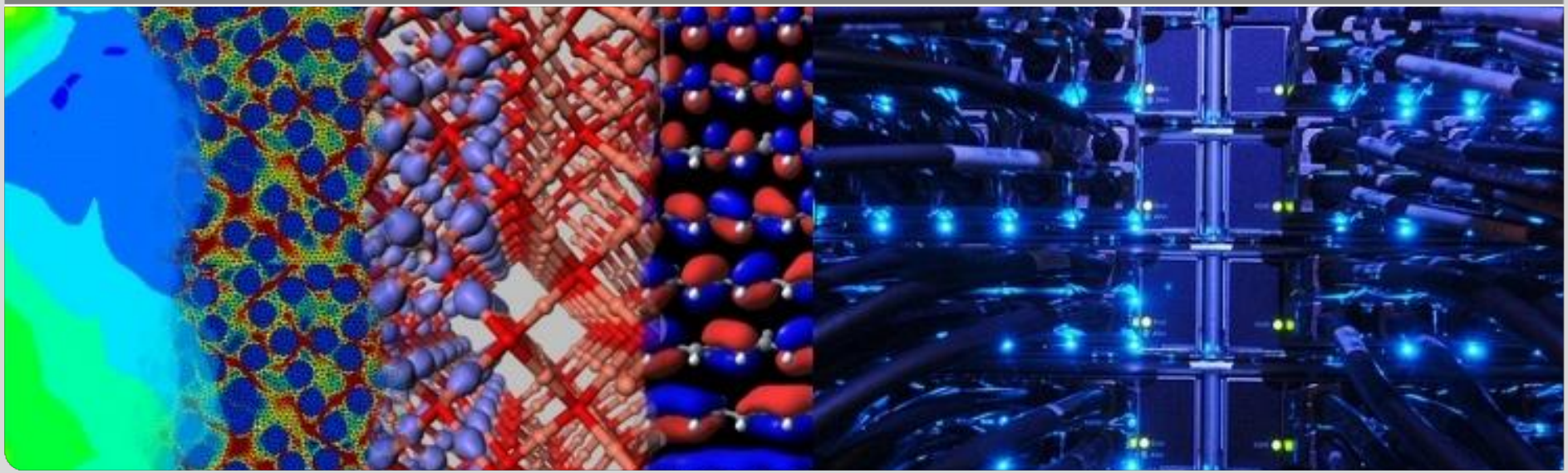
Karlsruhe Institute of Technology

College on Multiscale Computational Modeling of Materials for Energy Applications: Tutorial

Ivan Kondov

STEINBUCH CENTRE FOR COMPUTING - SCC



Acknowledgements

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Thanks to all partners in the project who have contributed to this tutorial!

Outline

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  - Exercise 1: Morphology in polymer electronics
  - Exercise 2: Morphology and donor-acceptor pairs in small-molecule semiconductor
- Tutorial 2: Using Fireworks and ASE
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  - Exercise 2: ForeachTask
  - Exercise 3: Charge transfer in dimers: sequential workflow
  - Exercise 4: Charge transport in disordered structures
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    - Parallel workflow
  - Exercise 5: Adding data analysis: Extending an existing workflow

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Tutorial 1
Using the MMM@HPC Framework

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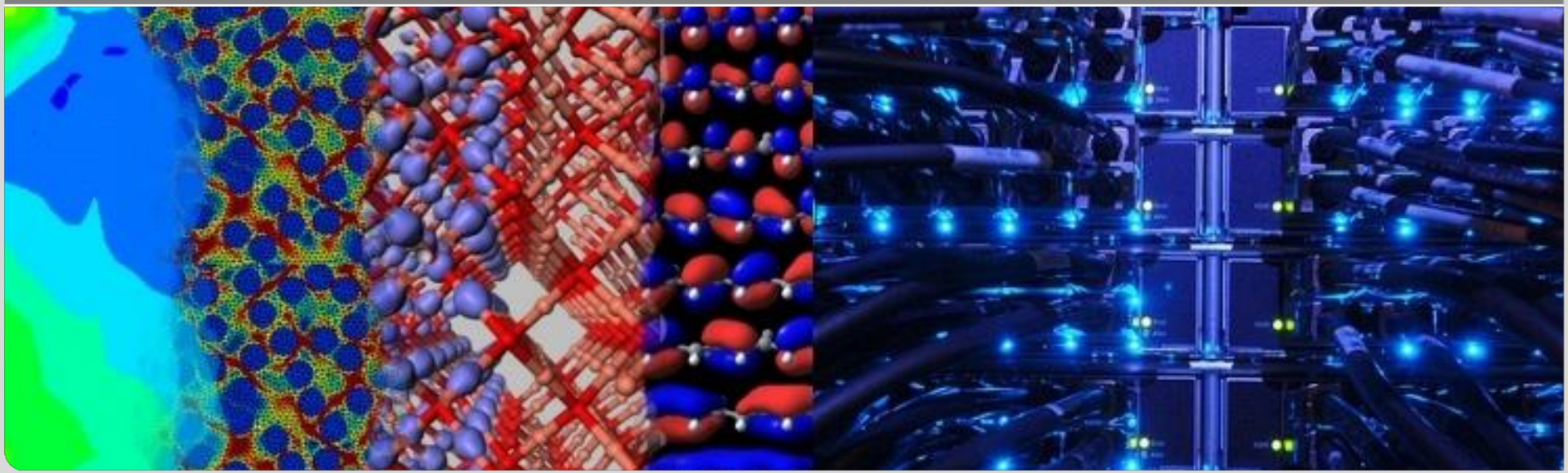
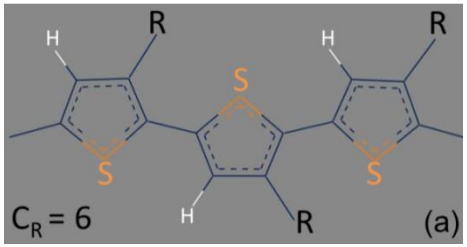


Charge transport in polymer-based devices

Task: Link between morphology protocols and charge transport protocols



***P3HT**: organic semiconducting polymer*

MOPHOLOGY

1 Generation of fully equilibrated atomistic structures and dynamics of model materials (Rr-P3HT, PQT)

amorphous

crystalline

CHARGE TRANSPORT

2 Computation of microscopic quantities, simulation of charge transport properties according to the physical model

hopping

band-like

Outcome: Charge transport rates inside crystalline and amorphous domains, in the interfacial area, and charge carrier mobilities through the entire material.

