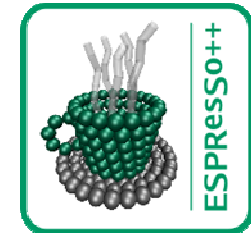
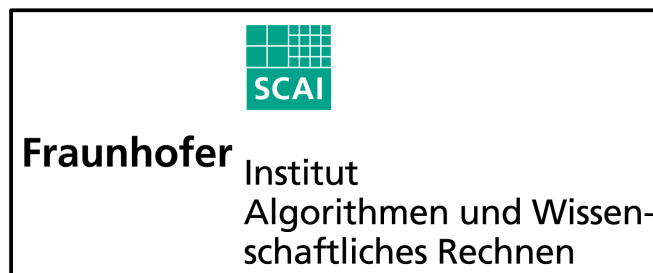

ESPResSo++: A Python-controlled, Parallel Simulation Software for Soft Matter Research



Axel Arnold
Thomas Brandes
Dirk Reith
Anton Schüller



Jonathan Halverson
Olaf Lenz
Torsten Stühn



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Molecular Dynamics (MD) Simulations

- **Modeling of systems with a large amount of particles: atoms, molecules or compounds thereof**
- **Computation of interactions between particles semi-empirically by force fields**
- **Representation over a short time scale (pico seconds)**
- **Statistical analysis of observables (macroscopic behavior)**



Focus of ESPResSo++

- **Physico-chemical molecular dynamics simulation of soft matter systems**
 - **Polymers**
 - **Liquid crystals**
 - **Colloidal suspensions**
 - **Bio-systems (e.g. bio-membranes)**
- **Too large to be simulated by classical all-atom molecular dynamics software (e.g. NAMD, GROMACS)**
- **“Coarse-grained” models reduce the number of degrees of freedom**
- **Great variability of methods**



Goals of ESPResSo++

- Development of **THE** reference software for coarse-grained many-particle simulations
- Research platform for new methods and models
 - Simple integration of new methods
 - Flexible combination of methods
- Production system
 - Parallelized, optimized core
 - Portable between workstations, clusters and HPC
- Implements modern methods: LB, AdResS, P3M, ...



Script Language + Extensibility



Script

Kernel

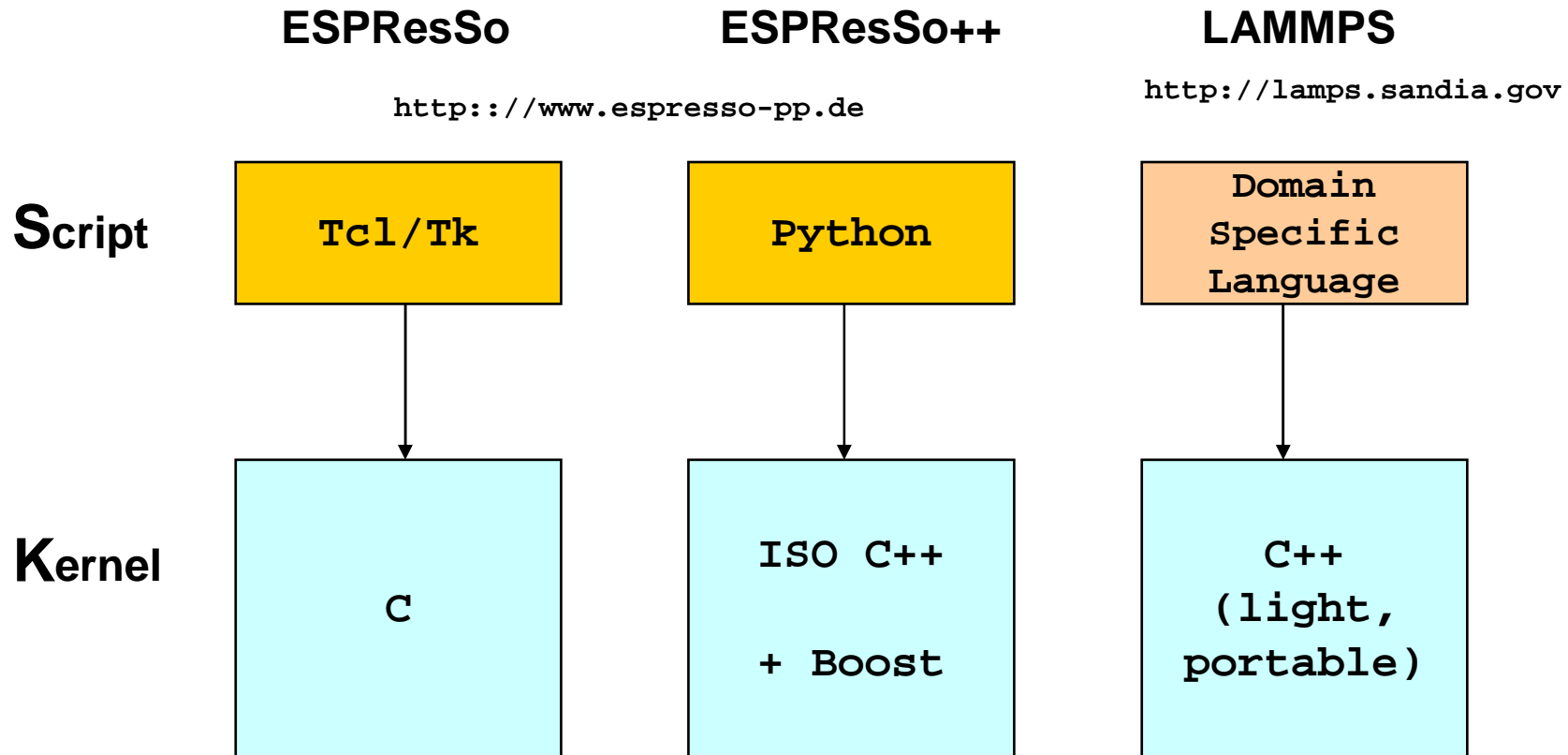
e.g.:
ESPResSo
ESPResSo++
LAMMPS
...



e.g.: NAMD, GROMACS



Programming Languages



Advantages of a Script Language / Python

- Variables
- Control structures
- Functions
- Combination with other functionality
 - E.g. Input / Output, GUI elements

Python is currently the most powerful script language

- Use of other modules: logging, matplotlib, numpy, scipy
- Derived classes for additional features
- Prototyping of new methods
- Support for parallel programming (MPI)



More about ESPResSo++

<http://www.espresso-pp.de>

**Parallel Method Invocation (PMI):
Lightning Talk of Olaf Lenz**

Thank you for your attention!

