University of Warsaw Lagrangian Cloud Model (UWLCM)
model formulation and stratocumulus simulations

Piotr Dziekan, Maciej Waruszewski, Hanna Pawłowska
Institute of Geophysics, Faculty of Physics, University of Warsaw

Sylwester Arabas, Anna Jaruga

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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: $\theta, q_v, u, v, w$
- anelastic approximation:

\[
D_t u = - \nabla \pi + kB + F_u,
\]

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

\[
D_t q_v = -C + F_{q_v},
\]

\[
\nabla \cdot (\rho^r_d u) = 0,
\]

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

**LAGRANGIAN**

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

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

\[
a_w (r, r_d, \kappa) = \frac{r^3 - r_d^3}{r^3 - r_d^3 (1 - \kappa)}
\]

- “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
  \[ r^2[n+1] = r^2[n] + \Delta t \frac{dr^2}{dt} \bigg|_{n+1} \]
- predictor-corrector advection of SDs
- calculated on GPUs
Time step sequence

for each timestep:

- calculate extrapolated advect field using \( u^{[n]} \) and \( u^{[n-1]} \)

- \(<\text{returns } u^{[n+1/2]}\>

- copy \( \theta^{[n]} \), \( q_v^{[n]} \), \( u^{[n+1/2]} \) to libcloudph++ memory

- \(<\text{launch SD condensation}\>
  
  - apply non-condensational explicit and semi-implicit RHS \( R_e^{[n]} \)

  - \(<\text{modifies } \theta, q_v, u\>
  
  - advect \( u \) with \( u^{[n+1/2]} \)

  - \(<\text{modifies } u\>

  - returns condensational RHS \( R_c^{[n]} \)

  - apply condensational RHS \( R_c^{[n]} \)

  - \(<\text{modifies } \theta, q_v\>

  - diagnose third moment of wet radius

  - returns post-condensational \( q_i \)

- \(<\text{launch SD coalescence and transport}\>
  
  - apply non-condensational explicit RHS \( R_e^{[n]} \) to \( q_i \)

  - \(<\text{modifies } q_i\>

  - advect \( \theta, q_v, q_i \) with \( u^{[n+1/2]} \)

  - \(<\text{returns } \theta^{[n+1]}, q_v^{[n+1]}, q_i^{[n+1]}\>

  - apply buoyancy term of RHS \( R_{[n+1]}^{[n+1]} \)

  - \(<\text{modifies } w, u\>

  - apply pressure solver

  - \(<\text{modifies } u\>

- if time for output:
  
  - get SD diagnostics

  - \(<\text{returns moments of the dry/wet size distribution}\>

  - save the output

- \(<\text{libcloudph++ (CPUs or GPUs)}\>

- \(<\text{solver (CPUs)}\>
Spatial discretization

\[ \theta, q_v, u, v, w \]

→ Courant numbers

\[ \text{SDs} \]
Condensation sub-stepping

• Scheme for integration of the condensation equation converges for $\Delta t \approx 0.1 \text{ s}$
• LES timestep $\Delta t \approx 1 \text{ s}$
• two algorithms tested:
  – *per-cell*
  – *per-particle*
no sub-stepping:

\[ q_v^{[n]} \]

\[ q_v^{[n-1]} \]

2 sub-steps:

\[ (q_v^{[n]} - q_v^{[n-1]}) / 2 \]

\[ (q_v^{[n]} - q_v^{[n-1]}) / 2 \]

\[ \text{condensation (Δt / 2)} \]

\[ \text{condensation (Δt)} \]

- **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
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

(a) LWP [g m\(^{-2}\)]

(b) Entrainment rate [cm s\(^{-1}\)]

(c) Max. \(w\) variance [m\(^2\) s\(^{-2}\)]

(d) Surface precip. [mm / day]

(e) \(N_c\) [cm\(^{-3}\)]

(f) Cloud base height [m]

- **2D, \(\Delta t=0.1s, N_{SD} = 40\), no substeps**
- **2D, \(\Delta t=1s, N_{SD} = 40\), 10 substeps for condensation, per-particle substepping**
- **2D, \(\Delta t=1s, N_{SD} = 40\), 10 substeps for condensation, per-cell substepping**
- **2D, \(\Delta t=1s, N_{SD} = 1000\), 10 substeps for condensation, per-particle substepping**
2D vertical profiles

(a) $\theta_l$ [K] vs. $z/z_A$
(b) $q_t$ [g/kg] vs. $z/z_A$
(c) $q_t$ [g/kg] vs. cloud fraction
(d) Precip. flux [W m$^{-2}$] vs. $z/z_A$

