Journey to a Digital Twin
Developing a Python based Digital Shadow at BESSY II

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12. Dezember 2023

Outline

Motivation

Experience @ BESSY II

- Tracy II, thor-scsi & self built / IOC
- experimenting field
- in parallel: measurement scripts on Bluesky

Accelerator community and beyond

- FRIB online model flame [1]
- LUME project of LCLS II
- Functional Mockup Interface
- Open simulation platform [2, 3]

MML Success

- MML success: *one* tool → many machines
- eng↔phys mapping: 1↔1

MML to next level

- eng↔phys mapping: many↔many aka FMI, OSP?
- modelling device(s) response time: aka Bluesky/ophyd UX ↑
- repo pattern: handling configuration data abstraction

Not all answers today: rather a proposal for journey to come

BESSY II twin: current developments

User requests

- *set-values*: magnets, cavities, . . .
- *beam parameters*: e.g. δP

Calculation response

- orbit $\rightarrow$ beam position monitor readings
- optics: twiss function

Current realisation

e.g. magnet setpoints

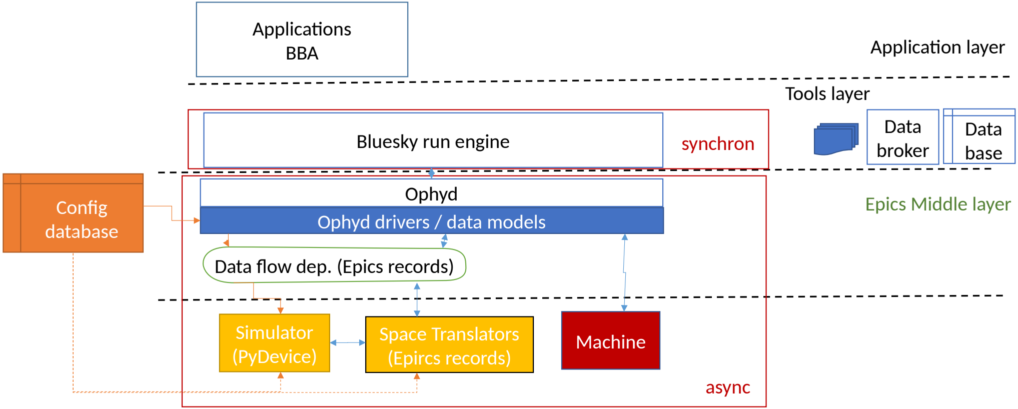
EPICS records

- virtual power converter per magnet
- connected to virtual power converter of “main supply”
- recalculation to main multipole $\leftarrow$ separate

PyDevice based engine

- engine: thor-scsi $\rightarrow$ PyAT
- current refactor: simplified design

BESSY II: overview



Handling configuration data

- Repository pattern
  - access of data
  - independent of storage: e.g. csv files, database, ...
- Identifier (pattern)
  - sole requirements: Hashable
  - PyAT → `typing.SupportsIndex`
  - dataclass: more readable?
- Datamodel?
  - express data structure to others
  - support by IDE's, etc
  - simplifies: storage, display (e.g. mongodb, RestAPI)

Loading parameters: repository pattern

```
class ParameterRepository(AbstractRepository):
    def get(self, reference: AbstractIdentifier) -> Any:
        return self.data[reference]

    def __init__(self, data):
        self.data = data
```

Inspiration

Basis identifier

```
class AbstractIdentifier(metaclass=abc.ABCMeta):
    @abc.abstractmethod
    def __eq__(self, other: AbstractIdentifier) -> bool:
        raise NotImplementedError

@dataclass(frozen=True, eq=True, kw_only=True)
class MMLIdentifier(AbstractIdentifier):
    family_name: str
    sector: int
    number: int
```

