University of Warsaw Lagrangian Cloud Model (UWLCM)

model formulation and stratocumulus simulations

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Agenda

- Model formulation
  - model equations
  - numerical implementation
- Stratocumulus simulations
  - 2D results
  - 3D results
- Cumulus simulations
- Chemistry ad
- Summary

LES model with SDM microphysics

EULERIAN

- Eulerian variables: θ, q_v, u, v, w
- anelastic approximation:

$$D_t \boldsymbol{u} = -\nabla \pi + \boldsymbol{k} B + \boldsymbol{F}_u,$$

$$D_t \theta = \frac{\theta^e}{T^e}\left(\frac{l_v}{c_{pd}} C\right) + F_\theta,$$

$$D_t q_v = -C + F_{q_v},$$

$$\nabla \cdot (\rho_d^r \boldsymbol{u}) = 0,$$

$$B = g\left[\frac{\theta - \theta^e}{\theta^r} + \epsilon\left(q_v - q_v^e\right) - \left(q_l - q_l^e\right)\right]$$

LAGRANGIAN

- Lagrangian representation of humidified aerosols, cloud droplets and rain drops
- κ-Köhler parametrisation of water activity

$$r\frac{dr}{dt} = \frac{D'_{\text{eff}}}{\rho_w}\left(1 - \frac{a_w\left(r, r_d, \kappa\right)\exp(A/r)}{\phi}\right),$$

$$a_w\left(r, r_d, \kappa\right) = \frac{r^3 - r_d^3}{r^3 - r_d^3\left(1 - \kappa\right)}$$

- “all-or-nothing” coalescence algorithm (Shima et al. 2009)

Numerics

EULERIAN

- advection with the MPDATA algorithm (libmpdata++)
- generalized conjugate residual pressure solver (libmpdata++)
- trapezoidal integration of buoyancy and pressure gradient
- Euler forward integration of other forcings
- calculated on CPUs

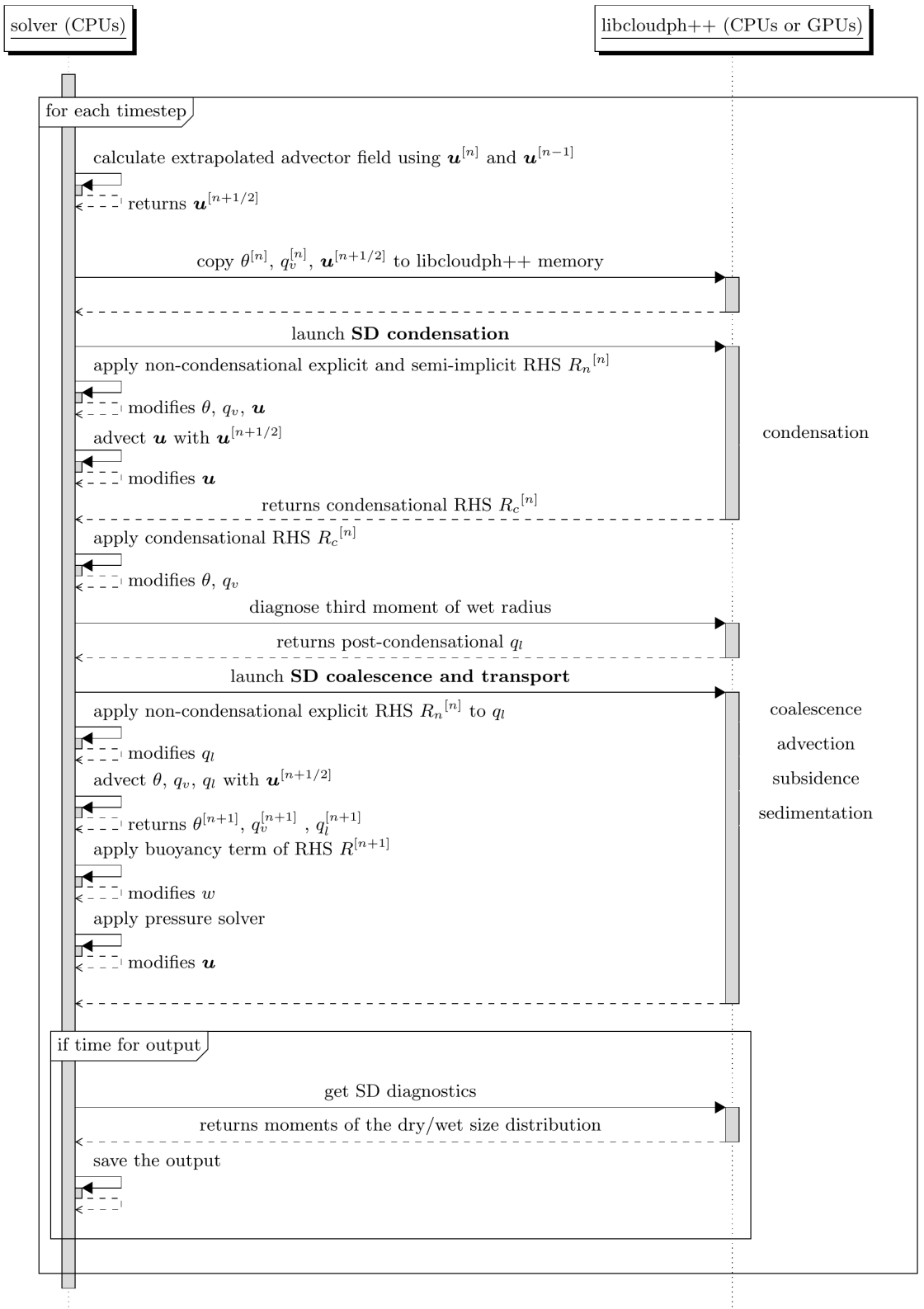
LAGRANGIAN

- Super-droplet method (libcloudph++)
- SD attributes: multiplicity, dry and wet radii, hygroscopicity
- integration of growth equation

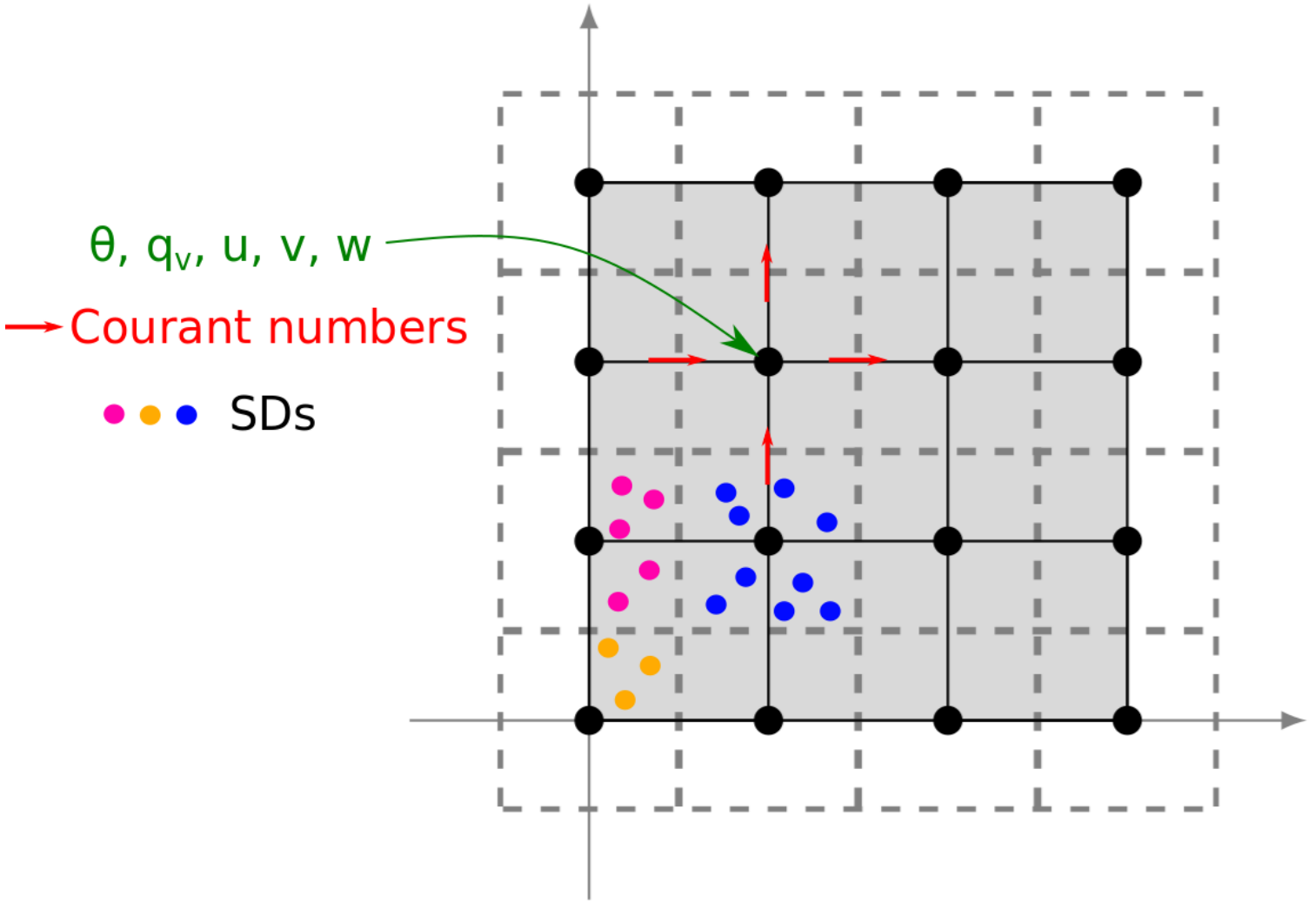
$$r^{2[n+1]} = r^{2[n]} + \Delta t \left. \frac{dr^2}{dt} \right|_{r^{2[n+1]}, q_v^{[n]}, \theta^{[n]}}$$

