Improvement of software infrastructure

Symposium on European PV Research Infrastructures

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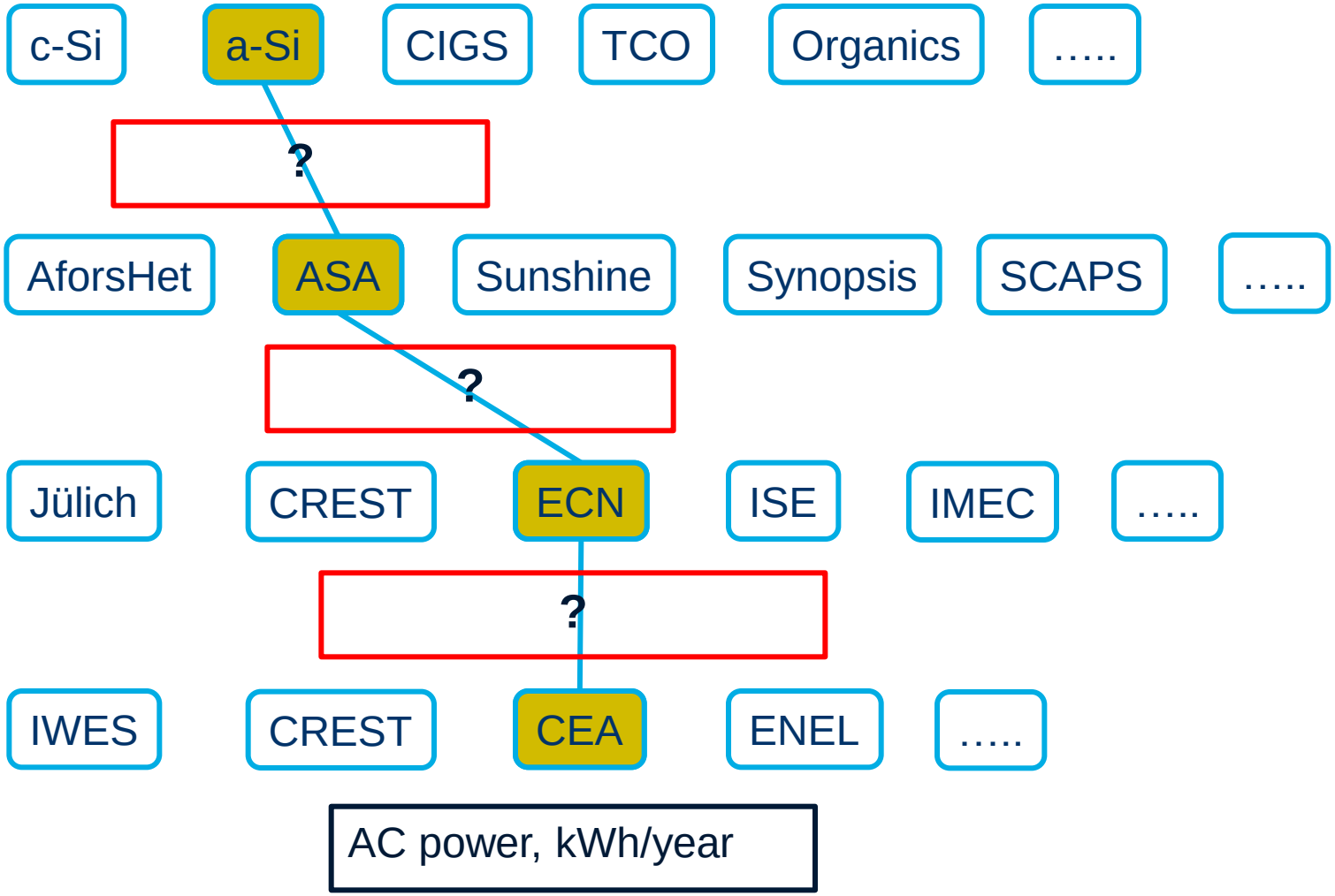
A European Project supported within the Seventh Framework Programme for Research and Technological Development

