University of Warsaw Lagrangian Cloud Model (UWLCM): LES with particle microphysics

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Agenda

1) Model overview
2) Particle microphysics
3) Fractal grid refinement
4) Software design
5) Computational performance

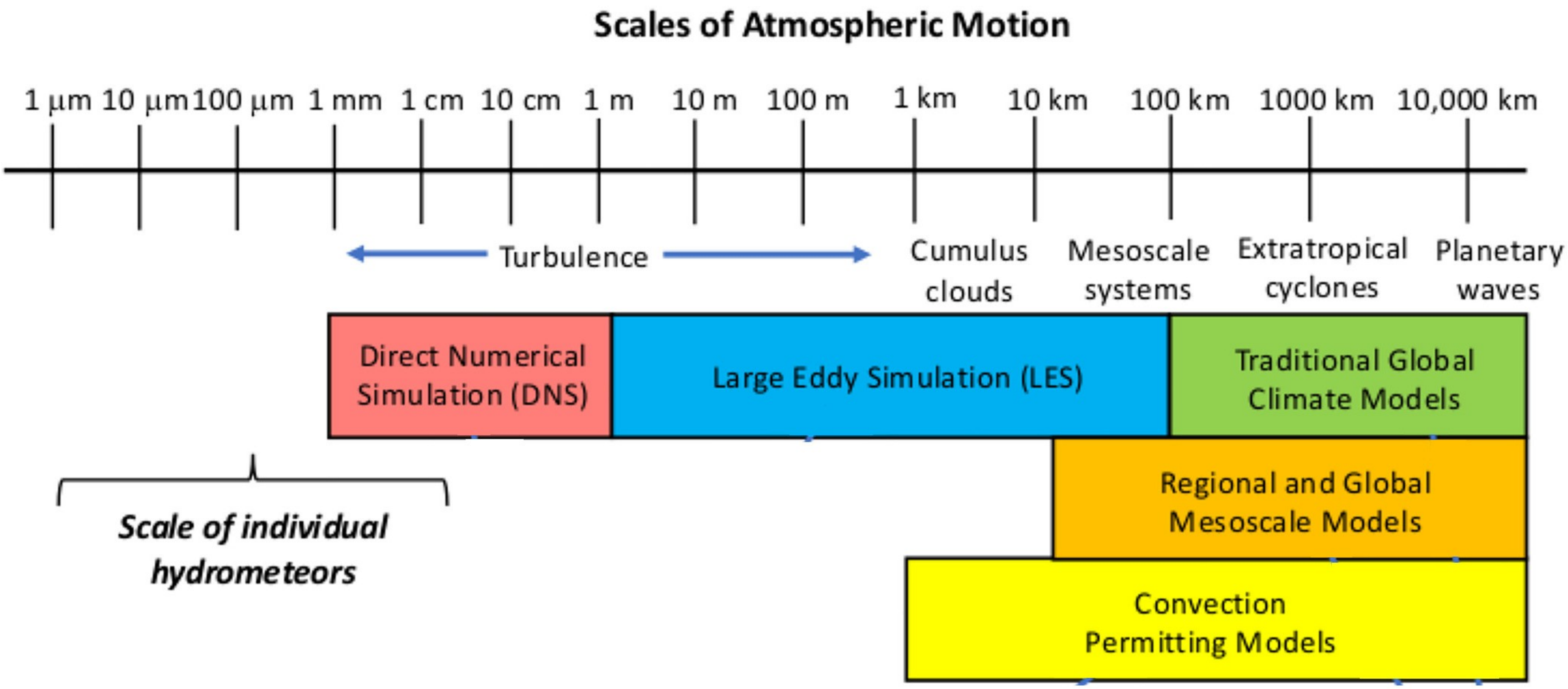
Agenda

1) Model overview

UWLCM basics

- Modeling air flow (2D or 3D):
  - Large eddy simulations: small-scale turbulence is parameterized

LES spatial scale



adapted from Morrison et al. *JAMES* (2020)

UWLCM basics

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- Modeling temperature and water vapor

