system of linear equations by LU factorization

All phones
By 2019
ENI 18.9PFlop/s

http://www.top500.org
Lists the top 500 supercomputers; Updated in 06/XX and 11/XX
The HPCG Benchmark

**HPCG on LoboCarneiro**
- Distributed Processes: 6048
- Global Problem Dimensions:
  - $nx$: 1040
  - $ny$: 1040
  - $nz$: 1456
- Number of Equations: 1,574,809,600
- Number of Nonzero Terms: 42,445,920,184
- GFLOP/s rating of: 4520.67 ~2.34% peak
- HPL: 193.09 Tflop/s

### Results from SC17 Nov 2017

<table>
<thead>
<tr>
<th>Rank</th>
<th>Site Description</th>
<th>Computer</th>
<th>Cores</th>
<th>Rmax Ptflops</th>
<th>HPCG Ptflops</th>
<th>HPCG Ptflops / HPL0</th>
<th>% of Peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>RIKEN Advanced Institute for Computational Science, Japan</td>
<td>K computer, SPARC64 VItlx 2.0GHz, Tofu Interconnect</td>
<td>705,024</td>
<td>10.5</td>
<td>0.60</td>
<td>5.7%</td>
<td>5.3%</td>
</tr>
<tr>
<td>2</td>
<td>NSCC / Guangzhou China</td>
<td>Tianhe-2 NUOT, Xeon 12C 2.2GHz + Intel Xeon Phi 57C + Custom</td>
<td>3,120,000</td>
<td>33.8</td>
<td>0.58</td>
<td>1.7%</td>
<td>1.1%</td>
</tr>
<tr>
<td>3</td>
<td>National Supercomputing Center in Wuxi China</td>
<td>Sunway Taihulight -- Sunway MPP, SW2610 260C 1.45GHz, Sunway, NSRCPC</td>
<td>10,649,600</td>
<td>93.0</td>
<td>0.48</td>
<td>0.5%</td>
<td>0.4%</td>
</tr>
<tr>
<td>4</td>
<td>Swiss National Supercomputing Centre (CSCS), Switzerland</td>
<td>Plit Daint -- Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries Interconnect, NVIDIA P100, Cray</td>
<td>361,760</td>
<td>19.6</td>
<td>0.48</td>
<td>2.4%</td>
<td>1.9%</td>
</tr>
<tr>
<td>5</td>
<td>Joint Center for Advanced HPC Japan</td>
<td>Oakforest-PACS -- PRIMERGY CX6000 M1, Intel Xeon Phi 7250 68C 1.4GHz, Intel OmniPath, Fujitsu</td>
<td>557,056</td>
<td>24.9</td>
<td>0.39</td>
<td>2.8%</td>
<td>1.5%</td>
</tr>
<tr>
<td>6</td>
<td>DOE/SC/IBN, NERSC USA</td>
<td>Cori -- XC40, Intel Xeon Phi 7250 68C 1.4GHz, Cray Aries, Cray</td>
<td>632,400</td>
<td>13.8</td>
<td>0.36</td>
<td>2.6%</td>
<td>1.3%</td>
</tr>
<tr>
<td>7</td>
<td>DOE/NNSA/LLNL USA</td>
<td>Sequoia -- IBM BlueGene/Q, PowerPC A2 16C 1.6GHz, 5D Torus, IBM</td>
<td>1,572,846</td>
<td>17.2</td>
<td>0.33</td>
<td>1.9%</td>
<td>1.6%</td>
</tr>
<tr>
<td>8</td>
<td>DOE/SC/Oak Ridge National Lab</td>
<td>Titan - Cray XK7, Opteron 6274 16C 2.20GHz, Cray Gemini Interconnect, NVIDIA K20x</td>
<td>560,640</td>
<td>17.6</td>
<td>0.32</td>
<td>1.8%</td>
<td>1.2%</td>
</tr>
<tr>
<td>9</td>
<td>DOE/NNSA/ANL, ANL</td>
<td>Trinity - Cray XC40, Intel E5-2698v3, Aries custom, Cray</td>
<td>301,056</td>
<td>8.10</td>
<td>0.18</td>
<td>2.3%</td>
<td>1.6%</td>
</tr>
<tr>
<td>10</td>
<td>NASA / Mountain View</td>
<td>Pleiades - SGI ICE X, Intel E5-2680, E5-2680v2, E5-2680v3, E5-2680v4, Infiniband FDR HPE</td>
<td>243,008</td>
<td>6.0</td>
<td>0.17</td>
<td>2.9%</td>
<td>2.5%</td>
</tr>
</tbody>
</table>