Communication handling: command pattern I/II

Motivation: abstract complex handling

- many tasks:
  - change devices
  - take data
  - analyse
- command interface:
  - e.g. CAD command line interface
  - e.g. Bluesky's RunEngine messages
  - device changes → command → record
  - twinning:
    - test on twin
    - replay to machine
  - optimisation applications, middle layer: → in different languages ← communication?

```
record(ao, "$(PREFIX):$(ELEMENT):Cm:set"){
    field(DTYP, "pydev")
    field(OUT,
      "@update(element_id='$(ELEMENT)',
              property_name='K', value=%VAL%)")
}

def update(*, element_id, property_name, value=None):
    with UpdateContext(...):
        elem_proxy = acc.get_element(element_id)
        elem_proxy.update(property_name, value)
class AcceleratorProxy(AcceleratorInterface):
    def get_element(self, element_id):
        return ElementProxy(self.acc[element_id])

class ElementProxy(ElementInterface):
    def __init__(self, obj):
        self._obj = obj
    def update(self, property_id: str, value):
        """complete the job"""
```

Communication handling: command pattern II/II

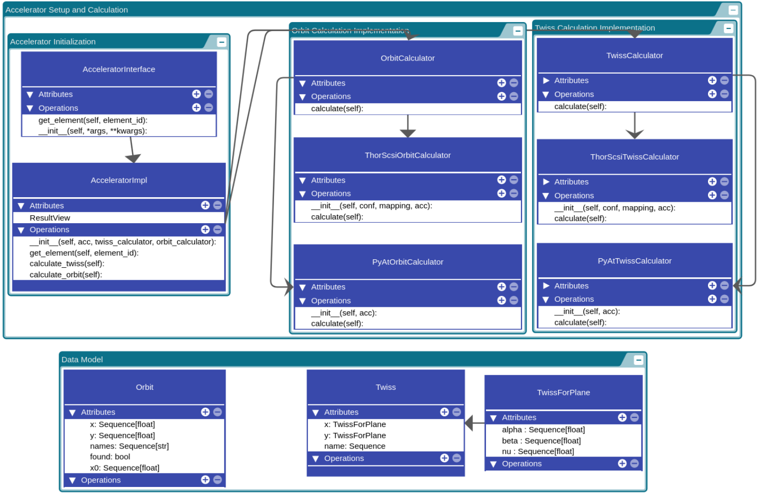
Motivation: abstract complex handling

Command interface

- *single entry point*
- $\rightarrow$ shadow
  - forward command arguments to shadow
  - callers $\rightarrow$ eavesdrop data they receive
    e.g. EPICS: register callbacks
  - slim interface: communication between languages?