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  - Bulk microphysics

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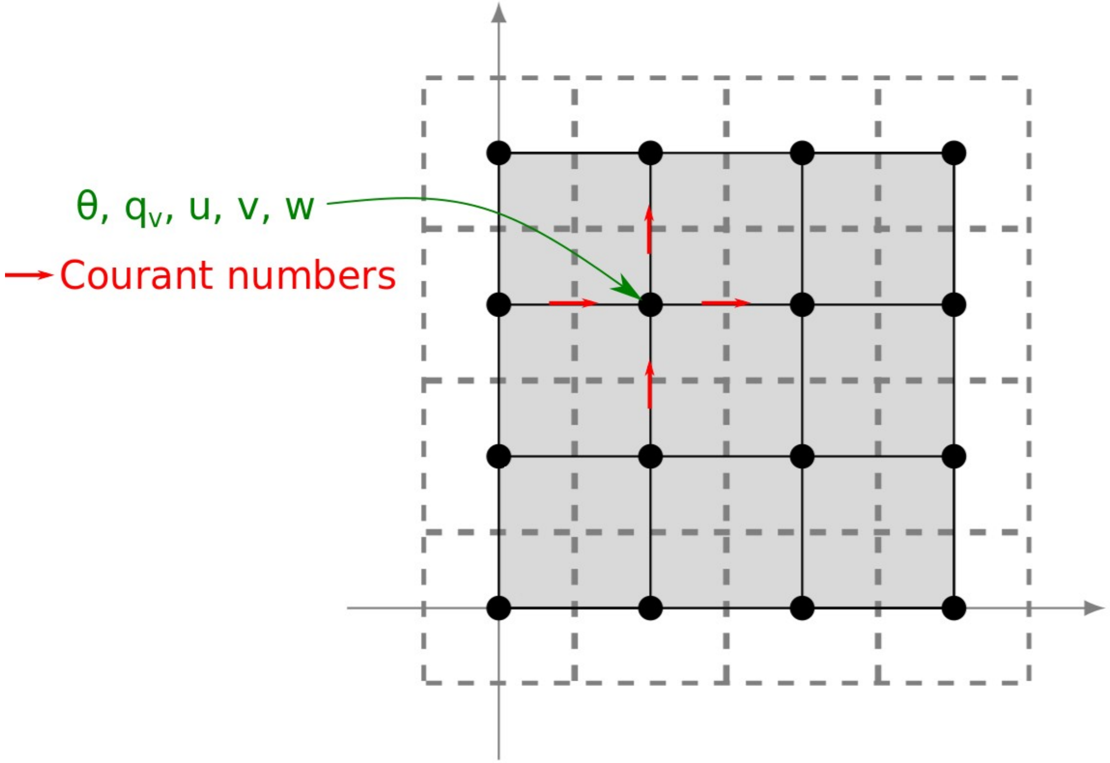
Eulerian

Eulerian variables

- Staggered rectangular grid with stretching
- Governed by anelastic equations
- Solved with MPDATA
- Subgrid-scale models:
  - Smagorinsky
  - Implicit LES



UWLCM basics

- Modeling air flow (2D or 3D):