Polymer: Morphology workflow

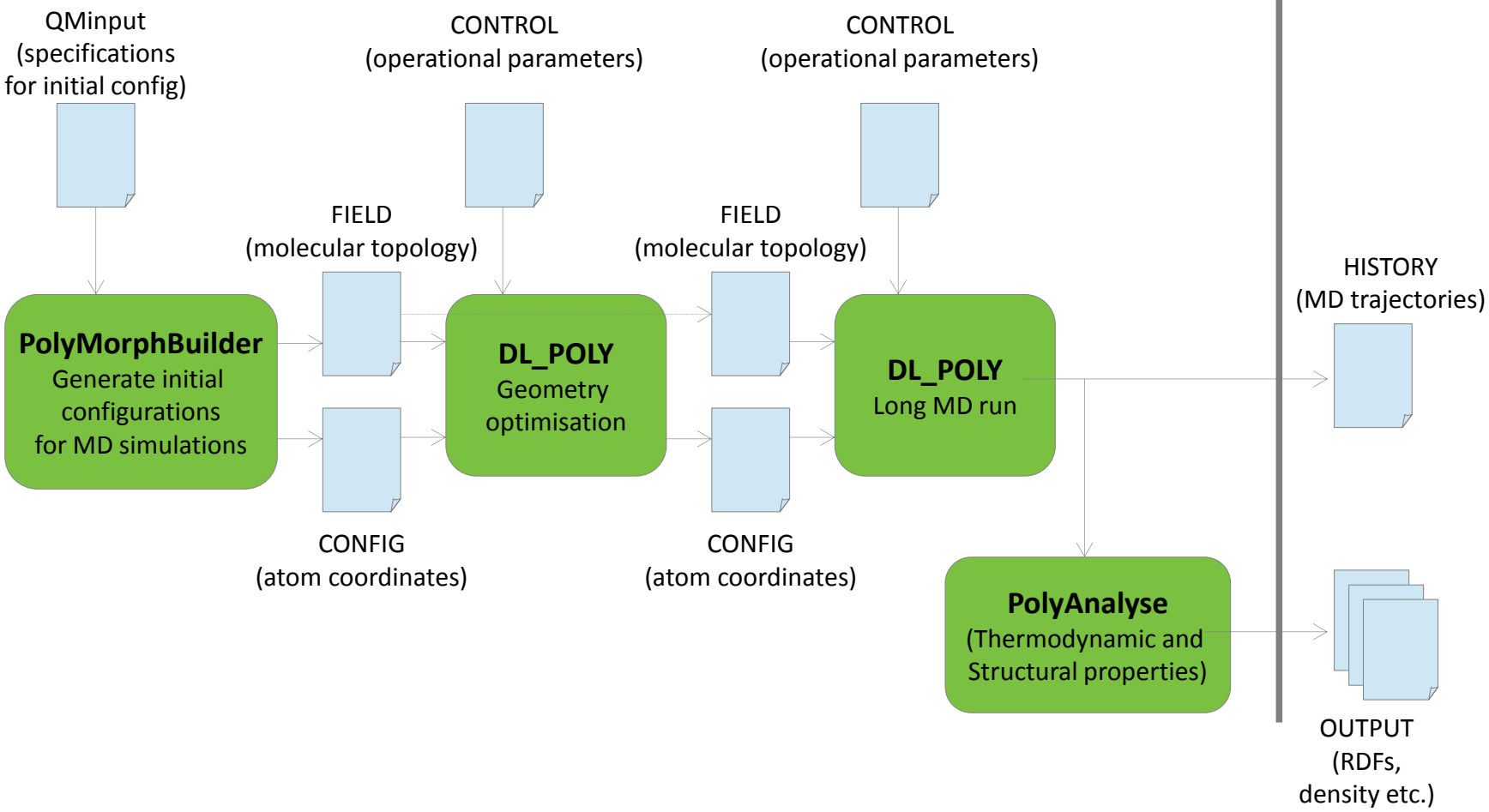
1. PolyMorphBuilder (building the initial morphology)
   - Initially combined with MAPS2 software platform for creating connectivity and assigning the corresponding force field.
   - Produces the input files for the MD simulation packages LAMMPS and DL_POLY and also for Monte Carlo home-made FORTRAN code.

2. DL_POLY (or LAMMPS)
   - Pre-equilibrated (geometry optimized)
   - Long all-atom Molecular Dynamics (and Monte Carlo) simulations using DL_POLY (or LAMMPS)

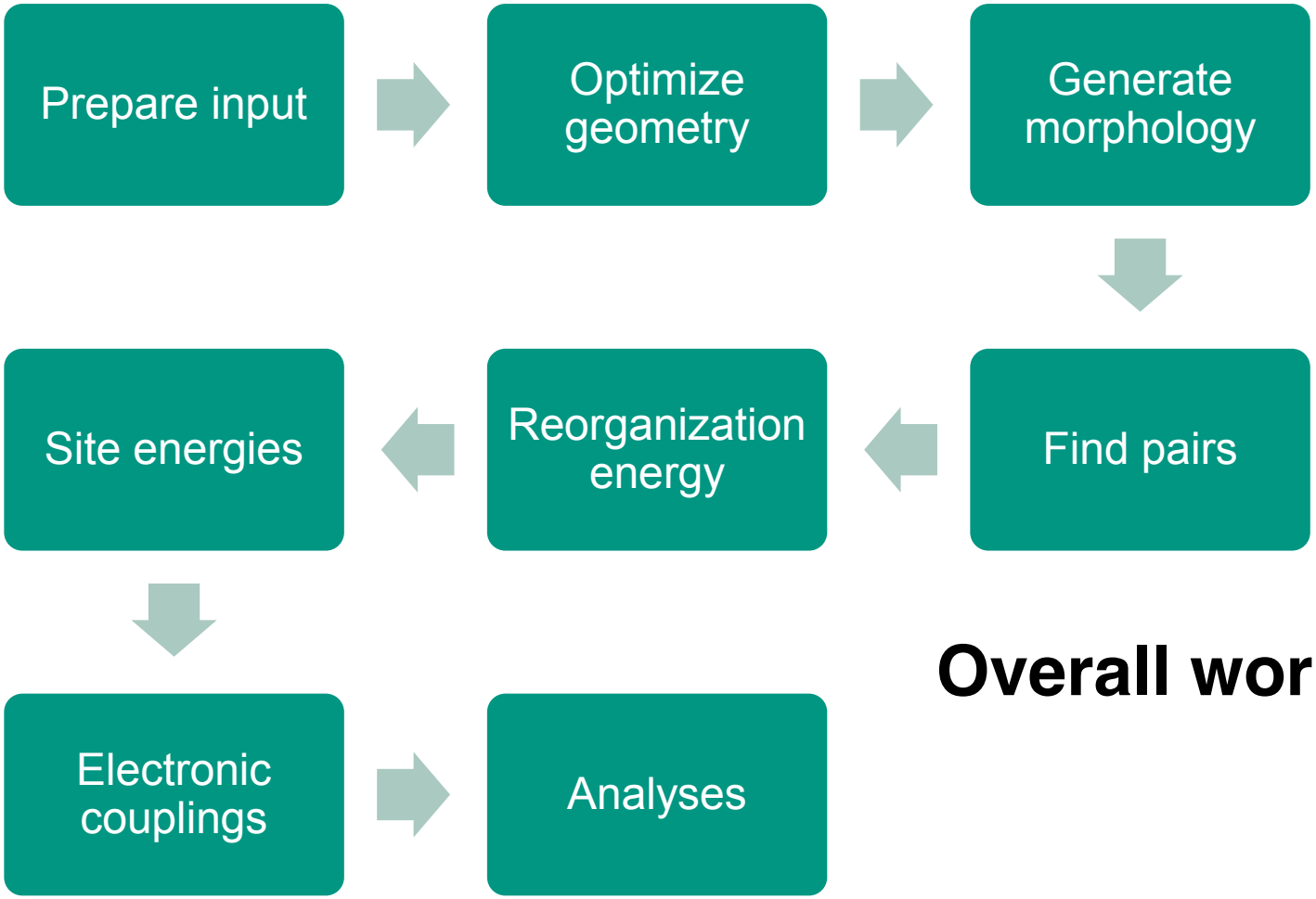
3. PolyAnalyse (home-made FORTRAN code)
   - Trajectories from step 2 are used for analysis to predict structural properties of interest.

