Hybrid Parallel Maximum Likelihood Fits on Many-Core Systems with MPI and OpenMP

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CERN openlab

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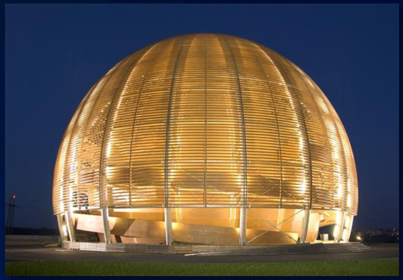
About CERN

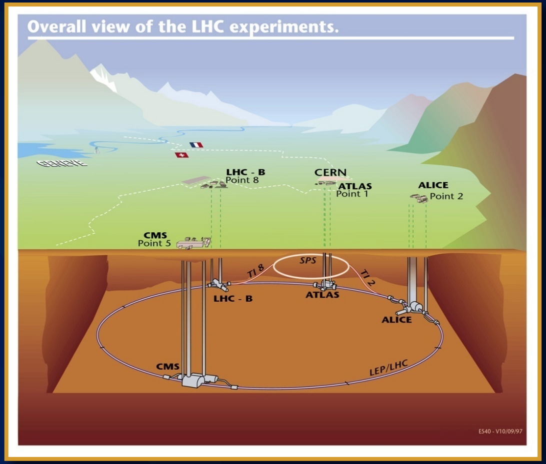


- **CERN is the European Organization for Nuclear Research in Geneva**
  - Particle accelerators and other infrastructure for high energy physics (HEP) research
  - Worldwide community
    - 20 members states (+ 3 foreseen members)
    - Observers: Turkey, Russia, Japan, USA, India
    - About 2300 staff
    - >10,000 users (about 5000 on-site)
    - Budget (2011) 1,000MCHF

- **Birthplace of the World Wide Web**

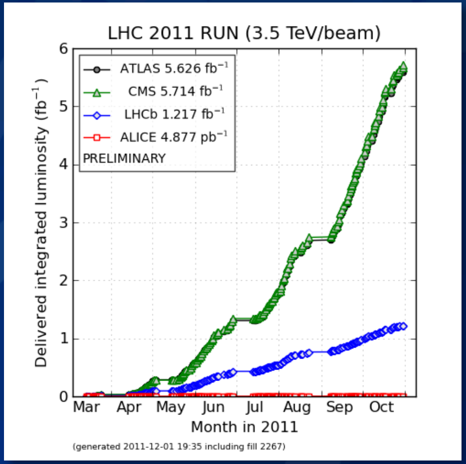
Large Hadron Collider (LHC)

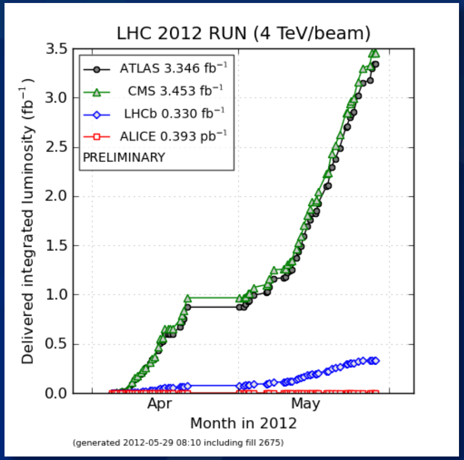
- **The biggest machine ever built**
  - 27 km, 100 meters below ground



- **Activities started in 2009**
  - Highest energy in an accelerator
  - Large data sample of recorded collisions (events) available for high energy physics (HEP) measurements

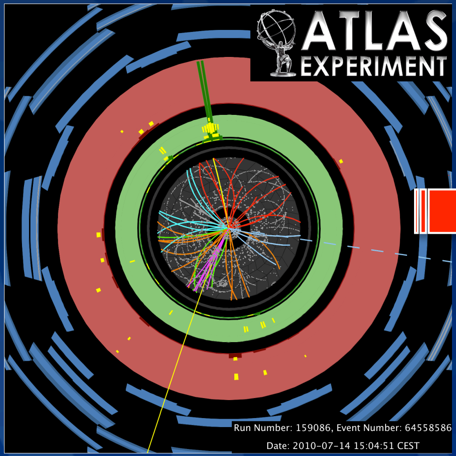
> 10^7 collisions per seconds, about 200-300 events recorded per second per experiment: **~300 MB/s (~5 PB/year)**

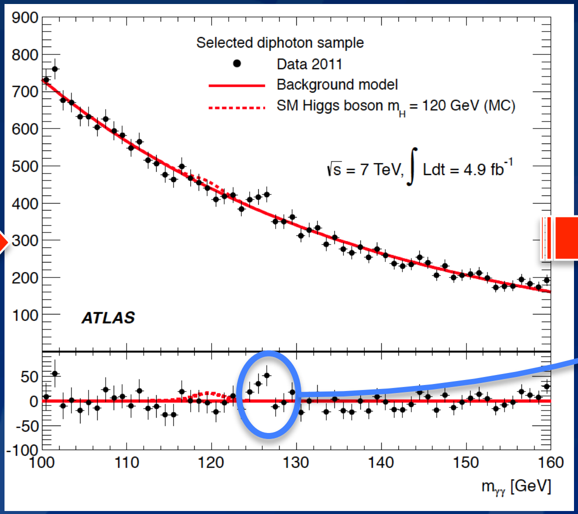


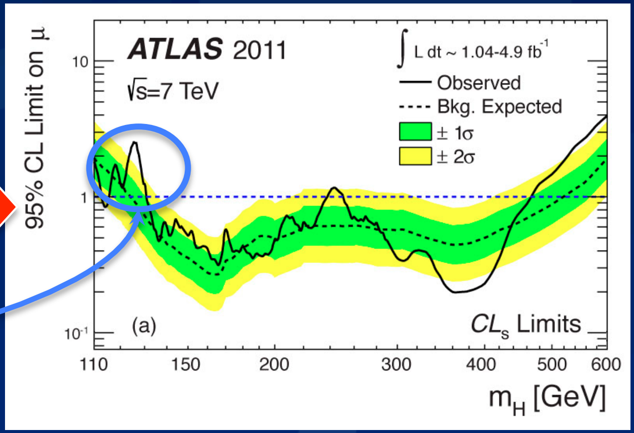


Data Analysis

- **Huge quantity of data collected, but most of events are due to well-know physics processes**
  - New physics effects expected in a tiny fraction of the total events: few tens
- **Crucial to have a good discrimination between interesting events and the rest, i.e. different species**
  - Data analysis techniques play a crucial role in this "fight"







Likelihood-based analysis

- **Specific variables (observables) combined by using multivariate analysis techniques, e.g. *Likelihood-based***
  - Each observable described by a probability density function $\mathcal{P}$
- **HEP package to build likelihood function models: ROOT/RooFit (http://root.cern.ch/drupal/content/roofit)**
  - C++ code
  - All data in the calculation are in double precision floating point numbers
- **We present the results based on a prototype of RooFit, that enables several optimizations and parallelization techniques applied to Maximum Likelihood fits**