  - Large eddy simulations: small-scale turbulence is parameterized
- Modeling temperature and water vapor
- Modeling liquid water
  - Bulk microphysics
  - Particle microphysics (super-droplet method)

Eulerian

Lagrangian

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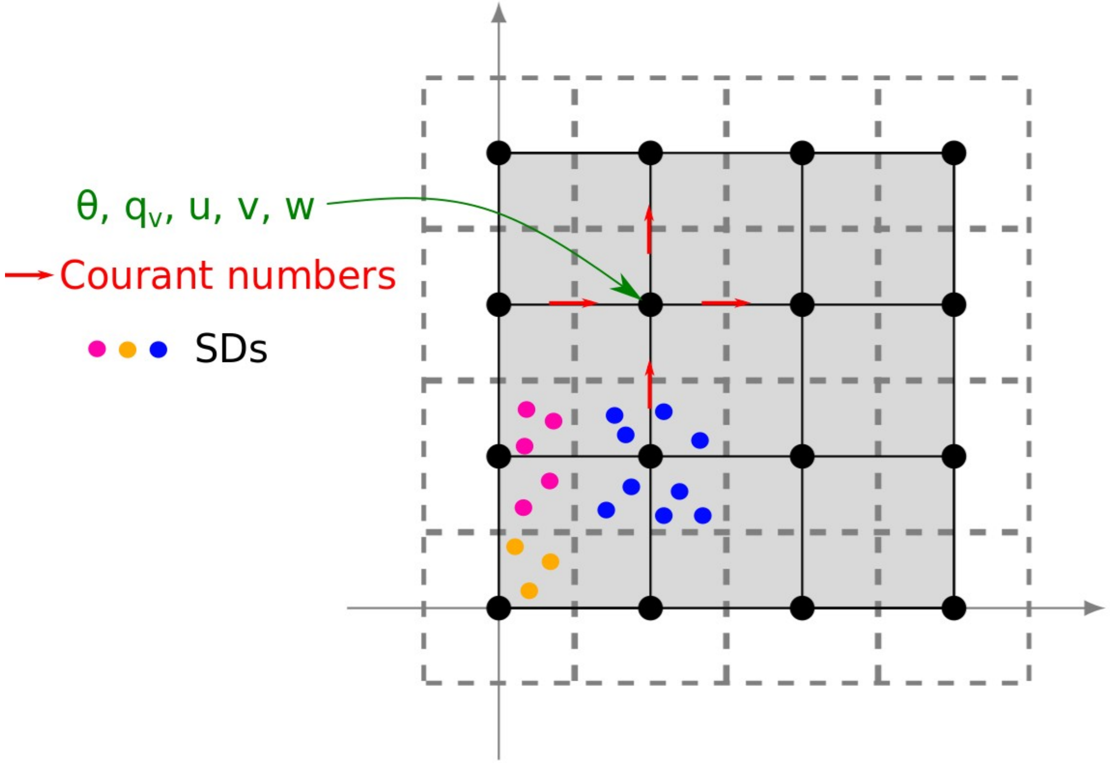
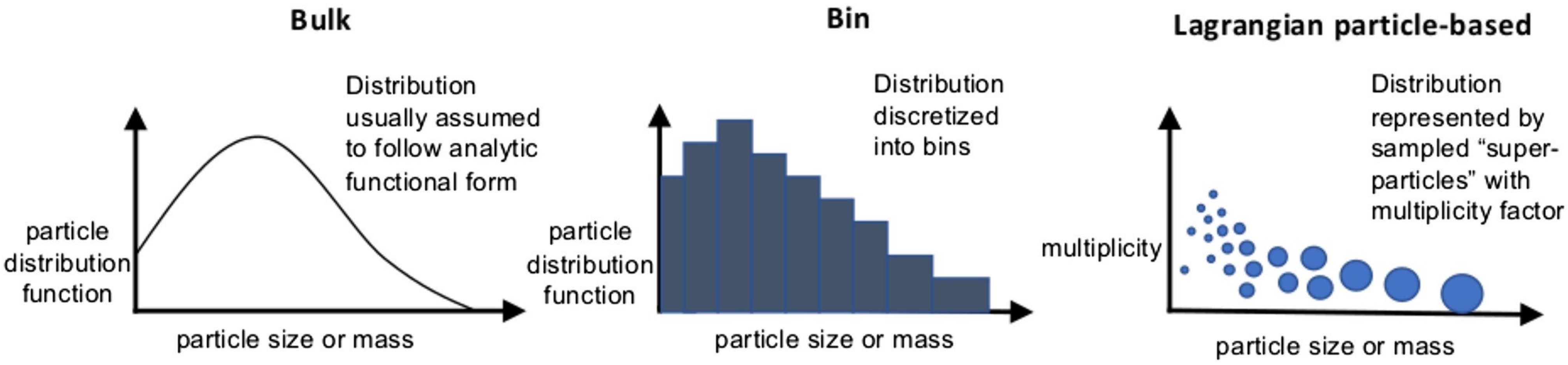
Super-droplets (SD)

