Employing HPC for Heterogeneous HEP Data Processing

AUGUST 2018

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Project Specification

project specification

Abstract

THIS IS MY ABSTRACT

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1. From physics to... Physics

Modern **High energy physics** (HEP) experiments require complex multistage infrastructure. To realize them several large scale objects are needed: from accelerators, detectors, data centers to the thousands of people involved to design and run the infrastructure.
The entry point of any **Large hadron collider** (LHC) experiment is the collision between proton-proton beams (although Pb beams are used) which trigger various physical processes. There are two kinds of processes, those that are not yet observed (**X**) and the observed ones (**Y**). The objective of LHC experiments is to expand our knowledge about elementary physical processes governing the universe by studying **X** through the observable particles that it produces. Unfortunately, interesting processes are quite rare, thus a huge amount of collisions are needed to produce one of them.
This creates a lot of difficult and interesting IT challenges because everything from data acquisition to data analysis has to scale to meet throughput and timing requirements. Faster data are processed, more collisions can be triggered quicker the research can proceed.
As computer scientists, our purpose here at CERN is to accelerate data processing by best exploiting the resources at our disposal, achieving the maximum efficiency using smart and creative approaches, in particular targeting **High Performance Computing** (HPC) environment.
The LHC infrastructure is designed to process huge amounts of data (hundreds of Pb/s). The data flow architecture illustrated in figure 1.1 is organized in four main stages. Staring from physical processes to the physics carried out by analyzing the data, with data acquisition and processing in the middle. Each of this step is complex and deserves a dedicated explanation.

Data generation The process starts with **particle collisions** this lead to particle interactions that create some **intermediate product**. This intermediate product can not be directly observed, bit it decays in **particles** that go through the detectors. This ones measure the charge of this particles. At the current time, this process is repeated every $25ns$. All data that is produced the sensor present installed inside the detectors is sent to the next level without any king of filtering operation.

Data aquisition Detectors are split in two levels: **physics detector level** and **electronics level**. The physics level takes in input sensor readouts and produces an analog signal. This analog signal is the digitalized by the electronics level. At this point data are too much to send them to the next stage. Models are used to distinguish between X and Y. Since these model are complex and the timing constraints are very strict, only a simplified version of them is implemented directly in hardware, on top of **asic**s and **fpga**s boards. Because the models are simplified there are a lot of Y events labeled as X.
The event that survive this first stage ends up dumped into **disks** and send to the **High Level Trigger** (HLT).
The HLT has more relaxed time constraints since it receive less events and his job is to distinguish between X and Y exploiting, a simplified implementation of the models, but with more feature with respect to the previous stage that allows more precise evaluations. Another important characteristic of the HLT is that is implemented in software and executed on a CPU based cluster with accelerators such as GPUs and FPGAs present in the hosts.

Data processing At this point, data that survive to all the triggers is used here to generate a dataset used for analytics purposes. To build this dataset the same models deployed inside the triggers are used, but with way more features. To extrapolate useful information and build the dataset **raw data** are sent through a complex multistage processing pipeline. This pipeline is offline so it does not share the timing constraints of the previous stage but, efficient exploitation of resources is needed because even after all the filtering data is still huge and models are very complex.
The first stage, called **local reconstruction**, transforms charges in physical quantities such as **energy**, **time**, and **position**. This operation is done channel by channel. This channels are independent form each other thus, this is an Embarrassingly parallel problem. This parallelism is exploited though multi-threading running this code on a cluster of multi-core machines, although other parallel architectures, such as GPUs, are currently tested to deploy them in future upgrades. Then, information coming from different channel of the same detector are combined by the **cross channel clustering** into **local detector cluster**s. The final step needed to obtain **particle object**s is the **cross detector clustering** in which data coming from different detector is combined. In the end, some particle object built. The set of all this particle objects forms the dataset used to push our understanding of physics over the horizon.

