Pathway to exascale: experiences in adopting more scalable algorithms in ESPResSo

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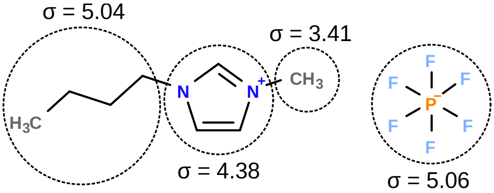
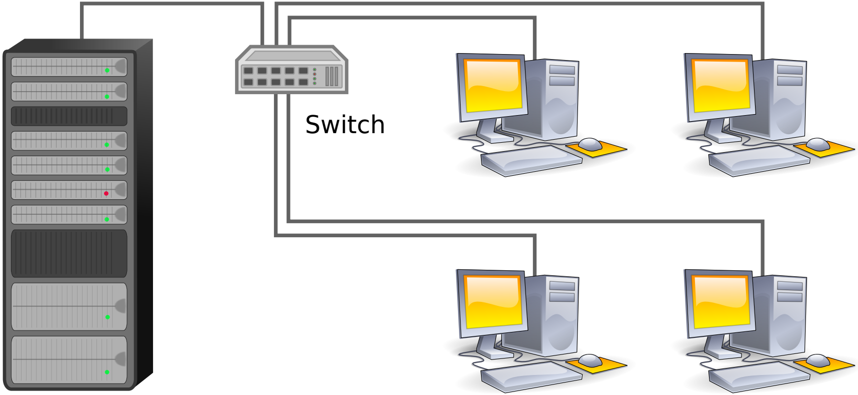
Multiscale modeling



(coarse-grained model of a ionic liquid)

(ink droplet injected in a nanopore filled with fluid)

High-throughput computing



Storage server

Switch

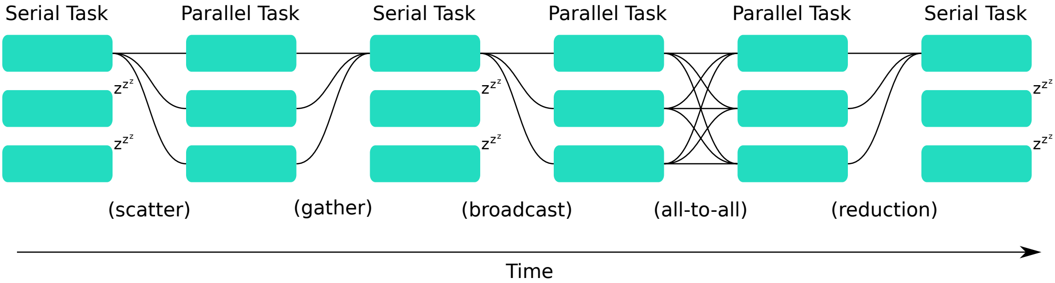
Coworker's workstations

Image credits: AJ, *Computer*, 2008; cyberscooty, *Switch-Hub*, 2012; Moini, *Server rack*, 2011; CC0, via Open Clipart.

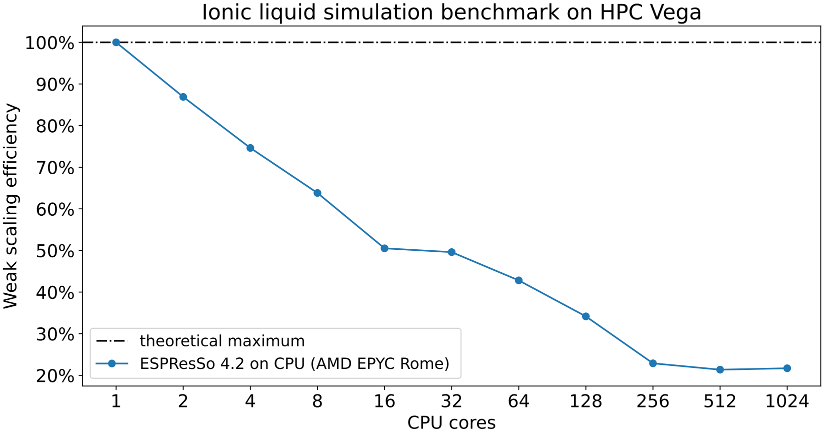
High-performance computing

Image credit: Erik And30, *Berzelius supercomputer LiU*, 2022, CC BY-SA 4.0, via Wikimedia Commons.

