Lightning Talk Efficient Scientific Computing School

Bruno Alves

Compact Muon Solenoid, CERN, Switzerland





Bertinoro, 21-26 October 2019

Personal overview

2012 - 2018: Master's in Physics Engineering, Instituto Superior Técnico, University of Lisbon Summer 2016: Summer Student at CERN Summer 2018: Image classification with machine learning: Leiden, Netherlands September 2018 – March 2019: Data analysis and generative machine learning (GANs): Melbourne, Australia From May 2019: Trainee at CERN, working in the HGCal group of the CMS experiment

CMS High Granularity Calorimeter



Performace studies of silicon partial wafers



Scientific computing interests

Dealing with CERN's huge datasets:

Parallelism:

how to best exploit all the available cores; best practices to avoid thread concurrent access;

learn TBB basics;

have the chance to apply CUDA to a realistic problem;

know which technology is better fit for each situation.

• C++ usage:

Efficient coding:

facilitate auto-vectorization, decrease cache misses, reduce memory usage, use special C++ keywords;

Scalability:

write more abstract code maintaining readability and efficiency to avoid long development times when changing small analysis details;

$\underline{C^{++17} \text{ and } C^{++20} \text{ features:}}$

avoid old C or C++ constructs when better options are available

Thank you!

About Me...

Name: Paolo Baldan Born: 25th June 1993, Rome Education:

- Bcs at University of Rome Tor Vergata (2015)
- Mcs at University of Rome La Sapienza (2017)
- Phd at University of Rome La Sapienza under the supervision of professor Giorgio Parisi (ongoing).

... and my Research

How similar are 3d amorphous materials to their infinite dimensional (Mean Field) counterpart?



Potential Energy Landscape at Jamming



Steep Increase in the Number of Thermodynamic States

States are Organized in a Hierarchical & Ultrametric way

Moving Forward

Upcoming Analyses

Push Compression Further Increase Dimensionality Increase Sample Size

Computational Challenges

- Steep Increase of the Relaxation Time $\tau \propto e^{E/(T-T_0)}$
- Very Mild increase of the Correlation Length

Beating the Timescale Problem

- Clever (Nonlocal) Montecarlo Moves
- Efficient Hardware Exploitation
 - Parallel Computing

Wanna Know More?

Come and See my Poster!



Konstantin Batkov

- Applied nuclear physicist
- Scientist at the MAXIV synchrotron light source

Lund, Sweden

- Neutronics (neutron transport through matter)
 - neutron production and moderation
- Radiation shielding calculations

- Extensive Monte Carlo
 - FLUKA, PHITS, MCNP
 - variance reduction
- Complex geometries built with a *bricolage* C++ framework



- Neutron production calculations for the European Spallation source (accelerator-based neutron source)
- Multidimensional optimisation
 - massive Monte Carlo calculations
 - variance reduction
 - MPI
- Low dimensional moderator concept
 - cold neutron brightness increased by a factor of 2.5





- Radiation shielding at the MAX IV synchrotron light source
- Realistic fully parameterised geometric models
- Variance reduction



Much more details in the poster



- Machine learning
 - ill-posed problems
- Development of large scale scientific applications with modern C++
- Variance reduction
 - quick and memory-efficient operations with tensors
- GPU programming
 - reverse ray-tracing
- MPI programming

Research Activities and Areas of Interest in Scientific Computing

Rajarshi Bhattacharya

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Outline

- Physics Analysis in CMS
 - \circ HH \rightarrow bbtt
 - $\circ~B_{_S} \rightarrow \phi \phi \rightarrow kkkk$ with L1 tracks for CMS Phase 2 Tracker
 - Optimization of isolation for electron and muon for $H \rightarrow ZZ \rightarrow 4$ leptons analysis
- Service to the experiment
 - Beam Test data analysis for the proposed 2S modules of the CMS Phase-2 outer tracker
 - Calibration of noisy channels for the current CMS tracker
 - Data quality monitoring for the current CMS tracker

