Review Calcolo ATLAS Italia

Settembre 2022

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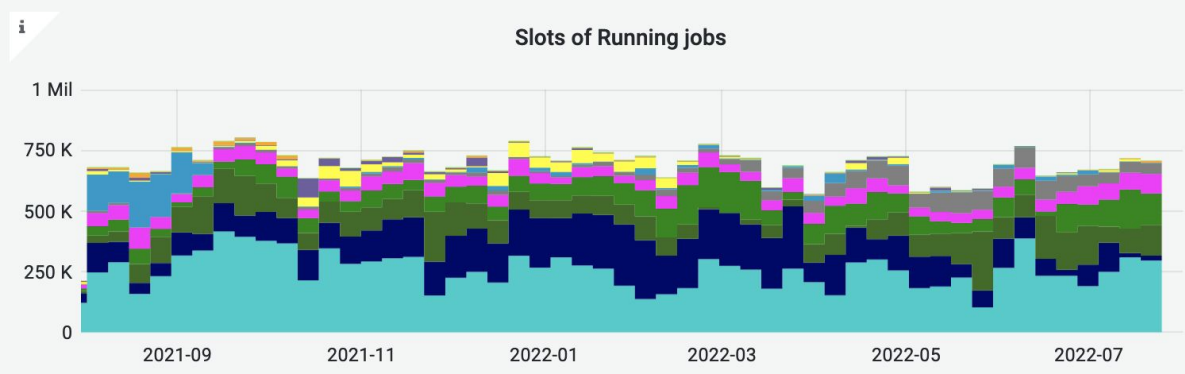
on behalf of the ATLAS-ITALIA computing group

Outline

- Andamento computing ATLAS e contributo ATLAS Italia (luglio 2021-luglio 2022).
- Overview sulle attivita' in corso e sviluppi futuri nel calcolo ATLAS
- Stato acquisti e richieste per il 2023

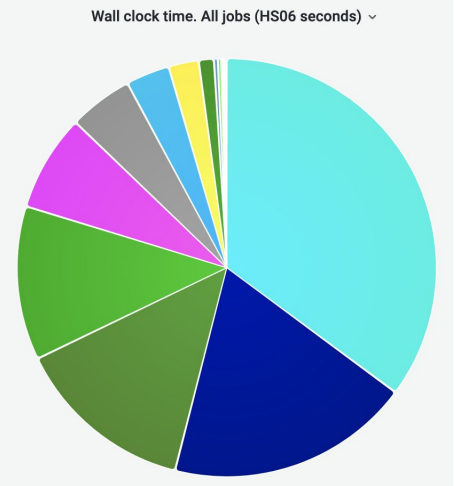
Utilizzo risorse ATLAS (luglio 2021 - luglio 2022) : CPU

- Circa 690k (average) computing slots ogni giorno per tutto il periodo in esame (pledged and unpledged, all Tiers resources together)
  - Importante sforzo che ricade su pochi esperti chiave (sia ADC dia DDM)



- Attivita' tipica di periodi di analisi (senza data taking): Intensa attivita' di produzione MC (~70% includendo generazione, simulazione e ricostruzione) e analisi dati (~25% tra derivations e analisi vera e propria)

	Value	Percent
MC Simulation Full	91 Tri	36%
MC Reconstruction	49 Tri	19%
MC Event Generation	36 Tri	14%
Group Production	31 Tri	12%
User Analysis	19 Tri	7%
Group Analysis	13 Tri	5%
MC Simulation Fast	9 Tri	3%
Data Processing	6 Tri	2%
MC Resimulation	3 Tri	1%



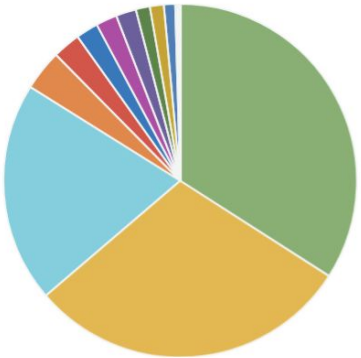
- Efficienza (HS06 seconds) ~ 90%

Utilizzo risorse ATLAS (luglio 2021 - luglio 2022) : disco e tape

- Tape occupato ~ 360 PB (250M files) su 390 PB: principalmente RAW data, AOD e HITS
- Disco occupato ~ 280 PB (850M files) su 290 PB: principalmente dati derivati (DAOD) e AOD

TAPE

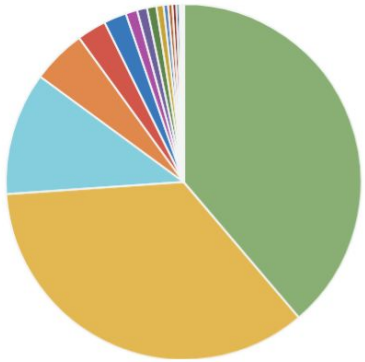
Tape size



	total	percentage
RAW	123 PB	34%
AOD	107 PB	30%
HITS	73 PB	20%
DRAW	13 PB	4%
DAOD	9 PB	3%
NTUP	7 PB	2%
ESD	7 PB	2%
DESD	7 PB	2%
no_name	5 PB	1%
EVNT	5 PB	1%
RDO	4 PB	1%

DISCO

Disk size



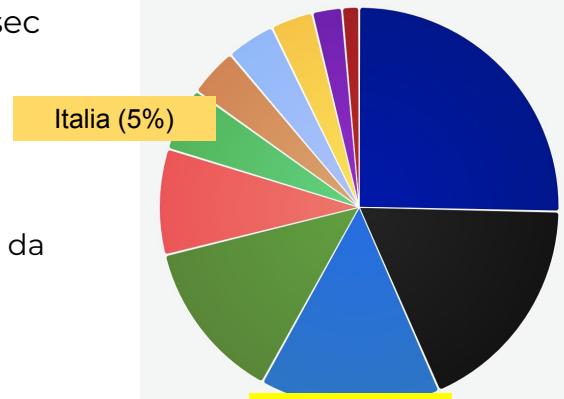
	total	percentage
DAOD	110 PB	39%
AOD	100 PB	35%
HITS	32 PB	11%
EVNT	14 PB	5%
RDO	8 PB	3%
RAW	6 PB	2%
log	3 PB	1%
no_name	3 PB	1%
ESD	2 PB	1%
DESD	2 PB	1%

Contributo italiano computing ATLAS (luglio 2021 - luglio 2022)

Contributo italiano alle attivita' di computing di ATLAS :

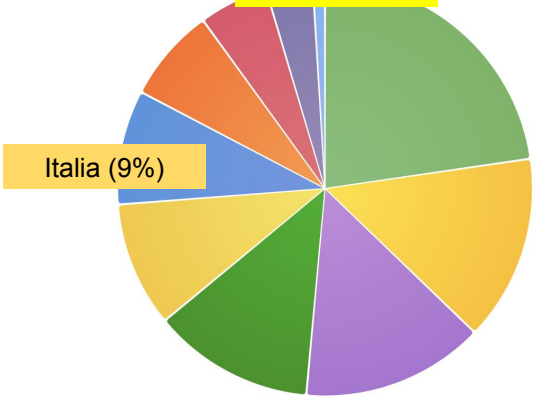
- CPU : overall ~ 5% wallclock time totale in HS06-sec (T1+T2+T3, solo risorse grid, T0 escluso)
  - sotto share : consistente overpledge di alcune cloud, sofferenza a inizio anno
- Disco occupato (datadisk, calibdisk, groupdisk e localgroupdisk) : overall ~6% (escludendo T0)
  - leggermente sotto share alcune risorse ancora da mettere il linea
- Tape (T1 only) : ~9%
  - perfettamente in linea con lo share (9%)

CPU



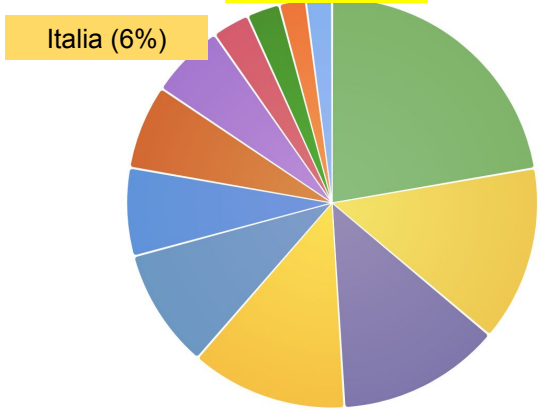
US	31 Tri	25%
DE	22 Tri	18%
FR	18 Tri	15%
UK	16 Tri	13%
CA	11 Tri	9%
IT	6 Tri	5%
NL	5 Tri	4%
ND	5 Tri	4%
ES	4 Tri	3%
RU	3 Tri	2%

TAPE



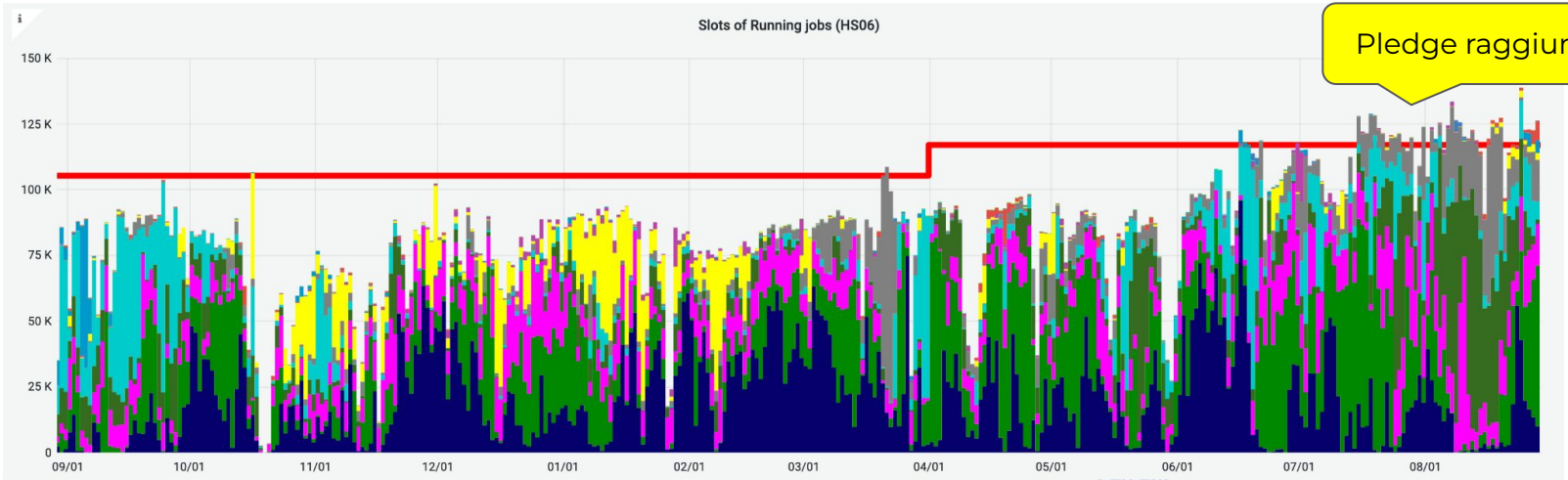
	Value	Percent
US	61 PB	23%
UK	39 PB	15%
FR	38 PB	14%
DE	34 PB	13%
CA	26 PB	10%
IT	24 PB	9%
NL	19 PB	7%
ND	14 PB	5%
ES	10 PB	4%

STORAGE



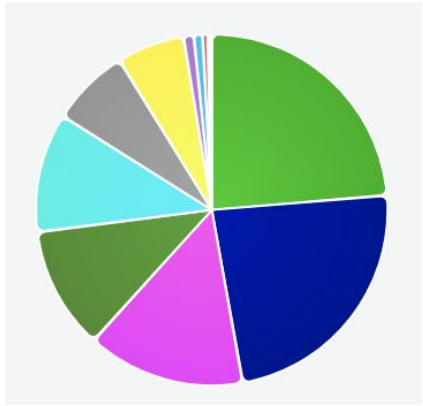
DE	41 PB	14%
FR	38 PB	13%
UK	37 PB	12%
CERN	28 PB	9%
ND	21 PB	7%
CA	20 PB	7%
IT	17 PB	6%
NL	9 PB	3%
ES	8 PB	3%
RU	6 PB	2%

Attivita' ATLAS al T1 : CPU

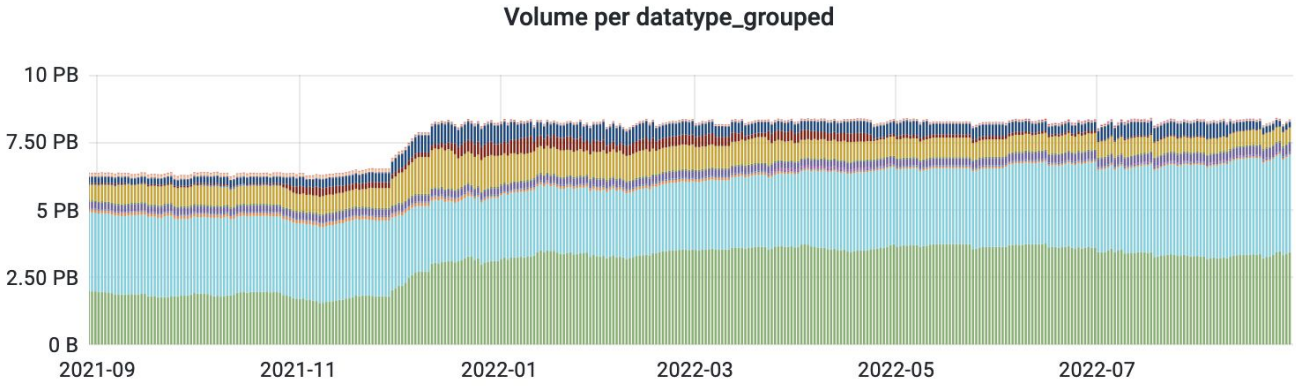


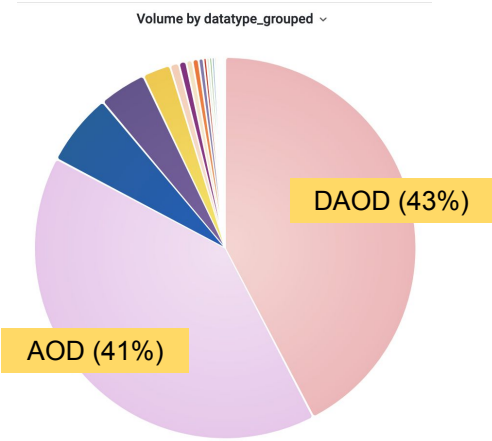
- Share tipico di un T1 per un periodo di analisi dati
  - preparazione dati secondari per l'analisi (group production),
  - analisi (user analysis)
  - produzione di MC
  - Reprocessing
- In sofferenza per problemi procurement delle risorse : average pledge 110 kHS06, computing power fornita 85 kHS06

