#### GPU APPLICATION IN HEP

#### M. Bauce

Sapienza Università di Roma

October 21, 2013







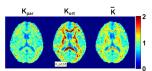
#### The GAP project

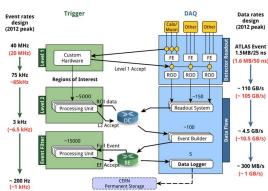


**GAP - GPU application project** for realtime in HEP and medical imaging, funded by the italian ministry of research.

- ► Interest in three different fields:
  - Low Level Trigger systems
  - High Level Trigger systems ◄◄
  - Real-time medical imaging





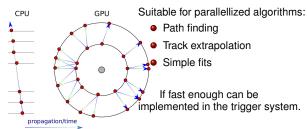


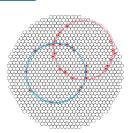
The Atlas trigger



#### Example of applications







### NA62 Low Level Trigger ring reconstruction from Cherenkov detector: $\sim$ 50 ns/ring at L0, $\sim$ 1.5 $\mu \rm s/event$ at L1



#### Alice HLTrigger

- Input: 300 Hz 30 GB/s
- 20k tracks to reconstruct
- All track reconstruction:
   CPU: 1 s → GPU: 300 ms

### Who i am?

### Riccardo Biondi

Born in Matelica (Mc), 26 years old, always fascinated by science and computers since i was i child, so i decided to be a physicist

### **Academic path:**

- Studied high energy theoretical physics at Università "La Sapienza" in Rome
- Final thesis on: neutrinoless double beta decay
- A numerical computation of nuclear matrix element
- Realistic description of neutron-neutron correlation function

### **PhD** Activity

### PhD student ad università dell'Aquila

- Phenomenology of Sterile Active Neutrino oscillations
- Dark Matter: Mirror Dark Matter models
- Phenomenology of Mirror Standard neutron oscillations
- Data analysis of UCN trapping experiment ad ILL

### Why am i here?

In my activity as PhD student i have to work with tools like:

- Numerical computation
- Experimental data Analysis
- Montecarlo simulations

I am here to improve my abilities in scientific computing and to learn new methodologies to use in my research activities.

#### A fast overview of ...

### New PFA techniques for Jet Energy Resolution improvement toward the ILC experiment. Preliminary study of the e+e- $\rightarrow$ H Z channel

#### Eté Rémi

Claude Bernard University Lyon 1 - Institut de Physique Nucléaire de Lyon (IPNL)

October 21th, 2013

**ESC 13** 







#### ILC experiment and the ILD detector

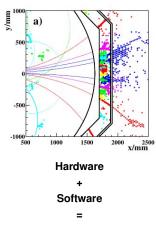
ILC : International Linear Collider ILD : International Large Detector

Particle Flow Algorithm: Global reconstruction algorithm that follows the particle through the entire detector and measure a given physical quantity in the most appropriated sub detector.

For instance: Measure the momentum in the Tracker (TPC) and the energy of particles in the calorimeters

Current reconstruction code, PandoraPFA:

- Follows the tracks from the TPC and find measure the energy of each particle in the calorimeters (ECal + Hcal).
- Cluster the remaining neutral fragments.
- Loop over the parameters of clustering algorithms and find the best configurations.



Particle Flow Algorithm!

Need a new reconstruction approach mainly for two reasons :

- Need at least one other reconstruction software to validate the event reconstruction
- A higher granularity can help to separate the contributions of the different particles in a better way → new clustering methods

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Studying the separation capability in the SDHCAL using new algorithms

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#### My PhD thesis consists in:

- Studying the separation capability in the SDHCAL using new algorithms
- Studying the efficiency of these algorithms in the ILD full detector and its impact on the jet energy resolution
- Apply this set of algorithms on a physics channel : e+e- → H Z and compare it with PandoraPFA

#### Why ESC13?

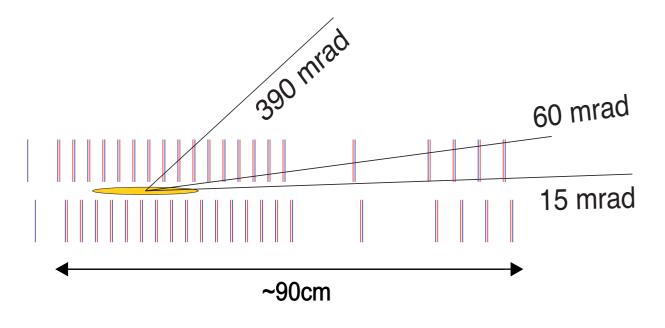
- Need a lot of C++ development and the code has to be really efficient!
- Parallel computing is more than needed. Thousands of calorimeter hits per event for the smallest energy of ILC!
- This school could help me for future choices after the PhD
- I like programming and this is best reason why I should come! ©