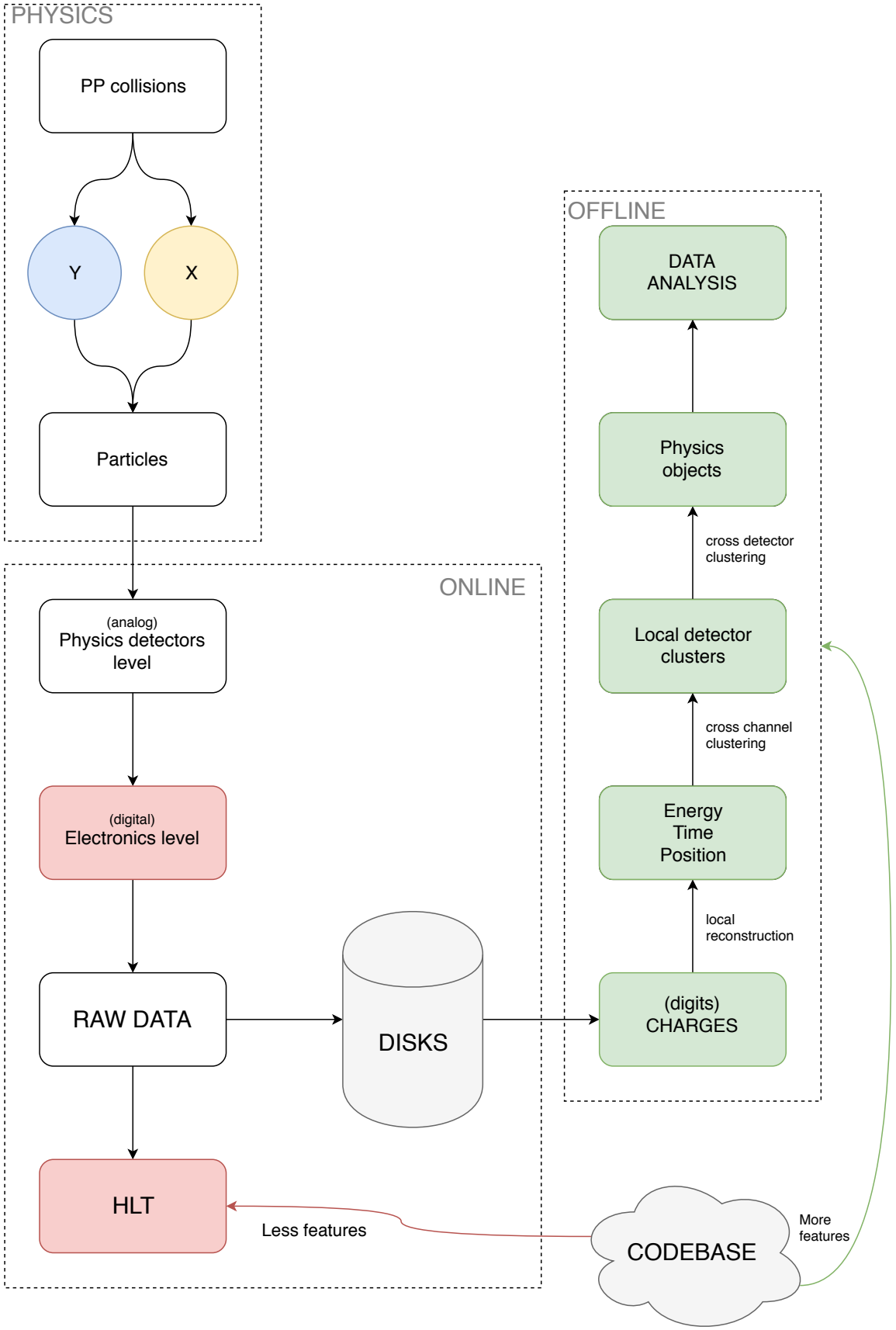
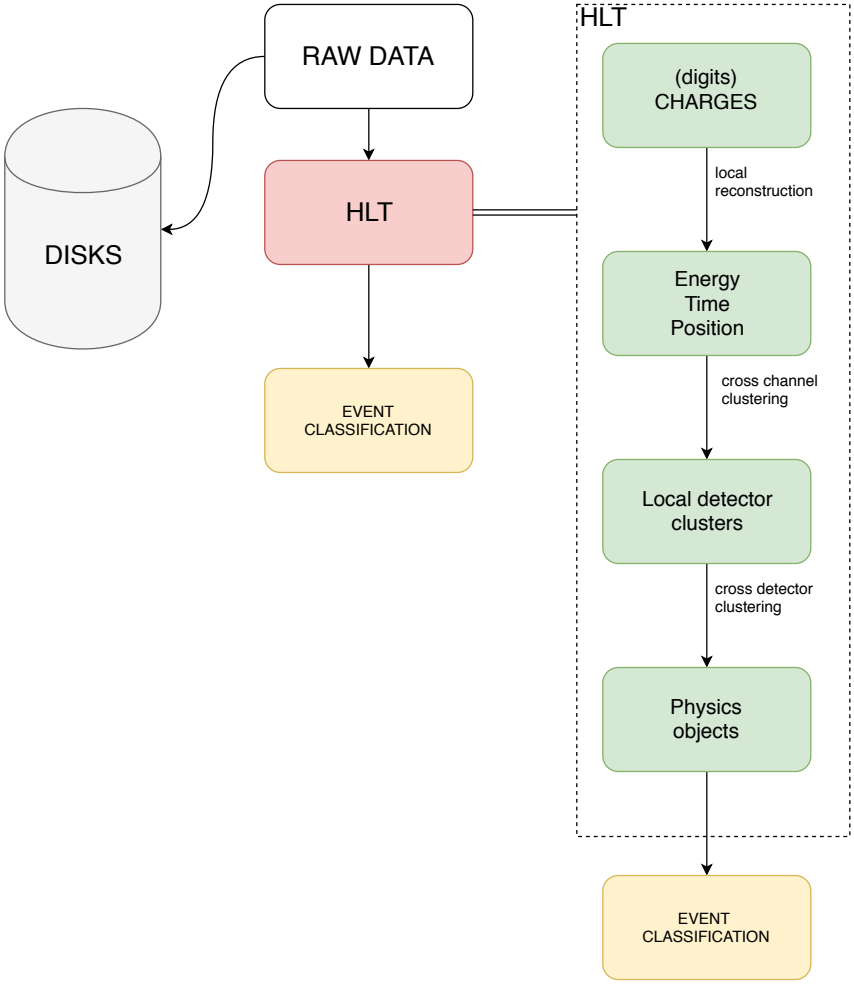