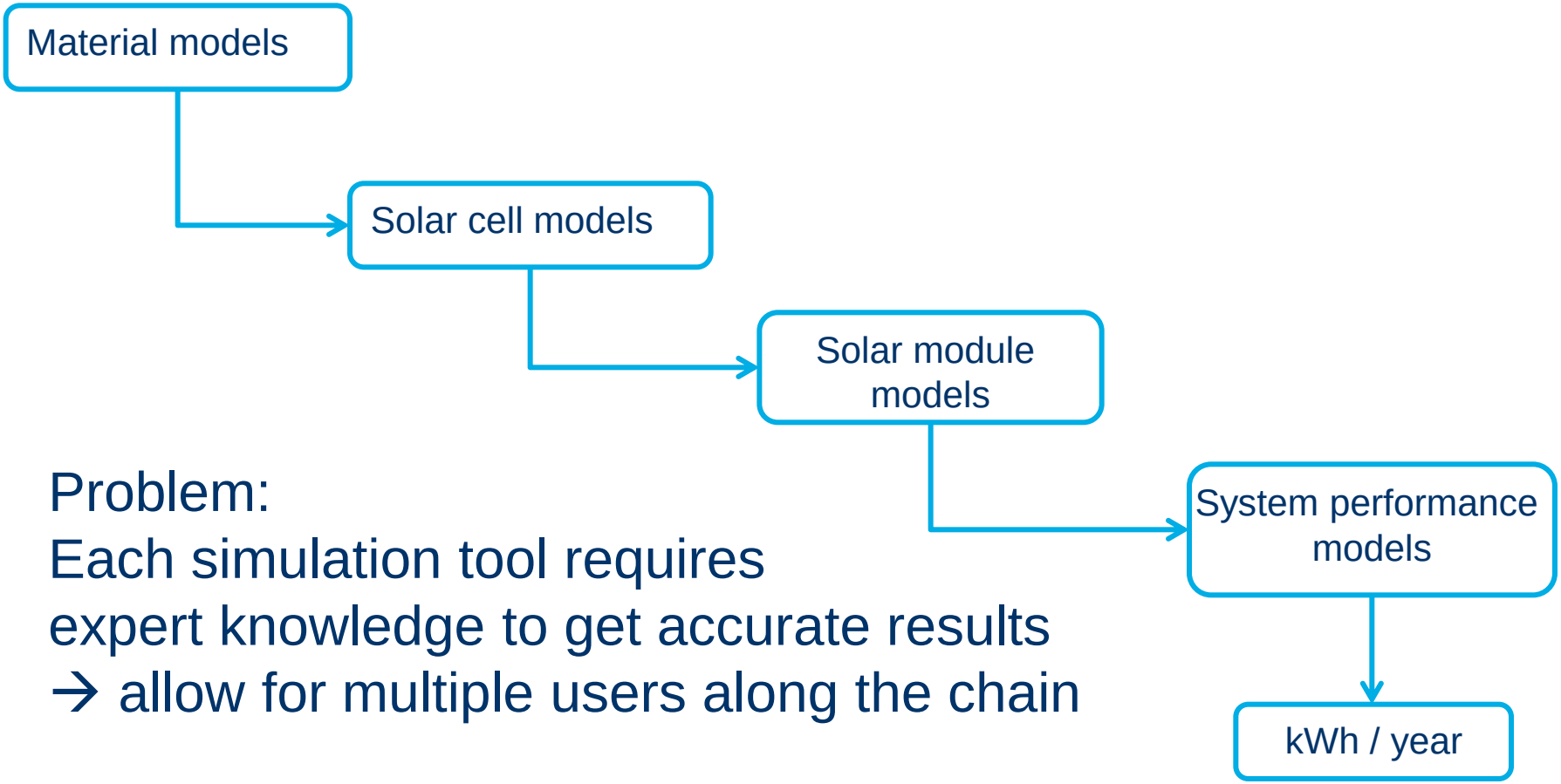
Vision for future software infrastructure

