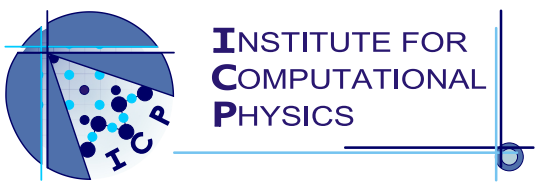
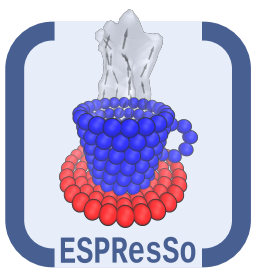
Managing sustainable and community-driven research software in physics

Jean-Noël Grad, Alexander Reinauer,
Rudolf Weeber, Christian Holm

Institute for Computational Physics, University of Stuttgart

September 15, 2022

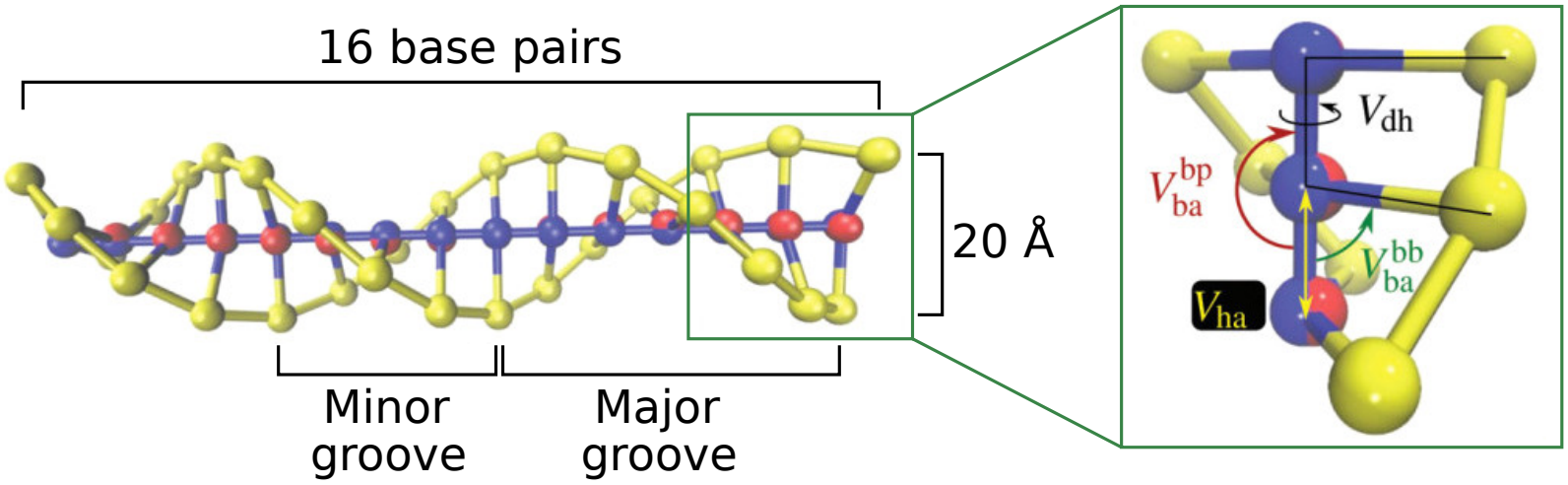




Funded by
DFG Deutsche Forschungsgemeinschaft
German Research Foundation

Particle-based simulations with coarse-grained models

- ESPResSo represents collections of atoms as single beads
- suitable for systems in which chemical detail can be ignored