- Computational particle-like objects called super-droplets represent:
  - Humidified aerosols
  - Cloud droplets
  - Rain drops



SD: Droplet size distribution

- Each SD represent multiple real hydrometeors (multiplicity) with same properties (e.g. radius)
- Evolution of the DSD is resolved, like in bin microphysics



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SD pros

- Easy to add new attributes
  - Chemistry
  - Aerosol hygroscopicity
- Scales down to DNS
- No numerical diffusion of droplet size distribution
- Stochastic collision-coalescence
- Activation without parameterization
- Solute effect after activation
- Straightforwad aerosol processing

SD cons

- Inconsitent results of collision-coalescence modeling with different implementations
- Increased spatial and temporal variances; requires averaging

SD use case 1: sea salt GCCN

- Solute effect is important for GCCN

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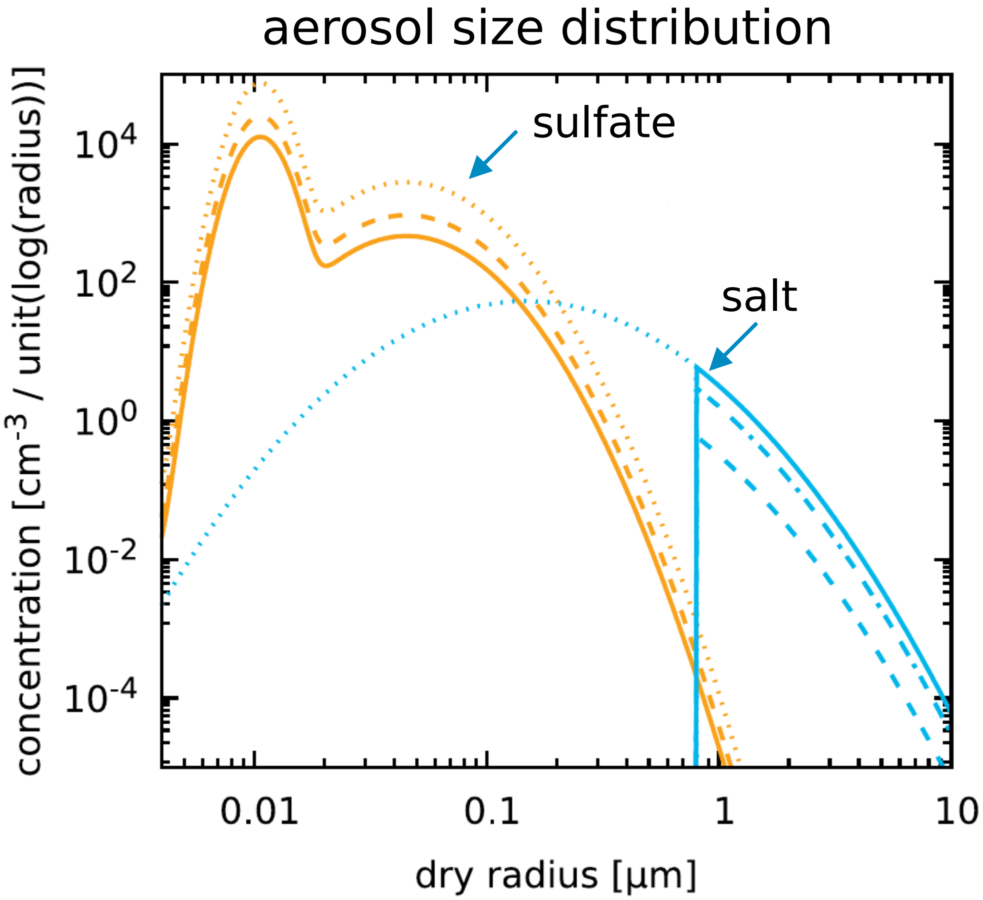
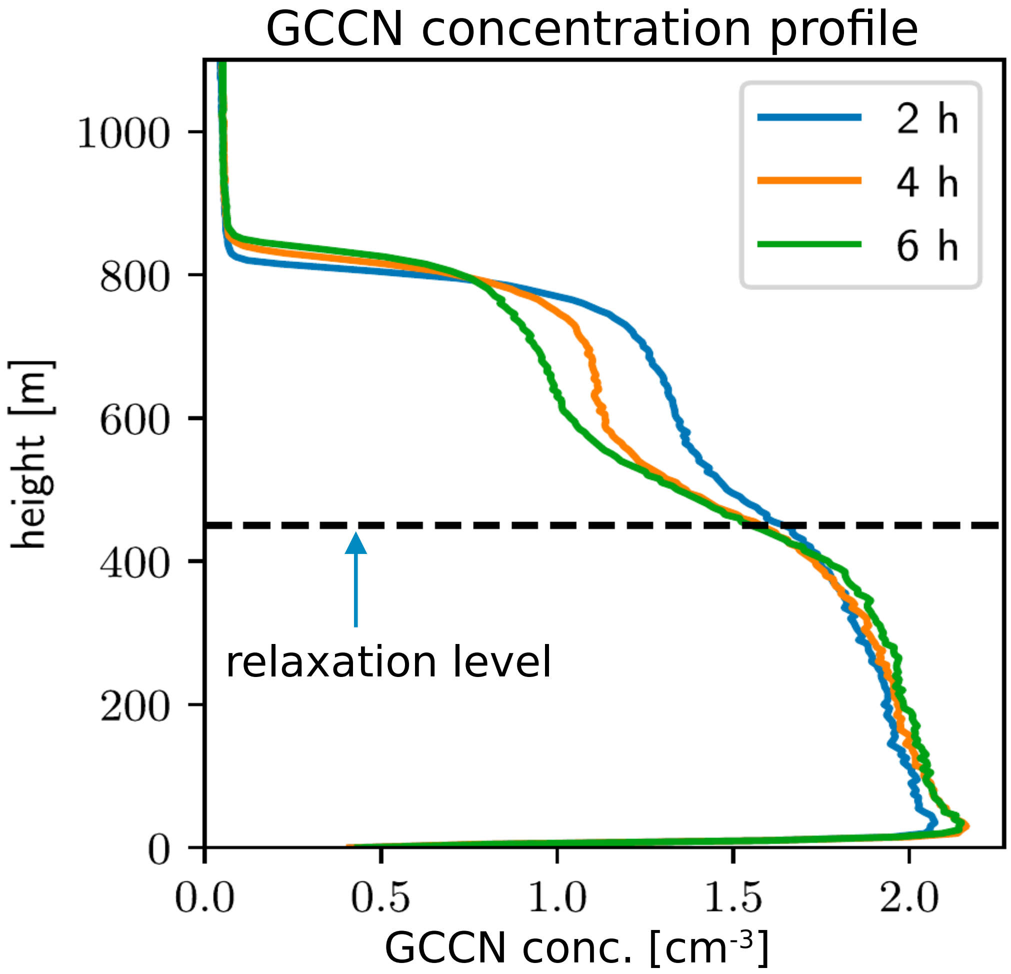
- Solute effect is important for GCCN
- Two types of aerosols: sulfate CCN and salt GCCN