Ready to use toolbox of software tools to talk with each other



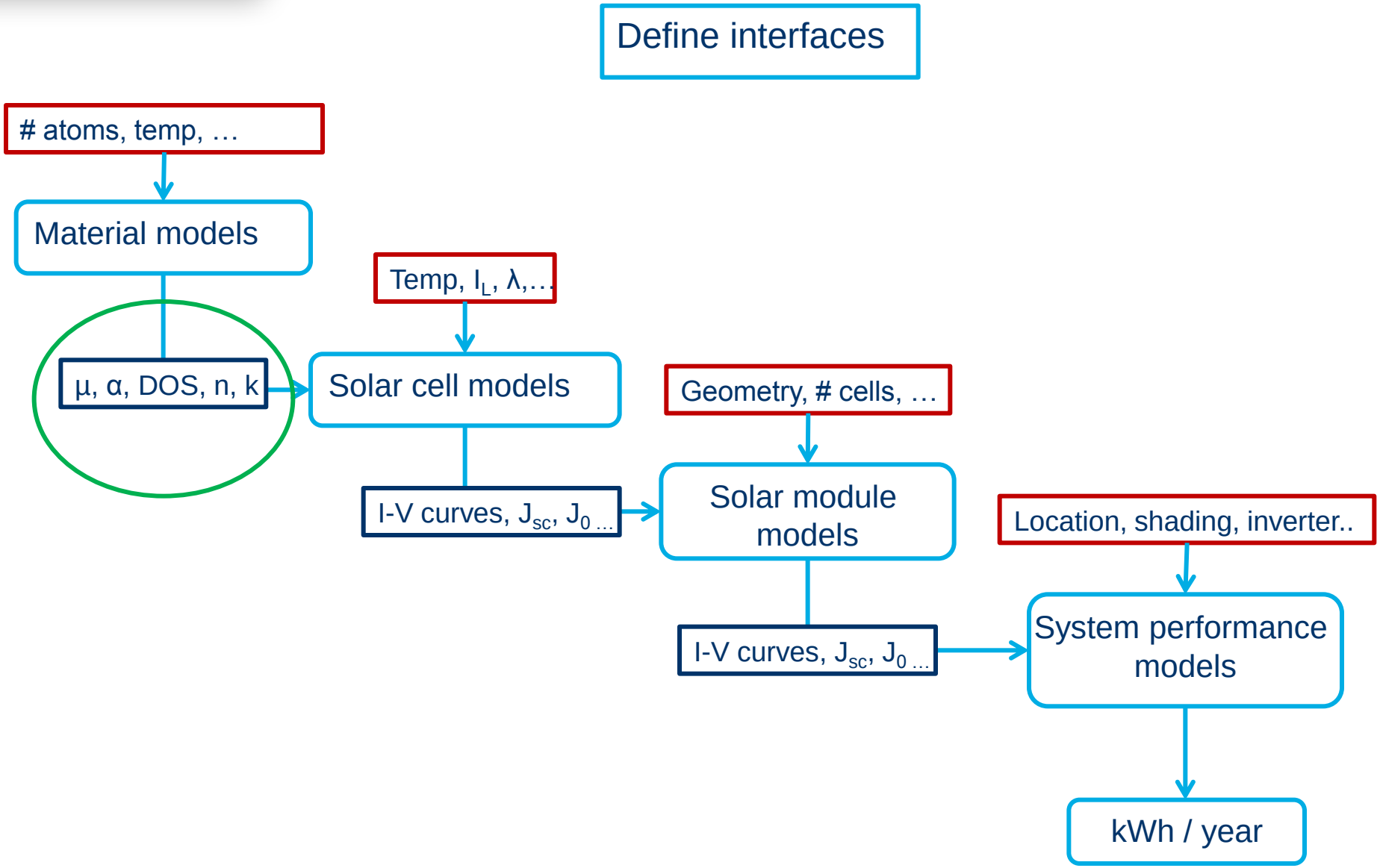
Aim of Sohpia JRA4

Aim: flexible, easily accessible material-system simulation chain



Problem:
Each simulation tool requires
expert knowledge to get accurate results
→ allow for multiple users along the chain