1. from: //software.sandia.gov/hpcg/
NACAD´s Mission

- High Performance Computing in Engineering and Computational Science – Interdisciplinary Area with Major in HPC since 1988
- To provide and operate an advanced infrastructure for computing
- Develop and support multidisciplinary R & D projects of relevance, especially in:
  - Energy: Oil and Gas, Electric
  - Civil, Mechanical and Materials Engineering
  - Environment, Meteorology and Oceanography
  - Computing, Database and Data Mining
  - Biological Sciences
COPPE’s new machine: LoboCarneiro
253 Compute Nodes 6072 Cores (506 Processors
Intel Xeon Haswell E5-2670V3 12-Cores
2.3GHz) 16.192GB Mem DDR4, 193 Tflop/s
Real life computations

Fluid-Structure Interaction: Wave reaching midship region, simulation and experiments visualization. Computed with FLUENT, Cluster Petrobras

Turbulent turbidity current simulation
FE-VMS, EdgeCFD, 30M tets, LoboCarneiro

SEM solution of full elastic wave equation in random heterogeneous media
Octree-based mesh generation: 75B elements
Joint work COPPE/CentraleSupelec

VIV on a rigid riser with strakes, Re=10K,
Computed with EdgeCFD 7M tet4, LoboCarneiro
ACM SIGHPC/Intel Computational & Data Science Fellowships 2017
The new paradigm

PREDICTIVE

COMPUTATIONAL SCIENCE
Predictive Science\textsuperscript{1}

Definition: Predictive science is the scientific discipline concerned with accessing the predictability of mathematical and computational models of physical events in the presence of uncertainties. It embraces the process of model selection, calibration, validation, verification, and their use in forecasting features of physical events with quantified uncertainty.

Models: mathematical constructions based on physical principles or empirical relations—generally based on inductive theories which attempt to characterize abstractions of physical reality.

\textsuperscript{1}J. Tinsley Oden, Ivo Babuska, and Danial Faghihi, Predictive Computational Science: Computer Predictions in the Presence of Uncertainty, Encyclopedia of Computational Mechanics, Wiley
Uncertain Rheology of Non–Dilute Currents

<table>
<thead>
<tr>
<th>Author</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Einstein (1906) [25]</td>
<td>$\nu_m = \nu_f (1 + 2.5c)$</td>
</tr>
<tr>
<td>Mooney (1951) [26]</td>
<td>$\nu_m = \nu_f \exp\left(\frac{2.5c}{c_m}\right)$</td>
</tr>
<tr>
<td>Krieger and Dougherty (1959) [7]</td>
<td>$\nu_m = \nu_f \left(1 - \frac{c}{c_m}\right)^{-2.0}$; $c_m = 0.74$</td>
</tr>
<tr>
<td>Batchelor (1977) [27]</td>
<td>$\nu_m = \nu_f \left(1 + 2.5c + 6.2c^2\right)$</td>
</tr>
<tr>
<td>Brady (1993) [28]</td>
<td>$\nu_m = 1.3\nu_f \left(1 - \frac{c}{c_m}\right)^{-2.0}$</td>
</tr>
<tr>
<td>Toda and Hisamoto (2006) [29]</td>
<td>$\nu_m = \nu_f \left(1 - 0.5c\right)^{-2}$</td>
</tr>
<tr>
<td>Toda and Hisamoto with k (2006) [29]</td>
<td>$\nu_m = \nu_f \left(\frac{1+0.5ke^{-2}}{(1-kc)(1-c)}\right)$; $k = 1 + 0.6c$</td>
</tr>
</tbody>
</table>

Computational Setup: closed channel with sustained current

- Channel dimensions, $x_c = 6$, $y_c = 0.4$, $z_c = 0.5$, inlet windows $yw = 0.4$ $zw = 0.04$. Computational setup inspired on a experimental one (calibration and validation)
- Initial relative concentration = 0.11 (normalization constant)
- Reynolds number $Re = 1.5 \times 10^4$, used to allow the formation of turbulent structures. Transient flow features.
- No-slip and no-penetration in all walls with inflow velocity = 0.5

Time: 24.0

μD colored by $\left(\sigma^D / \mu^D\right)$ in %

SGSC plus parallel SWMS engine with 257 samples

Toda and Hisamoto with k (2006) [29]
Uncertain Rheology of Non–Dilute Currents: Bayesian Calibration, Validation and Prediction

MCMC ran for 104521 samples with 50% burn-in, and for each step of the chain, 104522 samples for the Monte-Carlo integration.

