PSI Center for Scientific Computing, Theory and Data

Automated workflows

What I have learned from writing koopmans

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LMS Seminar, 12 March 2025

Outline

What I’ve learned after 5 years of trying to automate Koopmans functionals

A brief history of the `koopmans` code

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… but what have I learned throughout this process?

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Well not quite, but the intervening years have not been kind!

Interfacing with AiiDA

What I needed to do

- isolate into steps
- functional programming
- what is the best way of writing a workflow?

Common Workflow Language

Basic Concepts of CWL

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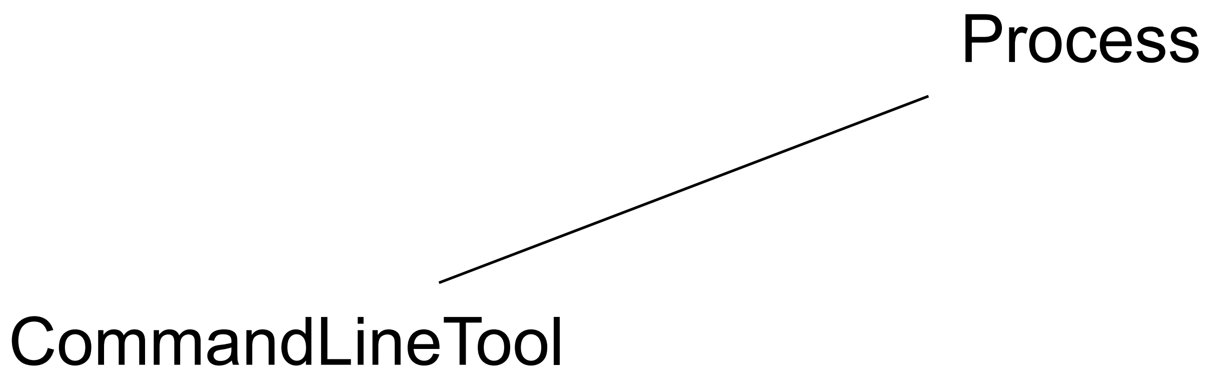
- mostly used by bioinformatics community