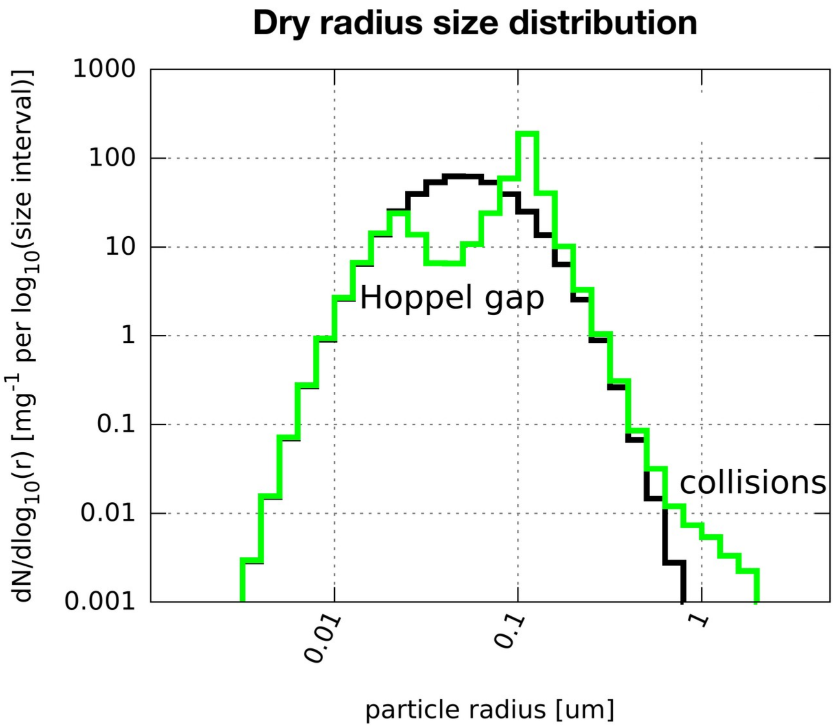


SD use case 1: sea salt GCCN

- Solute effect is important for GCCN
- Two types of aerosols: sulfate CCN and salt GCCN
- Strong GCCN washout and source near surface: relaxation



SD use case 2: chemistry



- Oxidation reaction is irreversible and affects the sizes of aerosol particles that served as condensation nuclei for cloud droplets
- As a result a gap in sizes between the activated and not activated aerosols is formed (Hoppel gap)
- Additionally a tail of larger aerosol particles is formed due to collisions between water drops

A. Jaruga

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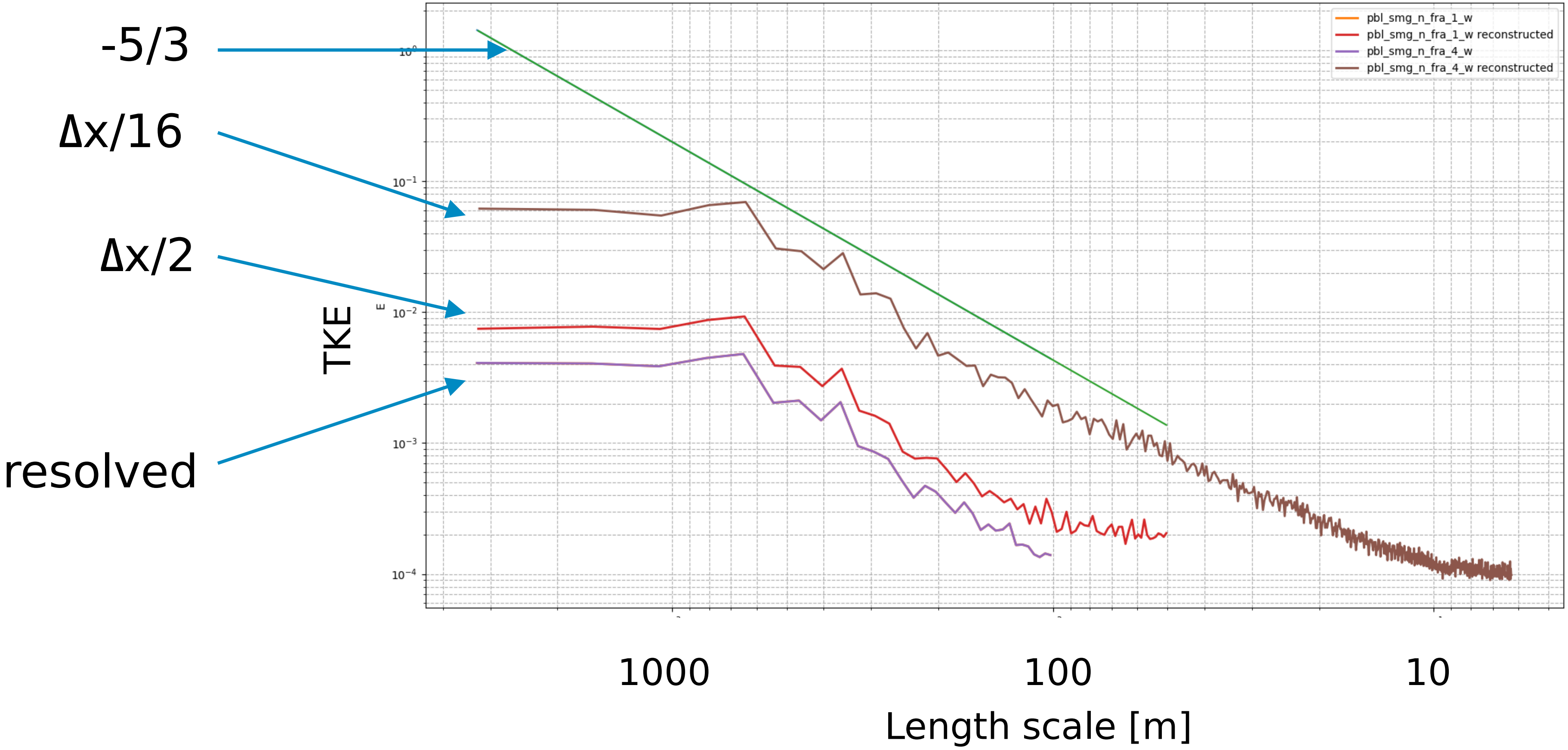
Reconstruction of SGS eddies

- Uses self-similarity of turbulence
- Applicable in the inertial range
- Each iteration doubles resolution, multiple iterations can be done

