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Running Run3 simulations

ALICE Analysis tutorial

First TF orbit 9689120 Date: Pri New 18 16 57 27 2022 Detectors: ITS.TPC.TRD.TDF.PHS.ENC.MFT.NCH.MIC

Outline

- Introduction to ALICE Run3 simulation ecosystem
- o2-sim and the events simulation.
- Available simulation configurations and possibilities
- The O2DPG workflow → the new working standard

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- Introduction to ALICE Run3 simulation ecosystem
- o2-sim and the events simulation.
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- The O2DPG workflow → the new working standard

Opening Remark

Introductory overview for practical MC generation.
Additional info in other PWGs tutorials or documentation

Contacts



How to get in touch with the simulation developers

- Simulation <u>e-group</u> (for meeting announcements) + <u>WP12 meetings</u>
- Collaborative Mattermost channels (preferred over private email): <u>O2-simulation</u> + <u>O2DPG</u>
- <u>JIRA tickets</u> for feature requests/bug reports (components simulation or O2DPG)

Where to find information about simulation

- New documentation project: https://aliceo2group.github.io/simulation/
- Previous documentation in AliceO2: DetectorSimulation.md
- Some info in O2DPG: WorkflowRunner.md
- Various examples at <u>O2/SimExamples</u> or <u>nightly-tests</u>

* still early stage:

- give feedback
- ask questions
- <u>contribute</u>

Software environment reminder

simplest local build (basic generators such as Pythia8)

aliBuild build O2 O2DPG --defaults o2

alienv enter O2/latest,O2DPG/latest

full local build (all generators, QC and O2Physics included)

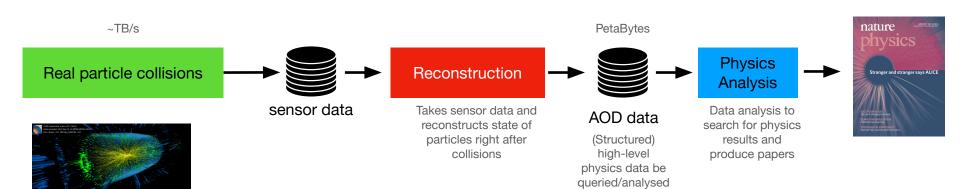
aliBuild build O2sim --defaults o2

alienv enter O2sim/latest

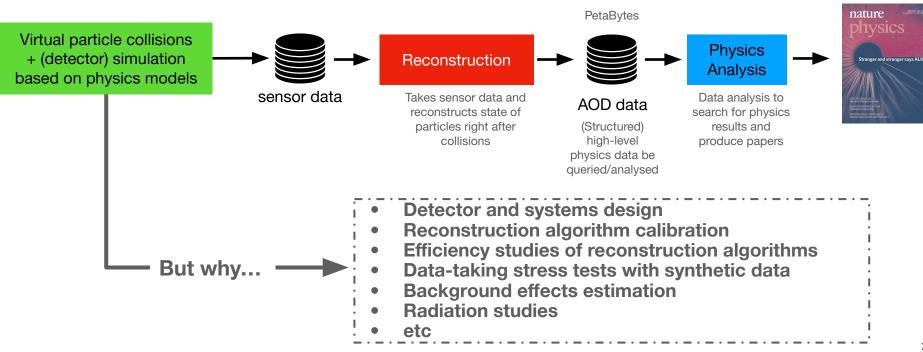
nightly precompiled builds (with CVMFS)