Figure 1.1: Cern data flow from collisions to analysis

2. Local energy reconstruction

The HLT shares the same code used for offline data processing, thus the processing pipeline is more or less the same. The fundamental difference is that the output is used to perform event classification instead of data analysis. The table 2.1 shows how much time is spent in every

Figure 2.1: HLT processing pipeline



single step of the reconstruction process. Most of it is spent into tracking but after it, the second more time consuming step is HCAL+ECAL local reconstruction that takes $113ms$ corresponding to 24% of the total time. Given the time needed to perform this reconstruction even achieving a speedup of two would reduce the total processing time of more than 10%. This is my focus in this project try to reduce it as much as possible.

Figure 2.2: Data processing time share

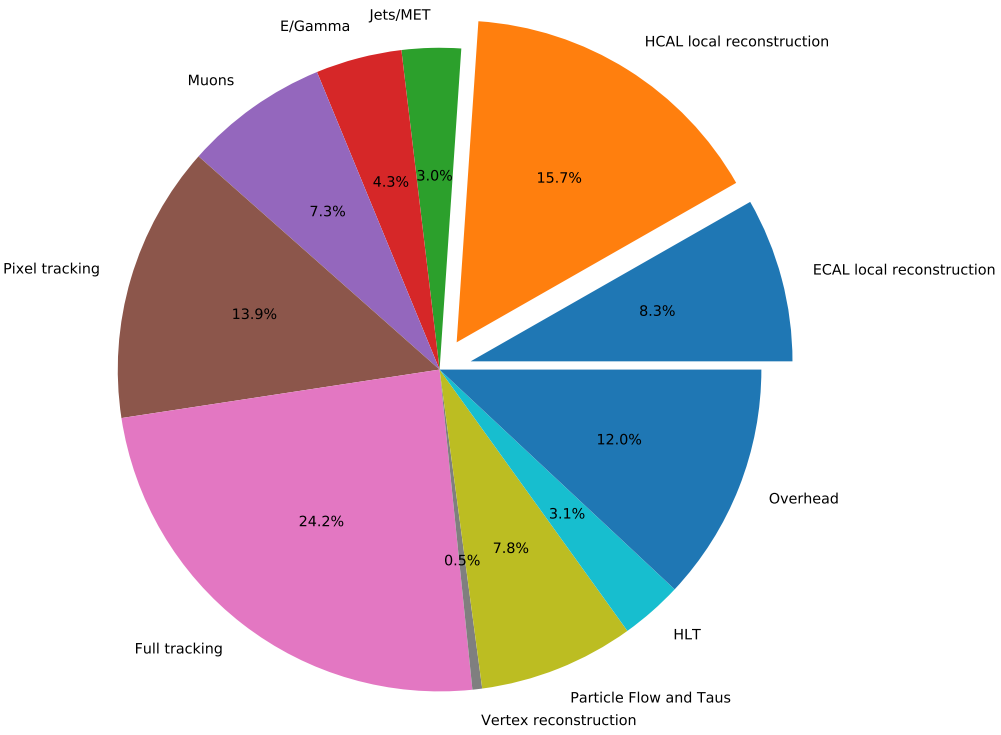


Table 2.1: Time spent into the various HLT reconstruction steps

Step	Real-Time	Percentage
ECAL local reconstruction	38.9 ms	8.25%
HCAL local reconstruction	73.9 ms	15.67%
Jets/MET	14 ms	2.97%
E/Gamma	20.4 ms	4.33%
Muons	34.2 ms	7.25%
Pixel tracking	65.7 ms	13.93%
Full tracking	114.2 ms	24.22%
Vertex reconstruction	2.3 ms	0.49%
Particle Flow and Taus	36.8 ms	7.8%
HLT	14.7 ms	3.12%
Overhead	56.4 ms	11.96%
Total	471.5 ms	100%

