Outline

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

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… but what have I learned throughout this process?

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Well not quite

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but the intervening years have not been kind – see permit photos)

Interfacing with AiiDA

What I needed to do

- isolate into steps
- functional programming

Common Workflow Language

Basic Concepts of CWL

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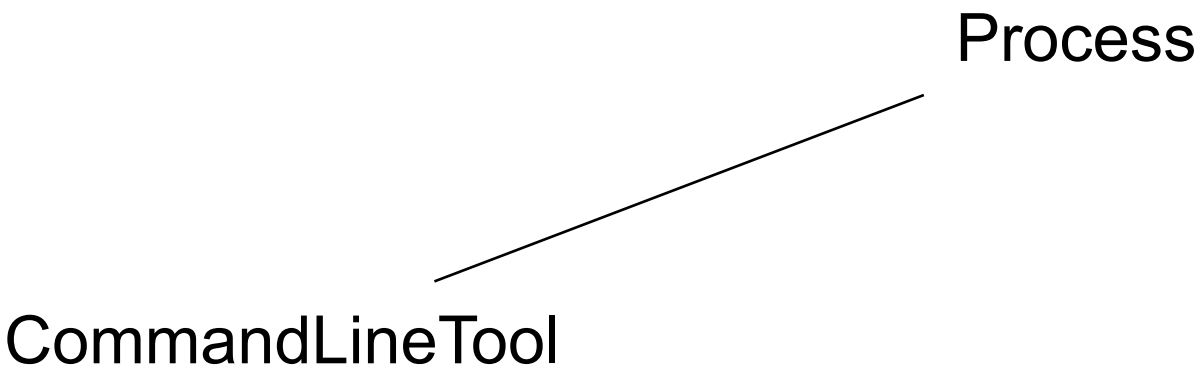
- mostly used by bioinformatics community