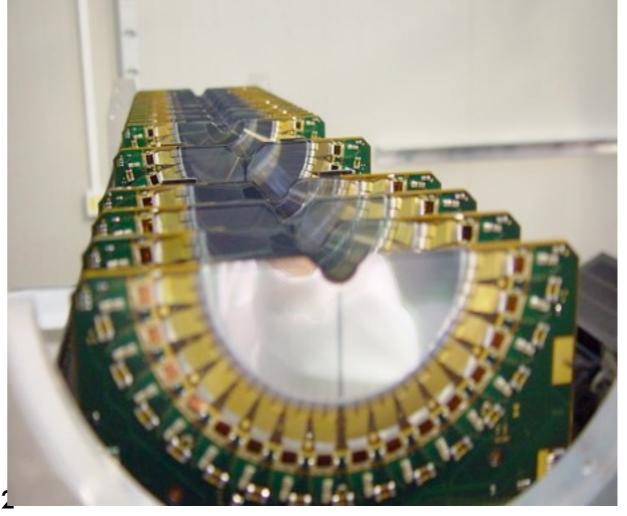
# Stefano Gallorini - University of Padua -

- I'm a member of the LHCb collaboration
- Part of my activity is dedicated to the porting of the tracking algorithm used in the High Level Trigger (HLT) to GPU

The algorithm reconstructs tracks inside the

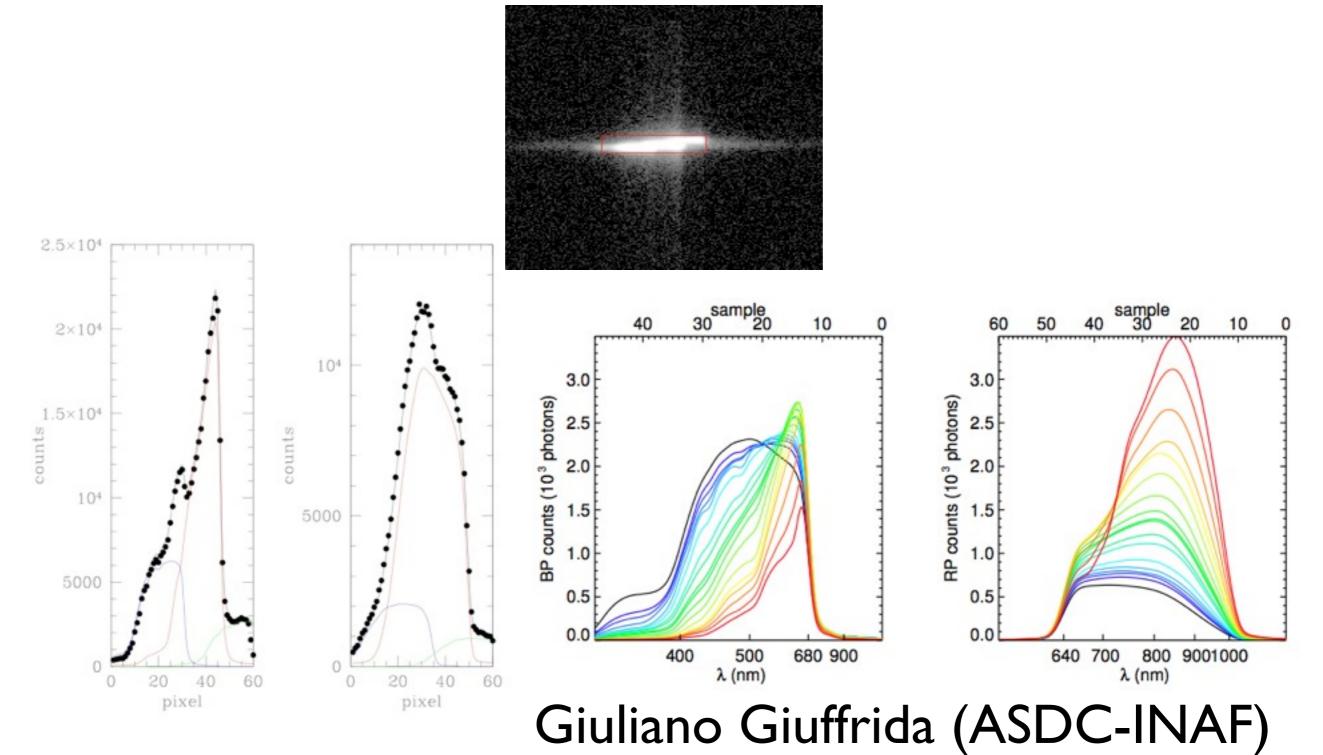
**VELO** detector





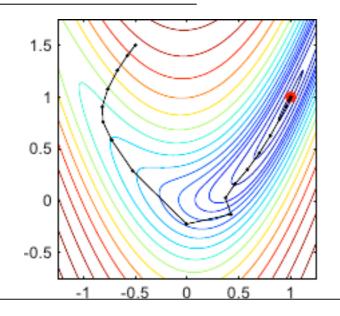
- In a future upgrade of the experiment, the use of GPUs in the HLT will allow to reduce computing time and implement more sophisticated selection algorithms
- Main requirements: high tracking efficiency > 99%, latency of few ms
- In Padua we have 2 GPUs (NVidia Titan & Tesla M2050). The work is just started...