(e) $\text{Var}(w)$ [m$^2$ s$^{-2}$] vs. $z/z_A$
(f) 3rd mom. of $w$ [m$^3$ s$^{-3}$] vs. $z/z_A$
(g) supersaturation [%] vs. $z/z_A$
(h) $N_c$ [cm$^{-3}$] vs. $z/z_A$

(i) $N_c$ [cm$^{-3}$] vs. Precip. flux [W m$^{-2}$]

(j) $N_c$ [cm$^{-3}$] vs. $\text{Var}(w)$ [m$^2$ s$^{-2}$]

Legend:
- 2D, $\Delta t=0.1s$, $N_{SD} = 40$, no substeps
- 2D, $\Delta t=1s$, $N_{SD} = 40$, 10 substeps for condensation, per-particle substepping
- 2D, $\Delta t=1s$, $N_{SD} = 40$, 10 substeps for condensation, per-cell substepping
- 2D, $\Delta t=1s$, $N_{SD} = 1000$, 10 substeps for condensation, per-particle substepping
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

- LWP [g m\(^{-2}\)]
- Entrainment rate [cm s\(^{-1}\)]
- Max. \(\omega\) variance [m\(^2\) s\(^{-2}\)]
- Surface precip. [mm / day]
- \(N_c\) [cm\(^{-3}\)]
- Cloud base height [m]

- 3D, \(\Delta t=0.1s, N_{SD} = 40\), no substeps
- 3D, \(\Delta t=1s, N_{SD} = 40\), 10 substeps for condensation, per-particle substepping
3D vertical profiles

- (a) $\theta_t$ [K]
- (b) $q_t$ [g/kg]
- (c) $q_t$ [g/kg]
- (d) Cloud fraction
- (e) Precip. flux [W m$^{-2}$]
- (f) Var($w$) [m$^2$ s$^{-2}$]
- (g) 3rd mom. of $w$ [m$^3$ s$^{-3}$]
- (h) supersaturation [%]
- (i) $N_c$ [cm$^{-3}$]

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- **3D, $\Delta t=0.1s$, $N_{SD} = 40$, no substeps**
- **3D, $\Delta t=1s$, $N_{SD} = 40$, 10 substeps for condensation, per-particle substepping**
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

Cloud water mixing ratio [g/kg] t = 120.00 min

(a) \( \langle r \rangle = 16.72 \, \mu m \), \( \sigma = 7.08 \, \mu m \), \( AF = 0.09 \)

(b) \( \langle r \rangle = 20.37 \, \mu m \), \( \sigma = 5.26 \, \mu m \), \( AF = 0.74 \)

(c) \( \langle r \rangle = 17.98 \, \mu m \), \( \sigma = 6.16 \, \mu m \), \( AF = 0.61 \)

(d) \( \langle r \rangle = 17.92 \, \mu m \), \( \sigma = 6.52 \, \mu m \), \( AF = 0.54 \)

(e) \( \langle r \rangle = 17.93 \, \mu m \), \( \sigma = 6.47 \, \mu m \), \( AF = 0.09 \)
Chemical reaction: oxidation of SO$_2$ by O$_3$ and H$_2$O$_2$

Included trace gases: SO$_2$, CO$_2$, O$_3$, H$_2$O$_2$, 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$_2$O$_2$
Example results

Dry radius size distribution

- 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:
  - homogeneous advection
  - source terms
  - prognosed velocity
  - pressure solver
  - subgrid-scale model

- boundary conditions
- concurrency handlers
- output handlers
Modern code structure: separation of concerns

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**libcloudph++**
- microphysical schemes:
  - single-moment bulk
  - double-moment bulk
  - Lagrangian
    - CPUs
    - GPUs
Modern code structure: separation of concerns

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UWLCM
- separation of features:
  - piggybacking
  - 2D / 3D
  - forcings (w/o microphysics)
  - microphysics
- plotting software

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- microphysical schemes:
  - single-moment bulk
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CPUs
GPUs
Modern code structure: separation of concerns

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libcloudph++
- microphysical schemes:
  - single-moment bulk
  - double-moment bulk
  - Lagrangian

- CPUs
- GPUs

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

- Code sections can be developed independently.
- Code are sections ready to be reused.
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:
    \( \text{opts} = \text{opts}::iga, \text{opts}::abs \)
  - non-oscillatory option:
    \( \text{opts} = \text{opts}::fct \)
  - third-order terms:
    \( \text{opts} = \text{opts}::tot \)
  - ...

- **Microphysics options**
  - coalescence kernel
  - terminal velocity
  - ...

- **Numerical precision**
  \( \text{real\_t} = \text{[float, double]} \)
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