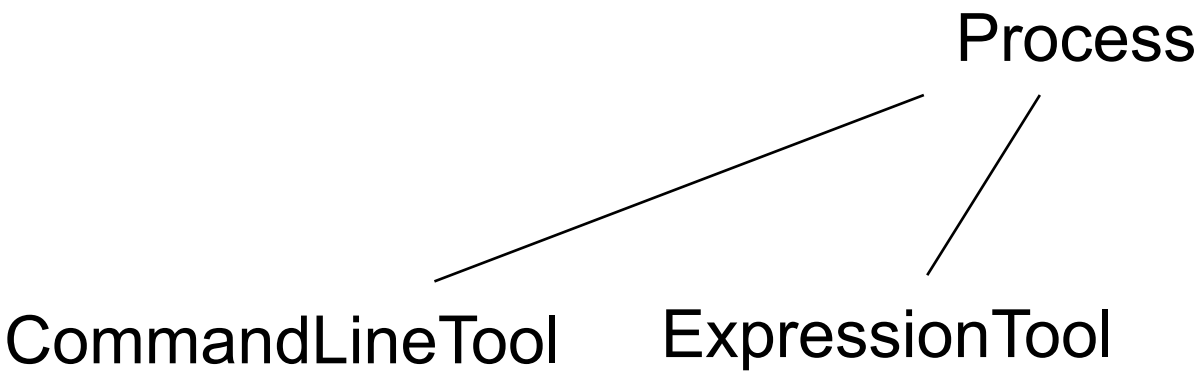
Basic Concepts of CWL

Process

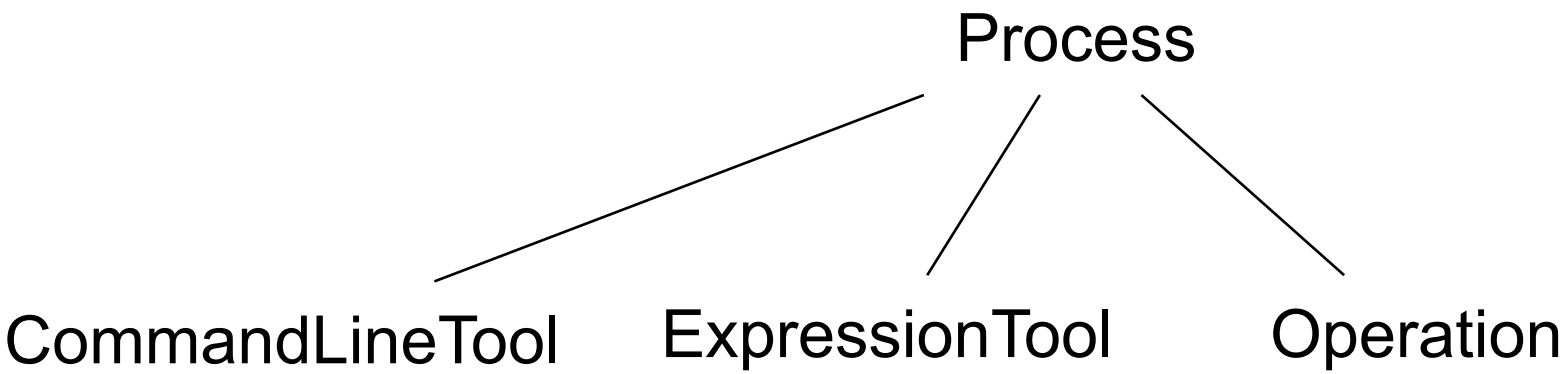
Basic Concepts of CWL



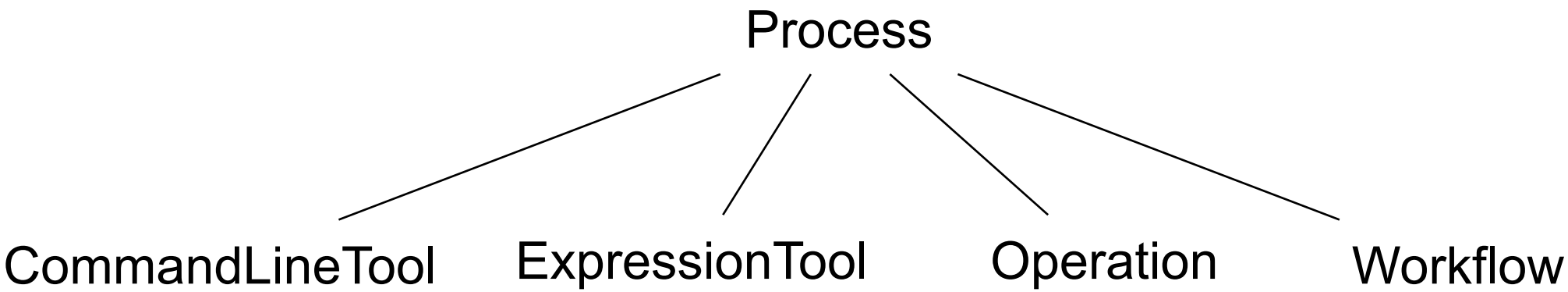
Basic Concepts of CWL



Basic Concepts of CWL



CommandLineTool



ExpressionTool

PSI

echo.cwl

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

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

outputs: []
```

Workflow

PSI

uppercase.cwl

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

inputs:
  message: string
outputs:
  uppercase_message: string

expression: |
```

Workflow

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

Pros and Cons

PSI

echo_uppercase.cwl

```yaml
cwlVersion: v1.2
class: Workflow

requirements:
  InlineJavascriptRequirement: {}

inputs:
  message: string

outputs:
  out:
```

