Writing workflows in AiiDA

A short introduction to AiiDA's engine

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AiiDA Workflow Tutorial May 22nd 2019

AiiDA

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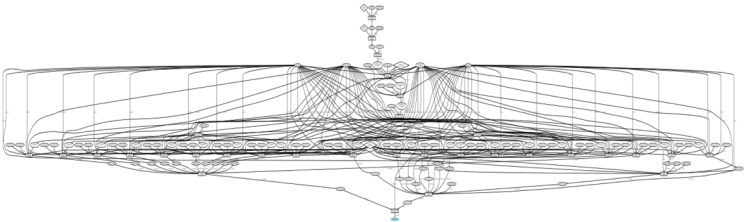

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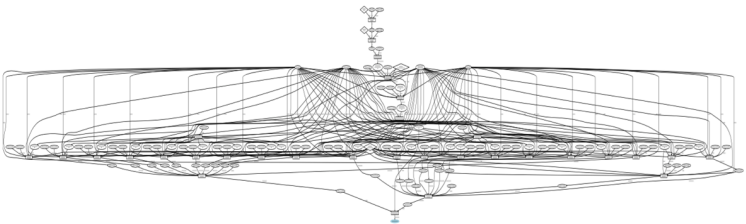

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AiiDA **Automated** Interactive Infrastructure and Database

AUTOMATED PROVENANCE: CALCULATIONS

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Add two numbers and multiply the sum by third

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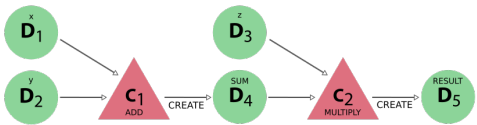

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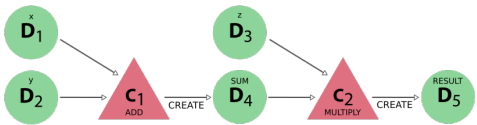

Directed **A**cyclic **G**raph

- Directed: inputs go in, and outputs come out
- Acyclic: causality principle forbids an output being its own input

AUTOMATED PROVENANCE: EXTERNAL CODES

But not all code is well-suited as python code:

What about running codes external to AiiDA?

```
#!/bin/bash
# Read two integers from file 'aiida.in` and echo their sum
x=$(cat aiida.in | awk '{print $1}')
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Implementation is different, but running very similar...

```
from aiida.engine import run
from aiida.orm import load_code, Int
from aiida.plugins import CalculationFactory

ArithmeticAddCalculation = CalculationFactory('arithmetic.add')

inputs = {
    'code': load_code('add@localhost'),
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run(ArithmeticAddCalculation, **inputs)
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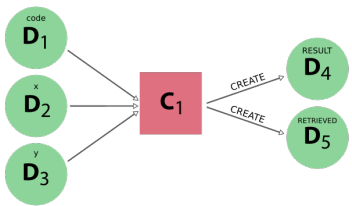

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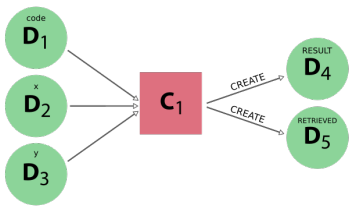

- Can be run on remote machines through job scheduler
- Implementation independent of job scheduler
- To change machine, just change the 'code' input
- Implementation focus of one of work groups tomorrow

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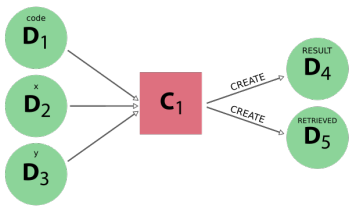
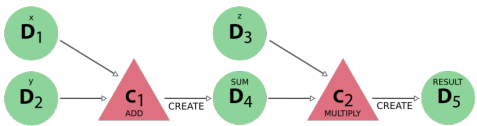


Let's go back to our add-multiple example



Individual sequence of calculations recorded...