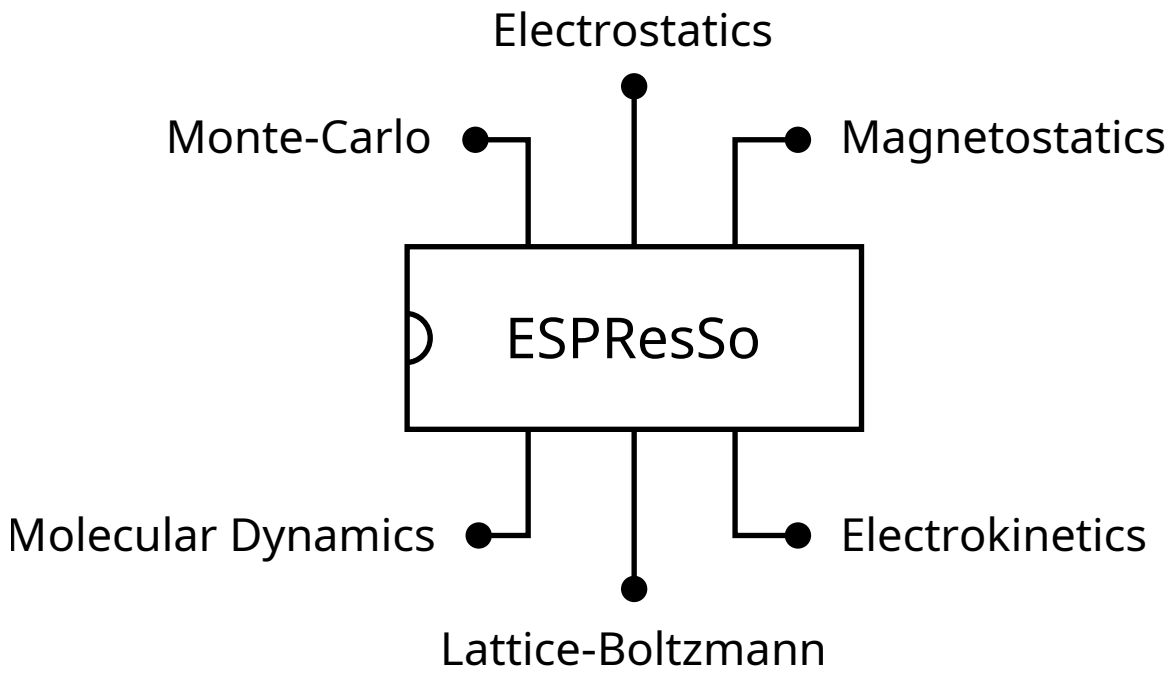


Computational fluid dynamics with lattice-Boltzmann

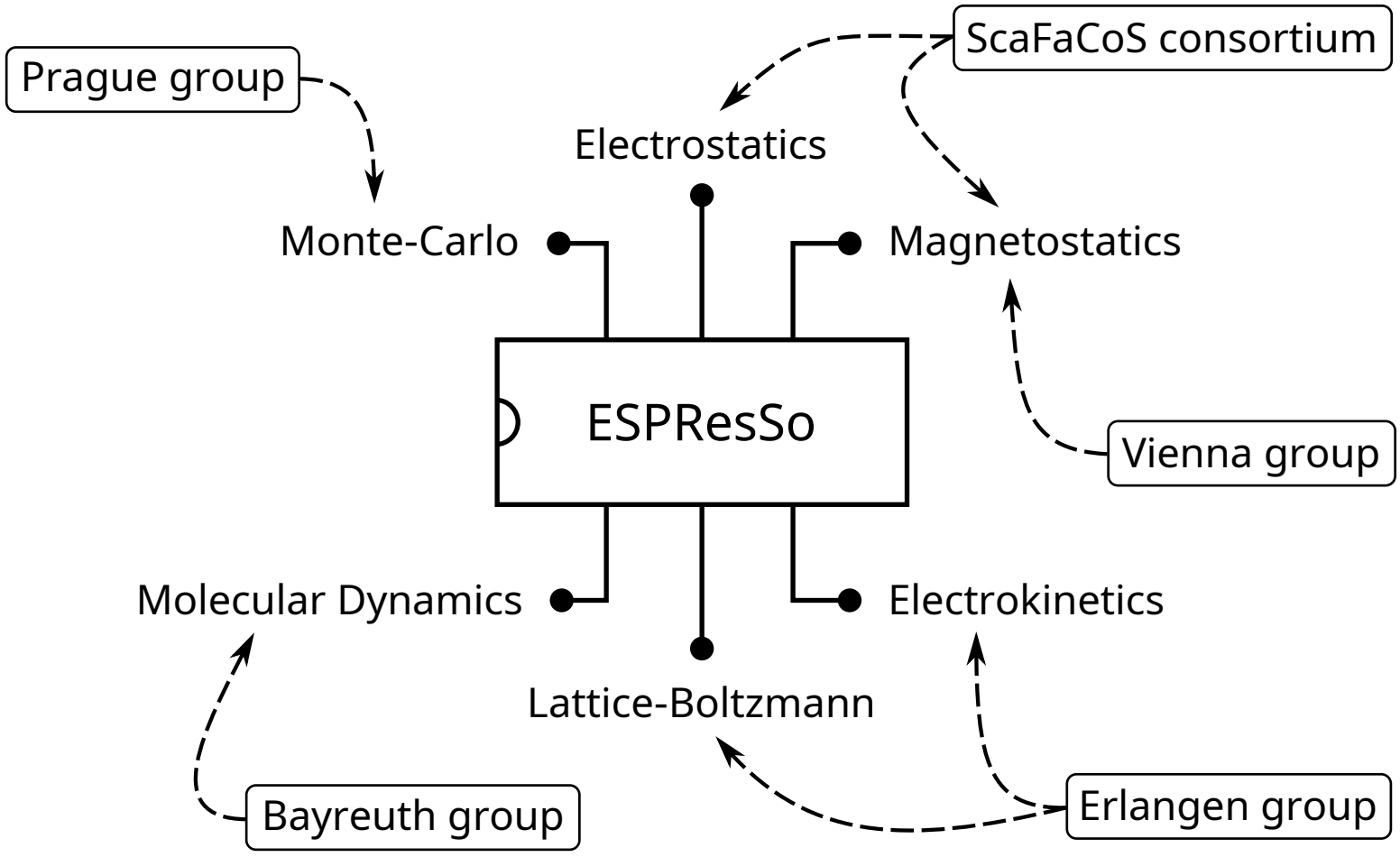
- established method to solve Navier–Stokes equations
- ESPResSo introduces coupling to particles
- advanced lattice-Boltzmann features:
  - diffusion-advection-reaction models
  - multiphase flow

(G. Rempfer, C. Holm; ink droplet in a carrier fluid moving around a solid obstacle)