- predictor-corrector advection of SDs
- calculated on GPUs

Time step sequence



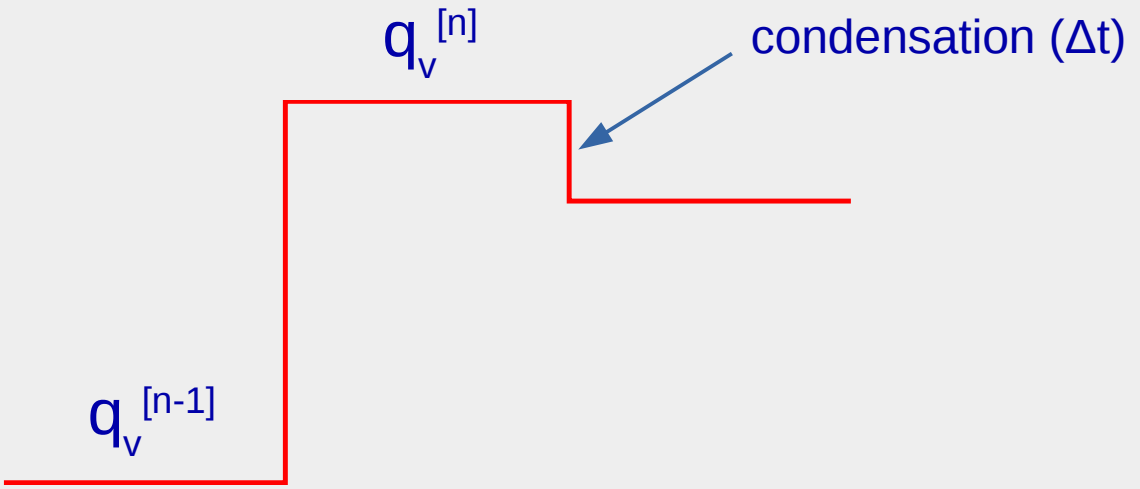
Spatial discretization



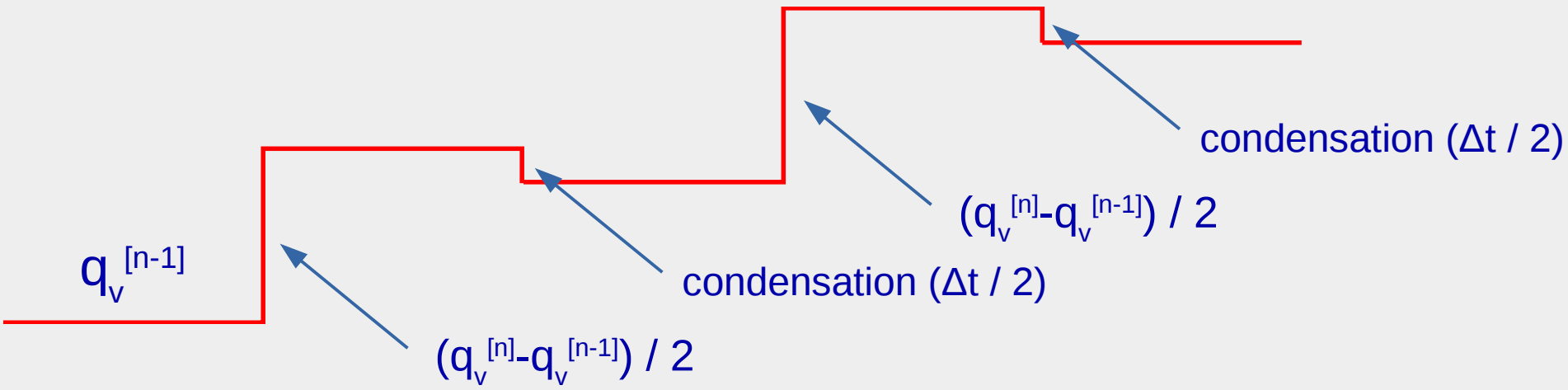
Condensation sub-stepping

- Scheme for integration of the condensation equation converges for $\Delta t \approx 0.1$ s
- LES timestep $\Delta t \approx 1$ s
- two algorithms tested:
  - *per-cell*
  - *per-particle*

no sub-stepping:



2 sub-steps:



- *per-cell*: $q_v^{[n-1]}$ comes from the cell in which the SD is at step n
- *per-particle*: $q_v^{[n-1]}$ comes from the cell in which the SD was at step n-1

Comparison with other models - DYCOMS RF02 stratocumulus simulations

- A drizzling marine stratocumulus
- Test UWLCM against 11 LES models from the Ackerman et al. 2009 intercomparison
- Microphysical schemes in other models:
  bin, single-moment bulk and double-moment bulk
- implicit LES in UWLCM, other models with explicit subgrid-scale schemes
- 2D and 3D simulations

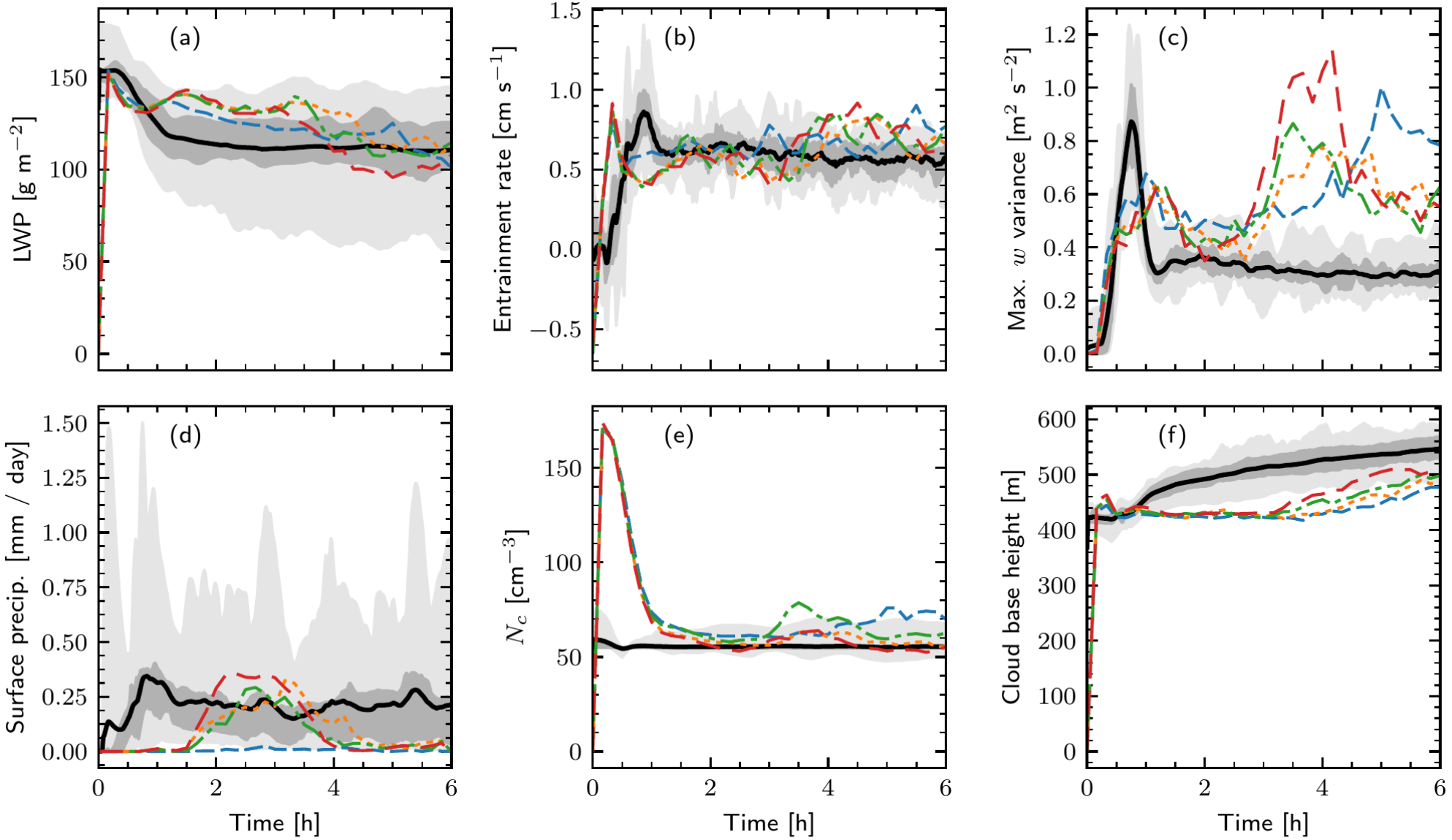
source: Angela Rowe
communitycloudatlas.wordpress.com

