Atmospheric modelling at AMCG: From the street to the clouds

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Air Quality and Health

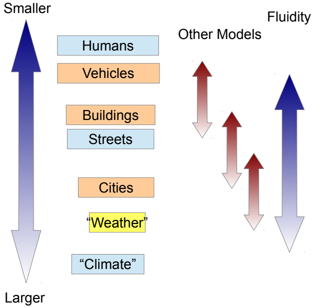
- Human activity has many impacts on the quality and health of the enviroment around us.
- Industry, transportation, cooking & other normal economic activities all increase quantities of aerosol pollutants in the air, both locally and globally
- Similar pollutants are also produced from natural sources; Volcanos, wild fires, biomass etc.
- Air quality has a direct impact on human health and quality of life.

Air Quality and Health

- Increased understanding of processes and distribution of pollutants important
  - Scientifically
  - For predicting and mitigating adverse health impacts
  - To satisfy regulatory bodies.
- Direct observation can be difficult, expensive or unfeasible
- In many cases the answer is numerical computation; modelling.

Atmospheric Modelling

- Air pollution has effects on many scales
  - human body (microns)
  - home/office (10 cm)
  - street (1 m)
  - district (100 m)
  - city (1 km)
  - region (10 km)
  - global (100 km)



Atmospheric Modelling

The important physics depends on the scales and sources of the pollutant:

Scale	Physical Processes
0-1m: Street scale	Dominated by local momentum forcing
1m-100m: District	Effects of buoyancy important
100m-1km: City	Chemical reactions important
1km-10 km: Regional	Wet deposition important
10km-100km: Global	Rotation dominated

Atmospheric Modelling

Existence of multiple scales is a classic opportunity for adaptive meshing:

- Model each area at the scale of interest
- Reduced need for nesting!
- Study behaviour of coupled system not forced system.
- Adaptivity example: movie

Also reduced order modelling; calculate only behaviour of primary degrees of freedom, very fast codes which exhibit the important behaviour to be modelled.

The Street Scale

- Flow modelled as a problem in Computational fluid dynamics.
- Primarily momentum driven.
- Two dimensional example from point source (D. Pavldids) : movie
- Reduced order model : movie
- Two dimensional comparison: (F. Fang & D. Pavldids) : movie
- Three dimensional comparison (full model & ROM): movie

Convective Scale modelling - ATHAM Fluidity

- ATHAM: The Active Tracer High-resolution Atmospheric Model. Originally developed at Max-Plank Institute, Hamburg. Used to study convective scale thunderstorm formation, volcanic plumes, wild fires etc.
- Fluidity: Advanced finite element Navier-Stokes solver with unstructured mesh and mesh adaptive capability.
- Synergy combines advanced numerics, modular form, simple GUI and adaptive capability of Fluidity with ATHAM's comprehensive library of microphysical process modules and parameterizations.

ATHAM: key Modelling Assumptions

Key modelling assumptions:

- Single temperature
- single pressure.
- Bulk momentum equation.

Materials sink/rise relative to bulk velocity parallel to gravitation

- Fall out a function of material only.

ATHAM-Fluidity

- Compressible bulk Navier-Stokes equations solved via iterated pressure correction method.
- Gas phase satisfies ideal gas law.
- Semi-Implicit formulation filters fast acoustic waves

$$\frac{\partial}{\partial t}(\rho u) + \nabla \cdot \rho u u = \nabla p - \rho g,$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho u = 0,$$

$$\frac{\partial \Theta}{\partial t} + \left(u + u'_{\Theta}\right) \cdot \nabla \Theta = S_{\theta},$$

$$p = \rho_g R_g T,$$

ATHAM-Fluidity

- Tracer equation for each material mass fraction
- Tracers advected by bulk flow (plus fallout velocity)
- Pressure obtained from ideal gas law for gas phase mixture.

$$\frac{\partial q_i}{\partial t} + \left(u + u_i'\right) \cdot \nabla q_i = 0,$$

$$p = \rho_g R_g T$$

ATHAM-Fluidity

- Bulk potential temperature related to in situ temperature through material heat capacities (sum of linearized entropies)
- Bulk density calculated from mass fraction weighted sum.

$$T = \frac{\left(c_{p,g} q_g + \sum_{\text{incomp}} c_{p,n} q_n\right) \Theta}{\left(\frac{p}{p_0}\right)^{\frac{R_g}{c_{p,g}}} c_{p,g} q_g + \sum_{\text{incomp}} c_{p,n} q_n}$$

$$\frac{1}{\rho} = \frac{q_g}{\rho_g} + \sum_{\text{incompressible}} \frac{q_n}{\rho_n},$$

Microphysics routines

- Microphysics (or "physics") routines parameterize phase changes on scale of raindrops (mm-cm) in terms of bulk dynamic variables.
    - Total material mass conserved through exchange,

$$\sum_i q_i = 1$$

    - ATHAM process pentagram for mass exchange

Herzog et al. (1998)

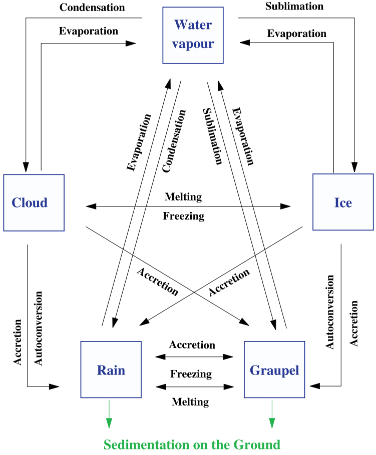


Fig. 1. Scheme of the microphysics for water.