Community-driven code development



Community-driven code development



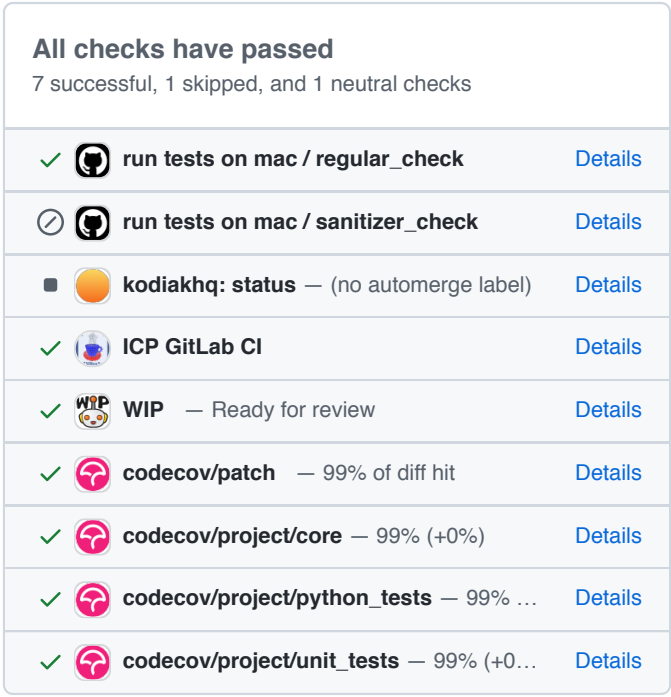
Development processes

Test-driven development

- new feature → write test on day 1
- enforced by continuous integration
  - tests on macOS, Ubuntu, Fedora
  - 99% code coverage is required
- merging is blocked if CI fails