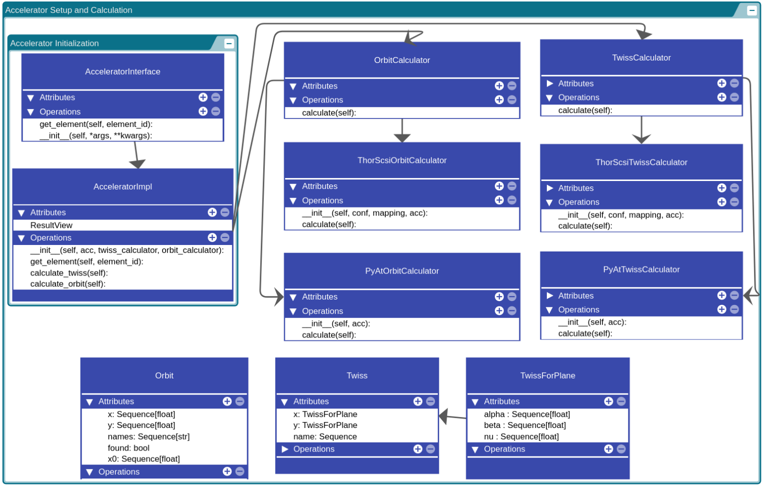
Different back-ends I/II

Proxy / dependency injection



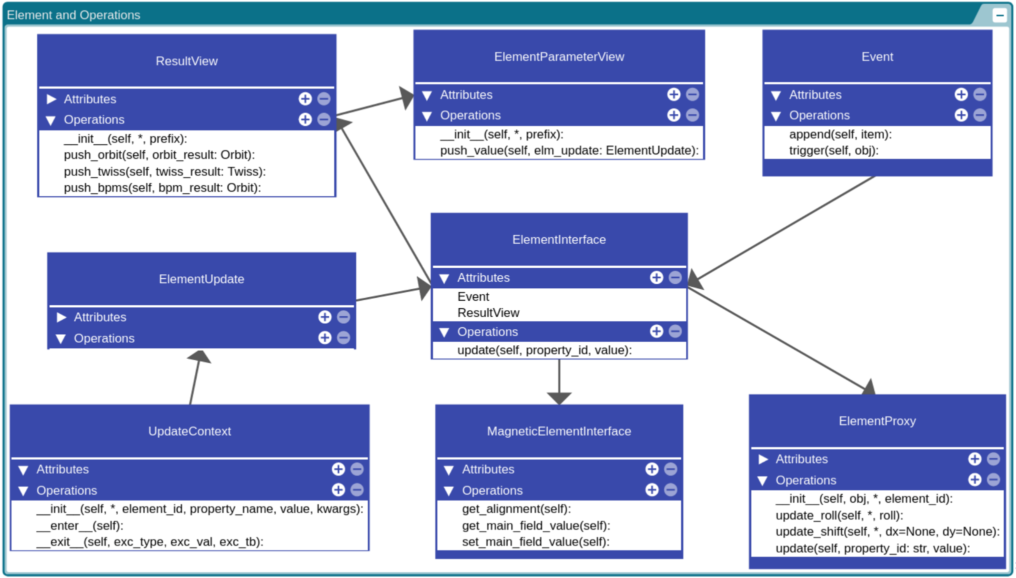
Different back-ends II/III

Proxy / calculators



Different back-ends II/II

Viewer



Waiting for results

Futures, promises and beer garden buzzers

- waiting for new data
- chaining asynchronous actions: e.g.
  - parallel setup
    - prepare injection automaton, injector chain
    - change optics
  - data taking
    - data arrived in device A
    - device B: only accept data after arrival in A
- alternative concepts
  - select
  - poll
  - threads: .run(), .join()

Ophyd: status

```python
class BPM(Device):
    """ensure to return only new data"""
    packed_data = Cpt(EpicsSignalRO, ":bdata")
    count = Cpt(EpicsSignalRO, ":count")
    timeout = Cpt(Signal, name="timeout",
                  value=3, kind=Kind.config)

    def trigger(self):
        def cb(value, old_value, **kwargs):
            # called when new packed data arrive
            # could check for value
            return True

        return SubscriptionStatus(
            self.packed_data, cb, run=False,
            timeout=self.timeout.get())
```

Timely device response: is it an issue?

Devices & time

- higher abstraction levels → automatation of more complex tasks: occasional failure → frequent occurance
- Modelling device response: Ophyd: timeout (settle time)
- → track response: report on failure → UX ↑

Real world example

dynamic aperture measurement / amplitude dependent tune shift

- diagnostic kicker
- turn by turn measurement: occasional failure
- time response superision: program failure when device failure → easier to track culprit

show what was don Python: dropping GIL: get prepared

Middle layer: layering, components

Middle layer: task

- conversion between spaces: eng $\leftrightarrow$ physics : OSP[1] *information layer*
- communication to: machine / simulation: OSP *communication layer*

Layers: advantage

- separation of responsibility / tasks $\rightarrow$ shadow as eavesdropper
- increase flexibility: e.g. communication layer (partly) control system dependent

Current design: review?

- MML engineering $\leftrightarrow$ physics: one to one
- FMU[2] many to many, units cross check

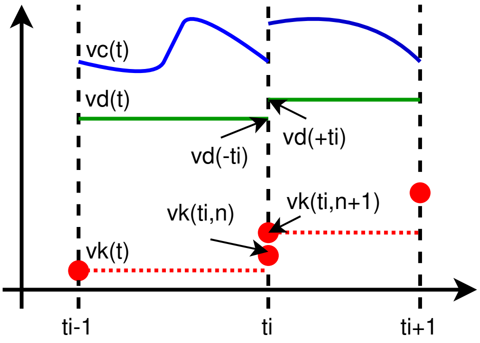
[1] **O**pen **S**imulation **P**latform [2, 3]
[2] **F**unctional **M**ockup **U**nit see https://fmi-standard.org