2.1 Problem statement

For each channel {given n charge readouts $\rightarrow$ reconstruct the energy}.

$$\begin{aligned} &\min(\chi^2) = \arg min_x(\|Px - b\|^2) \\ &\forall i : x_i \geq 0 \\ &\text{where:} \\ &\quad x = \text{energy vector} \\ &\quad P : ENERGY \rightarrow CHARGE = \text{feature matrix} \\ &\quad b = \text{charge vector} \\ &\quad n = 10 \text{ (in this particular case)} \end{aligned} \tag{2.1}$$

Which is a standard minχ^2 problem with additional positivity constraints. This constraint is present because physically speaking negative energy does not make sense.
As shown in [1] the statement above is incomplete. A perfect mapping from charges to energy does not exist because signal from the shower does not dissipate within one time slice ($25ns$). Adding the correlation term this problem becomes:

$$\begin{aligned} &\arg min_x(\left\|(Px - b)^T \Sigma(x)^{-1}(Px - b)\right\|^2) \\ &\forall x : x \geq 0 \end{aligned} \tag{2.2}$$

It is worth pointing out that Σ depends on x, meaning also Σ is unknown.
To compute Σ an iterative procedure is used:

1. Compute Σ.
2. Minimize χ^2.
3. If not convergence goto 1.

More precisely Σ is the covariance matrix representing the noise correlation between time samples i and j, obtained from data where no signal is present, and the single sample noise.
To solve the problem stated in 2.1 several algorithms exists, for example **lsqnonneg** illustrated in [4] and the **ffnls** illustrated in [2]. The one implemented is fnnls since as measured in [3] it is faster.
The problem presented in 2.2 is not a χ^2 problem but to solve it with nnls needs to be reduced into the canonical form. The redution exploits the Cholesky decomposition and is illustrated in 2.3.

$$\begin{aligned} &(Px - b)^T \Sigma(x)^- 1(Px - b) \\ \equiv \quad &\Sigma = LL^T, (AB)^{-1} = B^{-1}A^{-1} \\ &(Px - b)^T L^{-T} L^{-1}(Px - b) \\ \equiv \quad &(AB)^T = B^T A^T \\ &(L^{-1}Px - L^{-1}b)^T L^{-1}(Px - b) \\ \equiv \quad & \\ &(L^{-1}Px - L^{-1}b)^T (L^{-1}Px - L^{-1}b) \\ \equiv \quad &L^{-1}P = P', L^{-1}b = b' \\ &(P'x - b')^T (P'x - b') \end{aligned} \tag{2.3}$$

2.2 Fast non negative least square algorithm (FNNLS)

The nnls is an *active set iterative algorithm*. It uses two sets:

- **Passive set (P)**: the constraint is ”passive”, meaning that it is not satisfied.

- **Active set (R)**: the constraint is ”active”, meaning that it is satisfied.

The pseudo-code presented in algorithm 1, starts with a feasible solution (line 2), then checks for the positivity constraint. If there are some negative components it finds a non negative one that minimize the error, exploiting a gradient (line 5). More details can be found in [4]

Algorithm 1 NNLS

Input:
A real valued matrix of dimension $m \times n$
b real valued vector of dimension m
ϵ the maximum accepted error
K the maximum number of iterations
Output:
x the solution vector

1: **function** NNLS(A, b, ϵ, K)
2: $x \leftarrow 0$
3: $P = \varnothing$
4: $R = \{1, 2, ..., m\}$
5: $w = A^T(b - Ax)$ ▷ compute the gradient
6: **while** $R \neq \varnothing \wedge max(w) < \epsilon \wedge k < K$ **do**
7: $j \leftarrow max(w^P)$ ▷ $w^P \leftarrow \{w_j : j \in P\}$
8: Add j to P
9: Remove j from R
10: $A^P \leftarrow \{a_{ij} \in A : i \in P \wedge j \in P\}$
11: $s \leftarrow ((A^P)^T A^P)^{-1} A^P b^P$ ▷ s is a vector of the same dimension of P
12: **while** $min(s) \leq 0$ **do**
13: $\alpha = min_i\{\frac{x_i}{x_i - s_i} : i \in P \wedge s_i \leq 0\}$
14: $\forall i \in P : x_i \leftarrow x_i + \alpha(s_i - x_i)$
15: move to R all $i \in P : x_i \leftarrow 0$
16: $s \leftarrow ((A^P)^T A^P)^{-1} A^P b^P$ ▷ recompute s for the next iteration
17: $\forall i \in P : x_i = s_i$
18: $w \leftarrow A^T(b - Ax)$
19: $k \leftarrow k + 1$

This algorithm is slow because at each iteration it requires to calculate the pseudo-inverse (line 11). FNNLS, showed in algorithm 2, is faster because it reduces the computational burden of this operation. The idea is simple: instead of projecting the matrix A over P and then performing the transposition and multiplication, it saves $A^T A$ and performs the projection over P. Another operation avoided is the multiplication between A and b, also in this case the multiplication is performed in the preprocessing phase. At runtime, only the projection over P is performed.
This improvements reduces the computational making the it to run faster.

