

# Running productions with DIRAC

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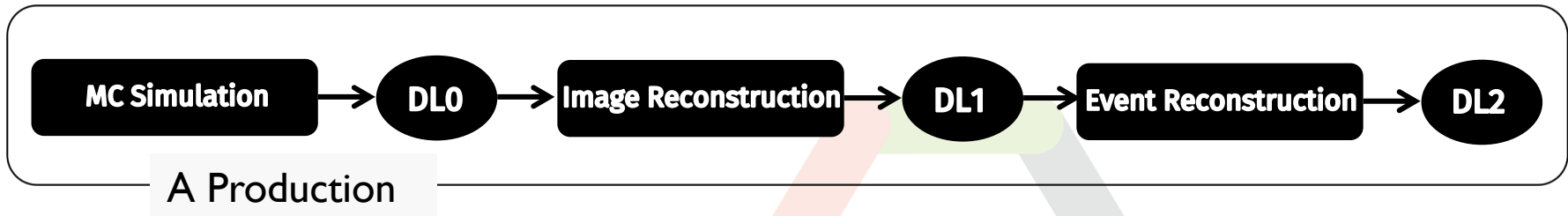


DIRAC & Rucio User Workshop

16<sup>th</sup> – 20<sup>th</sup> October 2023, KEK

- ▶ The DIRAC communities that need to manage massive productions with complex workflows use the Transformation System (see [doc here](#)) combined with a higher level system built on top of the it, called Production System
- ▶ Historically each of these communities has developed its own Production System
- ▶ Since v7r0 DIRAC provides its own Production System which is used by CTAO for now (see [doc here](#))
- ▶ We present here how CTAO and LHCb run their productions with DIRAC and LHCbDIRAC Production Systems

## Simple workflow example



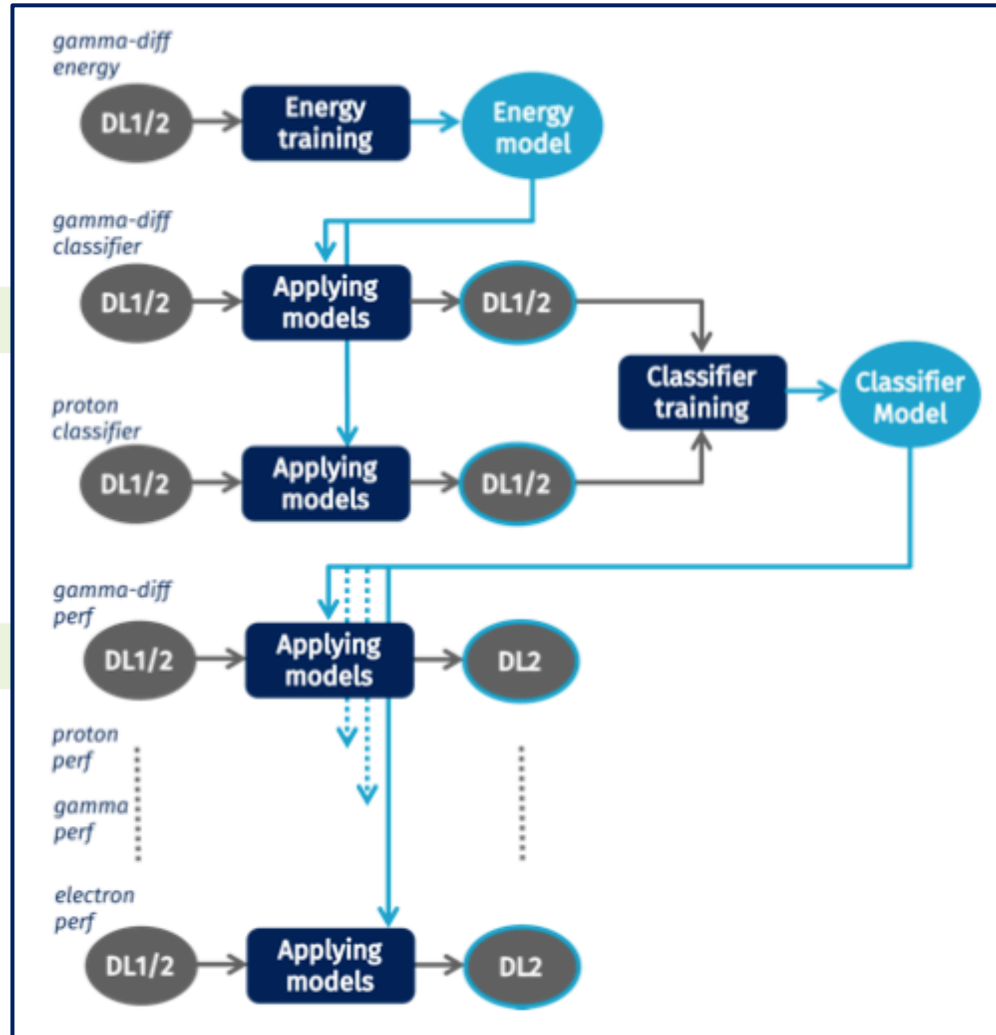
The Production System is a high-level system built on top of the Transformation System.