ANIMATION

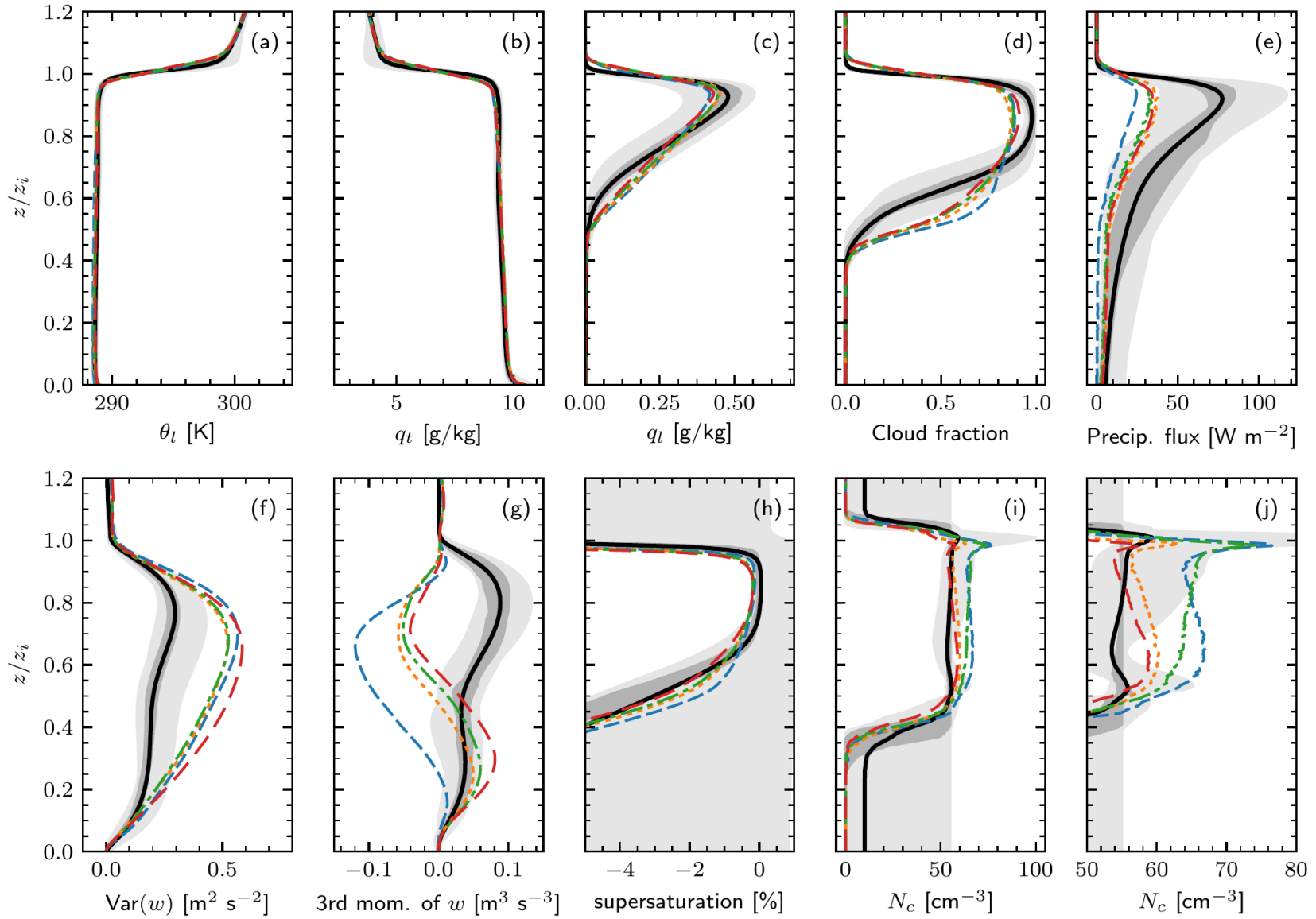
2D simulations

- Test the *per-cell* and *per-particle* sub-stepping algorithms
- Test different time step lengths
- Test different numbers of SDs,
  N_{SD} - initial number of SDs per cell
- Comparison with 3D results from Ackerman et al. 2008