$\text{HH} \rightarrow \text{bbtt}$

- Aim is to explore Higgs-self coupling and any presence of BSM physics
- Dominant production mode:
 - Gluon-gluon Fusion
 - σ_{HH} ~ 33 fb at 13 TeV
- Good compromise between yield and purity

My main contribution

DY background estimation



 b-Tagging efficiency measurement and b-Tagging weights calculation

<u>Results</u>

2016 Data (HIG-17-002), PLB

- SM HH production obs (exp) 31 (25) × σ_{SM}
- Both non-resonant and resonant searches



Triggering $B_S \rightarrow \phi \phi \rightarrow kkkk$ events using L1 tracks with the CMS Phase-2 Tracker



Rare process

- Br(B_s → $\phi\phi$) ≈ (1.84 ± 0.18) × 10⁻⁵ (PDG)
- BSM physics which are beyond the direct reach of the LHC may contribute

 $b \rightarrow sss penguin diagram$

- Fully hadronic final state
 - CMS can not study such final states with the current detector
 - At Phase-2, a new tracker with L1 tracking capabilities will allow one to trigger such final states efficiently
- Final state kaons are low p_T tracks, close to the L1 tracking threshold of 2 GeV
 - Major source of loss of efficiency

 B_s mass peak is clearly visible at the trigger level even with $\langle PU \rangle = 200$

14 TeV, 200 PU Normalized # of tracks CMS Phase-2 Upgrade Simulation 10-15 p_(GeV) candidates 14 TeV, 200 PU CMS Phase-2 Upgrade 0.2 Simulation — L1 signal B Mass ····· Offline signal L1 background 5.2 5.6 5.8 M_m (GeV)

30% signal efficiency can be achieved at a L1 rate of 15 kHz for <PU> = 200

Softest Track

Areas of Interest where efficient computing can be used

- High performance computing is becoming ever more important at the LHC
 - With increasing instantaneous luminosity which causes higher pile-up
 - With ever increasing data volume which require more efficient data access and analysis strategies
- Physics analyses are gradually moving from traditional cut based approach to Machine Learning based approach
 - GPU based computation can help a lot
- Use of GPUs may also improve Trigger latency significantly
- L1 tracking in CMS Phase-2
 - Complex trigger logic implemented in FPGAs
- Core software development
 - Requires expertise on efficient programming, e.g.
 - memory management
 - modern C++ idioms, tools and methodologies

Voids-Lensing Cross Correlation

Marco Bonici

Università degli Studi di Genova

October 21, 2019



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Euclid is an ESA space mission, whose launch is scheduled for 2022. Scientific objectives are

- Dark Energy, responsible of the universe acceleration
- Dark Matter, which drives structure formation
- The sum of neutrino masses







Lensing is a general relativistic effect, the light bending in gravitational field due to the universe mass distribution.



Voids are underdense regions, whose formation and evolution is sensitive to Dark Energy and Neutrinos.

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We want to forecast the Euclid sensitivity to cosmological parameters. The tool we use is the Fisher Matrix $F_{\alpha\beta}$, whose inverse gives the exptected parameters uncertainties. It is defined, in general, as

$$F_{\alpha\beta} = -\left\langle \frac{\partial^2 \ln P}{\partial \theta_{\alpha} \partial \theta_{\beta}} \right\rangle \tag{1}$$

where α and β span over the cosmological parameters, among which there are the neutrino masses M_{ν} and the Dark Energy equation of state parameters w_0 and w_a

$$w_{DE}(z) \equiv \frac{P_{DE}(z)}{\rho_{DE}(z)} = w_0 + w_a \frac{z}{1+z}$$
(2)

The Python code I am developing evaluates the Voids-Lensing Cross correlation Fisher Matrix. The code is divided in three parts:

- Lensing and Voids distribution evaluation for different values of the Cosmological parameters
- Evaluation of the Lensing and Voids distribution derivatives with respect to the Cosmological Parameters
- Fisher Matrix evaluation

The program can run on local machines, but there is the possibility to submit the different jobs in parallel to a computing facility.



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Achtung: preliminary result!