/cvmfs/alice.cern.ch/bin/alienv enter O2sim::v20241014-1

Classical pipeline in a HEP experiment: Experimental Data

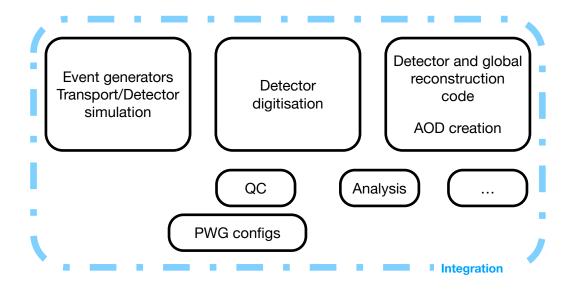


Classical pipeline in a HEP experiment: Simulation



The ALICE Run3 simulation ecosystem

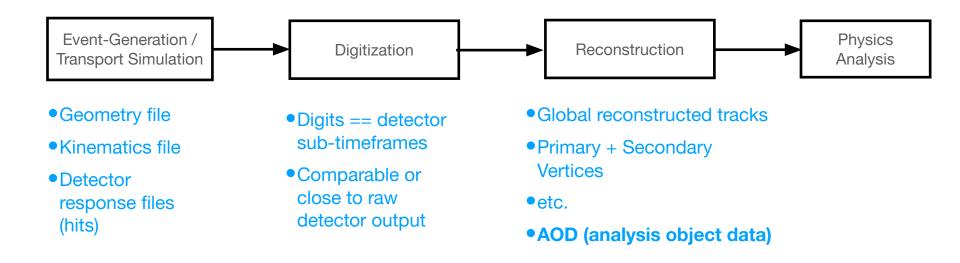
- Simulation ecosystem comprised of various components
- Core simulation part:
 - Event generation
 - Transport simulation
 - Digitization
- In addition, MC workflows may exercise all of
 - Reconstruction, QC, Analysis, etc.
- Individual parts maintained in <u>O2</u> and <u>O2Physics</u> repos



Integration and configuration of all parts into coherent workflows, done with:

- <u>O2DPG</u> repository (mainly for physics studies on GRID)
- <u>full-system-test</u> (mainly for data taking oriented simulations)

Data products in simulation pipeline



o2-sim: ALICE Run3 simulation tool

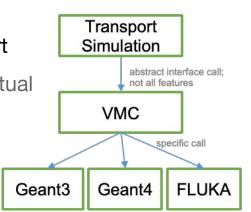
• o2-sim is the particle-detector simulator for ALICE Run3

Implements ALICE detector on top of well known particle-transport engines that implement actual physics models and particle transport

 Geant4, Geant3 and FLUKA interchangeably through use of Virtual Monte Carlo API

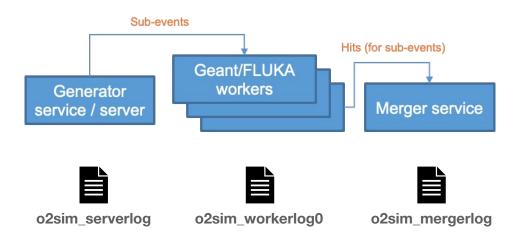
Main tasks of o2-sim:

- ALICE geometry creation
- Event generation (primary particle generation)
- Simulation of physics interaction of particles with detector material (secondary creation, etc.) and transport of particles until they exit detector or stop
- Creation of hits (energy deposits) as a pre-stage of detector response after particle passage



o2-sim: ALICE Run3 simulation tool

- New in Run3: scalable multi-core simulation with sub-event parallelism →allows to use big servers and obtain results for individual large events quickly
- Important: o2-sim treats events in complete isolation no timeframe concept (enters during digitization)
- o2-sim produces 3 internal log files \rightarrow in-depth description of each process and debug



Usage of o2-sim in examples

Examples of o2-sim usage

o2-sim -n 10 -g pythia8pp

o2-sim -n 10 -g pythia8pp -j 8 \
--skipModules ZDC --field 2 -e TGeant3

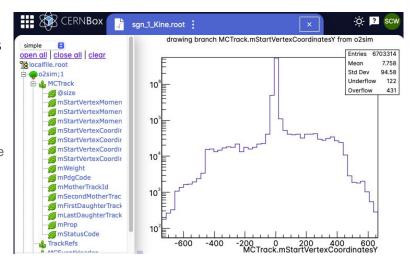
o2-sim -n 10 -g pythia8pp --noGeant

"Generate 10 default Pythia8 pp events and transport them through the complete ALICE detector" "Generate 10 default Pythia8 pp events and transport them with 8 Geant3 workers through everything but ZDC and use an L3-field of 2kGauss" "Just generate 10 default Pythia8 pp events and do nothing else (pure generator output)"

`o2-sim --help` lists the main options and shows default generation parameters

o2-sim: Kinematics output

- Kinematics output (default file o2sim_Kine.root) from transport simulation likely most interesting for physics analysis
 - contains creation vertices, momenta, etc of primary (generator) and secondary (transport) particles created in simulation
 - information on physics creation process, provenance (mother-daughter), etc.
 - Based on o2::MCTrack class, which is basically a more lightweight TParticle
- For each event, there is one entry of vector<MCTracks> in a TTree
- By default, kinematics is pruned (only relevant particles kept)
- In addition, event-level meta-information about each generated event is available in a separate file (o2sim_MCHeader.root)
 - for instance impact parameter of PbPb collision