Input / Output interfaces



Development of the material – cell interface:

Calculation of macroscopic material parameters, from the initial physical configuration of individual atoms.

Problem: This is a very difficult interface to standardise, owing to the large number of materials and material configurations involved.

1. Calculate atomic configuration (72 atoms)
2. Calculate the electronic structure, i.e. wave functions and (local) density of states (DOS).
3. Extraction of macroscopic parameters (absorption, mobility, or recombination rates) from DOS.
4. Repeat for different atomic configurations (approx. 3 months per configuration)
5. Repeat calculations (with different methodologies) for different materials.

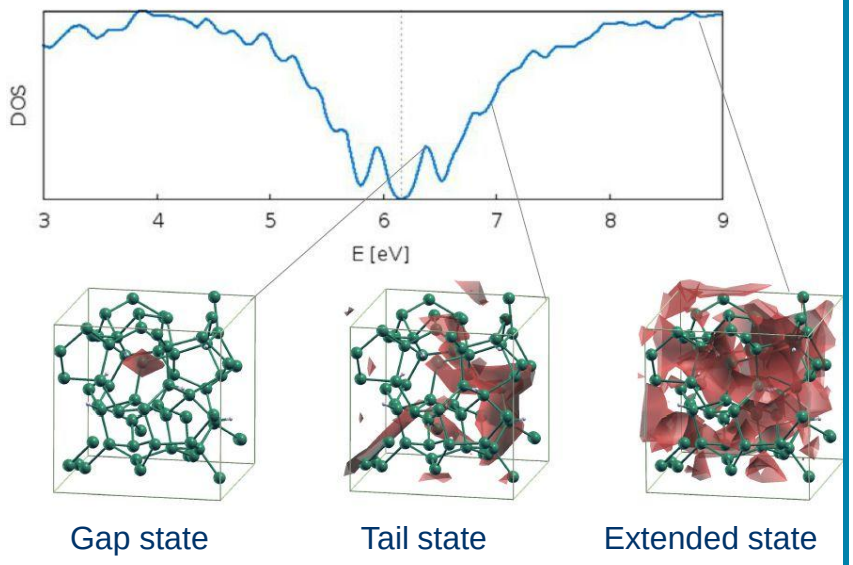
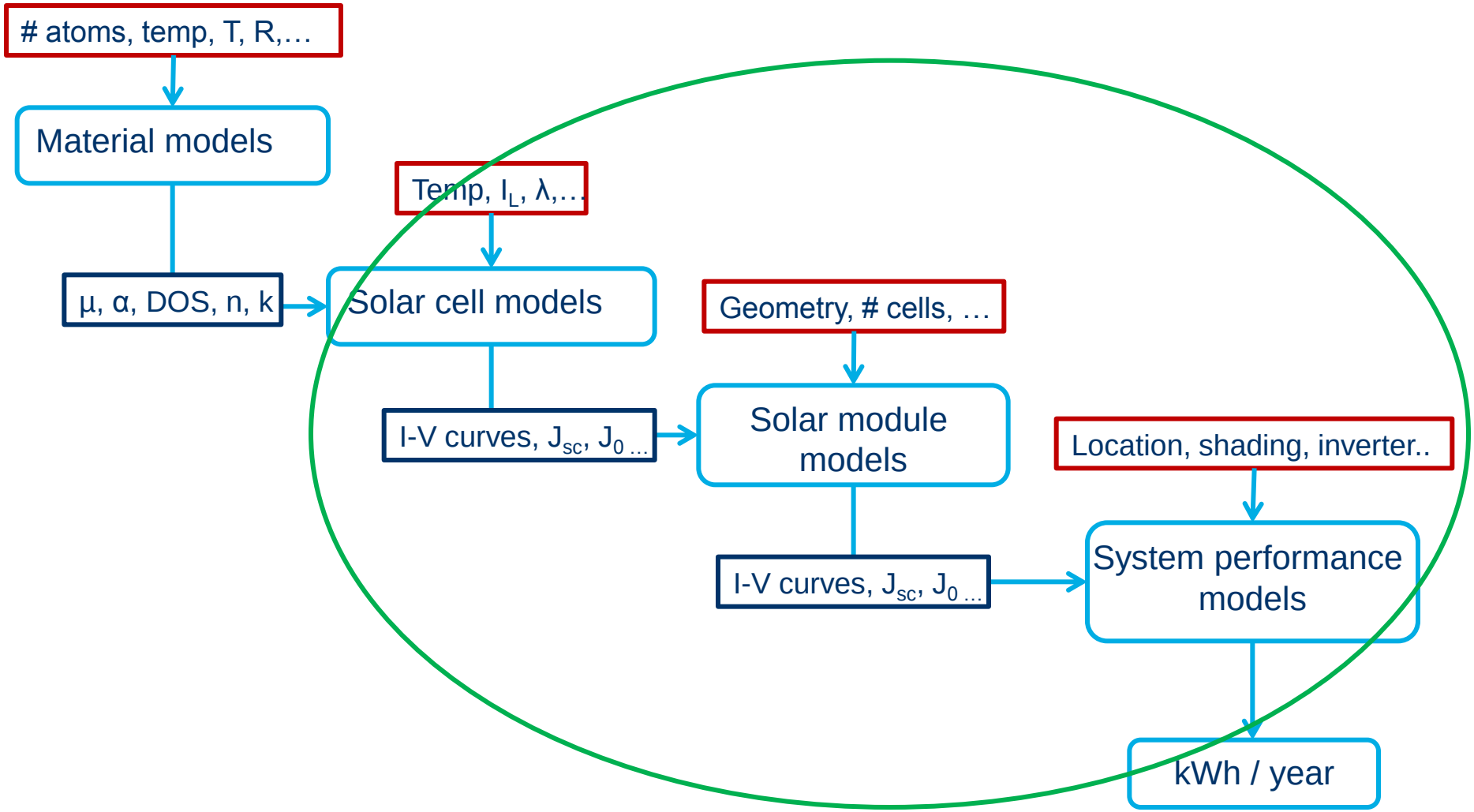


