Molecular Dynamics with i-PI

Joint with IMPRS-UFAST School

Electronic Structure Methods and Applications

The i-PI code

RESEARCH ARTICLE | AUGUST 14 2024

i-PI 3.0: A flexible and efficient framework for advanced atomistic simulations

Special Collection: Modular and Interoperable Software for Chemical Physics

Yair Litman; Venkat Kapil; Yotam M. Y. Feldman; Davide Tisi; Tomislav Begušić; Karen Fidanyan; Guillaume Fraux; Jacob Higer; Matthias Kellner; Tao E. Li; Eszter S. Pós; Elia Stocco; George Trenins; Barak Hirshberg; Mariana Rossi; Michele Ceriotti

+ Author & Article Information

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Connected Content

A companion article has been published: Updates to i-PI package improve performance in widely used atomistic simulation software

The i-PI code

- The (PI)MD engine does not need to know much about electronic structure:
  Only needs to *receive forces* and give *back positions*
- Same idea works for other “decoupled” ionic motion
  (geometry optimizers, classical MD, etc.)
- Often useful to use the electronic structure or machine learning as a simple driver (client)
  and have an external engine to control it

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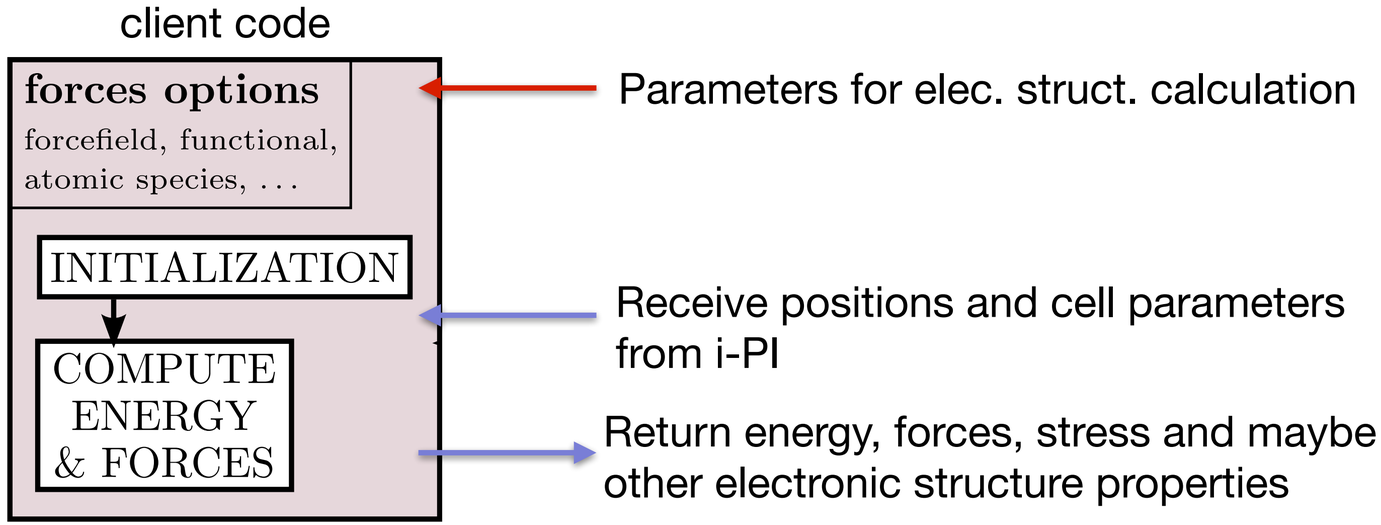
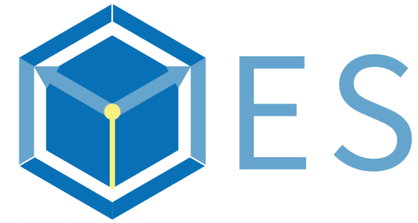