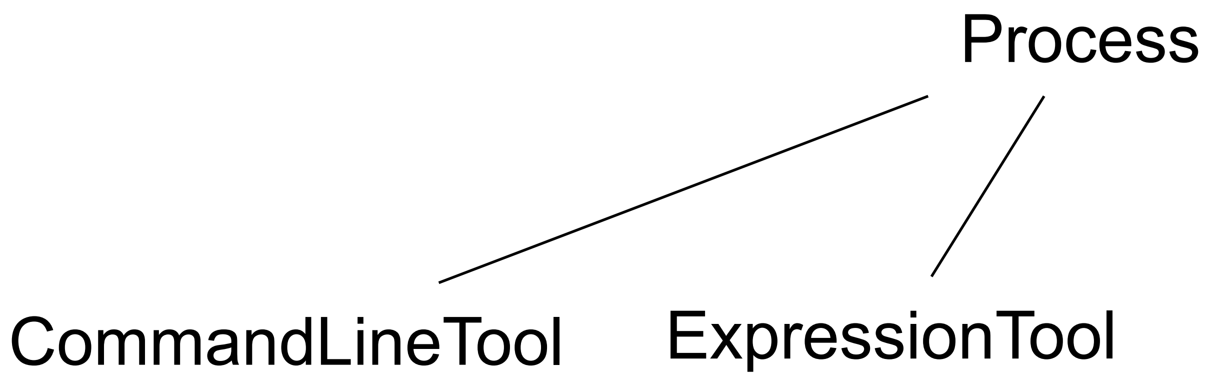
Basic Concepts of CWL

Process

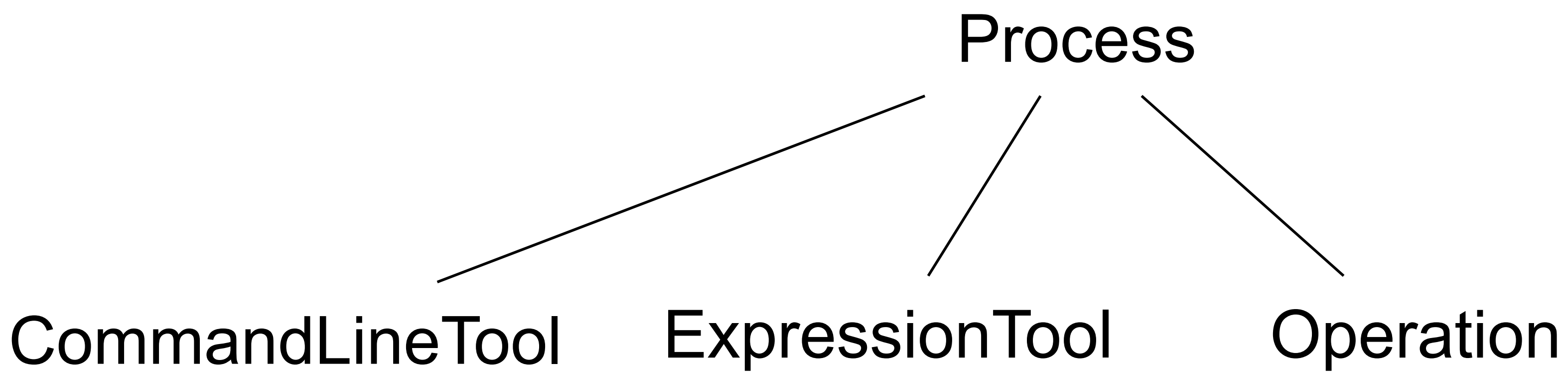
Basic Concepts of CWL



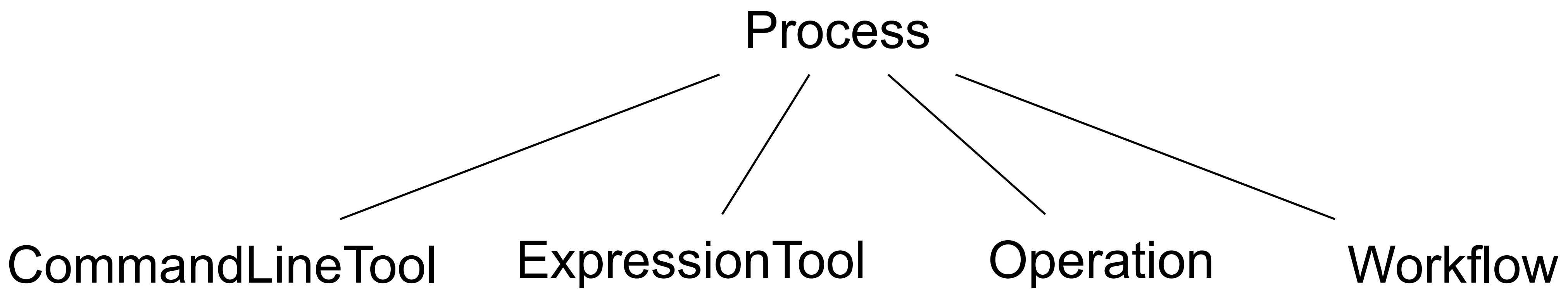
Basic Concepts of CWL



Basic Concepts of CWL



Basic Concepts of CWL



CommandLineTool

echo.cwl

```
cwlVersion: v1.2
class: CommandLineTool
baseCommand: echo

inputs:
  message:
    type: string
    default: "Hello World"
    inputBinding:
      position: 1
```

CommandLineTool

```
outputs: []
```

ExpressionTool

uppercase.cwl

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

inputs:
  message: string
outputs:
  uppercase_message: string

expression: |
```

ExpressionTool

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

Workflow

echo_uppercase.cwl