It automatically instantiates the different transformations that compose a Production.



Two transformations are connected if the output data of T1 intersects the input data of T2. The workflows are **data-driven**.

# CTAO processing workflow example





# CTAO processing workflow example (detailed view 1/2)

P1

DL0 gamma-diff  
Subset: energy training

DL0 gamma-diff  
Subset: classifier training

DL0 proton  
Subset: classifier training

DL0 gamma-diff  
Subset: performance

DL0 proton  
Subset: performance

DL0 gamma  
Subset: performance

DL0 electron  
Subset: performance

T1  
ctape-process

T2  
ctape-process

T3  
ctape-process

T4  
ctape-process

T5  
ctape-process

T6  
ctape-process

T7  
ctape-process

P2

DL1/2 gamma-diff  
Subset: energy training

DL1/2 gamma-diff  
Subset: classifier training

DL1/2 proton  
Subset: classifier training

DL1/2 gamma-diff  
Subset: performance

DL1/2 proton  
Subset: performance

DL1/2 gamma  
Subset: performance

DL1/2 electron  
Subset: performance

T8  
ctape-merge

T9  
ctape-merge

T10  
ctape-merge

T11  
ctape-merge

T12  
ctape-merge

T13  
ctape-merge

T14  
ctape-merge

DL1/2 gamma-diff  
Merged (intermediate)  
Subset: energy training

DL1/2 gamma-diff  
Merged (intermediate)  
Subset: classifier training

DL1/2 proton  
Merged (intermediate)  
Subset: classifier training

DL1/2 gamma-diff  
Merged (intermediate)  
Subset: performance

DL1/2 proton  
Merged (intermediate)  
Subset: performance

DL1/2 gamma  
Merged (intermediate)  
Subset: performance

DL1/2 electron  
Merged (intermediate)  
Subset: performance

T15  
ctape-merge

T16  
ctape-merge

T17  
ctape-merge

T18  
ctape-merge

T19  
ctape-merge

T20  
ctape-merge

T21  
ctape-merge

DL1/2 gamma-diff  
Merged (single file)  
Subset: energy training

DL1/2 gamma-diff  
Merged (single file)  
Subset: classifier training

DL1/2 proton  
Merged (single file)  
Subset: classifier training

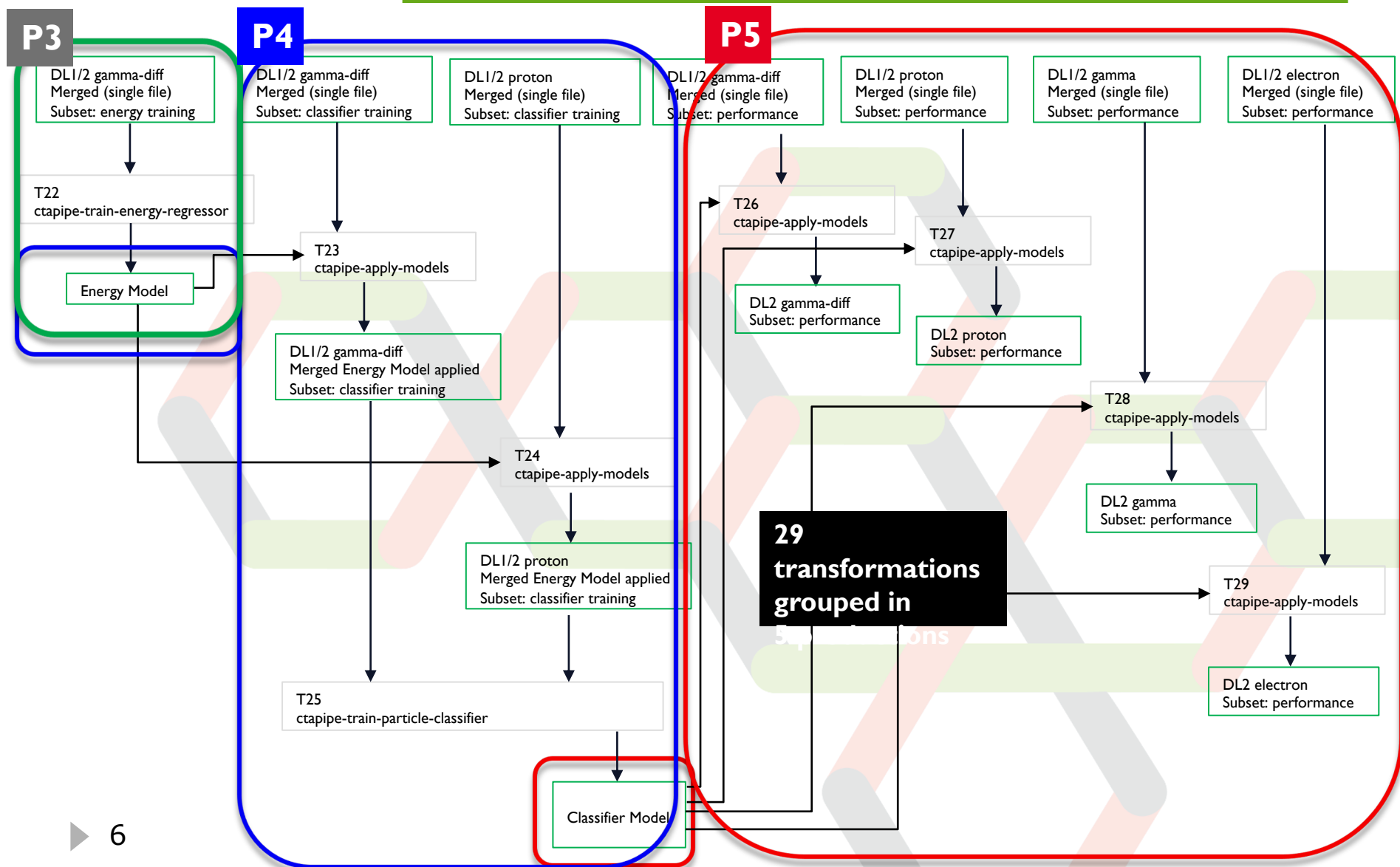
DL1/2 gamma-diff  
Merged (single file)  
Subset: performance