Polymer: Morphology workflow

Part A – Morphology generation: data interchange

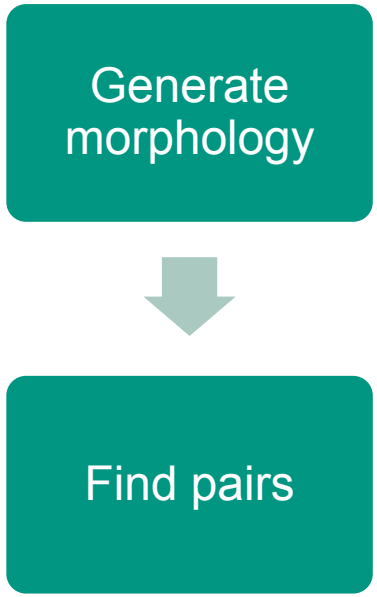


Exercise 2: Organic electronics workflow



Overall workflow

Exercise 2: Organic electronics workflow



On the Live CD

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Tutorial 2
Using FireWorks and ASE

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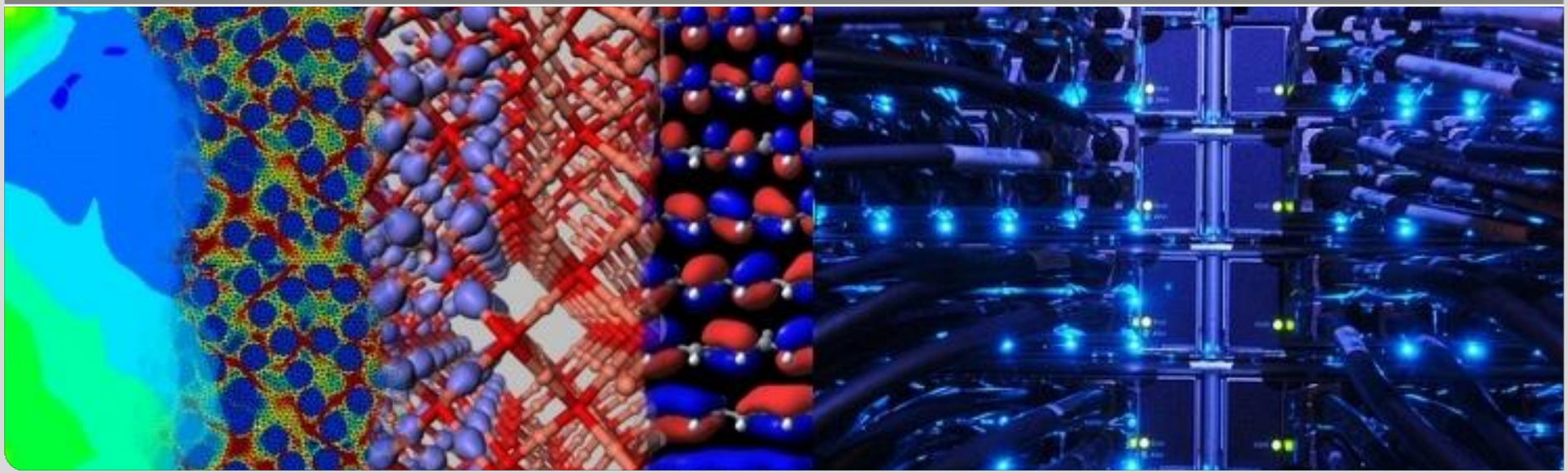


FireWorks general

- Define, manage and execute workflows
- Open source – a modified BSD license
- Website https://pythonhosted.org/FireWorks
- Used in the Materials Project http://www.materialsproject.org/

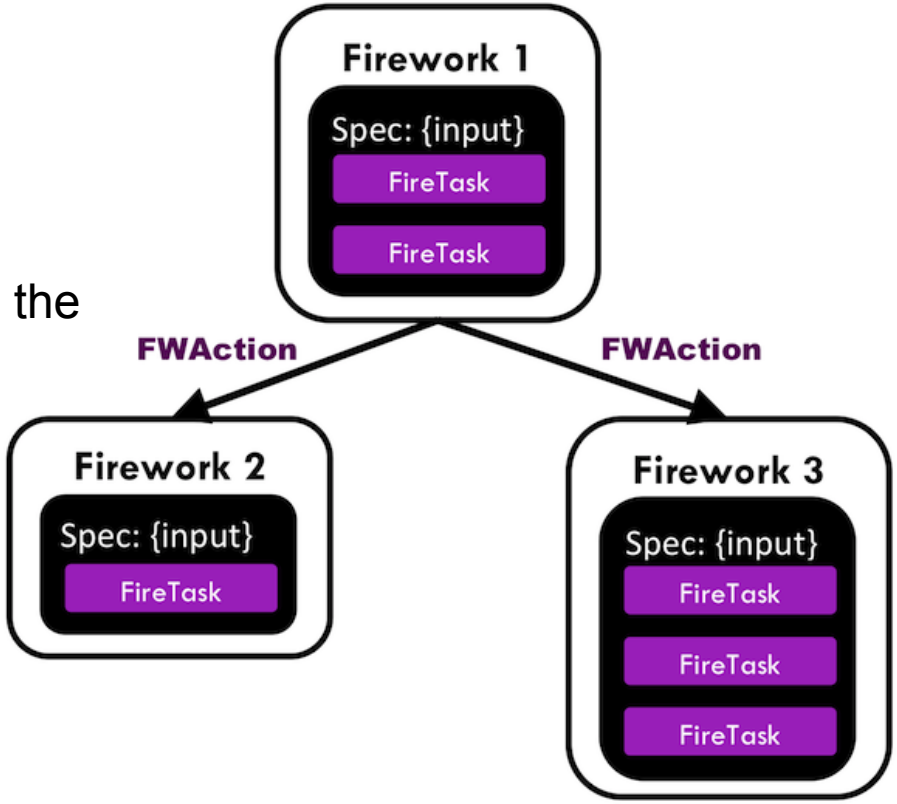
A. Jain et al., Concurrency and Computation: Practice and Experience 27, 5037 (2015)

FireWorks basics

- FireTask: an *atomic* computing job: one code, one script, one function

- FireWork:
  - Contains one or more FireTasks executed in a sequence
  - FireTasks in one FireWork share the same working directory
  - Includes bootstrap information: **spec**

- Workflow
  - A Directed Acyclic Graph (DAG) of FireWorks
  - **FWAction**



Source: https://pythonhosted.org/FireWorks

FireTasks

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Built-in FireTasks

- ScriptTask
- FileWriteTask, FileDeleteTask, FileTransferTask, CompressDirTask, ArchiveDirTask
- TemplateWriterTask
- PyTask

Custom FireTasks

- SingleTask
- ForeachTask
- JoinDictTask
- JoinListTask
- … write your own FireTasks!

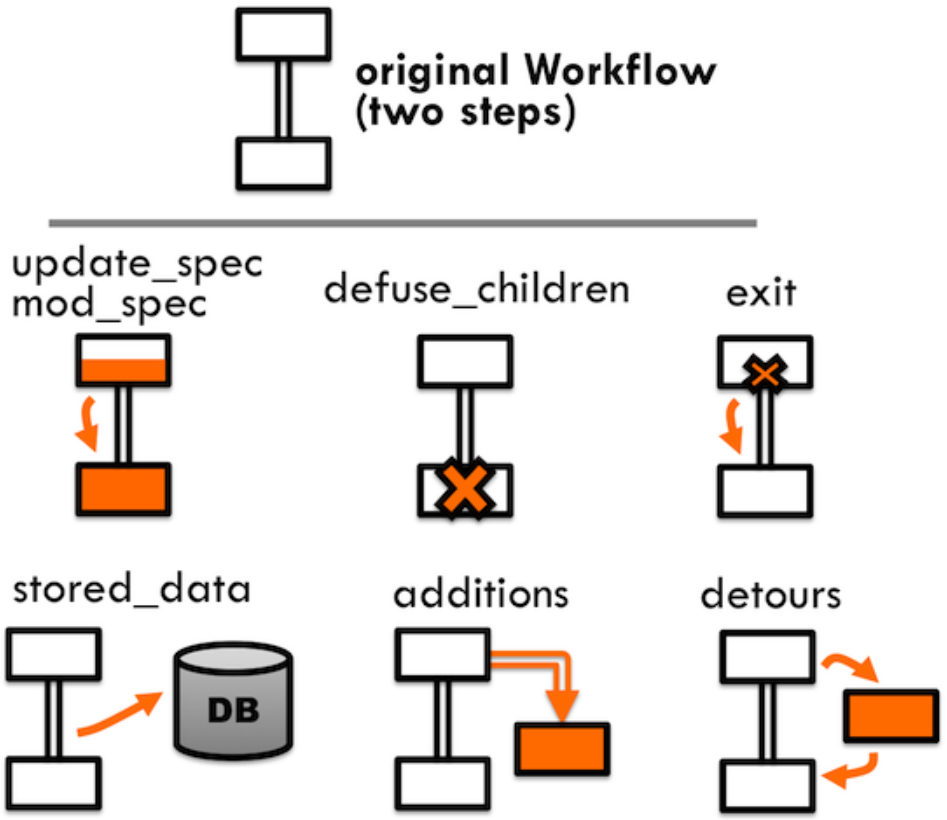
FWAction object

Returned by

- FireTasks
- Python functions called by PyTask

Purpose:

- Manage dataflow
- Dynamically change workflow



Source: https://pythonhosted.org/FireWorks

Using FireWorks (basic)

Create

- No workflow language
- No workflow editor available
- Write YAML or JSON manually
- Use Python scripts

Add

- LaunchPad: storage for all FireWorks objects
- Using command line:
  `lpad add`
- Use Python scripts

Launch

- FireWorker: computing resource
- Rocket launcher:
  `rlaunch`
- Multiple rockets launcher:
  `mlaunch`
- Execution via a batch system:
  `qlaunch`
- Use Python scripts

Query

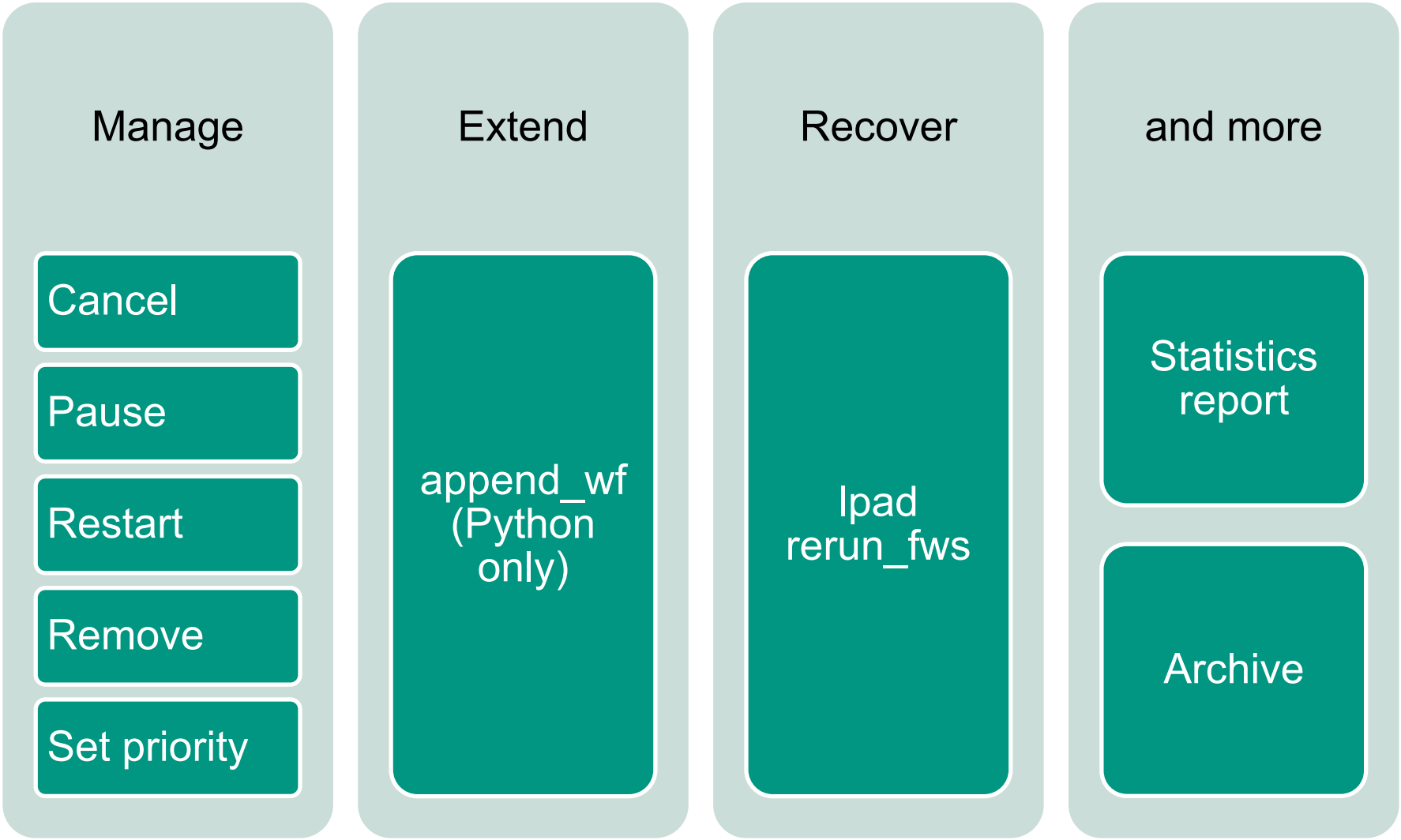
- Command line:

  ```
  lpad
  get_fws
  ```

  ```
  lpad
  get_wflows
  ```

- Use tracker
- Use web GUI
  `lpad webgui`
- Use Python scripts

Using FireWorks (advanced)



Using FireWorks productively

- Use FireWorks with batch systems
- Configure security
- Tune performance
- Consult the FireWorks documentation

Atomic Simulation Environment (ASE)

- Provides code integration infrastructure with calculator objects
- NWChem / Turbomole calculators in this tutorial
- Atoms class used for atomic structure data layout
- Dictionaries and lists (JSON serializable) used for all other data
- No data model
- Packages (in directory ictp-tutorial-fireworks/lib)
  - nwchem.py
    - basic wrapper, pre- and post-processor methods
  - transport.py
    - transport core methods
  - fw_task_functions_seq.py
    - reusable python functions needed for sequential workflows (one data entity)
  - fw_task_functions_par.py
    - reusable python functions needed for parallel workflows (multiple data entities)

wiki.fysik.dtu.dk/ase

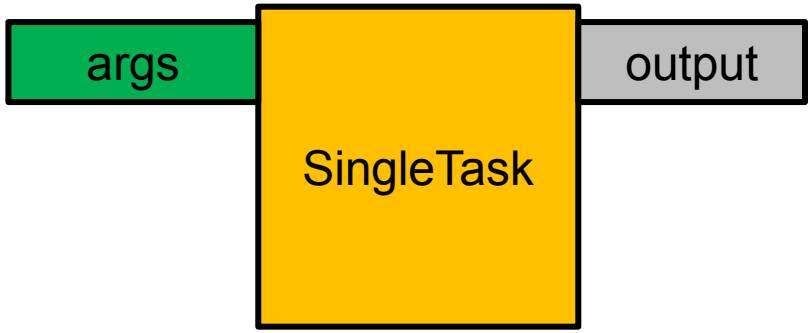
S. R. Bahn and K. W. Jacobsen, Comput. Sci. Eng. 4, 56 (2002)

SingleTask

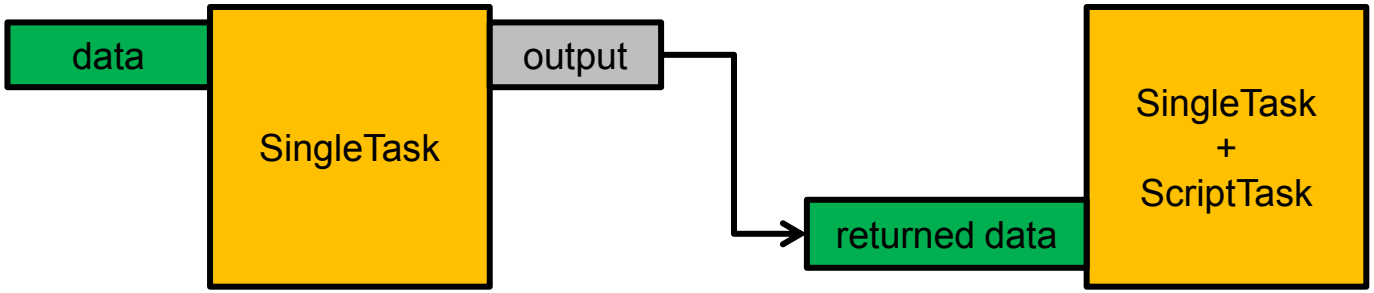
- Purpose: passes a list of data entities as positional arguments to a Python function and forwards the returned objects to the next FireWork via FWAction.