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REAL TIME DOSIMETRY IN IORT

Francesco Collamati INFN ROMA

ESC 2019 - Bertinoro (FC)

• TECHNIQUE RATIONALE:

 To deliver a high dose (~20 Gy) of radiation precisely to the target area, with minimal impact on surrounding healthy tissue

• HOW:

- The treatment is performed directly in the operating room, in one single shot
- Use of portable mobile linear accelerators
- Tipically using 5-10MeV (or 50kV X rays)



· PROs:

- A single application (≈min) replaces 30 days of standard RT treatment
 - Public health impact...
- Organs At Risk can be manually moved away/ protected
- Much reduced side effects to skin

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CONS

- Requires non trivial technical organisation
- Operating Room shielding, radio protection, multi disciplinary team, expensive machine
- Final global ≈10-15% uncertainty
- Misalignments, inhomogeneousity, material layers
- Same dose for every patient
- No "dosimetric report" after treatment

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TREATMENT PLANNING SYSTEM

- Its the system at the base of Radio Therapy, that allows it to be effective on the tumor while sparing healthy organs as much as possible
 - Everything starts from patient **CT**, that provides:
 - Shape of the patients
 - Density and material composition
 - A "virtual patient" is built
 - The effect of the beam on it is simulated, varying possible parameters (beam number and position, energy, absorbers...) to find the optimal configuration:
 - Desired dose @ the tumor
 - Minimal dose @ healthy tissue
 - After the treatment, it also provides a "dosimetric report": how much dose to the given organ





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Nothing similar exists today for IORT

No intraoperative "CT" image

Altered anatomy





TOWARDS A TPS IN IORT !?

INTRA OPERATIVE IMAGE

• Fuse pre operative CT + Intra operative image



TOWARDS A TPS IN IORT !?

INTRA OPERATIVE IMAGE

• Fuse pre operative CT + Intra operative image



FAST MONTE CARLO

- Image fed to Monte Carlo program for beam simulation
- A very fast simulation could allow real time dosimetry
 - ... GPU?


Presentation of research activity

ESC 2019 Architectures, Tools and Methodologies for Developing Efficient Large Scale Scientific Computing Applications Mattia Faggin

PhD school in Physics

Physics and Astronomy Department "Galileo Galilei" University of Padova







Dipartimento di Fisica e Astronomia Galileo Galilei



Main research activities

- PhD topic: "Measurement of heavy-flavor decay electron and heavyflavour baryon production with ALICE"
 - 1. Inclusive measurement of electrons from HF hadron decays (HFe) in Pb-Pb collisions

 \rightarrow paper committee chair of the article "Measurement of electrons from heavy-flavour hadron decays at mid-rapidity in pp and Pb-Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV"

 \rightarrow final rounds of collaboration review

- 2. Measurement of $\Xi_c^+ \to p K^- \pi^+$ in pp collisions
- Main goal of ALICE experiment: study of strongly interacting matter and of Quark Gluon Plasma (QGP)

 \rightarrow our universe thought to be in such state for the first few millionths of seconds after the Big Bang \rightarrow produced with ultra-relativistic heavy-ion collisions at LHC

- Charm and beauty quarks (HF) are produced in initial hard scattering (large Q^2) before the QGP formation (~ 1 fm/*c*)
- Unique probes, sensitive to the full QGP evolution



 $\sqrt{s_{NN}} = 5.02 \text{ TeV}$

HFe nuclear modification factor (R_{AA})

- HFe from inclusive electron spectrum
 → Statistical removal of hadron
 contamination
 - \rightarrow Subtraction of non-HFe background
- $p_{\rm T}^{\rm meas} \rightarrow p_{\rm T}^{\rm true}$ via unfolding
- In case of no medium effects: $R_{AA} = 1$
- Evident deviation from unity in central and semi-central Pb-Pb collisions
 → quark energy loss in the QGP



Nuclear overlap function: $\langle T_{AA} \rangle = \langle N_{coll} \rangle / \sigma_{pp}^{inel}$

Invariant cross section, pp @ $\sqrt{s_{\text{NN}}} = 5.02 \text{ TeV}$



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Charmed baryon production



- Baryon/meson for charmed hadrons in pp and p-Pb collisions at LHC higher than MC generators tuned to reproduce e^+e^- results
- Even higher values in Pb-Pb and Au-Au collisions at LHC and RICH
 - \Rightarrow charm hadronization not fully understood
 - 1. Heavy-quark hadronization influenced by surrounding hadronic environment?
 - 2. Possibility to hadronized via coalescence in QGP?