Figure 10: Predictive mean and confidence interval of deposition along the centerline in $x$ direction compared to observation (red dashed line).

Predicted deposition probability distribution obtained with inlet mixture velocity $Q_{inj} = 0.75$ compared to the observation (black vertical dashed lines)
CHALLENGES IN DATA ANALYSIS
Bringing High Performance Computing to Big Data Algorithms

Atop this hardware, the Apache Hadoop system implements a MapReduce model for data analytics. Hadoop includes a distributed file system (HDFS) for managing large numbers of large files, distributed (with block replication) across the local storage of the cluster. HDFS and HBase, an open source implementation of Google's BigTable key-value store, are the big data analogs of Lustre for computational science, albeit optimized for different hardware and access patterns.

Atop the Hadoop storage system, tools (such as Pig) provide a high-level programming model for the two-phase MapReduce model. Coupled with streaming data (Storm and Flume), graph (Giraph), and relational data (Sqoop) support, the Hadoop ecosystem is designed for data analysis. Moreover, tools (such as Mahout) enable classification, recommendation, and prediction via supervised and unsupervised learning. Unlike scientific computing, application development for data analytics often relies on Java and Web services tools (such as Ruby on Rails). Figure 1 (left) shows the mainstream Big Data system stack.

1.2 Application Areas

This chapter discusses HPC implementations of two mainstream Big Data algorithms. While the first one, Alternating Least Squares (ALS), has primarily commercial applications, the second one, Singular Value Decomposition (SVD), is uniformly applicable to a wide range of problems in science, engineering, and commerce.

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**Software Stack for HPC and Big Data**

<table>
<thead>
<tr>
<th>APPLICATION LEVEL</th>
<th>APPLICATIONS</th>
<th>MIDDLEWARE &amp; MANAGEMENT</th>
<th>SYSTEM SOFTWARE</th>
<th>CLUSTER HARDWARE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mahout, R and Applications</td>
<td>Hive, Pig, Sqoop, Flume, ZoomReduce, Storm</td>
<td>Virtual Machines and Cloud Services (optional)</td>
<td>Ethernet Switches, Local Node Storage, Commodity X86 Racks</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Hbase BigTable (key-value store), HDFS (Hadoop File System)</td>
<td>LINUX OS VARIANT</td>
<td>Infiniband + Ethernet Switches, SAN + Local Node Storage, X86 Racks + GPUs or Accelerators</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>DATA ANALYTICS ECOSYSTEM</td>
<td>COMPUTATIONAL SCIENCE ECOSYSTEM</td>
</tr>
</tbody>
</table>

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Why Data Management differs

**Business data**
- easy to understand
- text format
- all manipulation in SQL
- most of data stored is traversed for queries

**Scientific data**
- complex math / domain
- binary shared formats
- specific programs access
- only a small fraction of data is queried

Collapse of column with $\mu(I)$-rheology

Open Source Ecosystem

Spark
Using a D-DBMS to manage Predictive Models with data provenance

2. Scientific Application Modeling using Data-centric Workflows

1. Scientific Composition

3. Managed by a SWfMS and executed in HPC environments

4. Metadata from large volumes of data manipulated
   - Petabytes
   - Exabytes

5. Data Analyses

Souza et al, Data reduction in scientific workflows using provenance monitoring and user steering, FGCS, 2018
Putting the human in the loop

“In spite of the tremendous advances made in computational analysis, there remain many patterns that humans can easily detect but computer algorithms have a difficult time finding.”

Exploring the inherent technical challenges in realizing the potential of Big Data.

BY H.V. JAGADISH, JOHANNES GEHRKE, ALEXANDROS LABRINIDIS, YANNIS PAPAKONSTANTINOU, JIGNESH M. PATEL, RAGHU RAMAKRISHNAN, AND CYRUS SHAHABI

Big Data and Its Technical Challenges
Human In-the-Loop Challenges

Monitoring
- Define what data to monitor
- Provide data monitoring
- Give context (provenance) to data
- Show data at real time

Real Time Analysis
- Interact with data monitoring
- Define queries and visualization at real time

Fine-tuning
- Prepare execution to change
- Change the configuration at real time
- Keep data consistency
What AI has to say about HIL?

