COMMON WORKFLOW DESCRIPTION

AN EXPERIMENTAL VIEWPOINT

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IMD-1: Microstructure and Properties of Materials

NFDI MatWerk

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ALLOW FOR COMPARISON AND REUSE OF WORKFLOWS

Experiments 1

1. Prepare Al sample
2. Measure sample
3. Tensile test
4. Analyze curves
5. Calculate Modulus

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Experiments 2

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Simulations

1. Build model
2. Apply forces
3. Calculate
4. Predict curves
5. Calculate Modulus

Use same workflow steps were possible

MANY WORKFLOW LANGUAGES EXIST

Dedicated workflow languages

- Common workflow language
- Snakemake
- Nextflow
- Nexus
- Kadi4Mat – json
- pyiron-workflow

...

Programming languages:

- C
- python
- bash

...

TASK: PICK ONE AND USE FOR SIMULATIONS AND EXPERIMENTS

FORMAL WORKFLOW DESCRIPTION EXISTS

BUSINESS PROCESS MODELING

- Visual representation
- Process analysis
- Communication and documentation
- Simulation and automation

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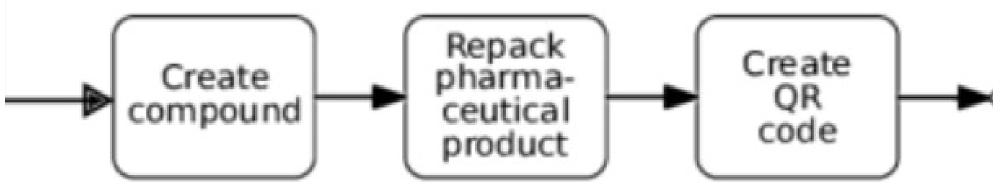


Two layers of information:

- Top level: short description
- Bottom level: details

Di Ciccio, et. al 10.1007/978-3-319-94214-8_4

GOAL: WORKFLOW STANDARDIZATION

Experiments have two layers:

- Workflow step incl. description as top layer

- Instrument has Standard Operating Procedure

Simulations have two layers:

- Function calls as top layer

- Each function is a graph node

WORKFLOW EXAMPLE

Header

```
from common_workflow_description import Storage, Sample, step
from analysis_steps import plot_curves, calc_E
```

Define workflow

```
wf = Workflow('Sandia Fracture Challenge 3')
proceduresLibrary = urlparse('https://…')
storage=Storage(proceduresLibrary)
```

Experiments

```
sample = Sample('AM_NA_05')
wf.step1 = step(storage, sample, 'metallography', {})
wf.step2 = step(storage, sample, 'tensile test', {})
…
```

Analysis

```
file_name = [v for k,v in list(wf....items())...][0][1]
wf.step6 = plot_curves(file_name, 'Strain (Gauge0)', 'Engr. Stress')
wf.step7 = calc_E(file_name, 'Strain (Gauge0)', 'Engr. Stress')
```

Footer

```
print('Output: ','\n '.join([f"{k}: {v}" for k,v in list(wf…)]))
wf.draw().render(filename="io_demo", format="png", cleanup=True)
```