DL1/2 proton  
Merged (single file)  
Subset: performance

DL1/2 gamma  
Merged (single file)  
Subset: performance

DL1/2 electron  
Merged (single file)  
Subset: performance

# CTAO processing workflow example (detailed view 2/2)



- ▶ The Production System user interface comprises a Python API a limited CLI
  - > Not very practical to configure and submit complex workflows
- ▶ For our convenience in CTADIRAC we have developed a YAML-based user interface (A. Faure)
- ▶ Currently it's specific to CTAO but it can be generalized and port it to vanilla DIRAC

# User interface for the Production System

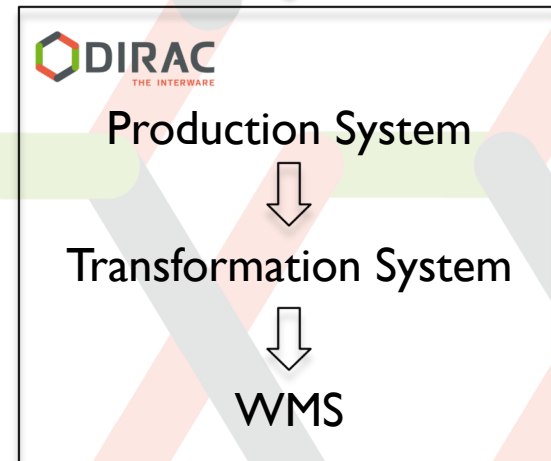
## Production description in YAML

```
ProdSteps:
- ID: 1
  input_meta_query:
    parentID:
      dataset: Prod5b-LaPalma_AdvancedBaseline_NS81x_electron_North_20deg_R1
  job_config:
    type: CtapipeProcessing
    version: v0.19.2
    array_layout: Alpha
    group_size: 2
    output_extension: DL2.h5
    data_level: 2
    options: --config v3/dl0_to_dl2.yml --config v3/prod5b/subarray_north_alpha.yml
- ID: 2
  input_meta_query:
    parentID: 1
    dataset:
  job_config:
    type: Merging
    version: v0.19.2
    group_size: 5
    output_extension: merged.DL2.h5
- ID: 3
  input_meta_query:
    parentID: 2
    dataset:
  job_config:
    type: Merging
    version: v0.19.2
    group_size: 2
    output_extension: alpha_train_en_merged.DL2.h5
    options: --no-dl1-images --no-true-images
    catalogs: DIRACFileCatalog

Common:
  MCCampaign: Prod5bTest
  configuration_id: 15
  base_path: /vo.cta.in2p3.fr/tests/prodsys/MC
```

## CLI User Interface

`cta-prod-submit <prodName> <workflow.yml>`



Computing resources

## Production description in YAML

```
ProdSteps:
- ID: 1
  input_meta_query:
    parentID:
      dataset: Prod5b-LaPalma_AdvancedBaseline_NS81x_electron_North_20deg_R1
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```

**A production is described by several steps, i.e. transformations**

Step 1

Step 2

Step 3

## Production description in YAML