... but not the 'how' or 'why'

AUTOMATED PROVENANCE: WORKFLOWS

Work function can be used to store *logical* provenance

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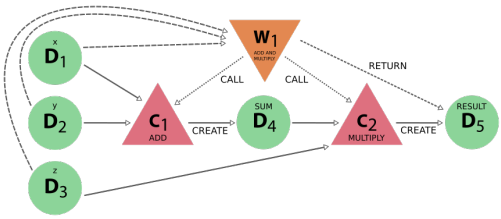

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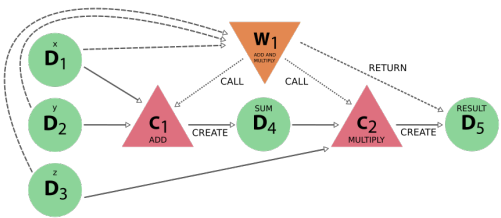

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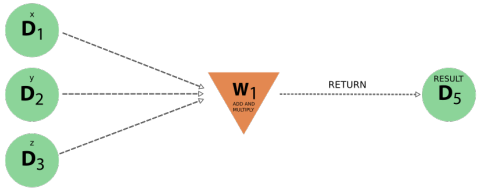

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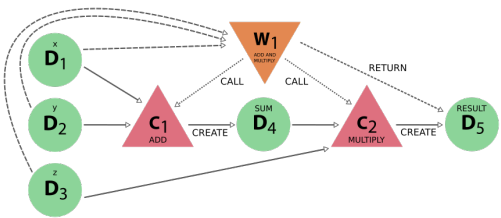

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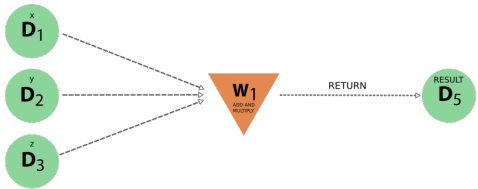
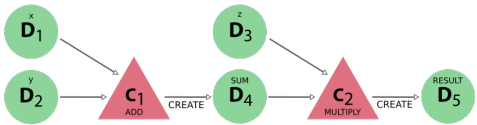


Or by ignoring it, retrieve the original data provenance



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Work chains achieve the same but save progress in between steps

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from aiida.orm import Int

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def multiply(x, y):
    return Int(x * y)

class AddAndMultiplyWorkChain(WorkChain):

    @classmethod
    def define(cls, spec):
        super(AddAndMultiplyWorkChain, cls).define(spec)
        spec.input('x')
        spec.input('y')
        spec.input('z')
        spec.outline(
            cls.add,
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    def add(self):
        self.ctx.sum = add(self.inputs.x, self.inputs.y)

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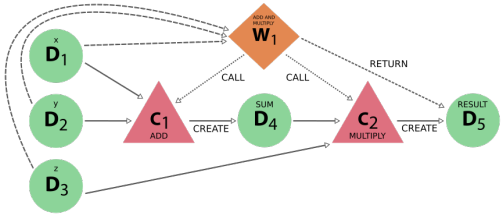

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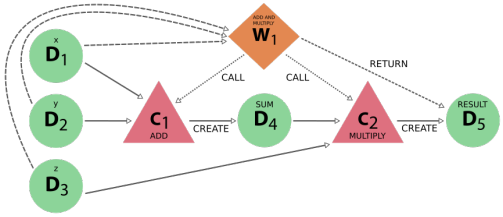
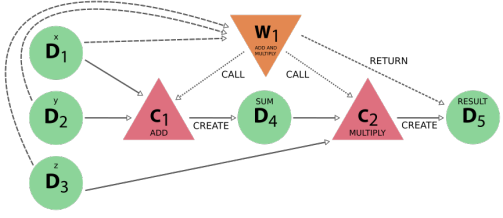


Only difference with work function solution is node type



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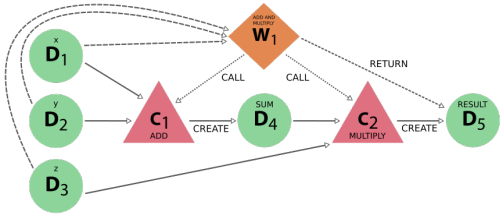