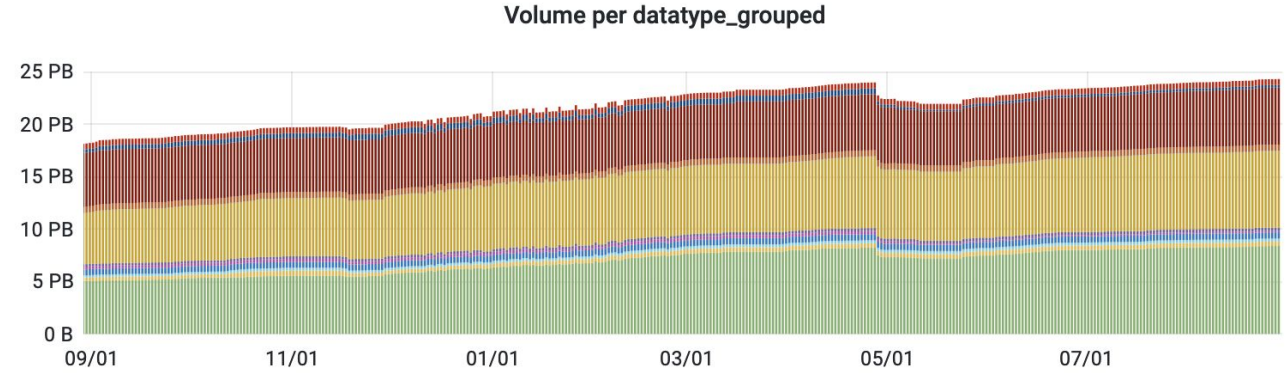
Group Production	24%
MC Reconstruction	24%
User Analysis	15%
MC Event Generation	11%
MC Simulation Full	11%
Group Analysis	7%
Data Processing	6%
MC Merge	1%
MC Simulation Fast	1%

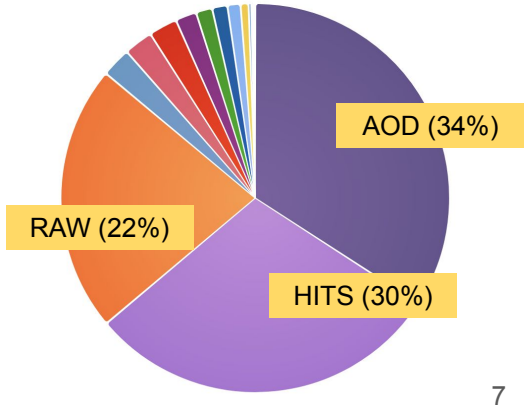


Attivita' al T1 : occupazione disco e tape

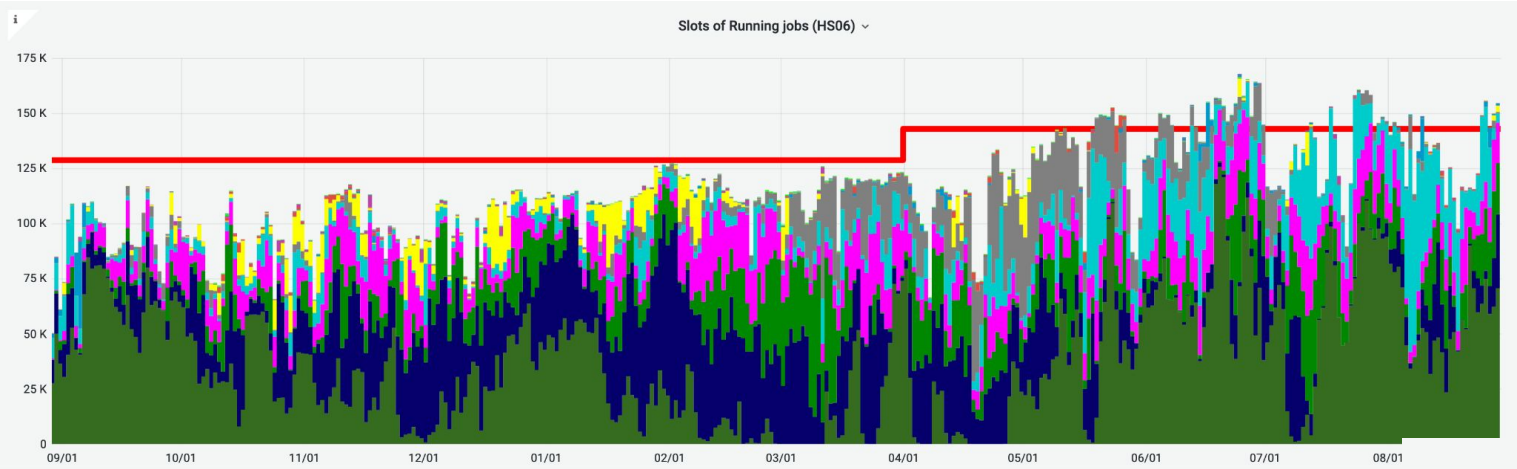




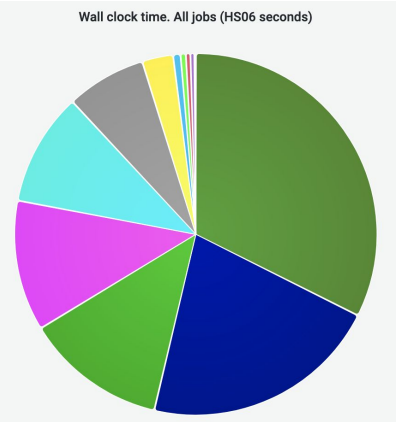




Attivita' ATLAS ai T2 : CPU



- Tipico share T2 :
  - MC (generation, simulation e reconstruction)
  - produzione di dati secondari (group production) e analisi utenti
-



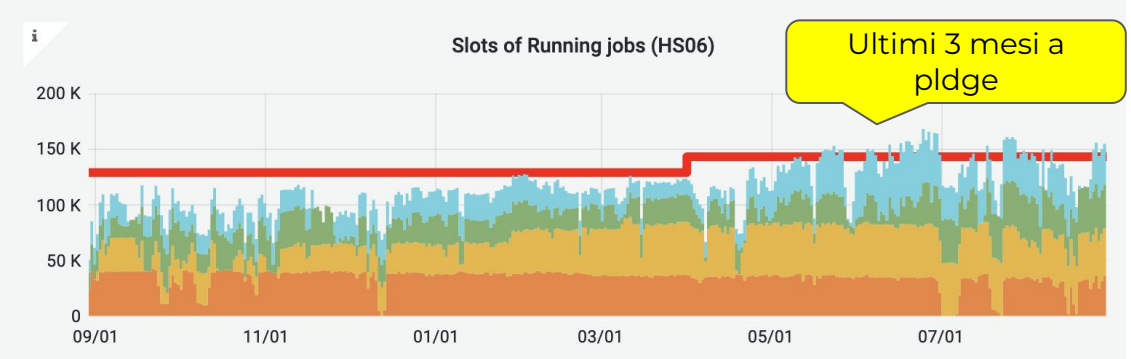
	Percent
MC Event Generatio	33%
MC Reconstruction	21%
Group Production	13%
User Analysis	12%
MC Simulation Full	10%
Group Analysis	7%
Data Processing	3%
MC Simulation Fast	1%
Testing	0%

Attivita' ATLAS ai T2 : CPU

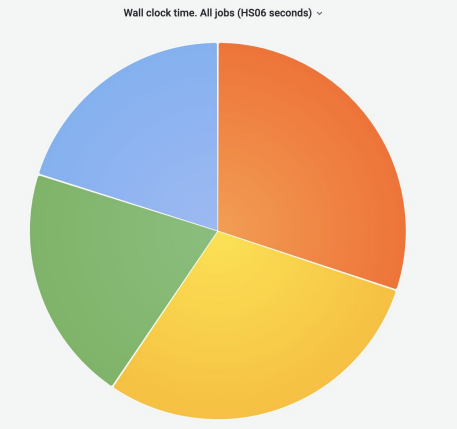
- In generale buon comportamento dei T2 italiani per l'ultimo anno di attivita'
  - reliability/availability ~ 95 %
  - Efficienza ~ 91%
  - Valori in linea con i migliori siti ATLAS

Leggero under-pledge (~15%) sulla CPU fornita (average pledge 135 kHS06, computing power fornita 114 kHS06)

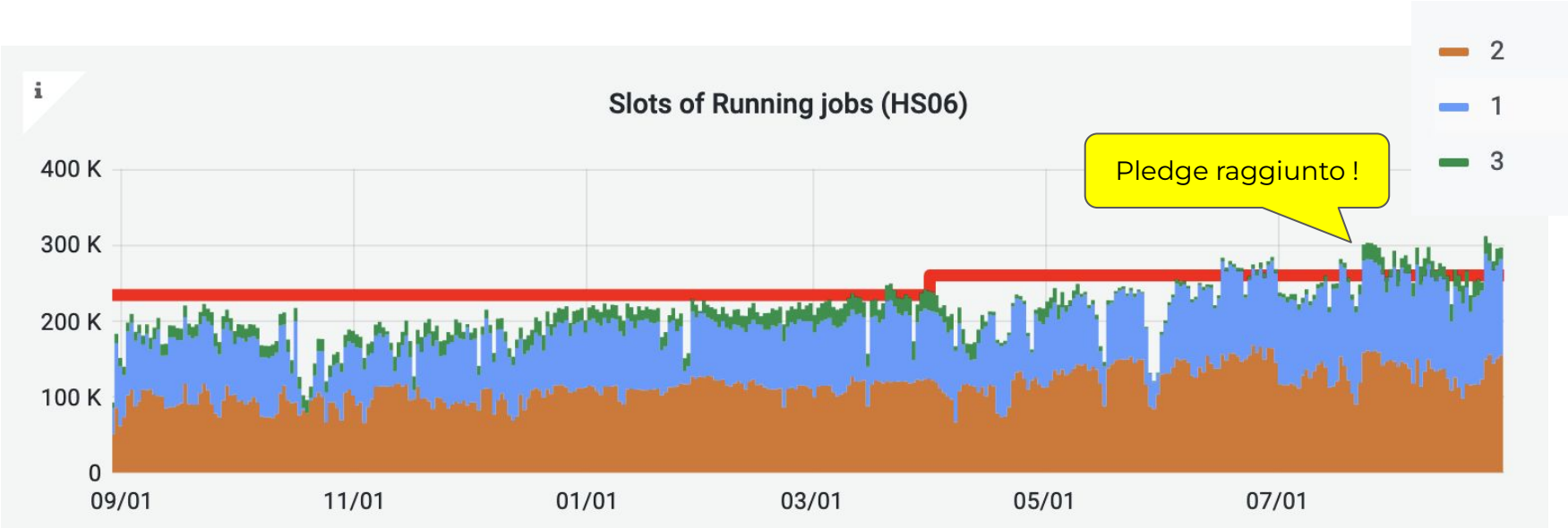
- Roma1 problema elettrico persistente con uno dei rack
- Milano ha lavorato alla sostituzione degli apparati di rete
  - Buona performance ma ristretta attivita' a task meno i/o intensive (generazione e simulazione)
  - Nell'ultimo mese riattivati tutti i workflow, non si sono piu' osservati problemi con lo storage (ma la statistica e' ancora piccola)



	Percent
INFN-FRASCATI	30%
INFN-NAPOLI-ATLAS	29%
INFN-ROMA1	20%
INFN-MILANO-ATLASC	20%



CPU performance summary (all sites)



Globalmente leggera sofferenza dei siti italiani

- 245 kHS06 pledge, 214 kHS06 delivered : T2 e T1, contributo dei T3 (15 kHS06, 6%) leggermente sotto la norma. Evidente recupero nell'ultimo periodo (ultimo mese 272 kHS06 delivered, 260 kHS06 pledge)
- Overall efficiency ~ 91% (in linea con l'efficienza della media dei siti ATLAS)

Situazione e disco e TAPE

	Disco occupato (PB) (dati luglio 2022)	Disco allocato (PB) (dati luglio 2022)
Frascati	1.42	2.43
Milano	1.47	1.68
Napoli	3.9	4.26
Roma	1.53	1.74
tot.	8.32	10.11

Importante intervento di IBISCO per crisi disco ATLAS

- Pledge 2022 : 9.94 PB

	Disco occupato (PB) (dati luglio 2022)	Disco allocato (PB) (dati luglio 2022)	Tape (PB) (dati luglio 2022)
CNAF	8.91	9.57	24.48

- Pledge 2022 (disco): 10.44 PB
- Pledge 20212(tape): 24.48

Responsabilita' calcolo italiani dentro ATLAS

ATLAS Italia partecipa alle attività di Atlas Distributed Computing (ADC) in diversi aspetti