- Mandatory arguments:
  - ‘function’: the name of the Python function

- Optional arguments (must be existing spec keys):
  - ‘args’: a string or list of names of data fields in the spec
  - ‘output’: a string or a list of names of fields for output



Exercise 1: SingleTask



Python:

```
cd exercise_1
cp ../demo/singletask_demo.py .
python singletask_demo.py

lpad reset
lpad add workflow.yaml
lpad get_fws -d all
rlaunch singleshot
rlaunch -s singleshot
rlaunch -s rapidfire
```

JSON/YAML:

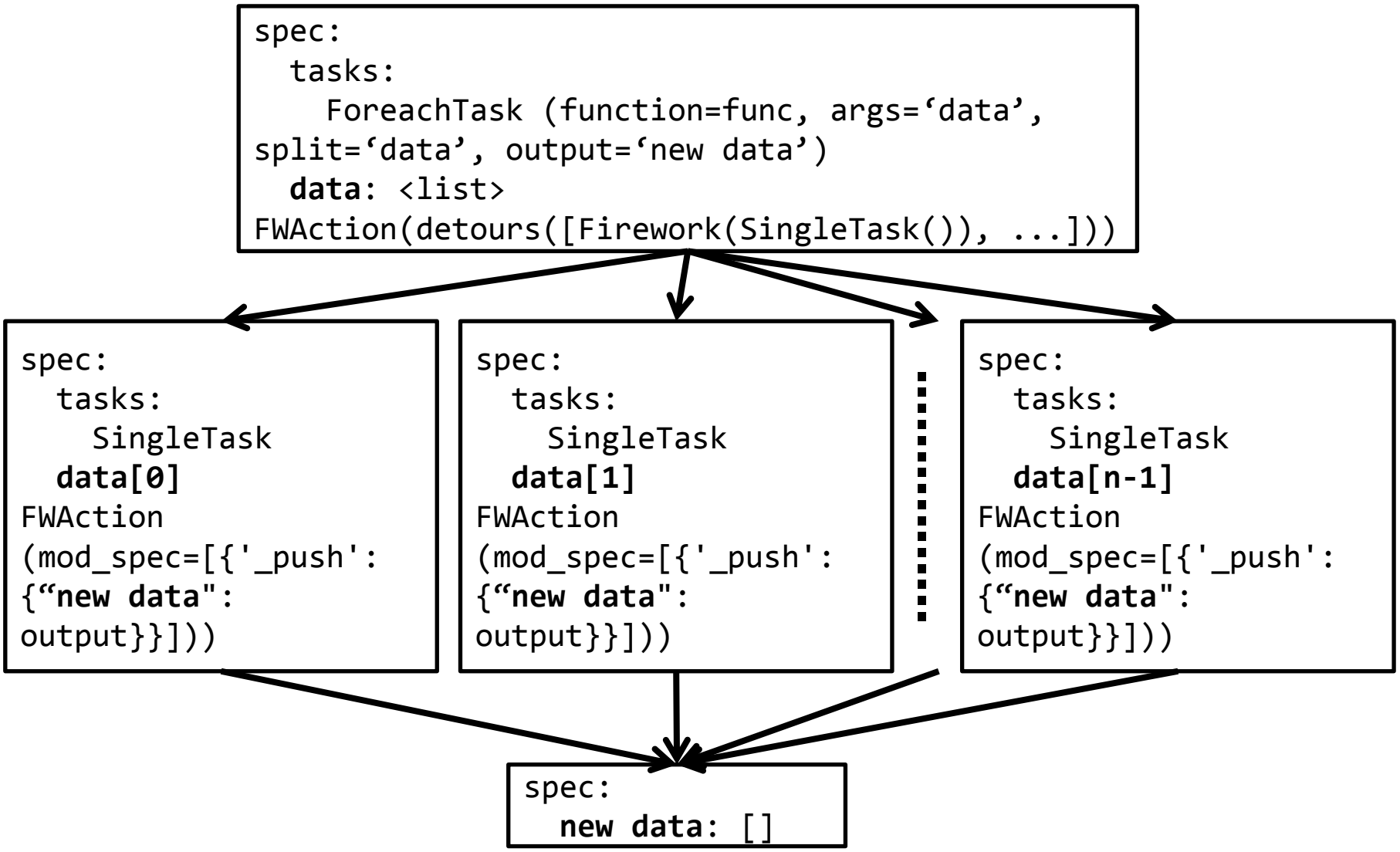
```
cd exercise_1
cp ../demo/singletask_demo.yaml .
cp ../demo/singletask_demo.json .
gedit singletask_demo.[json|yaml]

lpad reset
lpad add workflow.[json|yaml]
lpad get_fws –d all
rlaunch singleshot
rlaunch -s singleshot
rlaunch -s rapidfire
```

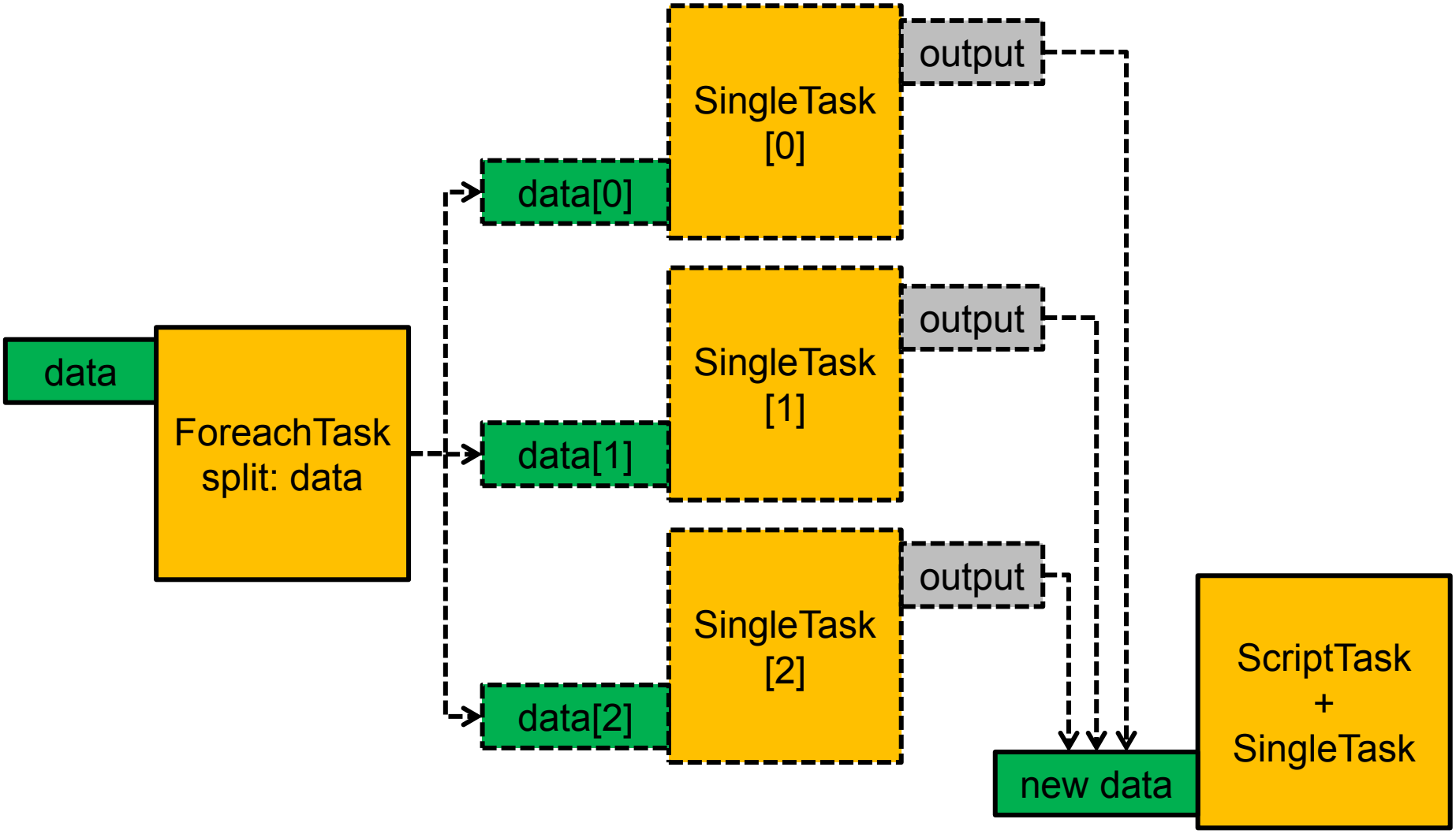
ForeachTask

- Purpose: realize a fork-join workflow model passing data through the spec
- Mandatory arguments:
  - ‘function’ is the name of the function
  - ‘split’ must be name of a list
  - ‘args’ must contain at least the ‘split’ argument
- Optional arguments:
  - ‘output’
- Arguments ‘args’ and ‘split’ must refer to existing spec keys