# Gaia BP/RP Deblending



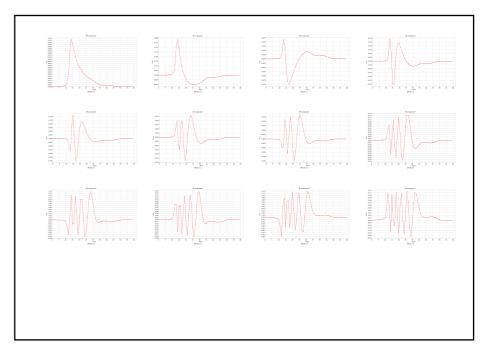
# Gaia BP/RP Deblending

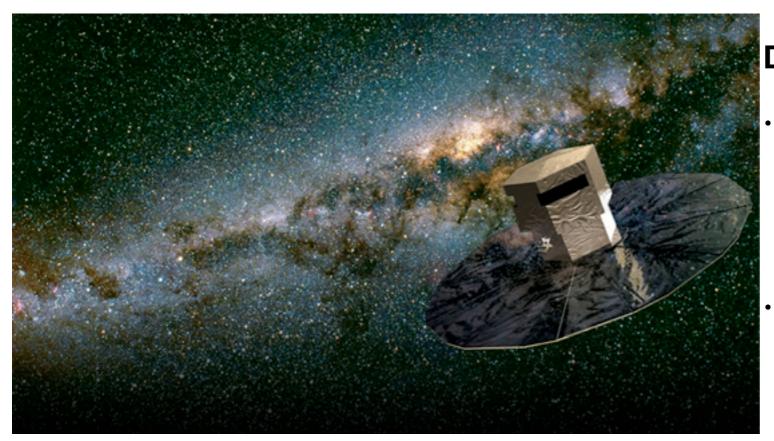
```
Algorithm 5: Levenberg-Marquardt algorithm
     input : f : \mathbb{R}^n \to \mathbb{R} a function such that f(\mathbf{x}) = \sum_{i=1}^m (f_i(\mathbf{x}))^2
                      where all the f_i are differentiable functions from \mathbb{R}^n to \mathbb{R}
                      \mathbf{x}^{(0)} an initial solution
     output: \mathbf{x}^*, a local minimum of the cost function f.
 1 begin
            k \leftarrow 0:
            \lambda \leftarrow \max \operatorname{diag}(\mathbf{J}^{\mathsf{T}}\mathbf{J});
           \mathbf{x} \leftarrow \mathbf{x}^{(0)};
           while STOP-CRIT and (k < k_{max}) do
                  Find \delta such that (\mathbf{J}^{\mathsf{T}}\mathbf{J} + \lambda \operatorname{diag}(\mathbf{J}^{\mathsf{T}}\mathbf{J}))\delta = \mathbf{J}^{\mathsf{T}}\mathbf{f};
                   \mathbf{x}' \leftarrow \mathbf{x} + \boldsymbol{\delta}:
                  if f(x') < f(x) then
                        \mathbf{x} \leftarrow \mathbf{x}';
 9
                      \lambda \leftarrow \frac{\lambda}{\nu};
10
11
                      \lambda \leftarrow \nu \lambda;
12
                  k \leftarrow k + 1;
13
            return x
14
15 end
```



### PCA Principal Component Analysis

$$S(pix) = \sum_{i=1}^{N} b_i * B_i(pix)$$





### Data set size:

- Entire sky scanned 70 times for 1 billion objects
  - images collected 10<sup>12</sup>
  - number of seconds processing time 108
  - collected data 150 Terabyte
  - total archive 1 Petabyte
- Nflops 10<sup>20</sup>–10<sup>21</sup>



NOSQL
Document oriented
Flexible "schemas"
Wire Protocol
Fast & Scalable
GeoIndexing



### Data analysis activity @ Borexino Experiment

Francesco Lombardi ESC13 - School Bertinoro 21-26 Oct 2013

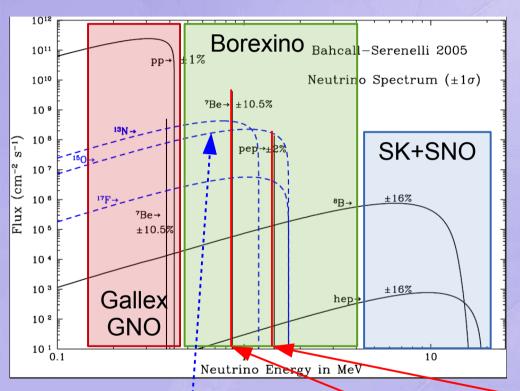
The Measurement of the CNO's neutrino fluxes with Borexino in very low S/N ratio conditions.