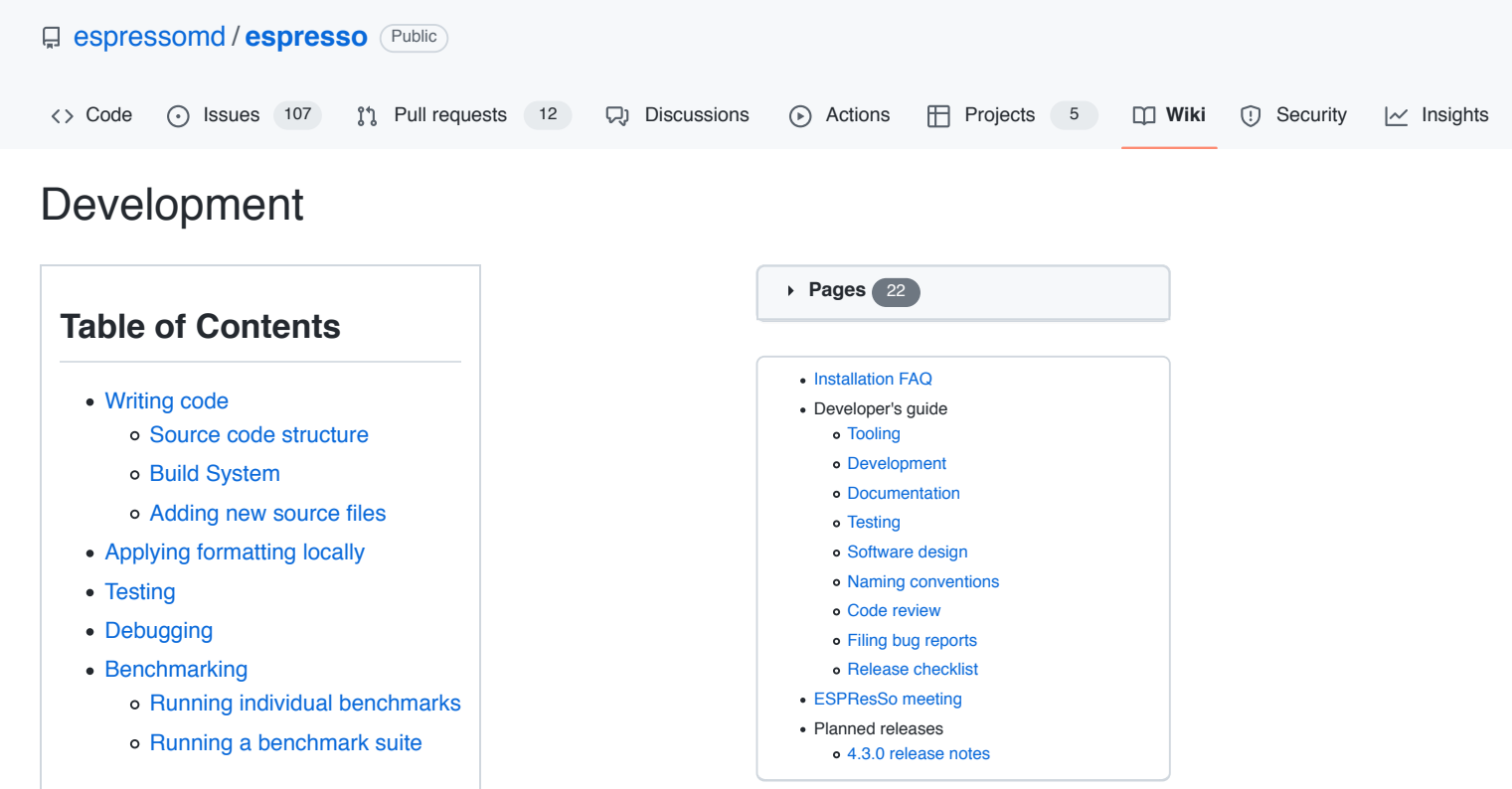
Documentation-driven development

- Doxygen, Sphinx, Jupyter notebooks
- documentation is tested in CI. . .
- . . . and automatically deployed online