```
ProdSteps:
- ID: 1
  input_meta_query:
    parentID:
    dataset: Prod5b-LaPalma_AdvancedBaseline_N5b1x_electron_North_20deg_R1
  job_config:
    type: CtapeProcessing
    version: v0.19.2
    array_layout: Alpha
    group_size: 2
    output_extension: DL2.h5
    data_level: 2
    options: --config v3/dl0_to_dl2.yml --config v3/prod5b/subarray_north_alpha.yml
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**A production is described by several steps, i.e. transformations**

**Each step is described by :**

- Input data query

## Production description in YAML

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    version: v0.19.2
    array_layout: Alpha
    group_size: 2
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**A production is described by several steps, i.e. transformations**

**Each step is described by :**

- Input data query
- Job configuration

**An input data query can be specified :**

- By a dataset



## Production description in YAML

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    parentID: 1
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    parentID: 2
    dataset:
  job_config:
    type: Merging
    version: v0.19.2
    group_size: 2
    output_extension: alpha_train_en_merged.DL2.h5
    options: --no-dl1-images --no-true-images
    catalogs: DIRACFileCatalog

Common:
  MCCampaign: Prod5bTest
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  base_path: /vo.cta.in2p3.fr/tests/prodsys/MC
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**A production is described by several steps, i.e. transformations**

**Each step is described by :**

- Input data query
- Job configuration

**An input data query can be specified :**

- By a dataset
- By a parent step (i.e. a query on the metadata of the outputs of the parent)

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```

**A production is described by several steps, i.e. transformations**

**Each step is described by :**

- Input data query
- Job configuration

**An input data query can be specified :**

- By a dataset
- By a parent step (i.e. a query on the metadata of the outputs of the parent)
- By a set of meta-data key-values

*Another  
production  
example*

```
ProdSteps:
- ID: 1
  input_meta_query:
    parentID:
      MCCampaign: PRODS
      array_layout: AlphaNectarcam
      site: Paranal
      particle: gamma-diffuse
      split: train_en
      thetaP: 20.0
      phiP: 0.0
      analysis_prog: ctape-merge
      analysis_prog_version: v0.19.3
      data_level: 2
      outputType: Data
      configuration_id: 8
      merged: 2
      moon: dark
  job_config:
    type: CtapipeTrainEnergy
    version: v0.19.3
    options: -c v3/train_energy_regressor.yml
```

## Production description in YAML

```
ProdSteps:
- ID: 1
  input_meta_query:
    parentID:
      dataset: Prod5b-LaPalma_AdvancedBaseline_NS81x_electron_North_20deg_R1
  job_config:
    type: CtapipeProcessing
    version: v0.19.2
    array_layout: Alpha
    group_size: 2
    output_extension: DL2.h5
    data_level: 2
    options: --config v3/dl0_to_dl2.yml --config v3/prod5b/subarray_north_alpha.yml
- ID: 2
  input_meta_query:
    parentID: 1
    dataset:
  job_config:
    type: Merging
    version: v0.19.2
    group_size: 5
    output_extension: merged.DL2.h5
```

**A production is described by several steps, i.e. transformations**

**Each step is described by :**

- Input data query
- Job configuration

**An input data query can be specified :**

- By a dataset
- By a parent step (i.e. a query on the metadata of the outputs of the parent)
- By a set of meta-data key-values

**For each step, the metadata of the outputs are automatically built from input data and job configuration**

*Another  
production  
example*

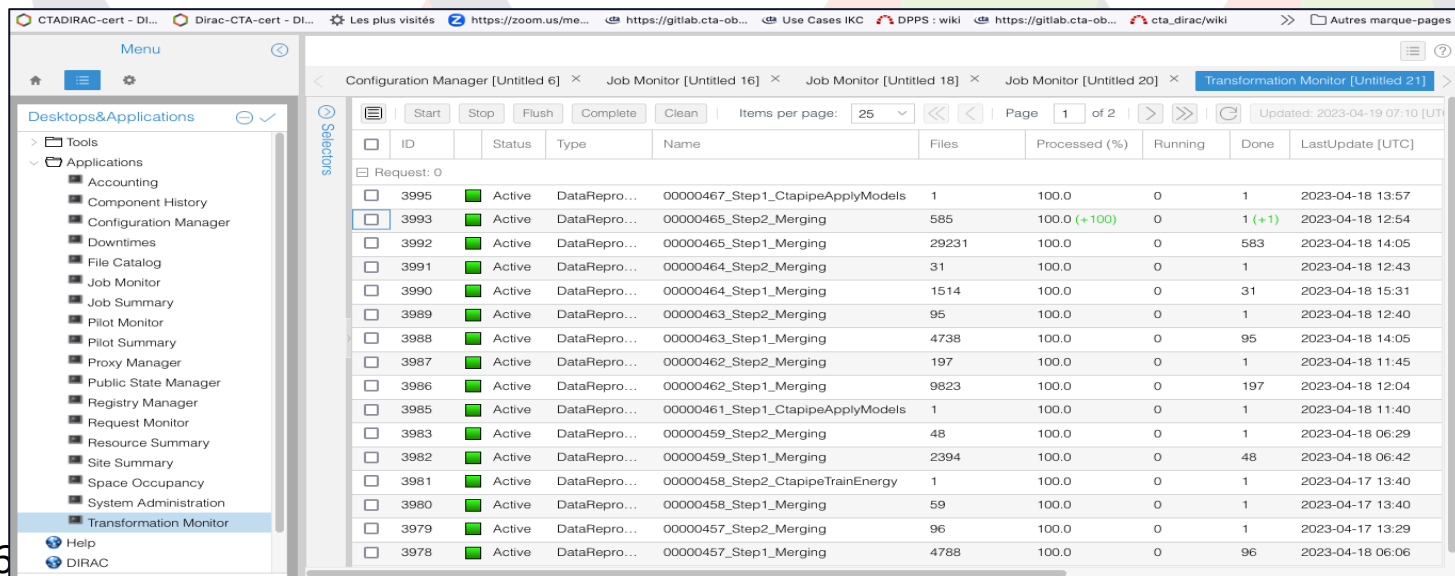
```
ProdSteps:
- ID: 1
  input_meta_query:
    parentID:
      MCCampaign: PRODS
      array_layout: AlphaNectarcam
      site: Paranal
      particle: gamma-diffuse
      split: train_en
      thetaP: 20.0
      phiP: 0.0
      analysis_prog: ctape-merge
      analysis_prog_version: v0.19.3
      data_level: 2
      outputType: Data
      configuration_id: 8
      merged: 2
      moon: dark
  job_config:
    type: CtapipeTrainEnergy
    version: v0.19.3
    options: -c v3/train_energy_regressor.yml
```