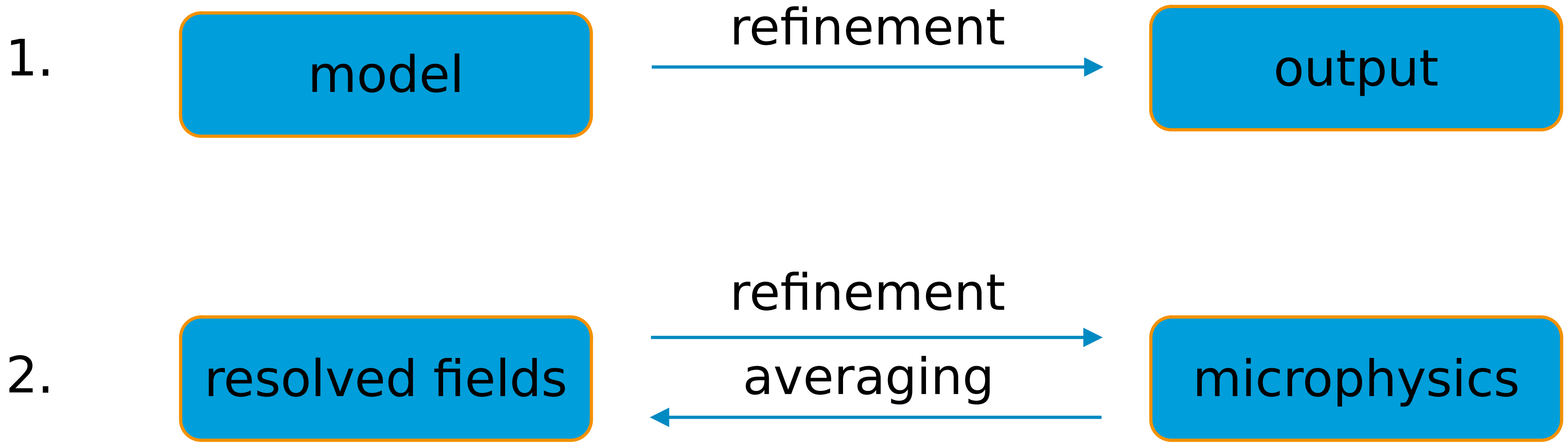
Reconstructed TKE spectrum



Grid refinement use cases

1.

Grid refinement use cases



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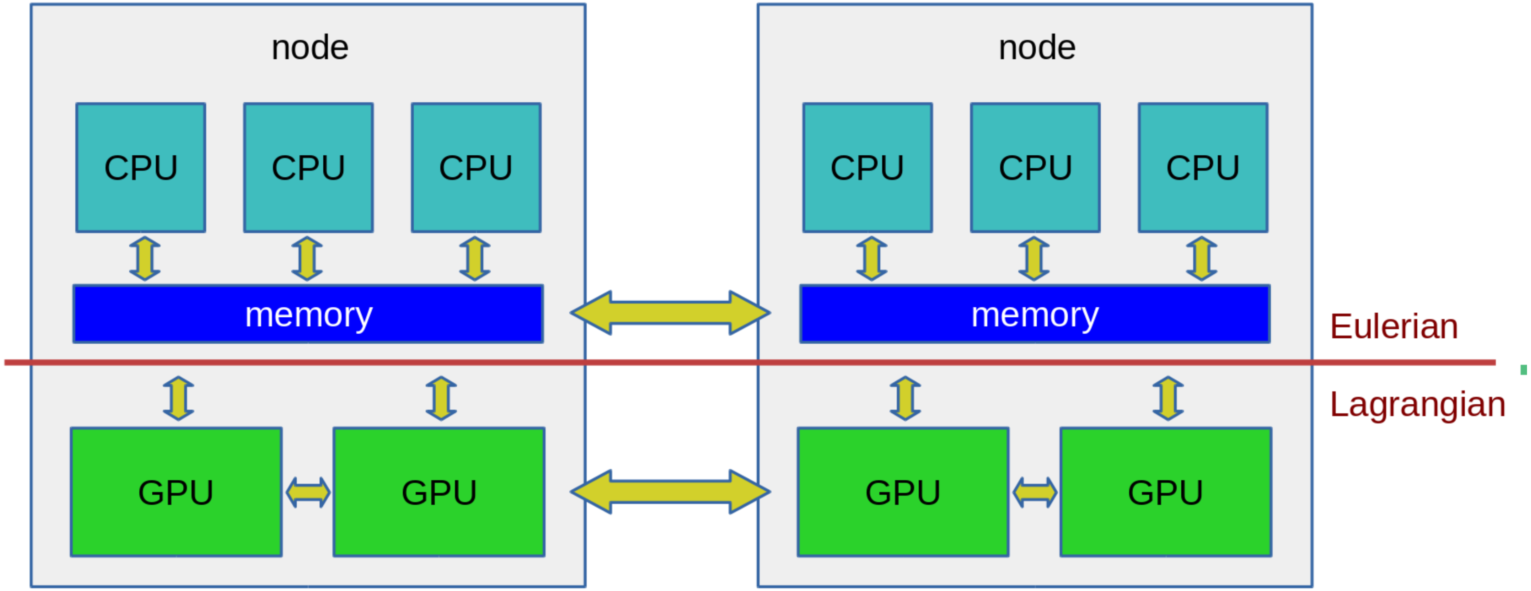
Design decisions