2D time series



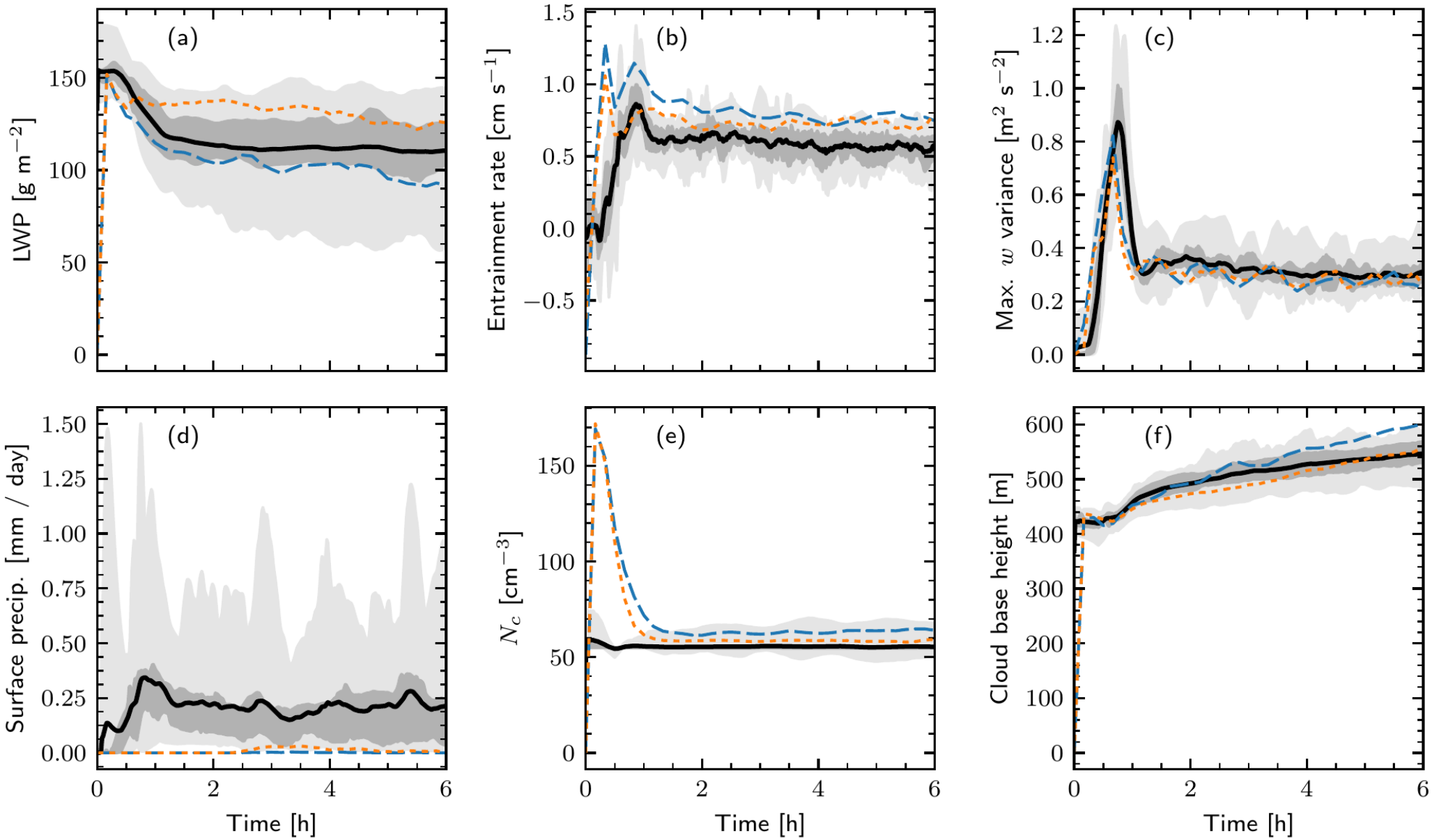
2D vertical profiles



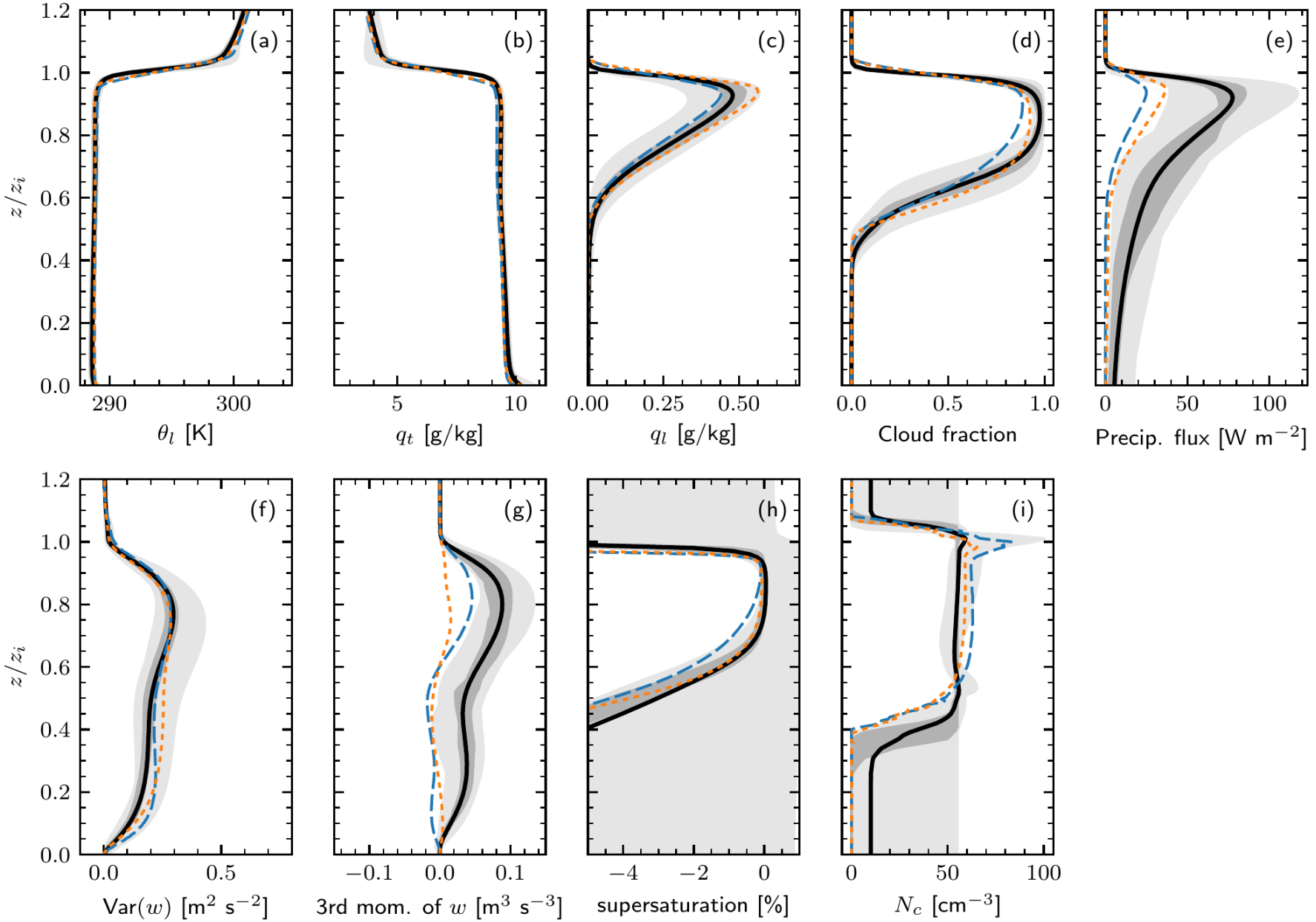
3D simulations

- Use the *per-particle* sub-stepping algorithm
- $N_{SD} = 40$
- Test for different time step lengths
- Comparison with 3D results from Ackerman et al. 2008