Pros and Cons

```
    type: string
    outputSource: uppercase/uppercase_message

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

Pros and Cons

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

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

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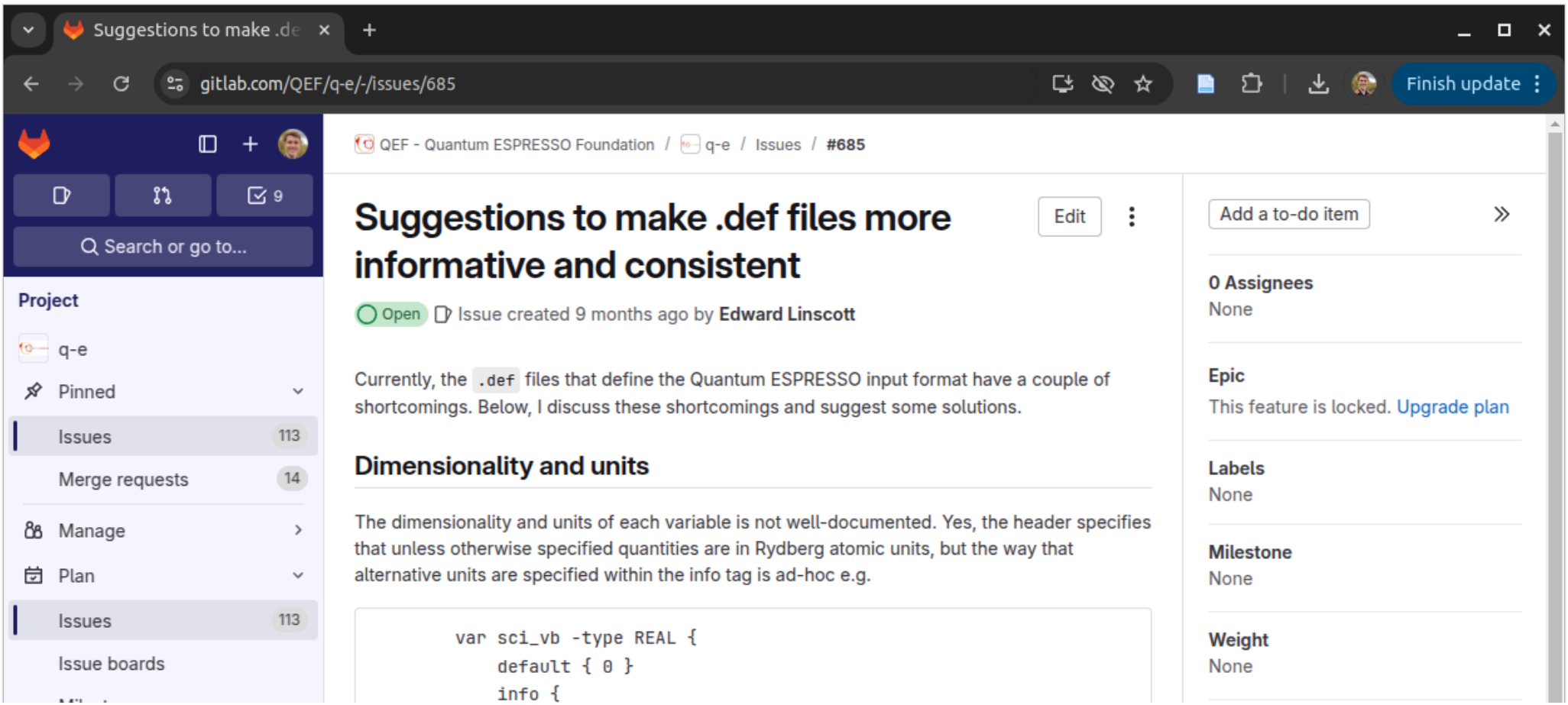
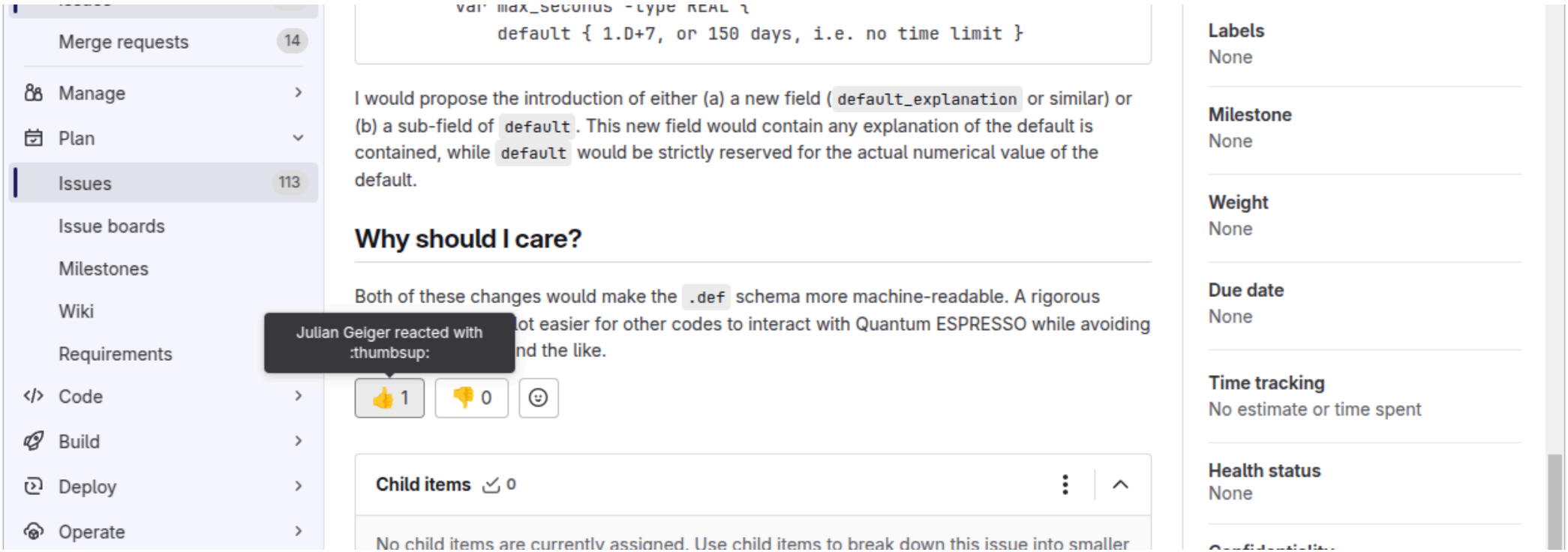


References


Merge requests 14
Manage
Plan
Issues 113
Issue boards
Milestones
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
ot 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