- Containers (docker, singularity) [A. De Salvo]
- Database (Frontier, Conditions) [A. De Salvo, L. Rinaldi]
- Harvester (evoluzione del WFMS di ATLAS) [A. De Salvo]
- International Computing Board [L. Carminati, L. Rinaldi]
- "S&C Financial Advisor" [D. Barberis]
- Installazione del software (CVMFS e distribuzione) [A. De Salvo]
- ADC Monitoring [dal 2017] [D. Barberis]
- ASCIG (ATLAS Software & Computing Infrastructure Group) [dal 2019] [D. Barberis]
- Network infrastructure (LHCONE) [Tutta la federazione italiana dei T1/T2/T3 italiana]
- distributed computing and storage evolution R&D [G. Carlino, A. De Salvo, A. Doria, E. Vilucchi]
  - Federazioni di xrootd e HTTPD, DPM, Storage Caching, ...
- VO management [A. De Salvo, E. Vilucchi]
- Chair computing speakers committee [L. Perini]
- EventIndex [D. Barberis]
- Tier2 :
  - Gestione infrastrutture, R&D, etc. [A. De Salvo, A. Doria, D. Rebatto, E. Vilucchi]
- Tier3 :
  - A. Budano, M. Corosu, A. Forte, A. Tarasio

Schedule

Intenso piano di lavoro per la comunita' computing per il 2022/2023

Data sample	Activity	2021				2022				2023			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Run 2 Data	DAOD Production and User Analysis												
	DAOD_PHYS Production												
	Reprocessing in Release 22												
Run 2 MC	New Production for Ongoing Analyses												
	DAOD_PHYS Production												
	Reprocessing in Release 22												
Run 3 Data	Tier-0 Reconstruction												
	Partial Reprocessing												
	Full Reprocessing												
	Delayed stream Reconstruction												
	DAOD Production and User Analysis												
Run 3 MC	Generation												
	Simulation												
	Reconstruction												
	Re-Reconstruction												
	DAOD Production and User Analysis												
Upgrade MC	Production and Analysis												
Heavy Ions	First pass Reconstruction												

Full steam Partial

Richieste 2023 da RRB

CERN-RRB-2022-050

ATLAS		2021			2022		2023		
		C-RSG recomm.	Pledged	Used	C-RSG recomm.	Pledged	Request	2023 req. / 2022 C-RSG	C-RSG recomm.
CPU	Tier-0	525	525	577	550	550	740	135%	740
	Tier-1	1170	1170	1340	1300	1300	1430	110%	1430
	Tier-2	1430	1430	2704	1588	1588	1747	110%	1747
	HLT	n/a	n/a	619	n/a	n/a	n/a	n/a	n/a
	Total	**3125**	**3125**	**5240**	**3438**	**3438**	3917	114%	3917
	Others			2388					
Disk	Tier-0	29.0	29.0	36.0	32.0	32.0	40.0	125%	40
	Tier-1	105.0	116.3	113.0	116.0	116.0	136.0	117%	136
	Tier-2	130.0	127.2	114.0	142.0	142.0	168.0	118%	168
	Total	**264.0**	**272.5**	**263.0**	**290.0**	**290.0**	**344.0**	**119%**	**344**
Tape	Tier-0	95.0	95.0	85.0	120.0	120.0	174.0	145%	174
	Tier-1	235.0	241.2	231.0	272.0	272.0	353.0	130%	353
	Total	**330.0**	**336.2**	**316.0**	**392.0**	**392.0**	**527.0**	**134%**	**527**

Richieste T1

ATLAS C-RSG recommended 2023

	ATLAS 2023 pledge	Italy share 2022	ATLAS IT 2023 pledge	Richieste 2023	Richieste 2023 (k€)	ATLAS 2022 pledge	Italy share 2022	ATLASIT 2022 pledge
CPU T1 (HS06)	1430000	0,09	128700	11700	175500	1300000	0,09	117000
Disco T1 (TB)	136000	0,09	12240	1800	252000	116000	0,09	10440
Tape T1 (TB)	353000	0,09	31770	7290	72900	272000	0,09	24480
Totale (k€)					500400			

- Richieste calcolate rispetto al pledge del T1 (non rispetto alle risorse effettive attualmente disponibili)
- Mantenuto lo stesso share per ATLAS-IT (9%)
- Obsolescenza non inclusa
- Fattori di conversione : 140 €/TBn (disco), 15 €/HS06 (cpu), 10 €/TBn (tape)

Richieste T2 complessive

ATLAS C-RSG recommended 2023

	ATLAS 2023 pledge	Italy share 2023	ATLAS IT 2023 pledge	ATLAS 2022 pledge	Italy share 2022	ATLASIT 2022 pledge
CPU T2 (HS06)	1747000	0,09	157230	1588000	0,09	142920
Disco T2 (TB)	168000	0,07	11760	142000	0,07	9940

- Mantenuto lo stesso share ATLAS-IT (9% CPU e 7% disco)

Stato risorse al 2022

- Storage:
  - La saga della gara unica da 2.2 PB (2020 !) si sta avviando a conclusione: ritardi (ed errori) nelle consegne. Risorse presso i siti, installazione prima dell'estate (Frascati e Roma), online a brevissimo. Installazione in corso a Milano
  - Acquisto singolo a Frascati 2021 terminato
  - Gara comune disco 2022 : capitolato pronto, partenza gara a brevissimo

- CPU :
  - Acquisti 2021 : ok a Roma1 in convenzione, Milano problemi con la convenzione (acquisto diretto)
  - Acquisti 2022 : non ancora finalizzati

Richieste dettagliate T2 : CPU

CPU	Frascati	Milano	Napoli	Roma1	Totale	Pledged
Finanziato 2022 (HS06)	36812	35781	34097	35204	141894	142920
Aggiornato 2022 (HS06) (*)	35312	36286	38886	30511	140995	
Obsolescenza 2023 (**)	16866 (8433/8433)	8004 (0/8003)	0	8004 (0/8003)	32874	
Obsolescenza 2022 non finanziata	0	422	0	6517		
Delta 2023	3000	3000	3000	3000	12000	
Totale richieste 2023 (HS06)	19866	11426	3000	17521	51813	
Totale CPU nel 2023 (HS06)	38312	39708	41886	40028	159934	157230

(*) numeri aggiornati dopo inserimento nuove risorse da gare in corso
(**) in parentesi (obsolescenza primo semestre 2023 / obsolescenza secondo semestre 2023)

Richieste dettagliate T2 : disco

Disco	Frascati	Milano	Napoli	Roma1	Totale	Pledged
Finanziato 2022 (TB)	2839	2432	2355	2432	10058	9940
Aggiornato 2022 (TB) (*)	3328	2489	4327	2624	12768	
Totale disco 2022 aggiornato (TB) senza LOCALGROUPDISK (**)	3148	2309	4147	2444	12048	
Obsolescenza 2023	0	0	0	0	0	
Delta 2023 (TB)	0	0	0	0	0	
Totale richiesta 2023 (TB)	0	0	0	0	0	
Totale disco 2023 (TB)	3148	2309	4147	2444	12048	11760

- (*) numeri aggiornati dopo inserimento nuove risorse da gare in corso
- (**) come al solito 180 TB a sito per LOCALGROUPDISK
- Napoli ha anticipato 2PB di disco IBISCO per crisi disco ATLAS

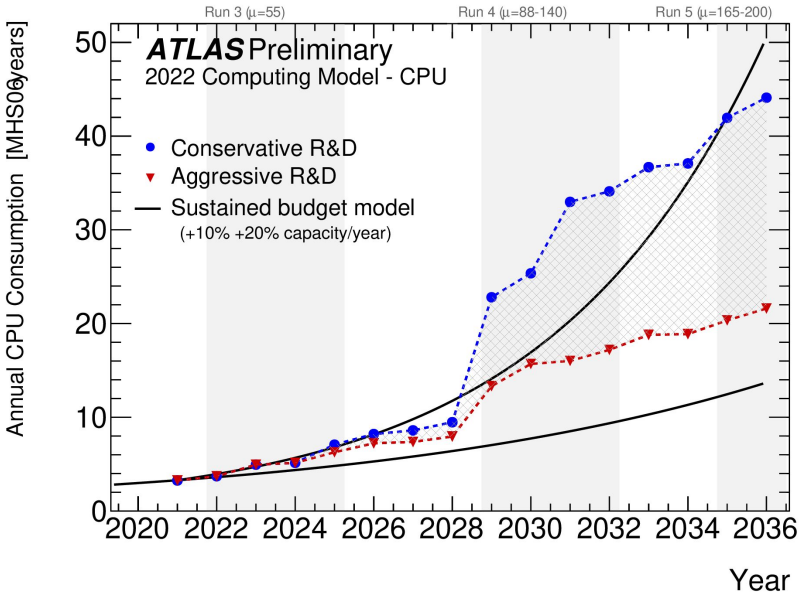
Richieste finanziarie T2

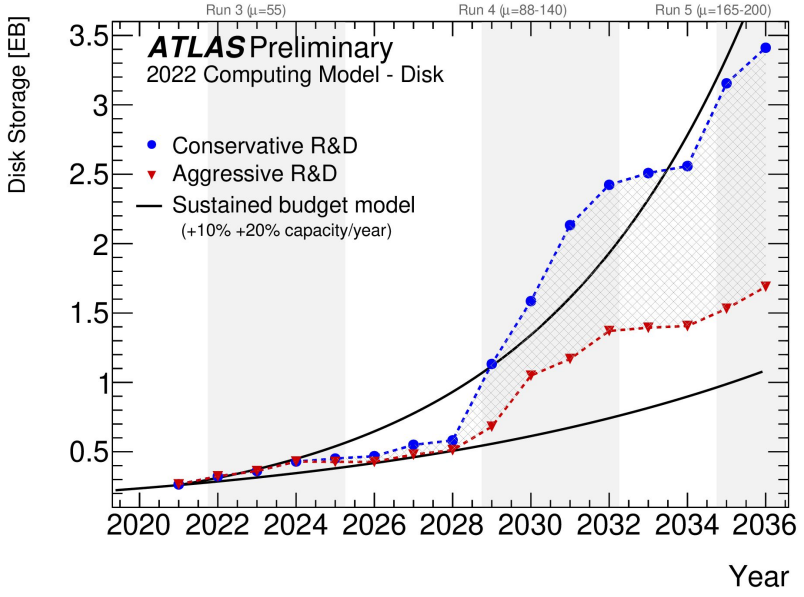
	Frascati	Milano	Napoli	Roma1	Totale
Richiesta CPU (k€)	297990	171390	45000	262815	777195
Richiesta Disco (k€)	0	0	0	0	0
Richiesta totale (k€)	297990	171390	45000	262815	777195
Overhead server (k€)	20859,3	11997,3	3150	18397,05	54403,65
Overhead rete (k€)	17879,4	10283,4	2700	15768,9	46631,7
Tot + TUTTI overhead	336728,7	193670,7	50850	296980,95	878230,35
Totale (escluso PON)	827380,35				
Totale (escluso PON e OH rete)	783448,65				

- Algoritmo per calcolo overhead : “server” : 7% del totale CPU + disco, “rete” : 6% CPU e 5% disco
- Fattori di conversione : 140 €/TBn (disco), 15 €/HS06 (cpu), 10 €/TBn (tape)

ATLAS Computing roadmap

ATLAS HL-LHC Computing Conceptual Design Report : projections of ATLAS computing requirements for Run3 and HL-LHC to fully exploit the machine physics potential is quite scaring !





Discussion started on possible strategies to meet the demanding requirements of HL-LHC

- optimisation (both speed and flexibility) of the experiment (e.g. reconstruction, simulation) and non-experiment (e.g. generation) software
- optimisation of the available hardware infrastructure usage

ATLAS Computing roadmap

- Exploitation of HPC resources : ATLAS has used up to 2.5 the computing pledge resources last year
  - Impressive contribution from HPC resources, mainly (~75% of the full HPC resources used by ATLAS) from opportunistic access to VEGA (Maribor, Slovenia within the EuroHPC program)
  - HPC jobs overall efficiency ~ 90%, very close to more 'standard' grid resource
  - VEGA very peculiar: able to run almost all workflows
- Data carousel in phase IV : use it for many workflows in parallel respecting computing share per workflow. Run Data Carousel jointly for more than one experiment
- Simulation optimisation :
  - Optimise G4 full simulation : expect up to 30% reduction
  - Pushing on fast calo simulation (ATLFAST III) : GAN based e/o parametrized CaloSim
  - Fast simulation for the ATLAS Tracker, FATRAS (FATRAS + FastCaloSim is ~50 times faster than pure Geant4).
  - More in general : build a chain of fast simulation tools (FastChain) for fast simulation, digitization and reconstruction, to be used interchangeably depending on the specific analyses need
- Reduce the impact of the analysis model on the storage : Introduced a new single DAOD_PHYS targeted for all (>~80%) physics analysis (~50 kB/event).
  - In addition a new smaller DAOD_PHYSLITE format (10 kB/event) will be introduced that contains already calibrated physics objects and will be centrally produced with frequent updates, typically every few months. A larger fraction of the AODs will be removed from disk and staged-in back from tape storage on demand in a so called data carousel mode of operation.

Conclusioni

- I siti italiani hanno continuato a lavorare in modo efficiente per tutto il periodo luglio 2021-luglio 2022. Siti affidabili (elevata reliability e availability) e con efficienza paragonabile ai migliori centri ATLAS
- Varie attivita' in corso dentro l'esperimento per ottimizzare l'uso delle risorse (G4 optimisation, fast simulation, nuovo analysis model, tape carousel, AthenaMT, integrazione di risorse HPC)
- Principali attivita' in corso nella comunita' italiana :
  - Studi per la migrazione dello storage (Frascati, Napoli, Roma) a DCache : preparazione di un testbed entro fine anno, migrazione effettiva il prossimo anno
  - Esplorazione attivita' di analisi su risorse INFN-Cloud recentemente partita (C. Marcon)
- Presentata la situazione delle risorse disponibili (gare) e le richieste per il 2023
  - Mantenuti gli stessi share delle scorse richieste
  - Nessuna azione immediata per quanto riguarda la crisi russa ma la situazione e' monitorata costantemente

ciao Laura !