Many advantages over work function

- Can be submitted to the daemon
- Progress is saved between steps in checkpoints
- Process specification gives succinct but clear summary
- Captures the scientific knowledge and can be re-run
- Can be re-used as building block in more complex workflows

AUTOMATED PROVENANCE: LOSING PROVENANCE

Workflows cannot *create* new data.
Doing so anyway, will cause loss of provenance

Take first example: add two numbers and multiply with third...
... but now compute the product *inside* the work function

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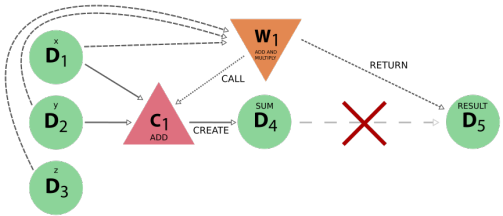

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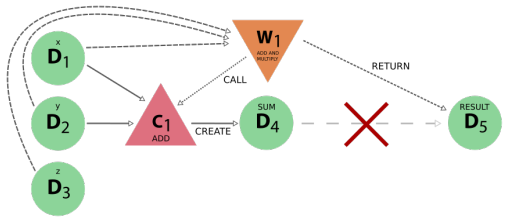

Why don't we just give the workflows the power to **create**?

WHY A DIFFERENCE BETWEEN CALCULATIONS AND WORKFLOWS?

Since workflows can return, they can also return their inputs

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from aiida.engine import workfunction
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@workfunction
def maximum(x, y, z):
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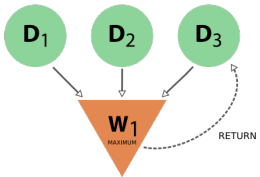

