LES and more...

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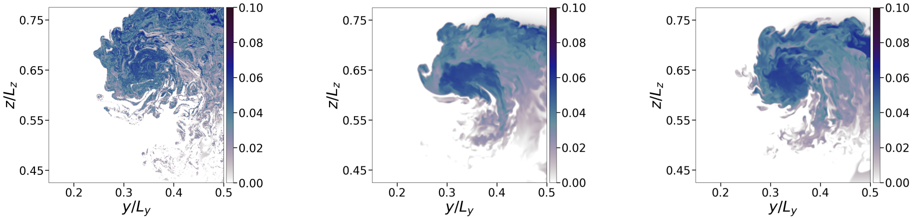


Contents

Not LES, not boundary layers (yet)

https://www.videvo.net/video/cumulonimbus-clouds-timelapse/4708/

Hybrid Lagrangian-Eulerian modelling

The basic conservation principles of fluid dynamics are most naturally expressed in a Lagrangian way: e.g. mass is conserved *following* fluid "particles".

However, certain fields are more naturally Eulerian in character, e.g. pressure. These fields are completely or largely determined by "integration", i.e. through inversion relations like Poisson's equation.

Conservation is Lagrangian. Inversion is Eulerian.

Computational methods exploiting this distinction may benefit from using a mixed, hybrid approach.

(semi)-Lagrangian modelling of the atmosphere

The idea goes back as far as Sawyer (1963): "A semi-Lagrangian method for solving the vorticity advection equation."

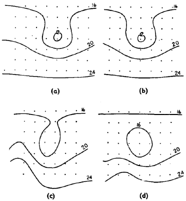
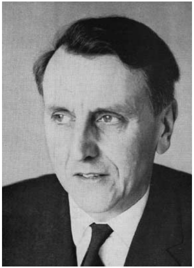


Fig. 3*a*. Correct stream function (or initial field displaced by 4 grid-lengths). *b*, Computed stream function by semi-Lagrangian procedure. *c*, Computed stream function by Eulerian (3–3–3) scheme. *d*, Computed stream function by Eulerian (3–5–3) scheme.



The UK Met Office uses Semi-Lagrangian (SL) advection for efficiency (however conservation is challenging).

Gadian (1989): simulations using fully Lagrangian smoothed particle hydrodynamics for **2D** cloud studies.

Shutts and Allen (2007): fast SL schemes inspired by gaming.

Moist Parcel-In-Cell (MPIC)

The new "Moist Parcel-In-Cell" (MPIC) algorithm goes further by representing the continuum by discrete "cloud parcels".

We use freely-moving parcels carrying *any number* of attributes (e.g. liquid water potential temperature θ_ℓ, specific humidity q, etc...)

The prototype model was developed for 3D incompressible flow (Boussinesq, no rotation):

$$\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = -\frac{\nabla p}{\rho_0} + b\hat{e}_z\,, \qquad \frac{\mathrm{D}b_\ell}{\mathrm{D}t} = 0\,, \qquad \frac{\mathrm{D}q}{\mathrm{D}t} = 0\,, \qquad \nabla\cdot\mathbf{u} = 0$$

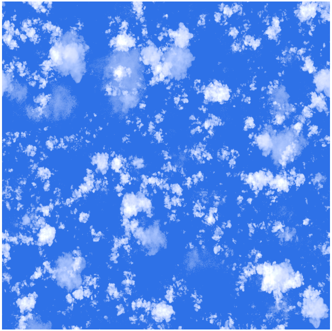
where the total buoyancy b is approximated by

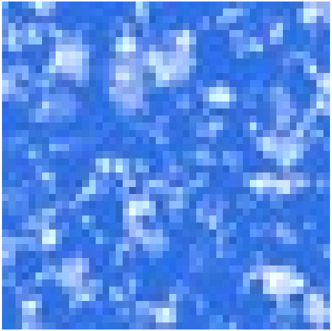
$$b = b_\ell + \frac{gL}{c_p\theta_{\ell 0}}\max\left(0, q - q_0 e^{-\lambda z}\right)\,.$$

Here, q_0 is a threshold saturation humidity, and λ is the inverse condensation scale height. L is the latent heat of condensation.

Motivation: grey zone

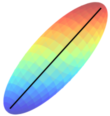
NWP/regional climate models now at 1-4 km resolution: turbulence poorly resolved. Large-Eddy Model resolution not affordable in medium long term.





