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Software Design in the Many-Cores era

A. Gheata, S. Hageböck

CERN, EP-SFT/IT

CERN School of Computing 2022

CPU Ninja

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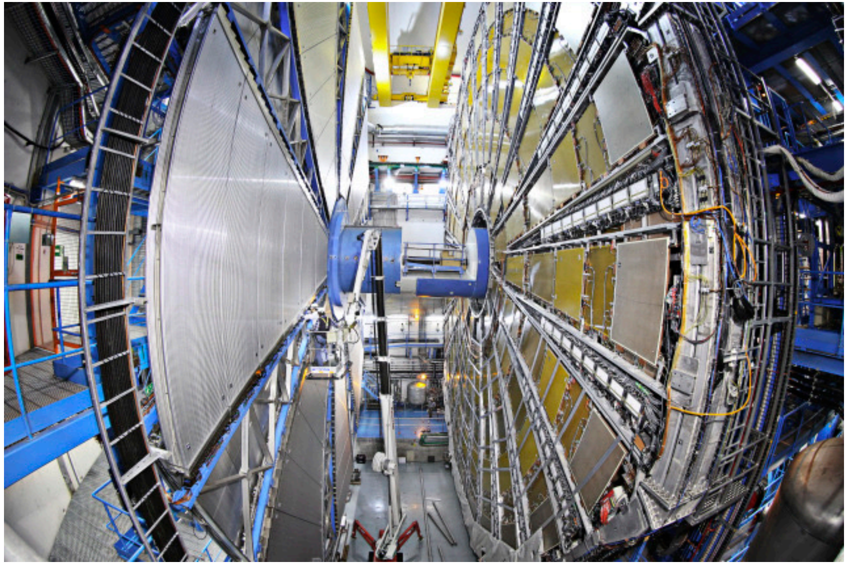

Lecture I

Parallelism in a Modern HEP Data Processing Framework

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Outline of This Lecture

The Goals:

1) *Understand why we need parallelisation*
2) *Understand the problem domain of physics processing*
3) *Break down big problems into work items that can be tackled in parallel*
4) *Be aware of the limitations for parallelisation*

- From sequential to parallel
- Experiment Frameworks: basic principles, design
- Laws of parallelism
- Concurrency Models: task-based parallelism

Hitting the Wall(s)

- Once upon a time, the life of software developers was much easier
  - Sequential programming
  - Want your program to run faster? Buy yourself a new machine!
- The fairy tale ended in the early 2000s
  - Processor manufacturers had to rethink CPU architectures
  - No more free lunch for software

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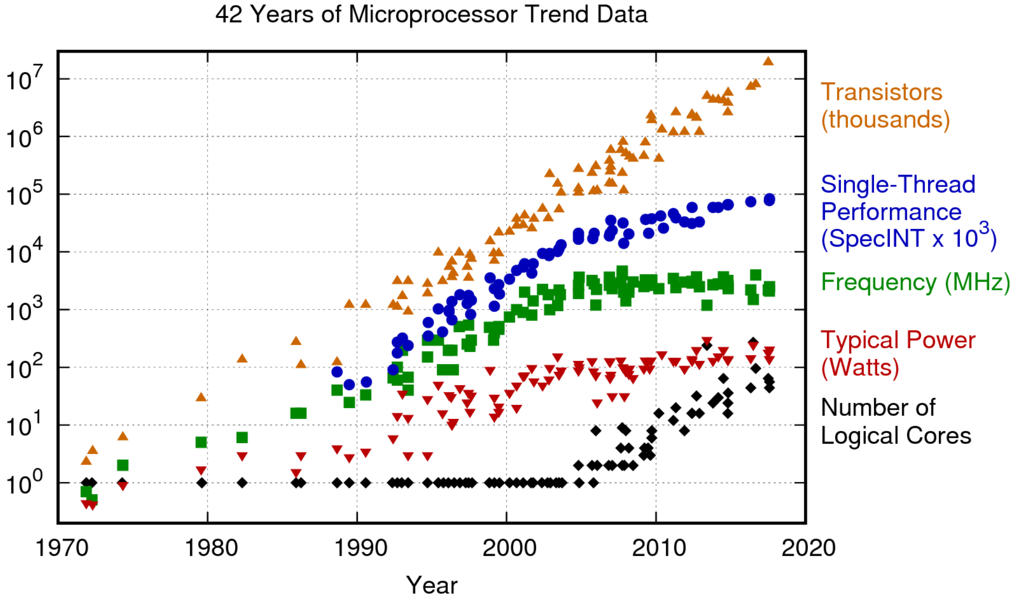
The Power Wall

- Manufacturers could not keep improving processor performance by increasing frequency
  - Not at the same rate at least
- **Power consumption and dissipation** became limiting factors
  - Higher clock rate could lead to overheating



https://www.karlrupp.net/2018/02/42-years-of-microprocessor-trend-data/

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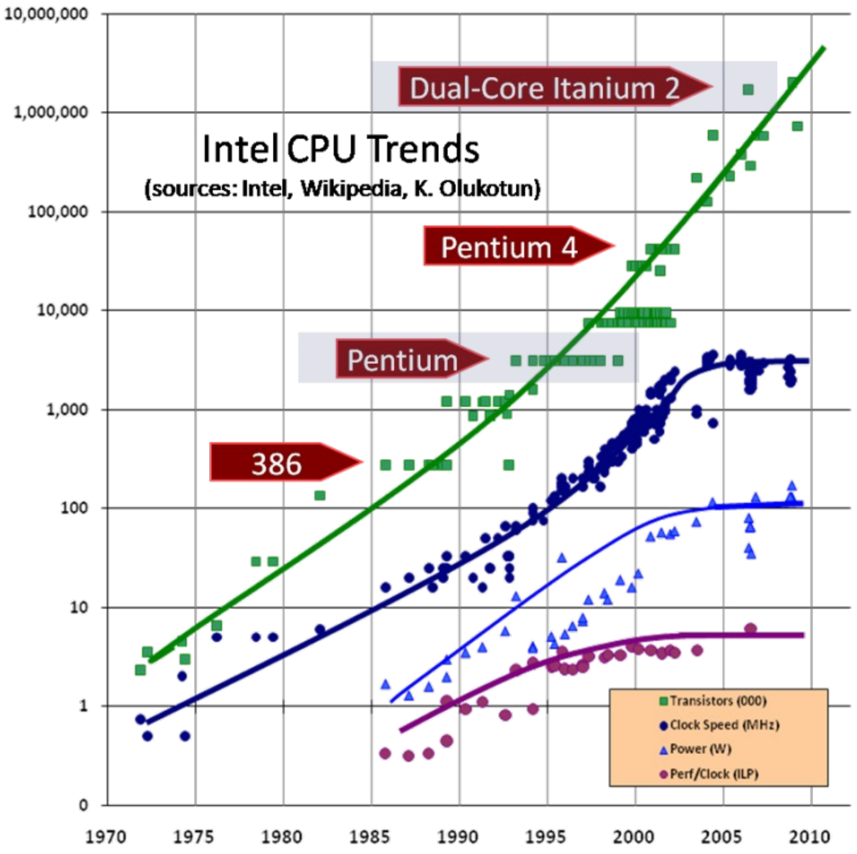
The ILP Wall