On autonomous cars (autonomous AI):

"But sometimes good verification and validation aren't enough to avoid accidents, because we also need good control: ability for a human operator to monitor the system and change its behavior if necessary. For such human-in-the-loop systems to work well, it's crucial that the human-machine communication be effective. In this spirit, a red light on your dashboard will conveniently alert you if you accidentally leave the trunk of your car open."

On general human AI interaction:

"As AI gets smarter, this will involve not merely building good user interfaces for information sharing, but also figuring out how to optimally allocate tasks within human-computer teams—for example, identifying situations where control should be transferred, and for applying human judgment efficiently to the highest-value decisions rather than distracting human controllers with a flood of unimportant information.

More on: https://futureoflife.org/
UQ with User Steering & Intervention

1. **Generate Geometric Mesh**
   - Mesh File \( \text{(mesh.msh)} \)
   - Geometry Parameters \( \text{(input.dat)} \)
   - **call** \( \text{MeshGen(input.dat)} \)

2. **Assign Initial Conditions**
   - Mesh File \( \text{(mesh.msh)} \)
   - Mesh Data \( \text{(MD)} \) set
   - **call** \( \text{MeshInit(mesh.msh, cp.in)} \)

3. **Do Mesh Partitioning**
   - Partitioned Mesh Data \( \text{(PD)} \)
   - **for each** mesh
   - **call** \( \text{MeshPre(mesh)} \)

4. **Run CFD Solver**
   - Output Data \( \text{(OD)} \) set
   - **for each** mesh
   - **call** \( \text{Solver(mesh)} \)

5. **Data Merger**
   - Merged Data \( \text{(GD)} \) set
   - **for each** output
   - **call** \( \text{Merge(output)} \)

6. **Extract Energy**
   - Data of interest \( \text{(ID)} \) set
   - **for each** result
   - **call** \( \text{Stat(result)} \)

7. **Average Energy for Current Level**
   - Average Vector \( \text{avg} \)
   - **call** \( \text{Average(ID)} \)

8. **Evaluates Norm Difference**
   - Solution
   - **call** \( \text{NormDiff(avg, avgOld)} \)

9. **Increase Interp. Level**
   - **call** \( \text{InterConf(currentLevel)} \)
   - \( \epsilon \) is true
   - **Online**
   - \( \epsilon \) is false
   - Results

**Provenance**

- Change
  - NormDiff
  - 0.001 to 0.01

**Compute the velocity at controlling points**

**Estimate if the variance at those points are greater than some tolerance previously set**

---

Parameter Online Tracking and Fine-tuning

In situ visualization with ParaView Catalyst

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Before adapt</th>
<th>After adapt</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow non-linear tolerance</td>
<td>1.0e-4</td>
<td>1.0e-3</td>
</tr>
<tr>
<td>Transport non-linear tolerance</td>
<td>1.0e-4</td>
<td>1.0e-3</td>
</tr>
<tr>
<td>Flow initial linear solver tolerance</td>
<td>1.0e-6</td>
<td>1.0e-1</td>
</tr>
<tr>
<td>Transport initial linear solver tolerance</td>
<td>1.0e-6</td>
<td>1.0e-1</td>
</tr>
</tbody>
</table>

**Table 1**

**libMesh-sedimentation workflow**

<table>
<thead>
<tr>
<th></th>
<th>Before</th>
<th>After</th>
<th>Reduction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Avg. Solver Time by iteration</td>
<td>3.82 min</td>
<td>2.21 min</td>
<td>42.14%</td>
</tr>
<tr>
<td>Avg. Number of elements</td>
<td>$2.4 \times 10^6$</td>
<td>$1.7 \times 10^6$</td>
<td>29.24%</td>
</tr>
<tr>
<td>Simulation time</td>
<td>(expected)</td>
<td>(real)</td>
<td>37%</td>
</tr>
</tbody>
</table>

~27 days              ~17 days
Data Science and Machine Learning Point of View

Fig. 1. A representation of knowledge discovery methods in scientific applications. The $x$-axis measures the use of data while the $y$-axis measures the use of scientific knowledge. Theory-guided data science explores the space of knowledge discovery that makes ample use of the available data while being observant of the underlying scientific knowledge.
Physical Analytics lies between IoT 1.0, physics-based modeling and big data analytics.