Maximum Likelihood Fits

- For estimating parameters over a data sample, by minimizing the Negative Log-Likelihood (NLL) function

$$NLL = \sum_{j=1}^{s} n_j - \sum_{i=1}^{N} \left[\ln \sum_{j=1}^{s} \left(n_j \prod_{v=1}^{n} \mathcal{P}_j^v (x_i^v | \hat{\theta}_j) \right) \right]$$

N number of events
$\hat{x}_i$ set of observables for the event i
$\hat{\theta}$ set of parameters
n observables
s species
n_j number of events belonging to the species j

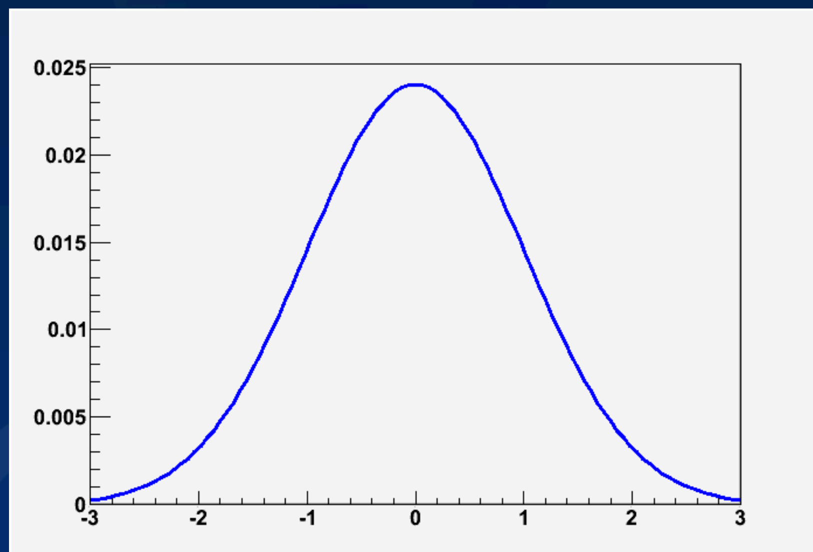
- The procedure of minimization can require several evaluation of the NLL
  - Depending on the complexity of the function, the number of observables, the number of free parameters, and the number of events, the entire procedure can require long execution time
  - **Mandatory to speed-up the evaluations of the NLL**

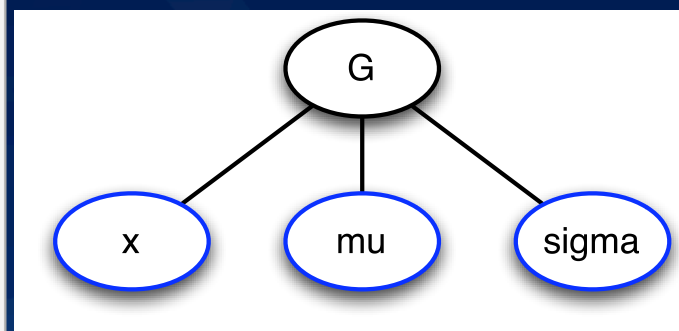
Examples

- **Simple case:**

Gaussian

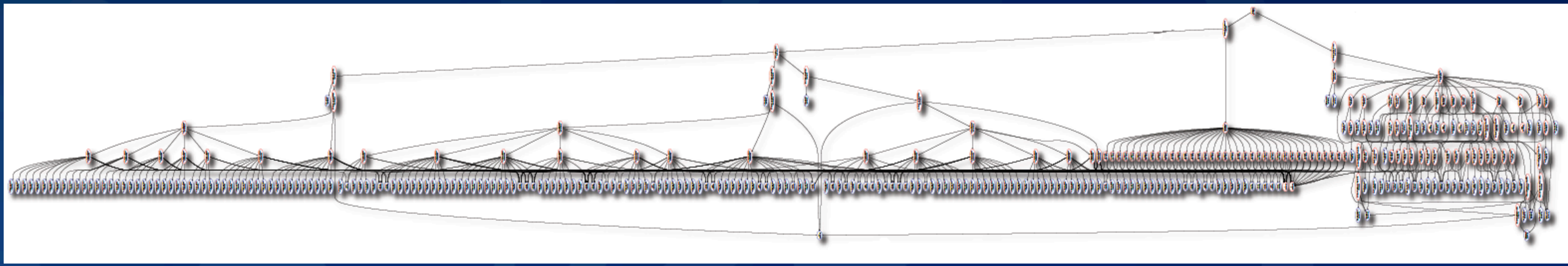
$$G(x|\mu,\sigma)$$





Examples

- **Higgs model:**
  - 12 observables
  - >200 parameters in the fit
  - Expected to increase its complexity in the next analyses



Algorithm Description (1)

- Recalling the NLL definition

③ ④ ② ①

$$NLL = \sum_{j=1}^{s} n_j - \sum_{i=1}^{N} \left[\ln \sum_{j=1}^{s} \left(n_j \prod_{v=1}^{n} \mathcal{P}_j^v(x_i^v | \hat{\theta}_j) \right) \right]$$

① Each $\mathcal{P}$ (Gaussian, Polynomial,…) is implemented with a corresponding class (basic PDF)
   – Virtual protected method to evaluate the function