- Processors apply multiple techniques to optimise the execution flow
  - Pipelining
  - Branch prediction
  - Out-of-order execution
  - …
- **Instruction-Level Parallelism growth also flattened**
  - Hard to squeeze more work out of a clock cycle



http://www.gotw.ca/publications/concurrency-ddj.htm

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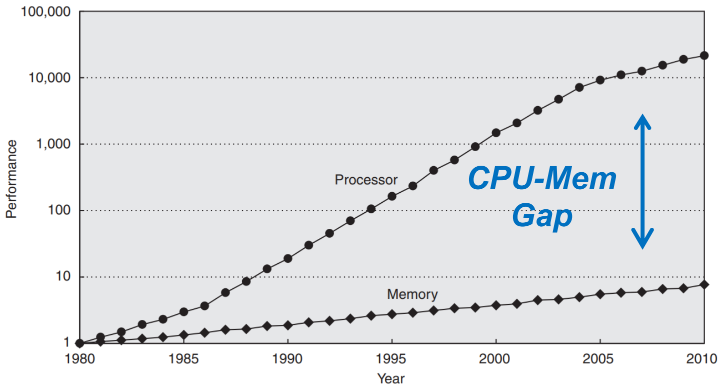
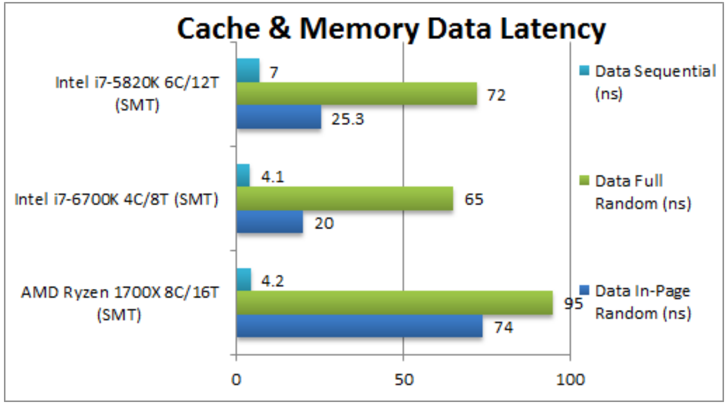
The Memory Wall

- Processor clock rates have been increasing faster than memory clock rates
- **Latency in memory access** is often the major performance issue in modern software applications
- **Larger and faster cache** memories help alleviate the problem but do not solve it
- Often the CPU is just waiting for data…





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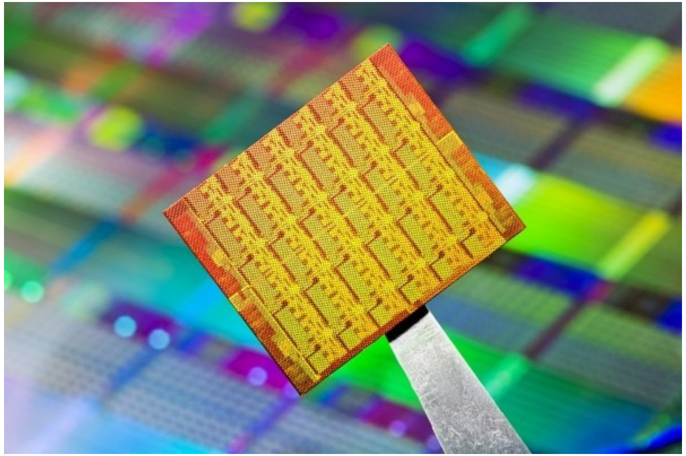
Multi/Many Core to the Rescue

- Let's change strategy
  - Grow by **combining simpler processing units**
  - Moore's law reinterpreted: number of cores per chip will double every two years

How to make the most of all these resources?



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From Single to Multi/Many core

	Irwin-dale	Wood-crest	Gaines-town	Haswell	Broad- well	Skylake	Ice Lake	AMD Epyc
Year	2005	2006	2009	2015	2016	2017	2021	2022
Cores	1	2	4	18	24	28	40	64 (128 SMT)
Freq (GHz)	3.8	3.0	3.33	2.1	2.2	2.5	2.3 (3.4 boost)	2.2 (3.5 boost)
LL Cache	L2 (2MB)	L2 (4MB)	L3 (8MB)	L3 (45MB)	L3 (60MB)	L3 (38MB)	L3 (60MB)	L3 (768MB)

Evolution of server processors
(https://ark.intel.com / https://amd.com)

Need for Parallelism

- Change of programming paradigm
  - Need to deal with systems with many parallel threads
  - Improvement in performance comes with **exploitation of concurrency**

- Will all programmers have to be parallel programmers?
  - Different levels of exposure: **explicit vs. implicit** parallelism
  - First step is to **change the way of thinking**!

Parallelism is here to stay

A Supercomputer

- Perhaps the most striking example of parallelism
  - top500.org: approaching 10M cores (Frontier 2021: 8.7M)
  - Parallelism intra-node and inter-node
  - Multi/many core, hybrid setups: CPU - GPU

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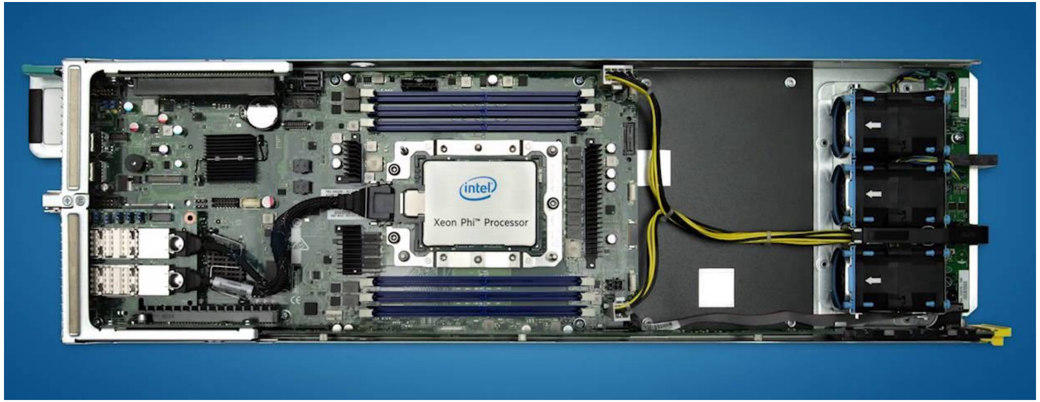
Parallel Hardware

Accelerators for massive parallelism



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How is Parallelism Achieved?