The i-PI code: Sockets Interface

- The i-PI code is a python interface for the calculation of (path integral *ab initio*) molecular dynamics
- i-PI communicates with the electronic structure codes through internet (or UNIX) sockets, making it extremely flexible
- Interfaced to many electronic structure codes: CP2K, DFTB+, LAMMPS, Quantum ESPRESSO, Siesta, FHI-aims, Yaff, deMonNano, plumed, ASE, TBE, CASTEP, AMS, …

Visit: https://ipi-code.org/

The i-PI code for nuclear dynamics



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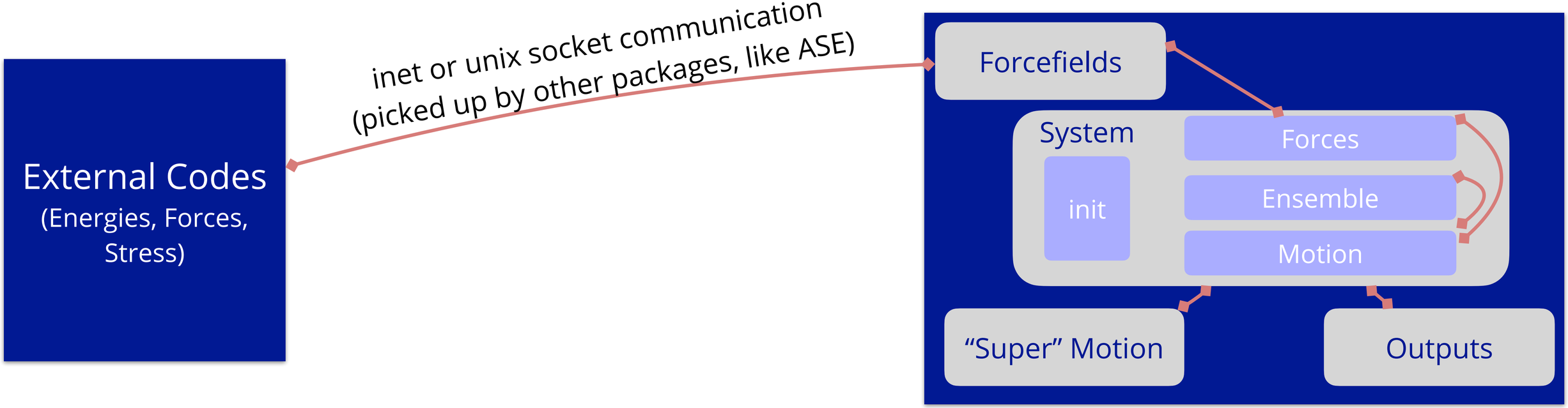

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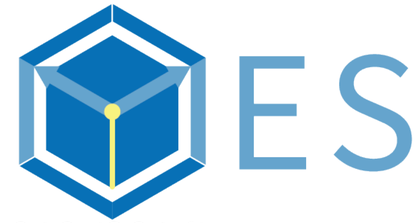