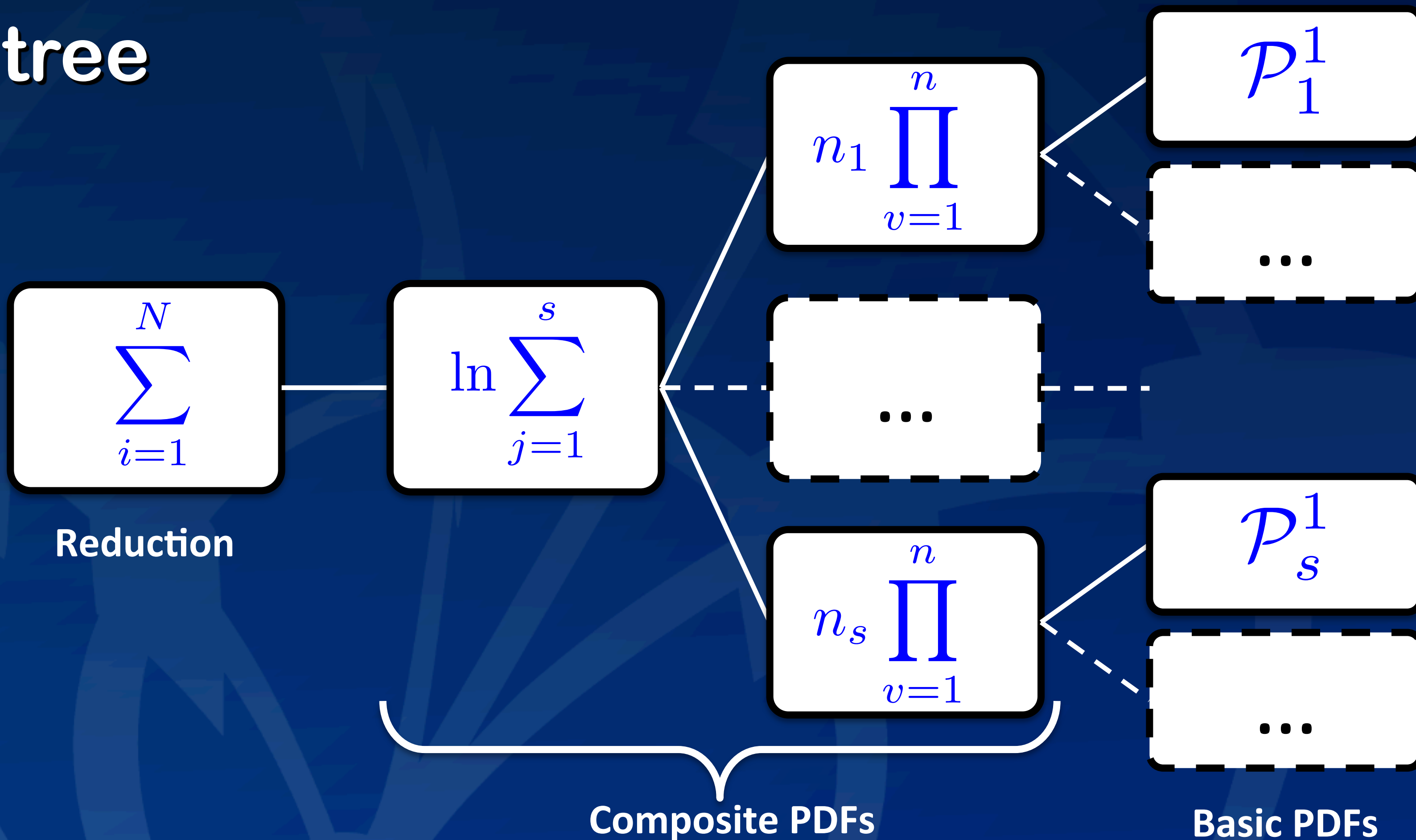
② Product over all observables (composite PDF)

③ Sum over all species (composite PDF)

④ Reduction of all values

Algorithm Tree

- We can visualize the NLL evaluation as a tree

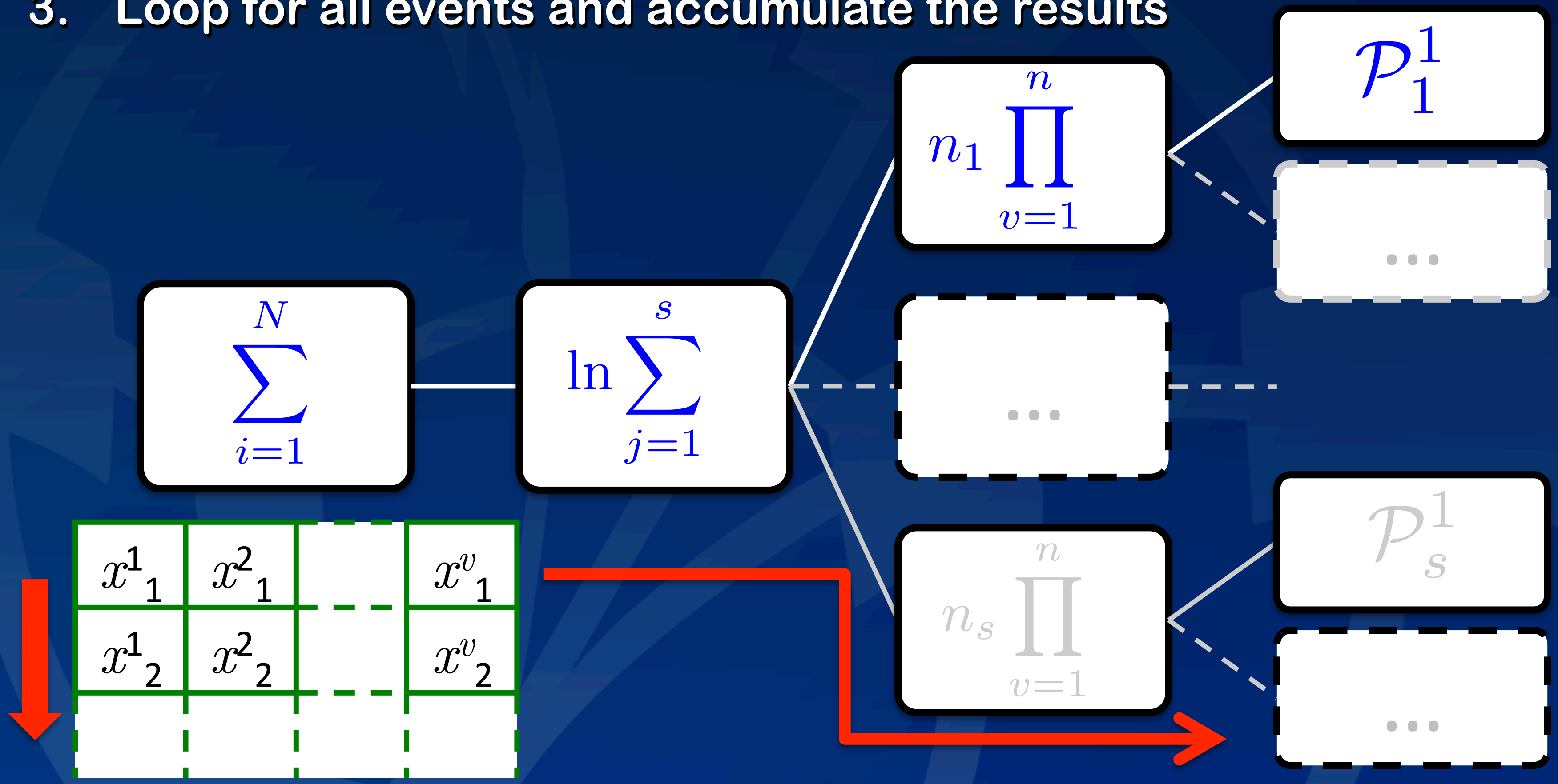


Algorithm Description (2)

- **Data are organized in memory in vectors**
  - A vector for each observable
  - Read-only during the NLL evaluation

RooFit Evaluation

1. **Read the observable values for a given event**
2. **Traverse the entire NLL tree**
   - Do the entire evaluation for each event
3. **Loop for all events and accumulate the results**