ForeachTask



ForeachTask



Exercise 2

Python:

```
python .py

lpad reset
lpad add workflow.yaml
lpad get_fws -d all
rlaunch singleshot
rlaunch -s singleshot
rlaunch -s rapidfire
```

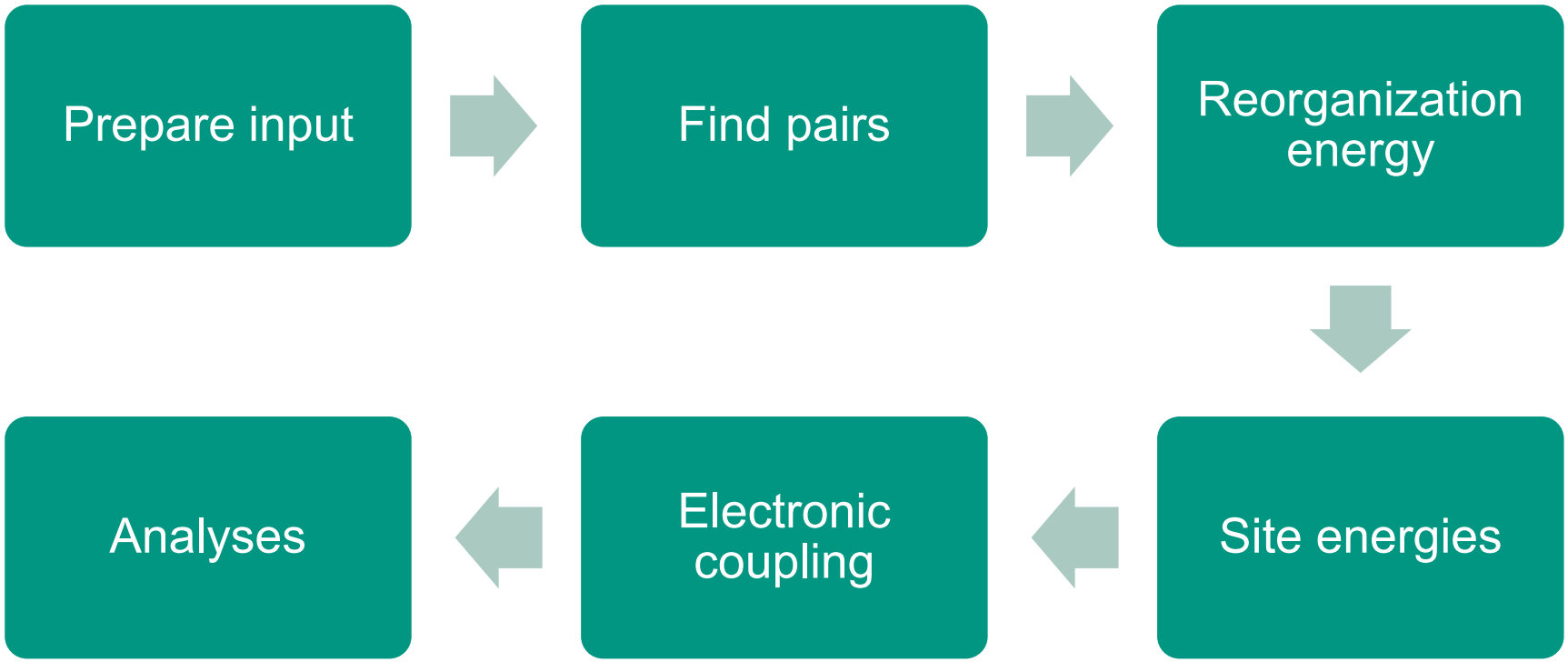
JSON/YAML:

```
gedit workflow.[json|yaml]

lpad reset
lpad add workflow.[json|yaml]
lpad get_fws –d all
rlaunch singleshot
rlaunch -s singleshot
rlaunch -s rapidfire
```