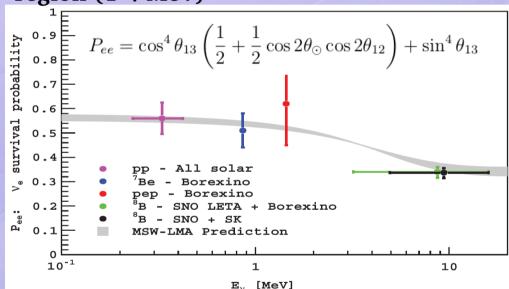
### Neutrino Fluxes Measurement (My Present Activity)



#### Solar Neutrino Fluxes from SSM



Measurement of the oscillation probability predicted by MSW theory. Borexino put the first point close the transition energy region (1-4 MeV)



New task, extremely challenge, will be to make the CNO's neutrino fluxes measurement.

The EXPECTED count rates are:

$$\Phi_{CNO}$$
 = 5.3 [cpd/100ton] from High-Z SM

$$\Phi_{\text{CNO}}$$
 = 3.8 [cpd/100ton] from Low-Z SM

SM=Solar Model

First Measurement of *pep* neutrino flux in  $\Phi_{pep} = 3.1 \pm_{(stat)} 0.5 \pm_{(sys)} 0.2 \text{ [cpd/100ton]}$ 

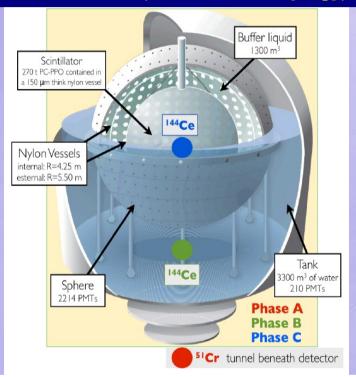
Measurement of *Be7* neutrino flux in  $\Phi_{\text{Be7}} = 46 \pm_{\text{(stat)}} 1.5 \pm_{\text{(svs)}} 1.6 \text{ [cpd/100ton]}$ 

## New prospective for data analysis and simulations with Parallel/Distributed calculations for SOX project



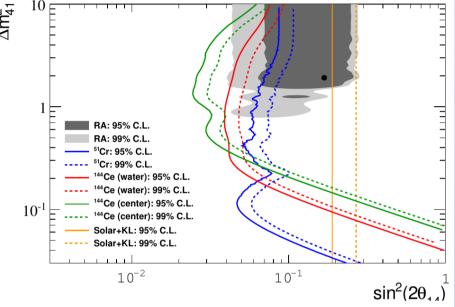
Simulation of a huge number of events (~10<sup>17</sup> events/sec)

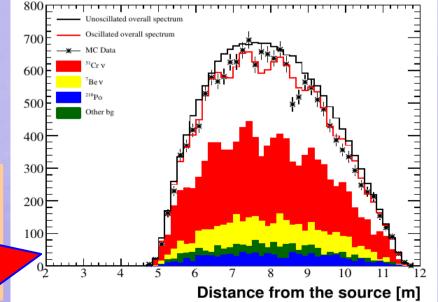
from source (<sup>51</sup>Cr A=200-400[PBq])



$$P_{ee} = 1 - \sin^2 2\theta_{14} \sin^2 \frac{1.27\Delta m_{41}^2 (eV^2)L(m)}{E(MeV)}$$

First Simulation of the Expected counts rate for anti-n moving the 51Cr source from Borexino center at 0.7MeV. The disappearance of anti-n expected is due to the existence of 4th neutrino family: the sterile neutrinos.







### Chemistry @ SNS

DREAMS is a Computational Chemistry and Biophysics group led by Prof. Vincenzo Barone. Research topics include:

- · ab initio methods, in particular models based on density functional theory (DFT)
- · <u>hybrid QM / QM and QM / MM methods, in both static and dynamic formulations</u>
- · Computational spectroscopy (electronic, vibrational, NMR, EPR ...)
- · molecular mechanics and classical molecular dynamics
- · ab initio dynamics, with specific focus on the "Atom centered Density Matrix Propagation"
- · Coarse-graining
- technological expertise for configuring and fully exploiting resources for high-performance computing and "grid" computing
- · Design of polymeric and nano-structured materials (in collaboration with the CNR)
- · Computational modeling of materials and meta-materials (in collaboration with INSTM)
- · Computational spectroscopy (in collaboration with LENS)
- · Computational modeling for cultural heritage and the 'soft matter' (in collaboration with CSGI)