- Study of $\Xi_c^+ \to pK^-\pi^+$ production in pp @ $\sqrt{s} = 13 \text{ TeV}$
 - \rightarrow topological selections and particle identification
 - \rightarrow next: possibility to adopt machine learning techniques to optimize the signal extraction



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Computing interests



 \rightarrow Even more challenging situation with Run 3 data

 \rightarrow I look forward to attending the lectures for many useful inputs

2. Explore new C++ standards and tools (still old-style C++ widely used)

3. Learn as much as possible!

Thank you!

The basics of efficient programming:











In-silico biomateriomics: efficient GPU acceleration and coarse-grained molecular dynamics approach

Federico Fontana

INFN-ESC 2019 21-26 October 2019

Tutor: **Prof. Francesco Nicotra** Supervisor: **Dott. Fabrizio Gelain**





Multiscale simulation of biomaterials



Length scale (m)





Molecular dynamics simulations (MD)

- MD consists in the solution of classical equation of motion (Newton's law) for studying the physical movements of atoms and molecules.
- MD simulations can be performed using different force-field and combining them together

GROMACS version 2016.3

- MPI and OpenMP
- Hybrid parallelization by making use of GPUs for the calculation of non-bonded force
- Multithreading with thread-MPI

Computational facility@CNTE

- 2 GPU NVIDIA® GeForce GTX 1080
- Cluster server: 4 nodes * 64 processors (AMD Opteron 6272)







MARTINI force-field

- Compatible with GROMACS simulation package
- 4 heavy atoms (or water molecules) \rightarrow CG grains
- Reduced computational costs
- **Monitor limited number of** events leading to **nanostructuring**, such as formation or breakage of H-bonds
- Fixed secondary structure parameters







GoMARTINI

- Mapping according to the MARTINI force-field philosophy
- No fixed secondary structure parameters
- Capture structural motion linked to folding or to particular catalytic activity.



AA representation of the protein 1UBQ (ubiquitin, left panel) and its CG representation in the ELNEDIN and GoMARTINI models as indicated.

Speed-up the MD simulations

Length scale (m)

Thank you for your attention

•Student:

Tonatiuh García Ch.

e-mail: tonaspiuck@gmail.com

 Student of PhD in the program: Language and Knowledge Engineering, LKE, at Benemérita Universidad Autónoma de Puebla, México.

First we start working with simulation, design, characterize and implementation of chaotic dynamical systems with analogous devices, in order to create random numbers. The idea was to enhance the chaotic behavior using an evolutionary algorithm to find the maximized the parameters to be set in the real circuit.

Important aspects:

- Good performance with basic test.
- Good characterization and enhancement of parameters.
- With serial or parallel interface with CPU is sufficient.
- Slow system for random bit generation.
- Difficult to do more demanding tests for the amount of bits needed. (million data per test)

Important aspects:

- Feasibility of carrying out more demanding tests.
- Good performance with less power consumption.
- Feasibility of collect millions of data in much less time.
- Adaptability, the entire system is full digital and programmable.

Topics:

- Muon tomography
- Muon radiography
- Cosmic ray detector for ALICE (ACORDE).[2]
- Particle trace reconstruction.
 - 1. Tesi di Dottorato di Giacomo Luca Bruno, The RPC detectors and the muon system for the CMS experiment at the LHC. Universit`a degli Studi di Pavia. 2000-2001.