- Full use of heterogeneous (CPU+GPU) clusters

Heterogeneous cluster schematic



- Eulerian component: resides in RAM, computed by CPUs
- Lagrangian component: resides in RAM, computed by CPUs
  or resides in GPU RAM, computed by GPUs

Design decisions

- Full use of heterogeneous (CPU+GPU) clusters
- Modular code design

Modular code design

- UWLCM uses two libraries:
  - libmpdata++ - collection of solvers that use MPDATA
  - libcloudph++ - collection of microphysics models
- Family of solvers – inheritance from simple to complex
- Benefits:
  - Improves code reusability
  - Simplifies code maintenance

Design decisions

- Full use of heterogeneous (CPU+GPU) clusters
- Modular code design
- Easy to use – Singularity image, multiple runtime options

Multiple single-line options

runtime options:

- number of dimensions:
  ./uwlcm --ny=[0, X]
- type of microphysics:
  ./uwlcm --micro=[blk_1m, lgrngn]
- where to calculate Lagrangian microphysics:
  ./uwlcm --backend=[serial, OpenMP, CUDA, multi_CUDA]
- model setup:
  ./uwlcm --case=[dycoms, bomex, ...]
- piggybacking:
  ./uwlcm --piggy=1 --vel_in=file
- number of CPU threads for dynamics:
  OMP_NUM_THREADS=X ./uwlcm
- MPI processes:
  mpiexec -np X ./uwlcm
- advection, coalescence, condensation timesteps
- number of super-droplets
- ...

compile time options:

- MPDATA options
  - variable-sign option:
    opts = [opts::iga, opts::abs]
  - non-oscillatory option:
    opts = [opts::fct]
  - third-order terms:
    opts = [opts::tot]
  - ...
- microphysics options
  - coalescence kernel
  - terminal velocity
  - ....
- numerical precision
  real_t = [float, double]

Design decisions

- Full use of heterogeneous (CPU+GPU) clusters
- Modular code design
- Easy to use – Singularity image, multiple runtime options
- Open-source code – hosted on Github
- C++ (CUDA and Python bindings in libcloudph++)
- use existing libraries (Boost, Thrust, blitz++, ...)
- Hybrid OpenMP + MPI parallelization
- Automated tests – Github Actions