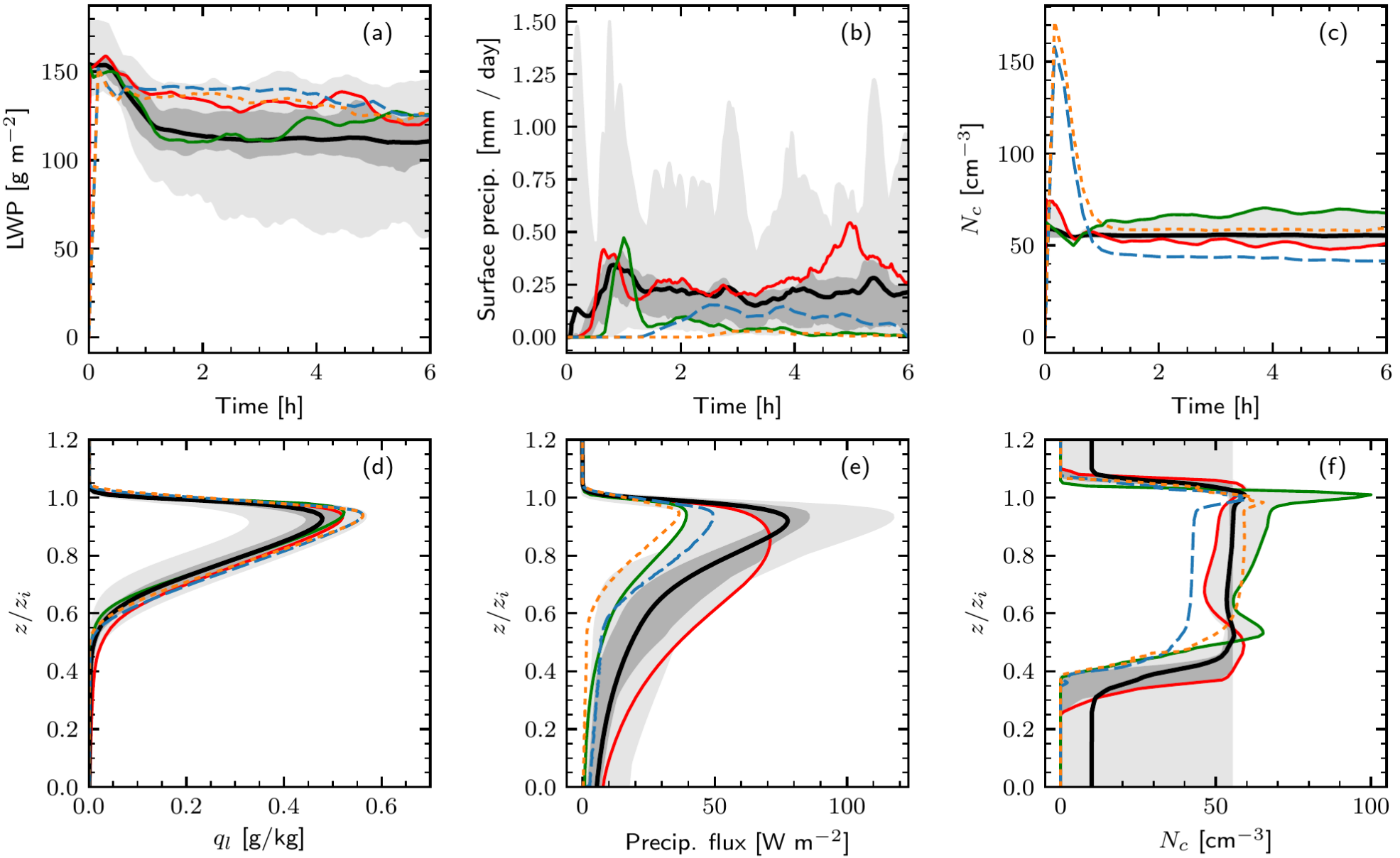
3D time series



3D vertical profiles



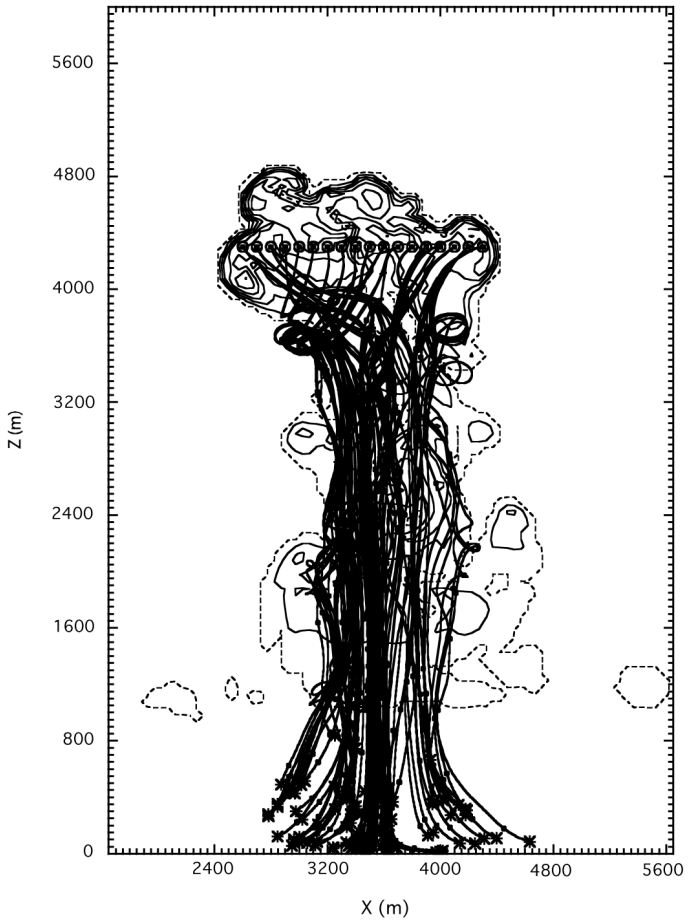
3D: comparison with bin microphysics

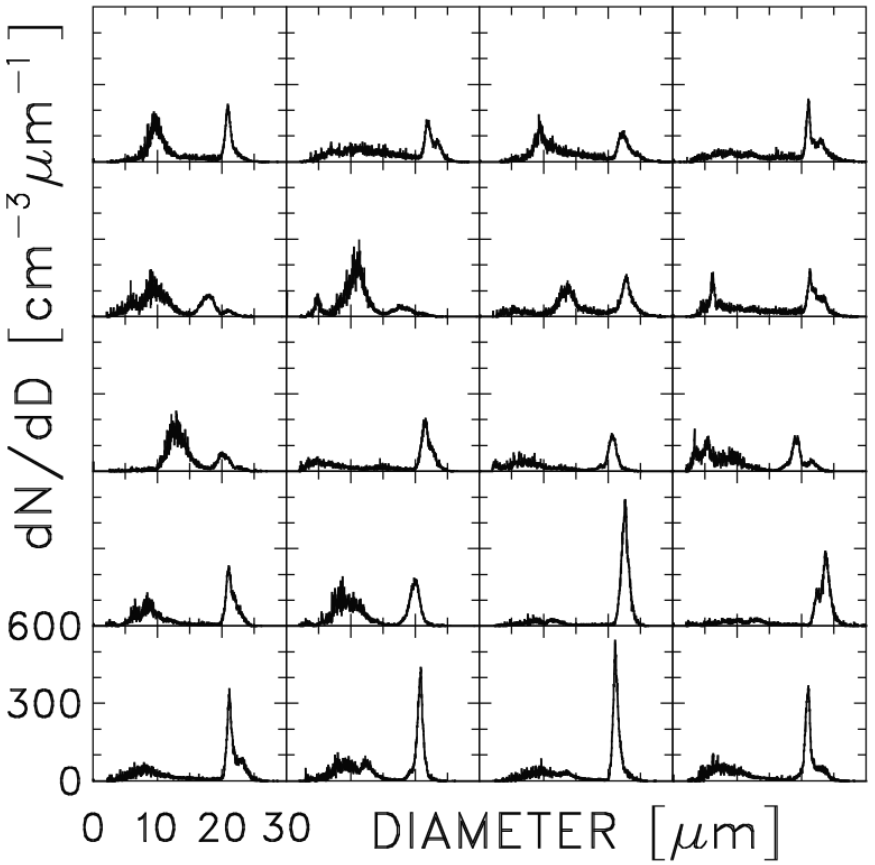


Stratocumulus modeling - conclusions

- General agreement between UWLCM and reference models
- Discrepancies in the third moment of vertical velocity (ILES vs SGS ?)
- Little rain in UWLCM
- N_{SD} = 40 same as N_{SD} = 1000
- *per-particle* sub-stepping necessary for correct activation
- 2D simulations convenient for testing and microphysics studies

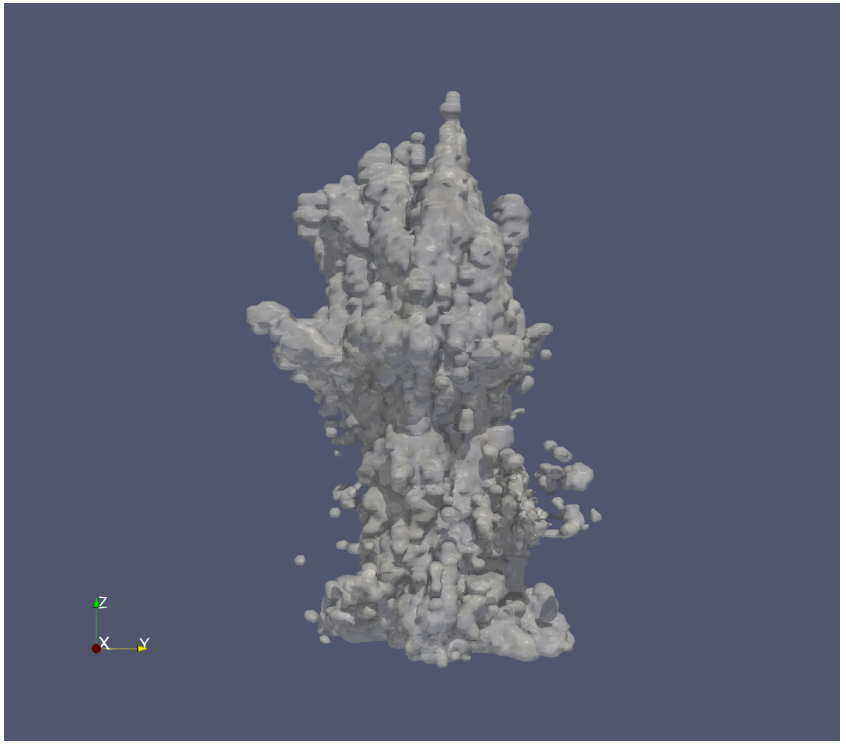
Advantages of particle-based microphysics: Cumulus simulations

