Towards ATHAM-Fluidity

Moist, compressible multimaterial physics in Fluidity

James R. Percival

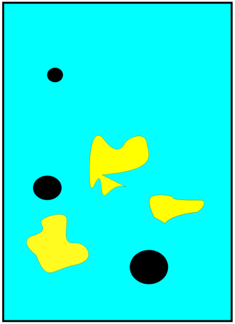
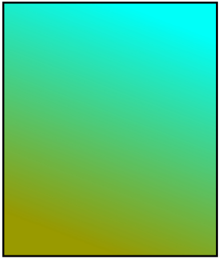
AMCG Seminar Series, June 2012

Describing the Atmosphere

Frame subtitles are optional. Use upper- or lowercase letters.

- Multimaterial, multiphase fluid
- Embedded liquid/solid phases in a (more) compressible gas
- Thermal behaviours of components differ
- Important materials undergo phase changes
    - water vapour $\Leftrightarrow$liquid water $\Leftrightarrow$ice

Multimaterial flow:

Difficult	Easier
	

Incompressible vs. Compressible flow

Incompressible	Compressible
Presure Lagrange multipler	Pressure function of state
Constraint $\nabla \cdot u = 0$	$p = p(\rho, T, \ldots)$
Volume preserving	Volumes change
No flow across ρ surfaces	No flow across entropy surfaces
	Conservation of mass momentum
Conservation of all passive tracers	Conservation of momentum
	Conservation of total energy

Entropy

- Nebulous concept as one of four thermodynamic variables (temperature, entropy, pressure, volume)
- Wikipedia: "establishes energy not available to work"
- 1st law of thermodynamics: for given unit of material

$$\underbrace{de}_{\text{specific internal energy}} = \underbrace{T}_{\text{temperature}} \times \underbrace{ds}_{\text{specific entropy}} - \underbrace{p}_{\text{Pressure}} \times \underbrace{d\left(\frac{1}{\rho}\right)}_{\text{specific volume}}$$

Entropy

- Relevant version: Definition of specific internal energy

$$e(\rho, s) = c_v T$$

- Material obeys ideal gas law

$$p = \rho \times \underbrace{R}_{\text{gas constant}=c_p - c_v} \times T$$

- Thermodynamic equation implies

$$p = \rho^2 \left.\frac{\partial e}{\partial \rho}\right|_s, \quad s = c_p \ln\left[T\left(\frac{p}{p_0}\right)^{\frac{R}{c_p}}\right] = c_p \ln[\Theta]$$

Internal Energy Equation

- Define $\frac{da}{dt} = \frac{\partial a}{\partial t} + u \cdot \nabla a$, material derivative.
- Thermodynamic equation in Lagrangian frame implies energy equation

$$\begin{aligned} \frac{de}{dt} &= \frac{\partial e}{\partial s}\frac{ds}{dt} + \frac{\partial e}{\partial \rho}\frac{d\rho}{dt} \\ &= 0 - \rho\frac{\partial e}{\partial \rho}\nabla \cdot u \\ &= -\frac{p}{\rho}\nabla \cdot u \end{aligned}$$

Fluidity Compressible algorithm

Pressure correction method. On each nonlinear iteration:

1. Update tracer equations
2. Update momentum equation
3. Solve continuity equation for intermediate density
4. Linearize momentum equation & equation of state to convert density update into pressure + velocity correction
5. Get final density update from equation of state.

A Brief History of ATHAM

- Active Tracer High Resolution Atmosphere Model
- Originally developed at Max Planck Institute
- Used for high energy plume modelling (Volcanoes! Wild fires)
- Dynamic core is finite difference with evolutionary pressure equation
- Fortran 77: Six letter variable names.
- Text file input, netcdf output.
- Code modification to select problem type

Key Dynamic Assumption

- Key modelling assumptions: Single temperature, single pressure.
- Bulk momentum equation.
- Materials sink/rise relative to bulk velocity parallel to gravitation only
- Fall out speed a function of the material state only.

ATHAM-Fluidity

- ATHAM microphysics and governing equations
  - ATHAM thermal equation
  - Source terms to
- Fluidity dynamic core & data structure
  - Fluidity compressible algorithm (pressure correction method)

ATHAM Dynamical Equations

- Bulk momentum equation

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

- Bulk mass continuity equation

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

ATHAM Dynamical Equations

- Individual tracer equations for the N mass fractions

$$\frac{\partial}{\partial t}(\rho q_i) + \nabla \cdot \rho q_i u_i = \nabla \cdot D_i \nabla q_i + F_i, \quad i \in [2, N]$$

- velocity = bulk + fall out

$$u_i = u + u_i' g$$

- Mass fractions sum to one!

$$q_1 = 1 - \sum_{i=2}^{N} q_i$$

Closures

- Equation of state for gas fraction

$$p = \rho_g R_g T$$

where

$$R_g = \frac{\sum_{i \in g} (c_{p,i} - c_{v,}) q_i}{\sum_{i \in g} q_i}$$

- Definition of bulk density,

$$\frac{1}{\rho} = \frac{V}{m} = \sum \frac{V_i}{m_i} \frac{m_i}{m} = \sum \frac{q_i}{\rho_i},$$

Closures

- Final equation of state

$$p = \frac{\sum_{i\in g} \rho \left(c_{p,i} - c_{v,i}\right) q_i T}{1 - \sum_{i\notin g} \frac{\rho q_i}{\rho_i}}, \quad \text{or} \quad \rho = \frac{p}{\sum_{i\in g} \left(c_{p,i} - v_{v,i}\right) T + p \sum_{i\notin g} \frac{q_i}{\rho_i}}$$

- Significantly more nonlinear than one-phase equation
- Important in solution algorithm.

Bulk Thermal equation

$$c_p\Theta = \left(\sum_{i\in g} c_{p,i}q_i + \sum_{n\notin g} c_n q_n\right)\Theta$$

$$= T\left(\left(\frac{p}{p_0}\right)^{\frac{\sum_{n\in g} R_n q_n}{\sum_{n\in g} c_{p,n} q_n}} \sum_{i\in g} c_{p,i}q_i + \sum_{n\notin g} c_n q_n\right)$$

$$\frac{\partial}{\partial t}(\rho c_p \Theta) + \nabla\cdot\rho c_p \Theta u_\Theta = \nabla\cdot D_\Theta \nabla\Theta,$$

$$u_\Theta = \frac{\sum_{n\in g} c_{p,n} u_n + \sum_{n\notin g} c_n u_n}{c_p},$$

Bulk Thermal equation

(Ought by rights to be)

$$\frac{\partial}{\partial t}\left(\rho c_p \ln\left(T\left(\frac{p}{p_0}\right)^{\frac{R_g q_g}{c_p}}\right)\right) + \nabla\cdot\left(\rho\left(\ln\left(T\left(\frac{p}{p_0}\right)^{\frac{R_g q_g}{c_{p,g}}}\right)\right) c_{p,g} q_g u_g + \sum_{i\notin g}$$

but probably too complicated.

Microphysics

- 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,
- Atham process pentagram for mass exchange

Herzog et al. (1998)

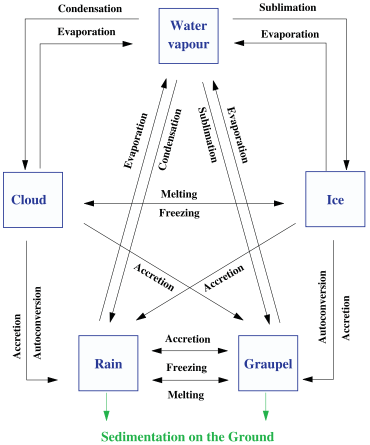


Fig. 1. Scheme of the microphysics for water.

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 fitting gives (other choices available)

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

- Obtain saturation mass fraction by considering gas phases 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 relaxation to saturation pressure over a timestep
- Mass removed from vapour phase

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

- Mass inserted into cloud water phase

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

Example: condensation onto cloud droplets

- Condensation a function of number of droplets and their size

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

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

Example: condensation onto rain droplets

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

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

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

Conversion: Cloud $\Longleftrightarrow$Rain$\Longleftrightarrow$Ice $\Longleftrightarrow$Graupel

- Many, many possible processes
- Currently implemented:
  - autoconversion (cloud drop clumping)
  - Accreation (sweeping)

Warm Bubbles

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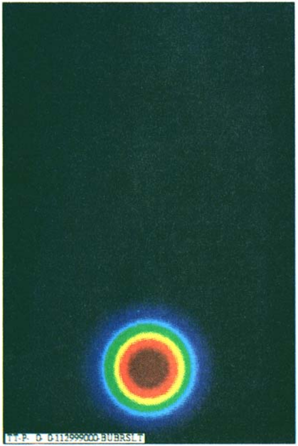
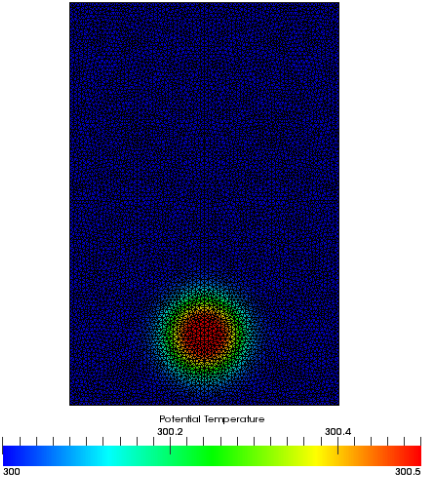
<tr><td></td><td>
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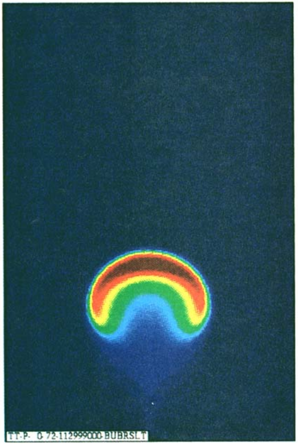	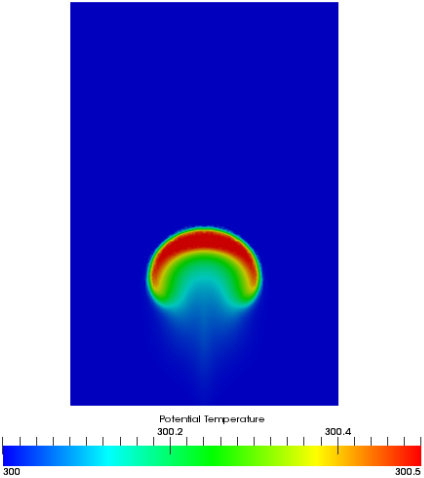

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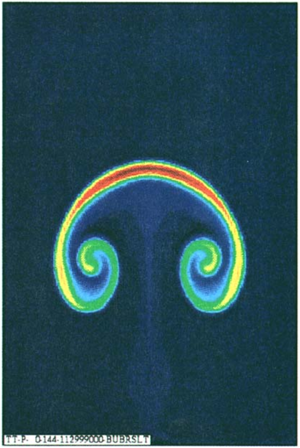
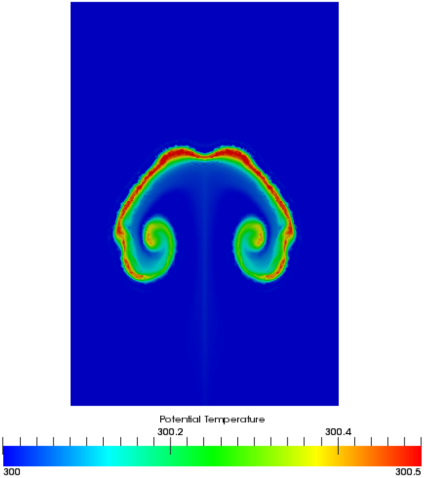
<tr><td>
</td><td>
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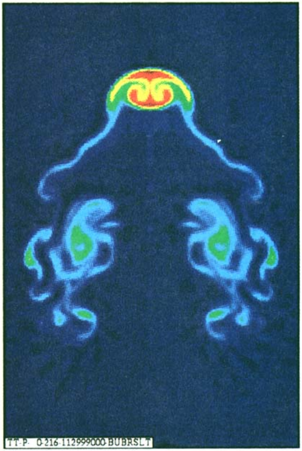

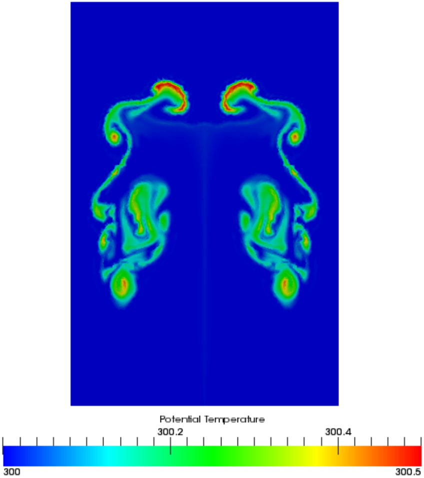

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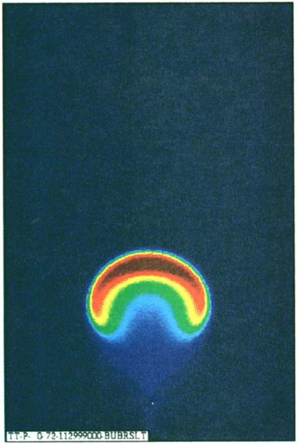	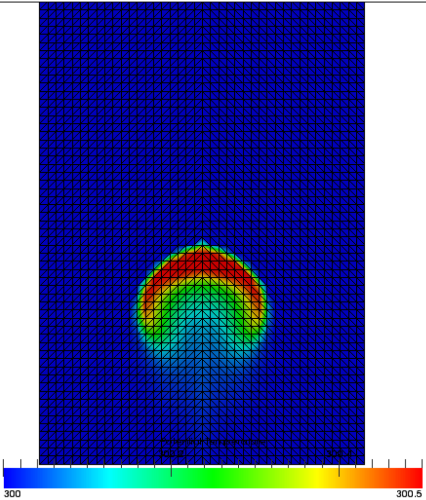

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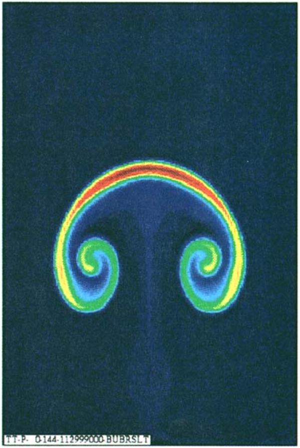	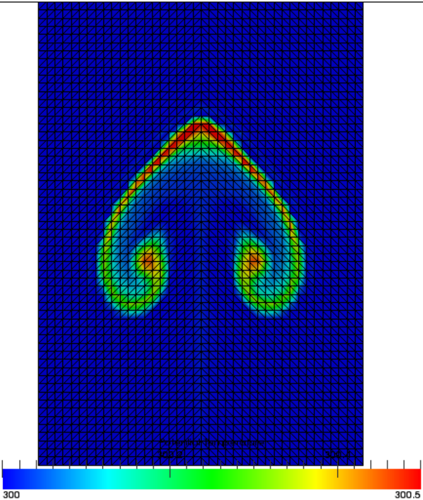

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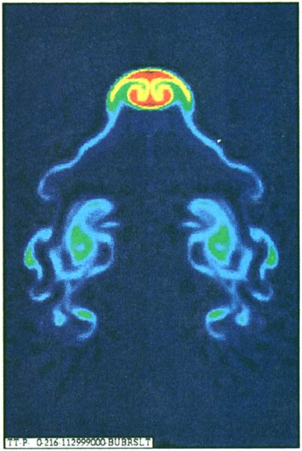
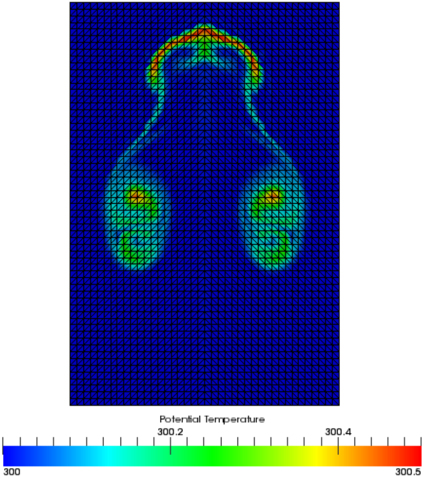


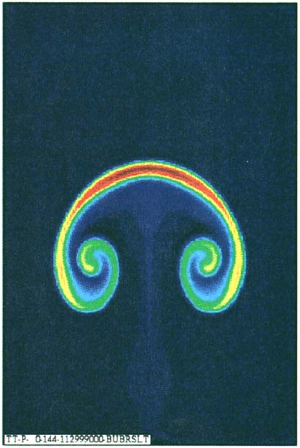


Multiphase Bubbles

Dry Bubble	Moist Bubble
Entropy perturbation	Material perturbation
$p^{\frac{c_{v,0}}{c_{p,0}}} = \frac{\rho R_0(\Theta_0+\delta\Theta)}{p_0^{\frac{R}{c_p}}}$	$p^{\frac{c_{v,0}+\left(c_{v,1}-c_{v,0}\right)\delta q}{c_p+\left(c_{v,1}-c_{v,0}\right)\delta q}} = \frac{\rho(R_0+(R_1-R_0)\delta q)\Theta_0}{p_0^{\frac{R_0+(R_1-R_0)\delta q}{c_p+\left(c_{v,1}-c_{v,0}\right)\delta q}}}$
$\frac{\partial}{\partial t}\delta\Theta + u\cdot\nabla\delta\Theta = 0,$	$\frac{\partial}{\partial t}\delta q + u\cdot\nabla\delta q = 0,$

If $\frac{c_{v,0}}{c_{p,0}} = \frac{c_{v,1}}{c_{v,1}}$, i.e. both diatomic/triatomic gases, or proportionate mixture, then can create "identical" problem with entropy or material phase.

Example

Roberts (Dry)	Fluidity (Moist)
	

Incompressible phase

- Unlike compressible phase can't be tested in comparison to dry core
- Must instead compare with original ATHAM code
- A work in progress

Example: a 2d Chimney and steam/ash rollers.

- To the movie

Summary

A compressible, single temperature, single pressure multimaterial model has been implemented in Fluidity. With simple microphysics

- Outlook
  - More microphysics to come through genuine ATHAM coupling
  - Still questions regarding adaptivity choices

For Further Reading I

- H. Byers
  Elements of Cloud Physics
  Univ. Chicago Press 1965
- J. M. Oberhuber, M. Herzog, H.-F. Graf, and K. Schwanke.
  Volcanic plume simulation on large scales.
  Journal of Volcanology and Geothermal Research, 87:29–53, 1998.
- M. Herzog, H.-F. Graf, C. Textor, and J. M. Oberhuber.
  The effect of phase changes of water on the development of volcanic plumes.
  Journal of Volcanology and Geothermal Research, 87:55–74, 1998.