same as pyiron-workflow style

UNIFIED WAY TO WRITE SOP: MARKDOWN+

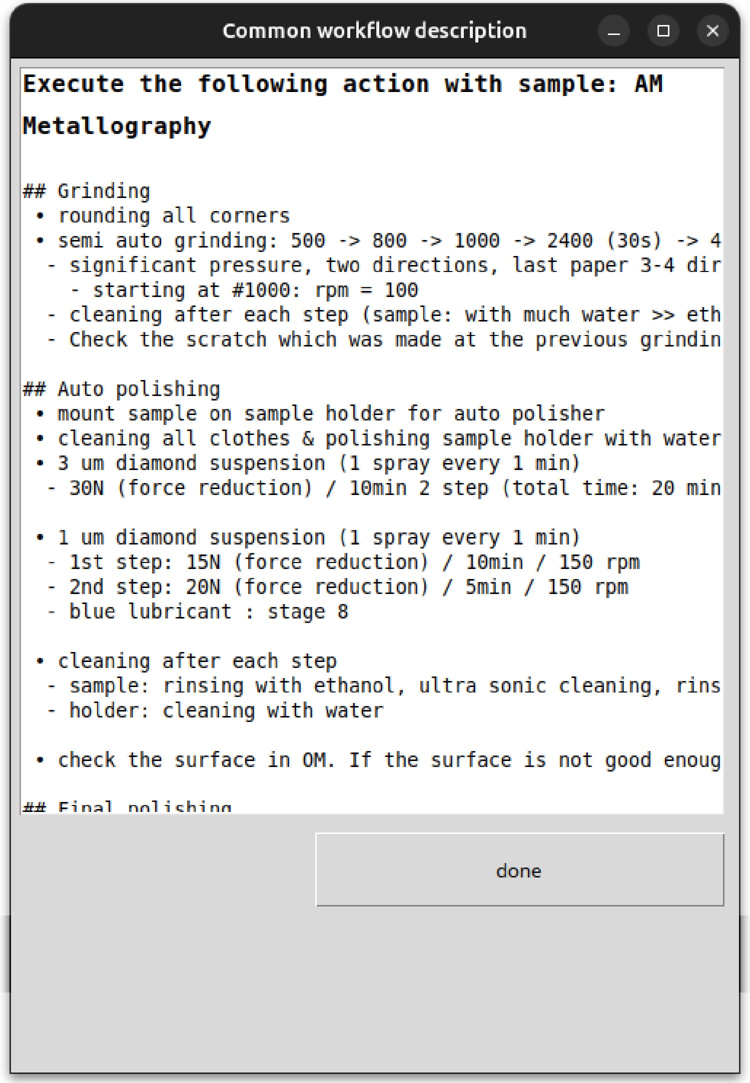
```
# Zeiss SEM
- Vent
- Open chamber
- Mount sample and close chamber
- Use it at |voltage|20| kV
- Use a aperture of |aperture|3|

Author: Steffen Brinckmann, IMD-1, FZJ
<!--- version:1.0 |filename|| -->
```

EXAMPLE: INSTRUCTIONS

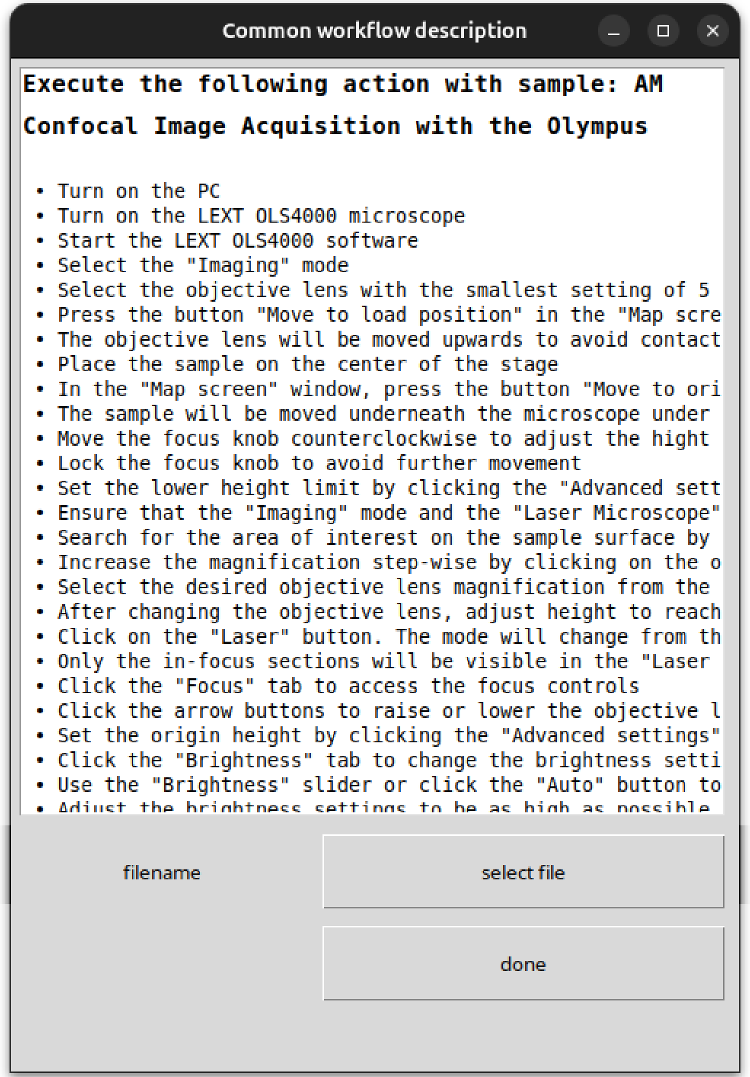
Instructions can have:

- no forms

- only ask for a file



```
Execute the following action with sample: AM

Metallography


## Grinding
 • rounding all corners
 • semi auto grinding: 500 -> 800 -> 1000 -> 2400 (30s) -> 4
  - significant pressure, two directions, last paper 3-4 dir
    - starting at #1000: rpm = 100
  - cleaning after each step (sample: with much water >> eth
  - Check the scratch which was made at the previous grindin

## Auto polishing
 • mount sample on sample holder for auto polisher
 • cleaning all clothes & polishing sample holder with water
 • 3 um diamond suspension (1 spray every 1 min)
  - 30N (force reduction) / 10min 2 step (total time: 20 min

 • 1 um diamond suspension (1 spray every 1 min)
  - 1st step: 15N (force reduction) / 10min / 150 rpm
  - 2nd step: 20N (force reduction) / 5min / 150 rpm
  - blue lubricant : stage 8

 • cleaning after each step
  - sample: rinsing with ethanol, ultra sonic cleaning, rins
  - holder: cleaning with water

 • check the surface in OM. If the surface is not good enoug

## Final polishing
```



```
Execute the following action with sample: AM

Confocal Image Acquisition with the Olympus


 • Turn on the PC
 • Turn on the LEXT OLS4000 microscope
 • Start the LEXT OLS4000 software
 • Select the "Imaging" mode
 • Select the objective lens with the smallest setting of 5
 • Press the button "Move to load position" in the "Map scre
 • The objective lens will be moved upwards to avoid contact
 • Place the sample on the center of the stage
 • In the "Map screen" window, press the button "Move to ori
 • The sample will be moved underneath the microscope under
 • Move the focus knob counterclockwise to adjust the hight
 • Lock the focus knob to avoid further movement
 • Set the lower height limit by clicking the "Advanced sett
 • Ensure that the "Imaging" mode and the "Laser Microscope"
 • Search for the area of interest on the sample surface by
 • Increase the magnification step-wise by clicking on the o
 • Select the desired objective lens magnification from the
 • After changing the objective lens, adjust height to reach
 • Click on the "Laser" button. The mode will change from th
 • Only the in-focus sections will be visible in the "Laser
 • Click the "Focus" tab to access the focus controls
 • Click the arrow buttons to raise or lower the objective l
 • Set the origin height by clicking the "Advanced settings"
 • Click the "Brightness" tab to change the brightness setti
 • Use the "Brightness" slider or click the "Auto" button to
 • Adjust the brightness settings to be as high as possible
```