"histogram of production vertex-y of all MCtracks (primary and secondary)"

Helper classes to access MC kinematics

- Reading and navigating manually through kinematics can be cumbersome ("ROOT-IO boilerplate")
- Offer 2 main utility classes making this easy for user
 - MCKinematicsReader Class to easily read and retrieve tracks for given event or a Monte Carlo label
 - MCTrackNavigator Class to navigate through mother-daughter tree of MC tracks and to query physics properties

```
using o2::steer;
using o2;

// access kinematics file with simulation prefix o2sim
MCKinematicsReader reader("o2sim",MCKinematicsReader::Mode::kMCKine);

// get all Monte Carlo tracks for this event
std::vector<MCTrack> const& tracks = reader.getTracks(event);

for (auto& t : tracks) {
    // analyse tracks; fetch mother track of each track (in the pool of all tracks)
    auto mother = o2::mcutil::MCTrackNavigator::getMother(t, tracks);
    if (mother) {
        std::cout << "This track has a mother'n";
    }

    // fetch the (backward first) primary particle from which this track derives
    auto primary = o2::mcutil::MCTrackNavigator::getFirstPrimary(t, tracks);
}
```

"Read all Monte Carlo tracks from stored kinematics file for event id 1. Then loop over all tracks and determine the direct mother particle and the primary ancestor in each case"

Generators: Basic

o2-sim has a couple of pre-defined generators (select with -g option)

o2-sim -g [pythia8pp | pythia8hi | boxgen | extkinO2 | hepmc] ...

Generators: Pythia8

- Pythia8 is more deeply integrated in O2 (compared to others) and it is recommended to use it whenever possible
- When Pythia8 is used, it can be fully configured via a special text file and the GeneratorPythia8 parameter
 - valid settings can be found in the <u>Pythia8 reference</u> manual
- we also provide a tool <u>mkpy8cfg.py</u> to help with the creation of the config file

```
### random
Random:setSeed = on
Random:seed = 130145275
### beams
Beams:idA = 1000822080
Beams:idB = 1000822080
Beams: eCM = 5020,000000
### processes
### heavy-ion settings (valid for Pb-Pb 5520 only)
Heavylon:SigFitNGen = 0
Heavylon:SigFitDefPar = 13.88,1.84,0.22,0.0,0.0,0.0,0.0,0.0
Heavylon:bWidth = 14.48
### decays
ParticleDecays:limitTau0 = on
ParticleDecays:tau0Max = 10.
### phase space cuts
PhaseSpace:pTHatMin = 0.000000
PhaseSpace:pTHatMax = -1.000000
```

run with this config

pythia8.cfg

o2-sim -n 10 -g pythia8 --configKeyValues "GeneratorPythia8.config=pythia8.cfg"

External Generators

- Apart from Pythia, direct (compiled) integration of specific generators is small in O2 in order to decouple PWG specific generator code and configs from data-taking
 - avoid recompile
- Rather, "external" generators can be interfaced in o2-sim by using just-in-time ROOT macros which implement, e.g., a GeneratorTGenerator class
 - setup generator at "use-time" in C++
 - generator setup becomes "configuration problem"
- This method is used to setup PWG specific generation in the O2DPG production system
 - e.g. <u>PWGDQ cocktail generator</u>

"call o2-sim with -g external option and reference the external file and function name"

o2-sim -n 10 -g external --configKeyValues
'GeneratorExternal.fileName=myGen.C;GeneratorExternal.funcName="gen(5020)"

"stub content of ROOT macro file myGen.C"

```
// my fully custom generator
class MyGen : o2::generator::GeneratorTGenerator {
  void Init() override;
  bool generateEvent() override;
};

FairGenerator* gen(double energy) {
  return new MyGen(energy);
}
```

HepMC generation

 Many generators allow by default to output HepMC formatted data → universal and convenient way of storing information from MC event generators



