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Transport modelling

Part 1 Eulerian approach Mesoscale modelling Better and better !

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Part 2 Chemistry Lagrangian Trajectories (for water vapour studies) Eulerian + Lagrangian $d\overline{\mathbf{V}}/dt + fk \times \overline{\mathbf{V}} + \nabla\overline{\phi} = \mathbf{F},$ $d\overline{T}/dt - \kappa \overline{T}\omega/p = Q/c_p,$ $\nabla \cdot \overline{\nabla} + \partial \overline{\omega} / \partial p = 0,$ $\partial \overline{\phi} / \partial p + R\overline{T} / p = 0,$ $d\bar{q}/dt = S_q$.

(horizontal momentum) (thermodynamic energy) (mass continuity) (hydrostatic equilibrium) (water vapor mass continuity)

Equation of motion F

Turbulent transport, generation and dissipation of momentum

Thermodynamic energy equation, Q Sources, Sinks (radiation/convective-scale phase change)

Water vapour mass continuity S

Sources / sinks of water mass

Transport

$$\frac{\partial n}{\partial t} = -\frac{\partial F_x}{\partial x} - \frac{\partial F_y}{\partial y} - \frac{\partial F_z}{\partial z} + P - L = -\nabla \cdot F + P - L$$

N=number of molecules of ...

F=nUdxdy / dxdy (normalized)

$$\frac{\partial n}{\partial t} = -\nabla \bullet (n\boldsymbol{U}) + P - L$$



 $\frac{\partial}{\partial t} \bar{n} = -\nabla \cdot (\bar{F}_{A} + \bar{F}_{T}) + \bar{P} - \bar{L}$ Fick's law: $F_{T} = -nD \text{ grad}(n)$ $= -\nabla \cdot (\bar{n}\bar{U}) + \nabla \cdot (Kn_{a}\nabla \cdot \bar{C}) + \bar{P} - \bar{L}$

Discretization

$$A \cdot n(\boldsymbol{X}, t_o) = n(\boldsymbol{X}, t_o) + \int_{k}^{k_{outd} \Delta k} \left[\frac{\partial n}{\partial t}\right]_{advection} dt$$

 $n(\mathbf{X}, t_o + \Delta t) = C \cdot T \cdot A \cdot n(\mathbf{X}, t_o)$

$$\begin{split} n(i, j, k, t_o + \Delta t) &= n(i, j, k, t_o) \\ + \frac{u(i-1, j, k, t_o)n(i-1, j, k, t_o) - u(i, j, k, t_o)n(i, j, k, t_o)}{\Delta x} \Delta t \\ + \frac{v(i, j-1, k, t_o)n(i, j-1, k, t_o) - v(i, j, k, t_o)n(i, j, k, t_o)}{\Delta y} \Delta t \\ + \frac{w(i, j, k-1, t_o)n(i, j, k-1, t_o) - w(i, j, k, t_o)n(i, j, k, t_o)}{\Delta z} \Delta t \end{split}$$

A= advection T= turbulent transport C= Chemistry



Hypothesis: C, T, A can be separated

A question of scales

- Impossible to explicitly resolve all physical processes
- Necessary to parametrize it function of model variables
- The parametrization depends on the spatial and temporal scales
- Issue: complexity and computing time !



Time

For a grid of atmospheric columns:

- 'Dynamics': Iterate Basic Equations
 Horizontal momentum, Thermodynamic energy,
 Mass conservation, Hydrostatic equilibrium,
 Water vapor mass conservation
- 2. Transport 'constituents' (water vapor, aerosol, etc)
- Calculate forcing terms ("Physics") for each column Clouds & Precipitation, Radiation, etc
- Update dynamics fields with physics forcings
- 5. Chemistry
- 6. Gravity Waves, Diffusion (fastest last)
- Next time step (repeat)