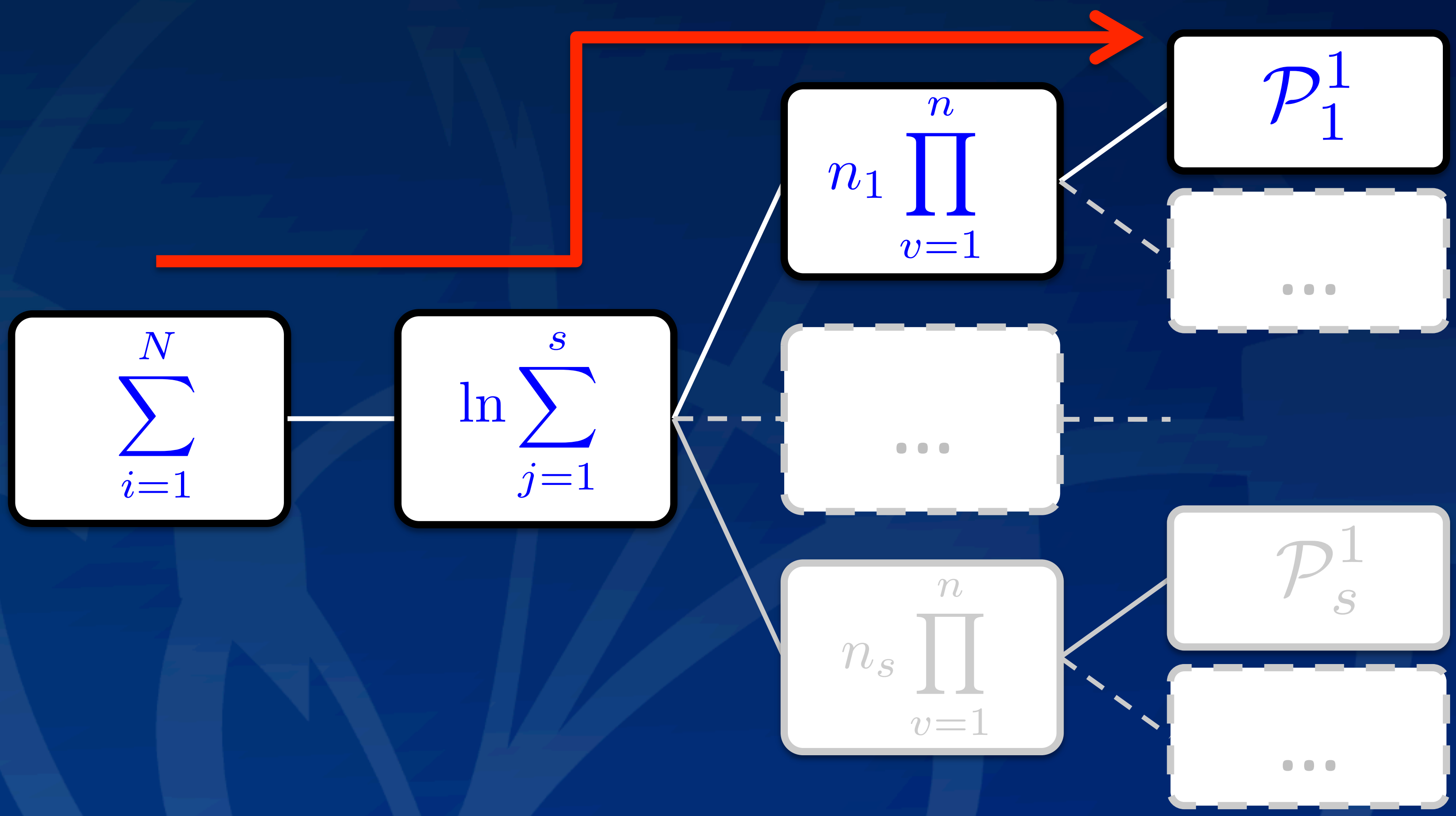


New Algorithm Design

- **Values of the PDFs evaluated with loops**
  - One loop per each PDF over the values of the observables
    - A loop iteration per each input event
  - Use Intel compiler for the **auto-vectorization** of the loops (using Intel SVML library)