Example: Condensation of Supersaturated Water

- Gvien enough cloud condensation nuclei, water vapour condenses out of air when water vapour partial pressure is higher than saturation pressure over flat liquid surface
- Empirical curve gives

$$p_{\mathrm{sat(vap)}} = 611.2 \exp\left(\frac{17.62\,(T - 273)}{T - 30}\right)$$

- Obtain saturation mass fraction by considering partial pressure of water vapour only.

$$q_{\mathrm{sat}} = q_g \frac{p_{\mathrm{sat}}}{\rho_g R_v T},$$

Example: Condensation of Supersaturated Water

- Relative humidity, $RH = \frac{q_v}{q_{sat}}$, between a bit above 0 and 1 and a bit.
- Assume superaturated water relaxes to saturation pressure over single timestep
- Mass removed from vapour phase

$$\frac{dq_v}{qt} = -\frac{q_v - q_{\mathrm{sat}}}{\Delta t} \mathscr{H}(q_v - q_{sat}) + \dots$$

- Mass inserted into cloud water phase

$$\frac{dq_c}{qt} = \frac{q_v - q_{\mathrm{sat}}}{\Delta t} \mathscr{H}(q_v - q_{sat}) + \dots$$

Example: condensation onto cloud droplets

- Condensation a function of number of droplets and their size

$$\mathrm{Con}\,C\left(\rho, p, T, q_g, q_v, q_c\right) = 4\pi \frac{q_g}{\rho_g} N_c r_c \frac{S_w - 1}{F_k + F_d}$$

$$\begin{aligned}
\rho_g =& \frac{\rho\, q_g}{1 - \sum_{n \neq g} \frac{\rho\, q_n}{\rho_n}} \\
N_c =& \frac{q_c}{\rho_w \pi r_c^3} \text{(number of cloud droplets/gas volume)}, \\
r_c =& 10\mu m \text{ (droplet radius)}, \\
S_w =& q_v / q_{sat} \\
F_k =& \left(\frac{L_v}{R_v T} - 1\right)\left(\frac{L_v}{K_a T}\right), \quad \text{(heat conduction)} \\
F_d =& \frac{R_v T}{p_{\mathrm{sat}} D_v}, \quad \text{(water vapour flux)}
\end{aligned}$$

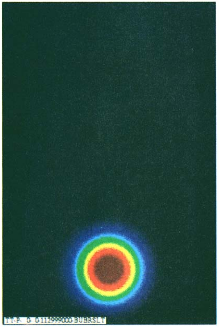
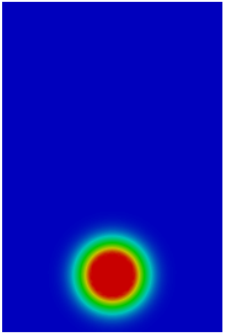
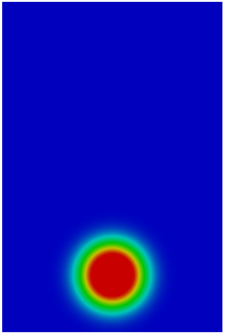
Example: condensation onto rain droplets

- Same idea as with cloud water, but rain drops assumed to be distributed around a mean radius, λ_r

$$
\begin{aligned}
\mathrm{Con}R &= 2\pi \frac{q_g}{\rho_g} N_{0,r} \frac{S_w - 1}{F_k + F_d}, \\
&\qquad \times \left(\frac{1}{\lambda_r^2} + 0.22\Gamma(2.75) \frac{\sqrt{a_r}}{\nu} \left(\frac{\rho_0}{\rho_g} \right)^{\frac{1}{4}} \frac{1}{\lambda_r^{11/12}} \right) \\
\lambda_r &= \left(\pi \frac{q_g \rho_w}{\rho_g q_r} N_{0,r} \right)^{1/4} \\
\rho_w &= \text{(water density)}
\end{aligned}
$$

- Rain fall out velocity assumed a function of radius (Newtonian terminal velocity).