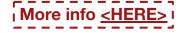
- o2-sim is capable of reading HepMC files out-of-the box → data from FIFOs can be read as well
 - HepMC3 is the default, but HepMC2.06 data
 are compatible as well ... --configKeyValues 'HepMC.fileName=/path_to/file.hepmc;HepMC.version=2"
- An additional feature of the tool is to spawn event generators using the cmd parameter of GeneratorHepMC → generators printing data in the stdout can be set to feed data automatically to o2-sim → no need for large local .hepmc files

Generation with local HepMC file or FIFO

o2-sim -n 10 -g hepmc --configKeyValues "HepMC.fileName=/path_to/file.hepmc"

Generation with automatic FIFOs using run/SimExamples/HepMC EPOS4

o2-sim -n 100 -g hepmc --seed 12345 --configKeyValues "GeneratorFileOrCmd.cmd=epos.sh;GeneratorFileOrCmd.bMax Switch=none;HepMC.version=2"





Generators: Triggering

- Event filtering or triggering is also flexibly supported on the generator level
 - e.g., only produce and simulate events of a certain property
- A user-configurable "external" trigger follows the "external" generator mechanism
 - one implements a trigger function in a separate ROOT macro and pass it to o2-sim with the `-t external` option
 - the trigger function inspects the vector of all generator particles
- Advanced: DeepTriggers allow to trigger on the collection of the primaries and further internal information of the underlying generator

"call o2-sim with pythia8pp generator put pass forward only events that satisfy the trigger condition given in file Trigger.C"

o2-sim -n 10 -g pythia8pp -t external --configKeyValues
'TriggerExternal.fileName=myTrigger.C;TriggerExternal.funcNa
me="trigger"

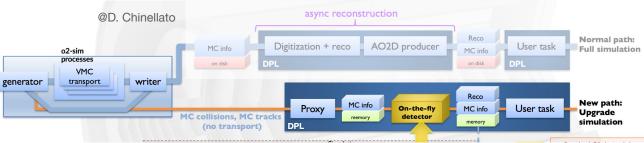
"stub content of ROOT macro file myTrigger.C"

```
// returns fully custom event trigger function
o2::eventgen::Trigger trigger()
{
  return [ ](const std::vector<TParticle>& particles) -> bool {
    return true; // triggered
  }
}
```



o2-sim as on-the-fly generator for analysis

- o2-sim can be used as generator service to inject events into a DPL (analysis) topology without intermediate storage
- useful for fast-simulation studies within analysis framework or for primary-only analysis tasks



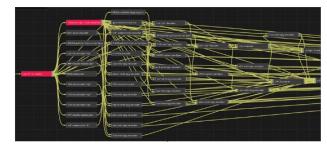
This method is used already by PWGs, such as for cocktail simulation in PWG-EM

Very basic example # Launch simulation o2-sim -j 1 -g pythia8pp -n 10 --noDiscOutput --forwardKine --noGeant &> sim.log & # Launch a DPL process o2-sim-mctracks-proxy -b --nevents 10 -lo2sim-pid \${SIMPROC}_I--aggregate-timeframe 1 &

- Crucial for on-the-fly analysis
- Can be omitted for single o2-sim process 20

Integrated workflows: O2DPG MC

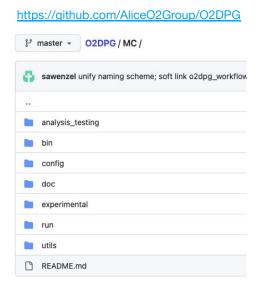
- In order to produce simulated AODs, we need to go beyond o2-sim and event generation and run the complete algorithmic pipeline including digitization and reconstruction steps
- This is a complex system, consisting of many executables or tasks, requiring consistent application and propagation of settings/configuration to work together
 - Example: full-system-test for data taking
 - hard to get right on your own → use a maintained setup!
- For ALICE Run3, the official production system targeting GRID productions is <u>O2DPG</u> repo (MC part)
- O2DPG also contains scripts/setup for data taking (DATA part)



"Interplay of algorithms is a complex system (DPL topology)"

02DPG ...