INSTRUCTION OPTIONS

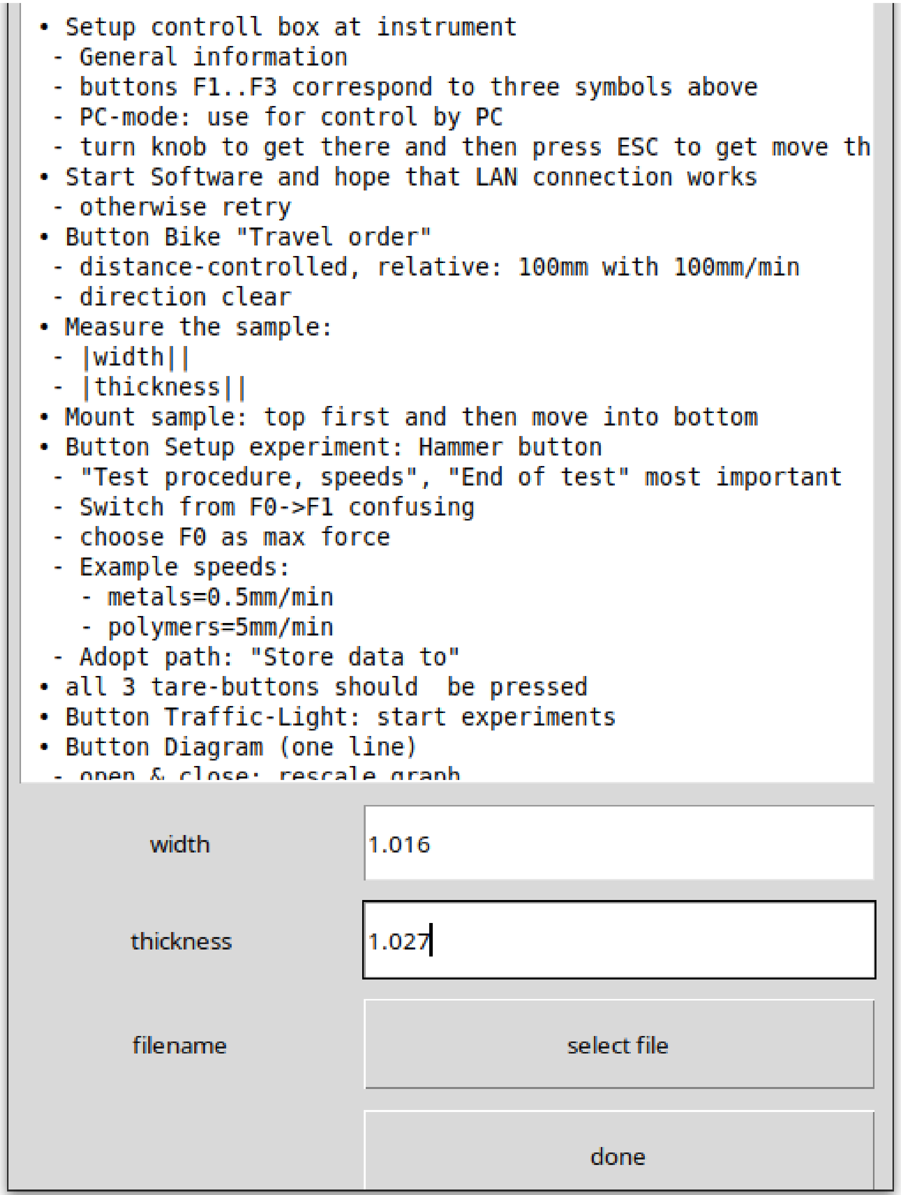
Instructions can include parameters

- geometry

- real process parameter

```
    prescribed flow rate: 16
    real flow rate: 10
```

- experimental metadata that is not in output file



```
• Setup controll box at instrument
 - General information
 - buttons F1..F3 correspond to three symbols above
 - PC-mode: use for control by PC
 - turn knob to get there and then press ESC to get move th
• Start Software and hope that LAN connection works
 - otherwise retry
• Button Bike "Travel order"
 - distance-controlled, relative: 100mm with 100mm/min
 - direction clear
• Measure the sample:
 - |width||
 - |thickness||
• Mount sample: top first and then move into bottom
• Button Setup experiment: Hammer button
 - "Test procedure, speeds", "End of test" most important
 - Switch from F0->F1 confusing
 - choose F0 as max force
 - Example speeds:
   - metals=0.5mm/min
   - polymers=5mm/min
 - Adopt path: "Store data to"
• all 3 tare-buttons should  be pressed
• Button Traffic-Light: start experiments
• Button Diagram (one line)
 - open & close: rescale graph
```

