SCYTHE: AN EXTRACTOR LIBRARY YOU MIGHT LIKE

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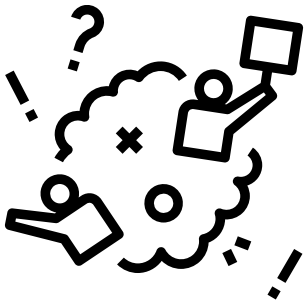
WHY DID WE MAKE SCYTHE?

Well, we first called it “MaterialsIO”

Both Citrine Informatics and the Materials Data Facility had *messy data files.*

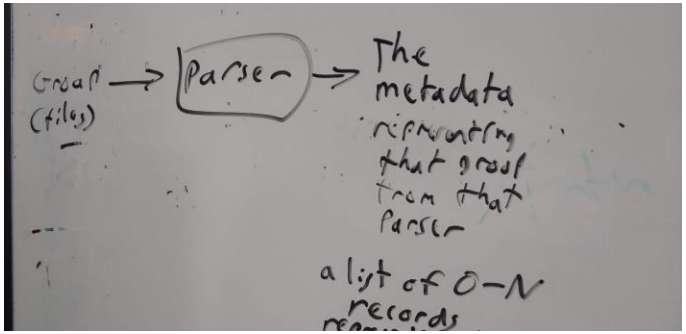
Each time the mess expanded
we created another tool
following whatever interface whomever felt like,



And did it *over and over again*

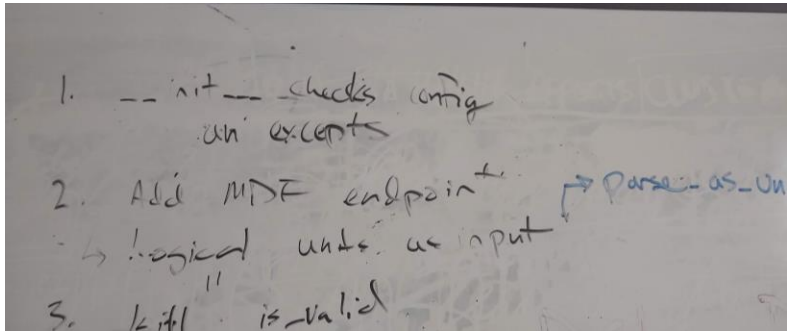
MERGING TOOK TALKING

We didn’t even have the same words for concepts, or goals



What is the operation we perform?

- Data to summary?
- Data to a new format (e.g., PIF)?

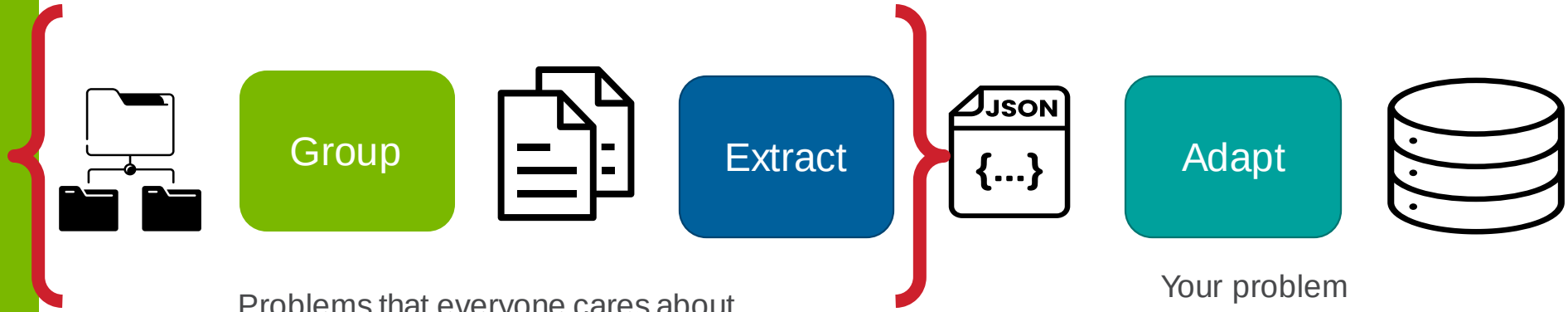


What is the interface?

- Where do file groups come from?
- Where do they go?
- What does the output look like?

SOME TIME LATER: A SYSTEM CHART

Between your files and your database



WHAT IS “GROUPING”

Scientists like many files, computers hate them

```
my_run\
   in.test
   out.test
   better.in
   better.out.3Oct94
   better.out.3Feb23
```

Group

```
[my_run\in.test
 my_run\out.test]
[my_run\better.in,
 my_run\better.out.3Oct94]
[my_run\better.in,
 my_run\better.out.3Feb23]
```

Grouping algorithms…

- use how files are arranged on filesystems
- to identify files that should be treated together
- for a <u>specific type of data extractor</u>

WHAT IS “EXTRACTING”

Turning trash into treasure

```
[my_run\better.in,
 my_run\better.out.3Feb23]
```

Extract

```
{
  ‘material’: ‘CuO’,
  ‘code_version’: asdf44,
  ‘temperature’: 1544,
   ...
```

Extracting algorithms…

- pull ugly scientific formats
- into a documentable format (JSON)
- that contains all data *anyone* cares about [note present tense!]

WHAT IS “ADAPTING”

Turning treasure back into *your preferred currancy*

```
{
   ‘material’: ‘CuO’,
   ‘code_version’: asdf44,
   ‘temperature’: 1544,
    ...
```

Adapt

```
<my_document>
   <material>CuO@1544</material>
   ...
</my_document>
```

Adapting functions…

- Take in the general-purpose, documented format
- and transform it into whatever you’d like
- so you can do whatever with it

THAT'S THE GENERAL PRINCIPLES

Now for the implementation

Our goals:

- Have the interface in Python
- Have a minimal interface that need be fulfilled
- Enable "file-system to database" in one line of code
- Make it work for >1 person

DOCUMENTATION TOUR

- Things to hit
  - Manifesto
  - Base classes
  - Utility operations
    - How Stevedore Makes it work
  - Adapter example for MDF

WHERE ARE WE AT?

It's still just a proof of concept

Who all is using it? No major users *yet*

- Not MDF (but its on the to-do list)
- Not Citrine (I'm not sure now that Citrination "open" is gone)

What are we actively doing?

- Revising the MDF extraction toolchain
- Explaining it to fine people (i.e., you) to see if it fits anywhere

What would I do next? [Given time]

- Finish up the documentation
- Strip out features to reduce dependencies (Py3.8+, stevedore is the goal)

WHAT'S NEXT

My question: Does this fit the model you need?

- If not, is there a small change we can try out?
- If so, how can we test to be sure?

My goals:

1. *Make it easier to use this groups' work in the MDF*
2. *Keep the interfaces for extractors as simple as possible, Pythonic*
3. *Save you all time*
4. *Puff my GitHub metrics 📈, get money 💰, retire early 🏖️*