This cycle breaks the acyclicity → no more DAG

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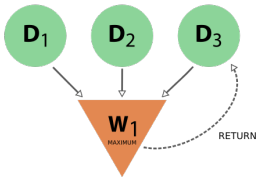
```



This cycle breaks the acyclicity → no more DAG

Two clearly distinct types of processes

CALCULATIONS

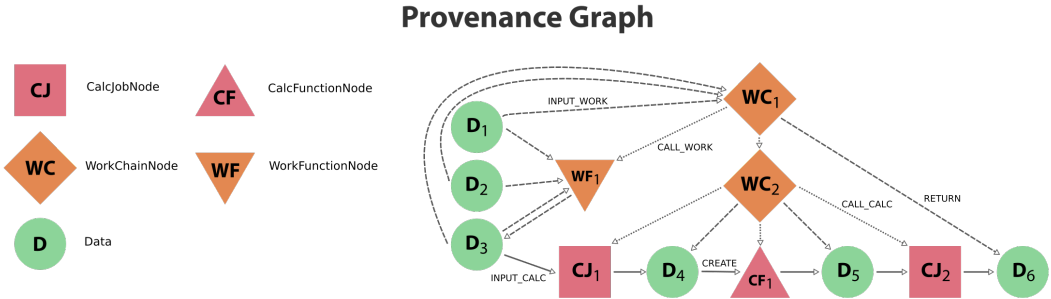
Can *create* new data

WORKFLOWS

Can *call* other processes

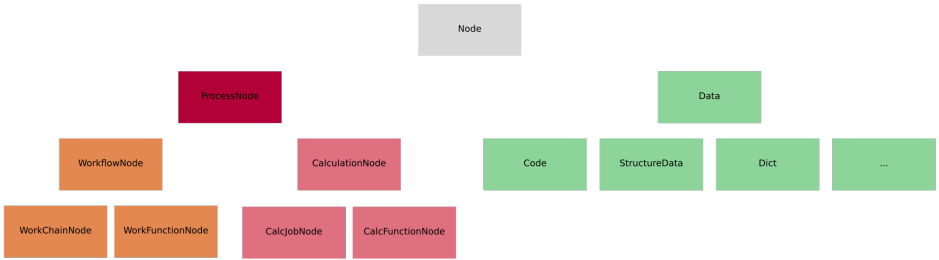
Can *return* existing data

PROVENANCE DESIGN: THE RULES



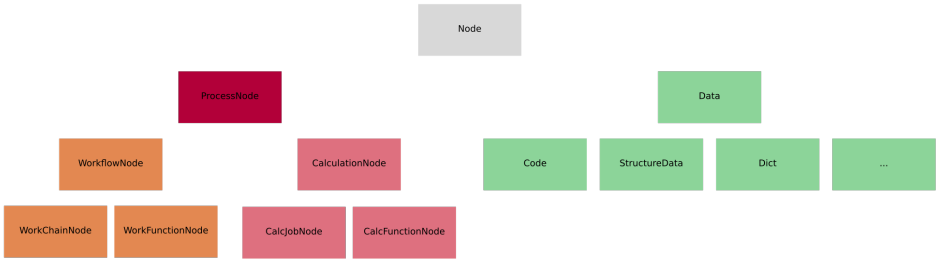
PROVENANCE DESIGN: THE RULES

ORM Hierarchy

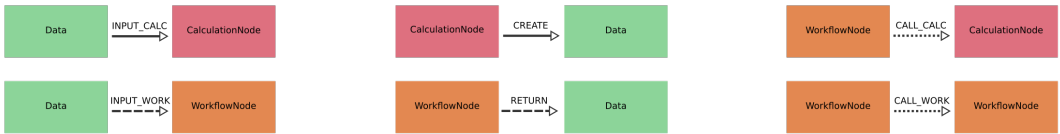


PROVENANCE DESIGN: THE RULES

ORM Hierarchy



Link Hierarchy



ENGINE: EVERYTHING IS A PROCESS

New processes to define calculations and workflows

Process class	Node class	Used for
`CalcJob`	`CalcJobNode`	Calculations performed by external codes
`WorkChain`	`WorkChainNode`	Workflows that run multiple sub processes
`FunctionProcess`	`CalcFunctionNode`	Python functions decorated with the `calcfunction` decorator
`FunctionProcess`	`WorkFunctionNode`	Python functions decorated with the `workfunction` decorator

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PROCESS STATE

Active	Terminated
Created	Killed
Running	Excepted
Waiting	Finished

ENGINE: EVERYTHING IS A PROCESS

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PROCESS STATE

Active	Terminated
Created	Killed
Running	Excepted
Waiting	Finished

PROCESS NODE ATTRIBUTES

Property	Meaning
`process_state`	Returns the current process state
`exit_status`	Returns the exit status, or None if not set
`exit_message`	Returns the exit message, or None if not set
`is_terminated`	Returns `True` if the process was either `Killed`, `Excepted` or `Finished`
`is_killed`	Returns `True` if the process is `Killed`
`is_excepted`	Returns `True` if the process is `Excepted`
`is_finished`	Returns `True` if the process is `Finished`
`is_finished_ok`	Returns `True` if the process is `Finished` and the `exit_status` is equal to zero
`is_failed`	Returns `True` if the process is `Finished` and the `exit_status` is non-zero

ENGINE: EVERYTHING IS A PROCESS

Four processes launchers with identical interface

`run`	Run blockingly and return result
`run_get_node`	Run blockingly and return result + node
`run_get_pk`	Run blockingly and return result + pk
`submit`	Submit to daemon and return node

ENGINE: EVERYTHING IS A PROCESS

Four processes launchers with identical interface

`run`	Run blockingly and return result
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`submit`	Submit to daemon and return node

Submit to the daemon

```
from aiida import orm
from aiida.engine import submit

ArithmeticAddCalculation = CalculationFactory('arithmetic.add')
node = submit(ArithmeticAddCalculation, x=orm.Int(1), y=orm.Int(2))
```

ENGINE: EVERYTHING IS A PROCESS

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Run blockingly in local interpreter

