Very common question: Why not just python (or bash)?

Example from DFT+DAMASK coupling
(more this afternoon)

```python
def get_elastic_constants_from_dft(chemical_element):
    ...
    return elasticity

def get_yield_stress_from_damask(elasticity, plasticity):
    ...
    return yield_stress

elasticity = get_elastic_constants_from_dft("Al")
yield_stress = get_yield_stress_from_damask(elasticity, plasticity)
```

Why?

```python
from pyiron_core import Workflow, as_function_node

@as_function_node
def get_elastic_constants_from_dft(chemical_element):
    ...
    return elasticity

@as_function_node
def get_yield_stress_from_damask(elasticity, plasticity):
    ...
    return yield_stress

wf = Workflow("damask")
wf.elasticity = get_elastic_constants_from_dft("Al")
wf.yield_stress = get_yield_stress_from_damask(wf.elasticity, plasticity
wf.run()
```

- *"I already have my code in Python/bash"*
- *"Anyway Python already delivers results I want"*

→ Why not just python/bash?

Why workflow? – Problems with bare python

No semantic meaning for computer

Please retrieve previous results

Likely: unorientable directory structure

```python
def get_elastic_constants_from_dft(chemical_element):
    ...
    return elasticity

def get_yield_stress_from_damask(elasticity, plasticity):
    ...
    return yield_stress

output = []
for element in ["Al", "Fe", "Cu", "Al"]:
    elasticity = get_elastic_constants_from_dft(element)
    yield_stress = get_yield_stress_from_damask(elasticity, plasticity)
    output.append([element, yield_stress])
```

Job submission: longer simulations to computer cluster

Intermediate results lost

Provenance: where did elasticity come from?

Very often: Once the author departs or after a few months, both workflow and results become unusable