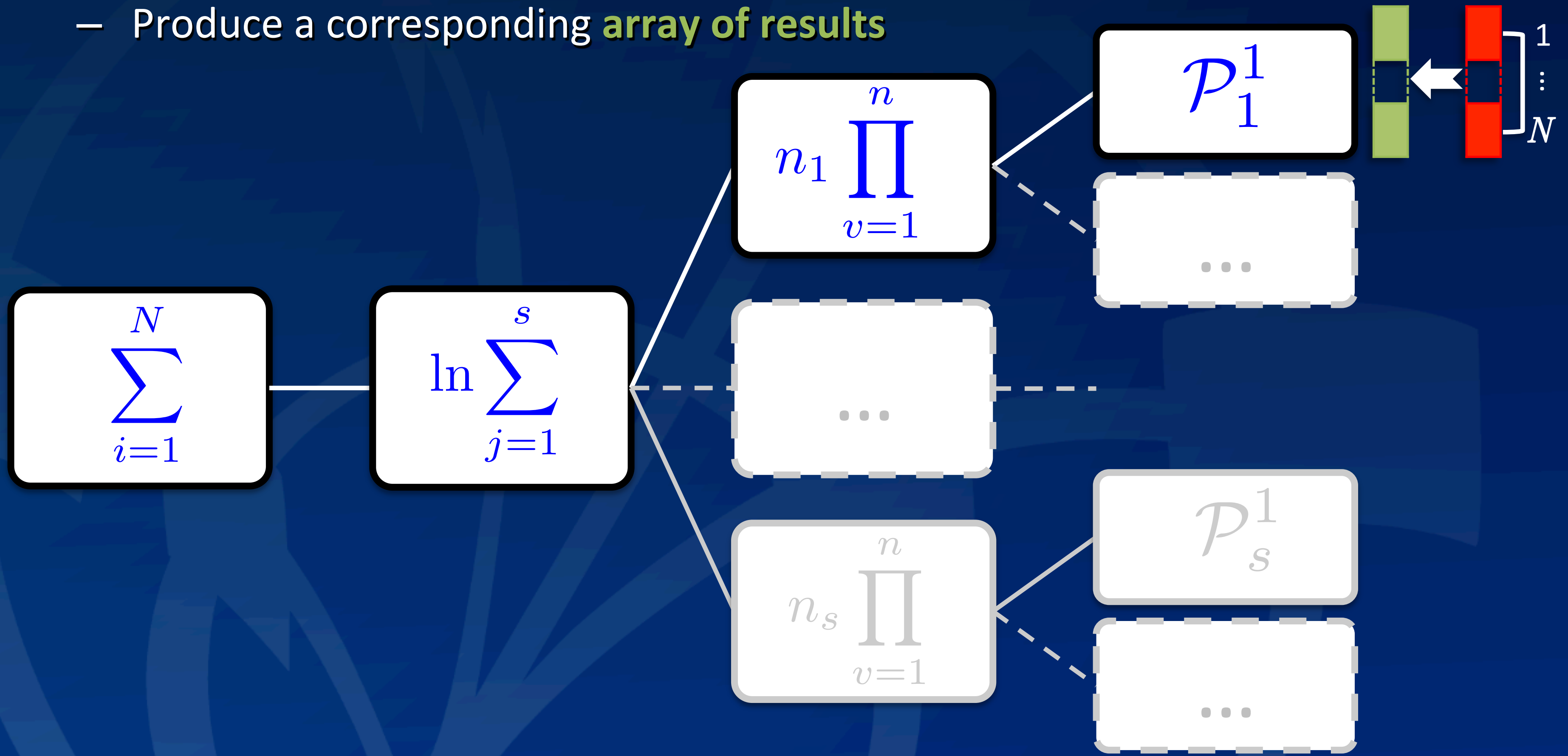
New Algorithm Evaluation

1. Traverse the NLL tree up to the first leaf (basic PDF)



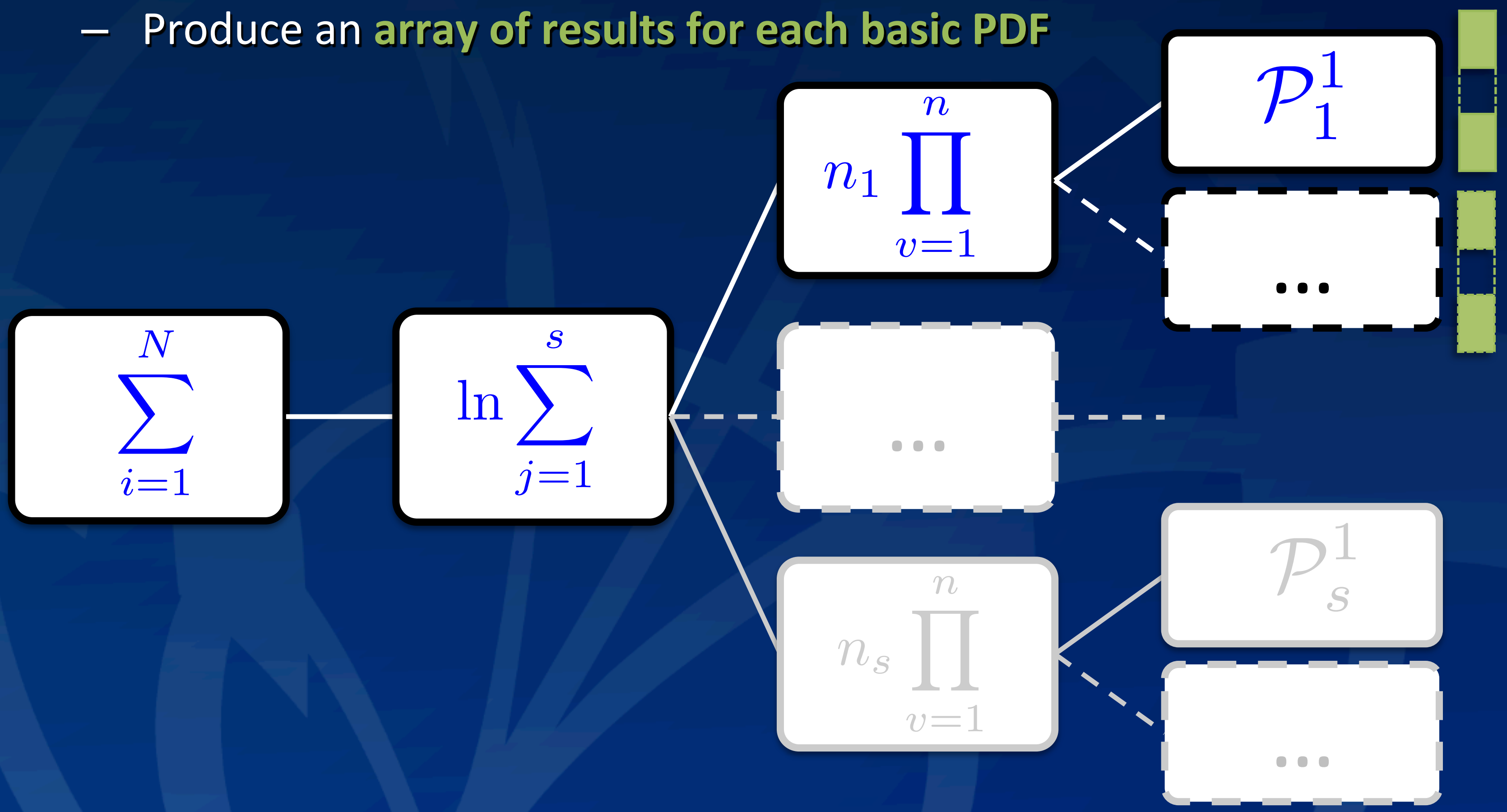
New Algorithm Evaluation

2. Loop over the *N* **events** and evaluate the PDF for each event
   – Produce a corresponding **array of results**



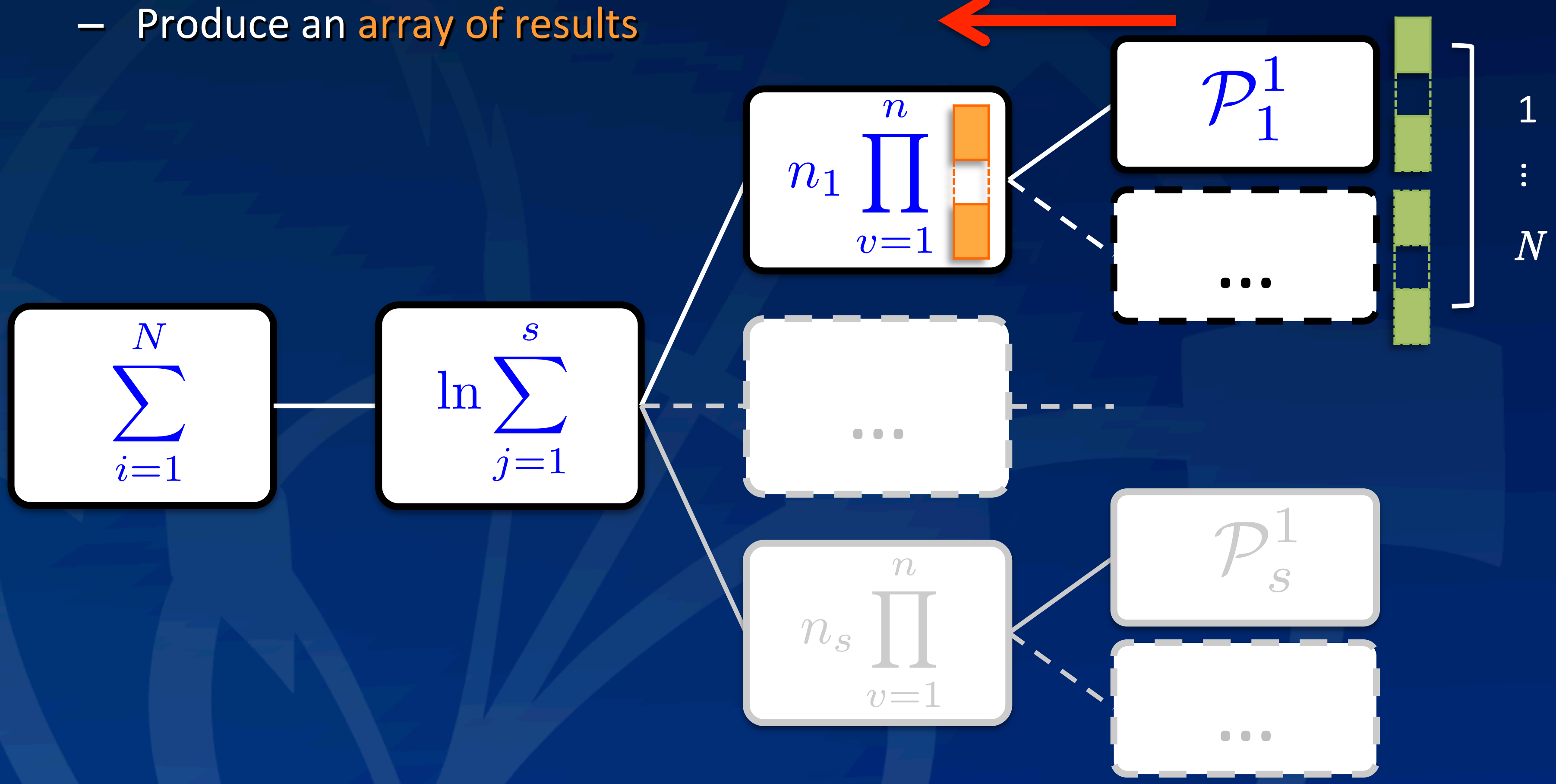