Communication patterns in ESPResSo

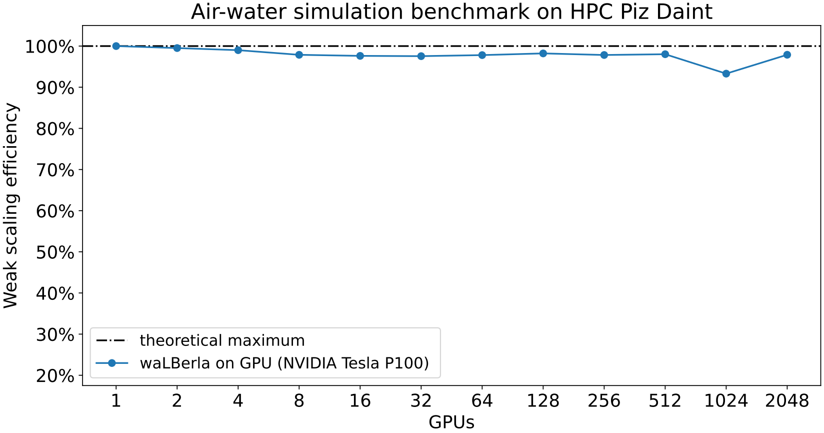


Benchmarking particle-based simulations



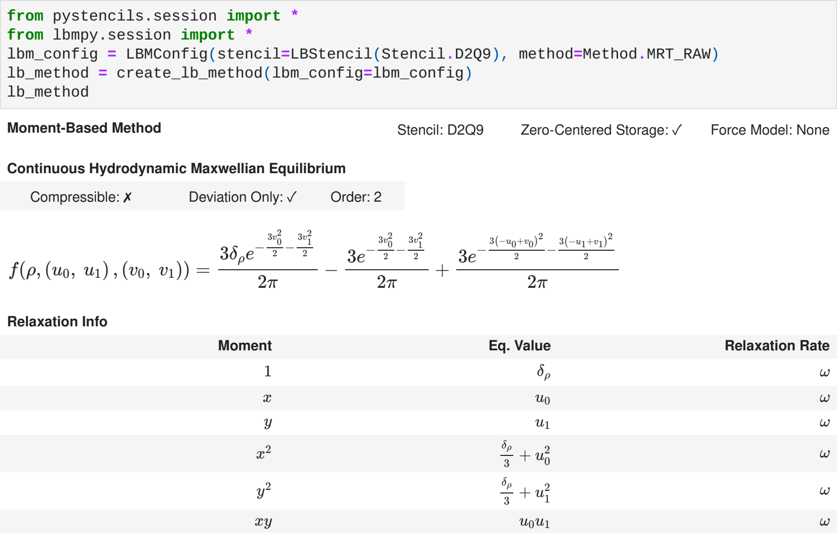
Grad, Weeber, *Report on the current scalability of ESPResSo and the planned work to extend it*, MultiXscale Deliverable 2.1, Zenodo, 2023, doi:10.5281/zenodo.8420222

Benchmarking grid-based simulations



Holzer, Bauer, Köstler, Rüde, *The International Journal of High Performance Computing Applications* 35(4):413, 2021, doi:10.1177/10943420211016525

Rapid prototyping in Jupyter Notebooks: automatic code generation



```
from pystencils.session import *
from lbmpy.session import *
lbm_config = LBMConfig(stencil=LBStencil(Stencil.D2Q9), method=Method.MRT_RAW)
lb_method = create_lb_method(lbm_config=lbm_config)
lb_method
```

Moment-Based Method Stencil: D2Q9 Zero-Centered Storage: ✓ Force Model: None

Continuous Hydrodynamic Maxwellian Equilibrium

Compressible: ✗ Deviation Only: ✓ Order: 2

$$f\left(\rho, \left(u_0,\ u_1\right), \left(v_0,\ v_1\right)\right) = \frac{3\delta_\rho e^{-\frac{3v_0^2}{2} - \frac{3v_1^2}{2}}}{2\pi} - \frac{3e^{-\frac{3v_0^2}{2} - \frac{3v_1^2}{2}}}{2\pi} + \frac{3e^{-\frac{3\left(-u_0+v_0\right)^2}{2} - \frac{3\left(-u_1+v_1\right)^2}{2}}}{2\pi}$$

Relaxation Info

Moment	Eq. Value	Relaxation Rate
1	δ_ρ	ω
x	u_0	ω
y	u_1	ω
x^2	$\frac{\delta_\rho}{3} + u_0^2$	ω
y^2	$\frac{\delta_\rho}{3} + u_1^2$	ω
xy	$u_0 u_1$	ω

Access scientific software anywhere with EESSI

```
jobs:
  ubuntu:
    runs-on: ubuntu-latest
    steps:
      - name: Setup EESSI
        uses: eessi/github-action-eessi@v3
        with:
          eessi_stack_version: "2023.06"
      - name: Checkout repository
        uses: actions/checkout@main
      - name: Run testsuite
        run: |
          module load ESPResSo/4.2.1-foss-2023a
          python3 -m venv --system-site-packages venv
          source venv/bin/activate
          python3 -m pip install -r requirements.txt
          make testsuite
          deactivate
```

EESSI

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

Acknowledgments

Links to projects:

- MultiXscale: www.multixscale.eu
- EESSI: www.eessi-hpc.org
- ESPResSo: espressomd.org
- waLBerla: walberla.net
- LbmPy: pypi.org/project/lbmpy

Social media:

- @MultiXscale / X
- @ICP_Stuttgart / X

YouTube:

- @MultiXscale
- @espressosimulationpackage7832

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