Proiezione obsolescenze

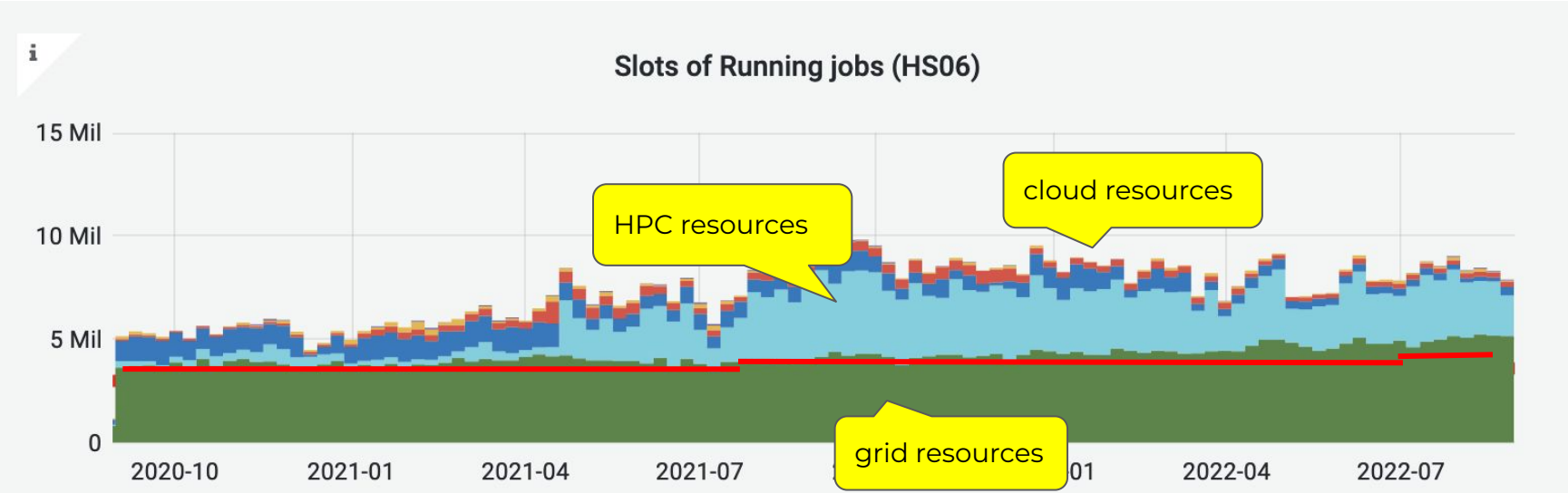
Proiezione obsolescenze CPU (HS06)

	2023	2024	2025	2026	2027	2028
Frascati	16866	10004		8440		
Milano	8003	5877			14000	8400
Napoli	0		2667			36200
Roma	8003			14000		8400
totale	32872	15881	2667	22440	14000	53000

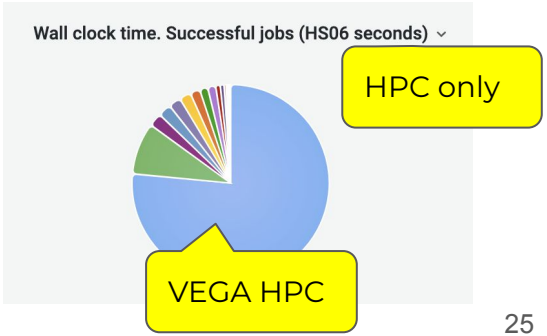
Proiezione obsolescenze disco (TBn)

	2023	2024	2025	2026	2027	2028
Frascati	0			561		1800
Milano	0	800		850		
Napoli	0			500		3500
Roma	0	800				
totale	0	1600	0	1911	0	5300

ATLAS Computing per type of resources



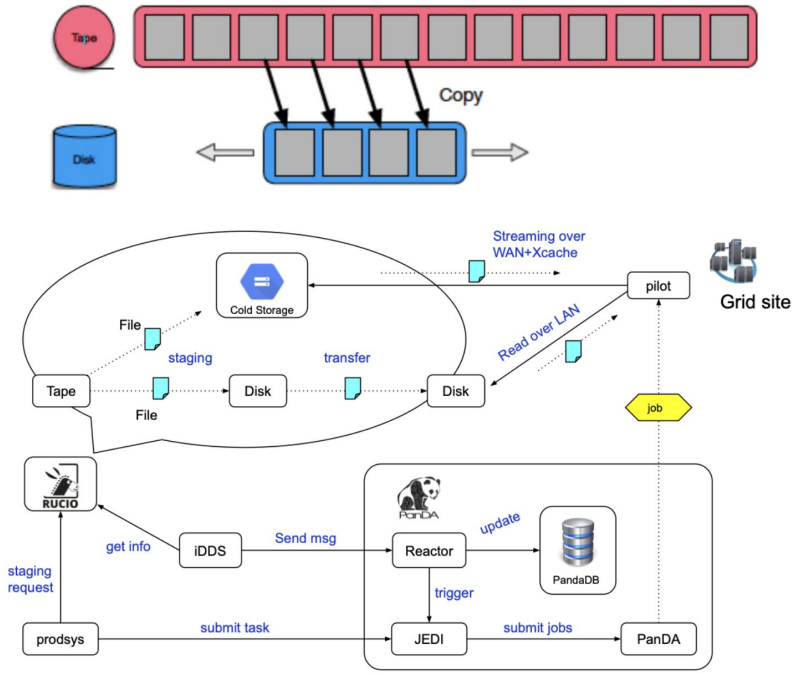
- ATLAS has used up to 2.5 the computing pledge resources last year
- Impressive contribution from HPC resources, mainly (~75% of the full HPC resources used by ATLAS) from opportunistic access to VEGA (Maribor, Slovenia within the EuroHPC program)
- HPC jobs overall efficiency ~ 90%, very close to more ‘standard’ grid resource
- VEGA very peculiar: able to run almost all workflows



The Tape Carousel model

The Data Carousel is the orchestration between the workflow management systems ProdSys2 and PanDA, the distributed data management system Rucio, and the tape services. It enables a bulk production campaign, with input data resident on tape, to be executed by staging and promptly processing a sliding window of a fraction of the input onto buffer disk such that only a percentage of the data are pinned on disk at any one time

- Phase I: Tape system performance evaluation at CERN and the WLCG Tier-1 centers.
- Phase II: Deeper integration between workflow, workload and data management systems (ProdSys2/PanDA/Rucio), and Identify missing software components
- Phase III: Run Data Carousel at scale in production for the selected workflows with an ultimate goal to have it operational before LHC Run 3 in 2022.
  - reprocessing of run2 data/MC
  - production of derived data
- Phase IV : use data carousel for many workflows in parallel respecting computing share per workflow. Run Data Carousel jointly for more than one experiment



Future of fast simulation : FastChain

- Optimise G4 full simulation : expect up to 30% reduction
- Pushing on fast (calo) simulation ATLFAST III : GAN based e/o parametrized CaloSim
- The next step will be a fast simulation for the ATLAS Tracker, FATRAS (within ACT : FATRAS + FastCaloSim is ~50 times faster than pure Geant4).
- More in general : build a chain of fast simulation tools (FastChain) for fast simulation, digitization and reconstruction, to be used interchangeably depending on the specific analyses need

HS06 x seconds

$\langle\mu\rangle$	Full Simulation	GEANT4 + FastCaloSim V2	FatRas + FastCaloSim V2 + GEANT4	pile-up Digitization	MC Overlay
140	5684	1137	114	3317	183
200	5684	1137	114	4233	202

Fast Calo simulation

Fast Calo + tracking simulation

RDO overlay

- Might also stop saving simulation output (HITS) as an intermediate format and go straight from EVNT to AOD in a single production step on the grid (save storage) .
- Aiming for production-readiness before the end of Run 3.

A new analysis model

- AODs and DAODs which are the two formats taking more than 70% of the disk space today
- Introduce instead a new single DAOD_PHYS targeted for all (>~80%) physics analysis (~50 kB/event).
- In addition a new smaller DAOD_PHYSLITE format (10 kB/event) will be introduced that contains already calibrated physics objects and will be centrally produced with frequent updates, typically every few months. A larger fraction of the AODs will be removed from disk and staged-in back from tape storage on demand in a so called data carousel mode of operation.
- Allow exceptions for performance groups, B-physics (separate stream), long lived particle searches....

	MC				Data			
	AOD	DAOD	DAOD PHYS	DAOD PHYS LITE	AOD	DAOD	DAOD PHYS	DAOD PHYS LITE
events	$3 \cdot 10^{10}$	$1 \cdot 10^{11}$	$3 \cdot 10^{10}$	$3 \cdot 10^{10}$	$2 \cdot 10^{10}$	$1 \cdot 10^{11}$	$2 \cdot 10^{10}$	$2 \cdot 10^{10}$
size/event [kB]	600	100	70	10	400	50	40	10
disk space [PB]	18.0	10.0	2.1	0.3	8.0	5.0	0.8	0.2
other versions	1.5	2	2	2	1.5	2	2	2
repl. fac.	0.5	1	4	4	0.5	2	4	4
Sum [PB]	13.5	20.0	16.8	2.4	6.0	20.0	6.4	1.6

50% of AOD on tape

4 replicas of derived data formats, 2 versions kept

- Run2 AM requires 132 PB
- Run3 AM would require ~85 PB

- The new model opens to the possibility of the creation of Analysis Facilities (few PB of disk space)

ATLAS Computing performance

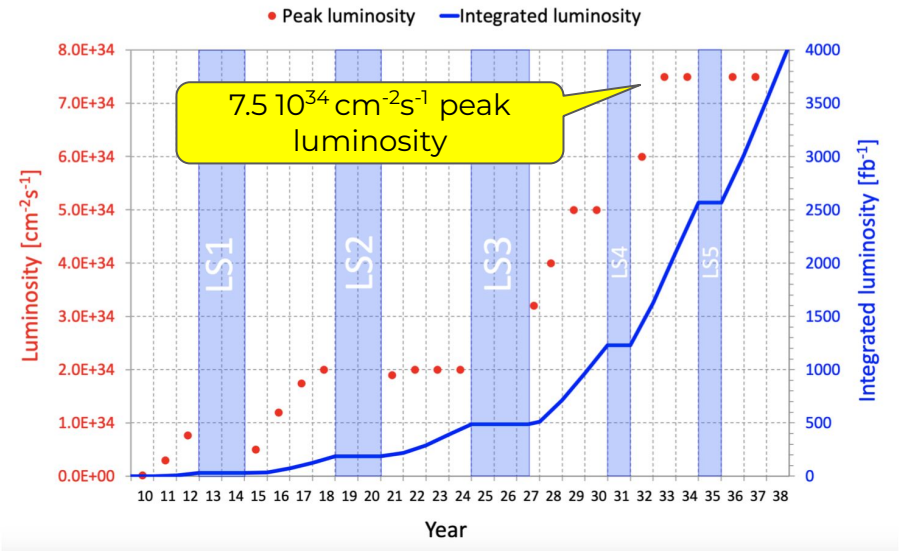
- Baseline: ATLAS implements the new data formats foreseen by the Run 3 analysis model, the multi-threaded software framework AthenaMT, and updates to the tracking code, but otherwise continues in largely the same way as in Run 2. In particular the CPU time per event for event generation, detector simulation and reconstruction is assumed to remain at the level currently achieved by applying the current software to the Phase-II detector simulation, and the mixture of generators and simulation remains the same;

- Conservative R&D: the research and development activities currently under way for Run 3 are assumed to be successful, including the data carousel, fast track reconstruction, lossy compression, and most of the detector simulation is done with fast simulation;

- Aggressive R&D: ATLAS implements new developments that very significantly improve the speed or storage volumes of workflows that currently are heavy consumers of resources, for example, porting of high-precision generators to GPUs, sharing events with CMS, or speeding up the full simulation either by software efficiencies or porting parts of the code to GPUs. Almost universal adoption by the physics groups of DAOD_PHYSLITE and development of very high quality fast simulation that could replace full simulation in almost all cases, would also fall into this category.

ATLAS Computing requirements for run3/4/5

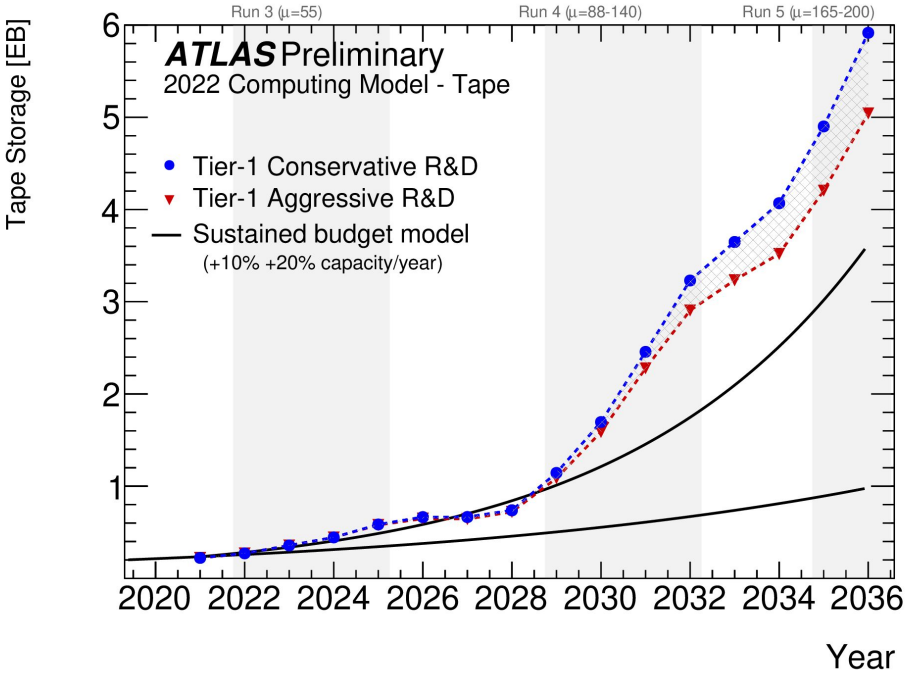
- The physics potential of HL-LHC is enormous, in 2034 expect 5 times the total statistic collected up to now in previous runs
- The amount of data and experimental conditions will pose severe challenges to the computing model



Parameter	unit	2023 Run3	2029 Run 4	2033 Run5
Interaction/crossing	max μ	55	140	200
Integrated luminosity	$fb^{-1}y^{-1}$	100	300	450
LHC ready for physics	10^6 s	7	7	7
Rate	kHz	1.4	10	10
Recorded events	10^9	10	70	70

- ATLAS HL-LHC Computing Conceptual Design Report : projections of ATLAS computing requirements for Run3 and HL-LHC to fully exploit the machine physics potential is quite scaring !