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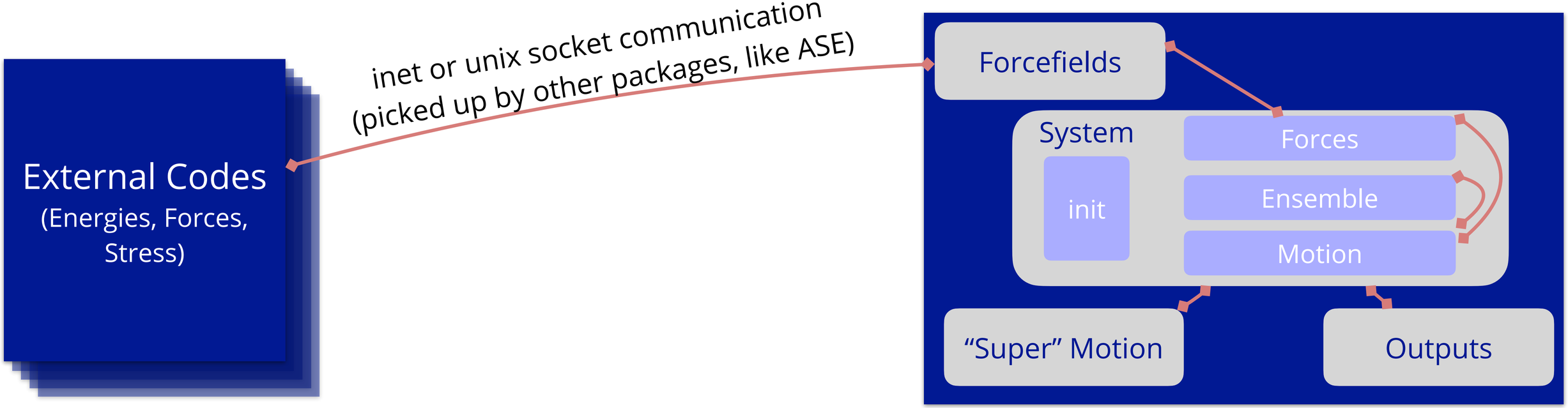

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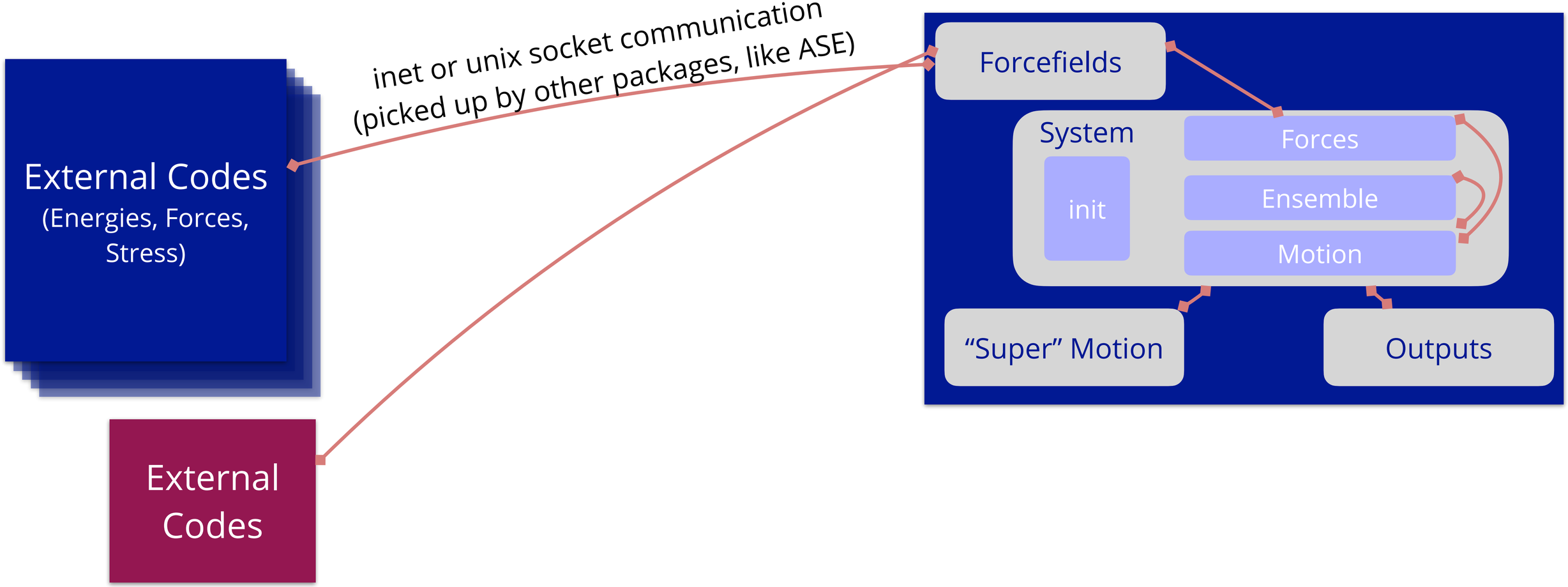