width 1.016

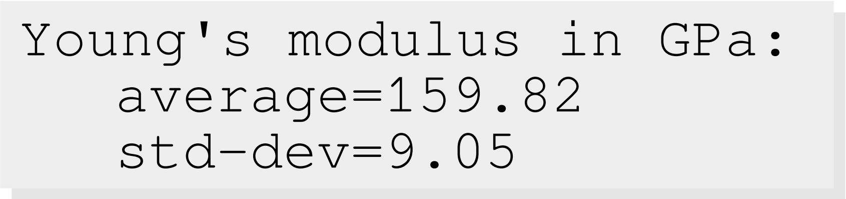
thickness 1.027

filename

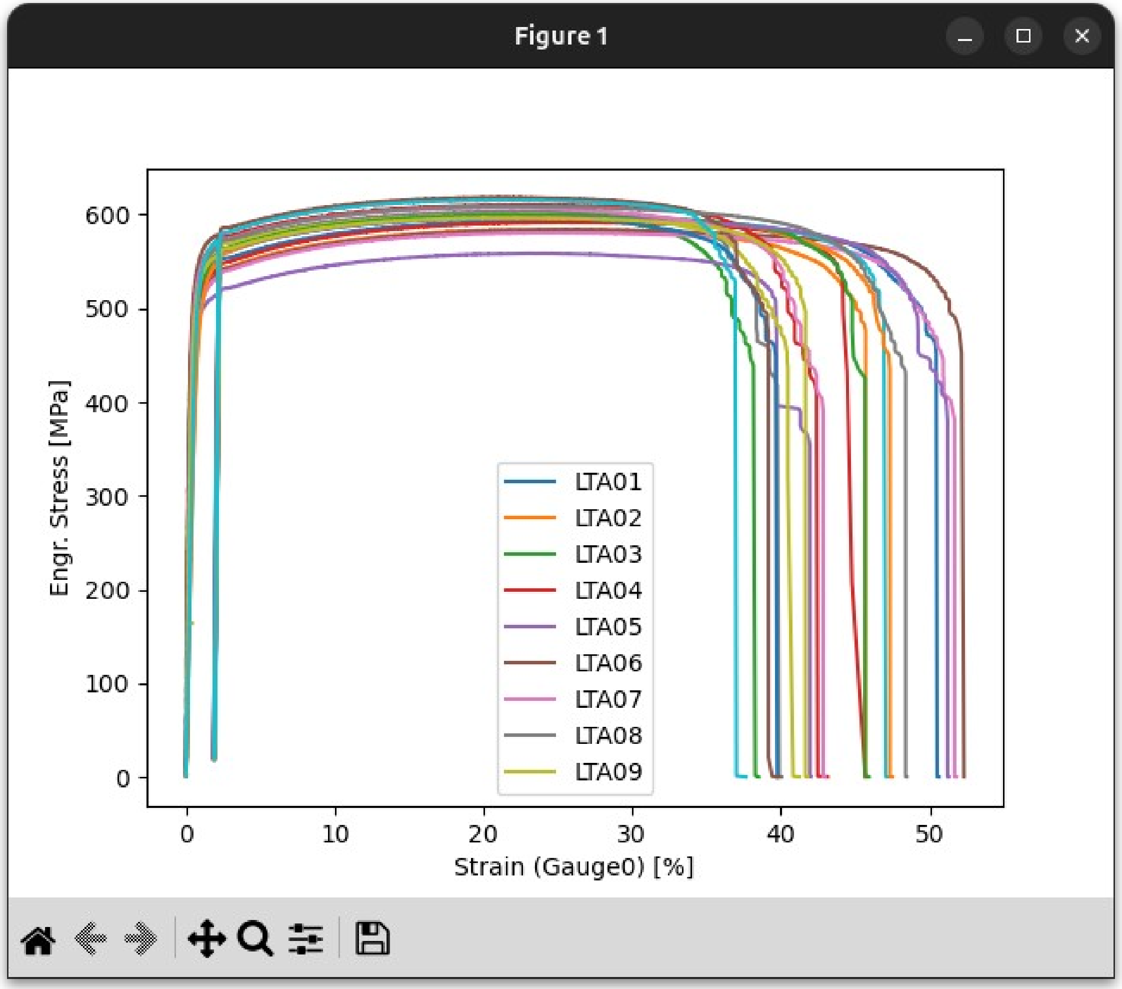
EXAMPLE: ANALYSIS STEP

All possibilities exist for:

- graphical plotting (tensile curves)
- calculating material properties
- simulation steps



```
Young's modulus in GPa:
   average=159.82
   std-dev=9.05
```



OUTPUT AND LOGFILE

```
Started minimalistic workflow engine
Output:
  step1: [Name: AM05,'',{}]
  step2: [Name: AM05,'',{'magnification': '5'}]
  step3: [Name: AM05,'....xlsx',{'width': '1.016'}]
  step4: [Name: AM05,'',{'magnification': '5'}]
  step5a:[Name: AM05,'',{'voltage':'30','aperture':'3'}]
  step5b:[Name: AM05,'',{'voltage':'30','aperture':'2'}]
```

```
08-22 10:52:39|INFO:Start workflow
08-22 10:56:31|INFO:Start step
  sample:{AM_NA_05}
  procedure-name:{tensile test}
  sha256:{ae9c351e9fcbd41fc39d0e3831d9dc8d3388bd7e714869aa050b870dc21ac341}
  Parameters: {{}}
08-22 10:57:40|INFO:Save step
  file-name:...LongitundinalTensileOverall.xlsx
  metadata: {"width": "1.016"}
08-22 10:57:40|INFO:End step
```

TWO ENGINES EXIST TO EXECUTE WORKFLOWS

On desktop computer, technical staff:

1) writes SOPs in Word, … saved in Markdown+

2) define the planned workflow with GUI saved as pyiron-workflow file

Workflow (incl. SOP) are executed in Android App or laboratory computer

Output and log-file are saved back into ELN

FUTURE GOAL

Pyiron-workflow:

- Many features: graphics, super-computer...

- Allow for adaptive workflows

Same output and logging files

Minimalistic engine:

- Can only run common-workflow-description

- No installation required

- people use reference to implement into own ELN, ...

A COMMON WORKFLOW DESCRIPTION EXISTS FOR EXPERIMENTAL AND NUMERICAL MATERIALS SCIENCE

- Most basic version exists
  - creates a receipt of all experimental steps
  - unified way to write procedures
- You can use pyiron-workflow to adopt it
- **GUI version with drag-drop will exist**

Looking for scientists feedback: What is missing?

NON UNIQUE DEFINITION: WHAT IS “A STEP” (same in simulations)

Smallest step that make scientific sense to execute individually (might depend on others)

- SEM

- EBSD (requirement of SEM before)

- EDX (requirement of SEM before)

Issue: requirements can only be resolved if there is step types (SEM procedures, …) → much more complicated (second version)

KNOWN SHORTCOMMING

Validation of experimental input:

“What happens if I enter a non-nonsensical value?”

Issue: How to integrate that into procedure that it is easy to write?

- allowed values

- only integers can be entered

- regex needed?

KNOWN SHORTCOMMING

Aborting a workflow: if sample breaks

NOT A SHORTCOMMING

Allow for comment / remark in each step?

- one can enter unforeseeable events

Very easy fix: just add “|comment||” at end of file

NOT A SHORTCOMMING

Do we need to have a common definition of the file? Likely yes.

But first we need a version that works, which can be tested.

Only then we find short-comings...

Development by prototyping (Wikipedia → Software prototyping)