



PSI

Center for Scientific Computing,
Theory and Data

How to write your workflow

Lessons I learned writing the koopmans package

Edward Linscott

LMS Seminar, 12 March 2025

A brief history of the koopmans code



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- (more recently) substantial changes to integrate with AiiDA (I'll discuss this later)

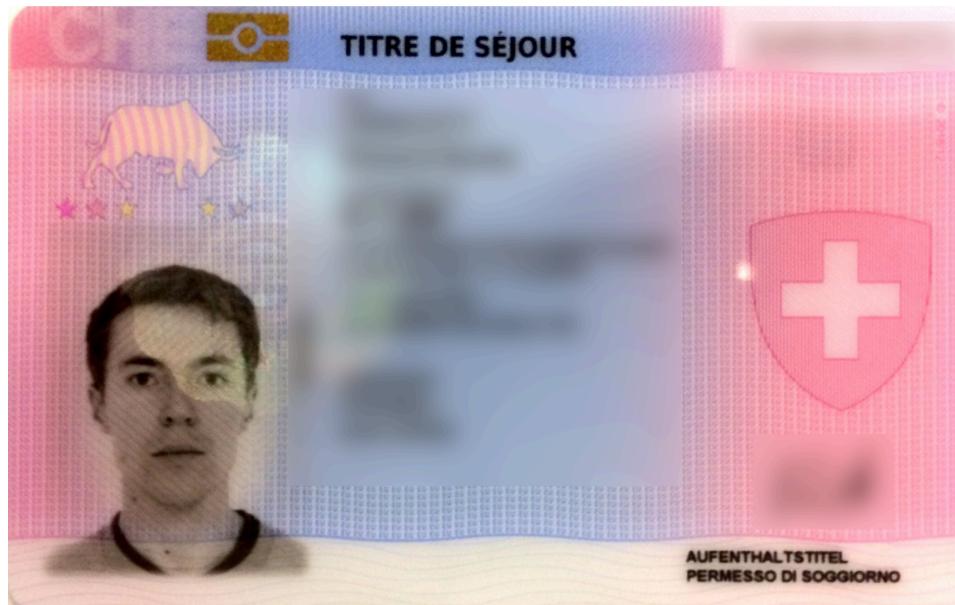
**.... but what have I learned
throughout this process?**



A scene from The Simpsons. Homer Simpson, wearing a tan shirt and grey pants, is standing on the left, gesturing with his hands while speaking. Bart Simpson, in his orange shirt, is looking up at him. In the foreground, the backs of two other characters are visible: a black-haired person in a blue shirt and a blonde person in a white shirt. The background shows a green hillside with a blue sky and clouds.

... not quite!

2019



2024



What I learned when interfacing koopmans with AiiDA

koopmans

Simple by design



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- local execution only



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- serial step execution (even when steps are independent!)



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We could really benefit from a lot of these features

Goals

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- UI should be as similar as possible
- old mode of running koopmans should still work
- minimal/no duplication of logic

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- ... and, more generally, many responsibilities are moved to the engine (reading/writing files, running calculations, checking the status of calculations, loading pseudopotentials, etc.)

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```
calc_nscf.parameters.outdir = calc_scf.parameters.outdir
```

becomes