Functional mockup interface

- split up: different components: standardised
- standard interface:
  - calculation / simulation engine → library
  - interface definiton → XML-file
- simulation engine:
  - differential equations *model exchange*
  - *co simulation*
  - simulation components *scheduled execution*
- concept of time: (including handling that states can switch)

split up simulation components in a standardised fashion

Concept of time



advancing time

Conclusion

- MML: prove many machines ← optimised by single toolkit
- python reimplementation: chance
  - revisit: OSP FMI, LUME,...
  - FMU: components, self describing, unit standard,...
  - OSP: layering: networking, information
  - software patterns: repository, dependency injection
- *target* keep flexibility, machine independence
- use patterns: simplify different use case implementations
- first points?
  - repo pattern ← configuration data management
  - time response: detect early when communication fails
  - shadow by eavesdropping

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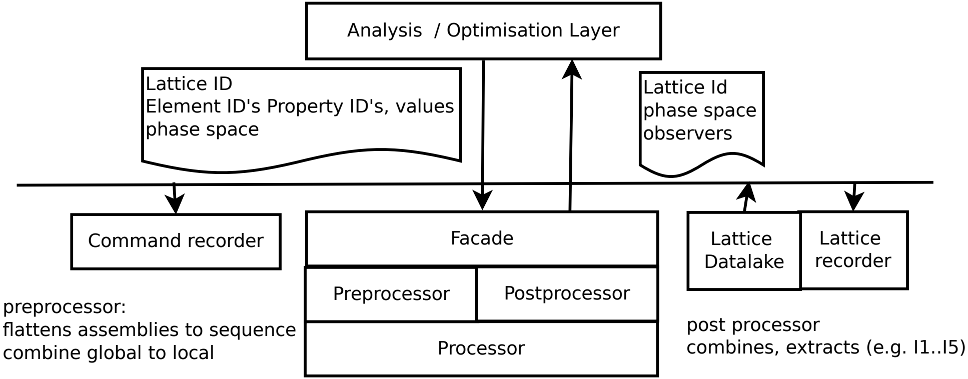
backup slides

Single particle dynamics: an architecture?

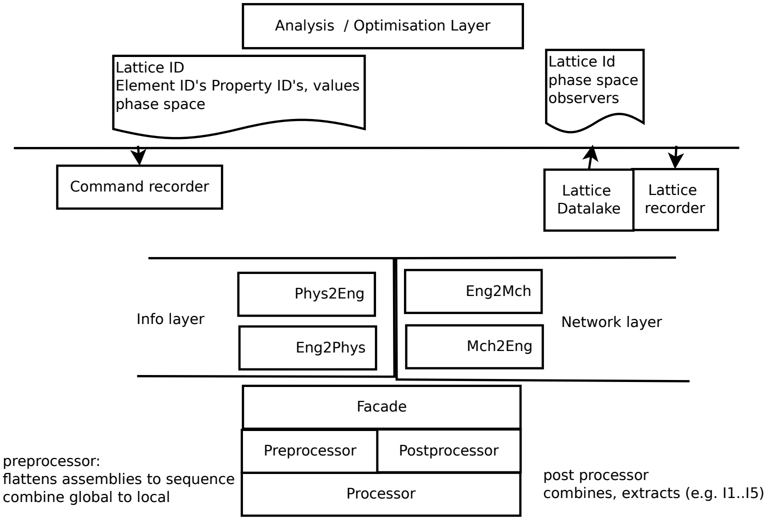
Proposal: overview



Details explained below, influenced by python architecture patterns [4]

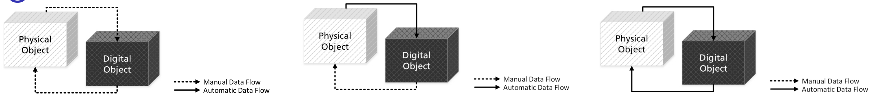
Single particle dynamics: an architecture?