Algorithm 2 FNNLS

1: $w \leftarrow (A^T b)(A^T A)x$
2: $s \leftarrow ((A^T A)^P)^{-1}(A^T b)^P$

2.3 Implementation details

This algorithm has several numerical issues coming from the pseudo-inverse computation (line 11 of pseudo-code 1 and line 2 of pseudo-code 2).
The original definition of the matrix A^P is $A^P = \{A.col(i) : \forall i \in P\} \cup \{0 : \forall i \in R\}$. While the definition of the vector b^P is $b^P = \{b_i : \forall i \in P\} \cup \{0 : \forall i \in R\}$. This results in a $m \times n$ matrix and a m dimensional vector. Calculating the pseudo-inverse with this matrix generates numerical issues, the results is a matrix containing some $-nan$.
One way to solve this problem is to reduce the number of operations needed to perform the computation. To achieve this there are three ways:

1. Invert the matrix through some decomposition.
2. Changing the definition of A^P to reduce the size of the matrix and the vector.
3. Combining both 1 and 2.

Decompositions The decompositions tested are **Cholesky** and **HouseHolder** with and without pivoting. These decompositions has been chosen following the advices present on this page of Eigen documentation. As a result all of them except the HouseHolder with pivoting were numerically unstable. But, the HouseHolder with pivoting is not fast enough to meet the time constraints so, other approaches has been tested.

$\boldsymbol{A^P}$ Observing the computations performed utilizing the original definition I noticed that a lot of useless operations containing 0 were present. Not only this slows down this is overhead but also increases the algorithmic error. Changing the definition to the one provided into the pseudo-code allowed also plain inverse and Cholesky to work without issues.

In the end the Cholesky without pivoting, applied on the modified A^P matrix, was chosen because it is proven in [5] to perform best.

2.4 GPU porting

Until now there are two version ported on GPU, the one taken from *cms-sw* codebase and the one implemented from scratch.
To exploit the parallelism provided by these devices a channel level parallelization is performed but, a dynamic parallelism inside the channel it to be studied.

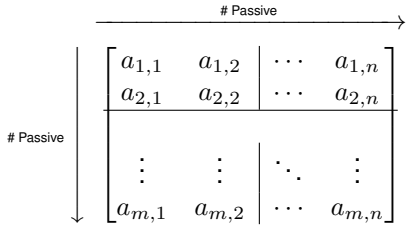
2.5 Optimizations

There are two kind of optimizations performed: numerical and algorithmic. In the first case some mathematical properties are exploited to reduce the number of operations, in the other case some architecture level knowledge is used to speedup the computation.

2.5.1 Numerical

The optimization performed here is to avoid using swap matrices and the P and R vectors. Studying the algorithm it is possible to notice that the P, R partitioning can be obtained in-place by

permuting the matrix A.



$$\begin{array}{c|cc|c} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \hline \vdots & \vdots & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,n} \end{array} \tag{2.4}$$

As shown in 2.4 the passive set grows from the top left corner. The size of this block is the same as P. This way, instead of a vector, a counter is enough to save the active set. Every time a variable enters in the active set the corresponding column and row are swapped accordingly and the $nActive$ counter is incremented.
Both the vector b and x are permuted, because otherwise they would not be aligned with the matrix.
A permutation matrix is used to keep track of all the swapping and the solution is reordered before being returned.
This optimization allows to reduce both memory allocation/de-allocation and cache faults resulting in a performance improvement of a factor of 2, as showed in 3.1.

2.5.2 Algorithmic

The optimization performed here is exploiting some pragmas to vectorise fixed iteration loops and to unroll the others, which have non constant number of iterations.
From the profiling performed can be noted that in case of fixed iteration loops the vectorization gives better performance results respect to the unroll. Also the compiler unroll vectorized loops combining the best of both approaches.
The unroll value has been determined empirically exploiting measurements like branch misprediction and cache faults for each value and used the one that minimize them.

3. Results

3.1 Test01: GPU vs CPU

The results of this test are used as baseline for further optimizations.
Test configuration:

- **CPU**: Intel(R) Core(TM) i7-4770K CPU @ 3.50GHz
- **GPU**: NVIDIA Tesla K40c

Implementations tested:

- **legacy_multifit_cpu**: plain *cms-sw* cpu code.
- **legacy_multifit_gpu**: plain gpu porting *cms-sw* cpu code.
- **multifit_cpu**: inplace fnnls cpu implementation.
- **multifit_gpu**: inplace fnnls gpu implementation.
- **multifit_cpu_swap**: fnnls cpu implementation with swapping matrices.
- **multifit_gpu_swap**: fnnls gpu implementation with swapping matrices.