ATLAS Computing requirements



The re-simulation workflow

A new workflow, MonteCarlo ReSimulation, was developed to minimize the resources needed to apply physics improvements to already generated FullSim HITS: the resources used by this workflow are 5-10% of the ones which would have been needed if we should have re-run the FullSim completely.

- Quasi-stable particles (b-hadrons, τ) not propagated correctly in Geant4 → impact on performance
- Resimulation of events with long living high-pT particles. Only a fraction of the events (varying for different samples) is processed
- Current status: total production: ~16 B events passed through re-simulation

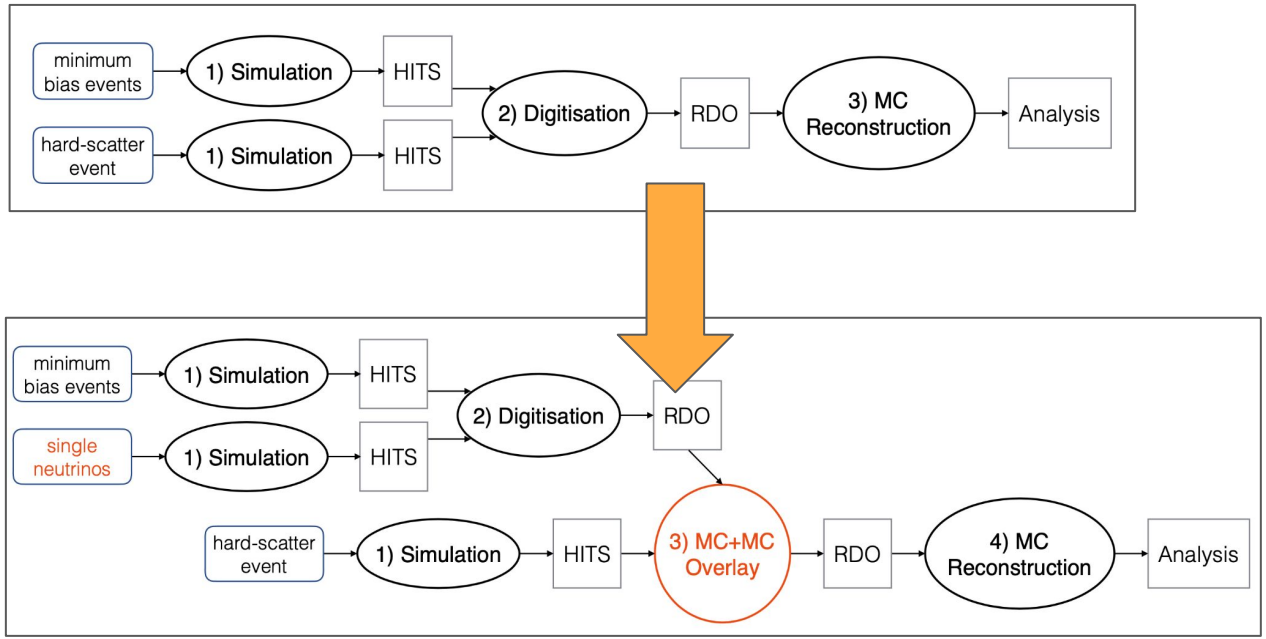
More on VEGA setup

- Vega site, 3 PQs, aCT push mode:
  - Vega (1GB/thread, 16-core)
  - Vega_largemem(4GB/thread, 16-core)
  - VEGA_MCORE (simul only, 64-core), testing 16-core as well
- NDGF-T1 storage endpoint
  - + CERN-PROD_DATADISK for simul inputs
- 2 ARC-CEs, 6 ARC data-delivery, 6 squids
  - Arex optimized (6.13 coming) for memory usage and transfer throughput
- Node outbound through 100 Gb/s NAT (ipv4, ipv6)
- Nodes: cvmfs + local nvme, 50GB file swap added for stability

New pileup modelling

The ATLAS detectors readout is sensitive to up to 39 LHC bunch-crossings (BCs) around the trigger BC.

- The average number of interactions that must be included is ~ 1560 (assuming 40 average interactions per bunch-crossing) : simulating this many extra interactions for each hard-scatter event would be prohibitive



- Simulate hard-scatter and minimum bias evts with G4
- Presampling: a large sample (1B) of combined pile-up events is produced from simulated minimum bias events during a separate digitisation step.
- Each simulated hard-scatter event is digitised and combined with an event sampled from these pileup datasets.
- CPU and I/O requirements of the digitisation are significantly lower and have almost no dependence on μ.
- Pre-mixed pile-up events can be reused for different hard-scatter samples

New pileup modelling

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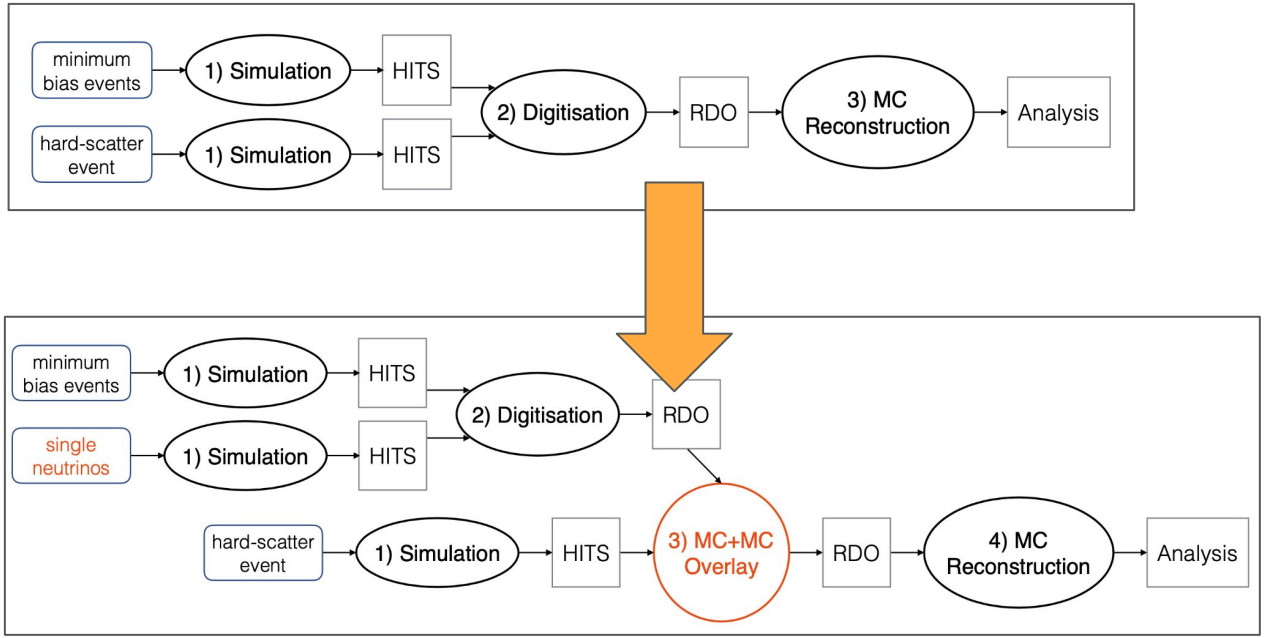
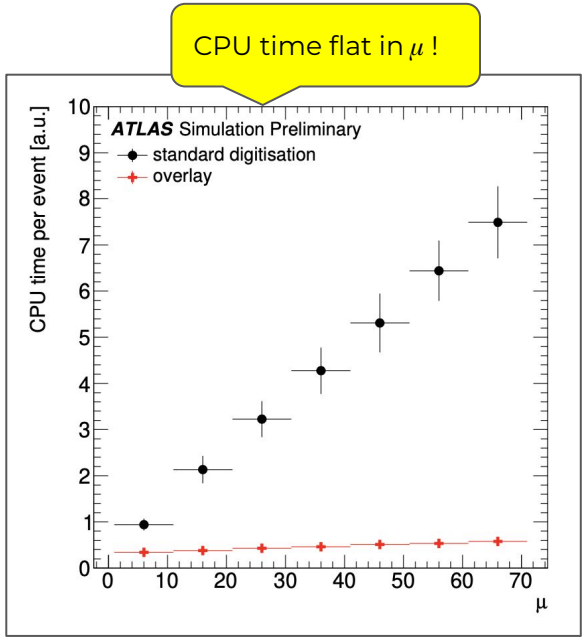
- The average number of interactions that must be included is ~ 1560 (assuming 40 average interactions per bunch-crossing) : simulating this many extra interactions for each hard-scatter event would be prohibitive

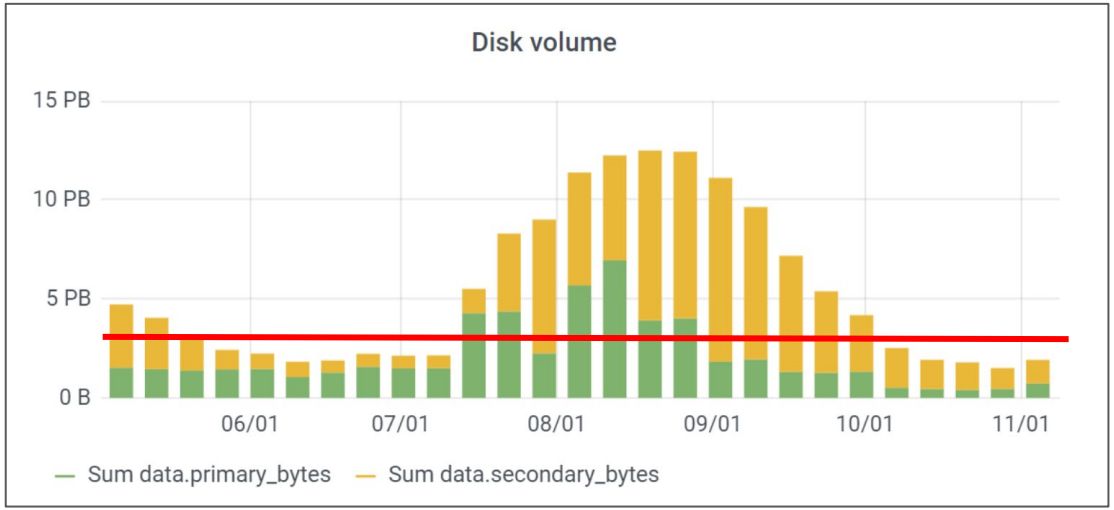




The Tape Carousel model

- Data Carousel for the reprocessing of all data collected by ATLAS in 2015-2018.
- The total data volume was close to 18.5 PB.
- Impressive improvement of the tape performance at T1 thanks to the work of local experts
- Target to keep on average 3 PB of data on disk (red line in the plot), generally achieved
- Several issue found and solved :
  - tuning of the algorithm of data replication in rucio
  - fixes in data pinning
  - introduced iDDS : allows JEDI to incrementally release tasks so tha tasks can start processing even if input data are only partially staged-in.

Sites	2018 Phase I Test (MB/s)	2020 Reprocessing (MB/s)
CERN (CTA Test)	2000	4300
BNL	866	3400
FZK	300	1600
INFN	300	1100
PIC	380	540
TRIUMF	1000	1600
CC-IN2P3	3000	3000
SARA-NIKHEF	640	1100
RAL	2000	2000
NDGF	500	600



Multi-threaded reconstruction software (AthenaMT)

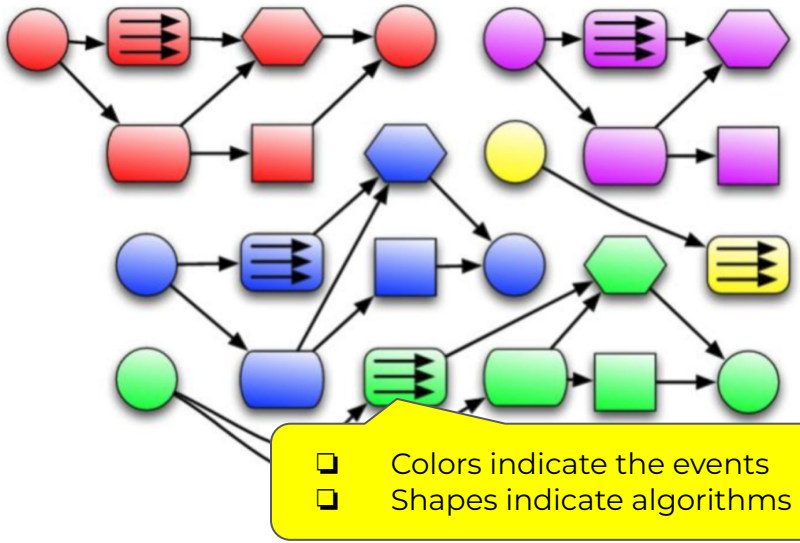
ATL-SOFT-PUB-2021-002

The new Athena release 22 (used since 2021 for reprocessing of Run 2 MC and data, as well as for Run3 data taking and MC simulations) is able to offer both multi-process and multi-thread parallelism.

- In multi-process (MP) parallelism, workers are forked from the primary process at a pre-configured stage during execution (e.g. before the first event is processed). Each worker also has its own unique memory space and produces its own outputs, which need to be merged via a post-processing step.

- In multi-thread (MT) threads are spawned and assigned some work (e.g. execute an algorithm). Single pool of heap memory shared across all threads. Various difficulties must be overcome:
  - multiple threads cannot write to the same memory at the same time;
  - threads must not attempt to read memory that is actively being written
  - algorithms must be scheduled such that all input is fully available before they run.