```
calc_nscf.link(calc_scf.parameters.outdir, 'tmp')
```

where

```
def link(self, src, dst):  
    self.engine.link(src=src, dst=self/dst)
```

Note: none of this refactoring
is specific to AiiDA!

At the AiiDA end



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- conversion of calculators from ASE to AiiDA and back
- verdi presto for simplified AiiDA setup
- verdi dump for dumping AiiDA database to a local file structure

**Writing workflows well is
hard...**

**Writing workflows well is
hard... how can it best be
done?**

Common Workflow Language

Basic Concepts of CWL



COMMON
WORKFLOW
LANGUAGE

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- introduced in 2014; version 1.2 released in 2020

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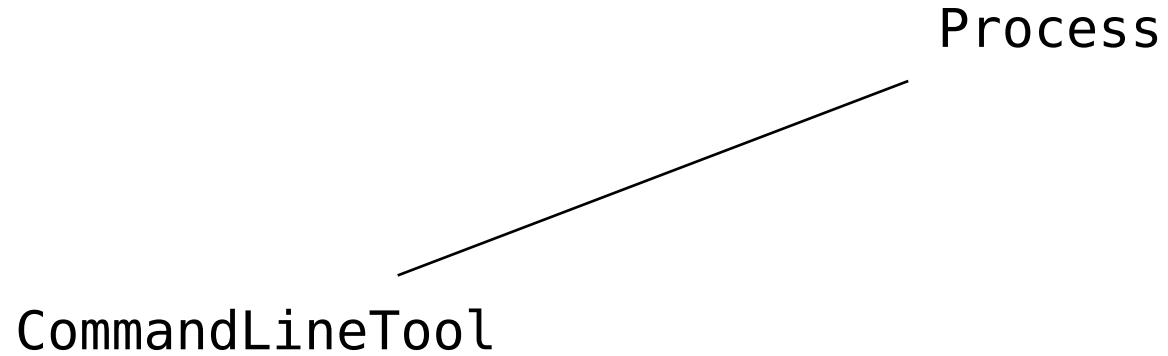