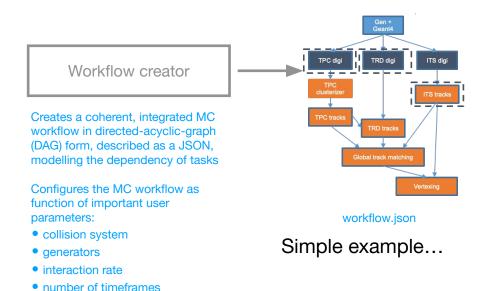
- provides authoritative setup for official MC productions for ALICE-Run3 and a runtime to execute MC jobs on GRID
- integrates all relevant processing tasks into a coherent and consistent environment to have a working pipeline from event generation to AOD and beyond
- maintains PWG generator configurations as versioned code
- performs testing / CI on PWG generator configurations

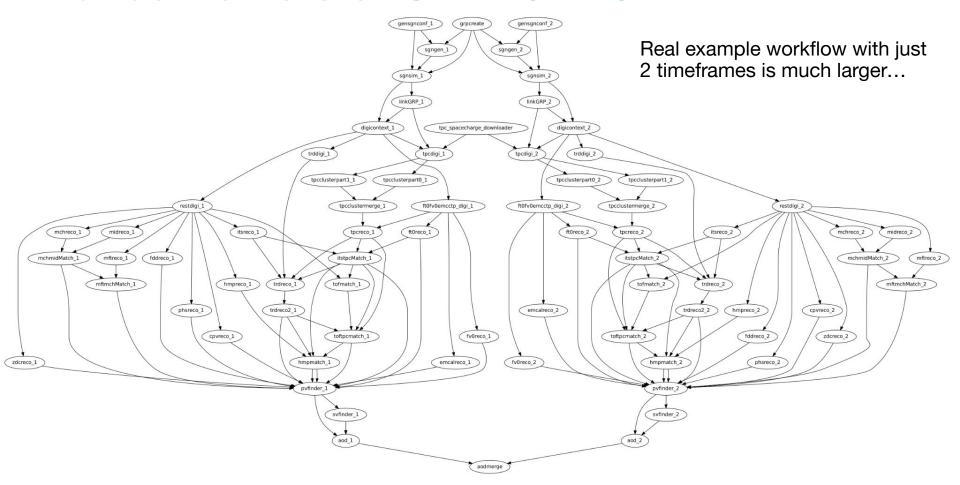


Important directories:

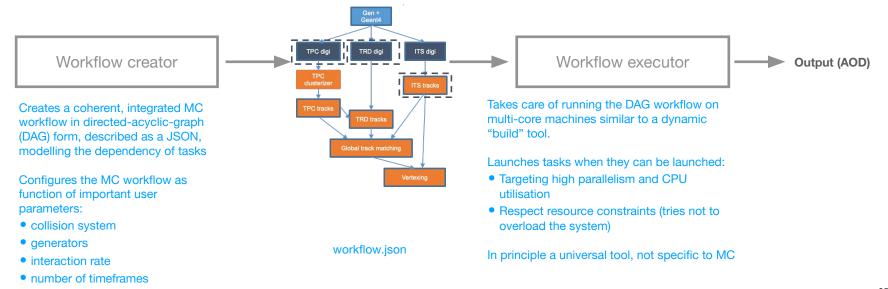
- MC/bin (workflow creation/execution)
- MC/run (PWG specific run scripts)
- MC/config (PWG specific generator configs)

- Running a MC job, is a two-fold process to decouple configuration logic from execution logic
 - Create a valid/configured description of a MC job == "workflow"

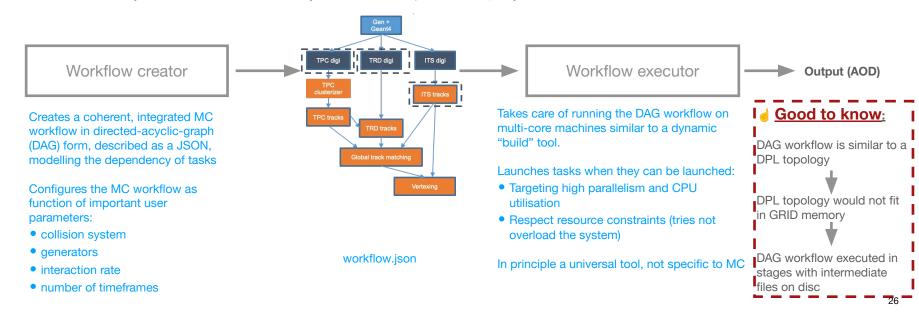




- Running a MC job, is a two-fold process to decouple configuration logic from execution logic
 - Step One: Create a valid/configured description of a MC job == "workflow"
 - Step Two: Run the MC job with a dynamic graph scheduler