```
from aiida import orm
from aiida.engine import run

ArithmeticAddCalculation = CalculationFactory('arithmetic.add')
result = run(ArithmeticAddCalculation, x=orm.Int(1), y=orm.Int(2))
```

ENGINE: EVERYTHING IS A PROCESS

Four processes launchers with identical interface

`run`	Run blockingly and return result
`run_get_node`	Run blockingly and return result + node
`run_get_pk`	Run blockingly and return result + pk
`submit`	Submit to daemon and return node

Run variants to get the process node or pk in addition to the result

```
from aiida import orm
from aiida.engine import run_get_node, run_get_pk

ArithmeticAddCalculation = CalculationFactory('arithmetic.add')
result, node = run_get_node(ArithmeticAddCalculation, x=orm.Int(1), y=orm.Int(2))
result, pk = run_get_pk(ArithmeticAddCalculation, x=orm.Int(1), y=orm.Int(2))
```

ENGINE: EVERYTHING IS A PROCESS

Four processes launchers with identical interface

`run`	Run blockingly and return result
`run_get_node`	Run blockingly and return result + node
`run_get_pk`	Run blockingly and return result + pk
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Variants are available as attributes on `run` launcher requiring only single import

```
from aiida import orm
from aiida.engine import run

ArithmeticAddCalculation = CalculationFactory('arithmetic.add')
result = run(ArithmeticAddCalculation, x=orm.Int(1), y=orm.Int(2))
result, node = run.get_node(ArithmeticAddCalculation, x=orm.Int(1), y=orm.Int(2))
result, pk = run.get_pk(ArithmeticAddCalculation, x=orm.Int(1), y=orm.Int(2))
```

ENGINE: EVERYTHING IS A PROCESS

Four processes launchers with identical interface

`run`	Run blockingly and return result
`run_get_node`	Run blockingly and return result + node
`run_get_pk`	Run blockingly and return result + pk
`submit`	Submit to daemon and return node

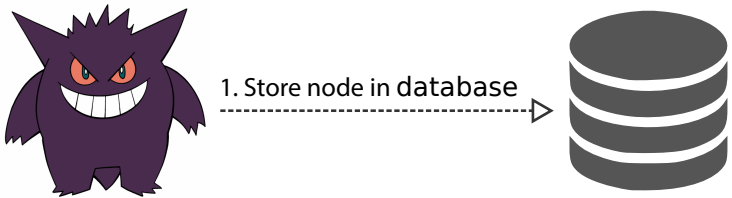
Syntactic keyword expansion for big input dictionaries