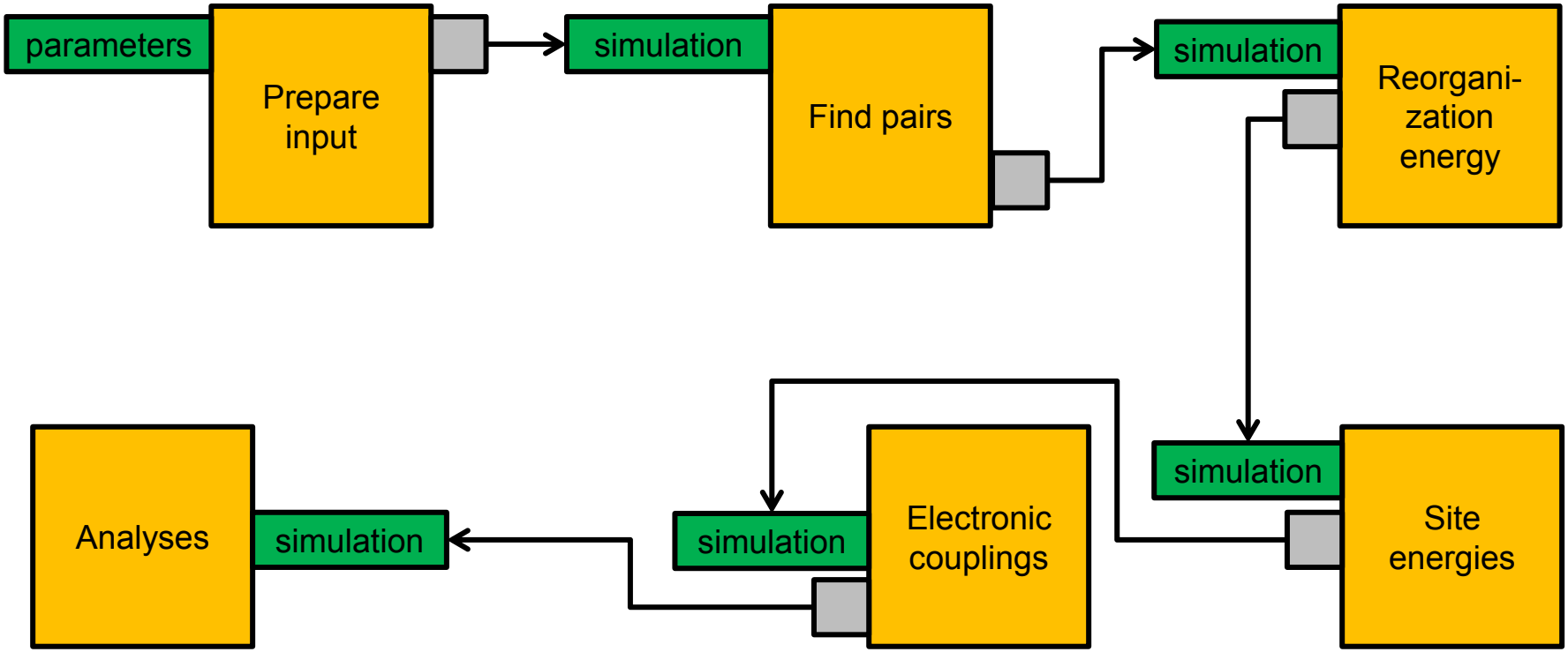
Charge transfer in dimers

- Control flow



Charge transfer in dimers

- Sequential dataflow



Exercise 3

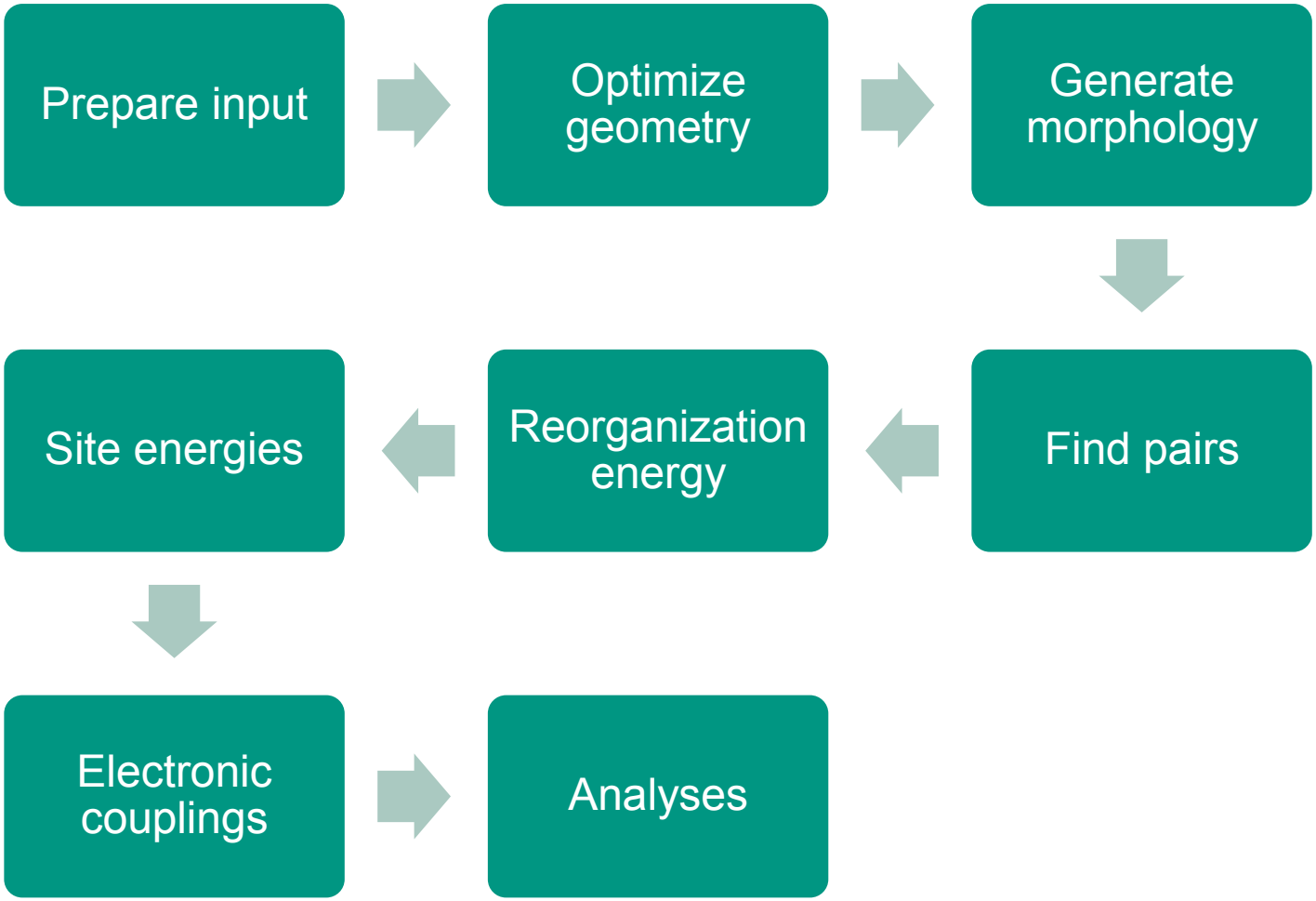
- For different dimers, for both A^+D and D^-A, calculate:
  - Internal reorganization energy λ
  - Electronic coupling V
  - Marcus rate, k

Dimer	V, eV	λ (A^+D), eV	λ (D^-A), eV	k (A^+D), s^{-1}	k (D^-A) , s^{-1}
Formic acid					
T-shaped benzene					
Parallel-displaced benzene					
H-bonded uracil					
Uracil stack					
Alq_3					

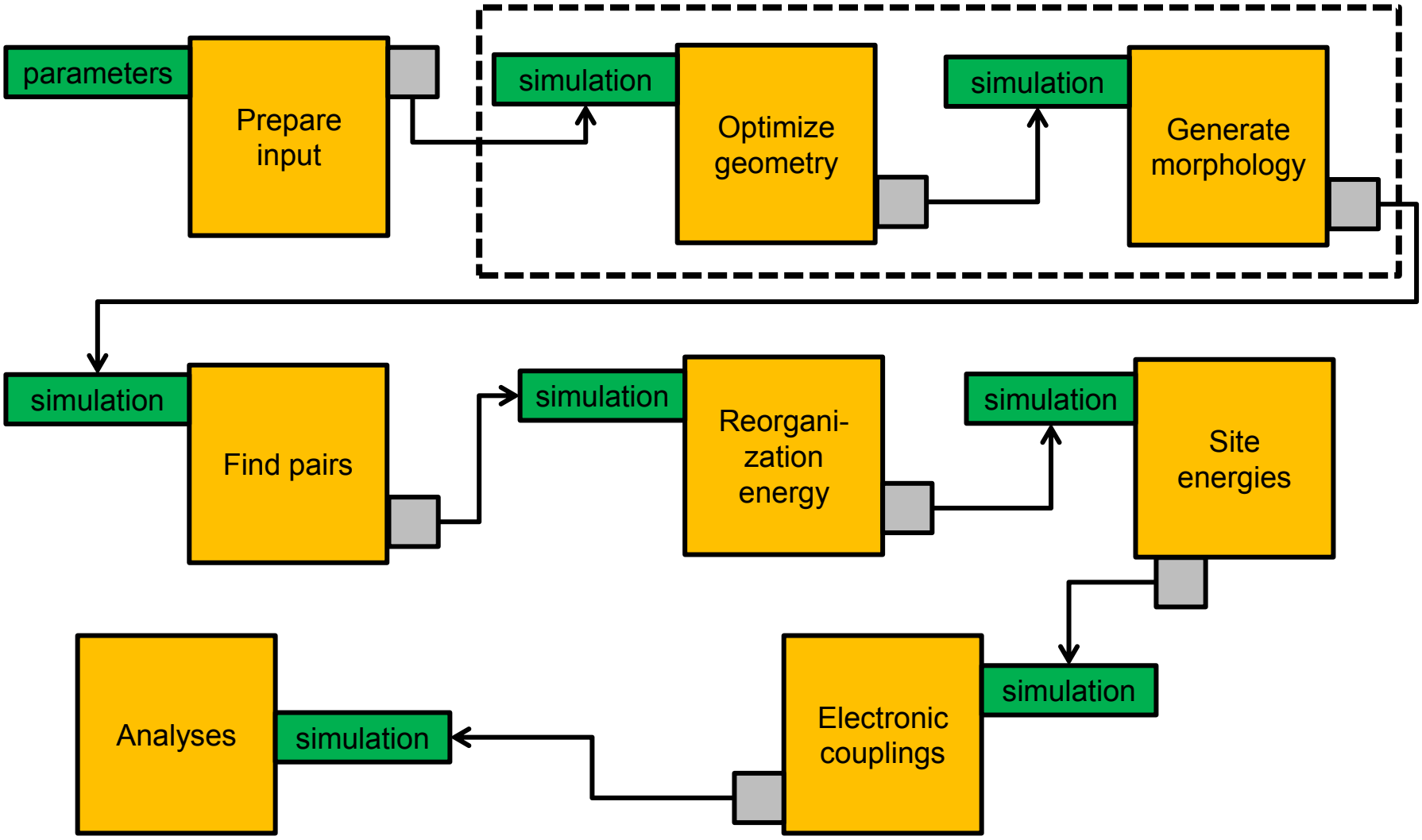
- Optional task: Repeat the calculation with the def2-SV(P) basis set.