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O2DPG-MC workflows: Requirements

- Valid AliEn-tokens are required to run (to access CCDB objects)
 - Experts may circumvent by using CCDB snapshots
- The O2DPG MC workflows are supposed to run in an 8-CPU core with 16GB RAM environment reflecting the default resources on the GRID
- This is also the requirement that you should fulfill when running locally on your laptop
- This translates into some defaults which are put in the workflow creation / execution
 - Transport simulation will use 8 workers
 - TPC + TRD digitisation 8 threads
 - The workflow runner will assume to have 8-cores available
- In turn, O2DPG MC workloads may lead to problems when run on hardware with less resources
 - But with a bit a tuning/adjustment it might be possible to run



O2DPG-MC workflows: Requirements

- Valid AliEn-tokens are required to run (to access CCDB objects)
 - Experts may circumvent by using CCDB snapshots
 - O2DPG MC workflow fetches automatically each object only once and caches them as snapshots
 - Default paths \${WORKDIR}/ccdb/<path>/<in>/<ccdb>/snapshot.root

Moreover...

The path can be also set manually

```
export ALICEO2_CCDB_LOCALCACHE=/<your>/<path> or by running
```

```
ALICEO2_CCDB_LOCALCACHE=${YOURPATH} o2_dpg_workflow_runner.py ... allowing usage of existing cache
```

A script in O2 is available for CCDB files download:

```
${O2_ROOT}/bin/o2-ccdb-downloadccdbfile --host http://alice-ccdb.cern.ch -p TPC/Calib/CorrectionMapRef --timestamp <timestamp> --created-not-after 3385078236000 -d ${YOURPATH}
```

O2DPG-MC step 1: workflow creation

- ALICE Run3 MC workflow creation done by script O2DPG/MC/bin/o2dpg_sim_workflow.py
- Configures the MC workflow as function of important (user) parameters (collision system, generators, interaction rate, number of timeframes, transport engine, etc.)
 - `o2dpg_sim_workflow.py --help` →documentation with all available options

```
${O2DPG_ROOT}/MC/bin/o2dpg_sim_workflow.py -eCM 14000 -col pp -gen pythia8 -proc cdiff -tf 5 —ns 2000 -interactionRate 500000 -run 302000
```

"Generate an ALICE-Run3 Monte Carlo workflow for a 5 timeframe simulation, with 2000 events per timeframe, at interaction rate of 500kHz for 14TeV pp collisions using Pythia8 that has special process cdiff enabled..."

I description | Important options:

-gen, -tf, -n, -eCM, -interactionRate, -run, -col Optionally: -field, -seed, -proc

Workflow creation: Run numbers

- The use of a run number is mandatory as it will be used to determine a timestamp needed to fetch conditions from CCDB
- So run numbers should be used even for non-data-taking anchored simulations
- A list of pre-defined run numbers for MC has been documented here: https://twiki.cern.ch/twiki/bin/view/ALICE/O2D PGMCSamplingSchema
- For example, for a PbPb simulation with field
 -0.5T, a run number of 310000 can be used
 - Should in principle fetch CCDB objects good for PbPb

Туре	Collision System	Energy	Magnetic field	Run no. Range	Time range (in EPOCH seconds)	JIRA Ticket
Local testing				300000-300099	1546300800-1546343770	
Run 5 ALICE3	Pb-Pb pp	5.5 TeV 14 TeV	0.5T 2T	300100-300999	1546343800-1546730770	O2-2572 ☑ (LHC21d9[x]
Run 3	рр	900 GeV	0.2T	301000-301499	1546730800-1546945770	LHC21i1_nightly LHC21i1[a-c] LHC21i3[b, d-g]
			-0.2T	301500-301599	1546945800-1546988770	
			unassigned	301600-301999	1546988800-1547160770	
Run 3	рр	13.6 TeV	-0.5T	302000-302999	1547160800-1547590770	O2-2679 (LHC21k6) LHC21i3[a, c]
			0.5T	303000-303999	1547590800-1548020770	
			unassigned	304000-309999	1548020800-1550600770	
Run 3	Pb-Pb	5.02 TeV	-0.5T	310000-310999	1550600800-1551030770	O2-2773 (LHC22b2) O2-2779 (LHC22b6)
			0.5T	311000-311999	1551030800-1551460770	
			unassigned	312000-319999	1551460800-1554900770	