Twinning aspects



Influenced by FMI[2], / OSP[3]

Digital twin: nomen clature



model shadow twin

Status

- different beam dynamics models available ← interaction
- **M**atlab **M**iddle **L**ayer [5] + **A**ccelerator **T**oolbox: [6] similar simulation many different ring light sources
- further online model implementations for ring light sources: DIAMOND [7], NSLS II [8], SLS [9] Solaris [10],
- FLAME: FRIB online model [1]

Need to go further?

- 20 years → experience gained
- software industry → Futures ("beer garden" buzzers), async, μ-services
- compare: iso standard , functional mock-up interface

split up [11], iso standard [12]

Excurs: Bluesky dynamic aperture check

Kicker delay

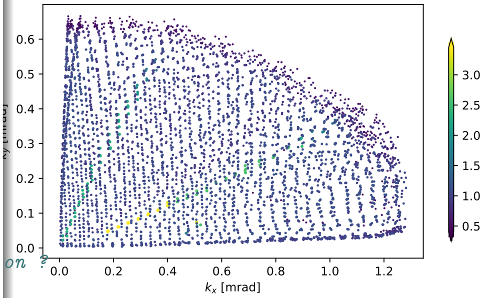
```python
class Delay(Device):
    '''Delay of kicker pulse to trigger'''
    #: delay after the trigger
    offset = Cpt(EpicsSignal, ':offset')

    #: switch the kicker on or off
    switch = Cpt(EpicsSignal, ':switch')

    def stage(self):
        assert(self.switch.get()) # is kicker on ?
        return super().stage()

    def unstage(self):
        return super().unstage()

    def set(self, value):
        return self.offset.set(value)
```



Devices

- kicker: delay,

Excurs: Bluesky dynamic aperture check

Kicker power converter

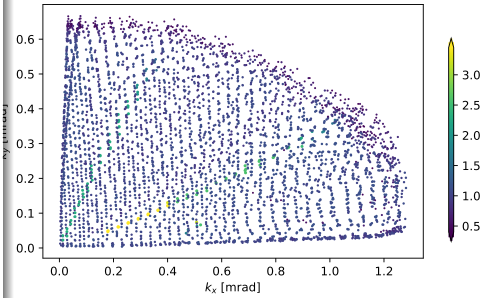
```python
class KickerPS(PVPositioner):
    '''Power converter of the kicker'''
    setpoint = Cpt(EpicsSignal, ':set')
    readback = Cpt(EpicsSignalRO, ':rdbk')
    done = Cpt(EpicsSignalRO, ':done')

    powered = Cpt(EpicsSignalRO, ':stat1')
    hv_on = Cpt(EpicsSignalRO, ':stat2')

    def stage(self):
        assert(self.powered.get())
        assert(self.hv_on.get())
        return super().stage()

    def unstage(self):
        return super().unstage()

    def stop(self, success=False):
        stat = self.setpoint.set(0)
```



Devices

- kicker: delay, pc

Excurs: Bluesky dynamic aperture check

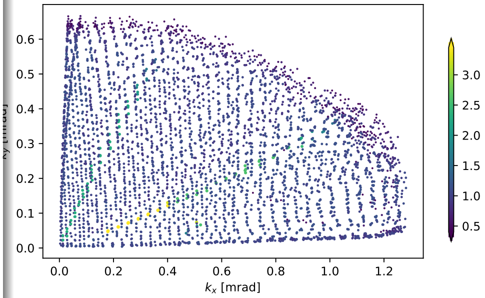
Hor & vert kicker

```
class HKicker(Device):
    '''Horizontal kicker supply and delay
   '''
    delay = Cpt(Delay, 'KDHKR', name='delay')
    ps = Cpt(KickerPS, 'PKDHKR', name='ps',
             timeout=30) # NB: limit

    def set(self, value):
        return self.ps.set(value)

class VKicker(Device):
    '''Vertical kicker supply and delay
    '''
    delay = Cpt(Delay, 'KDVKR', name='delay')
    ps = Cpt(KickerPS, 'PKDVKR', name='ps',
             timeout=30)

    def set(self, value):
        return self.ps.set(value)
```



