



Unified Framework for Discrete Integrations of Compressible and Soundproof PDEs of Atmospheric Dynamics



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Part I: Analytic Formulations:

Introduction;

Eulerian & Lagrangian reference frames;

Atmospheric PDEs;

Nonhydrostatic (all-scale) PDEs;

Perturbation forms;

Unified framework;

Conservation law forms;

Generalised coordinates;

Examples

Part II: Integration Schemes:

Forward-in-time integrators, E-L congruence;

Semi-implicit algorithms;

Elliptic boundary value problems;

Variational Krylov solvers;

Preconditioning;

Boundary conditions

Part I: Analytic Formulations

Meteorology has a large portfolio of diverse analytic formulations of the equations of motion, which employ variety of simplifying assumptions while focusing on different aspects of atmospheric dynamics.

Examples include: shallow water equations, isosteric/isentropic models, hydrostatic primitive equations, incompressible Boussinesq equations, anelastic systems, pseudo-incompressible equations, unified equations, and fully compressible Euler equations.

Many of these equations can be written optionally in Eulerian or Lagrangian reference frame and in terms of various dependent variables; vorticity, velocity or momentum for dynamics, and total energy, internal energy or entropy for thermodynamics.

However, with increasing computational power the non-hydrostatic (i.e., all-scale) systems come into focus, thus reducing the plethora of options.

Two reference frames



Eulerian



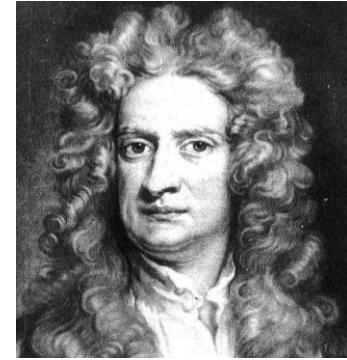
Lagrangian

$$\frac{\partial G\Psi}{\partial t} + \nabla \cdot (\mathbf{v}\Psi) = GR$$

(the archetype problem, AP)

$$\frac{d\Psi}{dt} = R$$

The laws for fluid flow --- conservation of mass, Newton's 2nd law, conservation of energy, and 2nd principle of thermodynamics --- are independent on reference frames → the two descriptions must be equivalent, somehow.



$$\dot{\mathbf{x}} \equiv \frac{d\mathbf{x}}{dt} := \lim_{\delta t \rightarrow 0} \frac{\mathbf{x}(\mathbf{x}_o, t + \delta t) - \mathbf{x}(\mathbf{x}_o, t)}{\delta t} = \mathbf{v}$$

physics (re measurement)

$$\frac{d\psi}{dt} := \lim_{\delta t \rightarrow 0} \frac{\psi(\mathbf{x}(\mathbf{x}_o, t + \delta t), t + \delta t) - \psi(\mathbf{x}(\mathbf{x}_o, t), t)}{\delta t}$$

math (re Taylor series)

$$\begin{aligned} &= \lim_{\delta t \rightarrow 0} \frac{1}{\delta t} \left([\mathbf{x}(\mathbf{x}_o, t + \delta t) - \mathbf{x}(\mathbf{x}_o, t)] \cdot \nabla \psi \Big|_{\mathbf{x}(\mathbf{x}_o, t), t} + \delta t \frac{\partial \psi}{\partial t} \Big|_{\mathbf{x}(\mathbf{x}_o, t), t} + \mathcal{O}(\delta t^2) \right) \\ &= \lim_{\delta t \rightarrow 0} \frac{\mathbf{x}(\mathbf{x}_o, t + \delta t) - \mathbf{x}(\mathbf{x}_o, t)}{\delta t} \cdot \nabla \psi \Big|_{\mathbf{x}(\mathbf{x}_o, t), t} + \frac{\partial \psi}{\partial t} \Big|_{\mathbf{x}(\mathbf{x}_o, t), t} + \lim_{\delta t \rightarrow 0} \mathcal{O}(\delta t) \\ &= \left(\mathbf{v} \cdot \nabla \psi + \frac{\partial \psi}{\partial t} \right)_{\mathbf{x}(\mathbf{x}_o, t), t}, \quad \forall_{\mathbf{x}(\mathbf{x}_o, t), t} \end{aligned}$$

$$\nabla = (\partial_x, \partial_y, \partial_z)$$



$$\frac{d\psi}{dt} = \frac{\partial \psi}{\partial t} + \mathbf{v} \cdot \nabla \psi$$

physics (relating observations in the two reference frames)

More math:

$$\vartheta_{\mathbf{x}(\mathbf{x}_o, t)} = \vartheta_o \frac{\mathcal{G}}{\mathcal{G}_o} \frac{\partial x^1, \dots, \partial x^M}{\partial x_o^1, \dots, \partial x_o^M} \equiv \vartheta_o J$$

parcel's volume evolution;
 $0 < J < \infty$, for the flow to
 be topologically realizable

$$\frac{1}{\mathcal{G}} \nabla \cdot \left(\mathcal{G} \frac{d\mathbf{x}}{dt} \right) := \lim_{\vartheta \rightarrow 0} \frac{1}{\vartheta} \frac{d\vartheta}{dt} = \frac{d}{dt} \ln \frac{\mathcal{G}}{\mathcal{G}_o} \frac{\partial x^1, \dots, \partial x^M}{\partial x_o^1, \dots, \partial x_o^M} = \frac{d}{dt} \ln J$$

flow divergence, definition

flow Jacobian



Leibniz, 1646-1716



Euler, 1707-1783

Euler expansion formula,

$$\frac{d}{dt} \ln J = \frac{1}{\mathcal{G}} \nabla \cdot (\mathcal{G} \mathbf{v})$$

and the rest is easy →

Lamb, H., 1945: *Hydrodynamics*. Dover, 738 pp.
 Truesdell, C., 1966: *The Mechanical Foundations of Elasticity and Fluid Dynamics*. Gordon and Breach, 218 pp.
 Chorin, A. J., and J. E. Marsden, 1984: *A Mathematical Introduction to Fluid Mechanics*. Springer-Verlag, 205 pp.

$$\rho \vartheta = m_o \Rightarrow \frac{d\rho}{dt} \vartheta_o J + \rho \vartheta_o \frac{dJ}{dt} = 0 \implies \text{mass continuity}$$

$$\frac{d\rho J}{dt} = 0 \Leftrightarrow \rho = \rho_o J^{-1} \Leftrightarrow \frac{d\rho}{dt} = -\frac{\rho}{\mathcal{G}} \nabla \cdot (\mathcal{G}\mathbf{v}) \Leftrightarrow \frac{\partial \mathcal{G}\rho}{\partial t} + \nabla \cdot (\mathcal{G}\mathbf{v}\rho) = 0$$

$$\left. \begin{aligned} \frac{d\psi}{dt} &= \frac{\partial \psi}{\partial t} + \mathbf{v} \cdot \nabla \psi \\ \frac{d\rho}{dt} &= -\frac{\rho}{\mathcal{G}} \nabla \cdot (\mathcal{G}\mathbf{v}) \Leftrightarrow \frac{\partial \mathcal{G}\rho}{\partial t} + \nabla \cdot (\mathcal{G}\mathbf{v}\rho) = 0 \end{aligned} \right\} \text{key tools for deriving conservation laws}$$

$$\frac{d\psi}{dt} = R \Rightarrow \frac{\partial \mathcal{G}\rho\psi}{\partial t} + \nabla \cdot (\mathcal{G}\mathbf{v}\rho\psi) = \mathcal{G}\rho R$$



THEOREM XIII.22.1 (On Change of Variables). Let U and U' be open subsets in \mathbb{R}^n (in particular, it may be that $U = U' = \mathbb{R}^n$). Let Φ be a topological mapping of class C^1 of the set U onto U' .

If a function $f \in \mathcal{L}^1$ has the property that $f \subset U'$, then:

$$(2) \quad \int_{\mathbb{R}^n} f(y) d\lambda^n(y) = \int_{U'} f(y) d\lambda^n(y) = \int_U f(\Phi(x)) \cdot |\det \Phi'(x)| d\lambda^n(x) \\ = \int_{\mathbb{R}^n} f(\Phi(x)) \cdot |\det \Phi'(x)| d\lambda^n(x).$$

Elementary examples:

Shallow-water equations

$$\frac{\partial G\mathcal{D}}{\partial t} + \nabla \cdot (G\mathbf{v}^* \mathcal{D}) = 0,$$

$$\frac{\partial GQ_x}{\partial t} + \nabla \cdot (G\mathbf{v}^* Q_x) = G \left(-\frac{g}{h_x} \mathcal{D} \frac{\partial H}{\partial x} + fQ_y - \frac{1}{G\mathcal{D}} \frac{\partial h_x}{\partial y} Q_x Q_y \right),$$

$$\frac{\partial GQ_y}{\partial t} + \nabla \cdot (G\mathbf{v}^* Q_y) = G \left(-\frac{g}{h_y} \mathcal{D} \frac{\partial H}{\partial y} - fQ_x + \frac{1}{G\mathcal{D}} \frac{\partial h_x}{\partial y} Q_x^2 \right),$$