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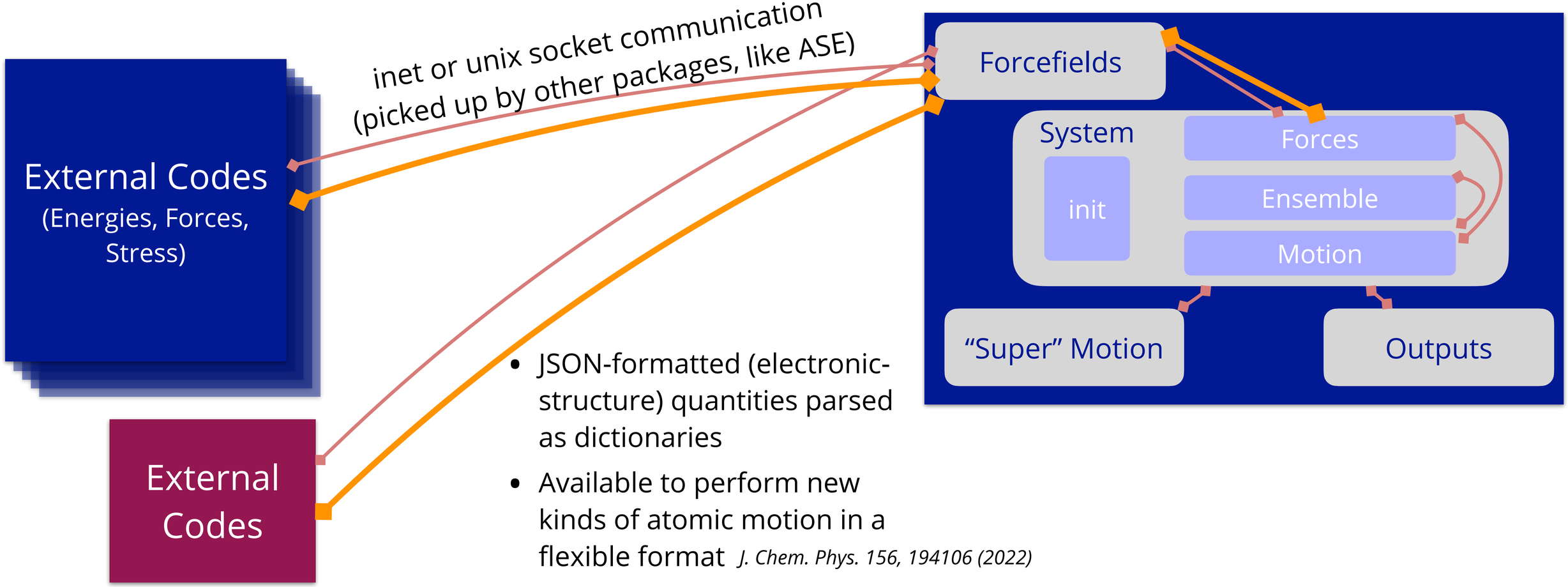

- JSON-formatted (electronic-structure) quantities parsed as dictionaries
- Available to perform new kinds of atomic motion in a flexible format *J. Chem. Phys. 156, 194106 (2022)*