Giordano Mancini Scuola Normale Superiore Pisa, Italy









### What I (try to) do (1)

### My research interests:

- 1)Development and implementation of algorithms for classical Molecular Dynamics, including polarizable force fields, NPBC and enhanced sampling
- 2)MD simulations of biological polymers (proteins, nucleic acids) and artificial molecular devices

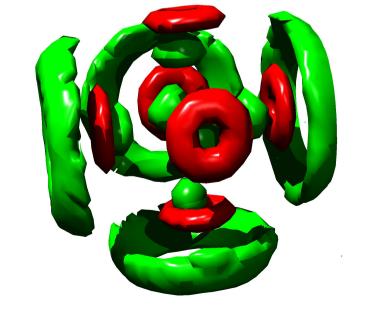
Coupling the Fluctuating Charge method, non periodic boundary conditions and enhanced sampling: aqua ions as case studies.

In preparation for J. Chem. Theor. Comput.

Giordano Mancini Scuola Normale Superiore Pisa, Italy

### **Acknowledgments:**

Prof. Vincenzo Barone Dr. Giuseppe Brancato Dr. Filippo Lipparini





### What I (try to) do (2)

MD simulations of biological enzymes: Cytochrome P450 2B4 versus F429H Mutant: New

Insights from Molecular Dynamics Simulations.

In preparation for J. Phys Chem. B

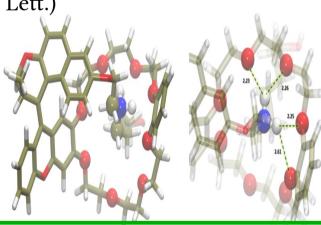
### **Acknowledgments:**

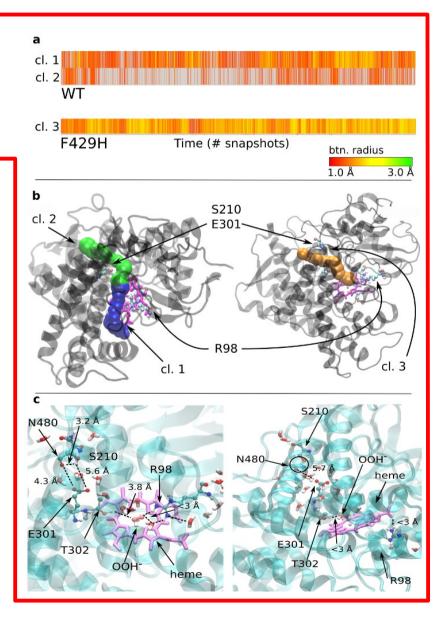
Prof. Vincenzo Barone
Dr. Giuseppe
Brancato
Dr. Costantino Zazza
Prof. Sason Shaik\*
Dr. Dandamundi\*
Usharani

Giordano Mancini Scuola Normale Superiore Pisa, Italy

#### Molecular Devices:

In silico study of molecular engineered nanodevices: a lockable light-driven motor in dichloromethane solution. (Submitted to J. Phys Chem Lett.)



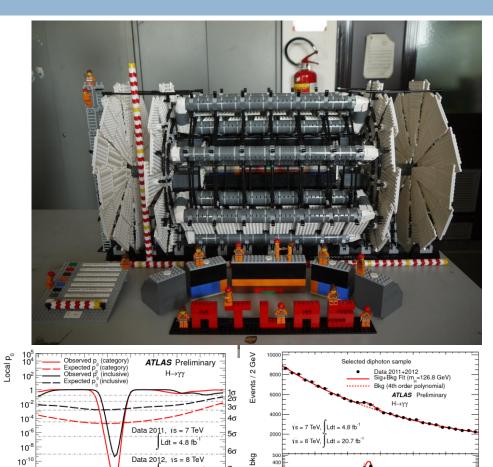


<sup>\*</sup>Institute of Chemistry and Lise Meitner-Minerva Center for Computational Quantum Chemistry, Hebrew University of Jerusalem

## HIGH ENERGY PARTICLE SEARCH AND TOOLS FOR ANALYSIS

### High energy physics research projects

- ATLAS collaboration
- Search of the Higgs boson in the diphoton plus missing transverse energy channel
  - Cutflow analysis (Event selection)
  - Performance of missing transverse energy
  - Higgs signal model fit (simultaneous fit using RooFit)
  - Building of background montecarlo model
  - Statistical analysis (maximum likelihood)
- Higgs mass precision measurement on the di-photon channel
- Future projects: search of graviton resonances in the di-photon channel
  - Randall-Sundrum and ADD model