(Szmelter & Smolarkiewicz, JCP, 2010)

anelastic system

$$\frac{d\mathbf{v}}{dt} = -\nabla \pi' - \mathbf{g} \frac{\theta'}{\theta} - 2\boldsymbol{\Omega} \times \mathbf{v}' + \mathbf{M}' + F_{\mathbf{v}},$$

$$\nabla \cdot (\bar{\rho} \mathbf{v}) = 0,$$

$$\frac{d\theta'}{dt} = -\mathbf{v} \cdot \nabla \theta_e + F_{\theta}.$$

See: Wedi & Smolarkiewicz, QJR, 2009, for discussion; and a special issue of JCP, 2008, "Predicting Weather, Climate and Extreme Events" for an overview of computational meteorology

All leading weather and climate codes are based on the *compressible Euler equations*, yet much of knowledge about non-hydrostatic atmospheric dynamics derives from the soundproof equations – descendants of the classical, reduced incompressible Boussinesq equations



Euler, 1707-1783



Boussinesq, 1842-1929

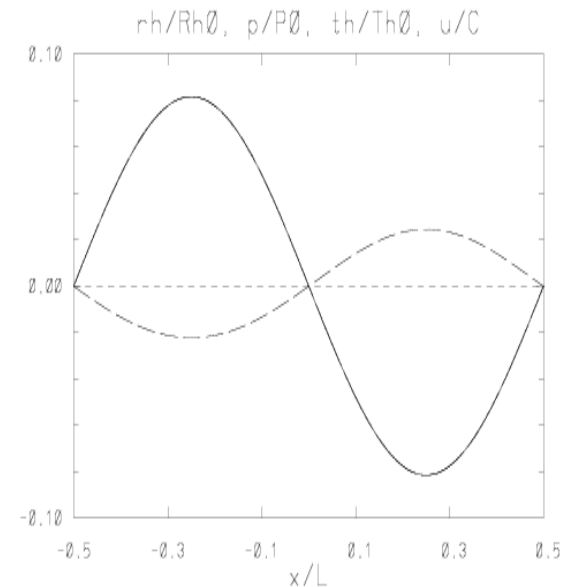
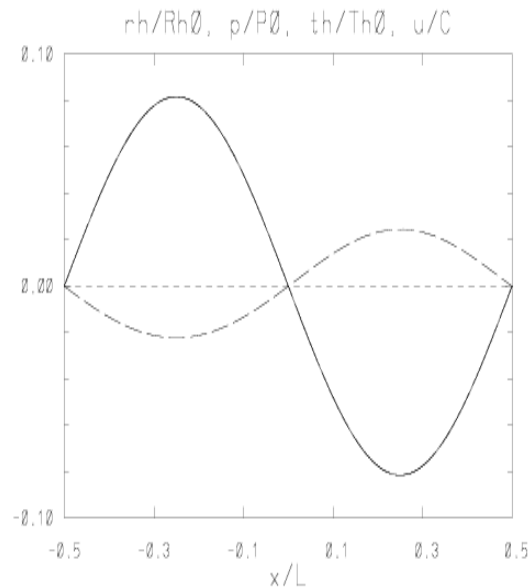
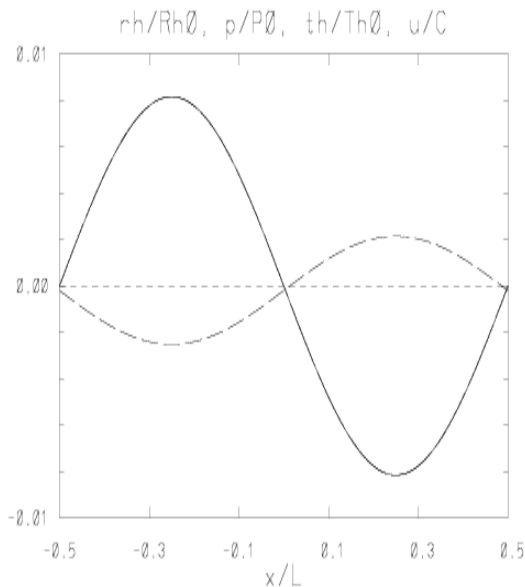
Why bother? Handling unresolved acoustic modes, while insisting on large time steps relative to speed of sound, makes numerics of non-hydrostatic atmospheric models based on the compressible Euler equations demanding

$$\rho \frac{du}{dt} = -\partial_x p$$

$$\frac{d\rho}{dt} = -\rho \partial_x u$$

$$p = \rho R_d T|_{T=T_0} = c_o^2 \rho$$

pressure and density solid lines, entropy long dashes, velocity short dashes



From compressible Euler equations to incompressible Boussinesq equations

$$\mathbf{g} = (0, 0, -g) = -g\nabla z$$

$$\rho \frac{d\mathbf{u}}{dt} = -\nabla p - g\rho\nabla z ;$$

3D momentum equations under gravity

$$\frac{d\rho}{dt} = -\rho\nabla \cdot \mathbf{u} ; \quad \frac{d\theta}{dt} = 0$$

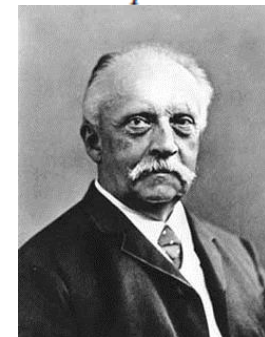
mass continuity and adiabatic entropy equations $ds = c_p d \ln \theta$

perturbation about static reference (base) state:

$$\rho = \rho_b(z) + \rho'(\mathbf{x}, t) ; \quad 0 = -\nabla p_b - \rho_b g \nabla z$$

momentum equation, perturbation form:

$$\rho \frac{d\mathbf{u}}{dt} = -\nabla(p - p_b) - g(\rho - \rho_b)\nabla z \Rightarrow \frac{d\mathbf{u}}{dt} = -\frac{1}{\rho} \nabla p' - g \frac{\rho'}{\rho} \nabla z$$



**Helmholtz,
1821-1894**

for problems with small vertical scales and density perturbations:

$$\rho' \ll \rho_b = \text{cnst.} \Rightarrow$$

incompressible Boussinesq equations

$$\frac{d\mathbf{u}}{dt} = -\nabla \frac{p - p_b}{\rho_b} - g \frac{\rho - \rho_b}{\rho_b} \nabla z \equiv -\nabla \frac{p'}{\rho_b} - g \frac{\rho'}{\rho_b} \nabla z$$

$$0 = -\nabla \cdot \rho_b \mathbf{u}$$

Perturbation forms in the context of initial & boundary conditions

Take incompressible Boussinesq equations:

$$\frac{d\mathbf{u}}{dt} = -\nabla \frac{p - p_b}{\rho_b} - g \frac{\rho - \rho_b}{\rho_b} \nabla z \equiv -\nabla \frac{p'}{\rho_b} - g \frac{\rho'}{\rho_b} \nabla z$$
$$0 = -\nabla \cdot \rho_b \mathbf{u}$$

which also require initial conditions for pressure and density perturbations. Then consider an unperturbed ambient state, a particular solution to the same equations

$$\mathbf{u}_e = (u_e(z), 0, 0), \quad \rho_e = \rho_e(z), \quad p_e = p_e(z), \quad \theta_e = \theta_e(z)$$
$$0 = \frac{d_e \mathbf{u}_e}{dt} = -\nabla \frac{p_e - p_b}{\rho_b} - g \frac{\rho_e - \rho_b}{\rho_b} \nabla z$$
$$0 = -\nabla \cdot \rho_b \mathbf{u}_e$$

subtracting the latter from the former gives the form

$$\frac{d\mathbf{u}}{dt} = -\nabla \frac{p - p_e}{\rho_b} - g \frac{\rho - \rho_e}{\rho_b} \nabla z \equiv -\nabla \phi - g \frac{\rho'}{\rho_b} \nabla z$$
$$0 = -\nabla \cdot \rho_b \mathbf{u} = -\nabla \cdot \rho_b \mathbf{u}'$$
$$\frac{d\theta'}{dt} = -\mathbf{u} \cdot \nabla \theta_e$$

that takes homogeneous initial conditions for the perturbations about the environment !

Perturbation forms in terms of potential temperature and Exner function

$$\pi := (p/p_0)^{R_d/c_p} ; \quad \pi = T/\theta ; \quad \frac{1}{\rho} \nabla p = c_p \theta \nabla \pi$$



F.M. Exner,
1876-1930

compressible Euler equations

$$\rho \frac{d\mathbf{u}}{dt} = -\nabla p - g\rho \nabla z$$

$$\frac{d\mathbf{u}}{dt} = -\theta \nabla (c_p \pi) - g \nabla z$$

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{u}$$

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{u}$$

$$\frac{d\theta}{dt} = 0$$

$$\frac{d\theta}{dt} = 0$$



$$\rho = \rho_b(z) + \rho'(\mathbf{x}, t) ; \quad 0 = -\nabla p_b - \rho_b g \nabla z \quad \theta = \theta_b(z) + \theta'(\mathbf{x}, t) ; \quad 0 = -\theta_b \nabla (c_p \pi_b) - g \nabla z$$

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\rho} \nabla p' - g \frac{\rho'}{\rho} \nabla z$$

$$\frac{d\mathbf{u}}{dt} = -\theta \nabla (c_p \pi') + g \frac{\theta'}{\theta_b} \nabla z$$