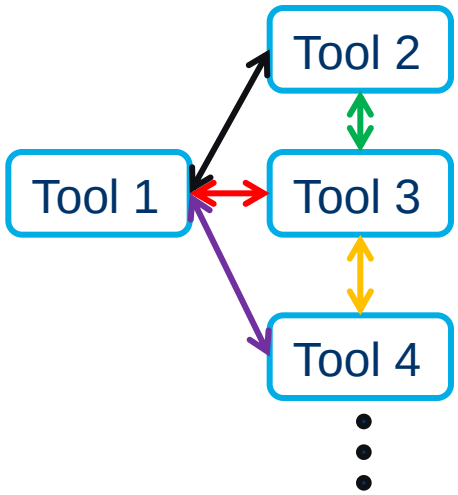
Image Courtesy Philip Czaja (Juelich)

Cell-System interaces



Development of cell to system interface

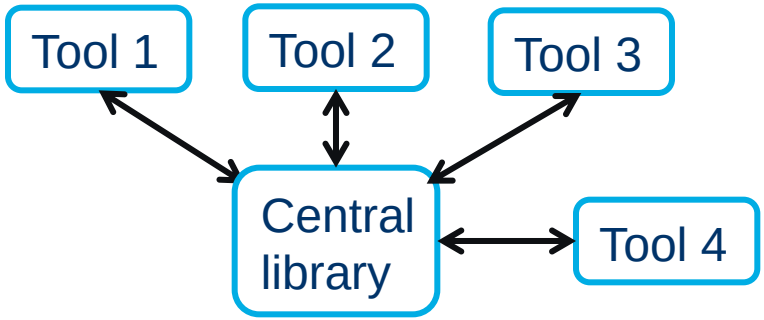
Multiple simulation tools need to communicate. Each simulation tool requires a *different* set and format of input data.



Solution:
1. Define standard interface data and data formats

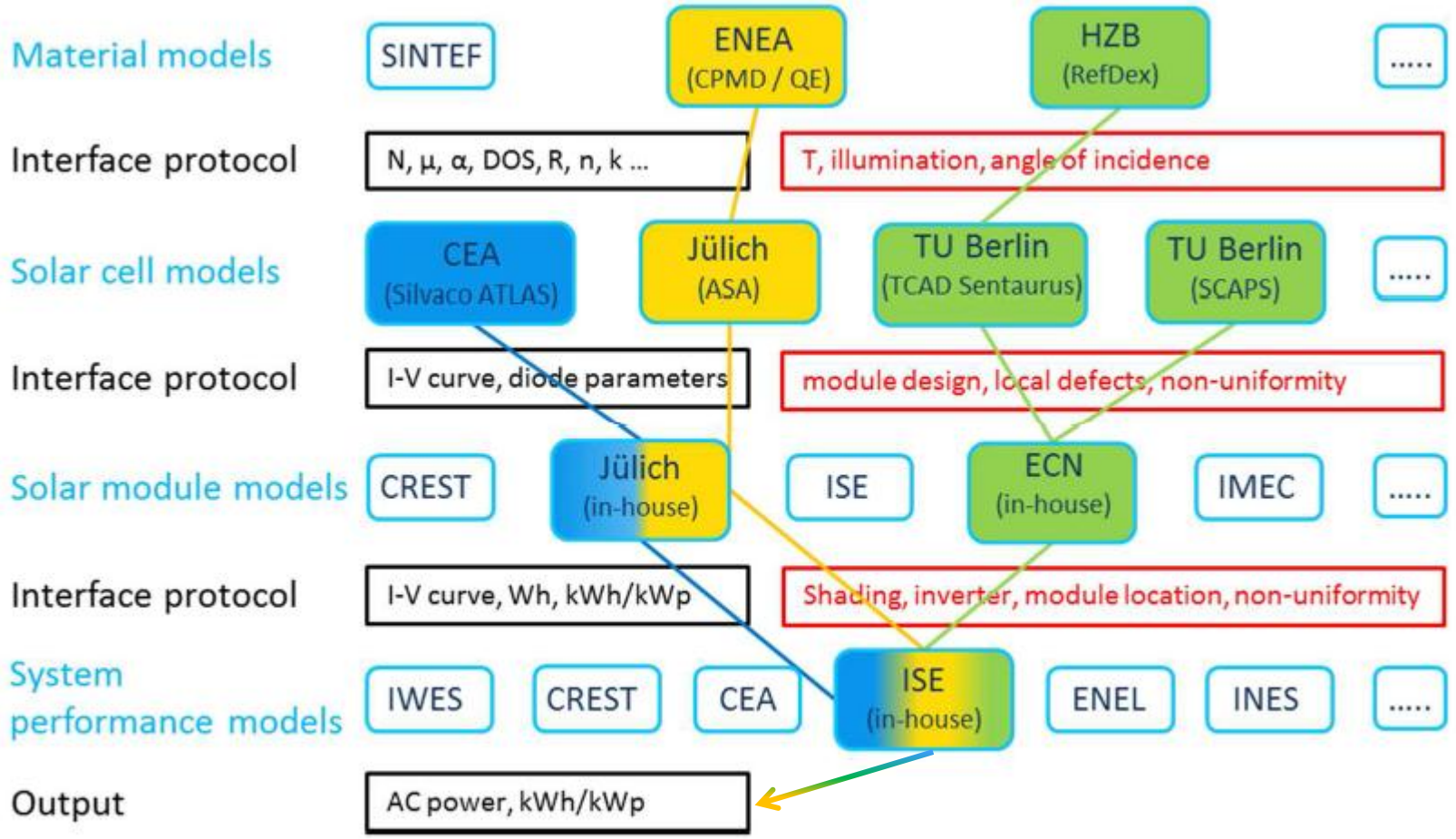
2. Development of a central library / interface