```
from aiida import orm
from aiida.engine import submit

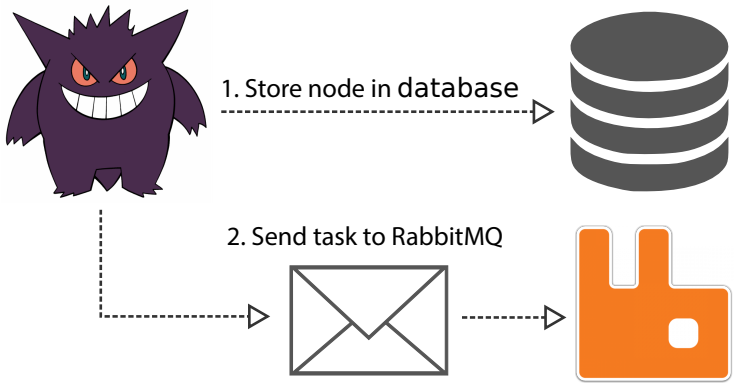
ArithmeticAddCalculation = CalculationFactory('arithmetic.add')
inputs = {
    'x': orm.Int(1),
    'y': orm.Int(2)
}
node = submit(ArithmeticAddCalculation, **inputs)
```

What happens when we submit a process?

What happens when we submit a process?

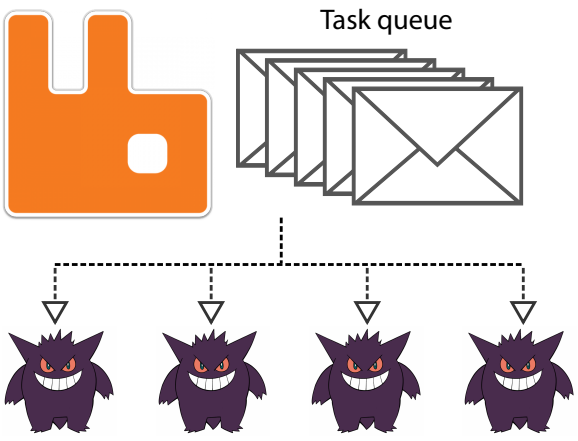


What happens when we submit a process?



What happens with those tasks?

What happens with those tasks?



ENGINE: RELYING ON A RESILIENT AND ROBUST RABBIT

The promise of RabbitMQ

- All tasks are persisted to disk
- Each task is guaranteed to be delivered
- Each task is guaranteed to be sent to only one listener at a time
- Each task is guaranteed to be completed

ENGINE: RELYING ON A RESILIENT AND ROBUST RABBIT

The promise of RabbitMQ

- All tasks are persisted to disk
- Each task is guaranteed to be delivered
- Each task is guaranteed to be sent to only one listener at a time
- Each task is guaranteed to be completed

This ensures that:

1. We can run multiple processes in parallel independently

2. Each launched task or "process" will eventually be completed

No matter what happens

ENGINE: EVERYTHING IS A PROCESS

`verdi process`: your one-stop-shop for inspecting and interacting with processes

ENGINE: EVERYTHING IS A PROCESS

`verdi process`: your one-stop-shop for inspecting and interacting with processes

`verdi process list`: list active and terminated processes

```
(aiida_3dd) aiida@theossrv5:~/code/aiida/env/3dd$ verdi process list -l 10
     PK  Created    State      Process label     Process status
-------  ---------  ---------  ---------------  --------------------------------
1285287  2D ago     ⏵ Waiting  PwRelaxWorkChain
1285535  2D ago     ⏵ Waiting  PwRelaxWorkChain
1286517  2D ago     ⏵ Waiting  PwRelaxWorkChain
1286913  2D ago     ⏵ Waiting  PwRelaxWorkChain
1287288  2D ago     ⏵ Waiting  PwBaseWorkChain
1287486  2D ago     ⏵ Waiting  PwRelaxWorkChain
1287517  2D ago     ⏵ Waiting  PwBaseWorkChain
1287937  2D ago     ⏵ Waiting  PwRelaxWorkChain
1289927  2D ago     ⏵ Waiting  PwCalculation     Waiting for transport task: update
1291148  2D ago     ⏵ Waiting  PwBaseWorkChain

Total results: 10

Info: last time an entry changed state: 43s ago (at 11:09:50 on 2019-03-22)
```

ENGINE: EVERYTHING IS A PROCESS

`verdi process`: your one-stop-shop for inspecting and interacting with processes

`verdi process status`: tree representation of call stack

```
(aiida_3dd) aiida@theossrv5:~/code/aiida/env/3dd$ verdi process status 1338418
PwRelaxWorkChain <pk=1338418> [ProcessState.FINISHED] [3:results]
    ├── PwBaseWorkChain <pk=1338525> [ProcessState.FINISHED] [4:results]
    │   ├── create_kpoints_from_distance <pk=1338529> [ProcessState.FINISHED]
    │   └── CalcJobNode <pk=1338569> [FINISHED]
    ├── PwBaseWorkChain <pk=1341443> [ProcessState.FINISHED] [4:results]
    │   ├── create_kpoints_from_distance <pk=1341445> [ProcessState.FINISHED]
    │   └── CalcJobNode <pk=1341463> [FINISHED]
    └── PwBaseWorkChain <pk=1341701> [ProcessState.FINISHED] [4:results]
        ├── create_kpoints_from_distance <pk=1341703> [ProcessState.FINISHED]
        └── CalcJobNode <pk=1341730> [FINISHED]
```

ENGINE: EVERYTHING IS A PROCESS

`verdi process`: your one-stop-shop for inspecting and interacting with processes

`verdi process report`: complete report of log messages and scheduler stdout/stderr