From Gettelman



Parameterization computes the changes in temperature and moisture (and possibly cloud water, momentum, etc.) Tendency, applied at each timestep The tendency can be calculated each n timestep (where τ_c is a convective timescale, typically 30min to 1hr)

momentum

$$\frac{du}{dt} + \frac{1}{\rho} \frac{\partial p}{\partial x} - fv = (P_{conv}) + P_{hdiff} + P_{vdiff} + P_{sfc}$$

$$\frac{\left. \frac{\partial \theta}{\partial t} \right|_{conv} = \frac{\theta_{final} - \theta_{initial}}{\tau_c} = P_{conv}$$

How Does the Feedback Occur Physics

At every grid point, predictive variables change at each time step Different processes concur to modify temperature and water vapour

temperature

$$\frac{d\theta}{dt} = P_{rad} + P_{conv} + P_{cond / evap} + P_{hdiff} + P_{vdiff} + P_{sfc}$$
water vapor
$$\frac{dq_{v}}{dt} = P_{conv} + P_{cond / evap} + P_{hdiff} + P_{vdiff} + P_{sfc}$$

Which processes goes into the regional scale ?

A large number of ways to parametrize processes in the models based on physical laws and empirical assumptions

BOLAM model (Bologna Limited Area)

Describe the parametrizations

Example that can be extended to mesoscale models

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GAW Overview of existing integrated Mesoscale meteorological and chemical transport models in Europe (available at www.cost728.org)

BOLAM Main Features: model dynamics (Buzzi et al, 1994)



Primitive equations with u, v, θ , q, ps as dependent variables (+ 5 microphysical variables);

- \blacktriangleright Rotated Arakawa C grid; σ vertical coordinate, recently hybrid $p=p_0 \sigma - (p_0 - p_s) \sigma^{\alpha} (\alpha > 1)$ on non uniform, staggered Lorenz grid;
- → Original forward-backward 3-D advection scheme (FBAS Malguzzi and Tartaglione, 1999) coupled with semi-lagrangian advection of hydrometeors; or WAF (Weighted Average Flux) scheme.
- ► Split-explicit time scheme (FB for gravity modes);
 - 4th order horizontal diffusion and 2nd order divergence diffusion;
- Davies-Kållberg-Lehmann relaxation scheme for lateral boundary conditions.



BOLAM Main Features Physical aspects

- Radiation: infrared and solar, interacting with clouds (Ritter & Geleyn and ECMWF *RRTM Rapid Radiative Transfer Model*).
- ➡ Vertical diffusion (surface layer and PBL parameterization) depending on the Richardson number (Louis scheme and -recently- E-l scheme).
- ➡ Soil and vegetation scheme, 4 layers (developed in coop. with the Hydrometeorological Institute of Russia Pressman, 2002; Drofa et al, 2003-2005).
- Explicit microphysical scheme with 5 hydrometeors (cloud ice, cloud water, rain, snow, hail/graupel), modified from Schultz (1995) and Drofa (2001). Global database available.

Convective parameterization: Kain-Fritsch (Kain, 2004), allowing interaction with the microphysical scheme.





WAF (weighted area flux) Billet and Toro 1997



$$\begin{split} f_{i+\frac{1}{2}} &= \frac{1}{\Delta x} (\rho_i u \frac{1}{2} \Delta x + \rho_i u \frac{1}{2} u \Delta t + \rho_{i+1} u \frac{1}{2} \Delta x - \rho_{i+1} u \frac{1}{2} u \Delta t) \\ &= \frac{1}{2} \rho_i u + \frac{1}{2} \rho_i u (u \frac{\Delta t}{\Delta x}) + \frac{1}{2} \rho_{i+1} u - \frac{1}{2} \rho_{i+1} u (u \frac{\Delta t}{\Delta x}) \end{split}$$