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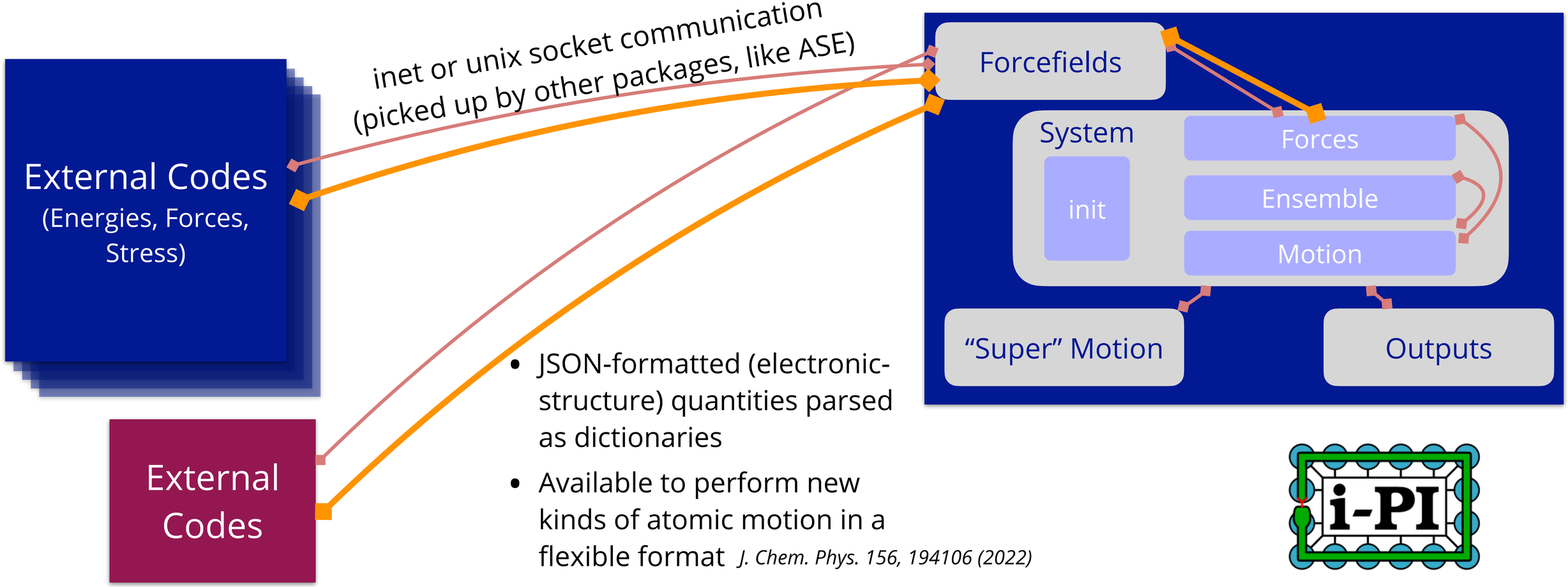