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2. A. Fernández, et. Al, ACORDE a cosmic ray detector for ALICE, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Volume 572, Issue 1, 2007, Pages 102-103, ISSN 0168-9002

Hígh mass dí-boson resonances ín semí-leptoníc fínal state @ ATLAS experiment

11th INFN ESC School

Bertinoro - 21st October 2019

Antonio Giannini

Outline

- I am a PhD @ Università Federico II in Naples (February 2017 -2020) involved in the ATLAS experiment.
- 3rd PhD year at CERN thanks to a simil-fellow contract.
- PhD activities:
 - semi-leptonic di-boson final state signatures for Standard Model measurements and searches of new physics with resonance interpretation, with particular interest in <u>Vector</u> <u>Boson Scattering (VBS)</u> and <u>Vector Boson Fusion (VBF)</u>.
 - Involved in the JetEtMiss team for developing of <u>Quark/</u> <u>Gluon jets</u> tagging techniques.
 - Responsibility in ATLAS derivation framework (data format).
- <u>Today:</u>
 - The ATLAS experiment.
 - A look to di-boson searches.
 - Machine Learning application in the searches of new physics with the development of a <u>Recurrent Neural</u> <u>Network (RNN)</u> for the VBF/ggF event classification.
 - Interest in scientific computing:
 - C++/python for analysis frameworks, plots and optimisation.
 - Python and Keras libraries for Machine Learning application.

The ATLAS experiment

- ATLAS is a multi-purpose experiment of high energy physics.
- The detector has a cylindrical symmetry around the direction of the colliding beams of protons.
- It is made of some sub-detector:
 - inner detector
 - electromagnetic calorimeter
 - hadron calorimeter
 - muon spectrometer
- A trigger system manage the rate of data acquisition.

Why di-boson searches?

Higgs boson discovery!

Diboson semi-leptonic channel ($X \rightarrow ZV \rightarrow Ilqq$) as signature for new physics

- 2 leptons improves the bkg rejection
- 2 quarks improve the decay rate of V boson

INFN ESC School 2019

VBF/ggF classification

based.

Move to a new approach Neural Network

Use the 4-momentum of jets:

low-level variables.

- Event classification according the production mechanism.
- Combination of 2 categories increases also the final sensitivity for exotic searches.

Recurrent Neural Network

INFN ESC School 2019

Interest in scientific computing

Backup

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Mathilde Himmelreich Baryonic decay channels of the Y4260

ESC 2019, Bertinoro, Italy

GSI, IHEP and BESIII

ESC 20019 | Bertinoro, Italy | Mathilde Himmelreich

Motivation

- Search and validation of QCD exotics
- Search for additional final states
- Search for isoscalar partners (I = 0)
- Explanation of measured states

PRL 110 252001 (2013)

Discovery of the $Z_c^{+/-}$ (3900) in the J/ $\psi \pi^{-/+}$ invariant mass spectrum in the decay Y(4260) $\rightarrow J/\psi \pi^+\pi^-$

Spectrum of charmonium – like mesons

Inclusive baryon analysis of the Y4260

$$e^{+} + e^{-} \to Y(4260) \to \begin{cases} \Lambda^{0}\overline{\Lambda^{0}} & +X & \Lambda^{0} \to p\pi^{-} + c.c. \\ \Sigma^{0}\overline{\Sigma^{0}} & +X & \Sigma^{0} \to \Lambda^{0}\gamma + c.c. \\ \Xi^{0}\overline{\Xi^{0}} & +X & \Xi^{0} \to \Lambda^{0}\pi^{0} + c.c. \\ \Omega^{-}X^{+} & \Omega^{-} \to \begin{cases} \Lambda^{0}\mathrm{K}^{-}(0.68) \\ \Xi^{0}\pi^{-}(0.24) \end{cases}$$

B€SⅢ

- Compute 4-vectors from reconstructed tracks
- Particle identification
- Particle selection
- Vertex fit (geometry)
- Optimisation of cut criteria
- Extract number of particles using mass plots
- Analysis of a high number of decay channels for an inclusive study requires many calculations → high performance required
- Single-Core Software in C++
- Cluster of ~10 k cores used and shared with other collaborations
- Local analysis of processed with ROOT