- “an open standard for describing how to run command line tools and connect them to create workflows”
- separate runners are required to execute the workflows; a CWL workflow only contains the logic of the workflows
- introduced in 2014; version 1.2 released in 2020
- mostly used by bioinformatics community

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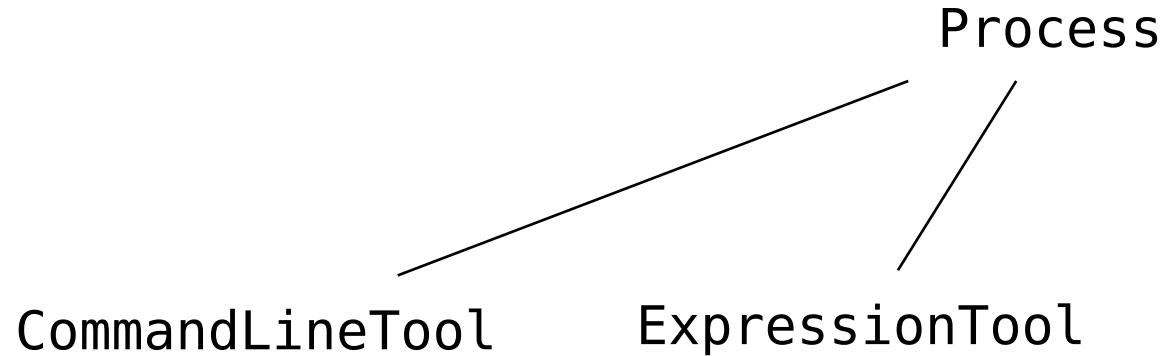


Process

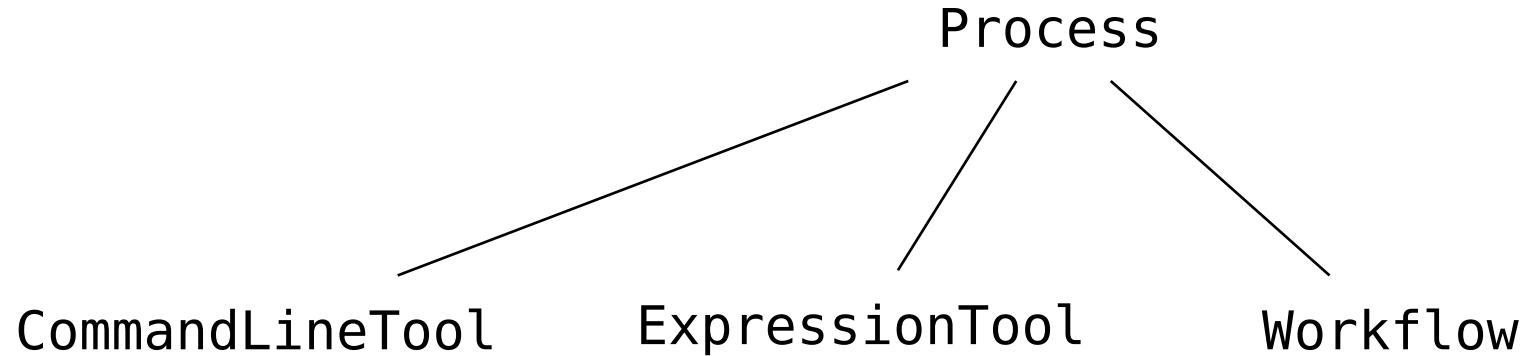
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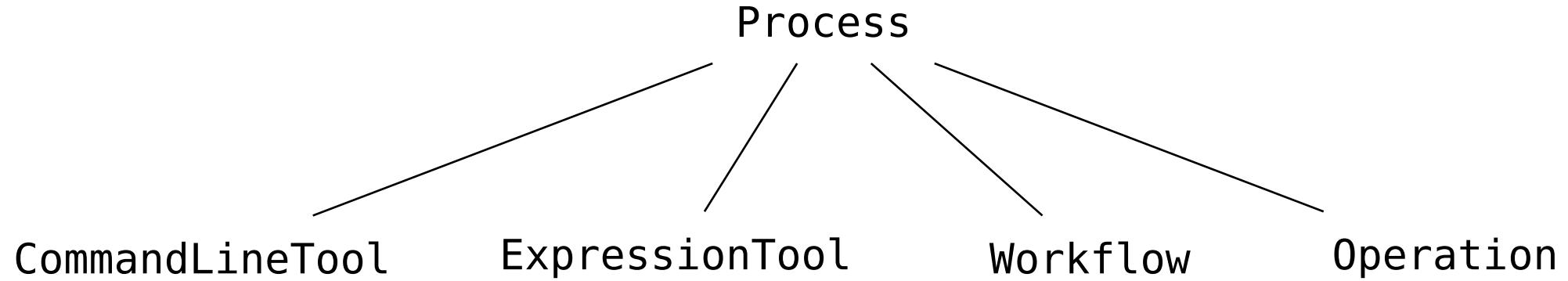
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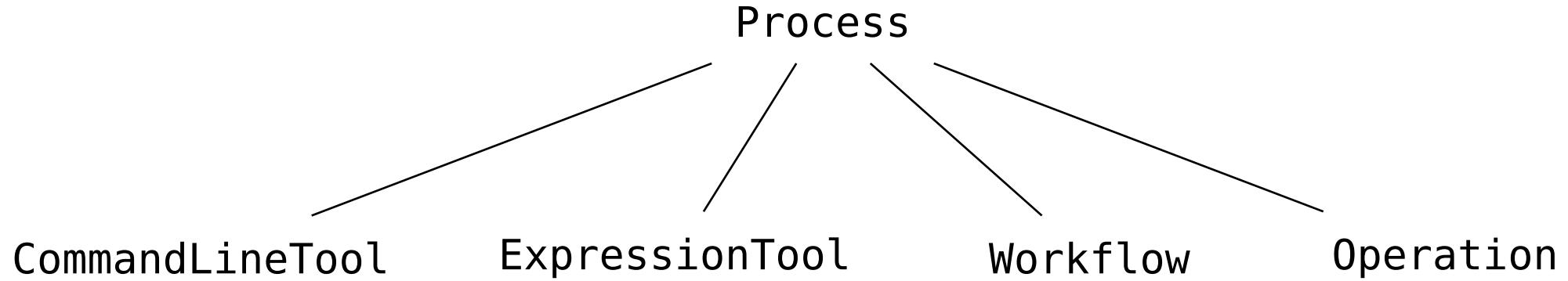
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Every Process has inputs and outputs

CommandLineTool