  However, the performance benefit from using a single pool of memory for all threads can be significant.

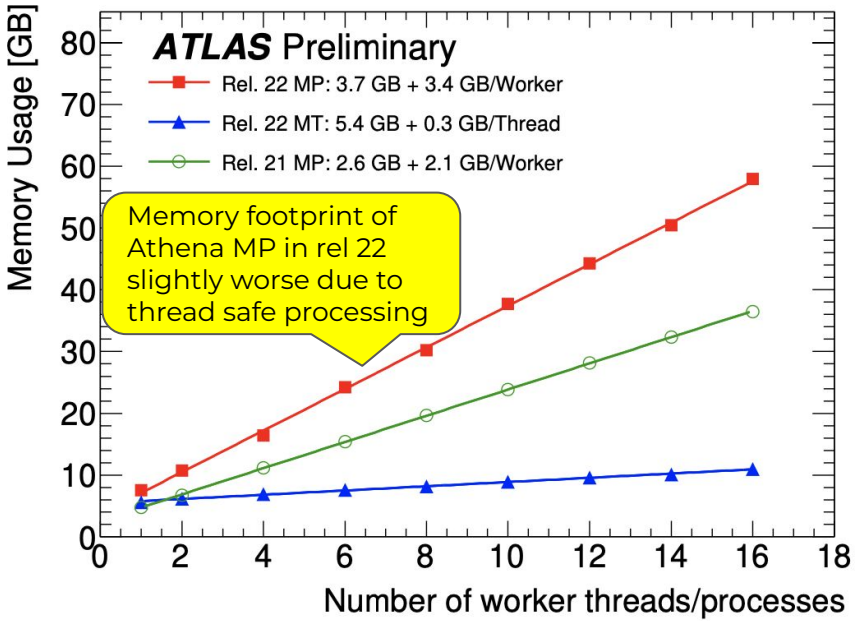


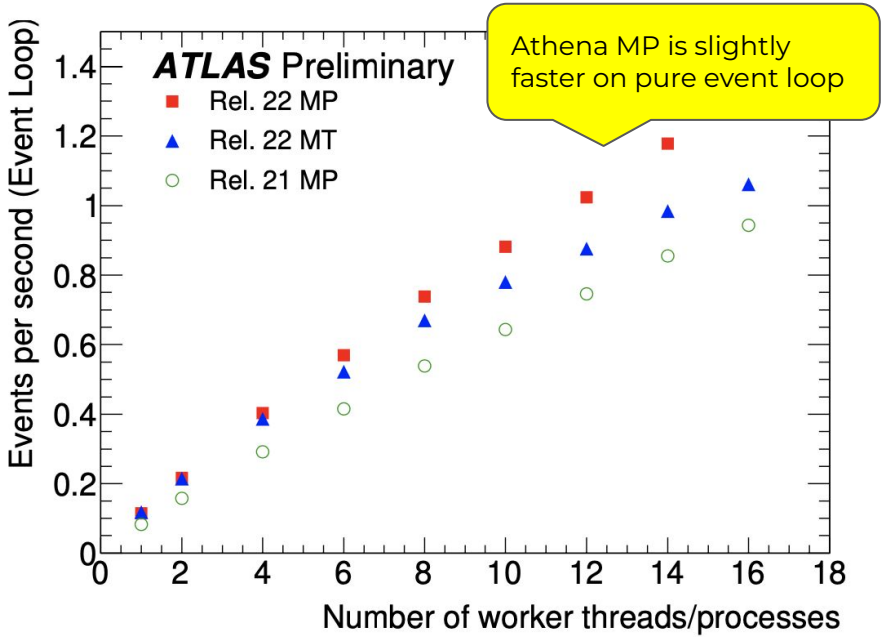
- Multi-threaded reconstruction software allows a better exploitation of opportunistic resources (eg HPC)

Multi-threaded reconstruction software (AthenaMT)

ATL-SOFT-PUB-2021-002

- The benchmark jobs use real data from run 357750 taken during 2018, with 250 events per worker process or thread.
- The data events have an average number of interactions per bunch crossing ⟨μ⟩ = 50, which is approximately that expected for the luminosity-leveling period during Run 3.
- Tests on an Intel®Xeon®CPU E5-2630 v3 at 2.40 GHz (16 cores no SMT) machine + 126 GB of memory.



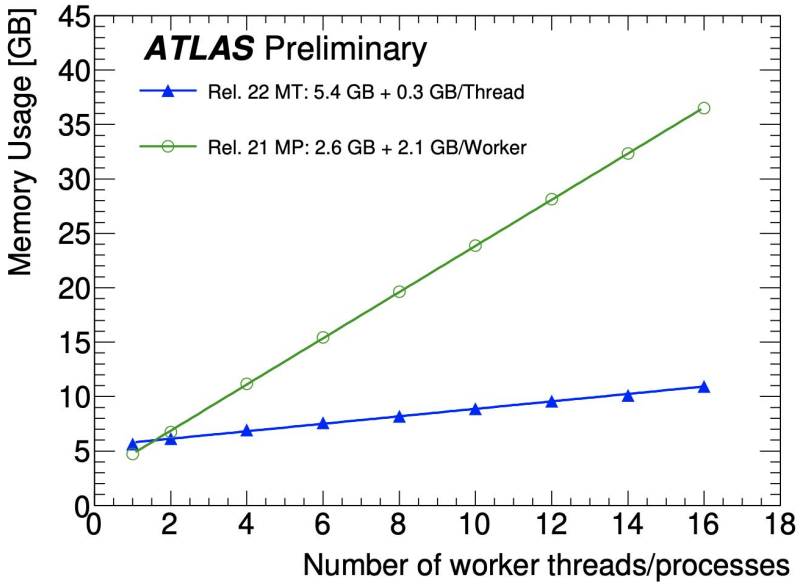


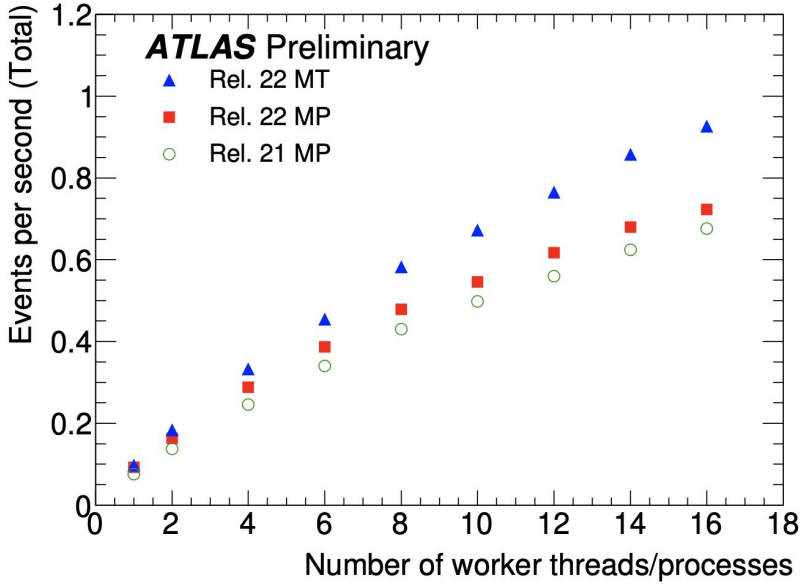
Highlights (I): AthenaMT

http://cdsweb.cern.ch/record/2771777/files/ATL-SOFT-PUB-2021-002.pdf

AthenaMT (MultiThreading) : uno degli achievement fondamentali degli sviluppi software degli ultimi anni

1. L'ultima release (rel 22) del software di ricostruzione di ATLAS (Athena) che verra' utilizzato di default per reprocessing run2 e per il run3 e' basata su multi-thread
2. Considerevole risparmio di memoria (all threads share the same allocated memory)





Highlights (II): simulation optimisation

1. A Geant4 (G4) Optimisation Task Force (TF) has been setup for optimising the performance of the ATLAS G4 simulation software:
   - 1.1. Taking advantage of **intrinsic performance optimizations** coming with newer Geant4 versions
   - 1.2. Optimization with **tuning of G4 parameters** (physics models, physics lists per regions)
   - 1.3. **Neutron** and **Photon Russian Roulette** + **EM range cuts** (ongoing physics validation)
   - 1.4. **Geometry** optimisations (new EMEC variants + R&D on ML guided steppers in geometry)
   - 1.5. **Magnetic field** tailored switch-off
   - 1.6. **Geant4 linking** as static library (a.k.a. Big library)

Stima : si riesce a ottenere un miglioramento della velocita' della fullsimulation ~ 20-25%

2. A new workflow, MonteCarlo ReSimulation, was developed to minimize the resources needed to apply physics improvements to already generated FullSim HITS: the resources used by this workflow are 5-10% of the ones which would have been needed if we should have re-run the FullSim completely. This workflow was applied on 16B events.

Highlights (III) : data carousel

- More dynamic use of the TAPE capabilities: “by ‘data carousel’, we mean an orchestration between workflow management (WFMS), data management (DDM/Rucio) and tape services whereby a bulk production campaign with its inputs resident on tape, is executed by staging and promptly processing a sliding window of X% (X~5%-10%) of inputs onto buffer disk, such that only X% of inputs are pinned on disk at any one time”
  - Retrieve a fraction of RAW data, process them, delete from disk, start again

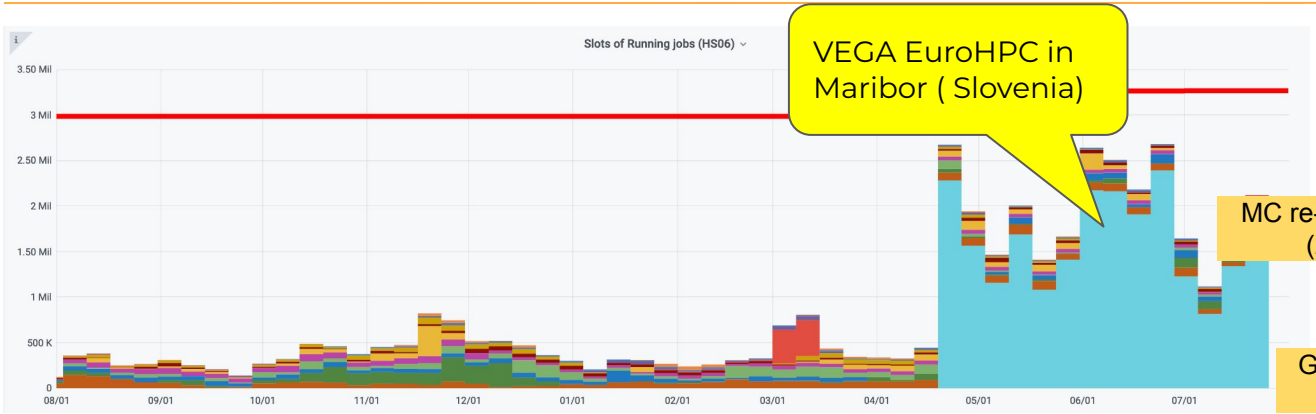
- ATLAS started the Data Carousel R&D in June, 2018, to study the feasibility to get inputs from tape directly, for various ATLAS workflows, such as derivation production and RAW data re-processing.
  - CNAF is actively (and very efficiently!) participating in the Data Carousel activities

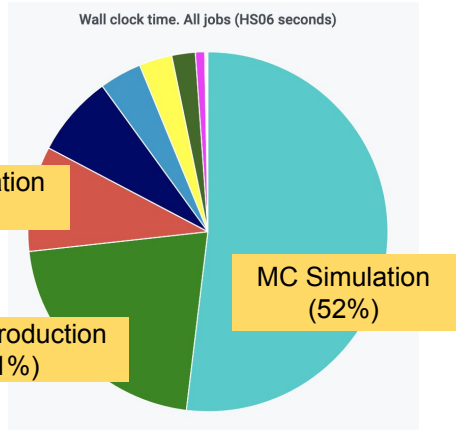
- Complete Run2 RAW (~18.5PB) reprocessing for long lived particles searches (DRAW_RPVLL) , staged & reprocessed, January~April, 2020
  - run at real scale: finished on time, no complains from data preparation group.
  - Much less disk space occupied (~2PB)

- Run in data carousel mode on AOD : they take 1/3 of ATLAS DISK space, move them to tape !?
  - Current goal : run derivation production in Data Carousel mode for Y2016-Y2018 datasets, produce DAOD_PHYS and DAOD_PHYSLITE for physics analysis