such that each simulation program must only communicate with only *one* interface, and can then communicate with all other simulation tools.



Successful demonstration of simulation chain

Testing of interfaces



Augarten 28th EUPVSEC (2013) Paris, France., pp.3949-3952, ISBN: 3-936338-33-7,

Central interface library

Task: Data transfer between PV simulation tools, from cell to system level.

✓ Proof of concept of this library written and tested

The library provides:

- a standard format to pass IV curve data, or IV parameters obtained from fitting
- One- and two- diode model fitting
- Option for spectral corrections
- Interpolation within the desired temperature and illumination range.

✓ Computationally intensive programs only simulate few data sets => interpolation

✓ simulated or experimental data can serve as input

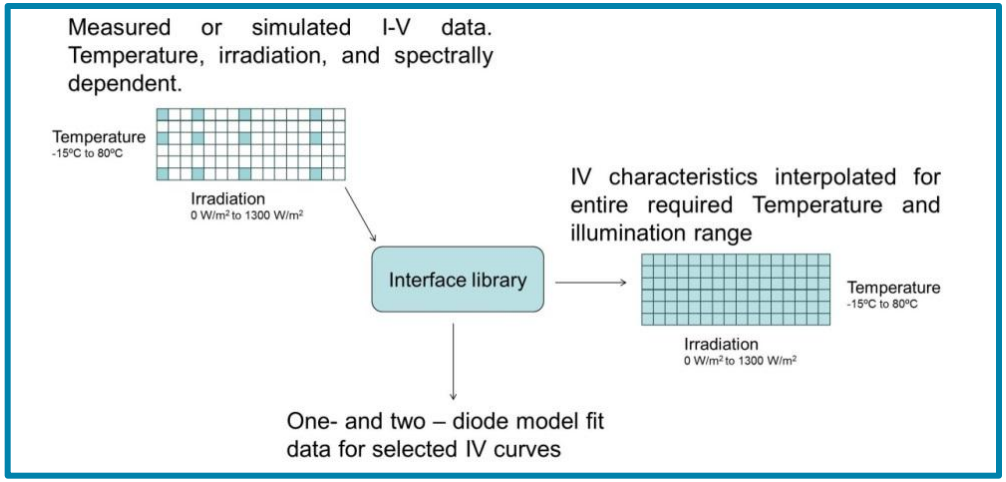


Figure 2: Schematic representation of the initial interface library developed in the Sophia project.

Conclusions and outlook

Conclusions

- PV-chain simulations using the central interface library demonstrated
  - more efficient
  - less error prone
  - “simple” investigation of impact on system performance from changes at the cell or module level.
- Everyone should use the central interface library => network of simulators

Outlook

- Development of a Central European modelling online database containing:
  - lists of tools, contacts, experts, ... **to be published and extended**
  - data exchange standards, central interface library tool **to be published soon**
  - Standardised data sets for material, cell data
  - Links to existing, referenced data sets, ….
- Development of “official” EU/worldwide standards for PV simulation tool data input/output formats and content
- Development of publically accessible, technology specific simulation chains to be accessed by researchers and industry

SOPHIA
European Research Infrastructure

THANK YOU!

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