Linear numerical schemes for solving partial differential equations (PDE's), having the property of not generating new extrema (monotone scheme), can be at most first-order accurate Godunov, 1959 $\varphi_{j}^{n+1} = \sum_{m}^{M} \gamma_{m} \varphi_{j+m}^{n}.$ (2) $\gamma_{m} \geq 0, \quad \forall m.$ (3)

$$\begin{array}{ll} f_{i+\frac{1}{2}} & = & \frac{1}{2}\rho_{i}u(1+\nu) + \frac{1}{2}\rho_{i+1}u(1-\nu) \\ \\ & \text{Since }\nu = u\frac{\Delta t}{\Delta x}; \end{array}$$





How to Parameterize convection

- Relate unresolved effects to grid-scale properties using statistical or empirical techniques
- Several schemes (Grell-Pan / Kain-Fritsch / Betts-Miller / Emanuel / ...)
- Mass-Flux: use simple cloud models to simulate rearrangements of mass in a vertical column

What properties of convection do we need to predict?

- convective triggering (yes/no)
- convective intensity (how much rain?)
- vertical distribution of heating and drying (feedback)

No scheme required if resolution high enough to reproduce updraft / downdraft (5 km)

When and where

Triggering (always requires positive area on a thermodynamic [e.g., Skew-T Log-P] diagram)

1.) mass or moisture convergence exceeding a certain threshold at a grid point, or

2.) positive destabilization rate, or

3.) perturbed parcels can reach their level of free convection, or

4.) sufficient cloud layer moisture





Т



And how much...

Convective intensity (net heating)

- proportional to mass or moisture convergence
- sufficient to offset large-scale destabilization rate
- sufficient to eliminate CAPE (constrained by available moisture)
- Vertical distribution of heating and drying
 - determined by nudging to empirical reference profiles
 - estimated using a simple 1-D cloud model to satisfy the constraints on intensity





Louis (1979): (simple but still used in CTMs)

$$\overline{w'C'} = -Kc \frac{\partial C}{\partial z}$$

PBL scheme (Holtslag and Boville, 1993)

$$\overline{w'C'} = -(Kc\frac{\partial C}{\partial z} - \gamma_c)$$

Here C: concentration, Kc: eddy diffusivity, z: Height, y reflects the nonlocal transport due to large eddy motion in the convective ABL. First term implies that scalar flux is always downgradient, the second term models the scalar flux as proportional to the strength of chemical flux of C from the surface





$$\Phi_{q} = \rho_{S}C_{D}\left(q_{SKIN} - q_{1}\right)$$

$$\Pi_{1} = -P_{RES} - P_{MELT} + \Phi_{SOIL} + \sum_{k=1} \Phi_{EVTR_{k}}$$

$$q_{1}^{G}(t + \Delta t) = q_{1}^{G}(t) + \frac{\Delta t}{\rho_{W}\Delta z_{1}}\left(-\Pi_{1} + \Pi_{2}\right)$$

$$\prod_{k=1}^{Lowest}$$

Schematic representation of the vegetation-soil scheme

F turb, is turbulent flux of entropy and water vapour, F rad, is flux of shortwave and longwave radiation, F precip, is flux of atmospheric precipitation, Fwc and Fwcv are hydraulic and vegetation fluxes of soil water content, Fsc and Fsw are conductivity and hydraulic fluxes of soil entropy

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Cloud processes





FIG. 1. Flow diagram for the NWP explicit microphysics algorithm; r is mixing ratio. The subscripts are v, vapor; p, cloud ice; lr, liquid saturation; ir, ice saturation. Schultz, 1995 Drofa, 2002

- Cloud / Ice / Rain / Snow / Graupel qc, qp, qr, qs, qi
- Condensation
- Collection dqr/dt=Ccrqrqc
- Melting
- Evaporation

- Fall

Very nice, but ... it works well ?

Models include a large number of parametrization of complex processes
We are often interested to problems that involve a large number of processes
And results are sensitive to (a lot) of them
How to improve them ?
Observations are the key
An example using a simple assimilation scheme