New Algorithm Evaluation

3. **Repeat the evaluation for all basic PDF in a composite PDF**
   – Produce an **array of results for each basic PDF**



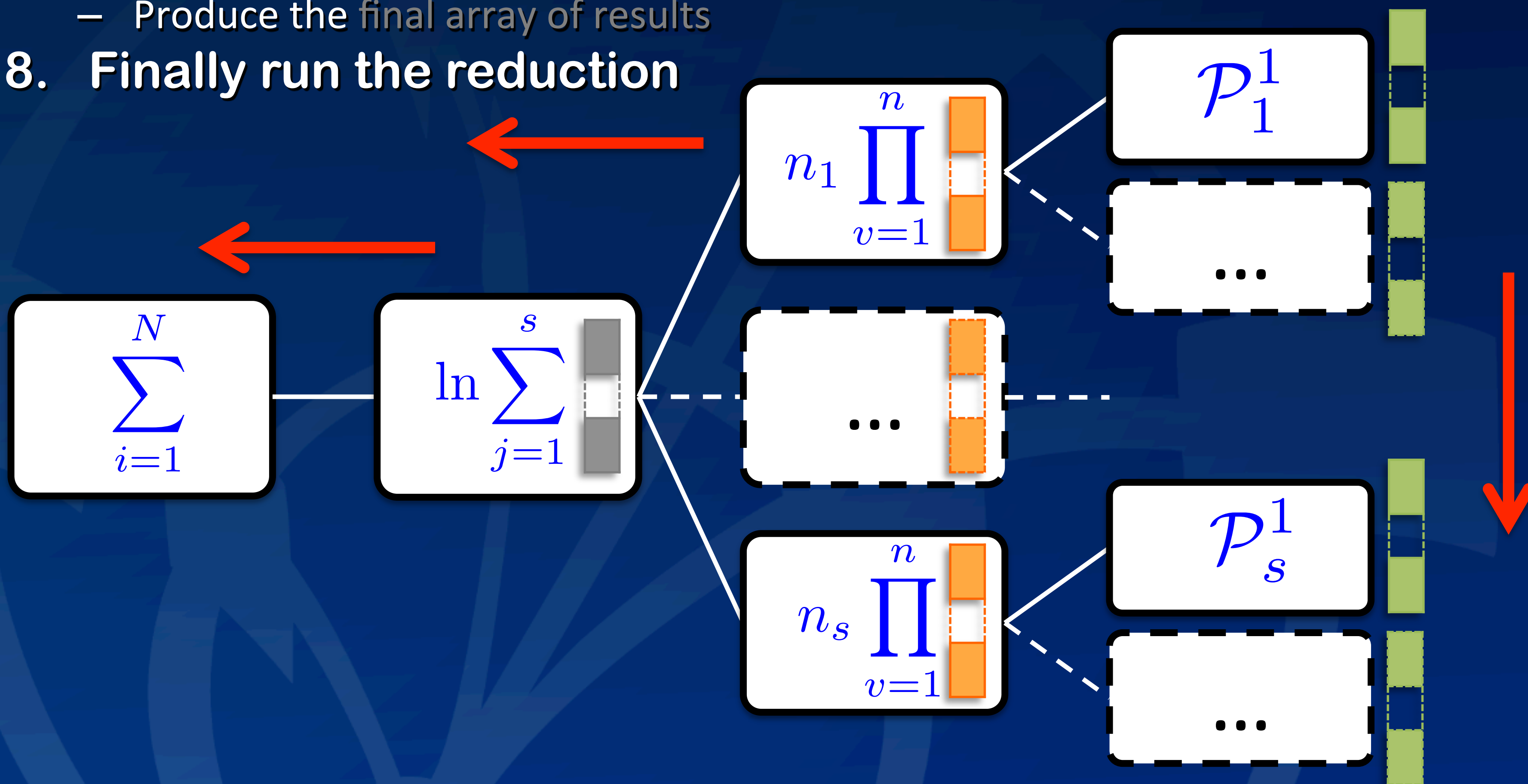
New Algorithm Evaluation

4. **Combine the array of results for the composite PDF**
   - Loop over the array of results of the basic PDF
   - Produce an array of results