```
(aiida_3dd) aiida@theossrv5:~/code/aiida/env/3dd$ verdi process report 1338418
2019-03-22 05:26:39 [553130 | REPORT]: [1338418|PwRelaxWorkChain|run_relax]: launching PwBaseWorkChain<1338525>
2019-03-22 05:28:02 [553147 | REPORT]:   [1338525|PwBaseWorkChain|run_calculation]: launching PwCalculation<1338569> iteration #1
2019-03-22 07:45:52 [554706 | REPORT]:   [1338525|PwBaseWorkChain|inspect_calculation]: PwCalculation<1338569> completed successfully
2019-03-22 07:45:52 [554707 | REPORT]:   [1338525|PwBaseWorkChain|results]: workchain completed after 1 iterations
2019-03-22 07:45:52 [554708 | REPORT]:   [1338525|PwBaseWorkChain|on_terminated]: remote folders will not be cleaned
2019-03-22 07:45:53 [554709 | REPORT]: [1338418|PwRelaxWorkChain|inspect_relax]: after iteration 1 cell volume of relaxed structure is 427.27585978
2019-03-22 07:45:54 [554710 | REPORT]: [1338418|PwRelaxWorkChain|run_relax]: launching PwBaseWorkChain<1341443>
2019-03-22 07:47:21 [554713 | REPORT]:   [1341443|PwBaseWorkChain|run_calculation]: launching PwCalculation<1341463> iteration #1
2019-03-22 08:00:47 [554854 | REPORT]:   [1341443|PwBaseWorkChain|inspect_calculation]: PwCalculation<1341463> completed successfully
2019-03-22 08:00:47 [554855 | REPORT]:   [1341443|PwBaseWorkChain|results]: workchain completed after 1 iterations
2019-03-22 08:00:47 [554856 | REPORT]:   [1341443|PwBaseWorkChain|on_terminated]: remote folders will not be cleaned
2019-03-22 08:00:48 [554857 | REPORT]: [1338418|PwRelaxWorkChain|inspect_relax]: after iteration 2 cell volume of relaxed structure is 427.275859777
2019-03-22 08:00:48 [554858 | REPORT]: [1338418|PwRelaxWorkChain|inspect_relax]: relative cell volume difference 5.54830030607e-12 smaller than convergence threshold 0.01
2019-03-22 08:00:49 [554859 | REPORT]: [1338418|PwRelaxWorkChain|run_final_scf]: launching PwBaseWorkChain<1341701> for final scf
2019-03-22 08:02:13 [554881 | REPORT]:   [1341701|PwBaseWorkChain|run_calculation]: launching PwCalculation<1341730> iteration #1
2019-03-22 08:11:19 [554931 | REPORT]:   [1341701|PwBaseWorkChain|inspect_calculation]: PwCalculation<1341730> completed successfully
2019-03-22 08:11:19 [554932 | REPORT]:   [1341701|PwBaseWorkChain|results]: workchain completed after 1 iterations
2019-03-22 08:11:19 [554933 | REPORT]:   [1341701|PwBaseWorkChain|on_terminated]: remote folders will not be cleaned
2019-03-22 08:11:20 [554934 | REPORT]: [1338418|PwRelaxWorkChain|results]: workchain completed after 2 iterations
2019-03-22 08:11:30 [554935 | REPORT]: [1338418|PwRelaxWorkChain|on_terminated]: cleaned remote folders of calculations: 1341730 1341463 1338569
```

ENGINE: EVERYTHING IS A PROCESS

`verdi process`: your one-stop-shop for inspecting and interacting with processes

`verdi process pause`: pause an active process