**Production System CLI** : start, stop, complete, monitor productions, etc.

```
$ dirac-prod-get-trans 649
```

|   | <b>TransformationName</b> | <b>Status</b> | <b>F_Proc.</b> | <b>F_Proc.(%)</b> | <b>TransformationID</b> |
|---|---------------------------|---------------|----------------|-------------------|-------------------------|
| 1 | 00000649_Step10_Merging   | Active        | 38             | 100.0             | 4468                    |
| 2 | 00000649_Step11_Merging   | Active        | 9977           | 100.0             | 4469                    |
| 3 | 00000649_Step12_Merging   | Active        | 139            | 100.0             | 4470                    |
| 4 | 00000649_Step13_Merging   | Active        | 5              | 100.0             | 4471                    |

## WebApp Transformation Monitor



CTADIRAC-cert - DI... Dirac-CTA-cert - DI... Les plus visités https://zoom.us/me... https://gitlab.cta-ob... Use Cases IKC DPPS : wiki https://gitlab.cta-ob... cta\_dirac/wiki

Menu

Desktops&Applications

- Tools
- Applications
  - Accounting
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  - Job Monitor
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  - Pilot Summary
  - Proxy Manager
  - Public State Manager
  - Registry Manager
  - Request Monitor
  - Resource Summary
  - Site Summary
  - Space Occupancy
  - System Administration
  - Transformation Monitor

Configuration Manager [Untitled 6] Job Monitor [Untitled 16] Job Monitor [Untitled 18] Job Monitor [Untitled 20] Transformation Monitor [Untitled 21]