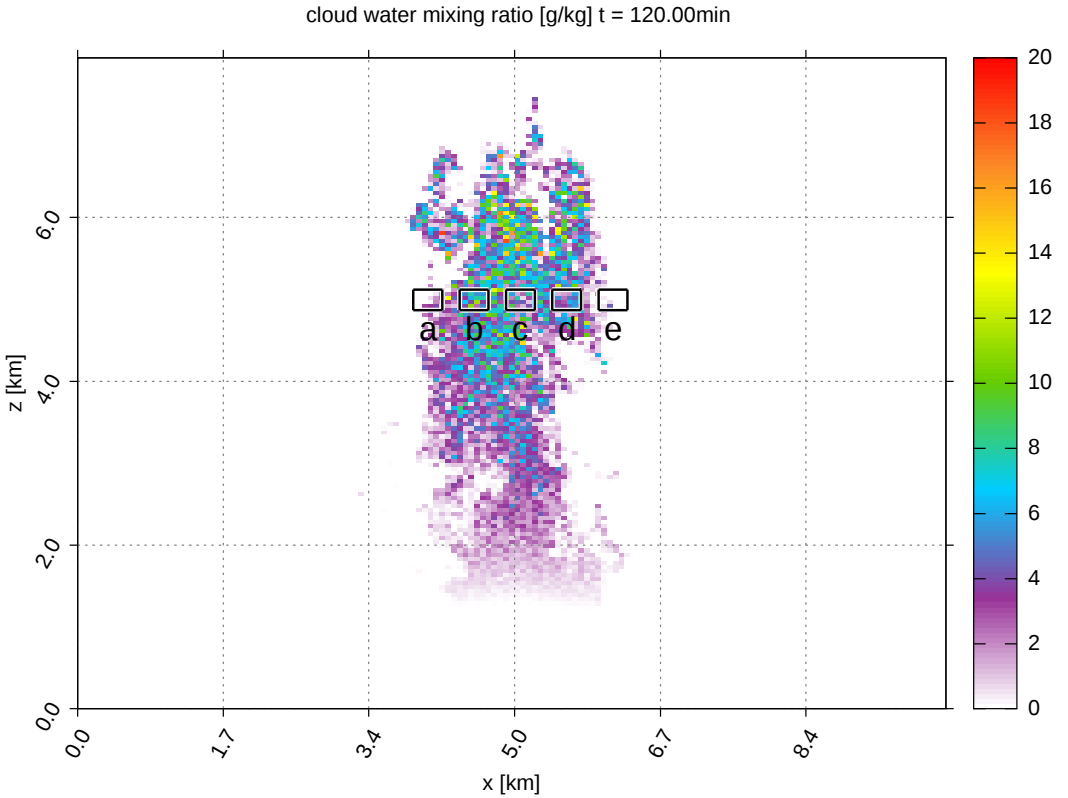


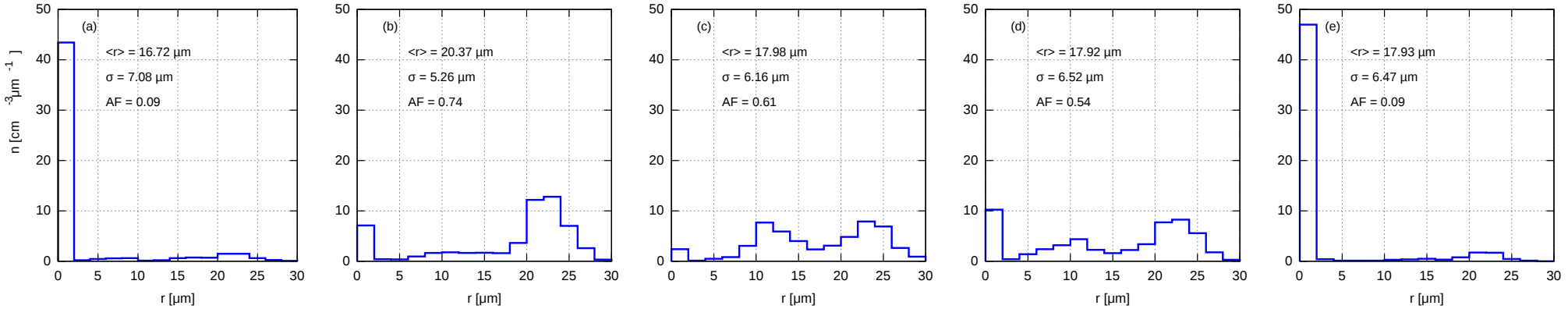


reproduced from Lasher-Trapp et al. *Q. J. R. Met. Soc.* 2005

UWLCM cumulus results







libcloudph++ 2.0: aqueous-phase chemistry extension of the particle-based cloud microphysics scheme

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Geoscientific Model Development

Geosci. Model Dev., 11, 3623–3645, 2018
https://doi.org/10.5194/gmd-11-3623-2018

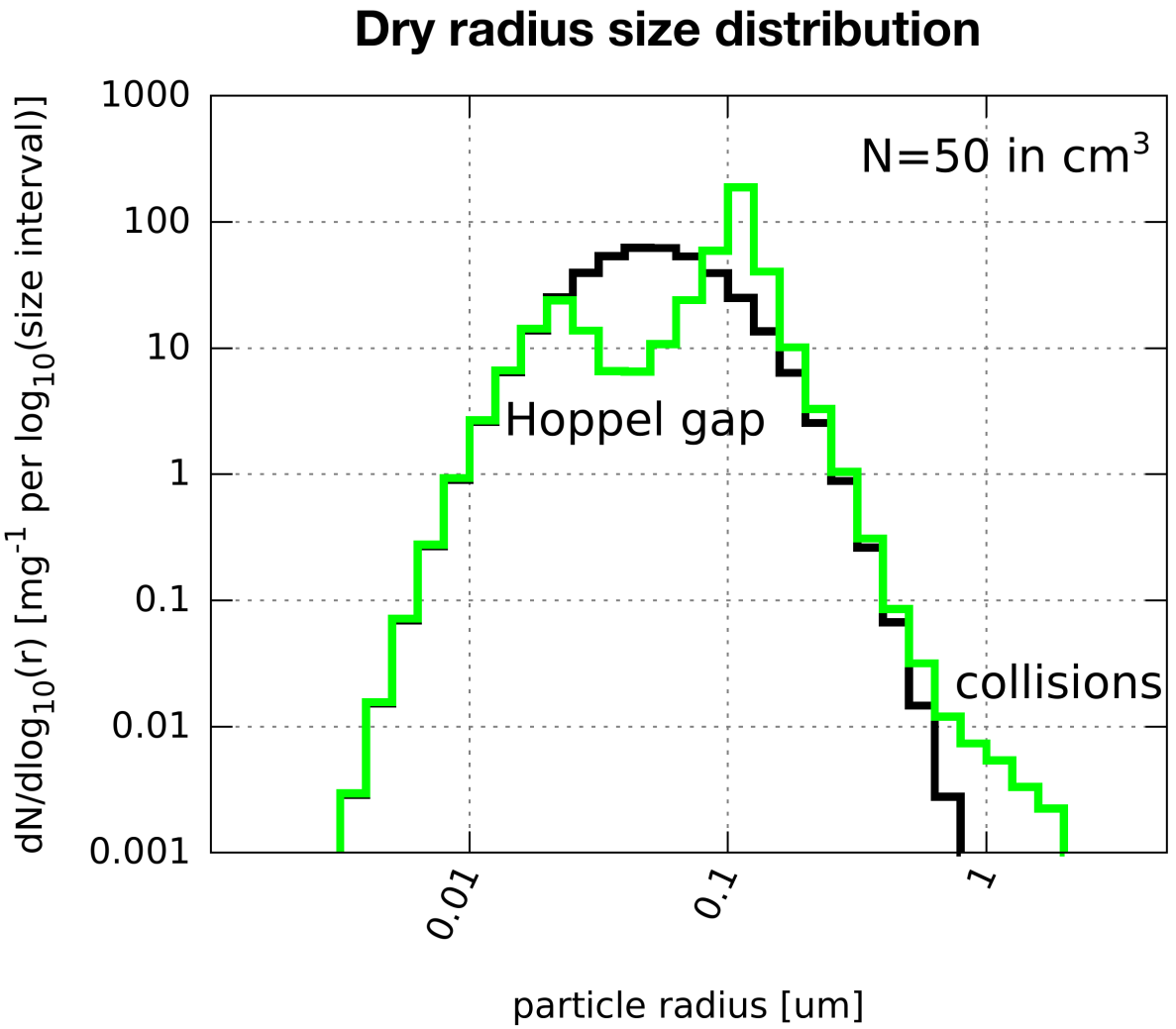
Chemical reaction: oxidation of SO_2 by O_3 and H_2O_2

Included trace gases: SO_2, CO_2, O_3, H_2O_2, NH_3, HNO_3

Processes:

- uptake of trace gases into droplets (modelled as a non-equilibrium process)
- dissociation into ions (iterative search for equilibrium pH of each super-droplet)
- oxidation of SO_2 by O_3 and H_2O_2