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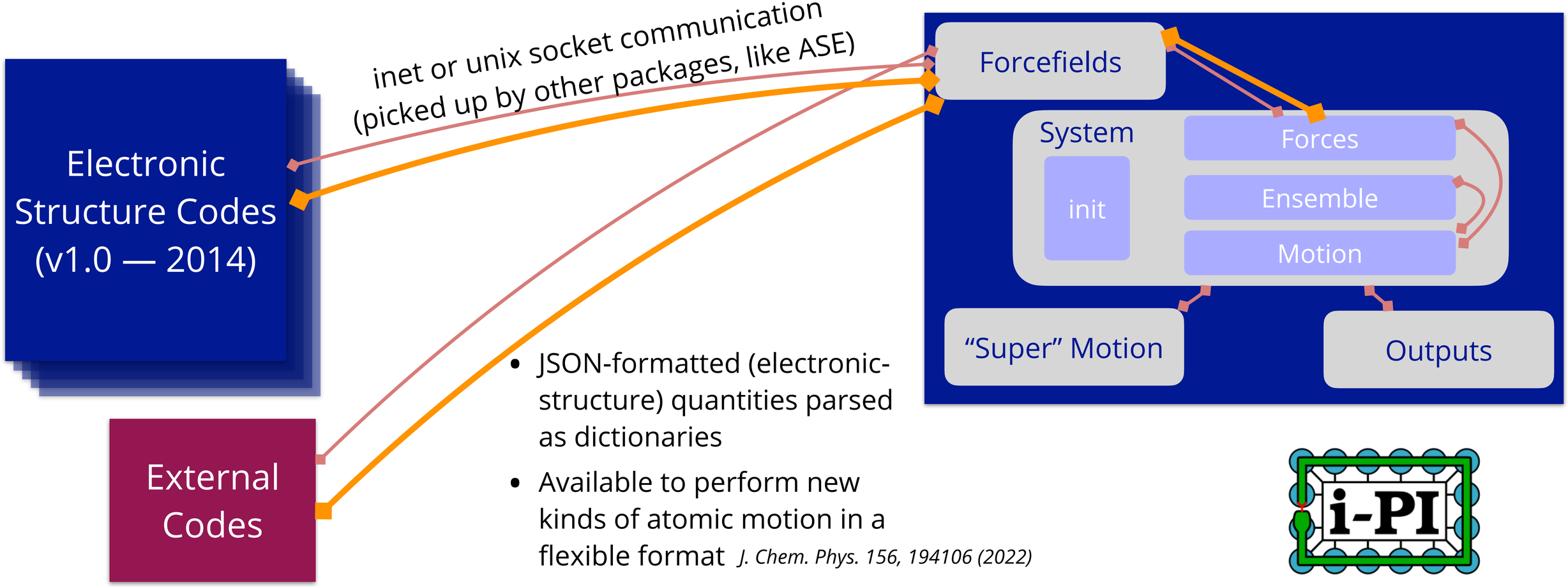

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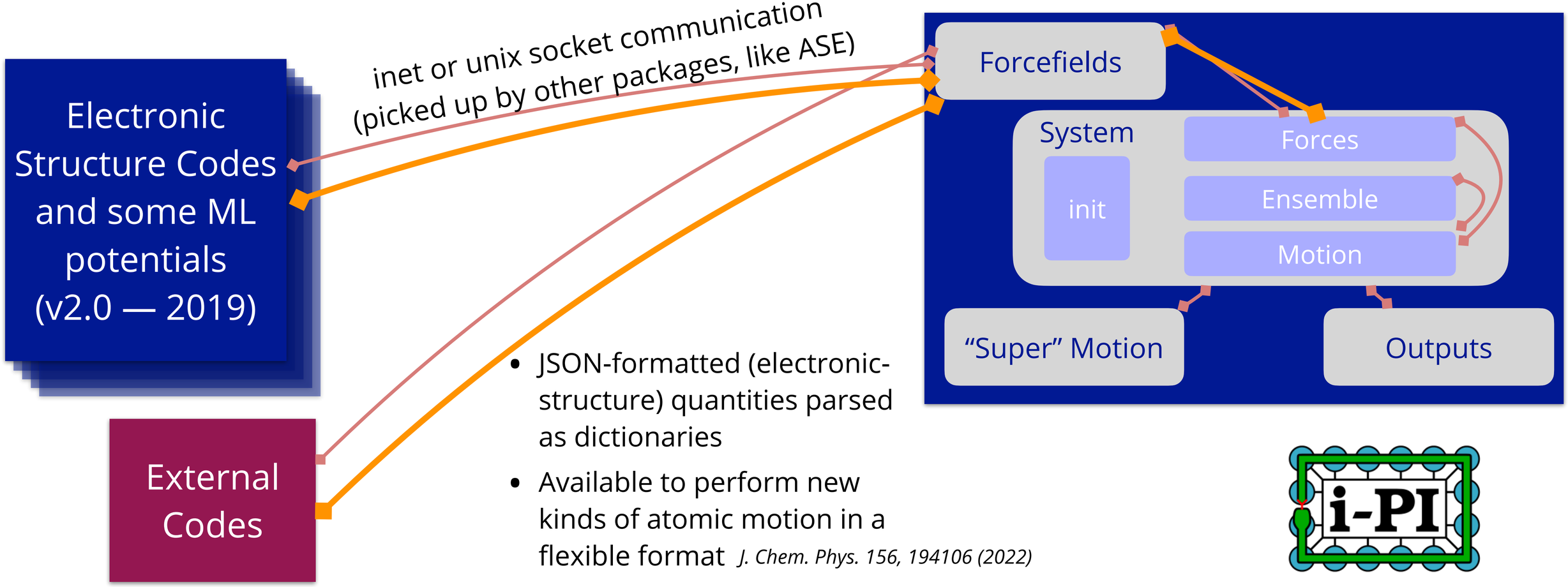