- Supercomputer design tailored for **High-Performance Computing**:
  - Homogeneous nodes (+ accelerators)
  - High-bandwidth low-latency networks (**InfiniBand**, Aries)
  - Parallel distributed file system (**Lustre**, GPFS)

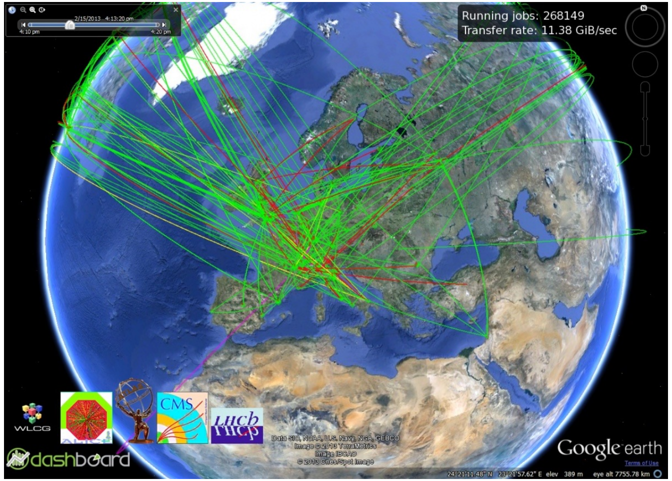
- **Explicit** low-level parallelism dominates
  - **MPI** for distributing processes, message passing
  - **OpenMP** inside a node (+ CUDA, OpenCL, SYCL)

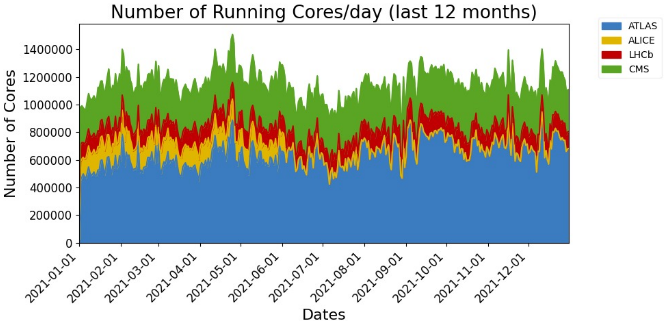
Parallelisation in HEP

LHC Computing Grid (WLCG)

- HEP is parallel since more than a decade
- Computations are distributed among hierarchically organised data centres spread around the globe
- Tens of billions of LHC events are processed per year, running on > 1M cores 24/7 365 days a year

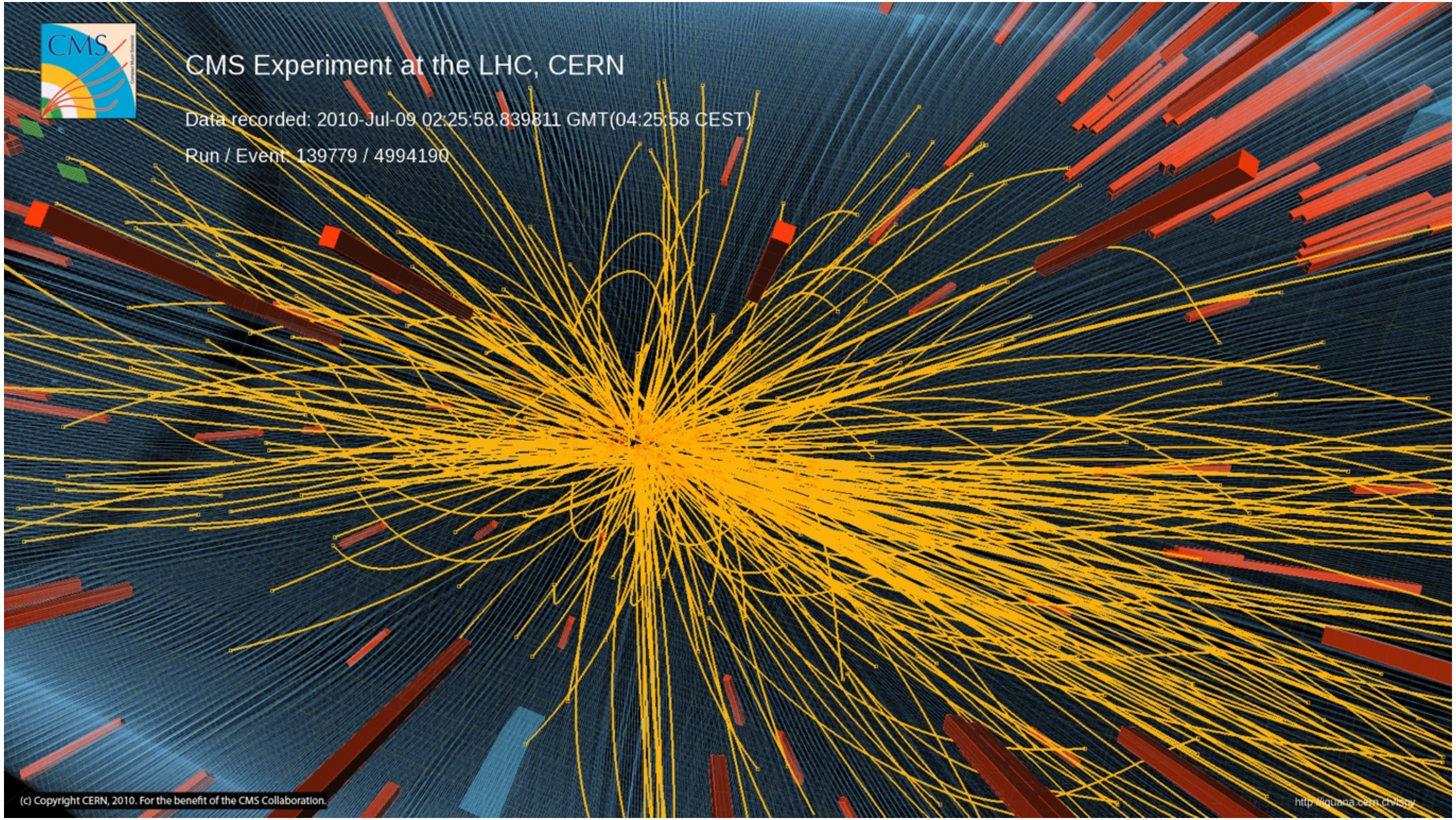
Huge parallel infrastructure!





https://wlcg.web.cern.ch/using-wlcg/monitoring-visualisation/monthly-stats

Physics Challenges



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Physics Challenges II

So why not treating every many-core computer in the WLCG as a computing centre of its own with many independent jobs on it?

- Due to the beam intensity (“luminosity”) at the LHC multiple proton-proton collisions take place at once (**pile-up**)
- Pile-up expected to increase further in Run 3 and especially in **HL-LHC**
- As a result, memory consumed by experiments’ reconstruction jobs will go up, making it hard to run many simultaneous jobs on a single computer
  - Independent jobs do not share memory!