Example results



- 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

Summary

- Particle-based Lagrangian microphysics used in LES give stratocumulus results in agreement with bulk and bin microphysics, except for lower precipitation.
- Implicit LES is in agreement with LES with subgrid-scale models, with the exception of skewness of the vertical velocity distribution.
- Thanks to the use of GPUs, sophisticated microphysics do not slow down simulations.
- LES code available for everyone: https://github.com/igfuw/UWLCM
- manuscript submitted to GMD

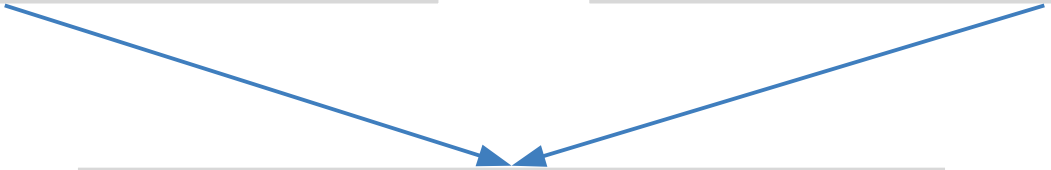
Software developed by our group

libmpdata++

- new implementation of MPDATA
- written in C++
- started ca. 5 years ago

libcloudph++

- cloud microphysics routines
- written in C++ with python bindings
- started ca. 5 years ago



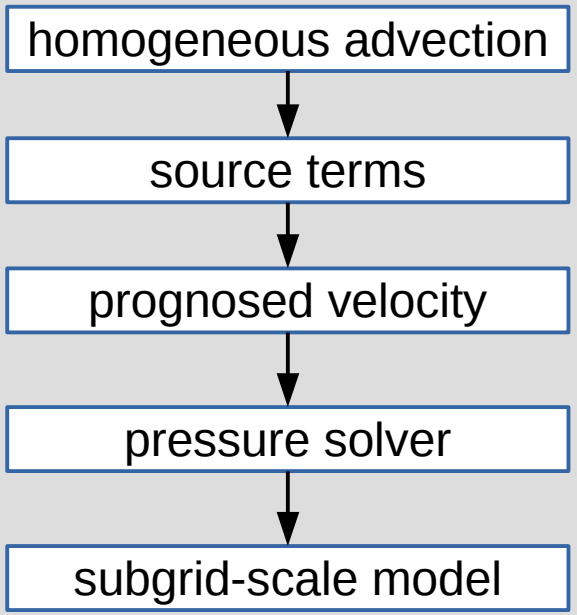
UWLCM

- Large Eddy Simulations of clouds using anelastic approximation
- written in C++
- started ca. 2 years ago

Modern code structure: separation of concerns

libmpdata++

- hierarchy of solvers:

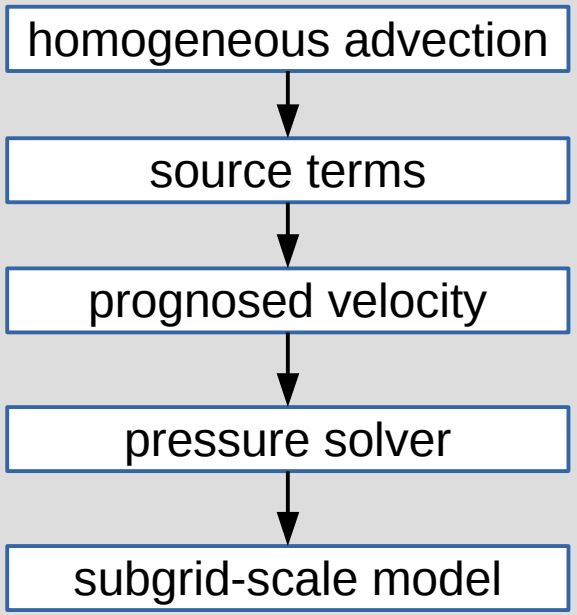


- boundary conditions
- concurrency handlers
- output handlers

Modern code structure: separation of concerns

libmpdata++

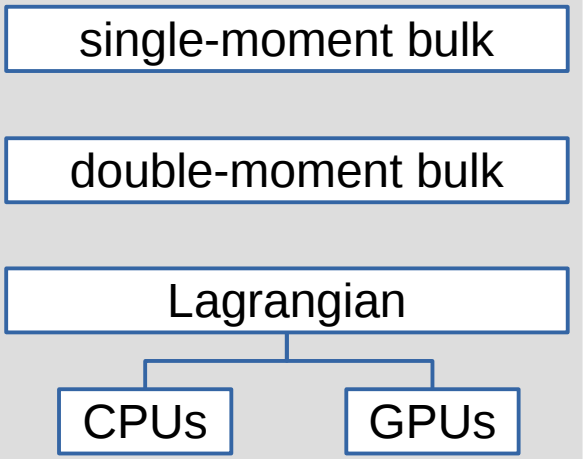
- hierarchy of solvers:



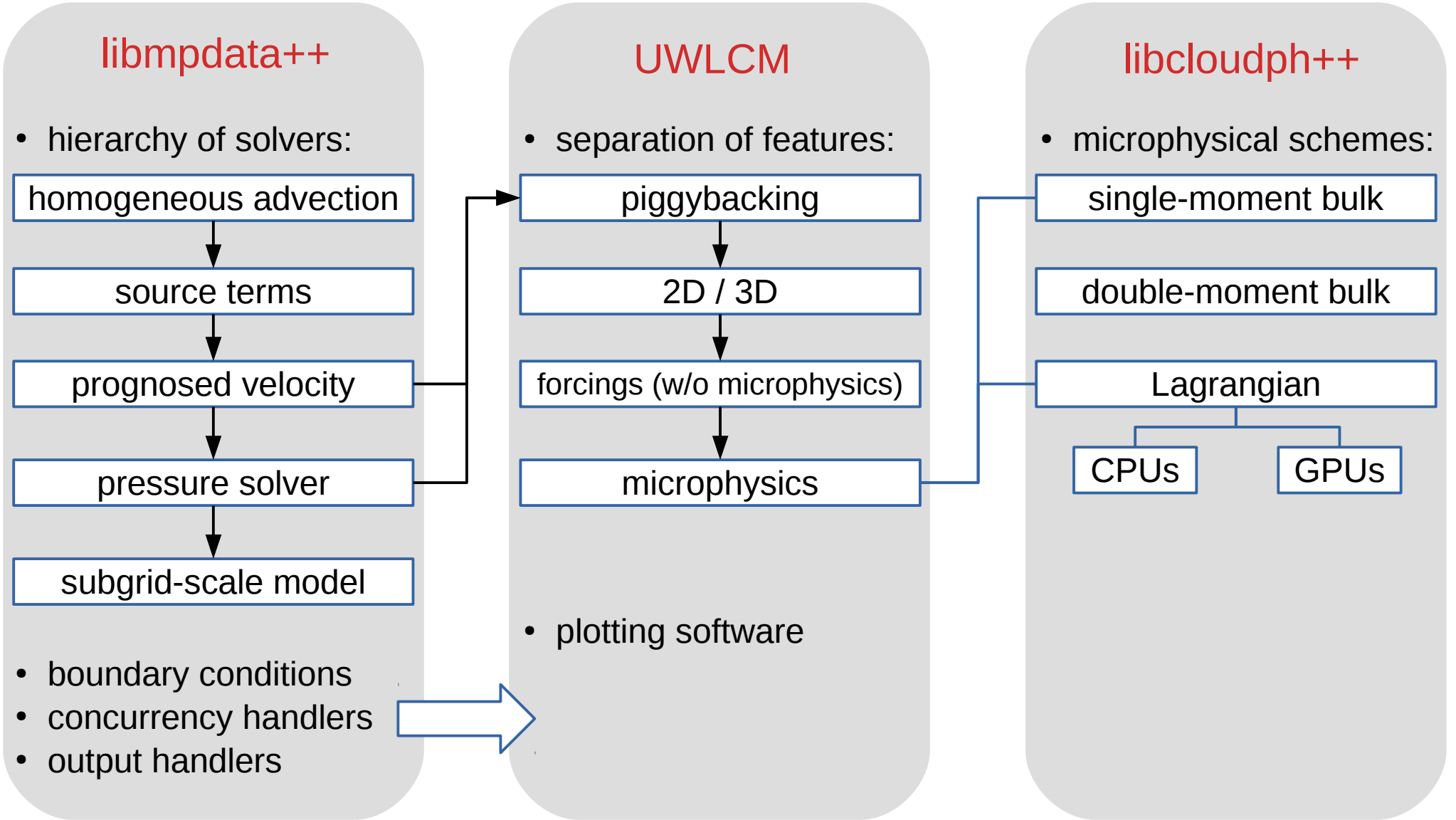
- boundary conditions
- concurrency handlers
- output handlers