The liquid-water buoyancy $b_\ell \equiv g(\theta_\ell - \theta_{\ell 0})/\theta_{\ell 0}$ where θ_ℓ is the liquid-water potential temperature and $\theta_{\ell 0}$ is a constant reference value.

In MPIC, each fluid parcel retains b_ℓ and q, *thereby exactly satisfying conservation*. Moreover, we evolve the vorticity $\boldsymbol{\omega} = \boldsymbol{\nabla} \times \mathbf{u}$ *on parcels* as 'vortons' (Novikov, 1983).



We use the equivalent form of the vorticity equation recommended in Cottet and Koumoutsakis (2001):

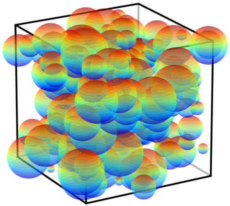
$$\frac{\mathrm{d}\boldsymbol{\omega}_i}{\mathrm{d}t} = \boldsymbol{S}(\mathbf{x}_i, t) \equiv (\boldsymbol{\nabla} \cdot \boldsymbol{F}, \boldsymbol{\nabla} \cdot \boldsymbol{G}, \boldsymbol{\nabla} \cdot \boldsymbol{H}) ,$$

for each parcel $i = 1, ..., n$, where

$$\boldsymbol{F} = \boldsymbol{\omega} u - b\hat{e}_y \quad ; \quad \boldsymbol{G} = \boldsymbol{\omega} v + b\hat{e}_x \quad ; \quad \boldsymbol{H} = \boldsymbol{\omega} w \, .$$

We must also attach a small volume V_i to each parcel in order to determine the contribution of each parcel to the fields of $\boldsymbol{\omega}$ and b represented on an underlying grid.

Interpolation: parcel $\rightarrow$ grid communication



Tri-linear interpolation is used to transfer parcel properties to gridded values.

For example, the value of the buoyancy b at each grid point $\bar{\mathbf{x}} = (\bar{x}, \bar{y}, \bar{z})$ is determined from

$$b(\bar{\mathbf{x}}) = \bar{V}^{-1} \sum_{i \in \mathcal{P}} \phi(\mathbf{x}_i - \bar{\mathbf{x}}) b_i V_i \quad \text{where} \quad \bar{V} = \sum_{i \in \mathcal{P}} \phi(\mathbf{x}_i - \bar{\mathbf{x}}) V_i$$

where the tri-linear weights ϕ are given by

$$\phi(\mathbf{x}_i - \bar{\mathbf{x}}) = (1 - |x_i - \bar{x}|/\Delta x)\,(1 - |y_i - \bar{y}|/\Delta y)\,(1 - |z_i - \bar{z}|/\Delta z)$$

and $\mathcal{P}$ is the set of all parcels within the 8 grid boxes surrounding $\bar{\mathbf{x}}$, while Δx, Δy and Δz are the grid lengths.

Advection: grid $\rightarrow$ parcel communication

The parcel motion is found by solving the simple ODEs

$$\frac{\mathrm{d}\mathbf{x}_i}{\mathrm{d}t} = \mathbf{u}(\mathbf{x}_i, t)$$

using the gridded velocity field $\mathbf{u}$ tri-linearly interpolated to the parcel position $\mathbf{x}_i(t)$.

The parcel velocity is given by

$$\mathbf{u}(\mathbf{x}_i, t) = \sum_{\bar{\mathbf{x}} \in \mathcal{G}} \phi(\mathbf{x}_i - \bar{\mathbf{x}})\mathbf{u}(\bar{\mathbf{x}}, t)$$

where $\mathcal{G}$ is the set of all grid points at the corners of the grid box containing parcel i.

Inversion: recovering the velocity field

The velocity field $\mathbf{u}$, needed to move the cloud parcels and to determine the vorticity source, is found by inverting $\boldsymbol{\omega}$ in a horizontally-periodic domain (in x and in y) bounded above and below by flat, free-slip boundaries at $z = L_z$ and $z = 0$.

To satisfy incompressibility ($\boldsymbol{\nabla} \cdot \mathbf{u} = 0$), we take $\mathbf{u} = -\boldsymbol{\nabla} \times \boldsymbol{A}$ where $\boldsymbol{A}$ is a vector potential. From the definition of vorticity, we find

$$\boldsymbol{\omega} = \boldsymbol{\nabla} \times \mathbf{u} = \nabla^2 \boldsymbol{A} - \boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \boldsymbol{A})\,.$$

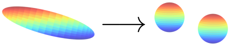
We are free to impose $\boldsymbol{\nabla} \cdot \boldsymbol{A} = 0$, leading to

$$\boldsymbol{\omega} = \nabla^2 \boldsymbol{A}\,,$$

Numerically, this is done in 'spectral space' after using Fast Fourier Transforms for accuracy and efficiency.