Furthermore:

- **Merging** of results of independent jobs takes significant amount of time

Another parallelisation strategy is needed!

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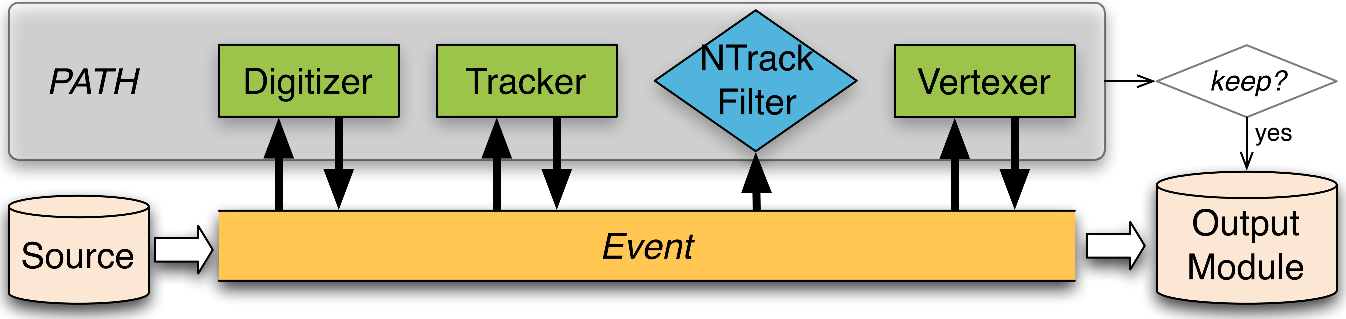
Framework Primer

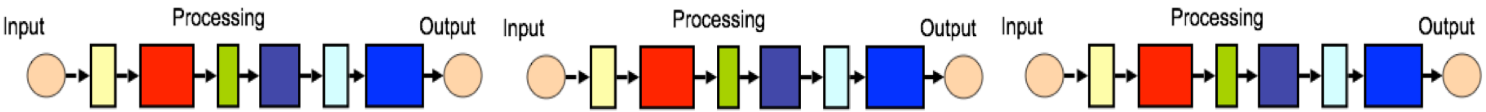
Experiment Software Follows the Idea of a Software Bus



Each experiment has software with about 5 million lines of code based on this model

Framework Primer II

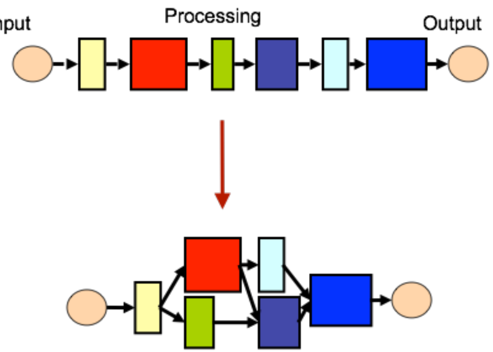
- Multiple events are being processed **sequentially**



- The result is being put into a single output file
- This keeps **only one core busy** at a time

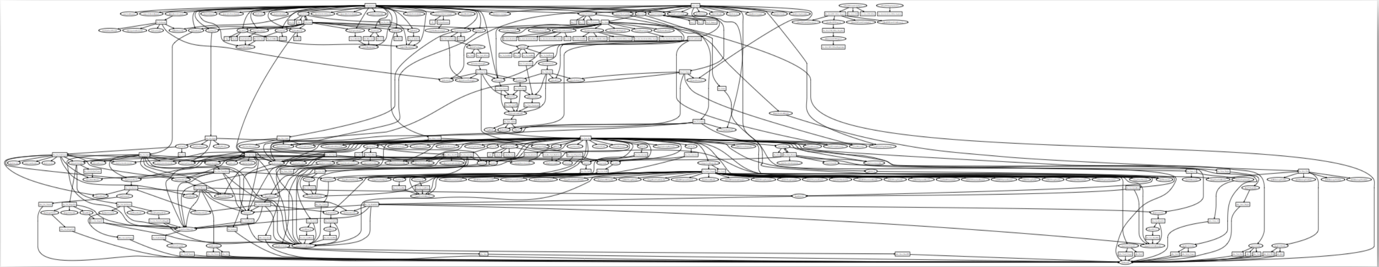
How to Introduce Concurrency

- The algorithms and their data dependencies form a **DAG** (directed acyclic graph)
  - Schedule the algorithms according to the DAG

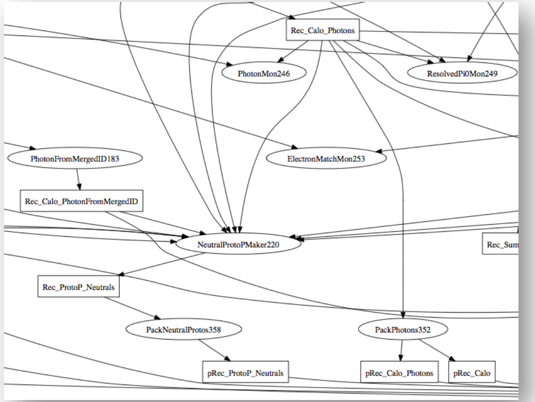


- Sounds more trivial than it is
  - Existing HEP software has many “backdoor” communication channels making the DAG non-obvious.

Real World Example



- Particular example taken from LHCb reconstruction program “Brunel”
- Gives an idea for the potential concurrency
- ATLAS and CMS just don’t fit on a slide…



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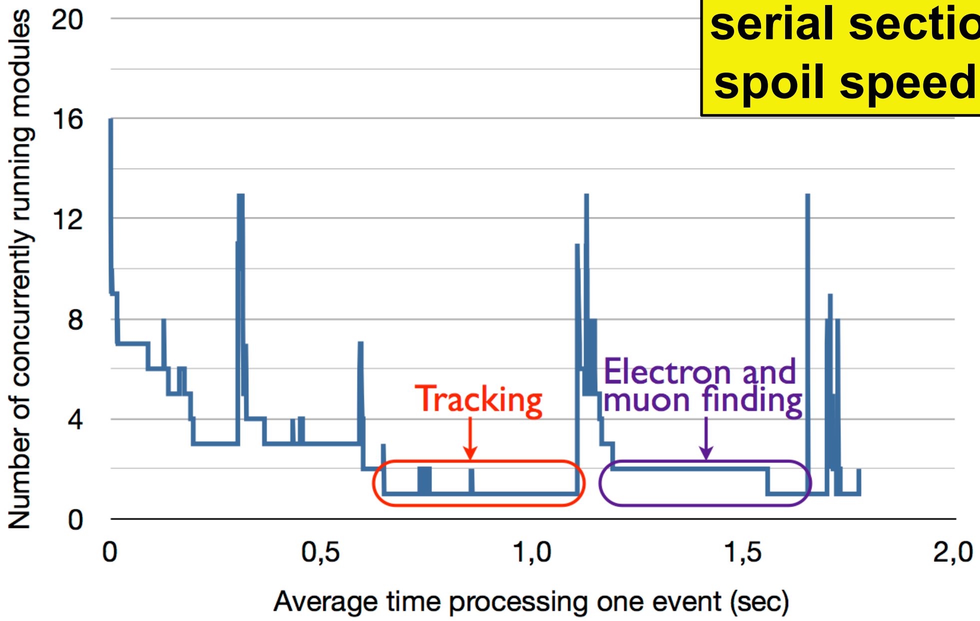
The DAG Can Get Narrower

Long serial sections spoil speedup!



