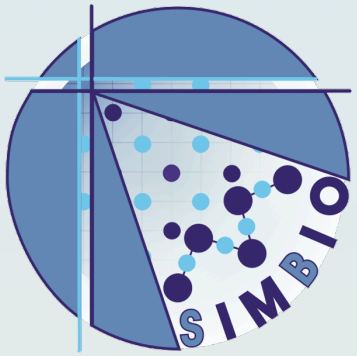



COMPUTATIONAL & THEORETICAL
SOFT MATTER and BIOPHYSICS

# ESPResSo

## Extensible Simulation Package for Research on Soft Matter

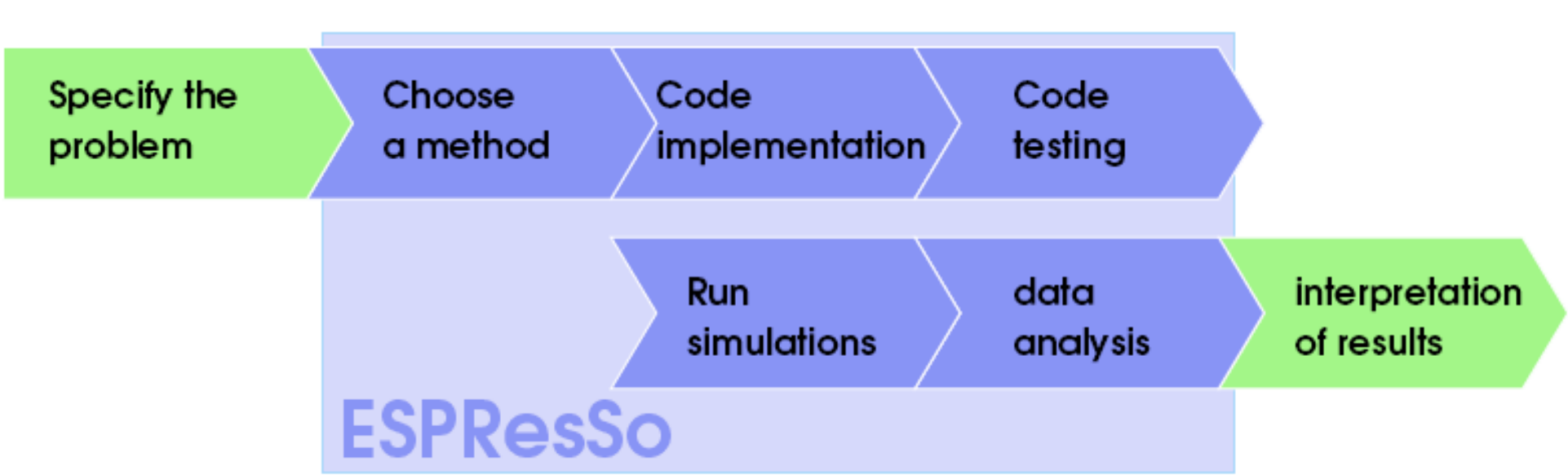
# Disclaimer

- Overview about the ESPResSo
- ESPResSo is under constant development
- I am mainly an ESPResSo user!
- Ask anytime if you want to know more!