Parcel splitting and mixing

Splitting is controlled by prescribing the maximum stretch γ (default: 4) a parcel may undergo. The stretch of each parcel i is defined by



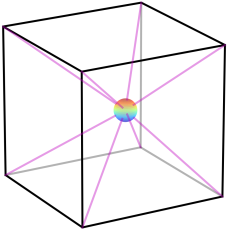
$$\gamma_i(t) = \int_{t_0}^{t} |\boldsymbol{\omega}_i \cdot \mathrm{d}\boldsymbol{\omega}_i/\mathrm{d}t|^{1/3}\mathrm{d}t$$

where t_0 is the time since the parcel last split, or otherwise the initial time.

Parcel removal is controlled by prescribing the minimum volume fraction $\hat{V}_{\min}$ (default: $1/6^3$) a parcel can have, i.e.

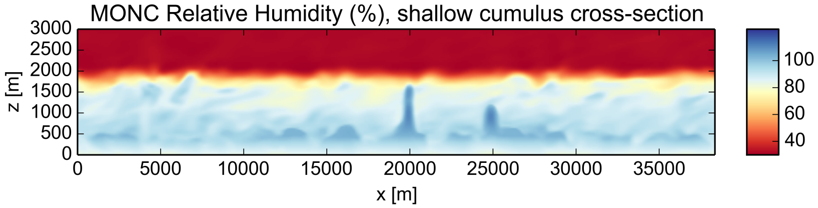
$$V_i/\Delta x\Delta y\Delta z \geq \hat{V}_{\min}.$$

Removal: the properties of surrounding parcels are adjusted to exactly conserve total volume, mass and liquid water content.



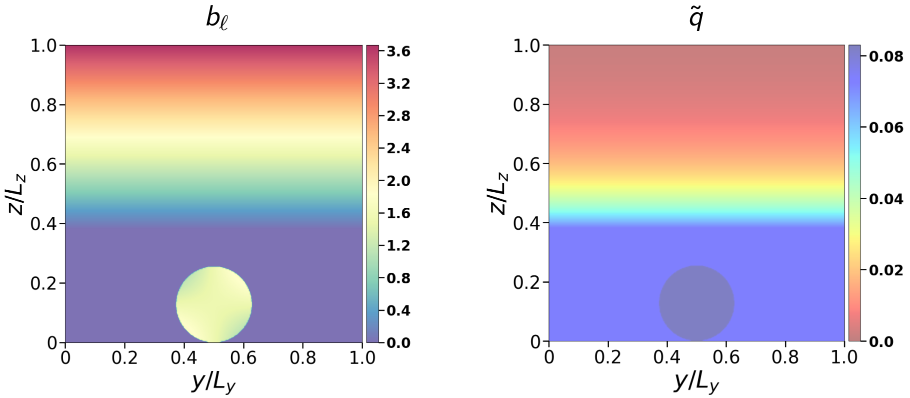
Reference model: MONC

MONC: Met Office Large-Eddy Model recently optimised for use on large parallel computers.
EPCC/Met Office collaboration.



Finite difference model on staggered grid. Smagorinsky subgrid model using nonlinear diffusion to account for unresolved turbulence OR monotonical integration using TVD advection.

We start with a spherical thermal of nearly uniform b_ℓ and $\tilde{q} \equiv q/q_0$ in a neutral layer near the ground, with a stratified zone aloft. Here $x = 0$ is shown.

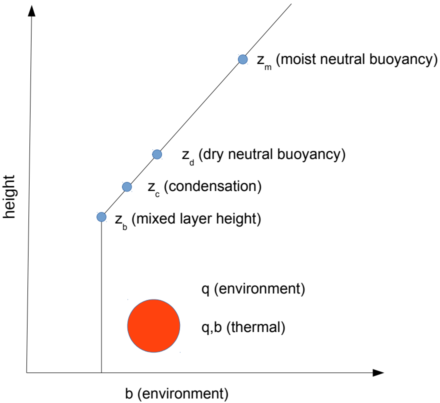


Vertical structure of the environment

The environment favours condensation (cloud formation) once the thermal rises past the lifting condensation level $z = z_c$.

This releases additional buoyancy, increasing the vertical acceleration, and takes the thermal past its level of dry neutral buoyancy $z = z_d$.

Only when the thermal encounters the level of moist neutral buoyancy $z = z_m$ (the nominal cloud top) is the upward acceleration arrested.

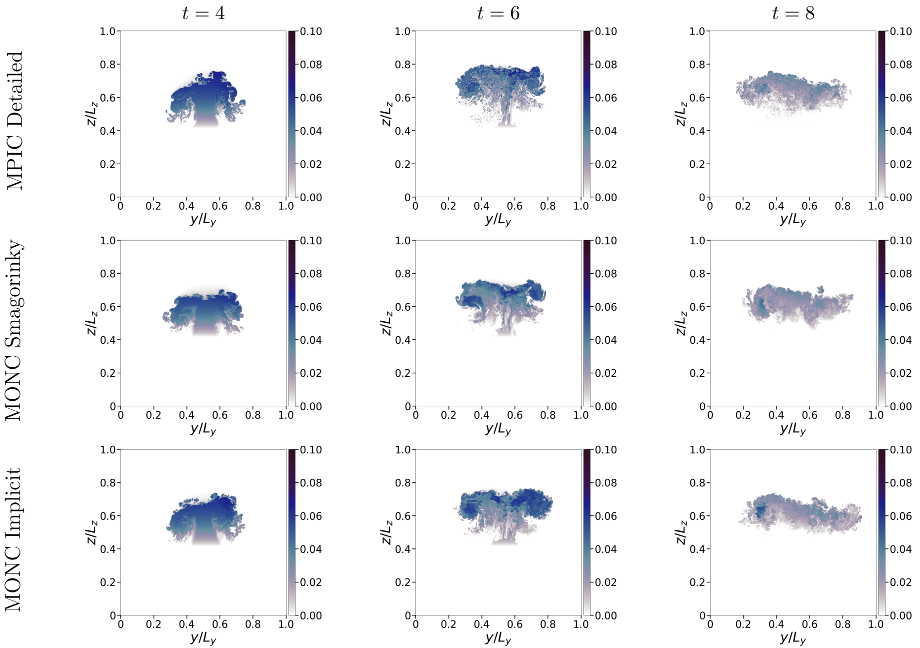


Reference simulations

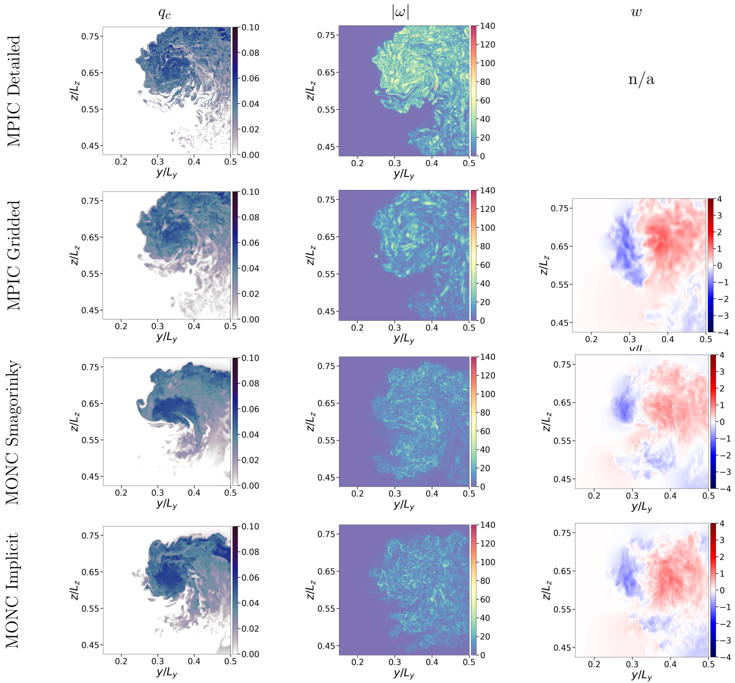
384^3 MPIC and 1024^3 MONC.

1) Evolution of liquid-water specific humidity.

2) Detailed zoom of liquid-water specific humidity, vorticity, vertical velocity at $t = 6$.



t = 4
t = 6
t = 8
MPIC Detailed
MONC Smagorinky
MONC Implicit
z/Lz
y/Ly

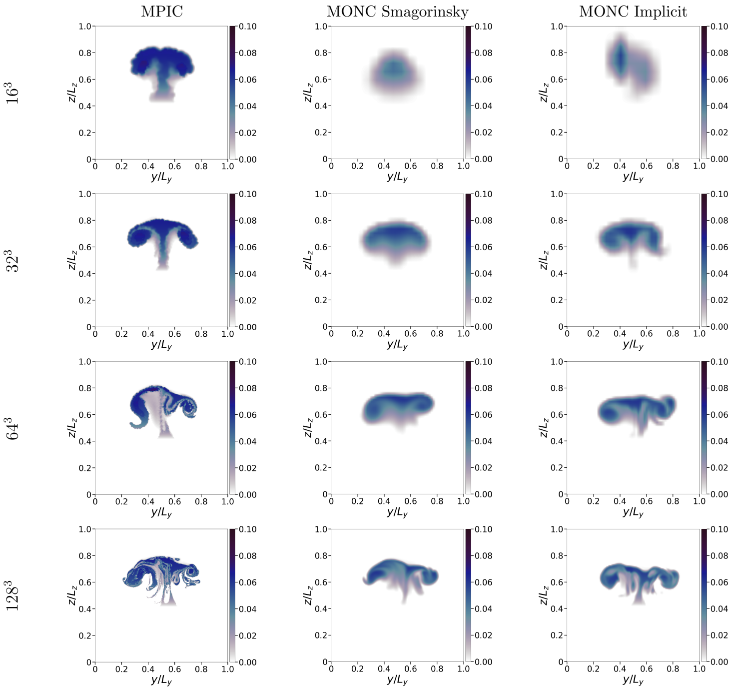


q_c
$|\omega|$
w
MPIC Detailed
MPIC Gridded
MONC Smagorinky
MONC Implicit
n/a
z/L_z
y/L_y

Resolution sensitivity

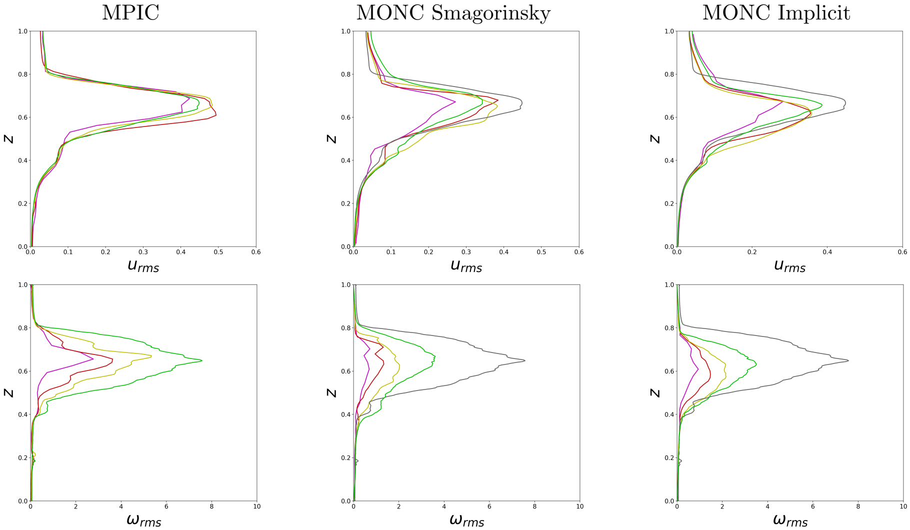
1) Liquid-water specific humidity at $t = 6$.

2) Convergence of bulk properties.