Charge transport in amorphous structures

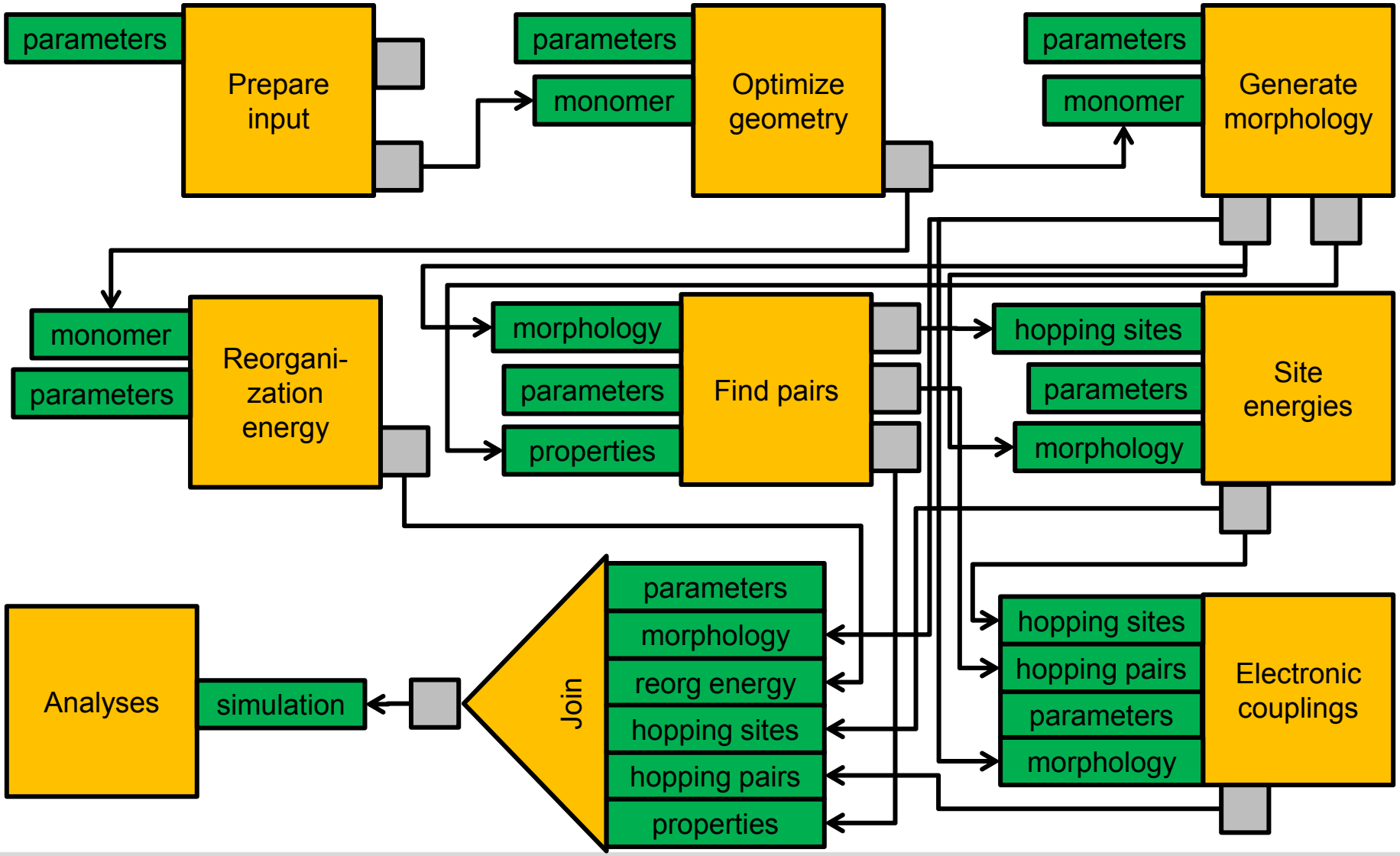
Sequential workflow



Charge transfer in amorphous structures



Charge transport in amorphous structures

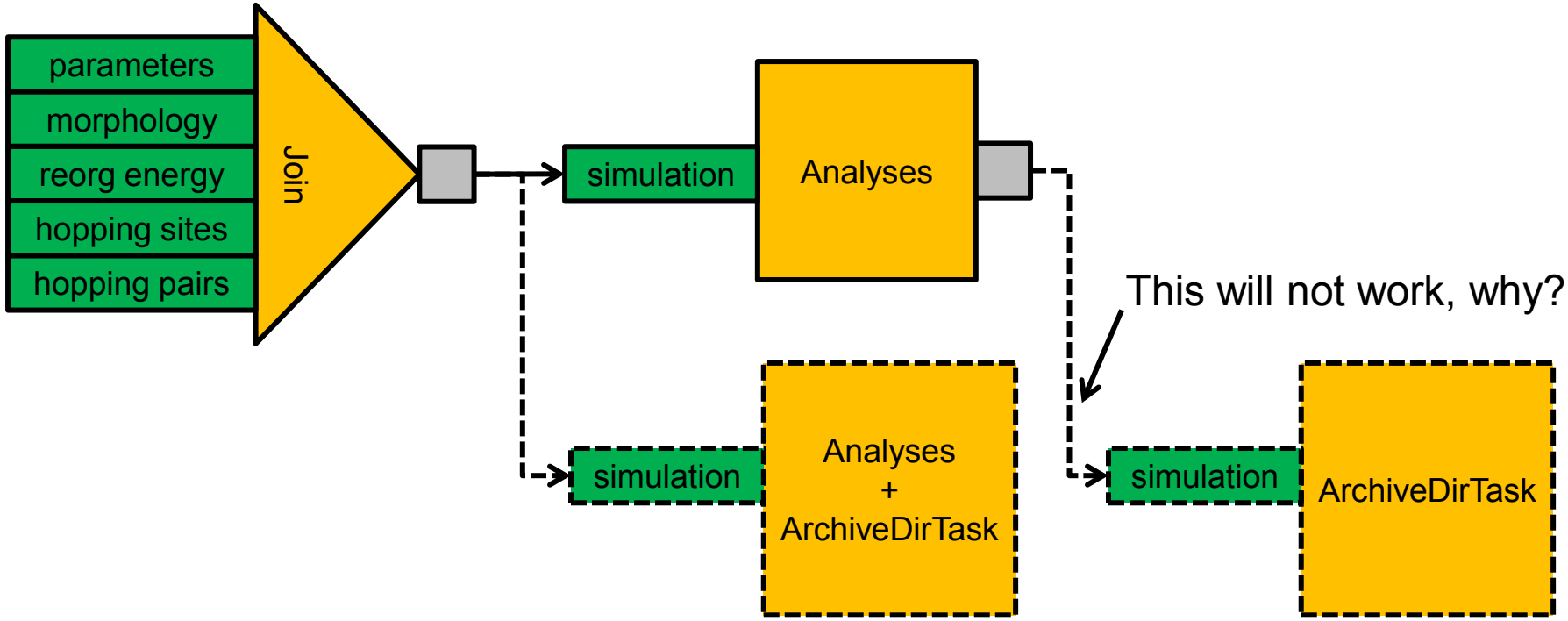


Exercise 4

- For Alq3 generate a morphology in a box with dimensions 40x40x40 Å.
- In the case of zero electric field and low carrier concentration, calculate:
  - Energy disorder σ
  - Mean electronic coupling $\langle V^2 r^2 \rangle$
  - Hole mobility μ^+

Appending fireworks / workflow

- Late extension in order to
  - Reuse simulation results in an other workflow
  - Repeat parts of the simulation with other parameters
  - Analyze / visualize / download results



Exercise 5

- Extend the completed workflow from Exercise 4 to visualize and download the results.

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