17/10/2013

ATLAS-CONF-2013-012

120 125 130 135 140 145

ATLAS-CONF-2013-012

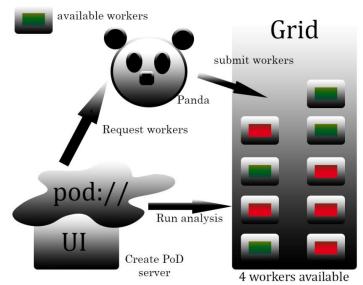
Simone Mazza - ESC13

### Particle physics analysis and computing resources

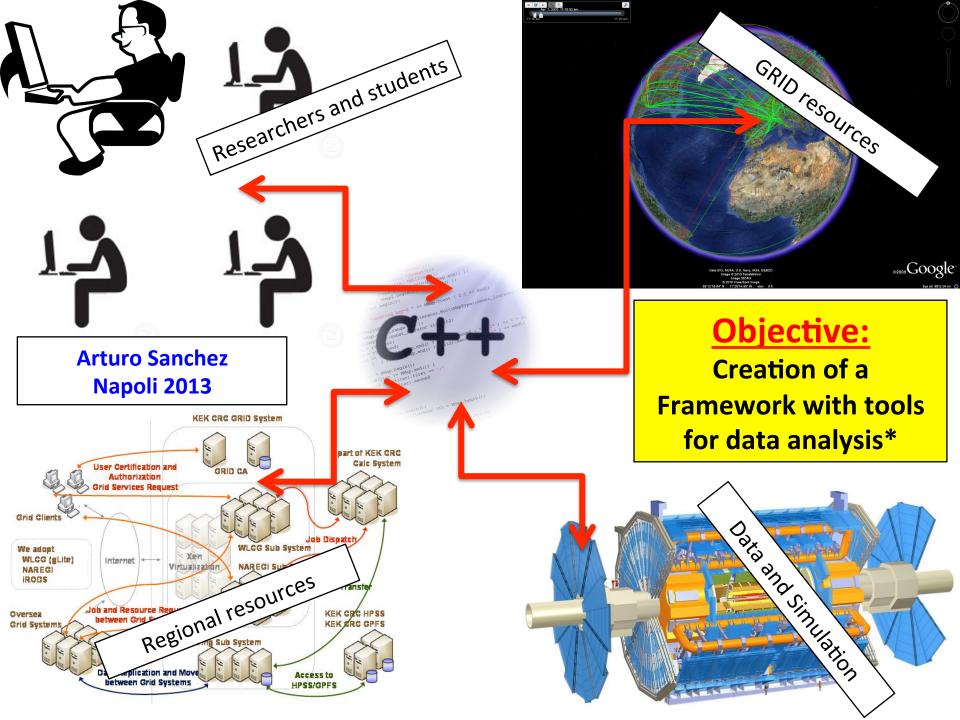
- Most of the time we have to analize huge amount of data that are placed somewere in the world (grid). To speed up the process we can
  - Send request for local copy and analyze locally: one core analysis, multicore analysis, local proof cluster
  - Send analysis job to the grid (where the datasets are) with a standard grid request
  - Pre-skimming of data on the grid, then copy and analyze locally
- Data analysis is a simple problem to parallelize
  - Few hundreds of operation for each event
- Optimizations
  - General code optimization
  - Proof/Prooflite for multicore analysis: computer clusters to analize data using proof (Milano: 192 cores)
  - Optimized data access (D3PDReader)
- What to do next?
  - OpenMP, MPI optimization
  - GPU analysis

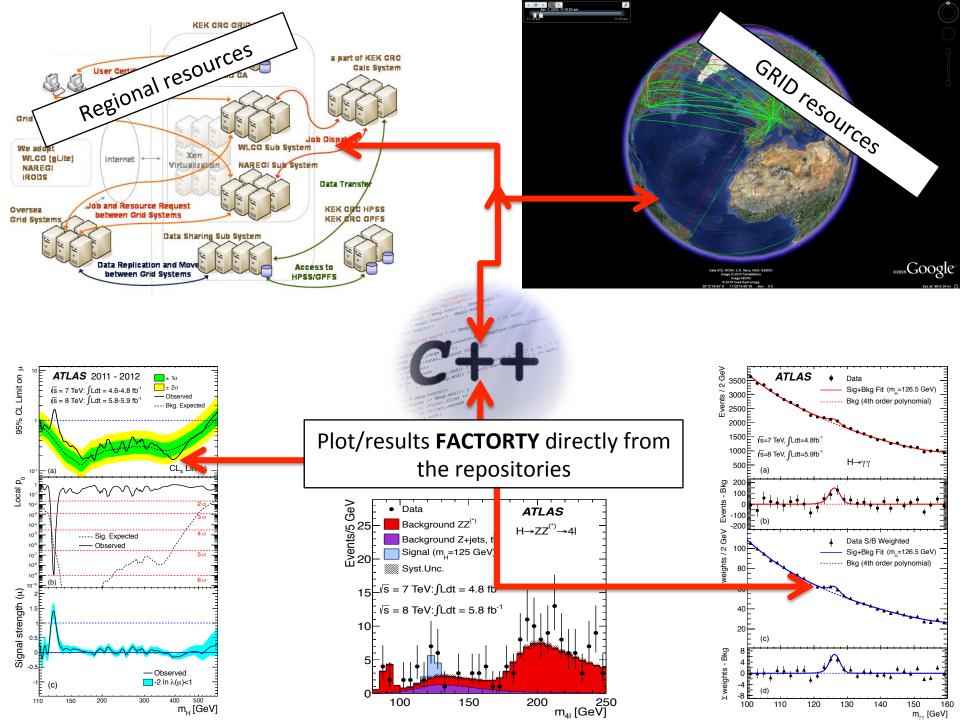
### Analysis test in a Grid facilities with the PanDA plugin for PoD