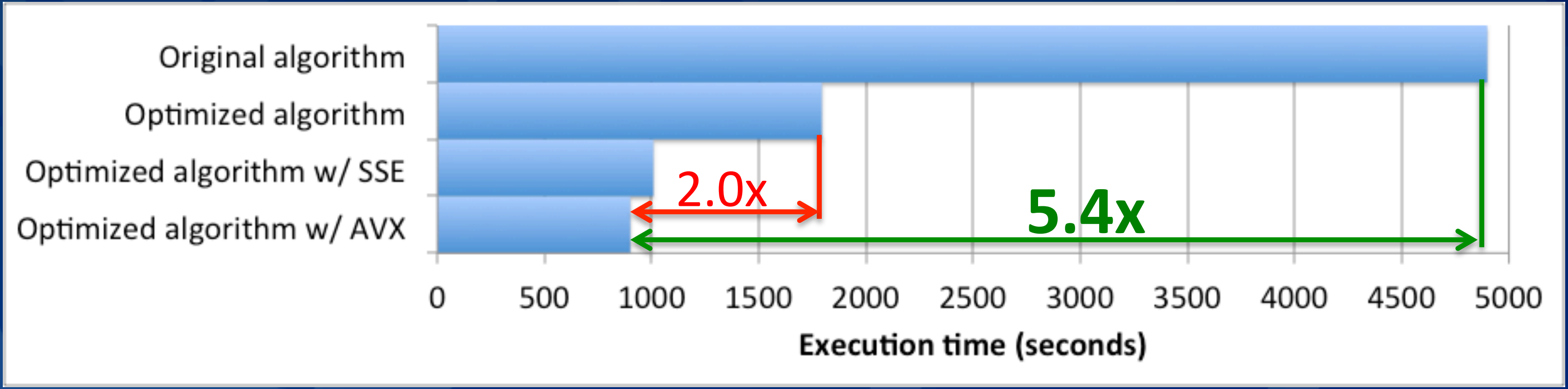
New Algorithm Evaluation

5. **Repeat for all composite PDFs**
7. **Loop over the array of results**
   – Produce the final array of results
8. **Finally run the reduction**



Sequential performance

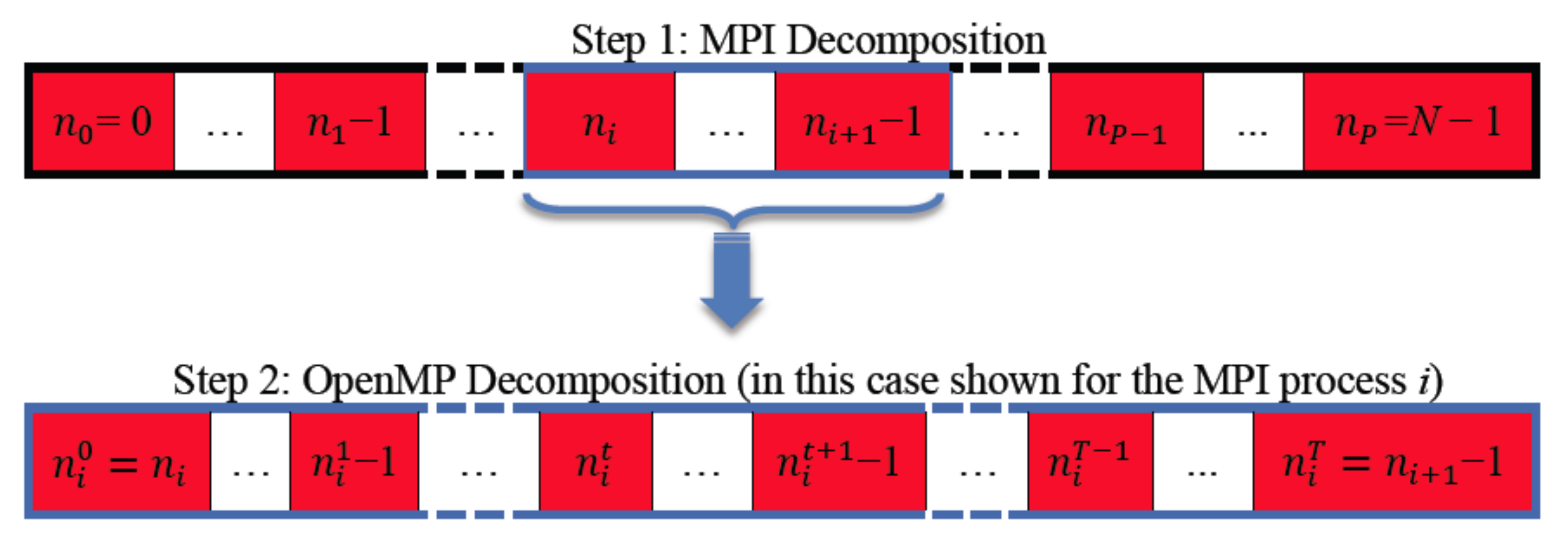
- Optimization with respect to original RooFit algorithm
  - Reduce the number of virtual functions calls
  - Inlining of the functions
  - Prefer data-flow rather than control-flow
- Testing on dual-socket Sandy Bridge-EP server, CPU E5-2680 @ 2.7GHz (Turbo OFF), dual socket, 8*2 cores
- Intel C++ compiler version 12.1.0
- Input data is composed by 1,000,000 events per 3 observables, for a total of about 24MB; results are stored in 29 vectors of 1,000,000 values, i.e. about 230MB



Parallelization: MPI+OpenMP

- **Each MPI process runs several OpenMP threads**
- **Decomposition of the input events (and corresponding loop iterations) in chunks**
  - Easy to balance: each chunk is composed by an equal number of events (maximum one event of difference)
  - Decomposition in two steps:
    - Step 1 for the MPI processes
    - Step 2 for the OpenMP threads belonging to each MPI process. A single OpenMP parallel region in common for all loops for each NLL evaluation
- **Input data are shared in memory between OpenMP threads**
- **Parallel reduction in two steps:**
  - Step 1 for the OpenMP threads belonging to each MPI process
  - Step 2 between the MPI processes (the only MPI communication based on `Allgather`)