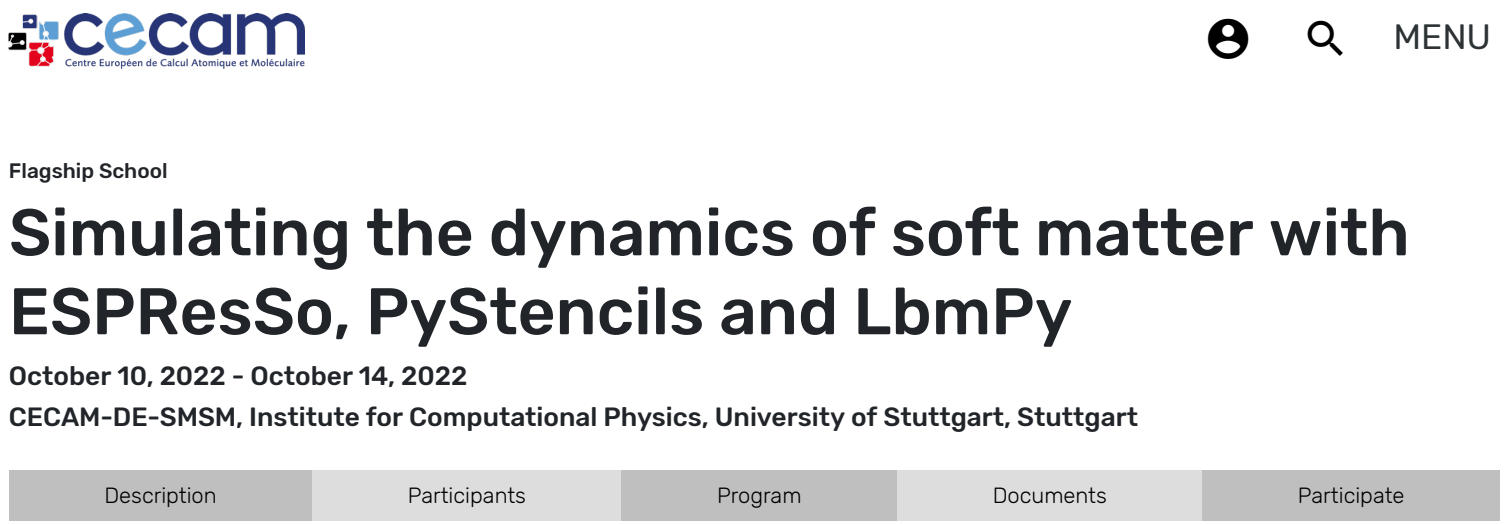
Onboarding

- wiki: good coding practices, tooling, processes
- online coding days every 3 months
  - pair programming and mentoring
  - collaboration with external contributors