# Outline

- Philosophy
- Design
- Methods
- Applications

# Computer simulations

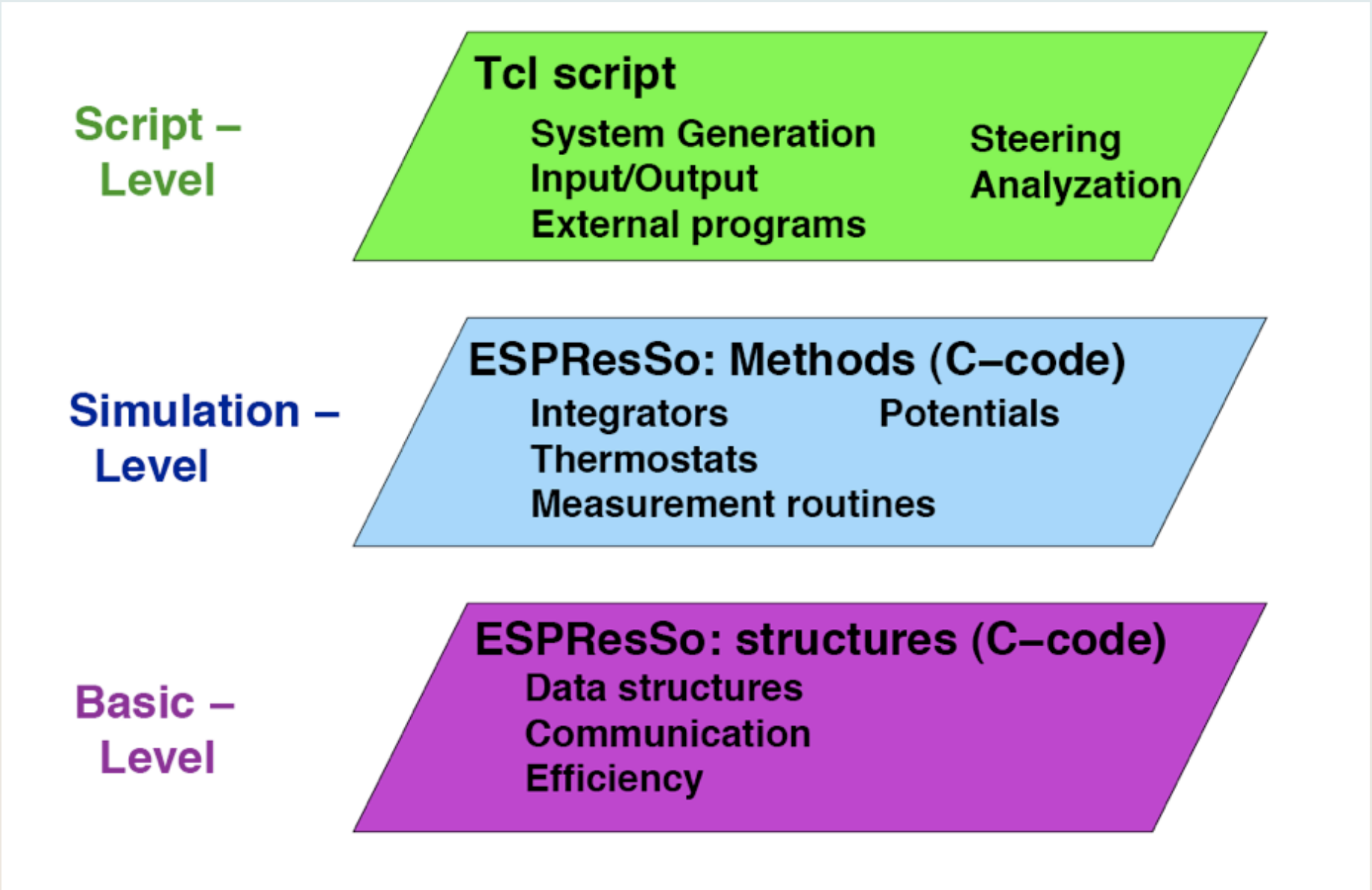



- ESPResSo is a simulation package for coarse-grained MD simulations
- strong on algorithms for long range interactions

# Design goals

- **Extensibility:** Easy implementation of new interactions and algorithms via simple interfaces
- **Flexibility:** Generality of implemented methods, simulation control via Tcl-script
- **Correctness:** Test suite checks numerical and physical correctness
- **Readability:** Beginners can start coding easily
- **Efficiency:** Usage of modern algorithms, such as P3M, ELC, LB and efficient MPI parallelization