Recommended way

- Documentation
- Official configuration folder

Workflow creation: Generator configuration

- Custom configurations can be specified to the generation workflow thanks to .ini files
 o2dpg_sim_workflow.py -gen pythia8 -ini <path/to/config.ini>
- They contain different sections for generator configurations but additional triggers for the produced particles can be added
- Official configurations can be found by default in

O2DPG/MC/config/<PWG>/ini/<config>.ini

and they are tested by a CI when modifications are requested via PR or new configurations are added

Snippet from PWGDQ configuration

 Configurations folder is linked to the O2DPG_MC_CONFIG_ROOT environment variable

Local configurations can be used, but also newer configurations can be tested with older O2DPG build and viceversa

[GeneratorPythia8]

config =

\${O2DPG_MC_CONFIG_ROOT}/MC/config/common/pythia8/generato
r/pythia8_hf.cfg
hooksFileName =

\${O2DPG MC CONFIG ROOT}/MC/config/PWGHF/pythia8/hooks/pyt

hia8_userhooks_qqbar.C hooksFuncName = pythia8_userhooks_ccbar(-4.3,-2.3)

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O2DPG-MC step 2: workflow execution

- Workflow runner/executor evaluates/builds a DAG workflow on a compute node
- Minimally, it takes the workflow file and a target as input

\${O2DPG_ROOT}/MC/bin/o2dpg_workflow_runner.py -f workflow.json -tt aod

"Execute workflow up to aod task (assuming 8-core CPU config)"

Checkpointing and incremental build

o2dpg_workflow_runner.py -f workflow.json -tt digi o2dpg_workflow_runner.py -f workflow.json -tt aod

 Convert DAG to simple shell script which could be run standalone "First execute until digitization ... and then continue until AOD (not doing tasks again which are already finished!)

o2dpg_workflow_runner.py -f workflow.json -tt aod --produce-script my_script.sh

"Create a simple shell script which can run everything sequentially up to AOD stage"

- ... many more useful features
 - As usual, o2dpg_workflow_runner.py --help, lists possible options

Run MC jobs on the GRID

 MC workflow can be run on the GRID up to the generation of AODs. → both O2DPG-MC steps will be run from a script

#!/usr/bin/env bash # Workflow creation: step 1 \${O2DPG_ROOT}/MC/bin/o2dpg_sim_workflow.py -eCM 13600 -col pp -gen_pythia8 -proc cdiff -tf 1 -ns 200 -e TGeant4 -interactionRate 500000 # Workflow execution: step 2 \${O2DPG ROOT}/MC/bin/o2dpg workflow runner.py -f workflow.json -tt aod

Jobs are submitted to the GRID via a script provided with the O2DPG package

--help to list all the available options

```
${O2DPG_ROOT}/GRID/utils/grid_submit.sh --script my_script.sh --jobname test --outputspec
"*.log@disk=1","*.root@disk=2" --packagespec "VO ALICE@O2sim::v20241014-1" --wait
--fetch-output
```

Options used:

example.sh O2DPG-MC script

--jobname: assigns a name to the task as appears on MonALISA --outputspec: specifies which files will be saved after the execution:

> @disk=2 denotes that 2 replicas will be saved of the file for security reasons

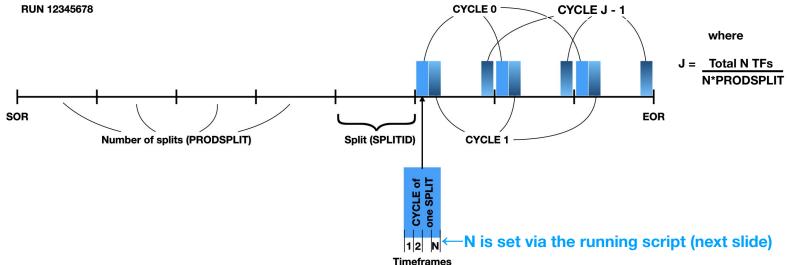
- --wait: your system will wait until the GRID jobs are done
- --fetch-output: downloads automatically the files of the local disk





Anchored MC productions

- Simulations in which conditions are set to match those during a real data taking run
 → LHC filling scheme, included ALICE detectors, dead channels, alignment, interaction
 rate etc.
- These productions are crucial for physics analyses to have realistic simulated samples
- One anchored MC run corresponds to one specific CYCLE of one SPLITID containing N timeframes of the total→ full RUN covered when all CYCLEs are produced for all SPLITIDs



Documentation

Anchored MC productions: how to?