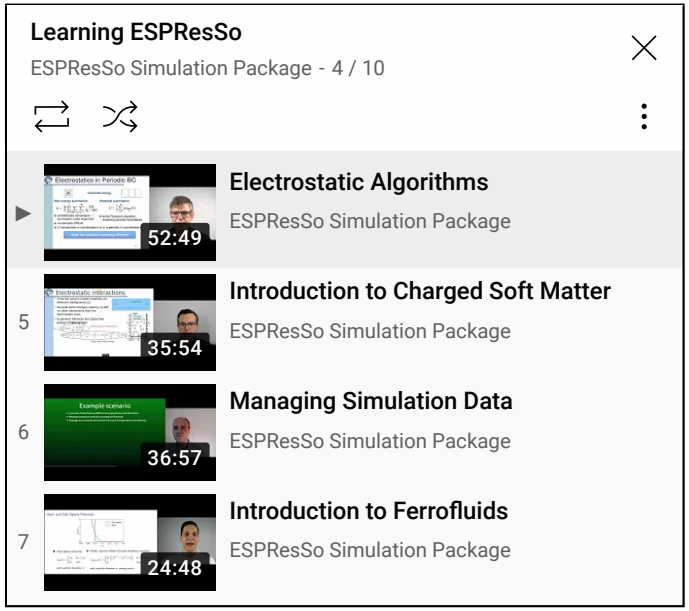
Outreach

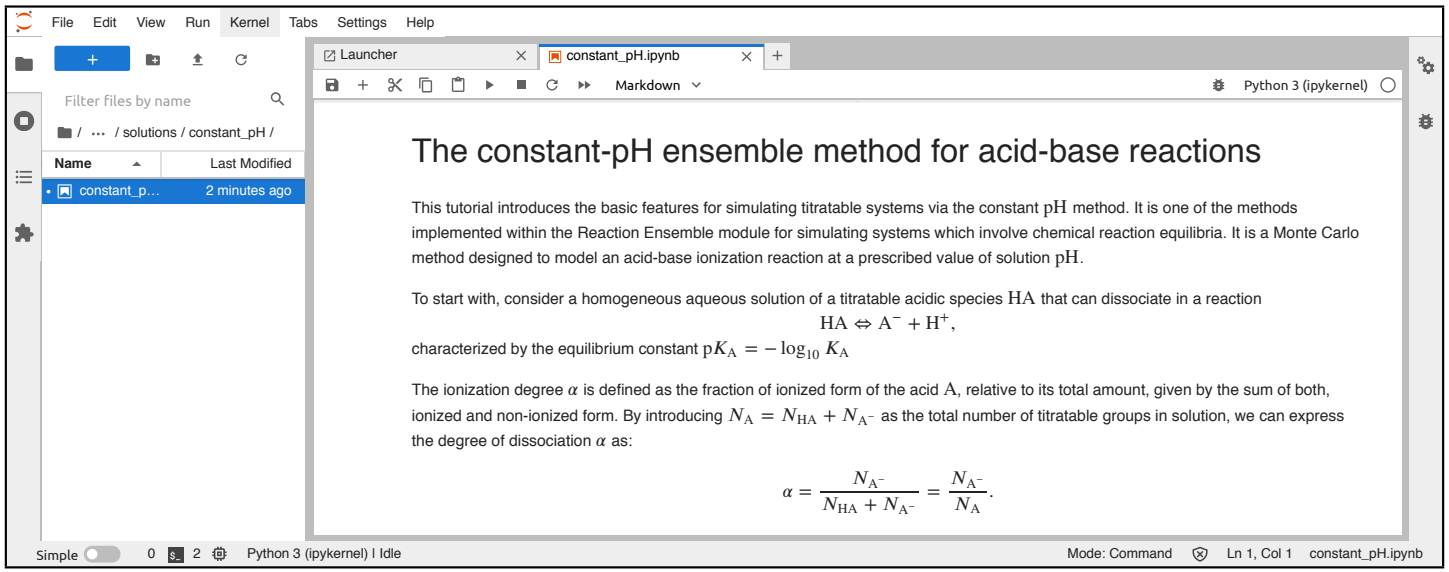
- annual 5-day CECAM school in October
  - train the next generation of contributors
  - discover ongoing projects in the community
- GitHub discussions, mailing list, community calls
- public notes from developer meetings



Dissemination

- packaging on Fedora, Ubuntu
- Singularity for HPC (planned)
- build environment on Gitpod
- run in the browser with Binder
- remotely executable teaching material, lectures on YouTube





Acknowledgments

- ESPResSo core team: A. Reinauer, R. Weeber, F. Weik, K. Szuttor
- Collaborators: S. Bindgen, P. M. Blanco, M. Holzer, D. Mostarac
- Funding: DFG Research Software Sustainability grant 391126171

- Gitpod integration: J. Scheunemann
- Jupyter consulting: A. Seeland
- Fedora packaging: C. Junghans