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Is Parallelisation Worth It?

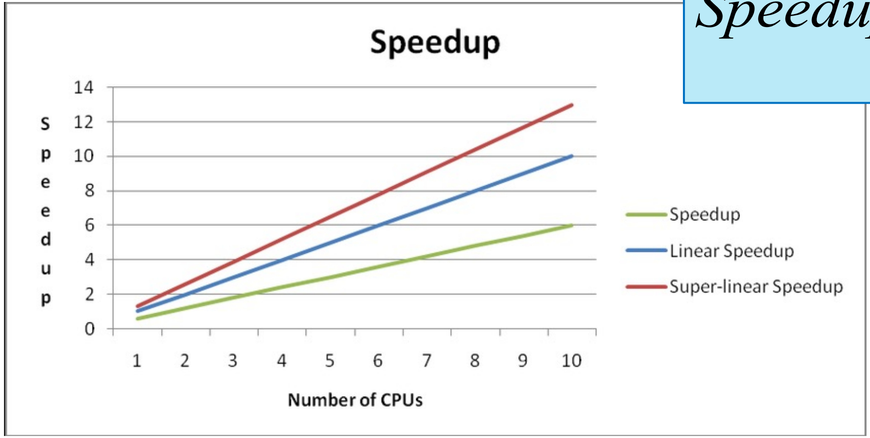
- We hit the wall very early – game over and that's it?
- Whenever thinking about parallelisation, one should spend some thoughts on whether the effort is worth it
  - The total cost of ownership of one additional box might be smaller than the design-implementation-maintenance costs
- What is the performance gain we can expect?

Amdahl's and Gustafson's laws can help you there!

Need for Speed(up)

- We parallelise because we want to run our application faster
- **Speedup**: how much faster does my code run after parallelising it?
  - Indicator of **scalability**

$$Speedup = \frac{Time_{serial}}{Time_{parallel}}$$



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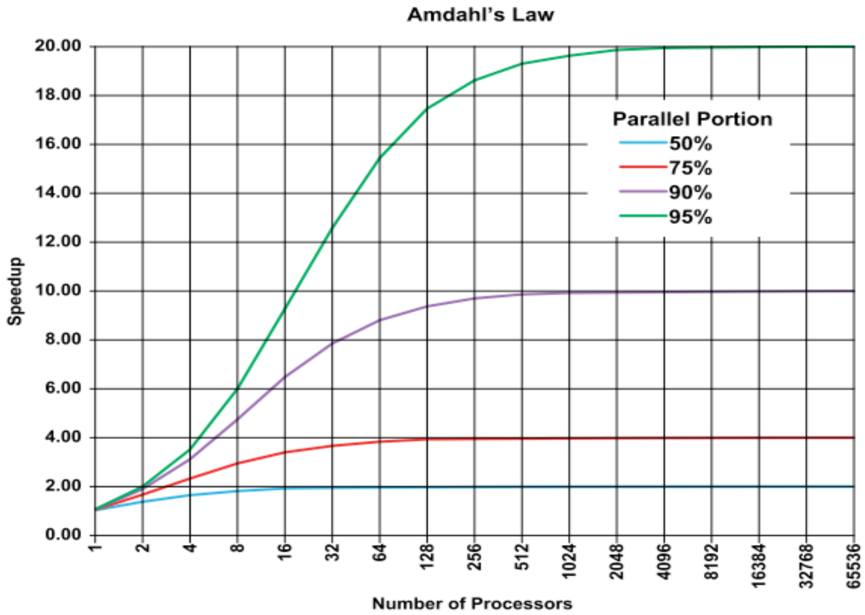
Amdahl's Law

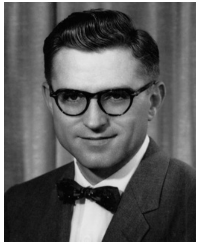
- It predicts the maximum speedup achievable given a problem of **fixed size**

$$Speedup = \frac{1}{(1-p)+\frac{p}{n}}$$

n: number of cores
p: parallel portion



"… the effort expended on achieving high parallel processing rates is wasted unless it is accompanied by achievements in sequential processing rates of very nearly the same magnitude." - 1967



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Gustafson's Law

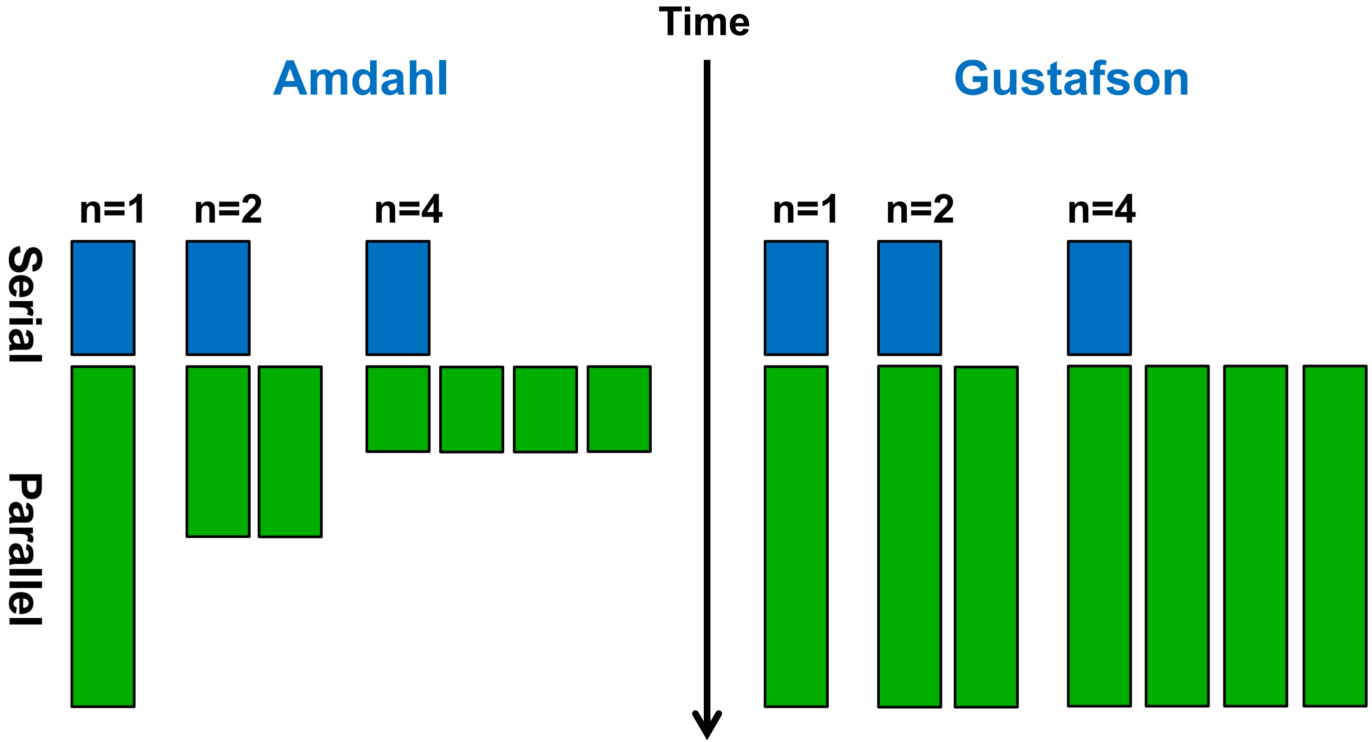
- Often **problem size increases**, while serial parts remain constant
- If problem size increases, so does the opportunity for parallelisation
- Solve bigger problems in the same amount of time by using more resources