Devices

- kicker: delay, pc $\rightarrow$ combined

Excurs: Bluesky dynamic aperture check

Turn by turn data

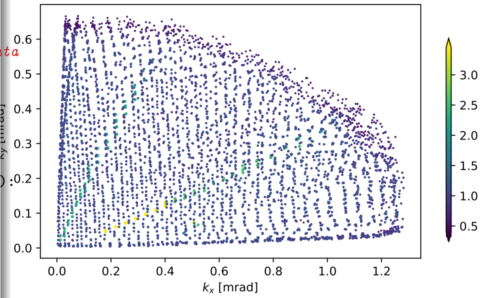
```
class Plane(Device):
    '''waveform and stats for one plane of the turn by turn data
    '''
    #: waveform
    wf = FC(EpicsSignalRO, '{self.prefix}:WF{self._coor}')
    #: peak to peak
    pp = FC(EpicsSignalRO, '{self.prefix}:PP{self._coor}')

    def __init__(self, prefix, coordinate_name=None, **kwargs):
        self._coor = coordinate_name
        super().__init__(prefix, **kwargs)

class SmallBuffer(Device):
    '''On the graphical user intrface: `Free run`
    '''
    x = Cpt(Plane, ':FR', coordinate_name='X')
    y = Cpt(Plane, ':FR', coordinate_name='Y')
    charge = Cpt(EpicsSignalRO, ':FR:WFS')

    def trigger(self):
        def cb(*, value, **kwargs): return True
        x_ready = SubscriptionStatus(self.x.wf, cb, run=False, ti
        y_ready = SubscriptionStatus(self.y.wf, cb, run=False, ti
        stat = AndStatus(x_ready, y_ready)
        return stat

class LiberaBox(Device):
    sht_buf = Cpt(SmallBuffer, prefix='bpmlbz2g', name='small_buffer')
    def trigger(self):  return self.sht_buf.trigger()
```



Devices

- kicker: delay, pc $\rightarrow$ combined
- turn by turn data: readout

Excurs: Bluesky dynamic aperture check

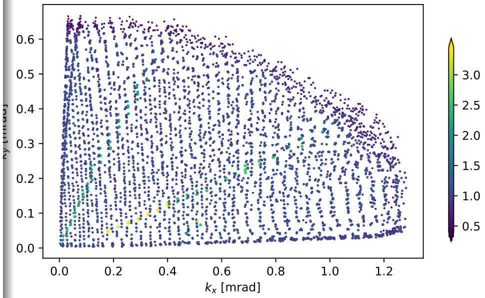
Plan (stub)

```
hk = HKicker(name='hk')
vk = VKicker(name='vk')
lb = LiberaBox(name='lb')

# excute on ray after the other
for ray_num in rays.coords['ray'].values:
    ray_data = rays.sel(dict(ray=ray_num))
    x = ray_data.sel(
        dict(coor='x', num=items)).values
    y = ray_data.sel(
        dict(coor='y', num=items)).values

    x_steps = cycler(hk, x)
    y_steps = cycler(vk, y)

    RE(
        bp.scan_nd(
            [lb, hk, vk], x_steps + y_steps
        )
    )
```



Devices

- kicker: delay, pc $\rightarrow$ combined
- turn by turn data: readout
- "rays from file" $\rightarrow$ plan $\rightarrow$ execute

Excurs bluesky: Lessons learned

Learning curve

- Device programmers
  - python experience: object oriented programming
  - event / call back patterns
  - personal recommendation: implement stop method (first)
- Plan programmers
  - python experience: generators
- Users
  - python experience: coding scripts

A little obstacle

- "epics.PV": for simple measurements → follow "manual work flow"
- Bluesky → "event" based → requires adaption

"Selling" Arguments

- Document structure → automatic storage
- Replay → life plot development
- Device drivers → make available
- Pay back:
  - Complex devices → details abstracted by standard interface
  - Large number of variables → device tree
  - Sophistcated plan stubs → reuse in different scripts