- Tape is becoming more and more important in the ATLAS reconstruction workflows

Highlights (IV) : HPC resources

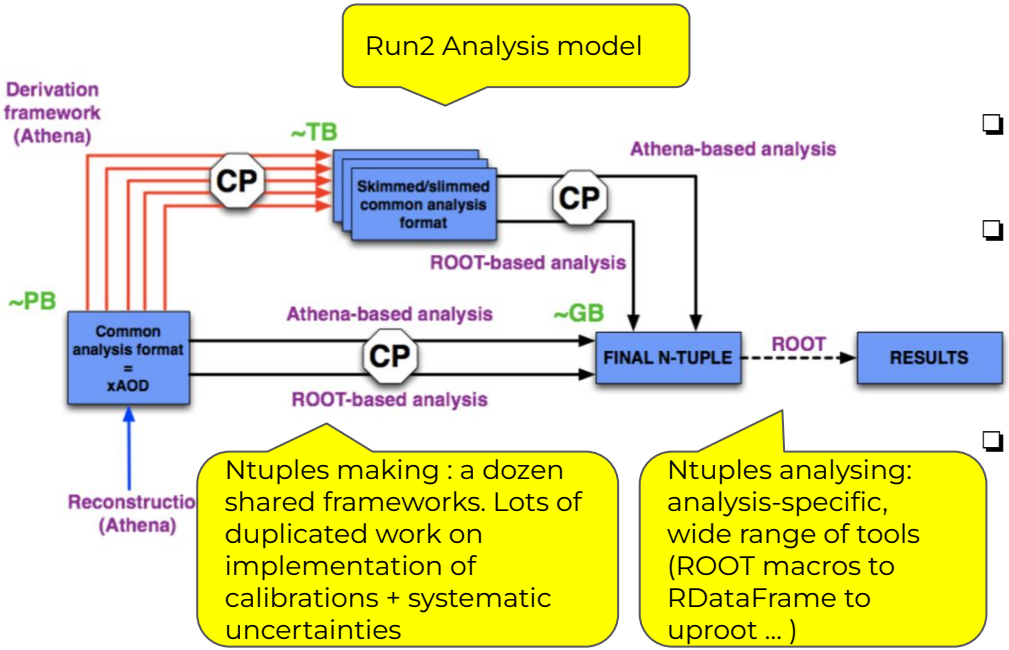




1. Risorse HPC : grande attenzione di ATLAS verso la possibilita' di utilizzare queste risorse (lo sforzo su AthenaMT va anche in questa direzione)
   1.1. il successo dipende fortemente dalla configurazione delle macchine (open/closed), dalla possibilita' di intervenire nel processo di definizione del progetto e dell'architettura e dalla disponibilita' di persone esperte dedicate
   1.2. su risorse 'open' (accesso dei wn alla rete esterna) si possono girare molti workflows di ATLAS
   1.3. Grant su VEGA (EuroHPC in Slovenia) : copre circa 50% del pledge ATLAS, quasi tutti i workflows (anche se principalmente MC)
2. In Italia ATLAS ha partecipato positivamente al grant CINECA 2020
   2.1. non chiaro se riusciremo a partecipare al nuovo grant Marconi 100 (non esiste un build del software ATLAS per Power9 serve manpower per costruirlo)

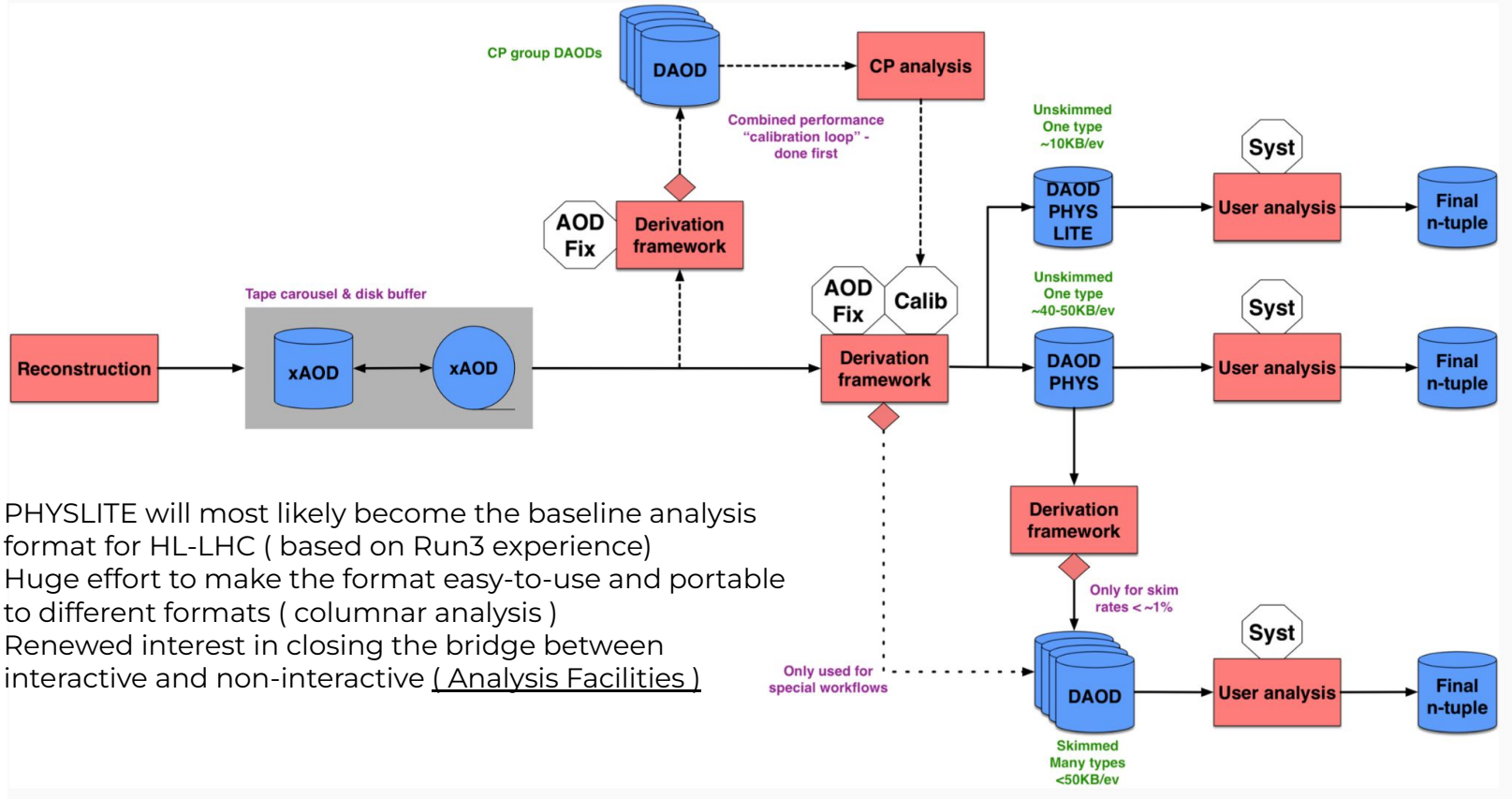
A new analysis model

The ATLAS Run-2 analysis model has been highly successful in the view of the productivity of ATLAS, but it has been expensive in terms of resource usage. The ATLAS Analysis Model Study Group for Run-3 (AMSG-R3) setup at the end of Run-2 was tasked to analyse the efficiency and suitability of the current model and to propose significant improvements.



- The output of the data and MC reconstruction is stored in Analysis Object Data (AOD) files and grouped in datasets on the various Grid sites.
- These datasets are processed in the derivation framework which produces about 80 different derived AOD (DAOD) formats that contain a subset of events and reduced reconstruction information tailored for specific physics analysis and performance groups.
- These DAOD types are processed by many individual analysers in a random manner who produce very condensed individual ntuples for further processing or final physics results

A new analysis model

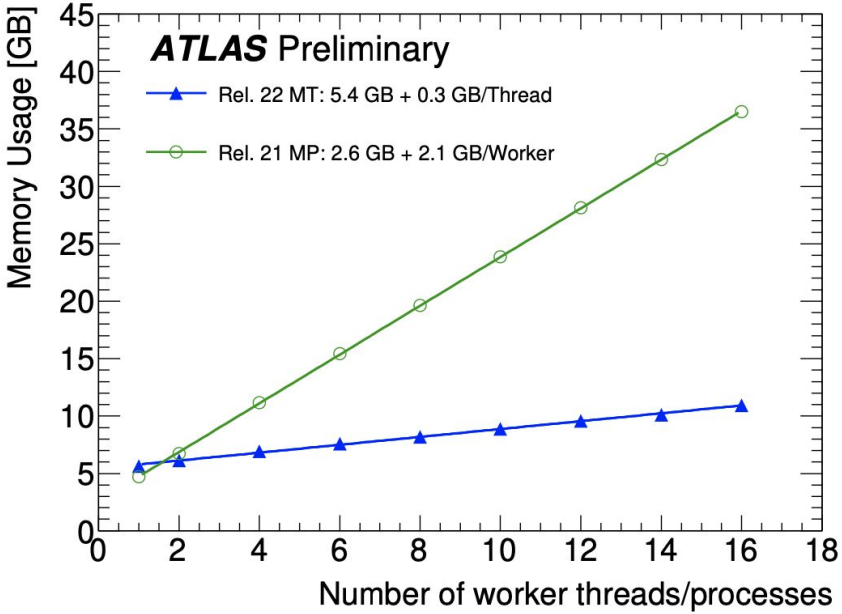


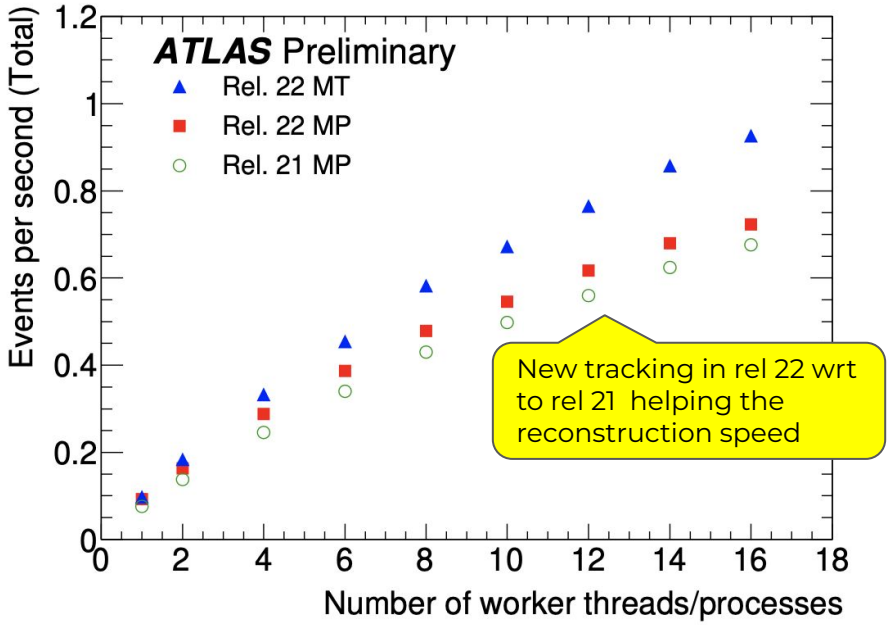
- PHYSLITE will most likely become the baseline analysis format for HL-LHC (based on Run3 experience)
- Huge effort to make the format easy-to-use and portable to different formats (columnar analysis)
- Renewed interest in closing the bridge between interactive and non-interactive (Analysis Facilities)

Multi-threaded reconstruction software (AthenaMT)

ATL-SOFT-PUB-2021-002

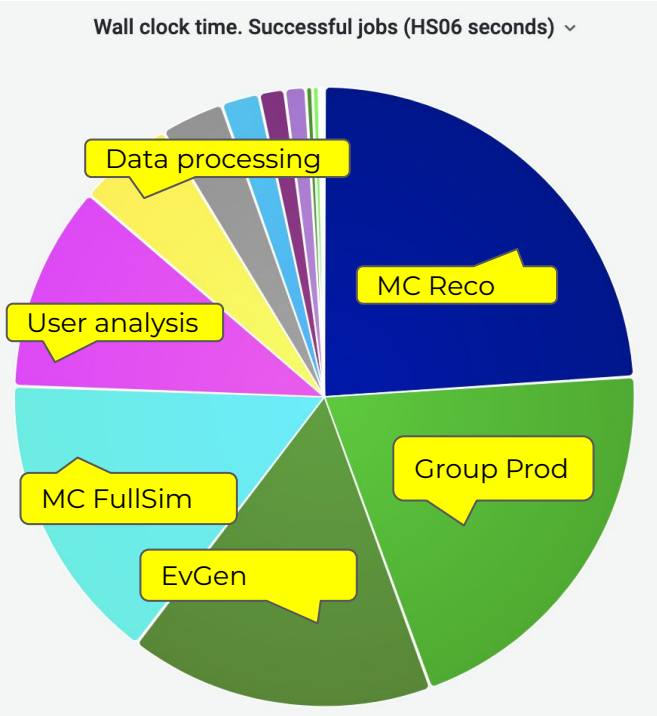
- The benchmark jobs use real data from run 357750 taken during 2018, with 250 events per worker process or thread.
- The data events have an average number of interactions per bunch crossing ⟨μ⟩ = 50, which is approximately that expected for the luminosity-leveling period during Run 3.
- Tests on an Intel®Xeon®CPU E5-2630 v3 at 2.40 GHz (16 cores no SMT) machine + 126 GB of memory.
- Multi-threaded reconstruction software allows a better exploitation of opportunistic resources (eg HPC)



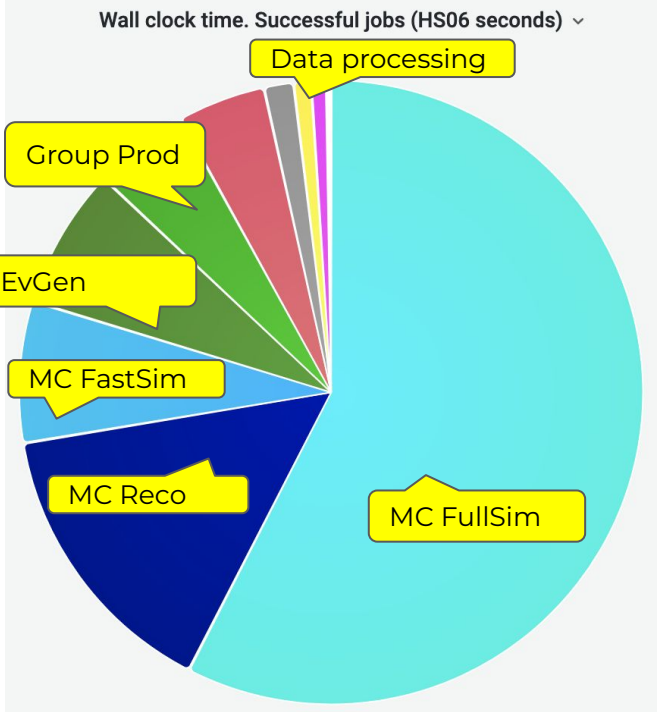


ATLAS Computing per type of resources

GRID RESOURCES



VEGA(HPC)



- Typical share of shutdown period (MC, analysis and reprocessing)
- VEGA (HPC) able to run all ATLAS workflows
- 1/16/64 threads jobs, 1GB/thread (4GB/thread queue available)
- CAVEATS (I): Opportunistic usage at the startup of the cluster, not guaranteed in the next years. Sharing with other users might introduce inefficiencies
- CAVEATS (II): lot of tunings (size, number of events etc) needed and still not optimal usage of the hardware.