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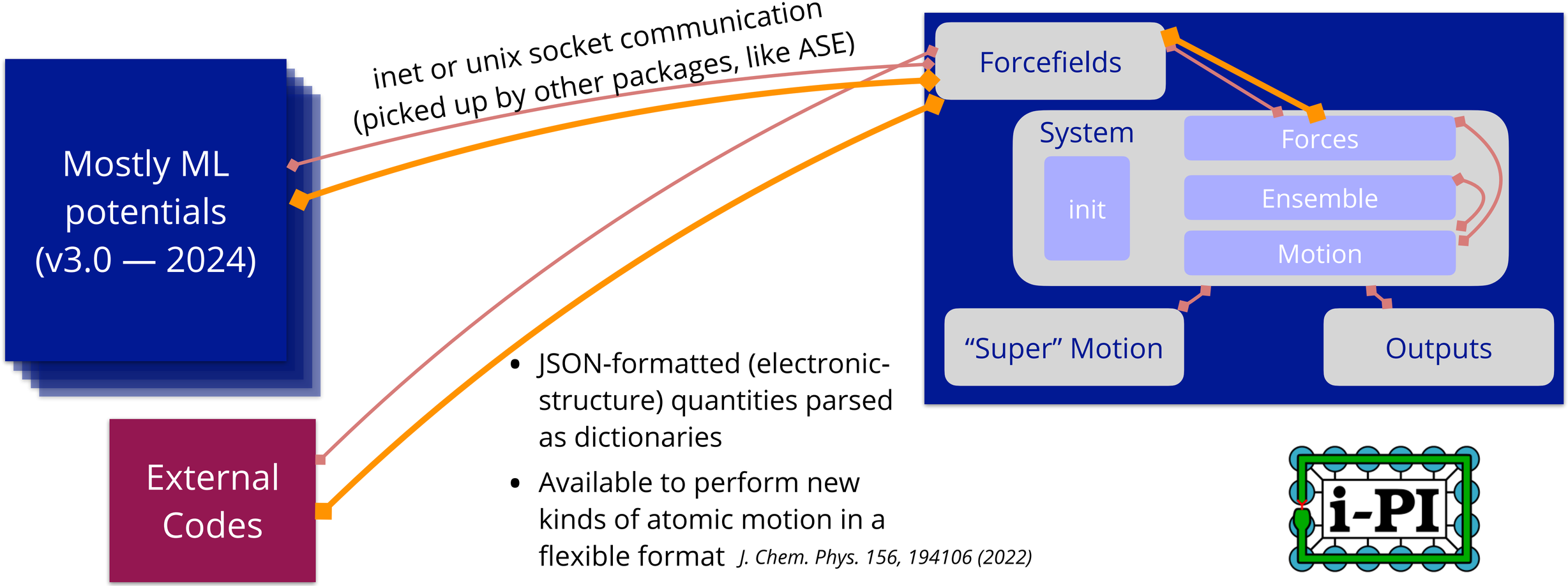

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Some Basics of Working with i-PI

- Installation:

```
pip install i-pi
```

- Let’s see how it connects: