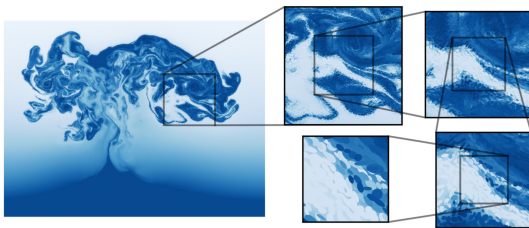


Organisation in parcel-based simulations of cumulus clouds

Steven Böing, Matthias Frey (St Andrews), David Dritschel (St Andrews), Alan Blyth and others.

July 9, 2024



Dritschel, D. G., Böing, S. J., Parker, D. J. and Blyth, A. M. (2018), *The Moist Parcel-in-Cell method for modelling moist convection*. *Q. J. R. Meteorol. Soc.*

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Frey, M., Dritschel, D., and Böing, S. (2023). *The 3D Elliptical Parcel-in-Cell (EPIC) method*. *J. Comp. Phys.*: X, 100136.

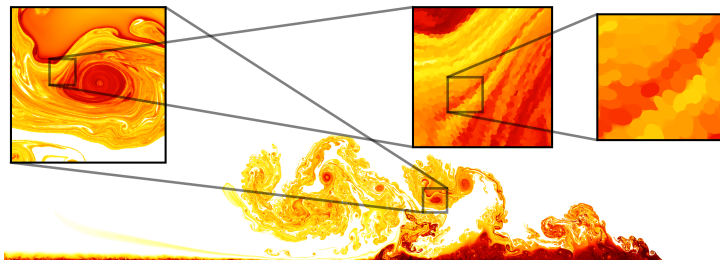
Supported by EPSRC grants EP/T025409/1 and EP/M008525/1, NERC grant NE/X018547/1

- These are (almost fully) based on parcels. Very different approach!
- Important: these parcels must interact (mix on small scale).
- Clean distinction between resolved dynamics and small-scale mixing.



Domantas Dilys, using EPIC's predecessor MPIC

- We use parcels carrying any number of (conserved) attributes and vorticity (evolved). Monotonic by design and globally conservative.
- Parcels have a volume V_i and a shape matrix \mathbf{B}_i in order to determine gridded fields needed to construct velocity on the grid.
- Incompressible, Boussinesq, evaporation and condensation but no precipitation yet.
- There are 2D (below) and 3D versions.



Mixing via splitting and merging

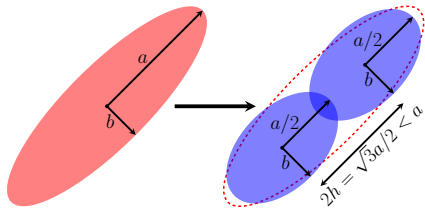
Splitting and merging conserve

- total centroid
- total area/volume
- total second moments (approximately)

Split criterion:

$$\lambda = \frac{a}{b} > \lambda_{\max} \quad [= 4]$$

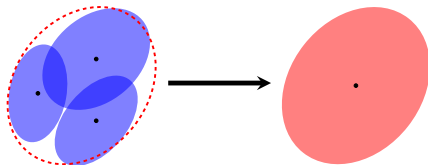
$$a_n > a_{\max}$$



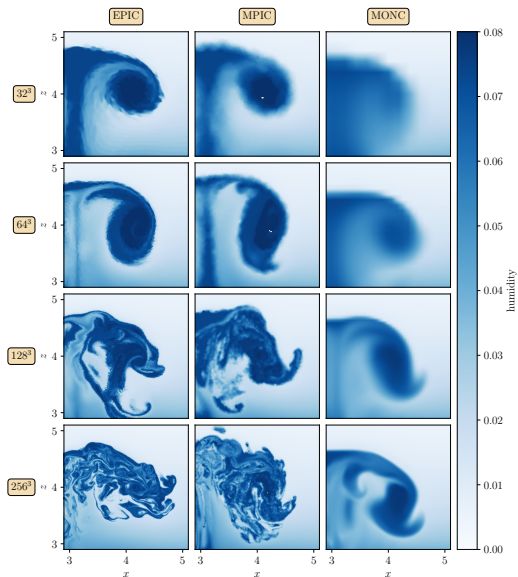
Merge criterion:

$$V_n < V_{\min}$$

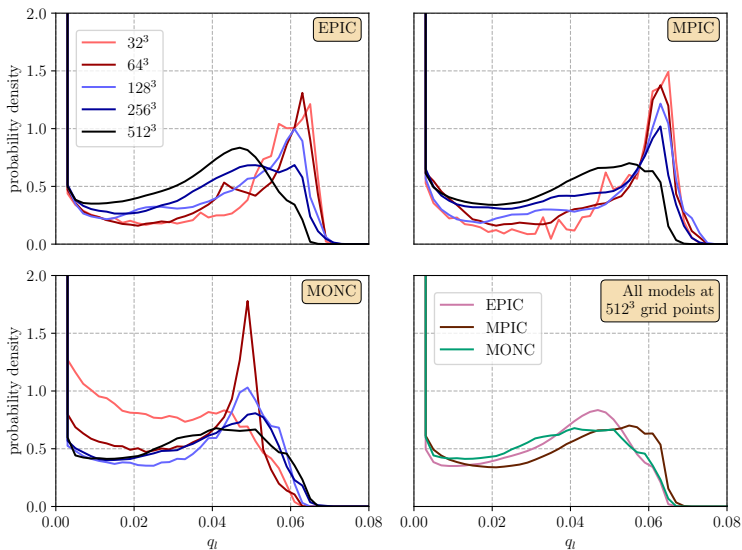
Nearest neighbour merging



Resolution dependence



Histograms of liquid water

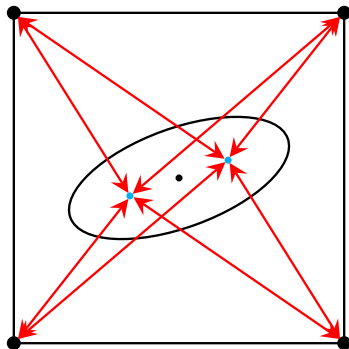


Enhanced mixing via the grid

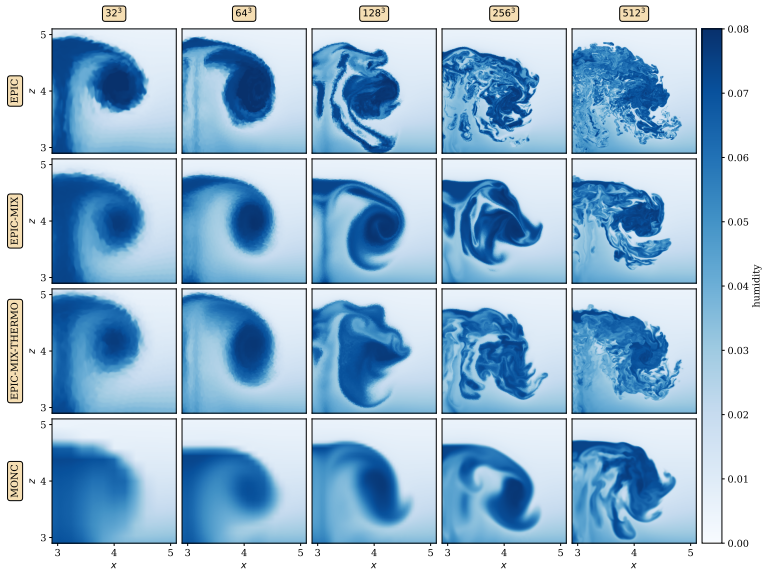
- Basic idea: nudge parcel value to grid value, which represents a mean of neighbours.

$$\phi' = \phi_p - \phi_g = \phi'(0)e^{-\beta|\mathbf{S}|t}$$

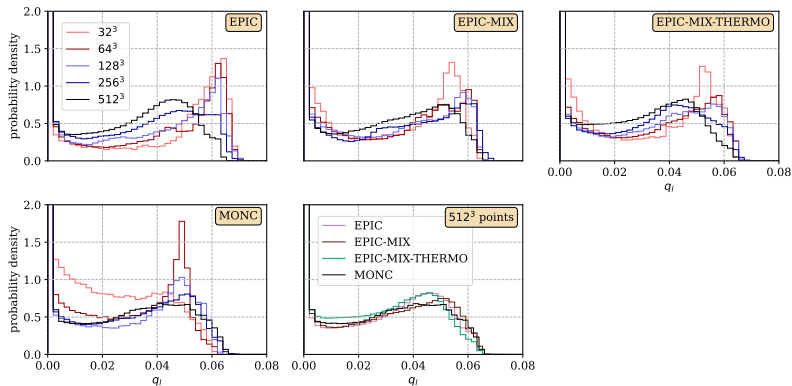
- β plays similar role to C_s in Smagorinsky scheme.
- Apply to grid point contributions to ensure conservation!



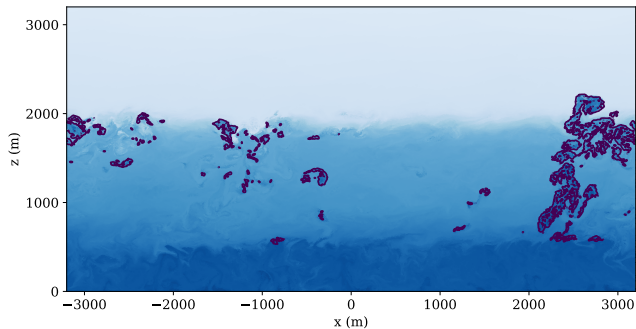
Application to moist thermal



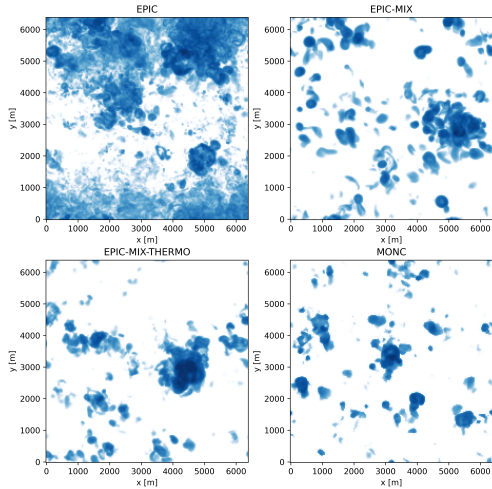
Moist thermal statistics



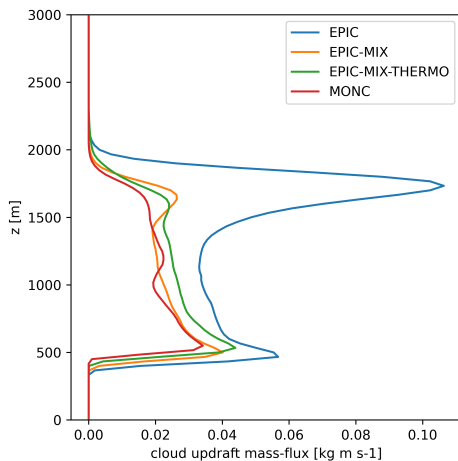
- Realistic **thermodynamics**: potential temperature, liquid water and water vapour.
- Includes large-scale forcings and **surface fluxes**.
- Mean velocity profile nudged at this point. 33m isotropic grid.



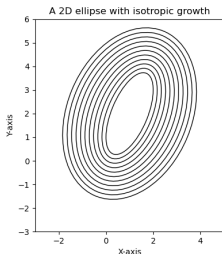
Liquid water path



Time-mean mass flux in BOMEX



- Clean separation between resolved dynamics and parameterised mixing.
- Turbulent mixing on small scales a challenge, even in Lagrangian models.
- Alternative approaches to be explored.



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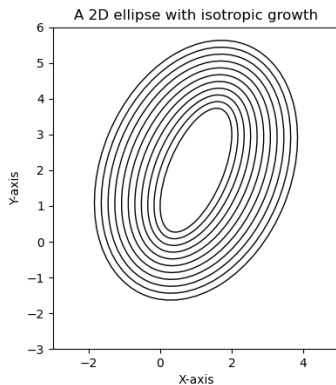
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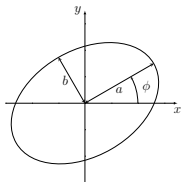
Supported by EPSRC grants EP/T025409/1 and EP/M008525/1, NERC grant NE/X018547/1

Alternative mixing formulations?

- Parcels grow and dilute over time.
- Parcels move stochastically (Brownian/Langevin/SDE).
- Parcels stretch stochastically (Brownian/Langevin/SDE for deformation tensor).
- Use parcel properties more efficiently?



Parcel-based model based on ellipses



Semi-major/-minor axes a and b

$$\mathbf{x}^T \mathbf{B}^{-1} \mathbf{x} = 1$$

where $\mathbf{B} = \begin{pmatrix} B_{11} & B_{12} \\ B_{12} & B_{22} \end{pmatrix}$ is symmetric.

Ellipse area preserved \Rightarrow Possible to store 2 (3D: 5) values per parcel (but may want one more for symmetry)!

Motion of a fluid ellipse in a linear background flow¹:

Given a linear background straining flow

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{S}(\mathbf{x}, t)\mathbf{x}(t)$$

where

$$\mathbf{S}(\mathbf{x}, t) = \nabla \mathbf{u}(\mathbf{x}, t) = \begin{pmatrix} u_x(\mathbf{x}, t) & u_y(\mathbf{x}, t) \\ v_x(\mathbf{x}, t) & v_y(\mathbf{x}, t) \end{pmatrix},$$

then reformulating the time derivative of the ellipse equation results in

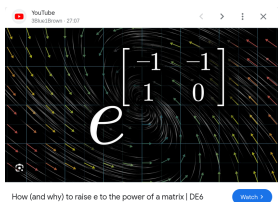
$$\frac{d\mathbf{B}}{dt} = \mathbf{B}\mathbf{S}^T + \mathbf{S}\mathbf{B}.$$

Note: This is also valid in 3D!

¹McKiver, W. J. & Dritschel, D. G. (2003). The motion of a fluid ellipsoid in a general linear background flow. *Journal of Fluid Mechanics*, 474, 147-173.

Deformation with matrix exponentials?

Computational cost is a challenge. Can we increase time step?



Tendency calculations, previously use RK4 directly on

$$\frac{d\mathbf{B}}{dt} = \mathbf{B}\mathbf{S}^T + \mathbf{S}\mathbf{B}.$$

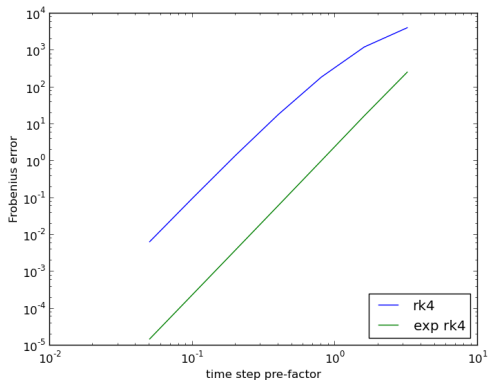
Solution for constant \mathbf{S} , which preserves volume (because \mathbf{S} is traceless)

$$\mathbf{B}(t + \Delta t) = e^{\mathbf{S}\Delta t}\mathbf{B}(t)e^{\mathbf{S}^T\Delta t}.$$

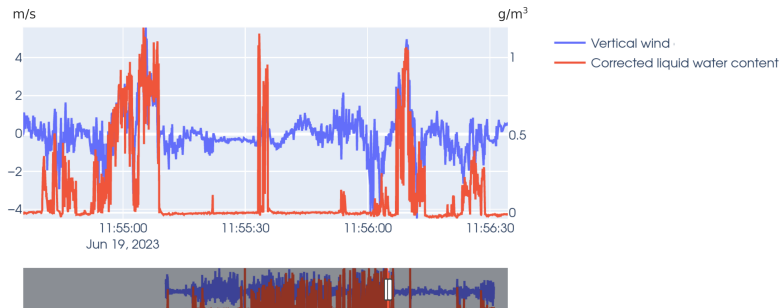
- Bit expensive, but can limit matrix multiplications needed to 3 for 8th order Taylor expansion (Bader et al. 2019).
- Possibly combine with scaling and squaring (Ward, 1977).
- Combines with low-storage RK schemes (Bazavov, 2020).

Test

- Pick random symmetric \mathbf{B} arrays.
- Pick random traceless $\mathbf{S}_{\text{start}}$ and \mathbf{S}_{end} arrays.
- Calculate time-step pre-factor (using worst case).
- Calculate error as function of time-step.



- Plan: **prognostic supersaturation** and **two-moment cloud droplets**.
- Non-precipitating vs. precipitating microphysics.
- Approach also suitable for approach using droplet bin sizes or superdroplets.
- Comparison against WOEST **flight data**.



The super-droplet method for the numerical simulation of clouds and precipitation: A particle-based and probabilistic microphysics model coupled with a non-hydrostatic model

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Meteorol Atmos Phys
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ORIGINAL PAPER

Investigation of droplet dynamics in a convective cloud using a Lagrangian cloud model

Junghwa Lee · Yign Noh · Siegfried Raasch ·
 Theres Riechelmann · Lian-Ping Wang

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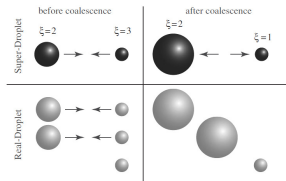


Figure 1. Schematic view of the coalescence of super-droplets. Two super-droplets with multiplicity 2 and 3 undergo coalescence (upper left panel). This represents the coalescence of two droplet pairs (lower panels). As a result, the super-droplet with multiplicity 2 becomes larger and the multiplicity of the other super-droplet decreases $3 \rightarrow 1$ (upper right panel).

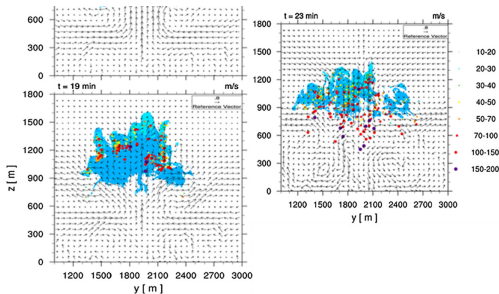
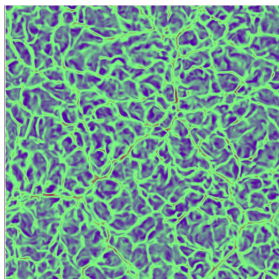


Fig. 7 Super-droplet distribution at the vertical cross section with the band thickness 100 m ($500 \text{ m} < x < 600 \text{ m}$). Vertical velocity field is overlapped for the AW case. Super-droplets are shown in different colors depending on its size ($t = 15, 17, 19, 21, 23 \text{ min}$)

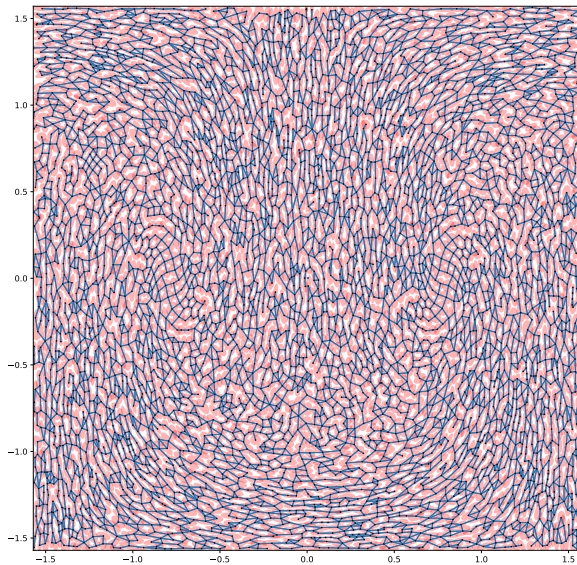
- Current simulations use free-slip boundary conditions, constant fluxes, and nudging of mean wind.
- Convective Boundary Layer study ongoing (Sam Wallace, St Andrews).



- Wind speed would determine interactive surface fluxes.
- It is not clear a priori how to implement atmospheric boundary conditions.
- Formulate Monin-Obukhov in terms of vorticity? Alternatives?

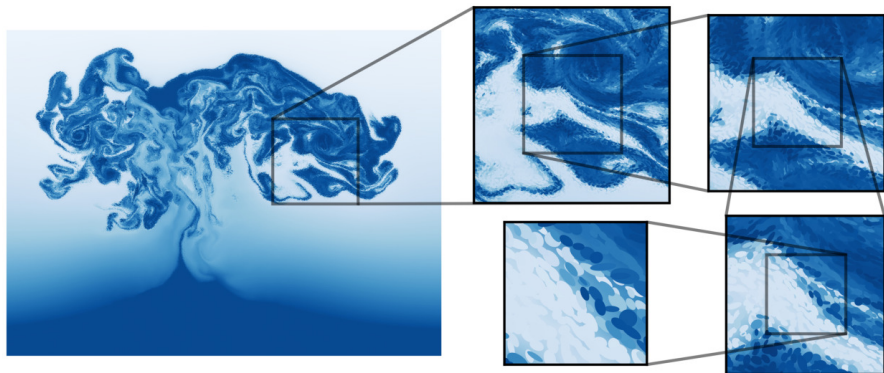
- Currently Cartesian grid, incompressible.
- However, in principle these aren't restrictions.
 1. Calculate flow field from parcel properties.
 2. Move and deform parcels.
 3. Split and merge parcels.
- Needs thinking about corrections. Local deviations from incompressible typically small in atmosphere.
- Hybrid gridded-Lagrangian options?

Exploit parcel (near) overlap?

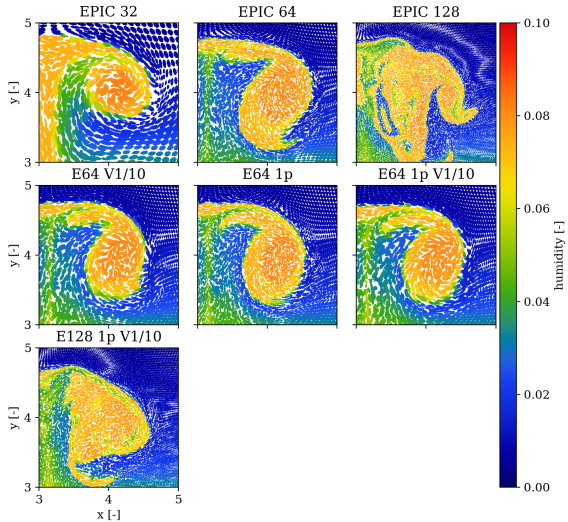


Uses algorithm of Gilitschenski and Hanebeck, IEEE, 2012

Parcel-level behaviour



Computational cost considerations



Number of grid cells	Energy loss (‰)	
	EPIC	PS3D
$48^2 \times 12$	0.310	0.514
$64^2 \times 16$	0.124	0.217
$96^2 \times 24$	0.040	0.065
$128^2 \times 32$	0.017	0.029
$256^2 \times 64$	0.002	0.005

Table 3: Relative total energy loss (in per mille) for the internal wave test case between the initial time $t = 0.0$ and the final time $t = 4\pi/\sqrt{2}$ versus the grid resolution. Note that the simulation values are interpolated to match the final time.