```
cwlVersion: v1.2
class: Workflow

requirements:
  InlineJavascriptRequirement: {}

inputs:
  message: string

outputs:
  out:
```

Workflow

```
    type: string
    outputSource: uppercase/uppercase_message

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

Workflow

```
    message:
      source: echo/out
  out: [uppercase_message]
```

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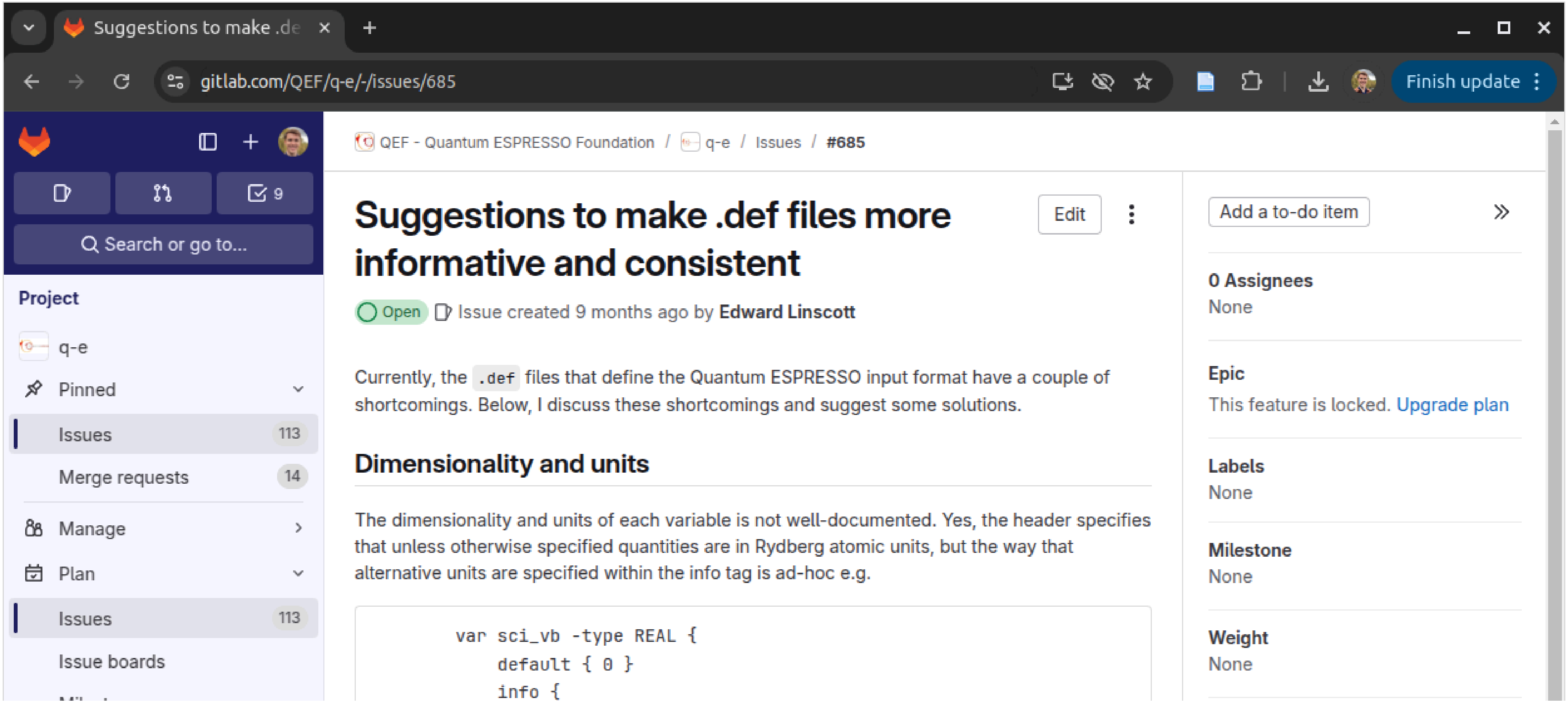
  - custom types do not permit defaults
  - rigorous schemas require willingness from the community

… willingness from the community?