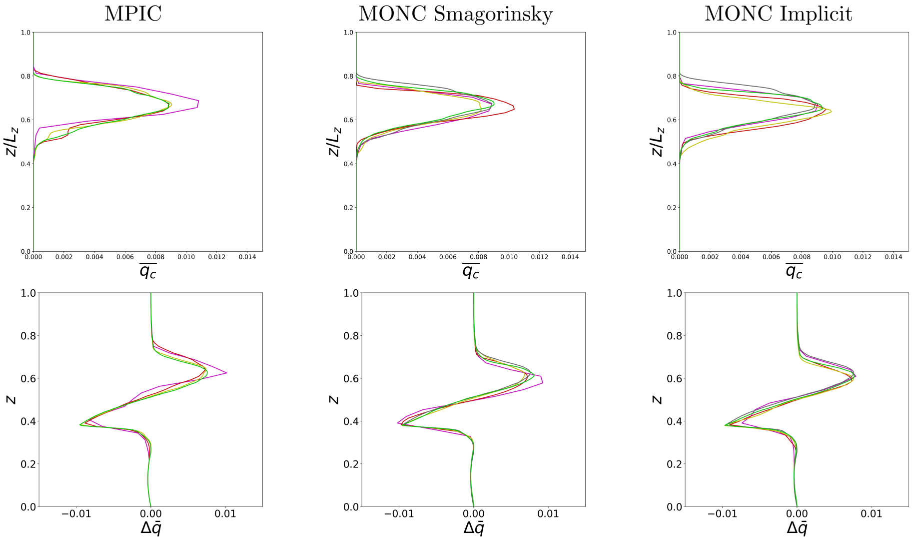


MPIC
MONC Smagorinsky
MONC Implicit
16^3
32^3
64^3
128^3
z/L_z
y/L_y
0
0.2
0.4
0.6
0.8
1.0
0.00
0.02
0.04
0.06
0.08
0.10

Vorticity converges slowly (influence of initial conditions?)
Much higher vorticity in MONC simulation (grey line: reference).

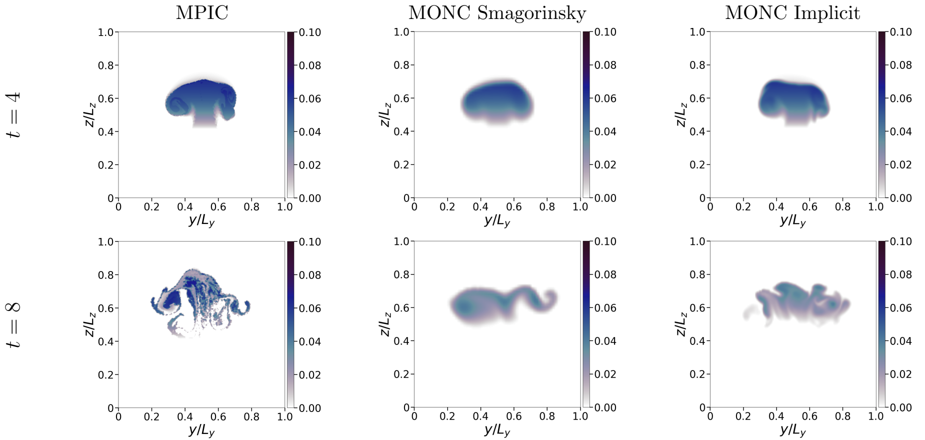


Top: liquid water at $t = 6$.
Bottom: change in total water content over the simulation.



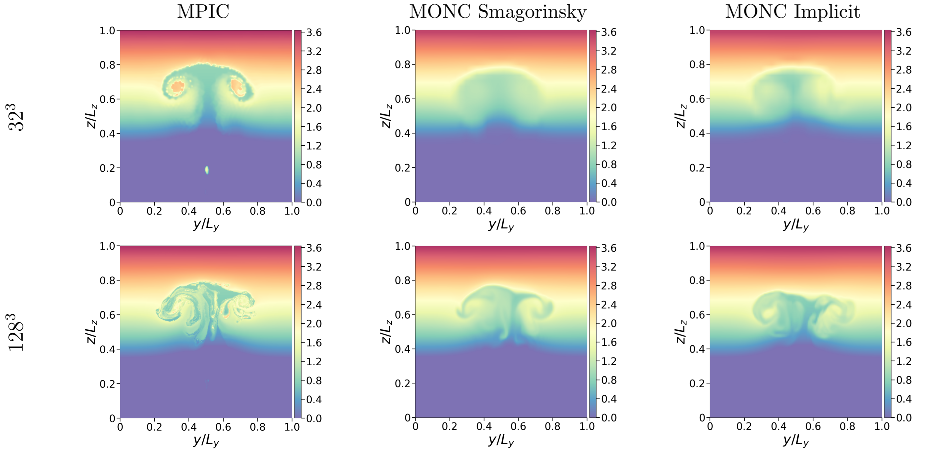
Time evolution of a marginally resolved simulation

Liquid water field: smooth in MONC, detailed in MPIC.