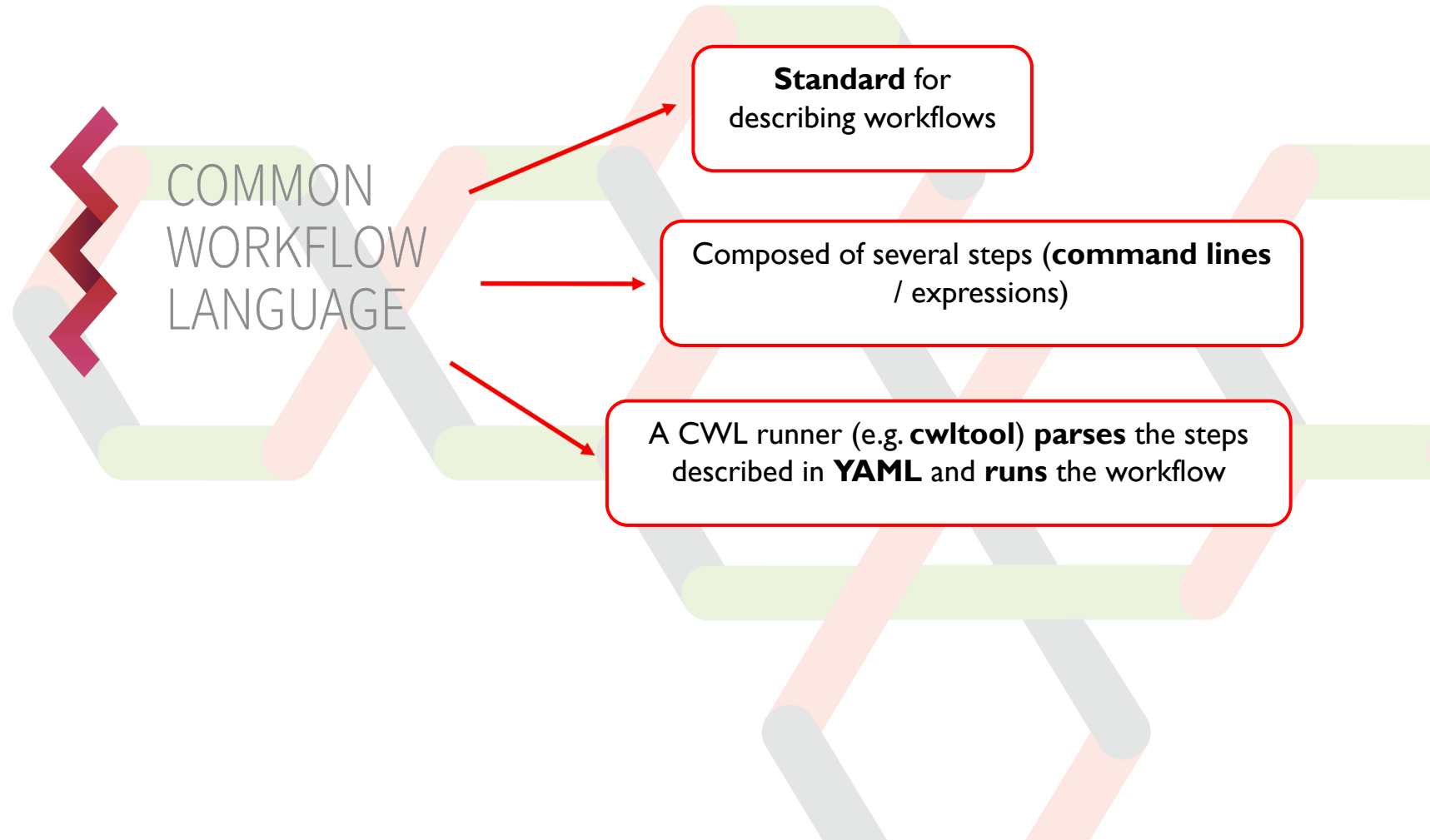
Start Stop Flush Complete Clean Items per page: 25 Page 1 of 2 Updated: 2023-04-19 07:10 [UTC]

| ID   | Status | Type         | Name                              | Files | Processed (%) | Running | Done   | LastUpdate [UTC] |
|------|--------|--------------|-----------------------------------|-------|---------------|---------|--------|------------------|
| 3995 | Active | DataRepro... | 00000467_Step1_CtapipeApplyModels | 1     | 100.0         | 0       | 1      | 2023-04-18 13:57 |
| 3993 | Active | DataRepro... | 00000465_Step2_Merging            | 585   | 100.0 (+100)  | 0       | 1 (+1) | 2023-04-18 12:54 |
| 3992 | Active | DataRepro... | 00000465_Step1_Merging            | 29231 | 100.0         | 0       | 583    | 2023-04-18 14:05 |
| 3991 | Active | DataRepro... | 00000464_Step2_Merging            | 31    | 100.0         | 0       | 1      | 2023-04-18 12:43 |
| 3990 | Active | DataRepro... | 00000464_Step1_Merging            | 1514  | 100.0         | 0       | 31     | 2023-04-18 15:31 |
| 3989 | Active | DataRepro... | 00000463_Step2_Merging            | 95    | 100.0         | 0       | 1      | 2023-04-18 12:40 |
| 3988 | Active | DataRepro... | 00000463_Step1_Merging            | 4738  | 100.0         | 0       | 95     | 2023-04-18 14:05 |
| 3987 | Active | DataRepro... | 00000462_Step2_Merging            | 197   | 100.0         | 0       | 1      | 2023-04-18 11:45 |
| 3986 | Active | DataRepro... | 00000462_Step1_Merging            | 9823  | 100.0         | 0       | 197    | 2023-04-18 12:04 |
| 3985 | Active | DataRepro... | 00000461_Step1_CtapipeApplyModels | 1     | 100.0         | 0       | 1      | 2023-04-18 11:40 |
| 3983 | Active | DataRepro... | 00000459_Step2_Merging            | 48    | 100.0         | 0       | 1      | 2023-04-18 06:29 |
| 3982 | Active | DataRepro... | 00000459_Step1_Merging            | 2394  | 100.0         | 0       | 48     | 2023-04-18 06:42 |
| 3981 | Active | DataRepro... | 00000458_Step2_CtapipeTrainEnergy | 1     | 100.0         | 0       | 1      | 2023-04-17 13:40 |
| 3980 | Active | DataRepro... | 00000458_Step1_Merging            | 59    | 100.0         | 0       | 1      | 2023-04-17 13:40 |
| 3979 | Active | DataRepro... | 00000457_Step2_Merging            | 96    | 100.0         | 0       | 1      | 2023-04-17 13:29 |
| 3978 | Active | DataRepro... | 00000457_Step1_Merging            | 4788  | 100.0         | 0       | 96     | 2023-04-18 06:06 |