$$Speedup = 1 - p + np$$

n: number of cores
p: parallel portion

"… speedup should be measured by scaling the problem on the number of processors, not by fixing the problem size." - 1988

Amdahl vs Gustafson



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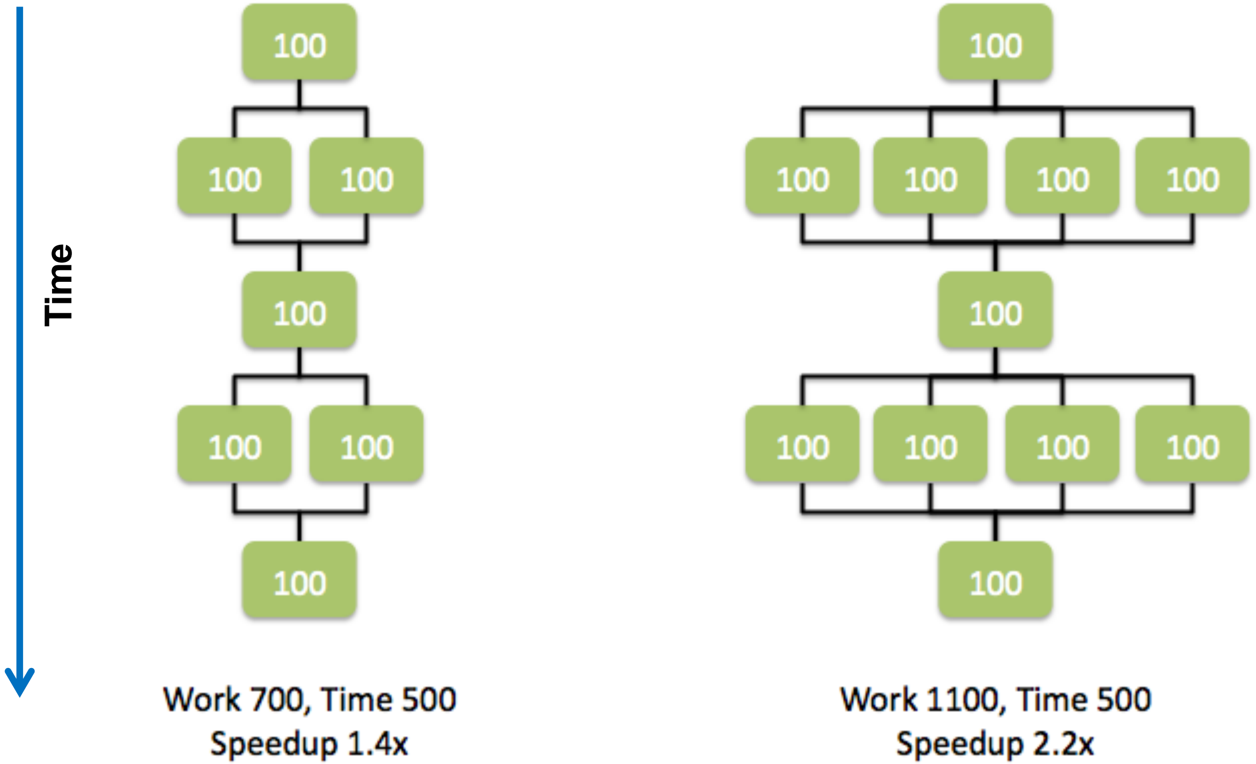
Increase the Problem Size!



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Strong and Weak Scaling

Case A

- A human is waiting in front of the terminal: **strong scaling**
- A problem of a fixed size is processed by an increasing number of processors
- Best modelled with **Amdahl's law**

Case B

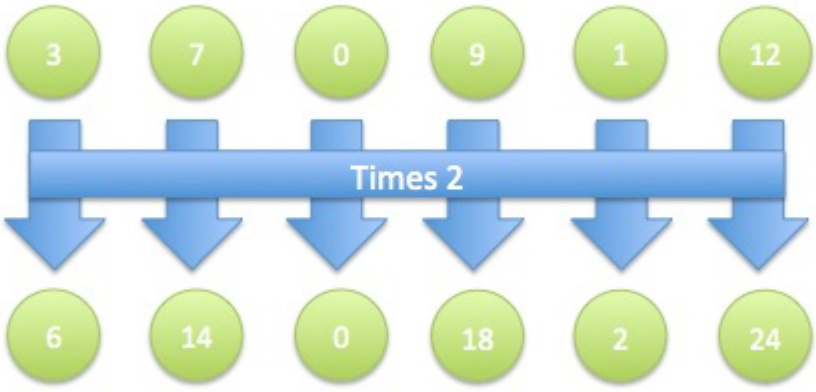
- Want to get the most done in a certain amount of time: **weak scaling**
- Every processor has a specified amount of work to do, and then when adding processors, we also add work
- Best modelled with **Gustafson's law**

Two sides of the same coin!

Data Parallelism

Definition: parallelism achieved through the application of the same transformation to multiple pieces of data

Example of pure data parallelism: multiplication of an array of values (ordinary administration for vector units and GPUs!)