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 {
```

0 Assignees
None

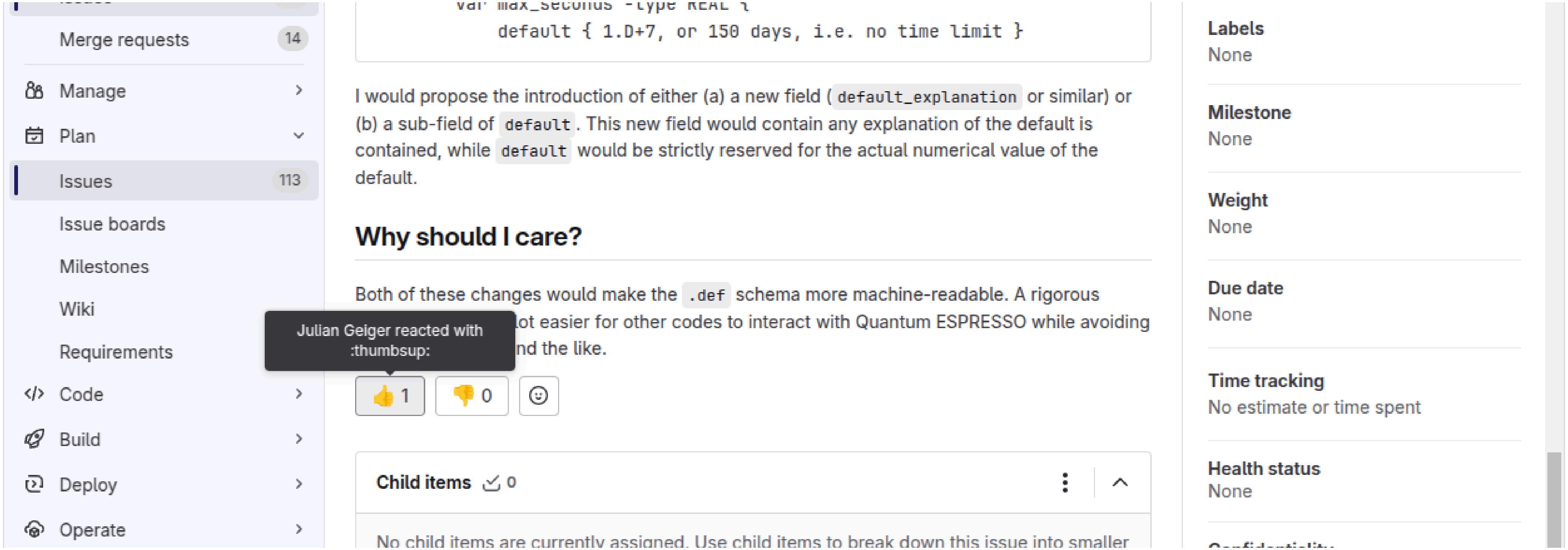
Epic
This feature is locked. Upgrade plan

Labels
None

Milestone
None

Weight
None

References



Merge requests 14
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Wiki
Requirements
Code
Build
Deploy
Operate

```
        default { 1.D+7, or 150 days, i.e. no time limit }
```

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.

Why should I care?

Both of these changes would make the `.def` schema more machine-readable. A rigorous … lot easier for other codes to interact with Quantum ESPRESSO while avoiding … nd the like.

Julian Geiger reacted with :thumbsup:

👍 1 👎 0

Child items 0

No child items are currently assigned. Use child items to break down this issue into smaller

Labels
None

Milestone
None

Weight
None

Due date
None

Time tracking
No estimate or time spent

Health status
None