```
echo.cwl

cwlVersion: v1.2
class: CommandLineTool

inputs:
  message:
    type: string
    default: "Hello World"
    inputBinding:
      position: 1
outputs: []

baseCommand: echo
```

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Called via \$ cwltool echo.cwl

ExpressionTool

```
uppercase.cwl
```

```
cwlVersion: v1.2
class: ExpressionTool
requirements:
  InlineJavascriptRequirement: {}

inputs:
  message: string
outputs:
  uppercase_message: string

expression: |
  ${ return {"uppercase_message": inputs.message.toUpperCase()}; }
```

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```

Called via \$ cwltool uppercase.cwl --message='goes to 11'

Workflow

```
echo_uppercase.cwl

cwlVersion: v1.2
class: Workflow

requirements:
  InlineJavascriptRequirement: {}

inputs:
  message: string
outputs:
  out:
    type: string
    outputSource: uppercase/uppercase_message
```

Workflow



```
steps:  
  echo:  
    run: echo.cwl  
    in:  
      message: message  
    out: [out]  
  uppercase:  
    run: uppercase.cwl  
    in:  
      message:  
        source: echo/out  
    out: [uppercase_message]
```

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```

Called via \$ cwltool echo_uppercase.cwl input.json

Operation

```
p_vs_np.cwl
```

```
cwlVersion: v1.2
```

```
class: Operation
```

```
inputs: []
```

```
outputs:
```

```
  result: bool
```

A less silly Operation

```
run_pw.cwl
cwlVersion: v1.2
class: Operation

inputs:
    input_file: File
    pseudopotentials:
        type: array
        items:
            type: File
outputs:
    output_file: File
```

Pros and Cons

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 - custom types do not permit defaults
 - rigorous schemas require willingness from the community

... willingness from the community?



The screenshot shows a GitLab issue page for a project named 'q-e'. The issue, titled 'Suggestions to make .def files more informative and consistent', was created by Edward Linscott 9 months ago and is currently open. The description discusses shortcomings in the .def files and suggests solutions. The sidebar on the left shows other issues and merge requests, while the right sidebar contains fields for assignees, epic, labels, milestone, and weight.

Suggestions to make .def files more informative and consistent

Open Issue created 9 months ago by Edward Linscott

Currently, the .def files that define the Quantum ESPRESSO input format have a couple of shortcomings. Below, I discuss these shortcomings and suggest some solutions.

Dimensionality and units

The dimensionality and units of each variable is not well-documented. Yes, the header specifies that unless otherwise specified quantities are in Rydberg atomic units, but the way that alternative units are specified within the info tag is ad-hoc e.g.

```
var sci_vb -type REAL {  
    default { 0 }  
    info {
```

... willingness from the community?

The screenshot shows a Jira interface. On the left is a sidebar with navigation links: Merge requests (14), Manage, Plan, Issues (113), Issue boards, Milestones, Wiki, Requirements, Code, Build, Deploy, and Operate. The Issues link is highlighted. The main content area shows a pull request with the title:

```
val INDEX_SECONDS -type REAL 1  
    default { 1.0+7, or 150 days, i.e. no time limit }
```

A comment below the code reads:

I would propose the introduction of either (a) a new field (`default_explanation` or similar) or (b) a sub-field of `default`. This new field would contain any explanation of the default is contained, while `default` would be strictly reserved for the actual numerical value of the default.

Below this is a section titled "Why should I care?". A tooltip from Julian Geiger says:

Julian Geiger reacted with :thumbsup:

Below the tooltip are three buttons: a thumbs up icon with the number 1, a thumbs down icon with the number 0, and a neutral face icon.

The Jira interface also includes sections for Child items (0), a summary note about child items, and various metadata fields on the right side:

- Labels: None
- Milestone: None
- Weight: None
- Due date: None
- Time tracking: No estimate or time spent
- Health status: None

Building ideas from CWL into koopmans

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koopmans is slowly being refactored into “CWL-inspired” Python

```
InputModel = TypeVar('InputModel', bound=BaseModel)
OutputModel = TypeVar('OutputModel', bound=BaseModel)

class Process(ABC, Generic[InputModel, OutputModel]):

    input_model: Type[InputModel]
    output_model: Type[OutputModel]

    def __init__(self, name: str | None = None, **kwargs):
        self.inputs: InputModel = self.input_model(**kwargs)
        self.outputs: OutputModel | None = None
        self.directory: Path | None = None

    def run(self):
        assert self.directory is not None, 'Process directory must be set before running'
        with utils.chdir(self.directory):
            self.dump_inputs()
            self._run()
            assert self.outputs is not None, 'Process outputs must be set when running'
            self.dump_outputs()

    @abstractmethod
    def _run(self):
        ...
```

A simple CommandLineTool

```

class Bin2XMLInput(IOModel):
    binary: File
    class Config:
        arbitrary_types_allowed = True

class Bin2XMLOutput(IOModel):
    xml: File
    class Config:
        arbitrary_types_allowed = True

class Bin2XMLPCommandLineTool(CommandLineTool[Bin2XMLInput, Bin2XMLOutput]):

    input_model = Bin2XMLInput
    output_model = Bin2XMLOutput

    def _pre_run(self):
        super()._pre_run()
        if not self.inputs.binary.exists():
            raise FileNotFoundError(f'{self.inputs.binary} does not exist')

        # Link the input binary file to the directory of this process as input.dat
        dst = self / "input.dat"
        dst.symlink_to(self.inputs.binary)

    @property
    def command(self):
        return Command(executable='bin2xml.x', suffix='input.dat output.xml')

    def _set_outputs(self):
        self.outputs = self.output_model(xml=self / "output.xml")

```

An example composite workflow

```
# Read and run the Koopmans workflow
wf = read('si.json')
wf.run_while()

# Merge the separate occ + emp projections into a set of projections that combines occ + empty
combined_proj_list = [p for block in wf.projections for p in block.projections]
combined_proj_obj = ProjectionBlocks.fromlist([combined_proj_list], ['up'], wf.atoms)

# Find the kcw.x output directory that contains the Hamiltonian to Wannierize
[kcw_ham_calc] = [c for c in wf.calculations if isinstance(c, KoopmansHamCalculator)]
kcw_outdir = File(kcw_ham_calc, kcw_ham_calc.parameters.outdir)

# Construct a Wannierize workflow for the joint occ + empty manifold
wann_wf = WannierizeBlockWorkflow.from_other(wf,
    block=combined_proj_obj[0],
    pw_outdir=kcw_outdir,
    write_tb=True,
    calculate_bands=True)
wann_wf.calculator_parameters['pw2wannier'].prefix = 'kc_kcw'
wann_wf.directory /= '02-joint-wannierize'

# Run the Wannierization
wann_wf.run_while()
```

So what?

koopmans + AiIDA

UI practically unchanged:

```
$ koopmans tio2.json
```

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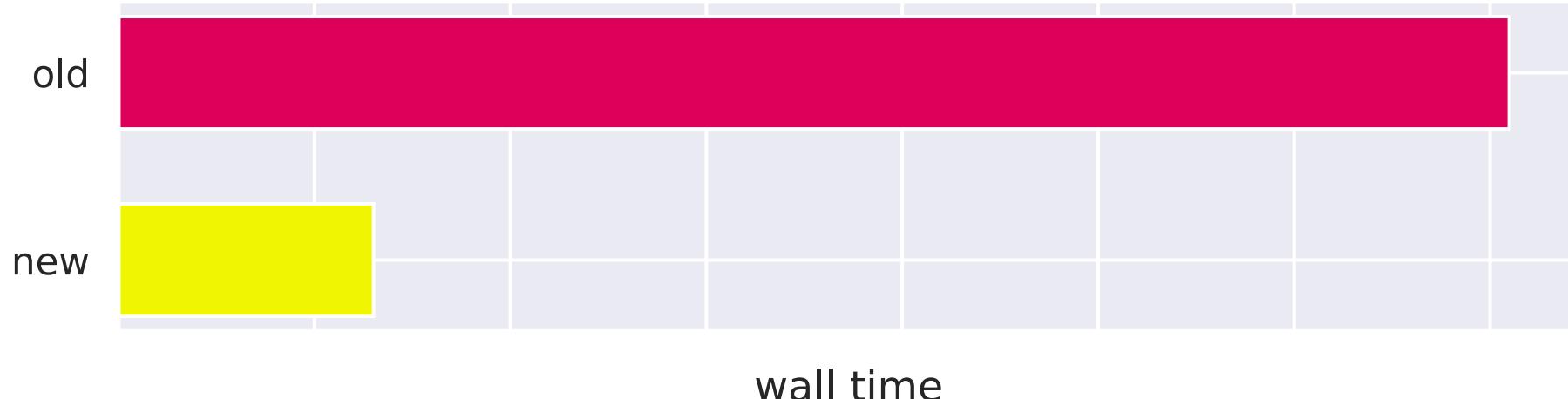
```
$ koopmans tio2.json → $ koopmans run --engine=aiida tio2.json
```

koopmans + AiiDA

UI practically unchanged:

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$ koopmans tio2.json → $ koopmans run --engine=aiida tio2.json
```

but executed remotely and in parallel:



Outlook

Workflow-runner-agnostic workflows?

A lot of the pain in koopmans + AiiDA derives from wanting to have two workflow runners:

- localhost (the original koopmans implementation)
- AiiDA

¹but still requires schemas, so not truly general

²S. P. Huber *et al.* *npj Comput Mater* **7**, 1–12 (2021)

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(cf. Do we want to write calculator-agnostic workflows?

- yes! See Common Workflows²)

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- make it easy for people to tweak and combine workflows
 - (should AiiDA be able to read and dump .cwl files?)
- for AiiDA , continue efforts to simplify

Fin

References



S. P. Huber *et al.* Common workflows for computing material properties using different quantum engines. *npj Comput Mater* **7**, 1–12 (2021).