Highly interdisciplinary with many interesting research topics:
- Statistical learning under physical constraints
- Model complexity reduction
- Situation-dependent, machine-learnt multi-model blending
- Graph theory and statistical physics
- Parallelizing physical models for data-intensive computation
- ...
- Feed learning back to improve understanding of the underlying physics
IBM Physical Analytics

Physical systems in different Industries

Cross Industry | Telecom | Oil and Gas | Health Care | Transportation & Travel | Utility | Agriculture | Public
---|---|---|---|---|---|---|---
Data Centers | High value Buildings | Network Offices | Pipelines & Fracking Operations | Hospitals | Bridges / Infrastructure | Solar farms | Vineyards, Wineries, Greenhouses | Environment

Links

Physical Analytics Platform

Massive Scalable Distributed Storage and Compute (PAIRS)

Real-time Data

Domain Data

Scalable Analytical Services

User Applications
Industry Point of View

GE 'Digital Foundries', where Physics + Analytics Intersect

Predix – A cloud-based platform for industry

Machine connectivity

Enterprise systems

Enhanced security

Asset optimization

Connectivity

Predix machine Software / Analytics

Services

Asset
Analytics
Data
Security
Operations
Cloud Foundry
Industrial Big Data
Predix Cloud
Gated community, purpose built for industry

Applications

UI / Mobile applications
A Word of Caution in Machine Learning

- Machine Learning (ML) are *Universal Approximators*
- Huge success in text mining, image recognition, etc.
- ML finds best solution minimizing some norm between *input* and *output* – standard solutions may be trapped within a local minimum, thus stochastic algorithms are preferred
- ML does not know about the problem being solved
  - In case of physical systems ML may reach unphysical solutions, that is, a solution for incompressible flows where velocity does not satisfy $\nabla \cdot \mathbf{u} = 0$
- ML learning should know about the physics: adding constraints to the formulation

Physics-Constrained Data Models

Karthik Duraisamy, Data-enabled, Physics-constrained Predictive Modeling of Complex Systems, SIAM NEWS, July-Aug, 2017

Figure 1. Example of data-augmented, physics-based modeling applied to turbulent flow prediction. Predictive improvement is achieved based on inferring force data over another airfoil and constructing machine-learned model augmentations. Left. Pressure over airfoil surface. Green: baseline physics model. Red: machine learning-augmented physics model. Blue: experimental measurements. Middle. Baseline flow prediction (pressure contours and streamlines). Right. Flow prediction using machine learning-augmented physics model. Image adapted from [8].

Navier-Stokes equation: Top: Predicted versus exact instantaneous pressure field \( p(t,x,y) \) at a representative time instant. This remarkable qualitative agreement highlights the ability of physics-informed neural networks to identify the entire pressure field, despite the fact that no data on the pressure are used during model training. Bottom: Correct partial differential equation along with the identified one obtained by learning \( \lambda_1, \lambda_2 \) and \( p(t, x,y) \).

Final Remarks and Discussion

- We see a synergy between HPC, Big Data, AI, and ML. We have learned that new machines open new possibilities → what will happen when we have exascale machines?
- Predictive Computational Science is the new paradigm
- CS&E and Data Science: we need them both
- Machines and Apps are becoming increasingly complex, how to manage all this? HPC, Storage, Networking and Visualization are becoming more integrated
- What’s AI role? How it will be integrated with PDE-based solvers? How to deal with the huge amount of data?
  - Los Alamos 2ND PHYSICS INFORMED MACHINE LEARNING, Jan 21-25, 2018
- International collaboration, like BR-EU H2020 will strengthen the field
- Digital Twins in Energy Industry
  - GE is promoting; Shell joined a JIP for digital twins in Oil&Gas in July, 2017
- The Brazilian government has sustained a successful R&D policy funding in the Energy area directly promoting partnerships involving the private sector, universities and research labs, supervised by the regulatory agencies ANP (oil & gas) ANEEL (electricity).
Our Team

**Faculty:**
- Civil Engineering: J. Alves, R. Elias, L. Landau
- Mechanical Engineering: F. Rochinha
- Computer Science: M. Mattoso
- Visitors: L. Franca (in memoriam), R. Cottereau (CNRS-Centrale), P. Valduriez (INRIA)

**Pos-Docs, Research Staff and Students:**

**Funding:** Petrobras, ANP, MCTIC, MEC

**Computer Resources:** NACAD/COPPE/UFRJ, SDumont/LNCC, TACC/UT Austin, Occigen/CINES, France, MN4-BSC, Spain

HPC4E team, Rio de Janeiro, 2017