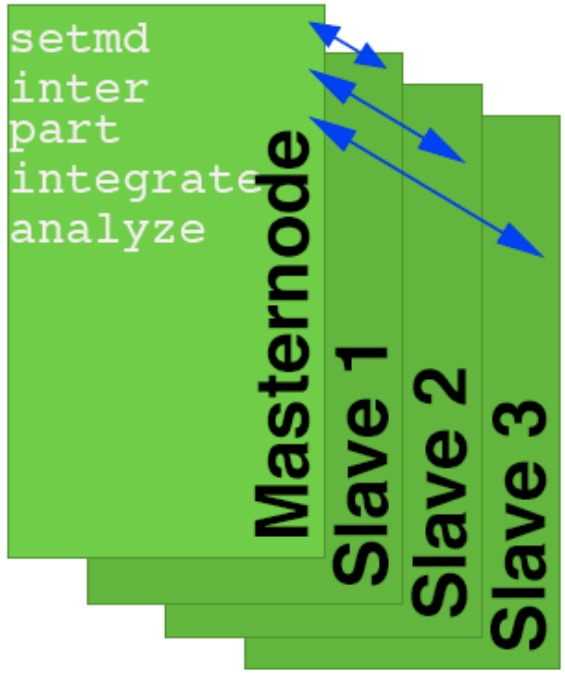
# Design


Script – Level
Tcl script
System Generation
Input/Output
External programs
Steering
Analyzation
Simulation – Level
ESPResSo: Methods (C–code)
Integrators
Potentials
Thermostats
Measurement routines
Basic – Level
ESPResSo: structures (C–code)
Data structures
Communication
Efficiency

# Design

- Tcl-Script
  - sets up particles and interactions
  - controls the simulation flow and the data analysis
- C-Simulation core
  - efficient data storage for particles and interactions
  - parallel MD integrators
  - analysis procedures

```
set box_length 10.7437
set density 0.7

setmd time_step 0.01
setmd skin      0.4
setmd box_l $box_length $box_length $box_length

set volume [expr $box_length*$box_length*$box_length]
set n_part [expr floor($volume*$density)]
for {set i 0} { $i< $n_part} {incr i} {
    part $i pos [expr $box_length*[t_random]] \
                        [expr $box_length*[t_random]] \
                        [expr $box_length*[t_random]] type 0
}

inter 0 0 lennard-jones 1 1 1.22 0.25 0
inter ljforcecap 20

thermostat langevin 1 1

for {set i 0} {$i < 1000} {incr i} {
    puts "step $i ftime=[setmd time] energy=[analyze energy total]"
    puts "temp = [expr [analyze energy kinetic]/(1.5*[setmd n_part])]"
    integrate 1000
}
```



# Advantages of the script interface

- easy and very robust implementation of complex simulation setups
- simulation procedure easily and quickly modifiable
- many advanced simulation schemes can be implemented in Tcl
- quick implementation and testing of specialized analysis methods
- full control at anytime during the simulation

# Basic features

- Integrators
  - Velocity–Verlet integration scheme (NVE ensemble)
  - Langevin or DPD thermostats (NVT ensemble)
  - constant pressure (NPT) integrator
- Cellsystems / particle organization
  - domain decomposition with or without Verlet–lists
  - atom decomposition ($O(N^2)$ interaction loop)
  - algorithm dependent specializations
- Analysis
  - Fundamental observables: force, energy and pressure
  - radius of gyration, center of mass
  - structure factors, distribution functions

# Interactions

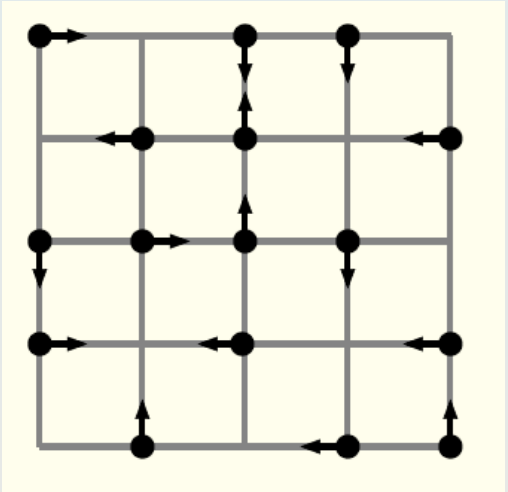
- Nonbonded interactions
  - generalized Lennard–Jones
  - Gay–Bernes
  - tabulated interactions
- Bonded interactions
  - FENE and harmonic pair bonds
  - angle and dihedral many body bonds
  - tabulated many body bonds
  - Constrained bonds using RATTLE
- Hydrodynamic interactions
  - Lattice-Boltzmann, DPD
- Electrostatic interactions