Warm Bubbles

Roberts (1993)	Low Resolution (DG unstructured)	High Resolution (CV quads)
		

Imperial College
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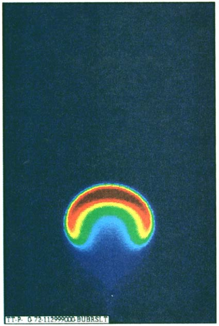
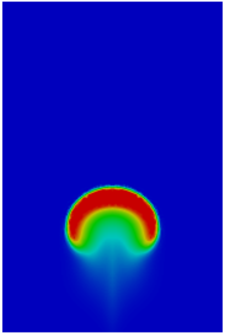
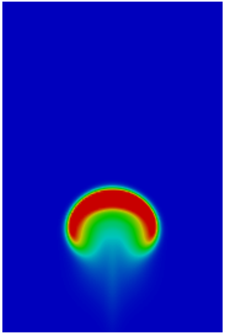
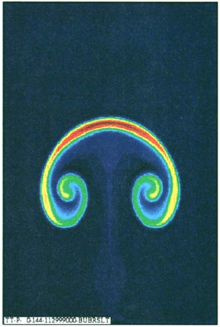
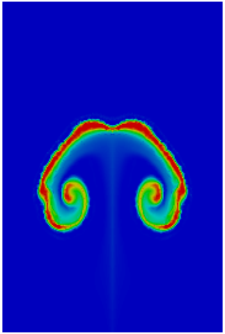
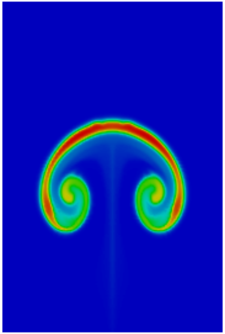
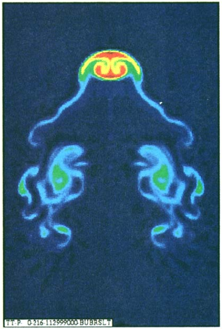
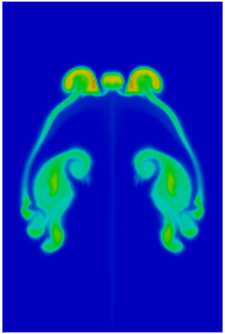
Warm Bubbles

Roberts (1993)	Low Resolution	High Res
		

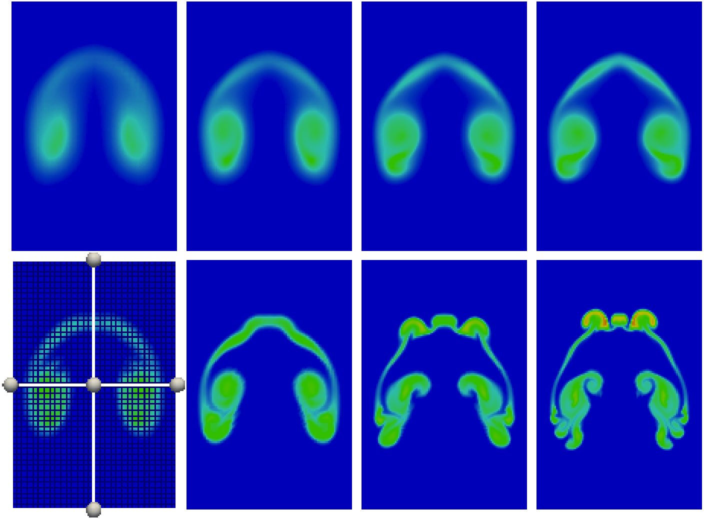
Warm Bubbles

Roberts (1993)	Low Res	High Res
		

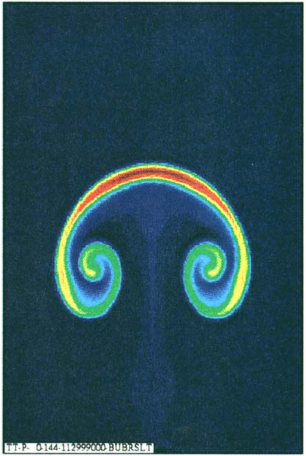
Warm Bubbles

Roberts (1993)	Fluidity
	

Warm Bubbles



Constituent driven rising Bubble

Roberts (Dry pot temp.)	Moist (density) Low resolution
	

Examples: Steam/ash rollers

- 2D problem showing adaptive meshing capability
- Moist (steamy) rising bubble below dense ash bearing cloud in neutrally balanced atmosphere.
- Rising/falling bubbles interact through tangling of trailing rollers
- Adaptive mesh adds resolution to capture vorticity filaments
- To the movie

2D Chimneys

- 2d problem with adaptive mesh (periodic domain)
- Warm, moist, polluted air introduced through chimney into a background flow.
- Buoyancy driven plume forms.
- Significant settling of model pollutant observed downstream of chimney due to lee effects.
- To the movie

3D Chimney/Power Station

- Using the Fluidity toolset, chimney example can be extended near trivially into 3 dimensions, or for complicated domains
- 3d model based on Battersea power station in London
- Interaction with background flow: movie
- Interaction with buildings: movie

Towards the future

- ATHAMFluidity: a moist, multimaterial model on unstructured and adaptive meshes
- Future: To produce full atmospheric model
  - Coupling to sun following radiative transfer model (RADIANT)
  - Advanced element choices
  - Addition of atmospheric/pollutant chemistry routines
  - Coupling to regional models & other fluidity components

For Further Reading I

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