The Moist Parcel-in-Cell (MPIC) method
Towards a physically realistic, parcels-based model

S. Böing
with D. Dritschel, D. Parker & A. Blyth
Universities of Leeds & St Andrews
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Essentially Lagrangian 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.
The idea goes back as far as Sawyer (1963): “A semi-Lagrangian method for solving the vorticity advection equation.”

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

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 $\theta_\ell$, specific humidity $q$, etc...)

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

$$
\frac{D\mathbf{u}}{Dt} = -\frac{\nabla p}{\rho_0} + b\hat{e}_z, \quad \frac{Db_\ell}{Dt} = 0, \quad \frac{Dq}{Dt} = 0, \quad \nabla \cdot \mathbf{u} = 0
$$

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 $\lambda$ is the inverse condensation scale height. $L$ is the latent heat of condensation.
The liquid-water buoyancy $b_\ell \equiv g(\theta_\ell - \theta_{\ell 0})/\theta_{\ell 0}$ where $\theta_\ell$ is the liquid-water potential temperature and $\theta_{\ell 0}$ is a constant reference value.

In MPIC, each fluid parcel retains $b_\ell$ and $q$, thereby exactly satisfying conservation. Moreover, we evolve the vorticity $\omega = \nabla \times u$ on parcels.

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

$$\frac{d\omega_i}{dt} = S(x_i, t) \equiv (\nabla \cdot F, \nabla \cdot G, \nabla \cdot H),$$

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

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

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 $\omega$ and $b$ represented on an underlying grid.
Tri-linear interpolation is used to transfer parcel properties to gridded values and vice versa. The parcel motion is found by solving

$$\frac{dx_i}{dt} = u(x_i, t)$$

using the gridded velocity field $u$ tri-linearly interpolated to the parcel position $x_i(t)$. 
The velocity field \( \mathbf{u} \), needed to move the cloud parcels and to determine the vorticity source, is found by inverting \( \omega \) in a horizontally-periodic domain (in \( x \) and in \( y \)).

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

\[
\omega = \nabla \times \mathbf{u} = \nabla^2 \mathbf{A} - \nabla(\nabla \cdot \mathbf{A}).
\]

We are free to impose \( \nabla \cdot \mathbf{A} = 0 \), leading to

\[
\omega = \nabla^2 \mathbf{A},
\]
Parcel splitting and mixing

Explicit equation for parcel stretching:

$$\gamma_i(t) = \int_{t_0}^{t} |\omega_i \cdot \frac{d\omega_i}{dt}|^{1/3} dt$$

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

Small parcels removed in conservative way
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 \( t = 6 \).
Vorticity converges slowly (influence of initial conditions?)
Much higher vorticity in MPIC simulation (grey line: MPIC at $256^3$).
Time evolution of a marginally resolved simulation

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

MPIC

MONC

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

Determine displacement from initial position for each parcel.

\[ t = 4 \quad t = 6 \quad t = 8 \]
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.
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, both for atmosphere and ocean applications. The option to look into detailed vortex interaction could provide new pathways to cold pool dynamics.
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!
Time evolution of a marginally resolved simulation

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

\[ t = 4 \]

\[ t = 8 \]
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)
- 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.

FFT Domain decompositions. Peter Sullivan, NCAR
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.
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.