MPI+OpenMP decomposition



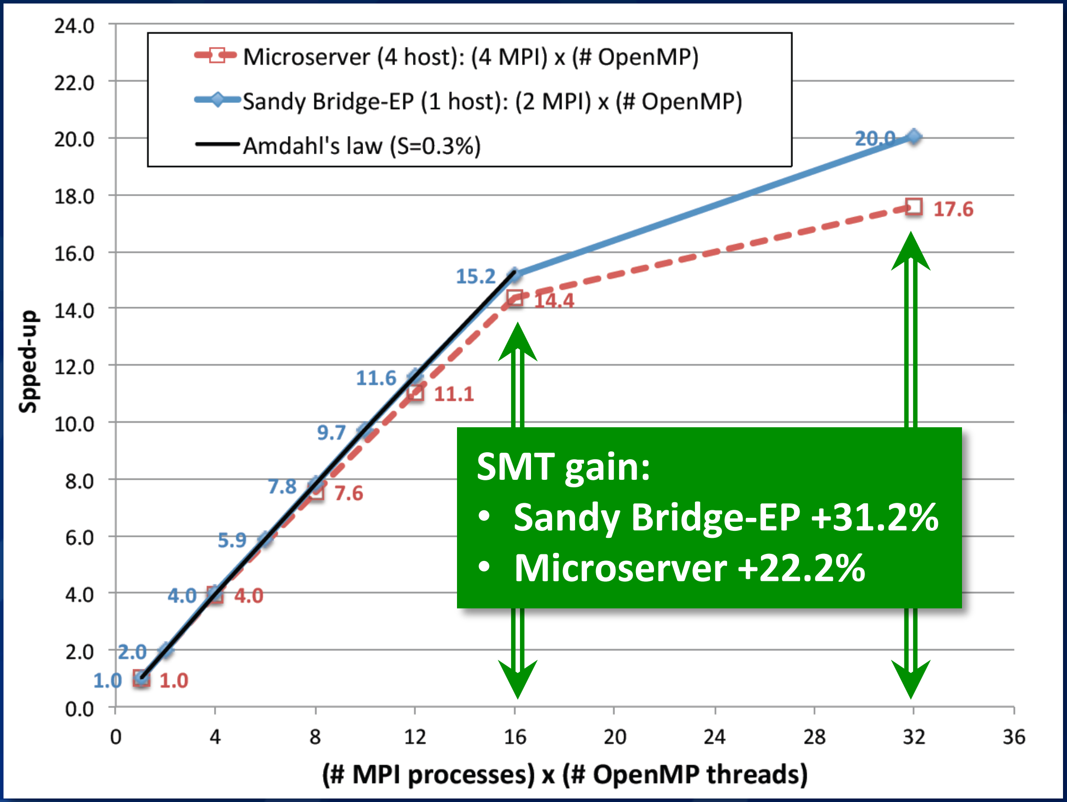
- P is the number of MPI processes involved, T is the number of OpenMP threads.
- OpenMP thread $t = 0,1,\ldots(T-1)$ of the MPI process $i = 0,1,\ldots(P-1)$ runs on the elements of the input data arrays with indices in the range $[n_i^t, n_i^{t+1}-1]$.

Parallel performance

- **Same example as before**
  - Sequential portion 0.3%
- **Intel MPI v4.0.3**
- **Testing on DELL C5220 Microserver, 4 hosts single-socket Sandy Bridge, CPU E3-1280 @ 3.50GHz (Turbo OFF), 4 cores, 8MB L3 cache (2MB per core)**
  - One Ethernet link per host @ 1Gb
- **Process topology to maximize the number of hosts, with a single MPI process per each host**
- **Comparison of the performance with the Sandy Bridge-EP system**
  - Same number of total cores (16)
  - 2 MPI processes with corresponding OpenMP threads pinned within the sockets
  - **Smaller L3 cache size on the CPU version (20MB, 2.5MB per core)**

Parallel performance

- **Perfect scalability: 14x-15x with 16 threads**
  - Using SMT threads: 20x for Sandy Bridge-EP, 18x for Microserver
- **Main limitation to scalability comes from the L3 cache size**
  - Negligible penalty for the Sandy Bridge-EP
  - Microserver: −4.5% per 12 threads, −5.5% per 16 threads
- **Analysis of the MPI communication time shows no penalty to the scalability**



Conclusion

- **Redesign the algorithm to exploit optimizations**
  - Data-flow versus control-flow
- **Vectorization is crucial to get performance**
  - A good compiler can help a lot
- **Good scalability, close to the expectation**
  - Low impact by MPI and OpenMP overheads
- **Code under validation by the HEP community**
- **Porting on Intel MIC using MPI as host-device communication approach, as part of the Intel-CERN openlab collaboration**
- **Some references:**
  - S. Jarp *et al.*, *Evaluation of the Intel Sandy Bridge-EP server processor*, March 2012, CERN-IT-Note-2012-005
  - S. Jarp *et al.*, *Parallel Likelihood Function Evaluation on Heterogeneous Many-core Systems*, August 2011, CERN-IT-2011-012

THANK YOU

Q & A

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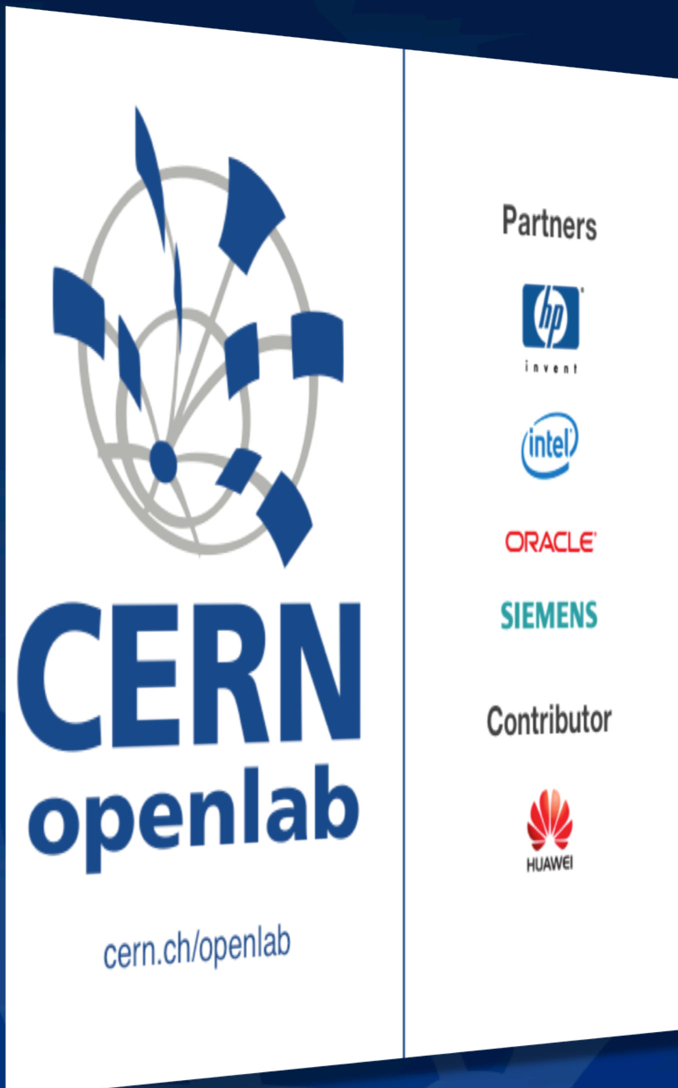

- **CERN openlab is a partnership between CERN and leading ICT companies**
  - Its mission is to accelerate the development of cutting-edge solutions to be used by the worldwide LHC community
- **The Platform Competence Center of the CERN openlab has worked closely with Intel for the past decade and focuses on:**
  - Many-core scalability
  - Performance tuning and optimization
  - Benchmarking and thermal optimization
  - Teaching