The grid_submit.sh script can be used to start anchored MC productions → a production script must be provided

example script for anchored pp production

```
export ALIEN_JDL_LPMANCHORPASSNAME=apass2
export ALIEN_JDL_MCANCHOR=apass2
export ALIEN JDL CPULIMIT=8
export ALIEN JDL LPMRUNNUMBER=535069
export ALIEN JDL LPMPRODUCTIONTYPE=MC
export ALIEN JDL LPMINTERACTIONTYPE=pp
export ALIEN_JDL_LPMPRODUCTIONTAG=LHC24a2
export ALIEN JDL LPMANCHORRUN=535069
export ALIEN JDL LPMANCHORPRODUCTION=LHC23f
export ALIEN JDL LPMANCHORYEAR=2023
export NTIMEFRAMES=1
export NSIGEVENTS=50
export SPLITID=100
export PRODSPLIT=153
export CYCLE=0
export SEED=5
export NWORKERS=2
${O2DPG_ROOT}/MC/run/ANCHOR/anchorMC.sh
```

test_anchor_2023_apass2_pp.sh

\${O2DPG_ROOT}/GRID/utils/grid_submit.sh --script test_anchor_2023_apass2_pp.sh --jobname test --outputspec "*.log@disk=1","*.root@disk=2" --packagespec "VO_ALICE@O2sim::v20241014-1" --wait --fetch-output

| | Important to know:

- All existing MC production listed in MonALISA→Production Info→MC production cycles (running, completed, software update, ...)
- Procedure to request Anchored MC production to O2DPG:
 - 1. Run a test on the GRID with your settings
 - 2. Provide estimate for running time, expected storage and number of events
 - 3. Provide link to GRID folder with tests and results configuration/JDL



Beyond here: Additional keywords

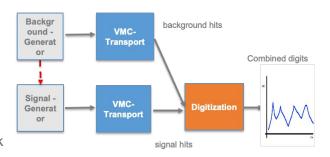
- Many more expert topics to be covered
- ... going beyond this basic set of slides ...
- Contact us for information!
- Help us improving the documentation which is still in an early stage!

Embedding CCDB-snapshots **FLUKA-studies** Configurable Params AEGIS GRID-jobs TroubleShooting QC-Tasks CaloFastSim Field CutTuning **GeneratorCocktails EmbeddingPattern** HepMC MCAnchoring xt GRP VMCReplay CollisionContext Alibi-testing TrackReferences TrackReproducibleSimulation ... and many more

Backup

Digitization, embedding (signal mixing)

- Digitization is likely less relevant for physics analysis purposes ... yet important to have heard about it
- Fundamental task of digitization is to
 - convert simple energy deposits into detector signals (digits) which finally resemble raw detector output
 - actually put individual generated events into a timeframe collection
 - account for pileup effects and triggering
- Digitization as signal embedding / mixing framework
 - Digitization can be used as an event-mixing / event-embedding framework
 - signal-background embedding allows to inject signal events into a repeated collection of background events (saves transport simulation time)
 - Can engineer sequences of event types within a timeframe (a signal event after every n-th min-bias event)



Embedding example in O2DPG:
PWGHF embedding

Estimate resources

 When running on GRID log files will show you the global runtime of your processes

```
**** Pipeline done success (global_runtime : 533.892s) *****
```

The expected running time in seconds is then:

$$\frac{N_{\rm events}^{\rm target}}{N_{\rm events}^{\rm test}} \times \Delta t_{\rm test} \times \frac{N_{\rm parallel\ workers}}{10\ 000} \qquad (N_{\rm parallel\ workers} = 8 \text{ on the GRID})$$

The storage resources instead are calculated with

$$\frac{N_{\text{events}}^{\text{target}}}{N_{\text{events}}^{\text{test}}} \times \text{size}_{\text{test}} \quad \text{where the size of the test is obtainable from} \\ \text{MonALISA} \rightarrow \text{add all stored files size}$$