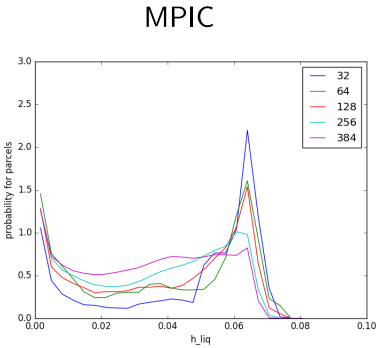
Time evolution of a marginally resolved simulation

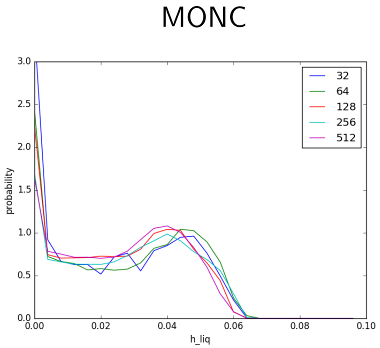
Relatively undiluted region in vortex ring at low resolution (MPIC).



Time evolution of a marginally resolved simulation

Liquid water PDF: MONC has better convergence here.
MPIC calculated directly from parcels (this matters!)

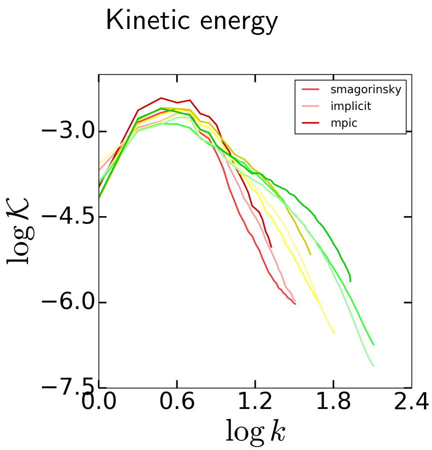


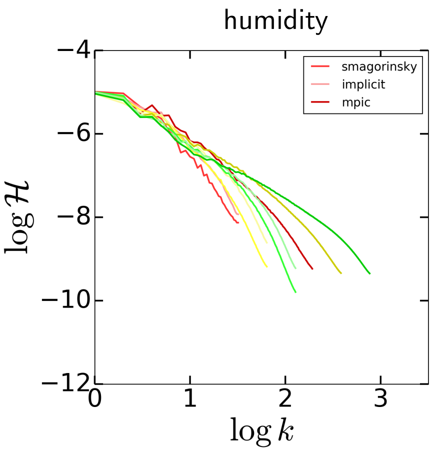


Is the resolved flow providing rapid enough mixing in MPIC? Do the unresolved scales play a crucial role?

Spectra

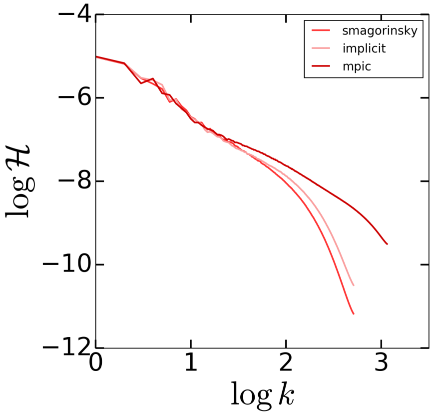
MPIC effectively doubles resolution!
Specific humidity spectra show a lot of detail (realistic?) on fine scales
Based on 64^3, 128^3, 256^3 grid points.





Spectra of humidity, reference simulations

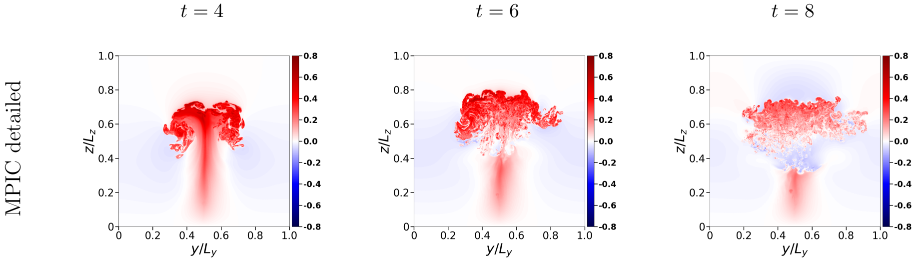
384^3 MPIC and 1024^3 MONC.
Small scale structures undampened in MPIC.



Current work: box counting and fractal dimension!

Example of Lagrangian diagnostics

Determine displacement from initial position for each parcel.