Highlights (V): new analysis model

1. Attualmente l'analysis model prevede ~80 diversi streams (DAOD) basati su skimming-menu diversi e con diverso contenuto a seconda dell'analisi

2. Analysis Model completamente diverso per run3 (e preparazione run 4)
   2.1. Solo un tipo di output (DAOD_PHYS) unskimmed con tutte le informazioni principali per il ricalcolo delle correzioni e sistematiche
   2.2. DAOD_PHYSLITE, pre-calibrati, possono essere riprodotti a partire da DAOD_PHYS
   2.3. open the discussion for analysis facilities

	MC size/event (KB/event)	Data size/event (KB/event)	Nominal MC events/year in run 3 (billion) from CDR*	Nominal data events/year in run 3 (billion) from CDR*	Total size/year/ version (PB)
PHYS	40	30	25	10	1.3
PHYSLITE	15	10			0.475

Default in Run4

Stima : assumendo 4 copie complete di DAOD_PHYS si passa da 60 PB (modello attuale) a ~ 32 PB (nuovo analysis model)

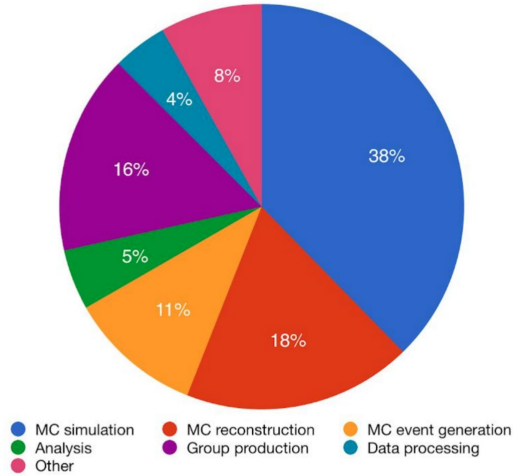
3. Produzione di DAOD_PHYS/PHYSLITE attraverso tape carousel !

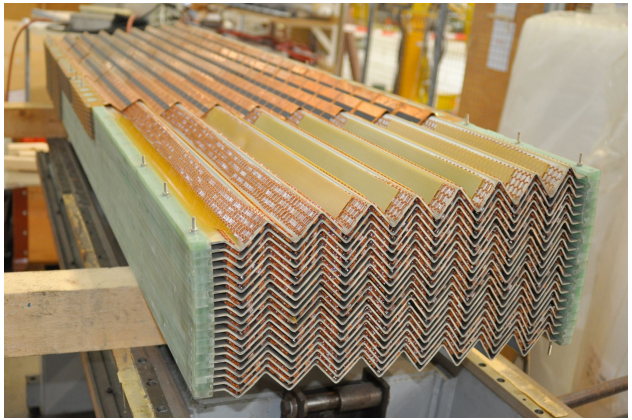
MC events production

ATL-SOFT-PROC-2021-017

Multipurpose experiments cover a wide ranging physics program from precision measurements to searches for new physics

- Monte Carlo events (both hard scatter and pile up) are functional to this process
- Typically the number of simulated MC events is ~ 2.5 the number of data events !
- Most of ATLAS CPU time used for MC detector simulation and ~80-90% of detector simulation time spent on calorimeters (complex geometries)



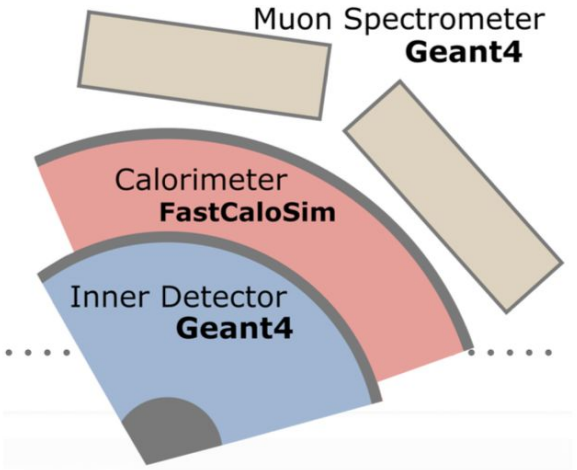


To reduce the impact of the preparation of MC events :

- Optimise G4 full simulation : expect up to 30% reduction
- Pushing on fast (calo) simulation
  - Reduce simulation time keeping as much accuracy as possible + memory efficiency
  - Increase the number of analyses using FastSim : Run 3: >50% events with fast simulation, Run 4: >75% events with fast simulation
- Part of the full-simulation on accelerators (e.g. GPUs)

Fast simulation : Atlfast-III

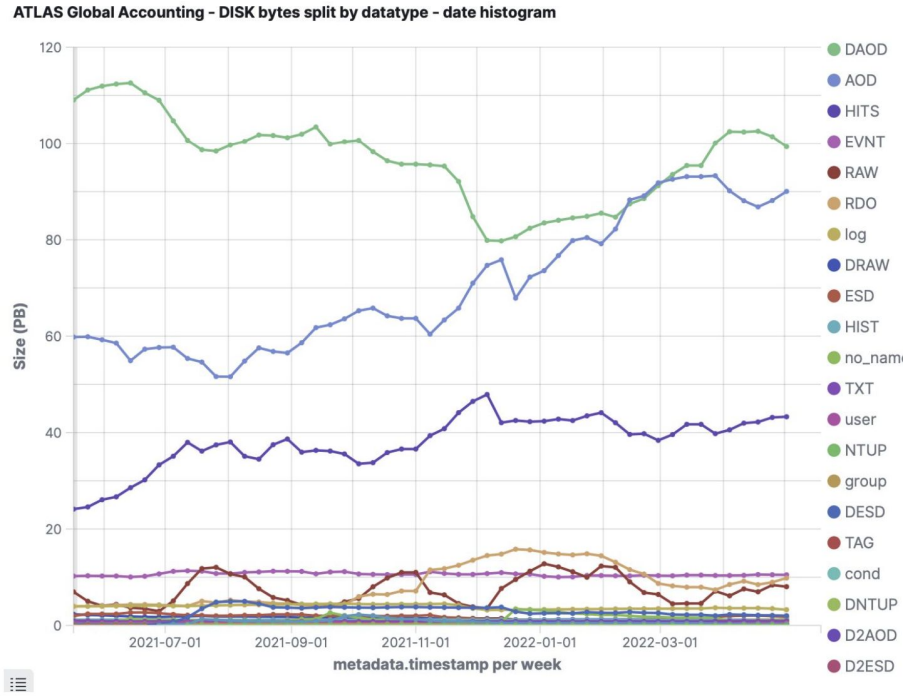
Fast Simulation : instead of simulating interactions of particle travelling through detector parametrise the detector response of single particles (Atlfast) : use electrons and photons for electromagnetic showers and pions for hadronic showers



- Atlfast-III (AF3) is the successor of the Atlfast-II (AF2) simulator
- Full simulation for tracking (ID + muons) and parameterized simulation of the calorimeter
- AF3 implements two distinct approaches of shower generation:
  - FastCaloSimV2: parameterized modelling (separate parameterisations of longitudinal and lateral shower developments)
  - FastCaloGAN: Generative Adversarial Network: GAN trained to reproduce voxels and energies in the layer as well as total energy in one single step
- Dedicated parameterization for punch through particles

A new analysis model

The ATLAS Run-2 analysis model has been highly successful in the view of the productivity of ATLAS, but it has been expensive in terms of resource usage. The ATLAS Analysis Model Study Group for Run-3 (AMSG-R3) setup at the end of Run-2 was tasked to analyse the efficiency and suitability of the current model and to propose significant improvements.

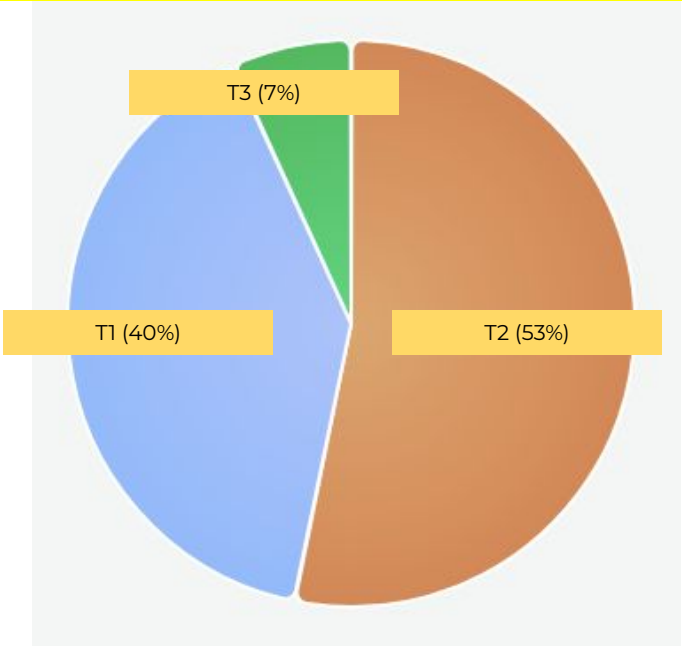


- The size/event for the AOD is about 600 kB
- Around 80 DAOD formats, size in the range of 40-450 kB depending on the type of the physics selection and the information retained.
- only 1-2 replicas of each dataset and campaign can be kept on disk.
- AODs and DAODs which are the two formats taking more than 70% of the disk space today
- As a rough Run-2 input parameter an initial sum of 132 PB of disk space used for AOD and DAOD format
- For the HL-LHC the projections of the ATLAS needs are significantly over the yearly flat budget increase. ATLAS is therefore investing significantly in methods to reduce the disk space needs in several areas

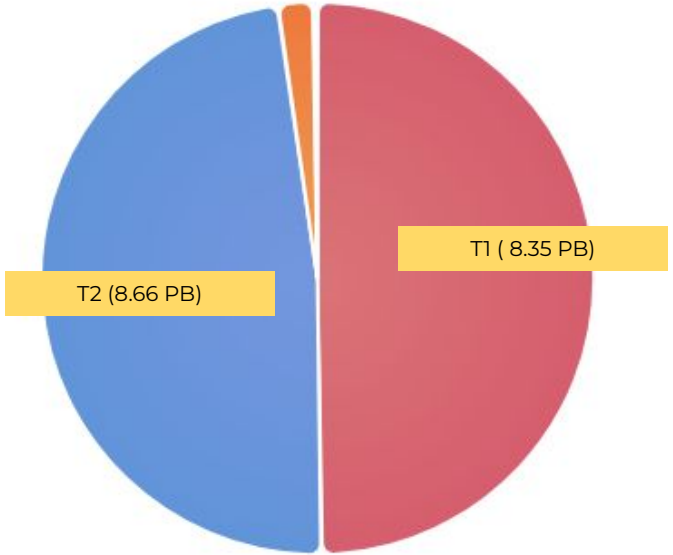
Distribuzione carico lavoro ATLAS in Italia

Lavoro distribuito sul T1 (CNAF), i quattro T2 (Frascati, Milano, Napoli e Roma1) e quattro T3 (Cosenza, Genova, Lecce, Roma3)

CPU

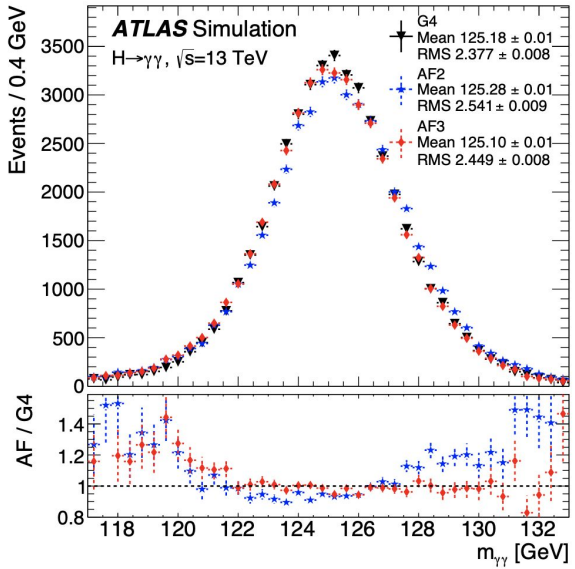


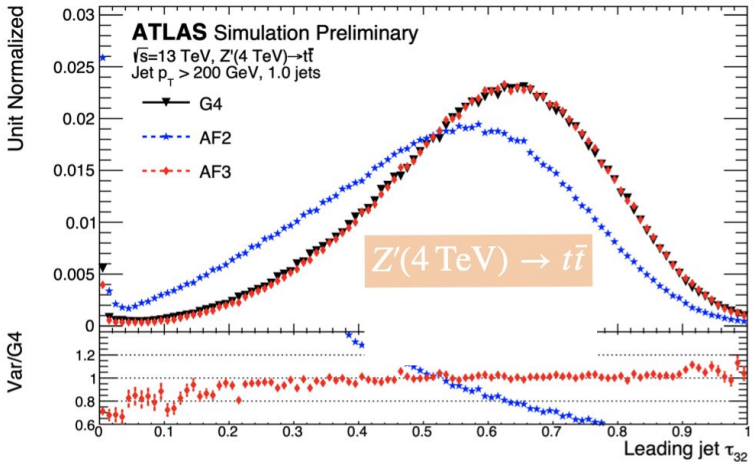
STORAGE



Fast simulation : Atlfast-III

Encompassing complex parameterized and deep learning algorithms, AF3 is the state of the art fast simulation in ATLAS and able to simulate a broad range of physics processes with high precision





- AF3 provides significant improvements in physics performance compared to AF2 while giving a speedup of $\mathcal{O}$ (5-10) compared to Geant4
- Improvements include better modelling of jet masses, constituents and substructure, better e/γ simulation and more
- AF3 was used for the re-processing of ~7 billion Run 2 events · Many more improvements expected for Run 3 and beyond