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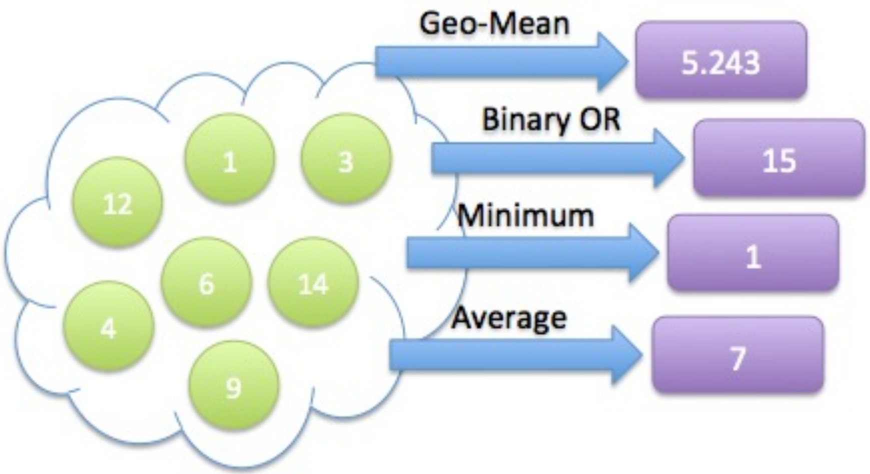
Task Parallelism

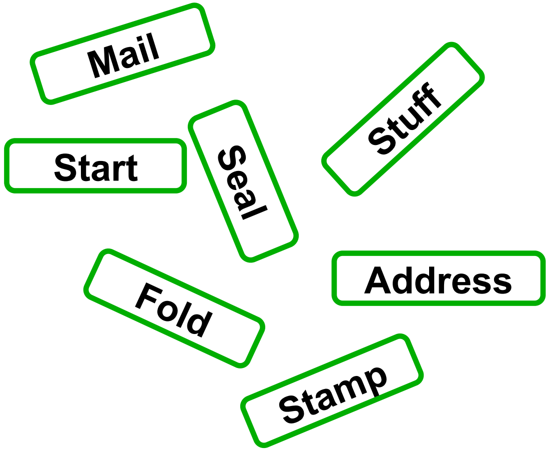
Definition: parallelism achieved through the partition of load in small work baskets consumed by a pool of resources.

Example of pure task parallelism: calculate mean, binary OR, minimum and average of a set of numbers



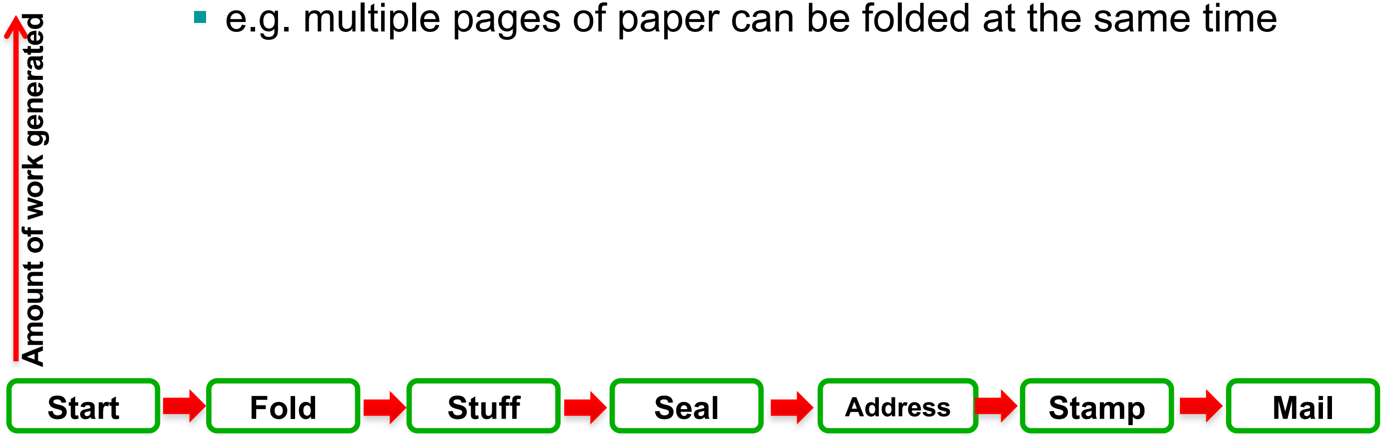
Mixed Solutions

Mandate: Build an efficient letter sending system mixing data and task parallelism



Mixed Solutions

- Fixed order of steps
- Data parallelism is already evident
  - e.g. multiple pages of paper can be folded at the same time



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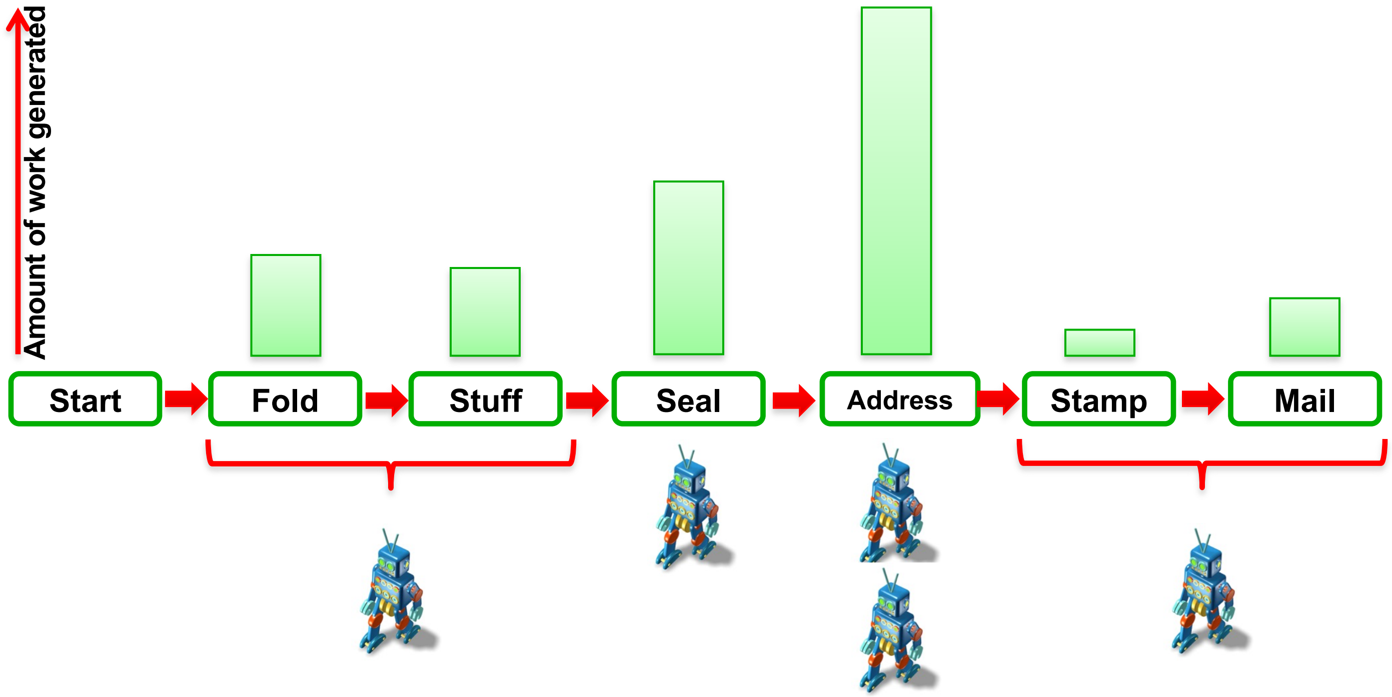
Mixed Solutions

- These operations require different amount of work though



Finding Concurrency

What can be executed concurrently?