Current plans

- Massive parallelism: project with EPCC.
- More flexible boundary conditions:
  Mean wind profile.
  Surface fluxes (heat, moisture, momentum). Vorticity damping?
  Inhomogeneous surface values.
- Further work on marginally resolved and subgrid-scale dynamics. Explicit representation of stretching, following McKiver and Dritschel (2003)? Minimize spectral filtering (first results promising)?
- Realistic thermodynamics and microphysics: proposed PhD project on prognostic droplet-size distribution, EPSRC proposal. From idealised to atmospheric model.
- Exploitation of vorticity diagnostics and Lagrangian analysis (with David Dritschel and Sam Wallace)

Parallelism

- Currently OpenMP. HPC trend to large distributed memory systems.
- Much more parcel data than grid data.
- Parcel data: local communication. Use derived types?
- Solver: requires global communication, but efficient algorithms exist.

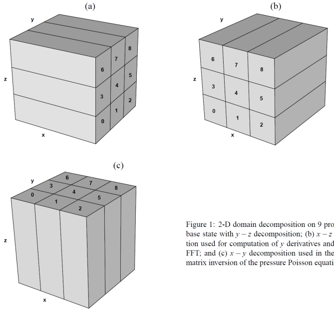


Figure 1: 2-D domain decomposition on 9 processors: (a) base state with $y-z$ decomposition; (b) $x-z$ decomposition used for computation of y derivatives and 2-D planar FFT; and (c) $x-y$ decomposition used in the tridiagonal matrix inversion of the pressure Poisson equation.

FFT Domain decompositions. Peter Sullivan, NCAR

eCSE project

A fully Lagrangian dynamical core for the Met Office NERC Cloud Model

St Andrews, Leeds, EPCC (Michèle Weiland, Nick Brown, Gordon Gibb)

Ideas:

- Harness MONC's parallelism.
- Poisson solver available. FFT-based solver hard to beat with limited grid data, but iterative solver also present.
- Approach: domain decomposition, number of parcels per subdomain will vary (simplicity versus optimal load balancing).
- Lagrangian diagnostics can feed back into standard MONC.
- Component testing using simplified code.

Objectives

(1) Introduce the Lagrangian dynamical core into the MONC framework: rewrite as independent components.

(2) Maintain the existing OpenMP in conjuction with MPI for the dynamical core: halo-exchanges and solver.

(3) Introduce parcel-based IO in the MONC framework: MONC's IO server fully asynchronous.

(4) Modernise MPIC code base: derived types, dynamic allocation.

Benefits

- First use of this type of model in atmospheric community.
- Massively parallel MPIC will make it more attractive for other problems, e.g. ocean mixed layer, idealised convection, density-laden flows.
- MPIC approach seems very well suited to mixed-mode parallelism.
- Alternative approaches will be available for MONC community.
- Lagrangian diagnostics currently lacking in MONC.
- BSD license.

Conclusions and future work

MPIC's parcel-based representation of variables has several advantages:

(1) it allows an *explicit* subgrid representation;

(2) it provides a velocity field which is *undamped* by numerical diffusion all the way down to the grid scale;

(3) it does away with the need for eddy viscosity parametrisations and, in their place, it provides for a natural subgrid parcel mixing;

(4) it is *exactly conservative* — there can be no net loss or gain of any theoretically conserved attribute; and

(5) it dispenses with the need to have separate equations for each conserved parcel attribute — attributes are simply labels carried by each parcel. Moreover, this advantage increases as more attributes are added, such as the distributions of microphysical properties, chemical composition and aerosol loading.

Conclusions and future work

Numerical tests demonstrate the robustness of the MPIC method as well as its ability to capture fine detail using only modest underlying grid resolutions.

The MPIC method is shown to compare well with a convection-permitting research model (MONC) run on a grid at least twice as fine in each coordinate direction.

Convergence of mixing in MPIC (parcel splitting and removal) remains an issue (i.e. for distributions of condensed water).

Many extensions are possible. An immediately viable one is to study sub-mesoscale ocean dynamics, particularly near the surface — no condensation is then required. This is a major topic in oceanography (Gula, Molemaker & McWilliams, 2014).

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Discussion points: methods

Experiences with monotonically integrated LES

Boundary conditions: law of the wall, roughness, transfer of momentum

Anisotropic subgrid models (walls, stratification)

Poorly resolved LES: parametrised versus explicit dynamics

Closures: Smagorinky, TKE, TKE+scalar variance, HOC

Time-stepping methods and advection schemes

Discussion points: test cases

Numerical tests

Testbeds settings: long-term LES

Experiences with topography in LES