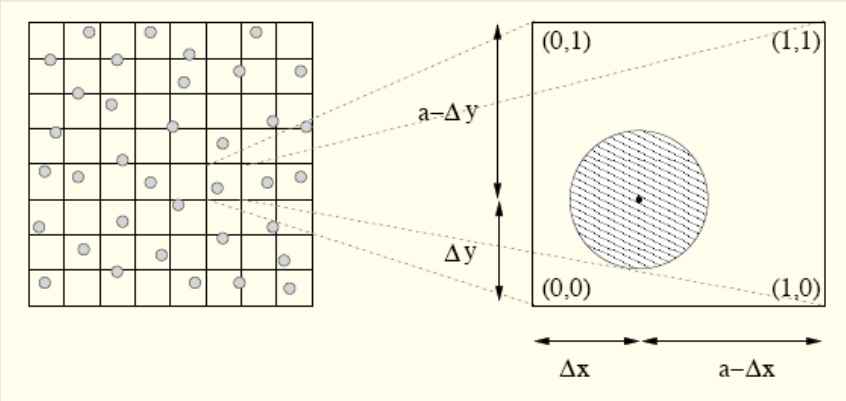
# Electrostatics

- Standard algorithms:
  - Coulomb: cut-off, (direct sum), Ewald
  - Debye-Hückel
- 3D periodic systems
  - P3M: Ewald sum with mesh–based Fourier space part
  - MEMD (Maggswell Equation MD): Maxwell equations solved on a lattice
- 2D+h periodic systems
  - MMM2D: non-Ewald method
  - ELC (Electrostatic Layer Correction): P3M + correction term
  - Treatment of dielectric discontinuities at interfaces
- 1D+2h periodic systems
  - MMM1D

# Hydrodynamics

- solving Boltzmann equation on a lattice
  - streaming and collision
  - discrete set of velocity populations
  - hydrodynamic fields from populations
- Frictional coupling of MD particles to LB fluid
  - Stokesian drag
  - momentum transfer (total momentum conserved