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# Support of CWL for describing transformations

- ▶ Initial support of transformations described in CWL (see Alice's talk at CHEP 2023)

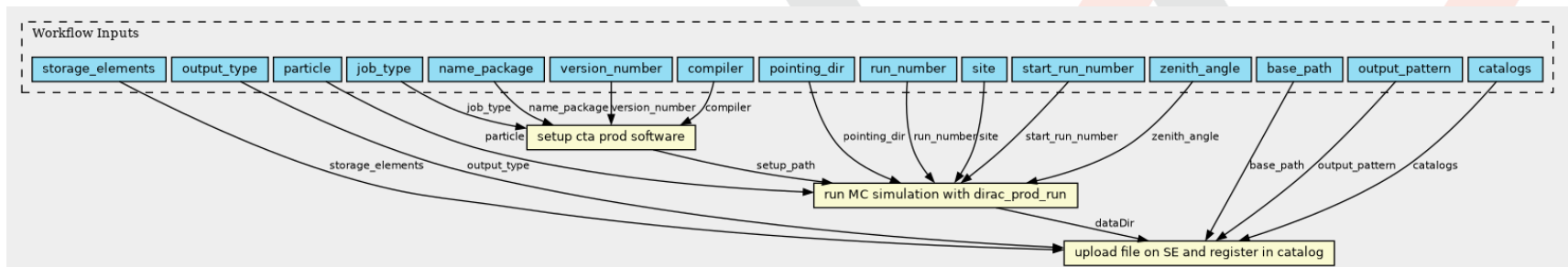


## ► Motivations

- Use a common workflow language both for local execution (e.g. by software developers for testing purpose) and execution through DIRAC

## ► Advantages of using CWL

- Standard language
- Syntax validation
- Workflow graph automatically generated



- ▶ In principle CWL could be used to describe workflows at different levels :
  - ▶ Job workflows : the different steps (executables) executed within a job
  - ▶ Production workflows : the different transformations composing a production

In CTADIRAC we have developed a tool :

***cta-prod-submit-from-cwl***

to parse CWL descriptions at job level and to submit transformations

## *cta-prod-submit-from-cwl*

1. Parses a workflow description in CWL using cwltool functions to extract the command lines and builds a DIRAC job (using DIRAC Job API)
2. From the job description, it builds and submits a transformation

### Transformation

```
trans = Transformation()
trans.setType("MCSimulation")
trans.setBody(job.workflow.toXML())
trans.addTransformation()
```

### DIRAC job

```
job.setExecutable("env setup")
job.setExecutable("run application")
job.setExecutable("data management")
```

```
name_package: corsika_simtelarray
version_number: "2022-08-03"
```

**Input YAML file**

### **CWL description**

```
cwlVersion: v1.2
class: CommandLineTool
label: setup cta prod software
baseCommand: cta-prod-setup-software

inputs:
  name_package:
    type: string
    inputBinding:
      prefix: -p
      position: 1
  version_number:
    type: string
    inputBinding:
      prefix: -v
      position: 2

outputs:
  dirac:
    type:
      type: array
      items: File
    outputBinding:
      glob: "dirac*"
```