All the cpu implementations are single-threaded. With 64k channels the GPU version achieves a speedup of 2.6. From 3.1 can be noted that the numerical optimizations allows to achieve a factor

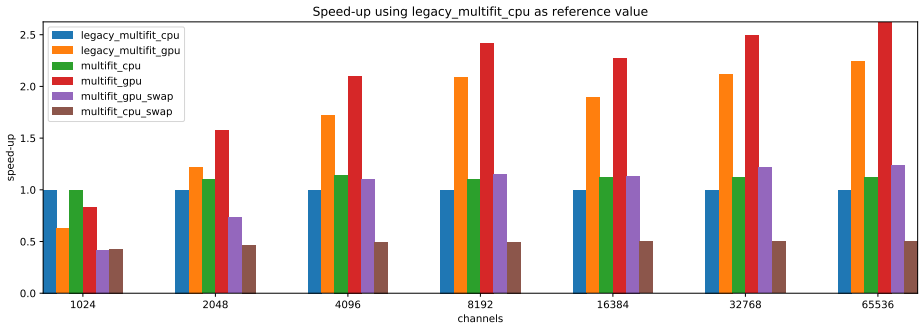


Figure 3.1: Speedup achieved with 10 iterations, log channel scale, higher is better

of 2 in speedup. The GPU performs twice as fast with respect to the CPU. Other optimizations like loop unrolling and branch reduction give a performance gain about 20% in CPU and 30% on GPU. From the plot present in 3.2 can be noted that, on GPU, the time increases faster at the beginning and around 15000 channels there is a change of slope and the increase becomes sub-linear. On the CPU, the increase is linear with respect to the channels. The plot in 3.3 makes more evident the difference between the different version of the algorithm. The GPU outperforms

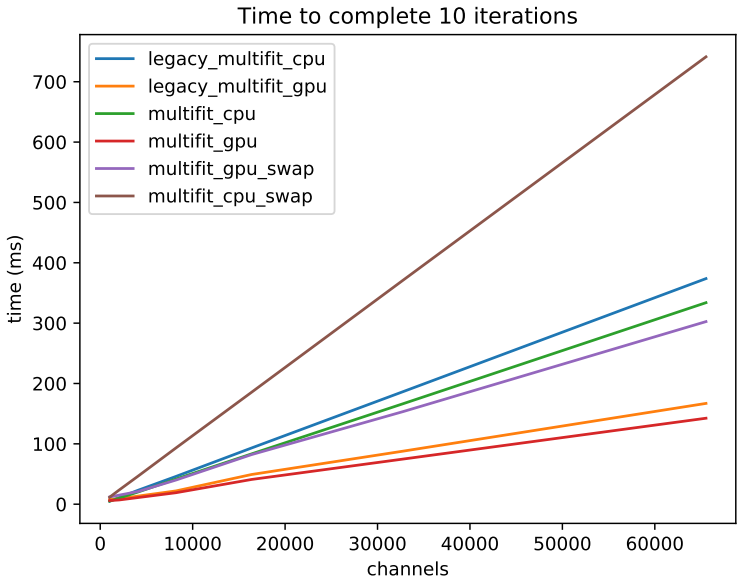


Figure 3.2: Time needed to complete 10 iterations, linear channel scale, lower is better

the CPU and it will be interesting to study what will happen if the number of channels increases even more.

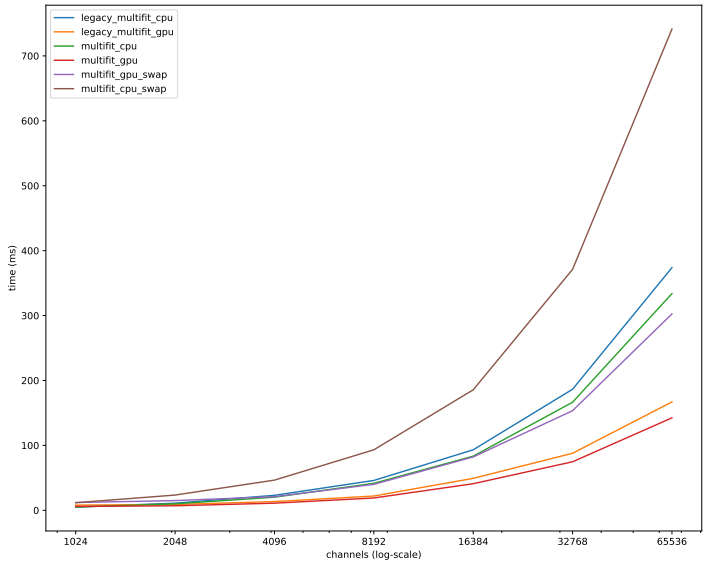


Figure 3.3: Time needed to complete 10 iterations, log channel scale, lower is better

4. Profiling and further optimizations

In order to further optimize the code some profiling is needed to identify the bottleneck and solve them... If possible.