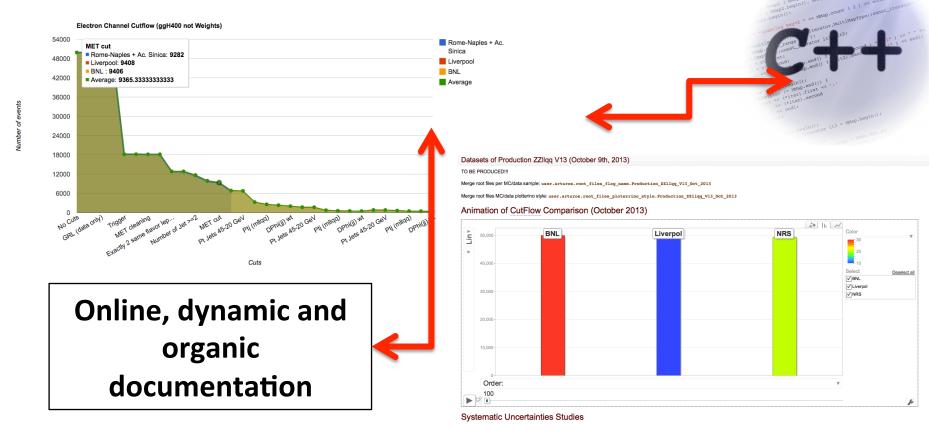
- Proof on Demand allows to enable a PROOF cluster on the Grid requesting workers trough Panda.
  - (Panda is the ATLAS workload management system to submit jobs on the grid)
  - We were able to obtain clusters with an high number of workers (up to 300 workers)
- Using a Proof-based analysis with optimized disk access
- Different from normal Grid jobs submitted to PanDA.
  - Once the requested PROOF cluster is available, the PROOFbased analysis can be directly send to the workers from the master (more interactive)
  - Same as a local proof cluster!

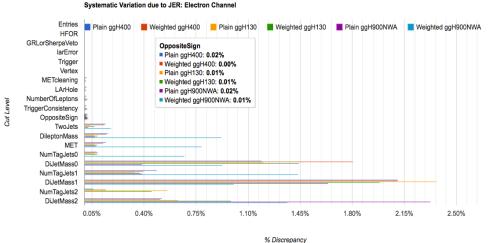


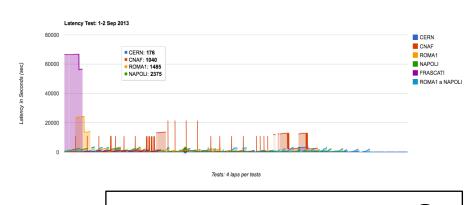
- Clusters can be enabled on any PanDA resource (Italian T2-T3 grid site)
  - Only one analysis (per site) can run at a time
- There are more possibilities
  - Proof based analysis on the proof cluster requested on grid with local data
  - Request workers and run analysis on a cluster where the datasets are
  - Run analysis in one site with data taken from another site via XrootD or http











\*Whatever data is.... ©

### Cristiano Santoni



- Research fellow at University of Perugia (from July 2013)
- Academic degree in computer science at University of Perugia (May 2013)
- Educational Grant at INFN Perugia
   (September 2010 August 2012)

### Scientific Computing experiences and activities

### • Thesis:

 Development of a GPU-based solver for Answer Set Programming

### Research:

- Feasibility study for integration of GPUcomputing and RTOS
- Development of GPU-based trigger algorithms for RICH and Charged Hodoscope detectors

(NA62 experiment and KLEVER project)

### Others activities

### Current:

 Design and development of a low level (L0) trigger algorithm for RICH and Charged Hodoscope detectors (NA62), based on multiplicity and average hit time, able to operate at tens of MHz

### • Past:

 Firmware development for various FPGAbased TDAQ systems for sensors (CMOS pixel, SiPM) readout

### **CRISTINA TRONCONI**

I work as an engineer at the Institute of
Atmospheric Sciences and Climate (ISAC) of the
Italian National Research Council (CNR) actively
collaborating with the Satellite
Oceanography Group.