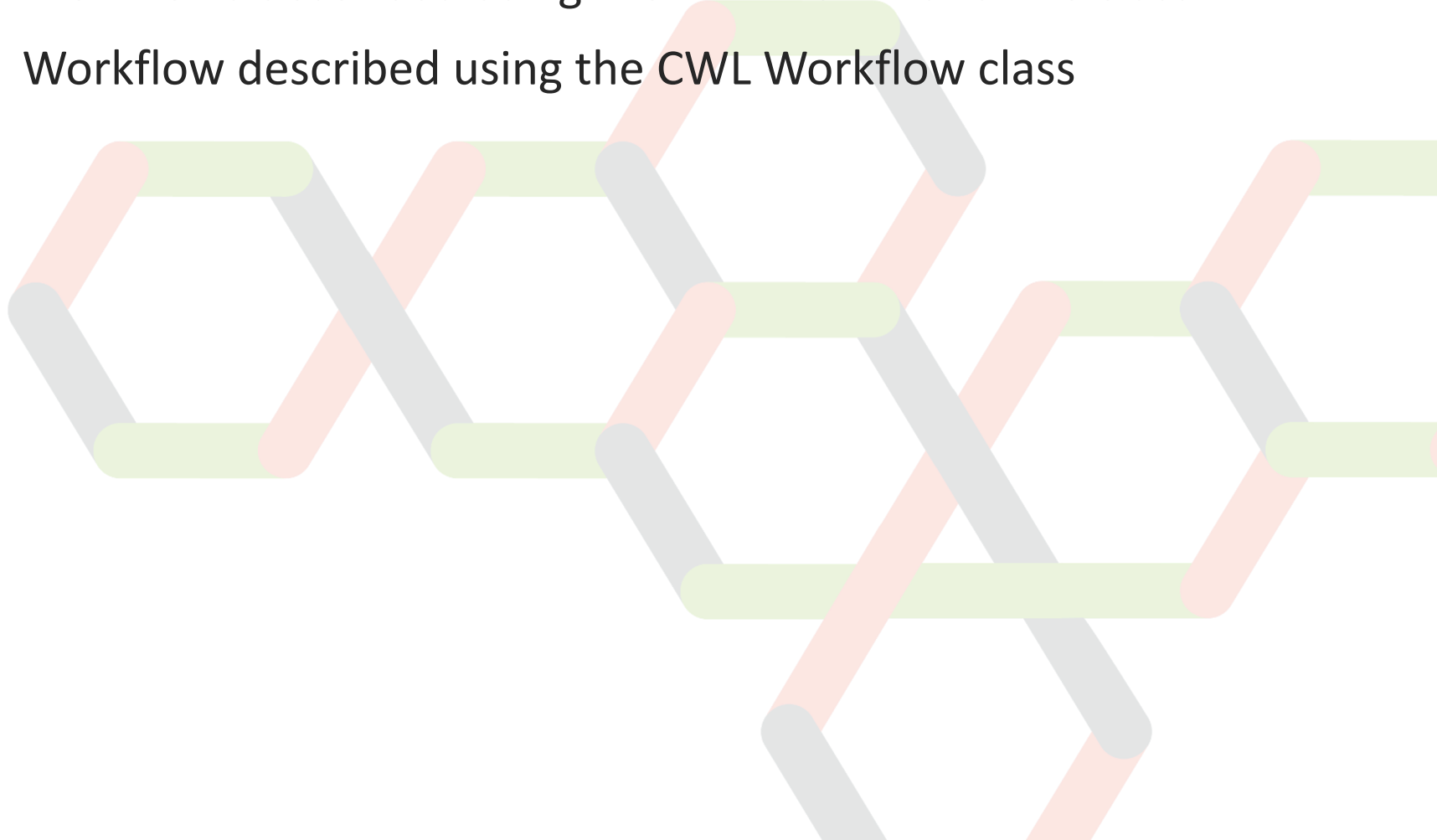


- ▶ We want to generalize our tool to build any kind of transformation
- ▶ We would like to explore the possibility to use CWL to describe DIRAC productions
- ▶ Explore how to take benefit from CWL scatter/gather functionality



# Backup

- ▶ ***cta-prod-submit-from-cwl*** supports
  - ▶ Workflows described using the CWL CommandLine class
  - ▶ Workflow described using the CWL Workflow class



## ***cta-prod-submit-from-cwl***

- ▶ Uses *cwltool* functions to generate the command lines from CWL description
- ▶ Builds DIRAC Jobs from the generated command lines

```
job.setExecutable( "command-line-1")  
job.setExecutable( "command-line-2")  
....
```

- ▶ Current limitations
  - ▶ It doesn't support Javascript expression
  - ▶ All inputs needed for the execution must be present in the command line, *e.g.* we don't support *initialWorkDirRequirement*

- ▶ A CWL workflow is made of different steps
  - ▶ The execution order depends on their I/O relations
  - ▶ If 2 steps are independent *cwltool* executes them in parallel

## ***cta-prod-submit-from-cwl***

- ▶ Determines the execution order using the same logic as *cwltool* and builds DIRAC jobs but with all steps in sequence

Step1

Inputs : *in1*, *in2*

Outputs : *out1*

Step2

Inputs : *out1*

Outputs : *out2*



```
job.setExecutable( "command-line-1")  
job.setExecutable( "command-line-2")  
....
```

## ▶ Current limitations

- ▶ The tool is not generalized yet to build any kind of transformation starting from CWL description
  - ▶ The Body of the transformation is built from CWL description, while the other attributes are not, i.e. Type, Group Size, InputDataQuery, etc.

## ▶ CWL functionalities not supported by our tool

- ▶ I/O of array type
- ▶ Sub workflows
- ▶ Conditional workflows
- ▶ Scattering workflows

- ▶ We could imagine a CWL description where
    - ▶ A CWL Workflow corresponds to a DIRAC production
    - ▶ CWL sub-workflows correspond to DIRAC transformations
  - ▶ In order to link the different transformations the Production System uses their Input and Output Queries
    - ▶ We could determine which sub-workflows are linked together based on their I/O
    - ▶ For each sub-workflow we build a transformation where the OutputQuery is built from the job parameters and the InputQuery is built from the OutputQuery
- > However this looks quite specific to each users community