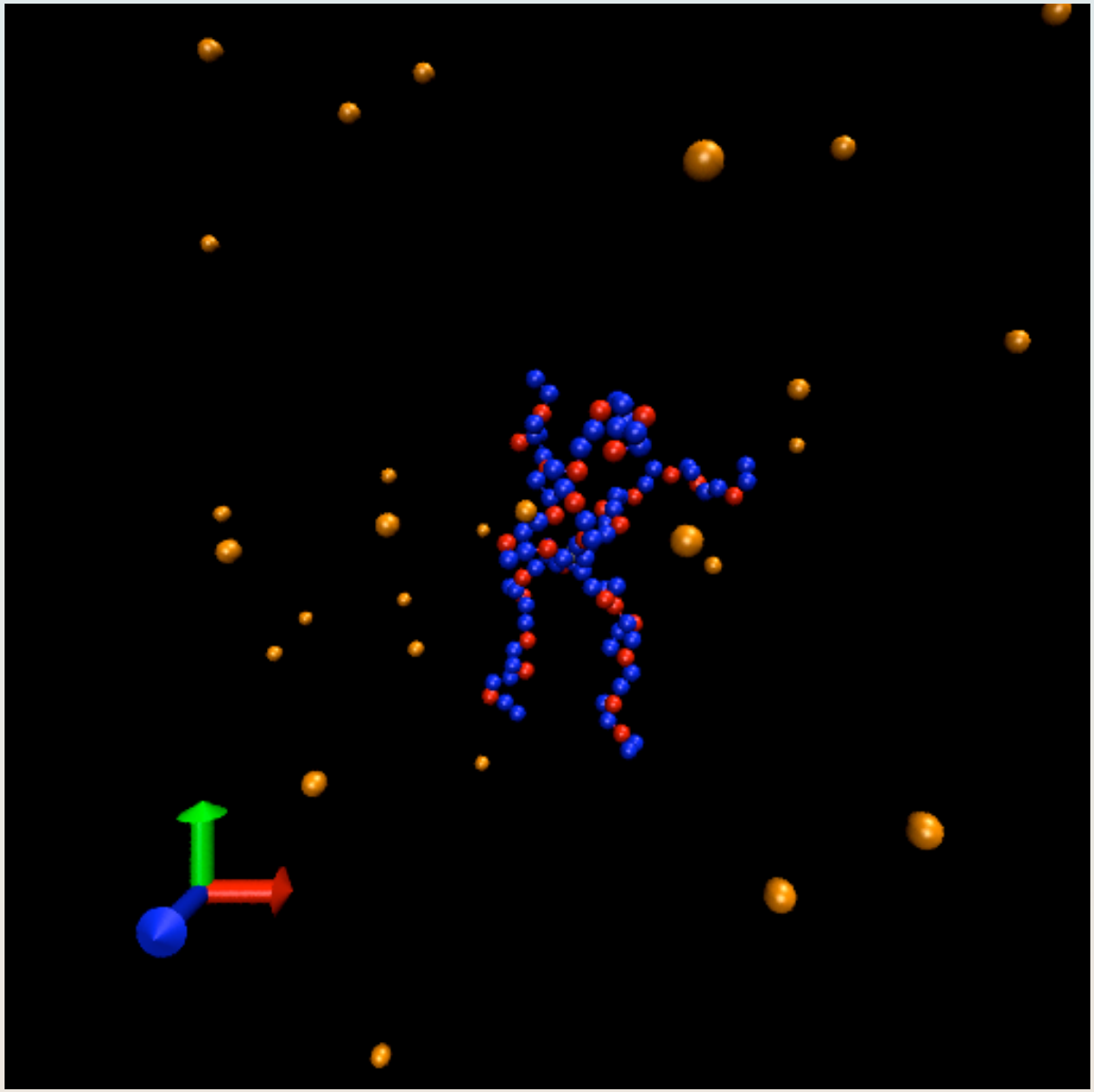



$$\mathbf{F} = -\zeta\left[\mathbf{V} - \mathbf{u}(\mathbf{R}, t)\right]$$

# Advanced features

- Interactive MD
- Graphical user interface supplied by TK/TCL interface
- (Online) Visualization using VMD

# ESPResSo in action



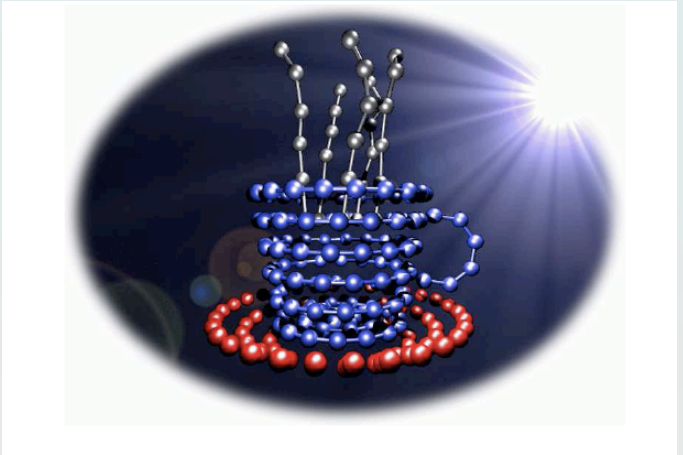
# ESPResSo in a nutshell

- Flexible and extensible simulation tool for particle models
- State–of–the–art algorithms
- easy to use
- easy to extend and to adapt
- efficiently parallelized
- many supported platforms

# Further info

- http://www.espresso.mpg.de/
- ESPResSo User Guide
- Tutorial - Q&A
- Email: espresso@fias.uni-frankfurt.de
- H.-J. Limbach, A.Arnold, B.A. Mann and C. Holm, in Comp. Phys. Comm. (2006), Volume 174, Issue 9, Pages 704-727.

# Credits



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- Additional ESPResSo developers:
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# Thank you!