4.1 Finding CPU hotspots

The methodology followed is to use **Intel VTune** on the entire regression. Profiling only the nnls portion of the code did not give reliable results because terminates too fast. Profiling the entire regression instead, gave interesting results; As showed in 4.1 and 4.2 there are two hotspots in the code.

```
48  #endif
49  void inplace_fnnls(const FixedMatrix& A,
50                                      const FixedVector& b,
51                                      FixedVector& x,
52                                      const double eps,
53                                      const unsigned int max_iterations) {          0.0% 0.
54    // Fast NNLS (fnnls) algorithm as per
55    // http://users.wfu.edu/plemmons/papers/Chennnonneg.pdf
56    // page 8
57
58    // FNNLS memorizes the A^T * A and A^T * b to reduce the computation.
59    // The pseudo-inverse obtained has the same numerical problems so
60    // I keep the same decomposition utilized for NNLS.
61
62    // pseudoinverse (A^T * A)^-1 * A^T
63    // this pseudo-inverse has numerical issues
64    // in order to avoid that I substituted the pseudoinverse whit the QR
65    // decomposition
66
67    // I'm substituting the vectors P and R that represents active and passive set
68    // with a boolean vector: if active_set[i] the i belogns to R else to P
69
70    // bool active_set[VECTOR_SIZE];
71    // memset(active_set, true, VECTOR_SIZE * sizeof(bool));
72
73
74    auto nPassive = 0;
75
76    // #ifdef __CUDA_ARCH__
77    // FixedMatrix AtA = transpose_wrapper(A);
78    // #endif
79    // #ifndef __CUDA_ARCH__
80    // FixedMatrix AtA = transpose_multiply(A);
81    // #endif
82    FixedMatrix AtA = A.transpose() * A;                                           37.6% 0
83    // assert(AtA == A.transpose() * A);
84    FixedVector Atb = A.transpose() *;                                             3.7% 0.
85
86    FixedVector s;                                                                 0.1% 0.
87    FixedVector w;                                                                 0.0%
```

Figure 4.1: VTune profiling of multifit_cpu. 37% of the total time is spent performing $A^T A$.

```
123     // swap AtA to avoid copy                                                                    
124     AtA.col(nPassive).swap(AtA.col(w_max_idx));                                          1.7%
125     AtA.row(nPassive).swap(AtA.row(w_max_idx));                                          1.8%
126     // swap Atb to match with AtA
127     Eigen::numext::swap(Atb.coeffRef(nPassive), Atb.coeffRef(w_max_idx));                0.1%
128     Eigen::numext::swap(x.coeffRef(nPassive), x.coeffRef(w_max_idx));                    0.1%
129     // swap the permutation matrix to reorder the solution in the end
130     Eigen::numext::swap(permutation.indices()[nPassive],                                 0.3%
131                         permutation.indices()[w_max_idx]);
132
133     ++nPassive;
134
135 #ifdef DEBUG_FNNLS_CPU
136     cout << "max index " << w_max_idx << endl;
137     std::cout << "n_active " << nActive << std::endl;
138 #endif
139
140 // inner loop
141 #pragma unroll VECTOR_SIZE
142     while (nPassive > 0) {
143       s.head(nPassive) =                                                                 34.5%
144           AtA.topLeftCorner(nPassive, nPassive).llt().solve(Atb.head(nPassive));
145
146       if (s.head(nPassive).minCoeff() > 0.) {                                            1.0%
147         x.head(nPassive) = s.head(nPassive);                                             1.3%
148         break;                                                                           0.0%
149       }
150
151 #ifdef DEBUG_FNNLS_CPU
152       cout << "s" << endl << s.head(nPassive) << endl;
153 #endif
154
155       auto alpha = std::numeric_limits<double>::max();
156       Index alpha_idx = 0;
157
158 #pragma unroll VECTOR_SIZE
159       for (auto i = 0; i < nPassive; ++i) {
160         if (s[i] <= 0.) {                                                                0.0%
161           auto const ratio = x[i] / (x[i] - s[i]);                                       0.0%
162           if (ratio < alpha) {
163             alpha = ratio;
```

Figure 4.2: Second bottleneck found using VTune. 34% of the time is spent calculating the Cholesky decomposition.