- The incompressible Boussinesq system is the simplest nonhydrostatic soundproof system. It describes small scale atmospheric dynamics of planetary boundary layers, flows past complex terrain and shallow gravity waves, thermal convection and fair weather clouds.
- Its extensions include the anelastic *equations* of Lipps & Hemler (1982, 1990) and the pseudo-incompressible equations of Durran (1989, 2008). In the anelastic system the base state density is a function of altitude; in the pseudo-incompressible system the base state density is a (different) function of altitude, and the pressure gradient term is unabbreviated.
- In order to design a common approach for consistent integrations of soundproof and compressible nonhydrostatic PDEs for all-scale atmospheric dynamics, we manipulate the three governing systems into a single form convenient for discrete integrations:

Unified Framework, combined symbolic equations:

$$\frac{d\mathbf{u}}{dt} = -\Theta \nabla \varphi - \mathbf{g} \Upsilon_B \frac{\theta'}{\theta_b} - \mathbf{f} \times (\mathbf{u} - \Upsilon_C \mathbf{u}_e) , \quad \Theta := \left[1, \frac{\theta(\mathbf{x}, t)}{\theta_0}, \frac{\theta(\mathbf{x}, t)}{\theta_0} \right] ,$$

$$\frac{d\theta'}{dt} = -\mathbf{u} \cdot \nabla \theta_e , \quad \Upsilon_B := \left[1, \frac{\theta_b(z)}{\theta_e(\mathbf{x})}, \frac{\theta_b(z)}{\theta_e(\mathbf{x})} \right] ,$$

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{u} . \quad \Upsilon_C := \left[1, \frac{\theta(\mathbf{x}, t)}{\theta_e(\mathbf{x})}, \frac{\theta(\mathbf{x}, t)}{\theta_e(\mathbf{x})} \right] ,$$

$$\rho := \left[\rho_b(z), \rho_b \frac{\theta_b(z)}{\theta_0}, \rho(\mathbf{x}, t) \right] ,$$

$$\varphi := [c_p \theta_b \pi', c_p \theta_0 \pi', c_p \theta_0 \pi'] , \quad \varphi = c_p \theta_0 \left[\left(\frac{R_d}{p_0} \rho \theta \right)^{R_d/c_v} - \pi_e \right] \text{ gas law}$$

conservation-law forms →

Combined equations, conservation form:

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \rho \mathbf{R}^{\mathbf{u}},$$

$$\frac{\partial \rho \theta'}{\partial t} + \nabla \cdot (\rho \mathbf{u} \theta') = \rho R^{\theta'}$$

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

$$\begin{aligned} & \left(\frac{d\psi}{dt} = R \right) \\ & \left(\frac{\partial \rho \psi}{\partial t} + \nabla \cdot (\rho \mathbf{u} \psi) = \rho R \right) \end{aligned}$$

specific vs. density variables

Accounting for curvilinear coordinates:

$$\frac{\partial \mathcal{G} \rho \psi}{\partial t} + \nabla \cdot (\mathcal{G} \rho \mathbf{v} \psi) = \mathcal{G} \rho R$$

$$\frac{\partial \mathcal{G} \rho}{\partial t} + \nabla \cdot (\mathcal{G} \rho \mathbf{v}) = 0$$

$\mathbf{v} = \dot{\mathbf{x}}$ not necessarily equal to \mathbf{u}
 $\mathcal{G}(\mathbf{x}, t)$ denotes the Jacobian
 \mathcal{G}^2 is the determinant of the metric tensor

$$\frac{\partial G \Psi}{\partial t} + \nabla \cdot (\mathbf{v} \Psi) = GR$$

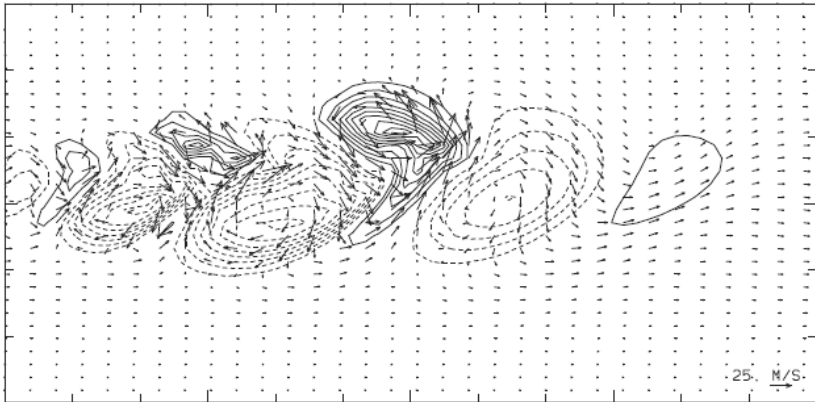


$$\frac{d\Psi}{dt} = R$$

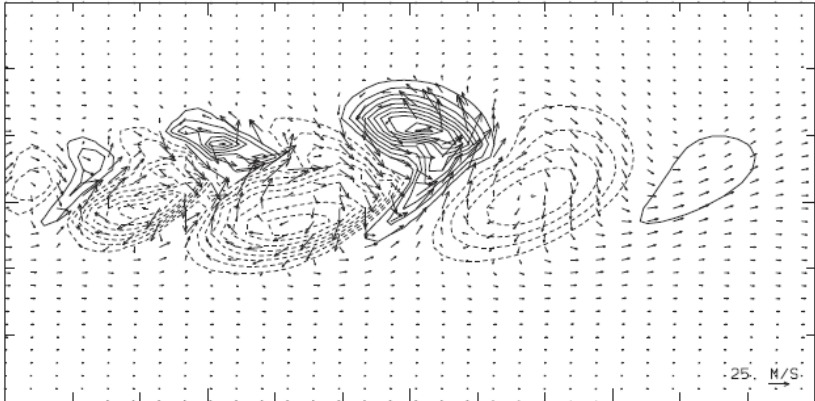
recall “the archetype problem, AP”

Global baroclinic instability; Smolarkiewicz, Kühnlein & Wedi (2014, J. Comput. Phys.)

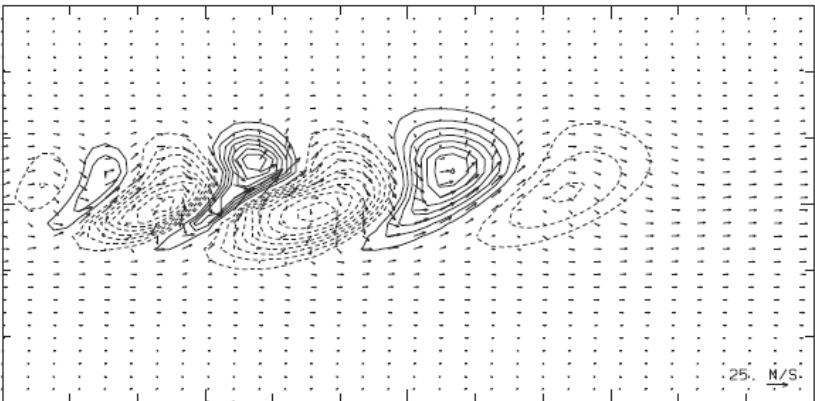
8 days, surface θ' ,
128x64x48 lon-lat grid,
128 PE of Power7 IBM



CMP, 2880 dt=300 s,
wallclock time=2.0 mns



PSI, 2880 dt=300 s,
wallclock time=2.3 mns,



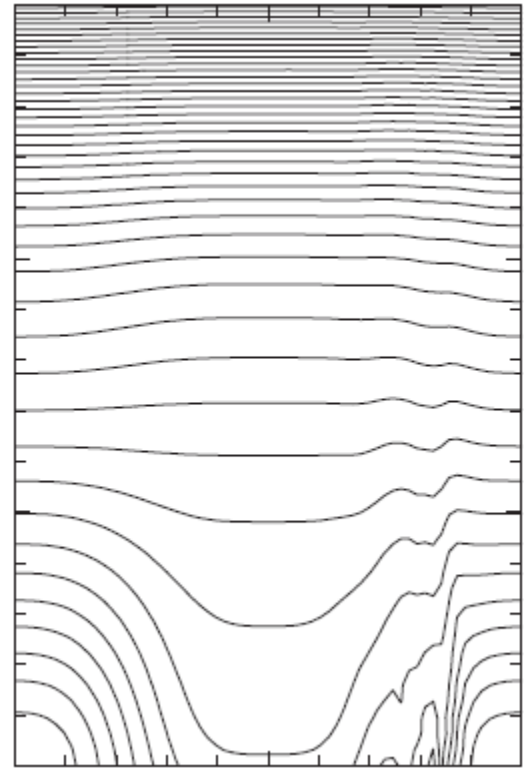
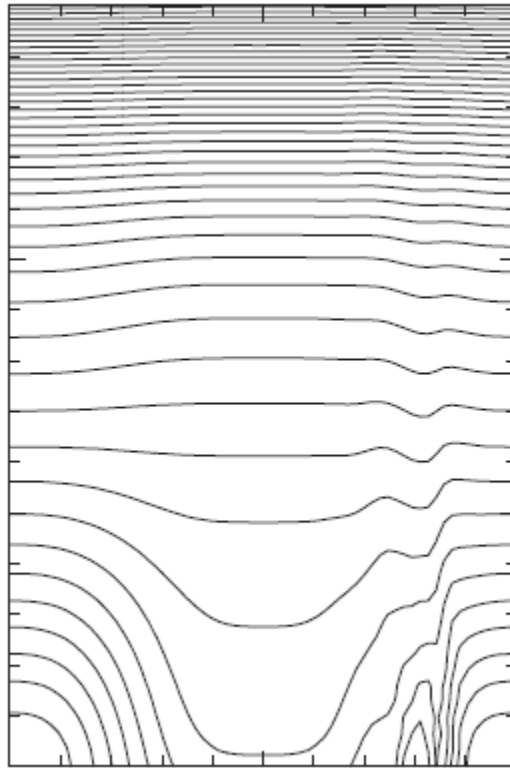
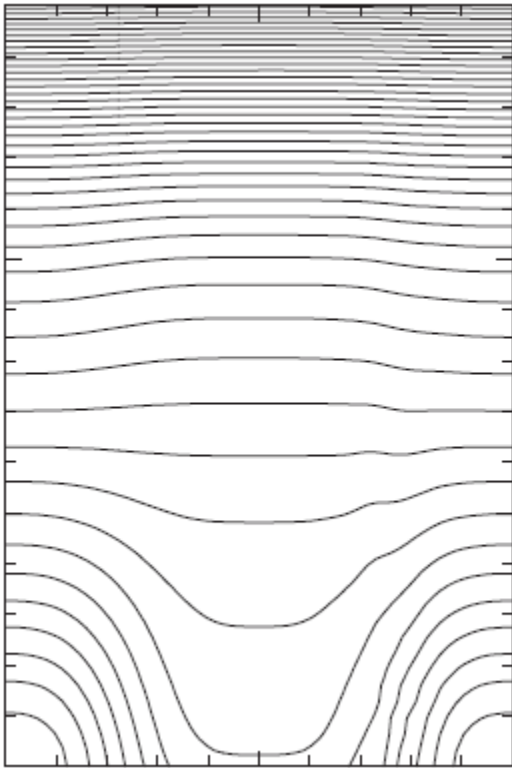
ANL, 2880 dt=300 s,
wallclock time=2.1 mns,

The role of baroclinicity

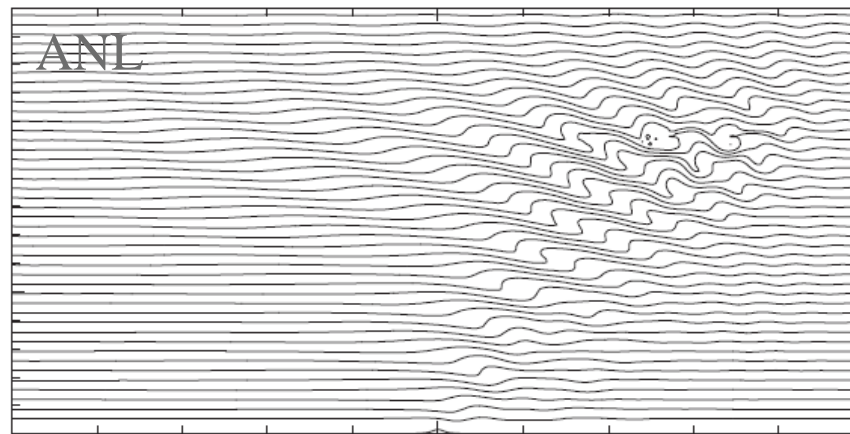
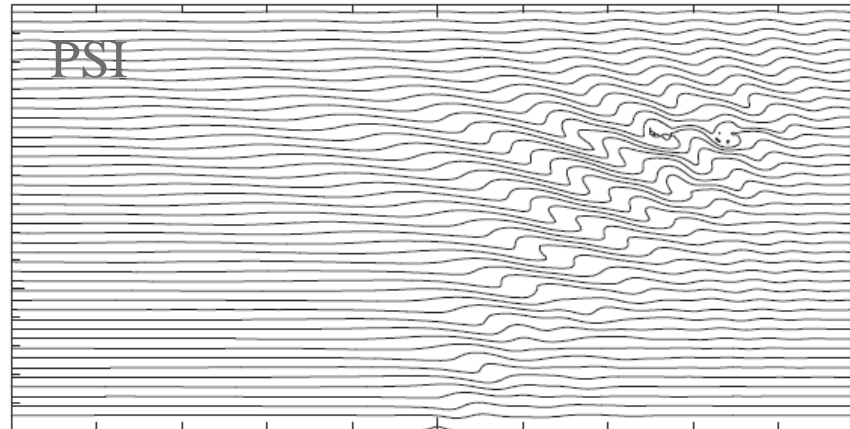
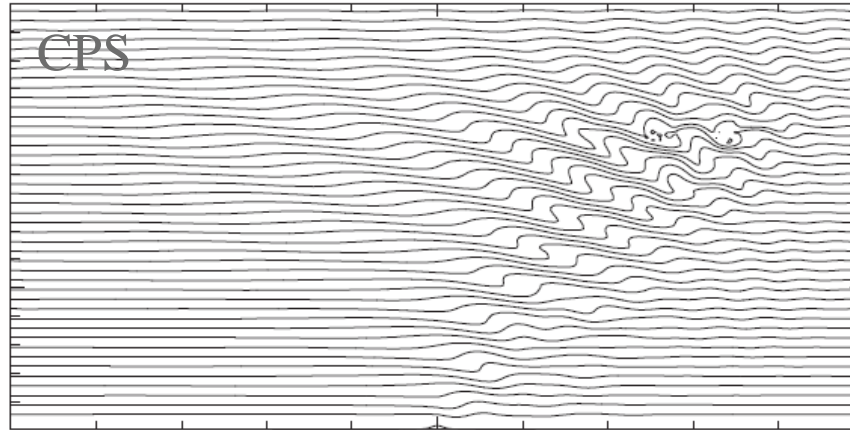
anelastic

pseudoincompressible

compressible

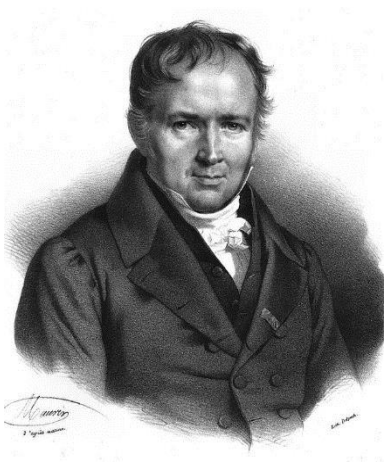


1.5h, surface $\ln\theta$, 320x160
Gal-Chen grid,
domain 120 km x 60 km
"soundproof" $dt=5$ s
"acoustic" $dt=0.5$ s
320 PE of Power7 IBM



Part II: Integration Schemes

- Generalised forward-in-time (FT) nonoscillatory (NFT) integrators for all scale, all speed flows PDEs (anelastic, pseudo-incompressible, acoustic; semi-implicit; flux-form Eulerian and semi-Lagrangian)
- Robust, variational Krylov-subspace solvers for generalised boundary value problems (BVP) of Poisson & Helmholtz type



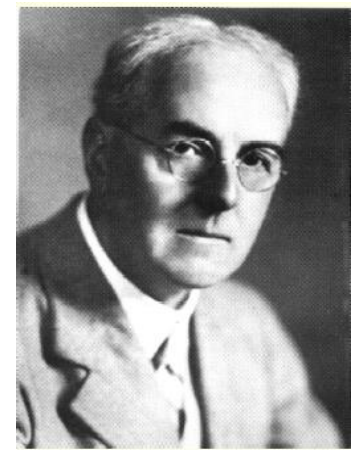
**Poisson,
1781-1840**



**Helmholtz,
1821-1894**



**Krylov,
1863-1945**



**Richardson,
1881-1953**

- Generalised forward-in-time (FT) nonoscillatory (NFT) integrators for the AP

Eulerian/LAGRangian congruence

Eulerian

$$\frac{\partial G\Psi}{\partial t} + \nabla \cdot (\mathbf{v}\Psi) = GR$$

Lagrangian (semi)

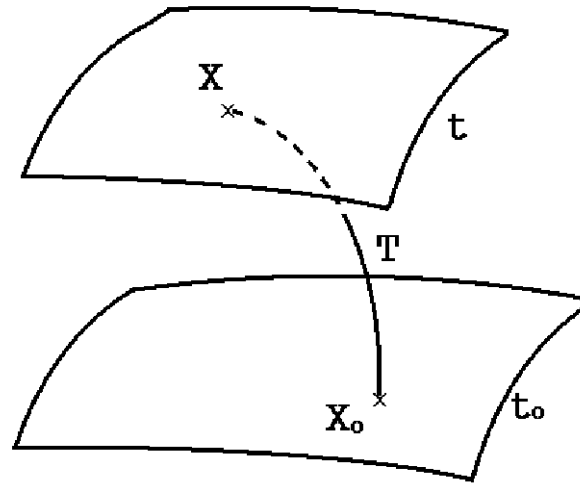
$$\frac{d\Psi}{dt} = R$$

$$\Psi_i^{n+1} = \mathcal{A}_i(\Psi^n + 0.5\delta t R^n) + 0.5\delta t R_i^{n+1}$$

Motivation for Lagrangian integrals

$$\Psi_i^{n+1} = \mathcal{A}_i (\Psi^n + 0.5\delta t R^n) + 0.5\delta t R_i^{n+1}$$

$$\frac{d\Psi}{dt} = R$$



$$\Psi(\mathbf{x}, t) = \Psi(\mathbf{x}_o, t_o) + \int_T R d\tau$$

$$\Psi_i^{n+1} = \Psi_o + 0.5\delta t(R_i^{n+1} + R_o) + \delta t\mathcal{O}(\delta t^2)$$

$$\Psi_i^{n+1} = (\Psi + 0.5\delta t R)_o + 0.5\delta t R_i^{n+1} + \mathcal{HOT}$$

Motivation for Eulerian integrals

$$\Psi_i^{n+1} = \mathcal{A}_i (\Psi^n + 0.5\delta t R^n) + 0.5\delta t R_i^{n+1}$$

$$\frac{\partial G\Psi}{\partial t} + \nabla \cdot (\mathbf{v}\Psi) = GR$$

forward-in-time temporal discretization:

$$\frac{G^{n+1}\Psi^{n+1} - G^n\Psi^n}{\delta t} + \nabla \cdot (\mathbf{v}^{n+1/2}\Psi^n) = (GR)^{n+1/2}$$

Second order Taylor expansion about $t=n\delta t$ & Cauchy-Kowalewski procedure →

$$\frac{\partial G\Psi}{\partial t} + \nabla \cdot (\mathbf{v}\Psi) = GR - \nabla \cdot \left[\frac{\delta t}{2} G^{-1} \mathbf{v} (\mathbf{v} \cdot \nabla \Psi) + \frac{\delta t}{2} G^{-1} \left(\frac{\partial G}{\partial t} + \nabla \cdot \mathbf{v} \right) \mathbf{v} \Psi \right] + \nabla \cdot \left(\frac{\delta t}{2} \mathbf{v} R \right) + \mathcal{O}(\delta t^2)$$

Compensating 1st error term on the rhs is a responsibility of an FT advection scheme (e.g. MPDATA). The 2nd error term depends on the implementation of an FT scheme

Given availability of a 2nd order FT algorithm for the homogeneous problem ($R \equiv 0$), a 2nd order-accurate solution for an inhomogeneous problem with “arbitrary” R is:

$$\Psi_i^{n+1} = \mathcal{A}_i \left(\tilde{\Psi}^n, \mathbf{V}^{n+1/2}, G^n, G^{n+1} \right) + 0.5\delta t \mathcal{R}_i^{n+1},$$

where

$$\tilde{\Psi}^n \equiv \Psi^n + 0.5\delta t \mathcal{R}^n.$$

“Banach principle”, an important tool for systems with nonlinear right-hand-sides:

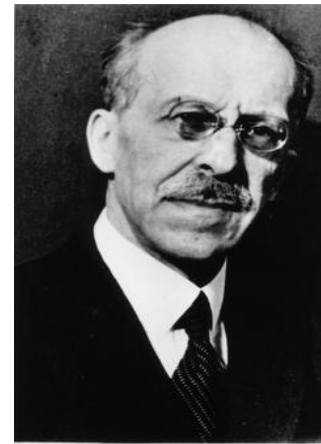
$$\forall_i \quad \Phi_i^{n+1, \mu} = \Phi_i^* + 0.5\delta t \mathbf{R}_i^{n+1, \mu-1}$$

$$\forall_i \quad \Phi_i^{n+1} = \Phi_i^* + 0.5\delta t \mathbf{R}_i^{n+1}$$

$$\begin{aligned} \|\Phi^{n+1, \mu} - \Phi^{n+1}\| &= 0.5\delta t \|\mathbf{R}(\Phi^{n+1, \mu-1}) - \mathbf{R}(\Phi^{n+1})\| \\ &\leq 0.5\delta t \sup \|\partial \mathbf{R} / \partial \Phi\| \|\Phi^{n+1, \mu-1} - \Phi^{n+1}\| \end{aligned}$$

Eulerian semi-implicit compressible algorithms → → →

Schur complement (solar MHD scenario)



J. Schur
Schur, 1875-1941

$$\left. \begin{aligned}
 \frac{d\mathbf{u}}{dt} &= -\nabla\pi' - \mathbf{g}\frac{\Theta'}{\Theta_o} + 2\mathbf{u} \times \boldsymbol{\Omega} + \frac{1}{\mu\rho_o}\mathbf{B} \cdot \nabla\mathbf{B}, \\
 \frac{d\Theta'}{dt} &= -\mathbf{u} \cdot \nabla\Theta_e + \frac{1}{\rho_o}\mathcal{H}(\Theta') - \alpha\Theta', \\
 \frac{d\mathbf{B}}{dt} &= \mathbf{B} \cdot \nabla\mathbf{u} - \mathbf{B}\nabla \cdot \mathbf{u}, \\
 \nabla \cdot \rho_o\mathbf{u} &= 0, \\
 \nabla \cdot \mathbf{B} &= 0.
 \end{aligned} \right\} \rightarrow \begin{aligned}
 \frac{\partial \rho^* \Psi}{\partial t} + \bar{\nabla} \cdot (\mathbf{V}^* \Psi) &= \rho^* \mathbf{R}, \\
 \Psi &= \{\mathbf{u}, \Theta', \mathbf{B}\}^T \\
 \mathbf{R} &= \{\mathbf{R}_u, R_{\Theta'}, \mathbf{R}_B\}^T
 \end{aligned}$$

$$\Psi_i^n = \mathcal{A}_i(\tilde{\Psi}, \tilde{\mathbf{V}}^*, \rho^*) + 0.5\delta t \mathbf{R}_i^n \equiv \widehat{\Psi}_i + 0.5\delta t \mathbf{R}_i^n$$

$$\Psi_i^{n,\nu} = \widehat{\Psi}_i + 0.5\delta t \mathbf{L}\Psi_i^{n,\nu} + 0.5\delta t \mathbf{N}(\Psi)|_i^{n,\nu-1} - 0.5\delta t \tilde{\mathbf{G}}\bar{\nabla}\Phi|_i^{n,\nu}$$

$$\Phi \equiv (\pi', \pi', \pi', 0, \pi^*, \pi^*, \pi^*)$$

$$\begin{aligned}
 \Psi_i^{n,\nu} &= [\mathbf{I} - 0.5\delta t \mathbf{L}]^{-1} \left(\widehat{\Psi} - 0.5\delta t \tilde{\mathbf{G}}\bar{\nabla}\Phi^{n,\nu} \right) \Big|_i \\
 \widehat{\Psi} &\equiv \widehat{\Psi} + 0.5\delta t \mathbf{N}\Psi|_i^{n,\nu-1}
 \end{aligned}$$

→ thermodynamic/elliptic problems for “pressures” Φ

$$\frac{\partial \mathcal{G} \varrho}{\partial t} + \nabla \cdot (\mathcal{G} \varrho \mathbf{v}) = 0, \quad \text{in some detail for compressible Euler PDEs}$$

$$\frac{\partial \mathcal{G} \varrho \theta'}{\partial t} + \nabla \cdot (\mathcal{G} \varrho \theta' \mathbf{v}) = -\mathcal{G} \varrho \tilde{\mathbf{G}}^T \mathbf{u} \cdot \nabla \theta_e,$$

$$\frac{\partial \mathcal{G} \varrho \mathbf{u}}{\partial t} + \nabla \cdot (\mathcal{G} \varrho \mathbf{v} \otimes \mathbf{u}) = -\mathcal{G} \varrho \left(\Theta \tilde{\mathbf{G}} \nabla \varphi + \mathbf{g} \Upsilon_B \frac{\theta'}{\theta_b} + \mathbf{f} \times (\mathbf{u} - \Upsilon_C \mathbf{u}_e) - \mathcal{M}'(\mathbf{u}, \mathbf{u}, \Upsilon_C) \right)$$

semi-implicit "acoustic" scheme:

$$\varrho_i^{n+1} = \mathcal{A}_i \left(\varrho^n, (\mathcal{G} \mathbf{v})^{n+1/2}, \mathcal{G}, \mathcal{G} \right) \implies \mathbf{V}^{n+1/2} = \overline{(\mathcal{G} \varrho \mathbf{v})}^{n+1/2}$$

$$\hat{\theta}'_i = \mathcal{A}_i \left(\tilde{\theta}', \mathbf{V}^{n+1/2}, \varrho^{*n}, \varrho^{*n+1} \right)$$

$$\hat{\mathbf{u}}_i = \mathcal{A}_i \left(\tilde{\mathbf{u}}, \mathbf{V}^{n+1/2}, \varrho^{*n}, \varrho^{*n+1} \right)$$

$$\varrho^{*n} := \mathcal{G} \varrho^n \text{ and } \varrho^{*n+1} := \mathcal{G} \varrho^{n+1}$$

$$\nu = 1, \dots, N_\nu \quad (\text{RE: Banach principle})$$

$$\theta'|_i^\nu = \hat{\theta}'_i - 0.5 \delta t \left(\tilde{\mathbf{G}}^T \mathbf{u}^\nu \cdot \nabla \theta_e \right)_i$$

$$\mathbf{u}_i^\nu = \hat{\mathbf{u}}_i - 0.5 \delta t \left(\Theta^{\nu-1} \tilde{\mathbf{G}} \nabla \varphi^\nu + \mathbf{g} \Upsilon_B \frac{\theta^\nu}{\theta_b} \right)_i - 0.5 \delta t \left(\mathbf{f} \times (\mathbf{u}^\nu - \Upsilon_C^{\nu-1} \mathbf{u}_e) - \mathcal{M}'(\mathbf{u}, \mathbf{u}, \Upsilon_C)^{\nu-1} \right)_i$$

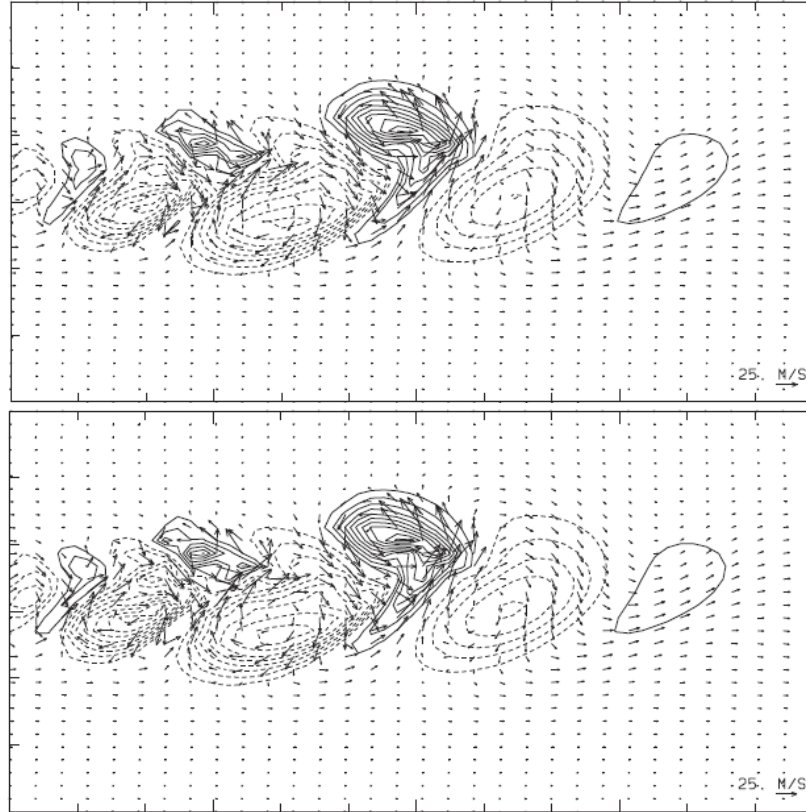
$$\varphi_i^\nu = c_p \theta_0 \left[\left(\frac{R_d}{p_0} \varrho^{n+1} \theta^{\nu-1} \right)^{R_d/c_v} - \pi_e \right]_i \quad (\text{RE: thermodynamic pressure})$$

$$\theta_i^\nu = \left(\hat{\theta}' - 0.5 \delta t \tilde{\mathbf{G}}^T \mathbf{u}^\nu \cdot \nabla \theta_e + \theta_e \right)_i \quad \theta_i^0 = \mathcal{A}_i \left(\theta^n, \mathbf{V}^{n+1/2}, \varrho^{*n}, \varrho^{*n+1} \right)$$

simple but computationally unaffordable; example →

Global baroclinic instability; Smolarkiewicz, Kühnlein & Wedi (2014, J. Comput. Phys.)

8 days, surface θ' ,
128x64x48 lon-lat grid,
128 PE of Power7 IBM



CPI2, 2880 dt=300 s,
wallclock time=2.0 mns

CPEX, 432000 dt=2 s,
wallclock time=178.9 mns

$$\begin{aligned}
 & \underbrace{\mathbf{L}\mathbf{u}^\nu}_{\text{elliptic pressure}} \\
 & \mathbf{u}^\nu + 0.5\delta t \mathbf{f} \times \mathbf{u}^\nu - (0.5\delta t)^2 \mathbf{g} \Upsilon_B \frac{1}{\theta_b} \widetilde{\mathbf{G}}^T \mathbf{u}^\nu \cdot \nabla \theta_e = \\
 & \hat{\mathbf{u}} - 0.5\delta t \left(\mathbf{g} \Upsilon_B \frac{\hat{\theta}'}{\theta_b} - \mathbf{f} \times \Upsilon_C^{\nu-1} \mathbf{u}_e - \mathcal{M}'(\mathbf{u}, \mathbf{u}, \Upsilon_C)^{\nu-1} \right) \\
 & - 0.5\delta t \Theta^{\nu-1} \widetilde{\mathbf{G}} \nabla \varphi^\nu \equiv \boxed{\hat{\mathbf{u}} - 0.5\delta t \Theta^{\nu-1} \widetilde{\mathbf{G}} \nabla \varphi^\nu} \quad \rightarrow \\
 & \boxed{\mathbf{u}^\nu = \check{\mathbf{u}} - \mathbf{C} \nabla \varphi^\nu} \quad \text{where } \check{\mathbf{u}} = \mathbf{L}^{-1} \hat{\mathbf{u}} \text{ and } \mathbf{C} = \mathbf{L}^{-1} 0.5\delta t \Theta^{\nu-1} \widetilde{\mathbf{G}}
 \end{aligned}$$

elliptic boundary value problems (BVPs):

Poisson problem in soundproof models relies on the mass continuity equation $\nabla \cdot (\varrho^* \mathbf{v}) = 0$

Because $\mathbf{v} = \widetilde{\mathbf{G}}^T \mathbf{u}$, acting with $\widetilde{\mathbf{G}}^T$ on both sides of $\mathbf{u}^\nu = \check{\mathbf{u}} - \mathbf{C} \nabla \varphi^\nu$ and ... \rightarrow

$$0 = -\frac{\delta t}{\varrho^*} \nabla \cdot (\varrho^* \mathbf{v}^\nu) = -\frac{\delta t}{\varrho^*} \nabla \cdot \left[\varrho^* \left(\check{\mathbf{v}} - \widetilde{\mathbf{G}}^T \mathbf{C} \nabla \varphi^\nu \right) \right]$$

diagonally preconditioned Poisson problem for pressure perturbation

Helmholtz problems for large-time-step compressible models also rely on mass continuity equation:

combine the evolutionary form of the gas law & mass continuity in the AP for pressure perturbation, to then derive the Helmholtz problem

where $\gamma \equiv R_d/c_v$

$$\frac{d\pi'}{dt} = -\gamma\pi\nabla \cdot \mathbf{u} - \mathbf{u} \cdot \nabla\pi_e \Rightarrow \frac{\partial\rho\pi'}{\partial t} + \nabla \cdot (\rho\pi'\mathbf{u}) = -\gamma\rho\pi\nabla \cdot \mathbf{u} - \rho\mathbf{u} \cdot \nabla\pi_e$$

$$\frac{\partial\rho^*\pi'}{\partial t} + \nabla \cdot (\rho^*\mathbf{v}\pi') = - \left[\gamma\rho^*\pi \frac{1}{\mathcal{G}} \nabla \cdot (\mathcal{G}\mathbf{v}) + \nabla \cdot (\rho^*\mathbf{v}\pi_e) - \pi_e \nabla \cdot (\rho^*\mathbf{v}) \right]$$

$$\ddot{\mathbf{v}} - \tilde{\mathbf{G}}^T \mathbf{C} \nabla \varphi^v$$

$$0 = -\delta t \left[\frac{1}{\mathcal{G}} \nabla \cdot (\mathcal{G}\mathbf{v}) + \frac{1}{\gamma} \frac{\pi_e}{\pi} \frac{1}{\rho^*\pi_e} \nabla \cdot (\rho^*\pi_e\mathbf{v}) - \frac{1}{\gamma} \frac{\pi_e}{\pi} \frac{1}{\rho^*} \nabla \cdot (\rho^*\mathbf{v}) \right] - \beta(\varphi - \hat{\varphi})$$



And how does one solve this “thing” ?



Notion of variational Krylov-subspace solvers:

$$d(p) - R = 0 \xleftarrow{t \rightarrow 0} \frac{\partial p}{\partial t} = d(p) - R$$

$$r := d(p) - R$$

$$\frac{\partial p}{\partial t} = r \implies \frac{\partial r}{\partial t} = d(r)$$

$$p^1 = p^0 + \delta t_0 r^0 \implies r^1 = r^0 + \delta t_0 d(r^0)$$

$$p^2 = p^1 + \delta t_1 r^1$$

$$\hookrightarrow p^2 = p^0 + (\delta t_0 + \delta t_1) r^0 + \delta t_1 \delta t_0 d(r^0)$$

$$\hookrightarrow r^2 = r^0 + \alpha d(r^0) + \beta d^2(r^0)$$

$$\frac{\partial}{\partial \alpha} \|r^2\| = 0 \wedge \frac{\partial}{\partial \beta} \|r^2\| = 0 \implies \alpha, \beta$$

e.g.

$$\frac{\partial}{\partial \alpha} \langle r^2, r^2 \rangle = 0 = \langle r^0 d(r^0) \rangle + \alpha \langle d(r^0) d(r^0) \rangle + \beta \langle d(r^0) d^2(r^0) \rangle$$

$$\frac{\partial}{\partial \beta} \langle r^2, r^2 \rangle = 0 = \langle r^0 d^2(r^0) \rangle + \alpha \langle d(r^0) d^2(r^0) \rangle + \beta \langle d^2(r^0) d^2(r^0) \rangle$$

$$- \begin{bmatrix} \langle d(r^0) d(r^0) \rangle, \langle d(r^0) d^2(r^0) \rangle \\ \langle d(r^0) d^2(r^0) \rangle, \langle d^2(r^0) d^2(r^0) \rangle \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \langle r^0 d(r^0) \rangle \\ \langle r^0 d^2(r^0) \rangle \end{bmatrix}$$

but for $k=0, \dots, n-1$

$$p^n = p^0 + \sum \gamma^k L^k(r^0);$$

$$r^n = r^0 + \sum \gamma^k L^{k+1}(r^0)$$

and

loop over $k = 0, \dots, n-1$

$$p^{k+1} = p^k + \delta t^k r^k$$

$$r^{k+1} = r^k + \delta t^k L(r^k)$$

with

$$\delta t^n = - \langle r^n L(r^n) \rangle / \langle L(r^n) L(r^n) \rangle$$

should do as well; at least for

$$\langle \zeta L(\xi) \rangle = \langle \xi L(\zeta) \rangle \text{ and}$$

$$\langle \xi L(\xi) \rangle < 0 \text{ for all } \xi, \zeta$$

Notion of preconditioning:

The best asymptotic convergence rate one can get from plain CG methods is in the inverse proportionality to (condition number)^{1/2} of the problem at hand

$$\alpha(p) - R = 0 \xleftarrow{\tau \rightarrow \infty} \frac{\partial P}{\partial \tau} = \alpha(p) - R$$

but also

$$\alpha(p) - R = 0 \xleftarrow{\tau \rightarrow \infty} \frac{\partial P(p)}{\partial \tau} = \alpha(p) - R$$

here $P \approx \alpha \Rightarrow$

$$\frac{\partial P}{\partial \tau} = P^{-1}(\tau) \approx e \quad \Big| \quad \alpha(p) - R = 0 \Rightarrow f(e) = \tau$$

$$\frac{\partial \tau}{\partial \tau} = \alpha(P^{-1}(\tau))$$

and the story continues

Preconditioners, $e \approx \mathcal{P}^{-1}(r)$, examples:

$$1) \quad \frac{e^{\mu+1} - e^\mu}{\Delta\tilde{\tau}} = \mathcal{P}^h(e^\mu) + \mathcal{P}^z(e^{\mu+1}) - r^{\nu+1} \quad \rightarrow \quad (\mathcal{I} - \Delta\tilde{\tau}\mathcal{P}^z)e^{\mu+1} = \tilde{R}^\mu$$

$$\tilde{R}^\mu \equiv e^\mu + \Delta\tilde{\tau}(\mathcal{P}^h(e^\mu) - r^{\nu+1})$$

$$2) \quad \frac{\mathcal{D}e^{\mu+1} - \mathcal{D}e^\mu}{\Delta\tilde{\tau}} = \mathcal{P}^h(e^\mu) - \mathcal{D}(e^{\mu+1} - e^\mu) + \mathcal{P}^z(e^{\mu+1}) - r^{\nu+1}$$

$\Delta\tilde{\tau} \rightarrow \infty$, block Jacobi

(-1) \mathcal{D} stands for the diagonal coefficient embedded within the matrix representing \mathcal{P}^h

$$3) \quad \frac{e^{\mu+1} - e^\mu}{\Delta\tilde{\tau}} = \mathcal{P}^h(e^\mu) + \mathcal{P}^z(e^{\mu+1}) - r^{\nu+1} \quad \rightarrow \quad \mathcal{P}^h(e^{\nu+1}) + \mathcal{P}^z(e^{\nu+1}) = r^{\nu+1}$$

$\delta\tilde{\tau} \rightarrow \infty$

$$e^{\nu+1} = \sum_{k,l} \hat{e}_{k,l}(z) \exp[i(k \cdot x + l \cdot y)]$$

$$r^{\nu+1} = \sum_{k,l} \hat{r}_{k,l}(z) \exp[i(k \cdot x + l \cdot y)]$$

$$\sum_{k,l} \left\{ \mathcal{C}_{k,l}(z) \hat{e}_{k,l} + \mathcal{B}_{k,l}(z) \frac{d^2 \hat{e}_{k,l}}{dz^2} - \hat{r}_{k,l} \right\} \exp[i(k \cdot x + l \cdot y)] \equiv 0$$

$$\forall_{k,l} \quad \left(\mathcal{C}_{k,l}(z) + \mathcal{B}_{k,l}(z) \frac{\delta^2}{\delta z^2} \right) \hat{e}_{k,l}(z) = \hat{r}_{k,l}(z)$$

Non-symmetric preconditioned generalized conjugate residual scheme GCR(k):

$$\frac{\partial^k \mathcal{P}(\Psi)}{\partial \tau^k} + \frac{1}{T_{k-1}(\tau)} \frac{\partial^{k-1} \mathcal{P}(\Psi)}{\partial \tau^{k-1}} + \dots + \frac{1}{T_1(\tau)} \frac{\partial \mathcal{P}(\Psi)}{\partial \tau} = \mathcal{L}(\Psi) - \mathcal{R}$$

For any initial guess Ψ_i^0 , set $r_i^0 = \mathcal{L}_i(\Psi^0) - \mathcal{R}_i$, $q_i^0 = \mathcal{P}_i^{-1}(r^0)$; then iterate:

For $n = 1, 2, \dots$ until convergence do

for $v = 0, \dots, k - 1$ do

$$\beta = -\frac{\langle r^v, \mathcal{L}(q^v) \rangle}{\langle \mathcal{L}(q^v), \mathcal{L}(q^v) \rangle},$$

$$\Psi_i^{v+1} = \Psi_i^v + \beta q_i^v,$$

$$r_i^{v+1} = r_i^v + \beta \mathcal{L}_i(q^v),$$

exit if $\| r^{v+1} \| \leq \epsilon^*$,

$$e_i = \mathcal{P}_i^{-1}(r^{v+1}),$$

$$\forall_i \text{ evaluate } \mathcal{L}_i(e) = \frac{1}{\rho^*} \nabla_i \cdot \mathbf{C} \nabla e,$$

$$\forall_{l=0, v} \alpha_l = -\frac{\langle \mathcal{L}(e), \mathcal{L}(q^l) \rangle}{\langle \mathcal{L}(q^l), \mathcal{L}(q^l) \rangle},$$

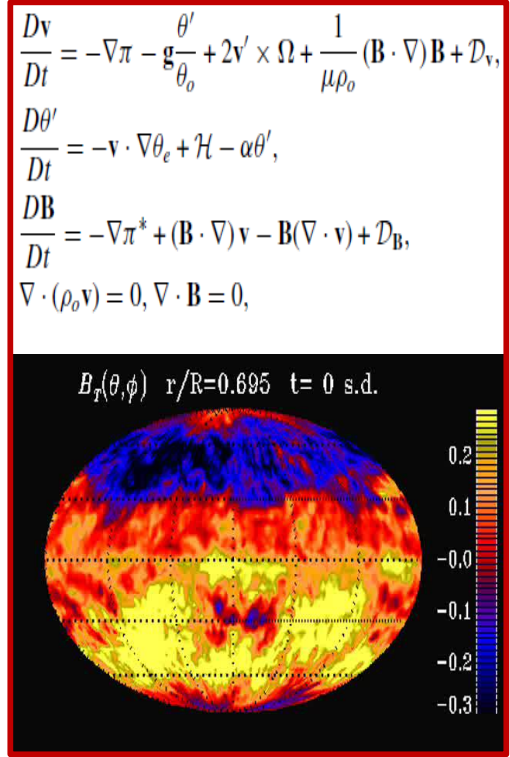
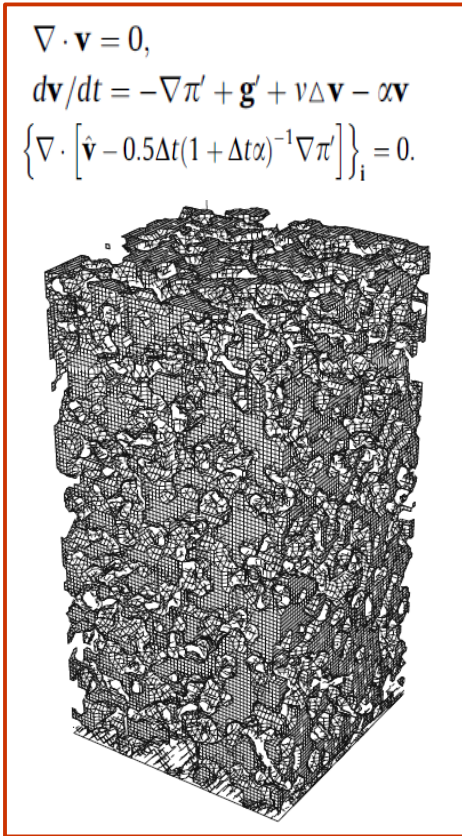
$$q_i^{v+1} = e_i + \sum_{l=0}^v \alpha_l q_i^l,$$

$$\mathcal{L}_i(q^{v+1}) = \mathcal{L}_i(e) + \sum_{l=0}^v \alpha_l \mathcal{L}_i(q^l),$$

end do,

reset $[\Psi, r, q, \mathcal{L}(q)]_i^k$ to $[\Psi, r, q, \mathcal{L}(q)]_i^0$,

end do.