```
(aiida_dev) sphuber@theos:~$ verdi process pause 804
Success: scheduled pause Process<804>
```

ENGINE: EVERYTHING IS A PROCESS

`verdi process`: your one-stop-shop for inspecting and interacting with processes

`verdi process pause`: pause an active process

```
(aiida_dev) sphuber@theos:~$ verdi process pause 804
Success: scheduled pause Process<804>
```

`verdi process play`: resume a paused process

```
(aiida_dev) sphuber@theos:~$ verdi process play 812
Success: scheduled play Process<812>
```

ENGINE: EVERYTHING IS A PROCESS

`verdi process`: your one-stop-shop for inspecting and interacting with processes

`verdi process pause`: pause an active process

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(aiida_dev) sphuber@theos:~$ verdi process pause 804
Success: scheduled pause Process<804>
```

`verdi process play`: resume a paused process

```
(aiida_dev) sphuber@theos:~$ verdi process play 812
Success: scheduled play Process<812>
```

`verdi process kill`: kill an active process

```
(aiida_dev) sphuber@theos:~$ verdi process kill 820
Success: scheduled kill Process<820>
```

ENGINE: EVERYTHING IS A PROCESS

`verdi process`: your one-stop-shop for inspecting and interacting with processes

`verdi process pause`: pause an active process

```
(aiida_dev) sphuber@theos:~$ verdi process pause 804
Success: scheduled pause Process<804>
```

`verdi process play`: resume a paused process

```
(aiida_dev) sphuber@theos:~$ verdi process play 812
Success: scheduled play Process<812>
```

`verdi process kill`: kill an active process

```
(aiida_dev) sphuber@theos:~$ verdi process kill 820
Success: scheduled kill Process<820>
```

`verdi process pause/play/kill`: fails if process is already terminated

```
(aiida_dev) sphuber@theos:~$ verdi process kill 812
Error: Process<812> is already terminated
```

ENGINE: ROBUSTNESS

Automatic retry for transport tasks with exponential backoff

```
(aiida_3dd) aiida@theossrv5:~/code/aiida/env/3dd$ verdi process list --paused
     PK  Created    State      Process label    Process status
-------  ---------  ---------  ---------------  ------------------------------------------------------------------------------------------
1343914  5h ago     ⏸ Waiting  PwCalculation    Pausing after failed transport task: retrieve_calculation failed 5 times consecutively

Total results: 1

Info: last time an entry changed state: 21s ago (at 16:10:08 on 2019-03-22)
```

ENGINE: ROBUSTNESS

Automatic retry for transport tasks with exponential backoff

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(aiida_3dd) aiida@theossrv5:~/code/aiida/env/3dd$ verdi process list --paused
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```

Rate limited connections to remote clusters per daemon worker

```
(aiida_3dd) aiida@theossrv5:~$ verdi computer configure show localhost
* safe_interval  0
```

ENGINE: ROBUSTNESS

Automatic retry for transport tasks with exponential backoff

```
(aiida_3dd) aiida@theossrv5:~/code/aiida/env/3dd$ verdi process list --paused
     PK  Created    State      Process label    Process status
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1343914  5h ago     ⏸ Waiting  PwCalculation    Pausing after failed transport task: retrieve_calculation failed 5 times consecutively

Total results: 1

Info: last time an entry changed state: 21s ago (at 16:10:08 on 2019-03-22)
```

Rate limited connections to remote clusters per daemon worker

```
(aiida_3dd) aiida@theossrv5:~$ verdi computer configure show localhost
* safe_interval  0
```

Rate limited scheduler state queries per daemon worker

```
(aiida_3dd) aiida@theossrv5:~$ verdi shell

In [1]: from aiida.orm import Computer

In [2]: computer = Computer.get(name='localhost')

In [3]: computer.get_minimum_job_poll_interval()
Out[3]: 30

In [4]: computer.set_minimum_job_poll_interval(60)

In [5]: computer.get_minimum_job_poll_interval()
Out[5]: 60
```

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FIN