4.1.1 Matrix multiplication

The first hotspot is the computation of A^TA that requires 37% of the total execution time. To solve this hotspot it is possible by exploiting the observations:

- The matrix A^TA is symmetric so it is enough calculate the one triangular portion and the copy the results back.
- The matrix is 10×10, it fits in L1 cache, thus cache efficiency is more important than algorithmic complexity.

Exploiting the hypothesis stated above the implementation illustraded in pseudo-code 3, specific for this case, has been provided.

This code is very simple but, in cache simple things are needed. The goal is to avoid useless computations, cache faults, and bubbles generated by branches. The main idea behind it is given that A^TA is symmetric compute only half of it and copy the values to the other part. Moreover, knowing that the multiplication is not between two random matrices but, between a matrix and his transpose, if the storage order is column major perform a column$\times$column dot product or a row$\times$row one in the other case. Since the storage order is column major there is another minor optimization that can be performed to gain the last drop of performance. This optimization is about the loop order. A careful choice minimizes jumps, for example in this particular case iterate over column generates no jumps neither cache misses, while iterating over rows generate a jump. A loop order of $row \rightarrow column \rightarrow dot\ product$ means that for each row there is one and only one jump. Instead, a loop order like $column \rightarrow row \rightarrow dot\ product$ generates $|columns| \times |rows|$

```
59    // FNNLS memorizes the A^T * A and A^T * b to reduce the computation.
60    // The pseudo-inverse obtained has the same numerical problems so
61    // I keep the same decomposition utilized for NNLS.
62
63    // pseudoinverse (A^T * A)^-1 * A^T
64    // this pseudo-inverse has numerical issues
65    // in order to avoid that I substituted the pseudoinverse whit the QR
66    // decomposition
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68    // I'm substituting the vectors P and R that represents active and passive set
69    // with a boolean vector: if active_set[i] the i belogns to R else to P
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71    // bool active_set[VECTOR_SIZE];
72    // memset(active_set, true, VECTOR_SIZE * sizeof(bool));
73
74
75    auto nPassive = 0;
76
77    // #ifdef __CUDA_ARCH__
78    // FixedMatrix AtA = transpose_wrapper(A);
79    // #endif
80    // #ifndef __CUDA_ARCH__
81    FixedMatrix AtA = transpose_multiply(A);                    16.1%
82    // #endif
83    // FixedMatrix AtA = A.transpose() * A;
84    // assert(AtA == A.transpose() * A);
85    FixedVector Atb = A.transpose() *b;                         5.3%  0.
86
87    FixedVector s;                                              0.0%
88    FixedVector w;                                              0.0%
89
90    Eigen::PermutationMatrix<VECTOR_SIZE> permutation;          0.1%
91    permutation.setIdentity();                                  0.3%
92
93  // main loop
94  #pragma unroll VECTOR_SIZE
95    for (auto iter = 0; iter < max_iterations; ++iter) {
96      const auto nActive = VECTOR_SIZE - nPassive;              0.0%  0.
97
98  #ifdef DEBUG_FNNLS_CPU
```

Figure 4.3: Cache efficient 10×10 matrix multiplication. The time needed to perform it is only 16.1% respect to the 37.6% spent by eigen implementation.

jumps, which is bad for performance.
This optimized version of the matrix multiplication, as showed in 4.3 takes only 16.1% of the total time, while the reference one takes 37.6% of it, giving a speedup of 2.33.
On the GPU side instead, is it possible to optimize this further by parallelizing this product with a kernel invocation.

4.1.2 Updating the Cholesky

The second bottleneck can be solved using the closed formula present in [6] to update the Cholesky without recomputing it in case of adding/removing one column and one row.
Given that nnls updates a components of the solution vector at the time, to reduce the number of iterations performed inside the regression it is possible to directly exploit this information to update the Σ matrix. That way the whole regression, that is intrinsically iterative might be executed in fewer iterations.

Algorithm 3 Cache efficient matrix transposition and multiplication. A column major storage order is assumed otherwise the index needs to be reversed.

Input:
A real valued matrix of dimension $m \times n$

Output:
$\boldsymbol{A^T A}$ Real valued matrix of size $m \times m$

```
1: function TRANSPOSE_MULTIPLY(A)
2:     m × m matrix B
3:     for i ← 0; i < m; ++i do
4:         for j ← i; j < m; ++j do                ▷ A^T A is symmetric, compute half of it
5:             B_ji ← 0
6:             for k ← 0; k < m; ++j do
7:                 B_ji += A_ik * A_jk
8:             B_ij ← B_ji                          ▷ Copy the result on the other half
       return B
```

5. Conclusions

Write your conclusions here.

Bibliography

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A. My First Appendix

In this file (appendices/main.tex) you can add appendix chapters, just as you did in the thesis.tex file for the 'normal' chapters. You can also choose to include everything in this single file, whatever you prefer.