Some techniques to figure this out:

- ***Data decomposition***
  - The partition of the data domain
- ***Recursive decomposition***
  - Divide and conquer
- ***Functional decomposition***
  - Split according to program functions
- ***Task decomposition***
  - Split according to logical tasks

DIVIDE
ET
IMPERA

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Mixed Data and Task Parallelism

- Pure task/data parallelism is difficult to achieve in reality
  - Sometimes close enough to real use cases!
- **Mixing data and task parallelism** is the key
  - Many different algorithms applied to a **stream of data**
  - Items processed in **stages** where data parallelism is expressed
  - Many items can pass through the **pipeline** simultaneously
  - Think of items as “collision events” and algorithms as “HEP data processing units”!

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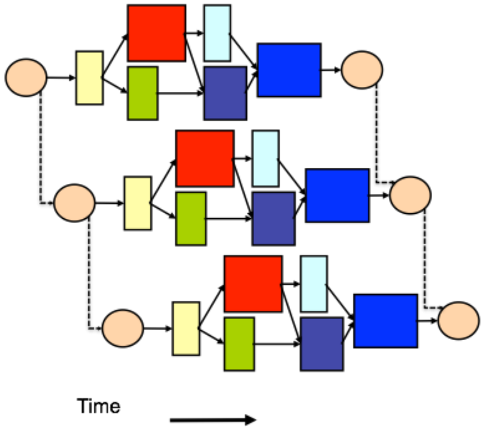
Rethinking the Parallel Framework

- **Need to change the problem size**
  - Process **multiple events concurrently**
  - Helps on tails of sequential processing
- **Contradicts a lot of the basic assumptions in existing code**
  - Code prepared to process only one event at a time in memory
  - But existing code can't be thrown away easily
  - Need to localise distributed states
- **Major effort ongoing in all LHC experiments**
  - Exciting times for curious programmers!



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A Glimpse on Complications

1. **The DAG is not known to its entirety**
   - Hidden dependencies
2. **Shared states are rarely safe**
   - “Caches” that do not behave like… well… caches
3. **Algorithms are not thread-safe**
   - E.g. track reconstruction cannot be run on two events concurrently
   - Making all algorithms thread-safe is an impossible task
4. **External libraries are not thread safe**
   - But independent parts of the framework access them
   - Not all of the libraries will be thread safe ever!

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Solutions?

We need a **smart scheduling** environment

1. **The DAG must be “fixed” by changing the existing code**
2. **Shared states are replaced by task-local data, avoid locks!**
   - More in the next lectures
3. **If an algorithm requires a non-thread safe resource, it has to ‘reserve’ it beforehand**
   - No two algorithms using the resource are scheduled at the same time

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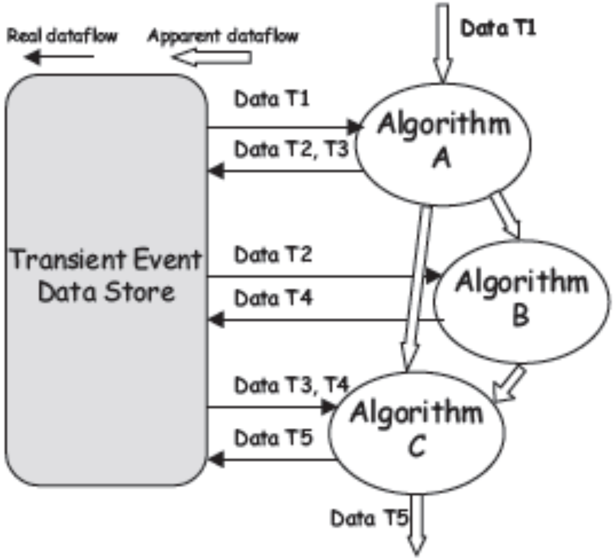
Scheduling Directions

Three ways of coding up a scheduler for the DAG:

- ***On demand***
  Start with the last algorithms in the DAG and invoke whatever algorithm is needed on-the-fly.
  (*backward scheduling*)

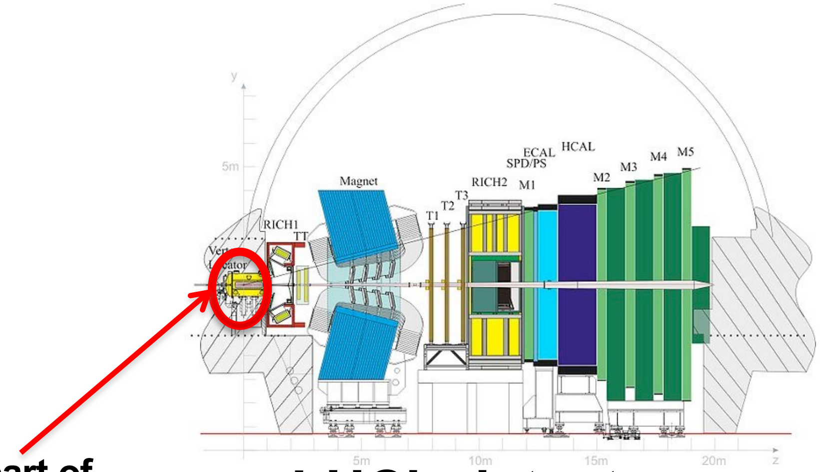
- ***Data driven***
  Start with the first algorithms in the DAG and start new algorithms whenever the necessary inputs are there.
  (*forward scheduling*)

- ***Global view***
  Analyse the entire DAG and schedule algorithms according to the dependency order (*graph scheduling*)



A Simplified Example

- **Such a parallel framework is not only theory**
- **They already exist for**
  - CMS offline software (CMSSW)
  - ATLAS/LHCb framework (Gaudi)
- **Let's have a look at an example workflow**
  - A slice of the LHCb reconstruction
  - Only the low level objects of the vertex locator (VELO)



This part of the detector

LHCb detector

The Velo Low-Level Reco DAG

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Take-Away Messages

- **Dealing with parallelism is inevitable**
  - Software must exploit parallel hardware
  - But there are different levels of exposure to parallelism
- **High energy physics has a history of parallelisation**
  - However, at a rather naïve level
  - The next steps require a harder approach
- **Parallelisation can be exploited in multiple ways**
  - Data parallelism and task parallelism
- **Amdahl's and Gustafson's laws** give a handle for scaling behaviour
- There is a clear strategy for parallelising HEP software
  - Use of a **task-based** approach