A few remarks on boundary conditions:

$$\sigma = \alpha(\phi) - R = \frac{1}{g^*} \nabla \cdot g^* (\nabla \phi - \phi \nabla \phi)$$

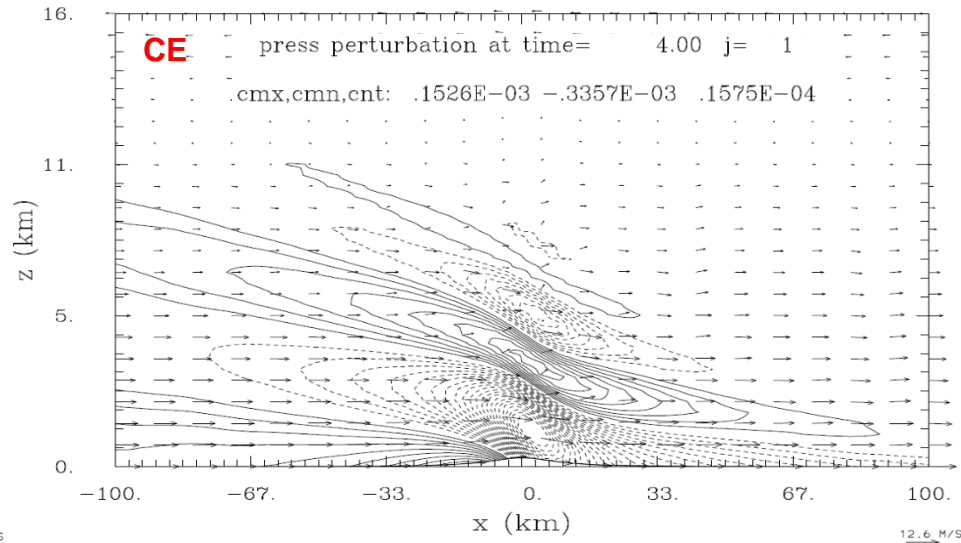
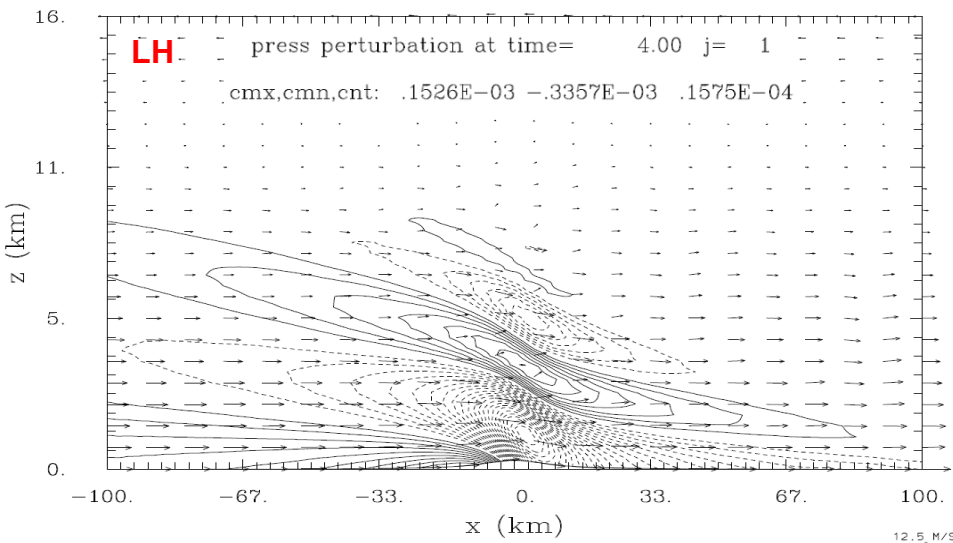
$$\phi^{v+1} = \phi^v + \beta^v \sigma^v$$

$$n \cdot \nabla \phi^{v+1} |_B = n \cdot \nabla \phi^v |_B + \beta^v n \cdot \nabla \sigma^v |_B$$

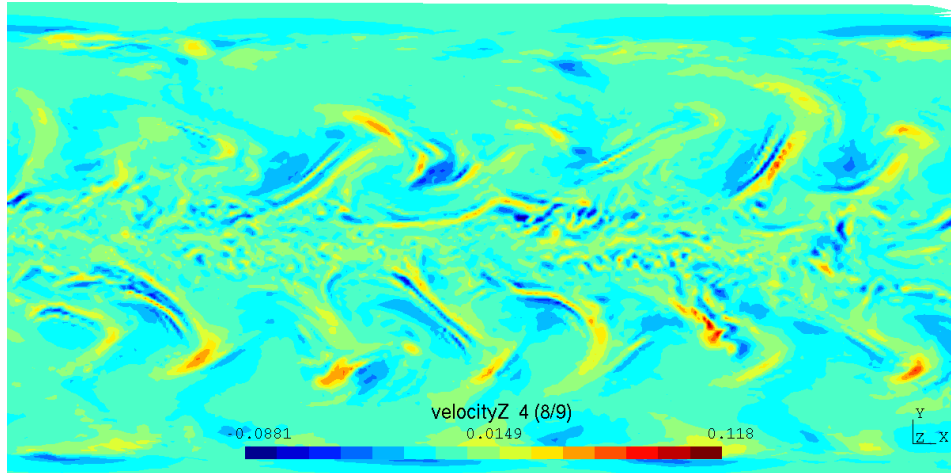
bc satisfied \forall if satisfied for $v=0$
 given $n \cdot \nabla \sigma^v |_B = 0$

$$\int \phi^{v+1} g^* d^3x = \int \phi^v g^* d^3x$$

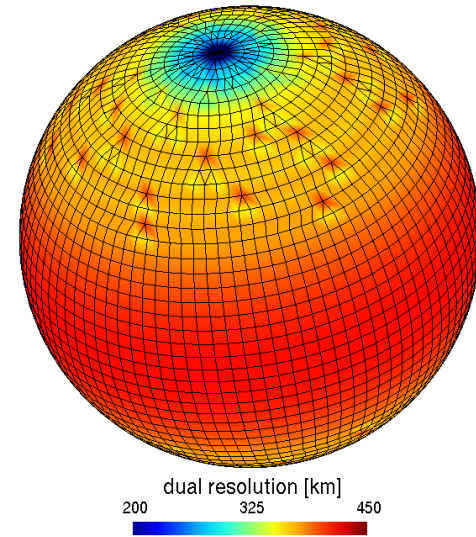
if $\phi = p - p_e$ and $\phi^0 = (p - p_e)^{n-1}$
 arbitrary constant is zero



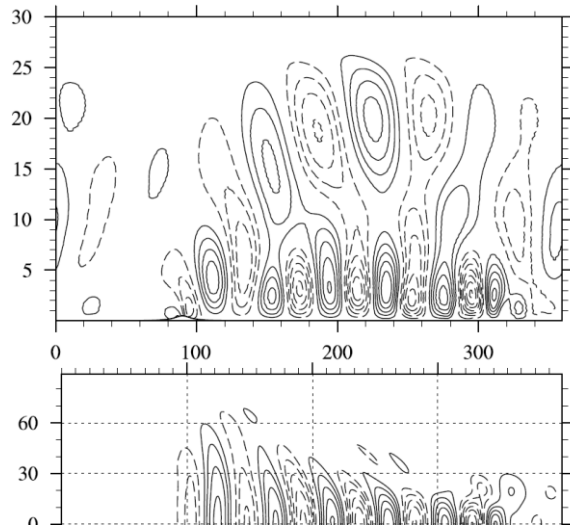
Pseudo-incompressible solution on the reduced T159 Gaussian grid



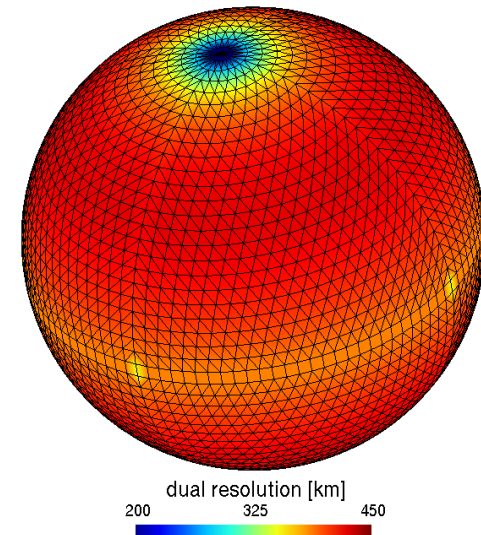
Held-Suarez climate benchmark; day 80 vertical velocity at $z=2.4$ km



Octahedral mesh built on the N255 reduced Gaussian grid



Trapped lee waves on a small planet; compressible solution





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Principal results

Soundproof and compressible nonhydrostatic models form complementary elements of a general theoretical-numerical framework that underlies non-oscillatory forward-in-time (NFT) flow solvers

The respective PDEs are integrated using essentially the same numerics

The resulting flow solvers can be available in compatible Eulerian and semi-Lagrangian variants

The flux-form flow solvers readily extend to unstructured-meshes

P.K. Smolarkiewicz, C. Kühnlein, N.P. Wedi, A consistent framework for discrete integrations of soundproof and compressible PDEs of atmospheric dynamics, *J. Comput. Phys.* 263 (2014) 185-205

M. Kurowski, W.W. Grabowski, and P.K. Smolarkiewicz, Anelastic and compressible simulations of moist deep convection, *J. Atmos. Sci.* 71 (2014) 3767--3787

P.K. Smolarkiewicz, W. Deconinck, M. Hamrud, G. Mozdzyński, C. Kühnlein, J. Szmelter, N. Wedi, A finite-volume module for simulating global all-scale atmospheric flows, *J. Comput. Phys.* 314 (2016) 287-304

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