libcloudph++

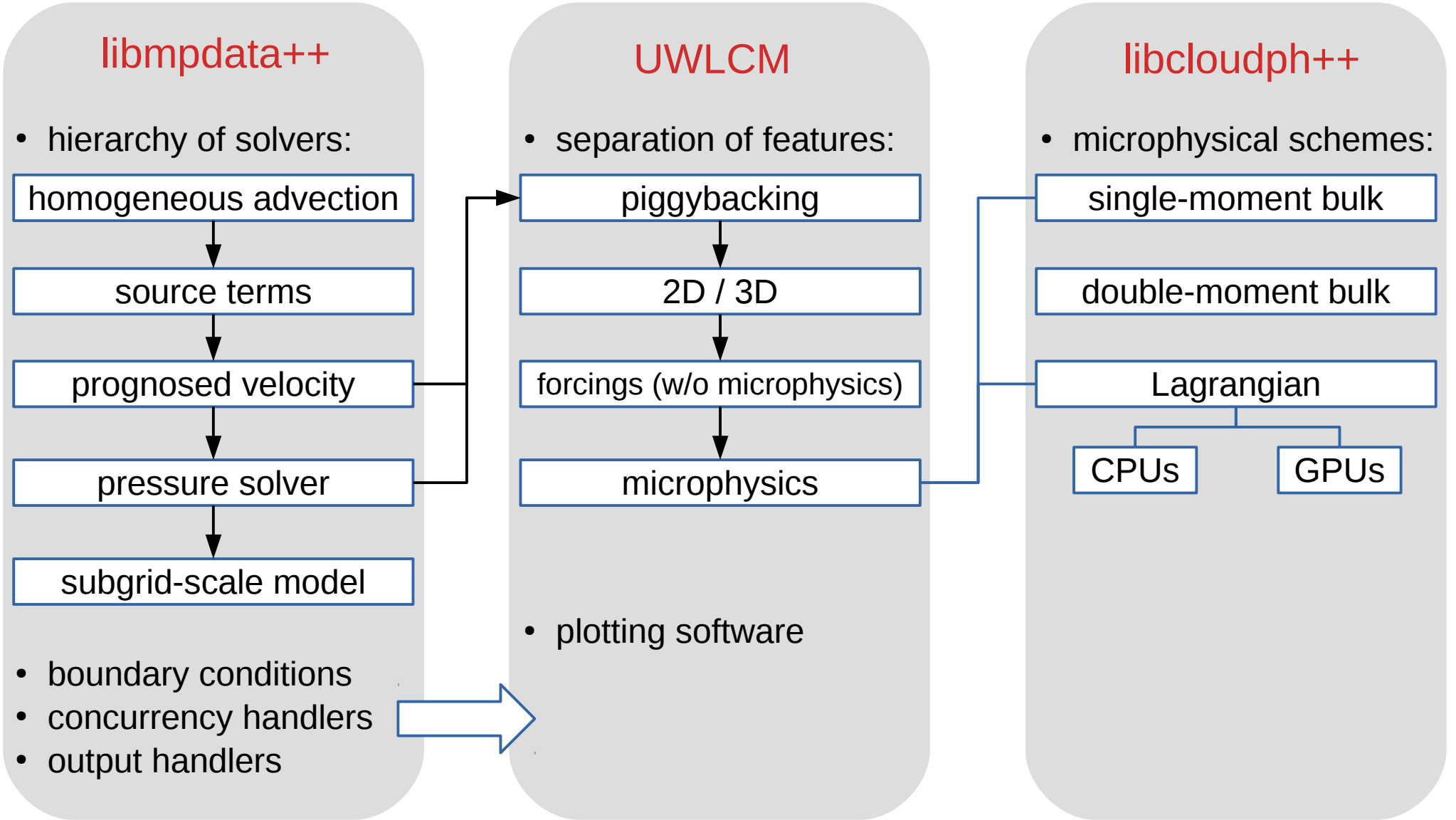
- microphysical schemes:



Modern code structure: separation of concerns



Modern code structure: separation of concerns



- Code sections can be developed independently.
- Code are sections ready to be reused.

- version control system
- automated tests
- open-source code hosted on github

Benefits of the modern code structure: one code, many models

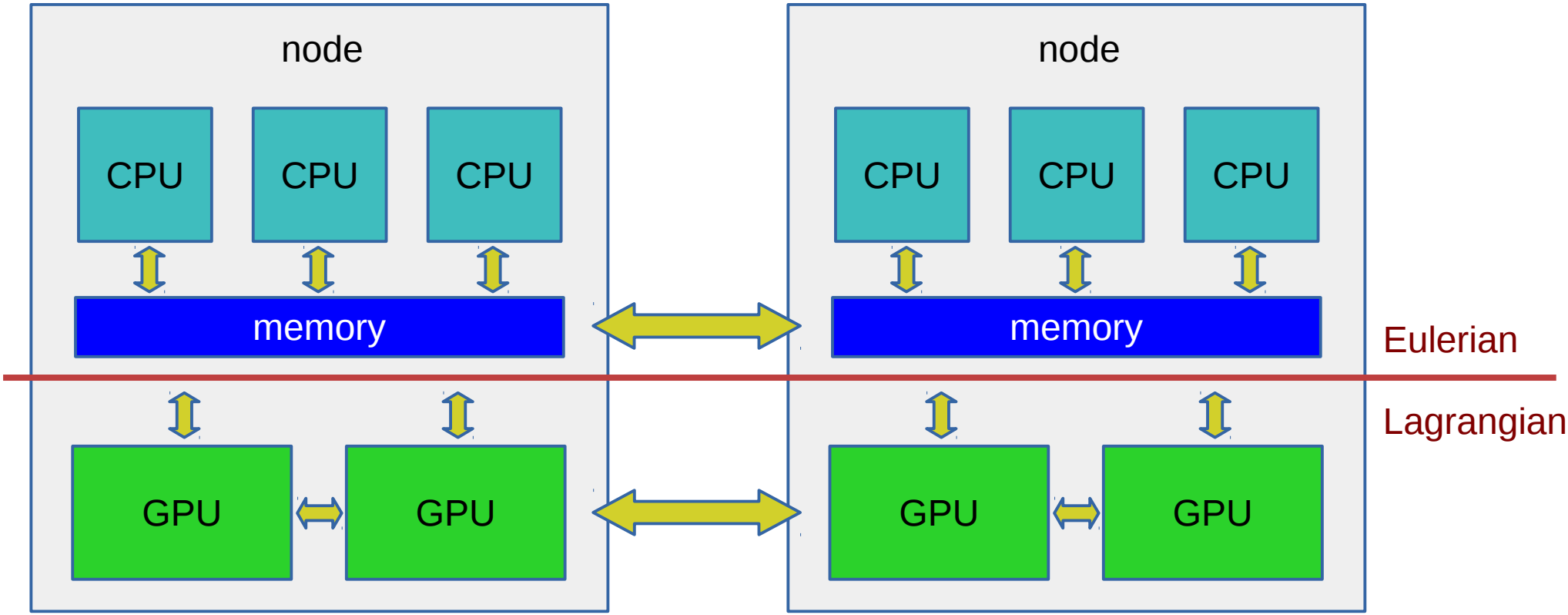
runtime options:

- number of dimensions:
  ./bicycles --ny=[0, X]
- type of microphysics:
  ./bicycles --micro=[blk_1m, lgrngn]
- where to calculate Lagrangian microphysics:
  ./bicycles --backend=[serial, OpenMP, CUDA, multi_CUDA]
- model setup:
  ./bicycles --case=[dycoms, bomex, ...]
- piggybacking:
  ./bicycles --piggy=1 --vel_in=file
- number of CPU threads for dynamics:
  OMP_NUM_THREADS=X ./bicycles
- distributed memory runs:
  mpiexec -np X ./bicycles
- 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]

Modern HPC architecture



- Domain decomposition between nodes
- Separate intra-node domain decomposition for CPU threads and GPUs
- Bulk microphysics computed on CPUs
- Lagrangian microphysics computed on CPUs or GPUs
- Simultaneous computations of fluid flow on CPUs and microphysics on GPUs synchronized only during condensation