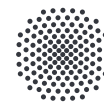# Load-Balanced, Large-Scale Soot Particle Agglomerations

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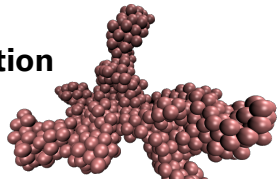Germany
Cluster of Excellence in Data-Integrated Simulation Science
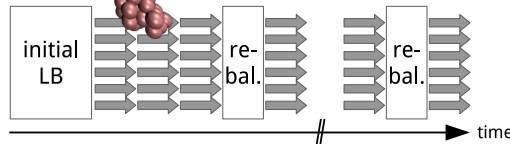Institute for Parallel and Distributed Systems / Scientific Computing

Challenges for Parallelization

- Lagrangian discretization
- Heterogeneity
- Dynamic behavior
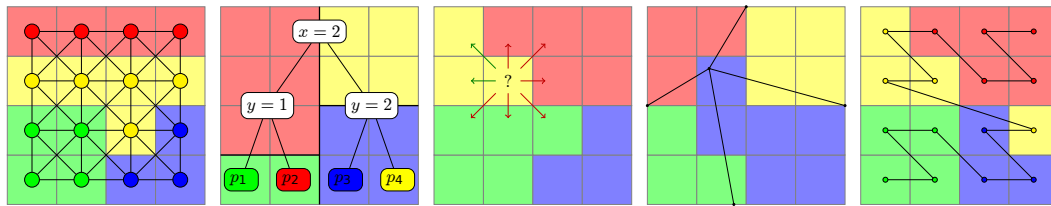- Coupled systems (multi-X)

Goals

- Efficient load-balancing
- Adaptive to dynamics

Methodology

- Method? Weights?
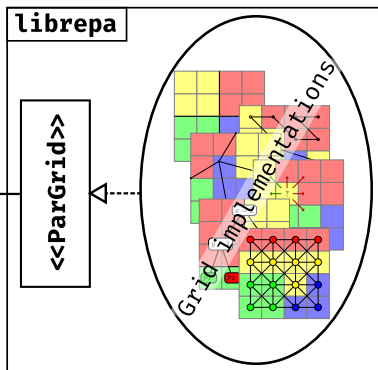- Points in time?

LibRepa

- Application oblivious
- Grid implemtations
- Load-balancing
- Communication hiding

ESPResSo

- Widely used MD package
- New module "Generic-DD"
- Bindings to libRepa
- Minimally invasive

```python
from espressomd.system import System

system = System(box_l=[100., 100., 100.])
dd = s.cell_system.set_new_dd("p4est")
# Setup simulation...

m = Metric("nforcepairs + 2*ndistpairs")

while not done:
    s.integrator.run(1000)
    if m.imbalance() > 1.1:
        dd.repart(m)
```
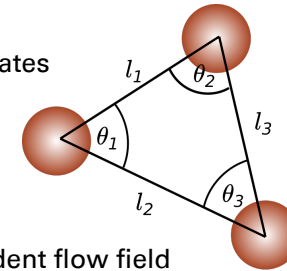
Cooperation with A. Kronenburg, ICT, U. Stuttgart

Soot Particles

- Morphology of aggregates
- Effectivity, toxicity, ...
- Thermal conditions

Model

- Langevin Dynamics
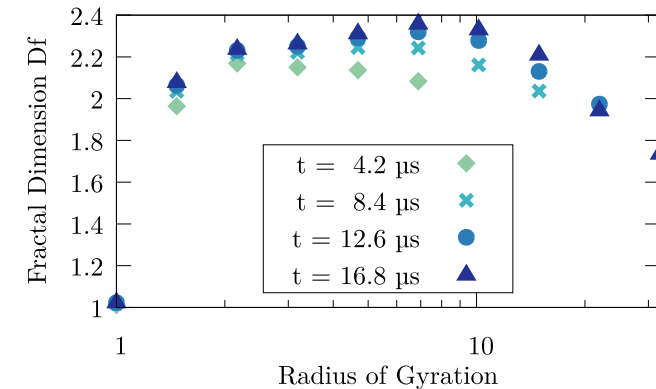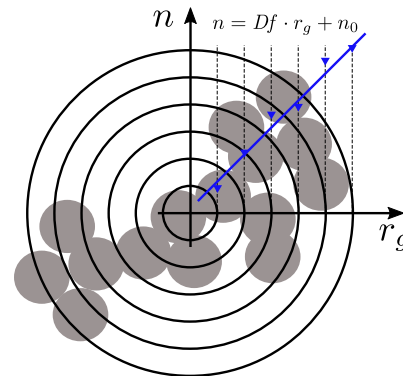- Turbulent, time-dependent flow field
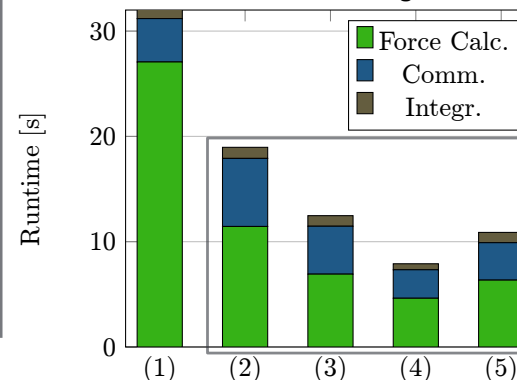- Dynamic bonding

Setup

- 109 mio. particles
- 15 mio. time steps

$$m\ddot{\mathbf{x}} = \mathbf{f} + \gamma(\dot{\mathbf{x}} - \mathbf{u}_{flow}(\mathbf{x})) + \mathbf{R}(t)$$

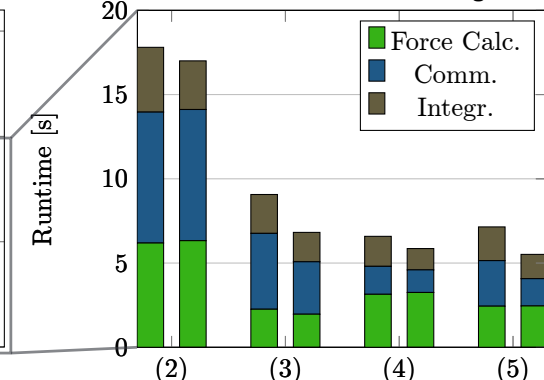$n = Df \cdot r_g + n_0$

SFC, different weights

SFC vs. GP, different weights

Preliminary evaluation for smaller 3.2 mio. particle scenario from [1, 2].

[1] S. Hirschmann et al. Adv. in Par. Comp. 32 (2017) 455–464
[2] S. Hirschmann et al., EPJST 227 (2019) 1779–1788

https://pvs.uni-stuttgart.de

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