I'm currently involved in the framework of national and international projects (MyOcean and SeaDatanet) whose main aim is the "Realization of European Interoperability in Ocean Science"



### Within these projects my work consists of:

- Development of satellite oceanographic remote sensing data applications based on grid infrastructure, in particular for what concerns SST (Sea Surface Temperature) data and Management of TDS (THREDDS Data Server)
- Optimization and parallelization of data processing chains
- Re-engineering of old processing chains
- Harmonisation of Data format (NetCDF) in the framework of the "Realization of European Interoperability"



### I'm deeply interested in this School in order to Improving:

- my skill in Software optimisation and Parallelisation,
- the knowledge of new Parallel programming techniques
- the perfomances of C++ codes

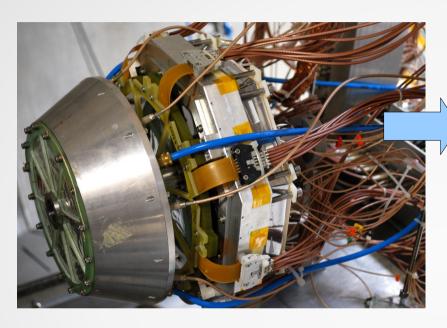




### Simone Valdré

- I graduated in Physics at Università degli Studi di Firenze in December 2009 and took the Master's degree in October 2012.
  - I did my thesis works inside an experimental nuclear physics collaboration (Nucl-Ex / FAZIA)
- Now I'm a PhD student at Università degli Studi di Firenze
  - I'm still working inside the Nucl-Ex / FAZIA collaboration
  - During the first year of PhD I took a course on programming in kernel space
- I've always been attracted by programming and I write simple programs for personal interest since I was young.

### Simone Valdré



- In our collaboration we use C++ programs to analyze data and to do simulations
- I work daily on the code to perform more advanced data analysis

```
class GAWorker GarfParticleMull: public GAWorker{
 GAWorker GarfParticleMull();
  //! In this method all the modules and aliases must be initialized.
  //! The list all modules in is ready and can be used.
  //! The list all modules out must be filled with ALL the parameters except
  //! name and connection, that will be adjusted later by GAAnalisi
  virtual int Init():
  //! this function will be called at the beginning of each run.
  //! it is a good place to load the calibration values.
  virtual int InitRun(char *run num);
  //! in this method data is processed.
  //! you can use the GAVirtualModule::is fired to see which of the
  //! input module(s) have been fired.
  //! don't forget to set is fired to 1 to the relevant output modules.
  //! IMPORTANT NOTE: you MUST manually reset all the output modules
        quantities that you do not compute!!! For example, if you use
        a GAVModule Ion, but you cannot identify the mass:
        ion->A=-1; ion->quality A=0;
  virtual int ProcessData();
 virtual ~GAWorker GarfParticleMull();
```

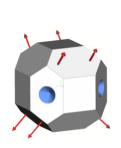
ESC13 - Bertinoro, 21-26/10/2013

### Simone Valdré

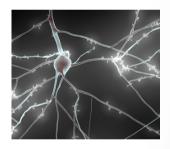
- ODIE is the main tool to calibrate data in our collaboration
  - It's entirely written and maintained in Florence.
  - It heavily uses object oriented features of C++
  - It has a modular structure that could be adapted to various experimental apparatuses
- GEMINI++ is a well known Monte Carlo simulation tool
- I actively contributed to develop a tool to analyze and compare ODIE and GEMINI++ outputs
- Here at ESC13 I expect to learn how to optimize at best our analysis software to improve our research

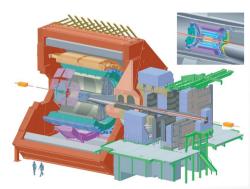
### Barthélémy von Haller

- Swiss, 32 yo, engineer in computer science
- Studied at EPFL (Lausanne)
  - Master on bio-inspired modular robotics
- Work(ed) at
  - CERN IT Administrative tools
    - Large Java web applications and Oracle DBs
  - EPFL Blue / Human Brain project
    - SDK: Common base for simulation, analysis and visualization
    - C++ with Python and Java bindings
  - CERN PH ALICE
    - Data Quality Monitoring (DQM)
    - C++ framework based on ROOT









### Barthélémy von Haller

- CERN PH ALICE (DQM continued)
  - 40 agents, 10000 objects, 1 update per minute
  - 24/7 use by DQM shifter
  - $\rightarrow$  Can we make our code better?
    - → Improve our practices & procedures ?
  - Analysis is demanding
  - → can we parallelize ? How ?
- ALICE Online-Offline framework (O2)
  - 2018/19 LHC 2<sup>nd</sup> Long Shutdown
  - Upgrade of several detectors -> continuous readout electronics for TPC and ITS
  - Architecture and R&D -> TDR -> Implementation