The BESIII Offline Software System (BOSS) is developed on the operating system of Scientific Linux CERN (SLC), using C++ language and GAUDI framework. The software uses some external HEP libraries such as CERNLIB, CLHEP, ROOT, Geant4 etc. The CMT is used as the software configuration management tool. MYSQL is used as database server.

http://english.ihep.cas.cn/bes/doc/2247.html

CP violation in charm physics

Serena Maccolini

19° Efficient Scientific Computing School October 21, 2019 - Bertinoro (FC)

CP violation

- CP is the combination of the charge conjugation C and parity transformation P
- If there is a difference between the ways nature treats matter and antimatter then CP is violated

 In our **universe**: matter is more abundant (baryon asymmetry)

The Standard Model

 The Standard Model (SM) describes three of the four known fundamental forces (the *electromagnetic*, *strong*, and *weak* interactions, and not including the gravitational force)

 Elementary particles include bosons (force carriers, *e.g. Higgs* particle or *gamma* rays) and **fermions** (matter and antimatter, *e.g. electrons* or *quarks*)

Why study charm physics?

- *CP* is naturally violated in weak interactions of *quarks* <u>but</u> the amount of baryon asymmetry which can be produced is too small
 → we hope that *CP*-violating **new physics** (NP) exists and we are looking for it
- The best way to search for NP is to study decays of particles containing the quark charm where small CP asymmetries are expected
- This year, CP violation in charm has been finally observed by the LHCb experiment!

The result is *compatible* with SM predictions but contributions from NP cannot be excluded at the moment. For this reason **more experimental inputs** are needed for theoretical tests.

Direct CP violation

Corresponds to

$$\mathcal{A}_{CP} = \frac{|A_f|^2 - |\bar{A}_{\bar{f}}|^2}{|A_f|^2 + |\bar{A}_{\bar{f}}|^2} \neq 0$$

 Most promising channels are suppressed decays where underlying physics could hide CP-violating interactions

Experimentally...

• *Raw asymmetry* between the **observed** yields:

$$A(D \to f) = \frac{N(D \to f) - N(\bar{D} \to \bar{f})}{N(D \to f) + N(\bar{D} \to \bar{f})}$$

Contributions other than Acp

Production asymmetry Detection asymmetry
$$A_P(D) = \frac{\sigma(D) - \sigma(\bar{D})}{\sigma(D) + \sigma(\bar{D})} \qquad A_D(f) = \frac{\epsilon(f) - \epsilon(\bar{f})}{\epsilon(f) + \epsilon(\bar{f})}$$

 The tough part is exploiting known decays (control channels) to correct these contributions and isolate A_{CP}

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Where is the computing?

- Computing power is becoming a limiting factor:
 - Need to handle huge data samples (hundreds of millions events)
 → efficient memory usage
 - Need to solve maximum likelihood estimation (MLE) problems with complicated probability density functions (PDFs)s → run on graphics processing units (GPUs)

Fit with "only" 55 free parameters and needs about 12 hours to be completed on a single CPU





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A new ECAL for LHCb experiment

Daniele Manuzzi 11th ESC, 20-26 October 2019, Bertinoro (IT)

The Large Hadron Collider







Frontier of energy



Frontier of "luminosity"



LHCb experiment



A new ECAL for LHCb experiment





LHCb experiment





A new ECAL for LHCb experiment





Electromagnetic Calorimeter



- Problems for the future: Radiation hardness • Overlapping showers Large combinatoric background
- Future ECAL design: Smaller cell size O Smaller Moliere's Radius

A new ECAL for LHCb experiment

• It is a wall, made of cells able to detect electrons and photons (identity, position, energy)



- **O** Time information
- New Reco. Algorithms







What I am studying now

Cluster Monitor



A new ECAL for LHCb experiment

t [1/200 ps]



Current Computing tasks

• LHCb:

• Full software trigger *new!* Huge need of resources for simulation

• Me:

- Need to increase the performance of my code (time and memory consuming jobs)
- Learn to write clearer scripts to be integrated in LHCb standard software

A new ECAL for LHCb experiment