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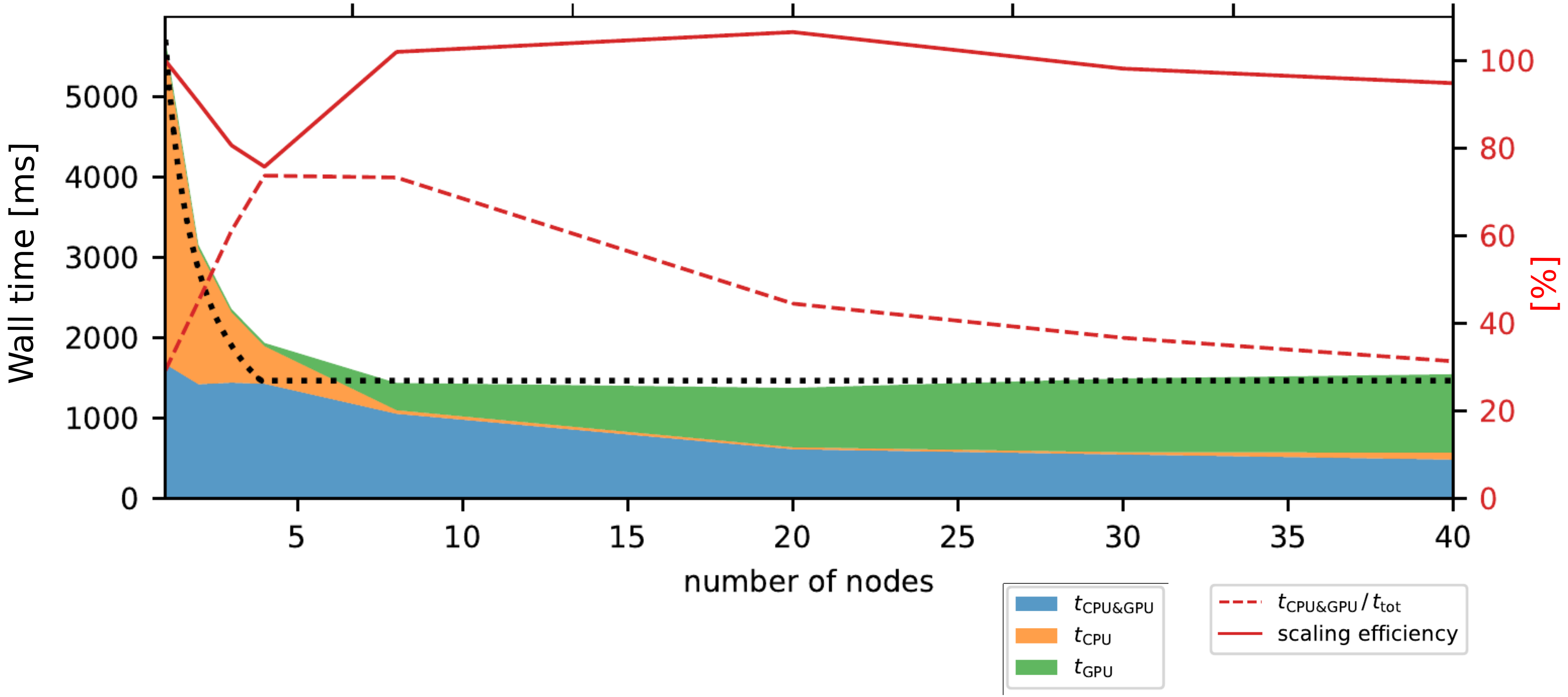
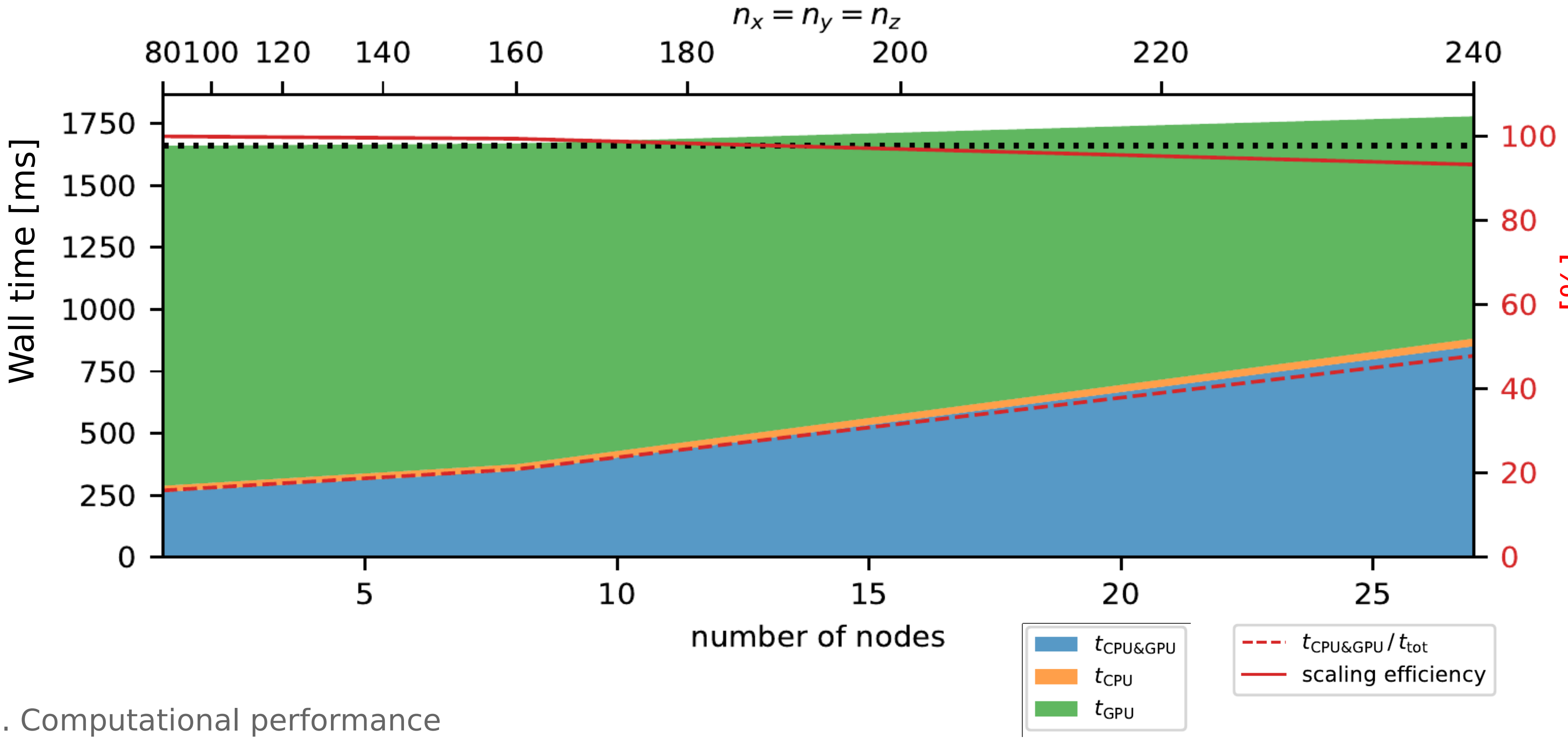
CPU strong scaling, GPU weak scaling



Weak scaling



Summary

- UWLCM is a tool for LES modeling of clouds with a focus on detailed representation of cloud microphysics
- UWLCM in nextGEMS
  - Simulations of EUREC4A domain
    - Setup: open / periodic boundaries? EUREC4A-MIP?
    - Comparison with ICON-LES
  - Other ideas?
    - Warm cloud parameterization?