March 2019, Reading

Unified Framework for Discrete Integrations of Partial Differential Equations of Atmospheric Dynamics

European Research Council
Established by the European Commission
Supporting top researchers from anywhere in the world

ECMWF

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-subspace solvers;

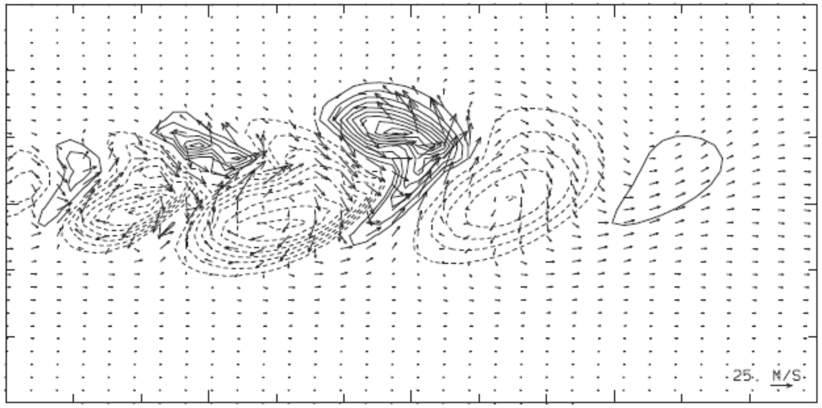
Preconditioning;

Boundary conditions

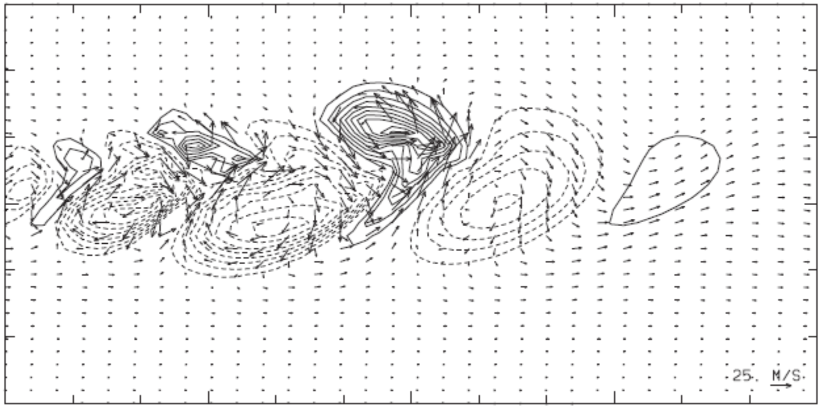
Preamble:

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

This huge computational-efficiency gain comes at the cost of increased mathematical/numerical complexity

ECMWF

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.

ECMWF

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.

Fundamentals:

Newton, 1642-1727

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

physics (re measurement)

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

math (re Taylor series)

$$= \lim_{\delta t \to 0} \frac{1}{\delta t} \left(\left[\mathbf{x}(\mathbf{x}_o, t+\delta t) - \mathbf{x}(\mathbf{x}_o, t)\right] \cdot \nabla\psi\Big|_{\mathbf{x}(\mathbf{x}_o,t),\,t} + \delta t \frac{\partial \psi}{\partial t}\Big|_{\mathbf{x}(\mathbf{x}_o,t),\,t} + \mathcal{O}(\delta t^2) \right)$$

$$= \lim_{\delta t \to 0} \frac{\mathbf{x}(\mathbf{x}_o, t+\delta t) - \mathbf{x}(\mathbf{x}_o, t)}{\delta t} \cdot \nabla\psi\Big|_{\mathbf{x}(\mathbf{x}_o,t)\,t} + \frac{\partial \psi}{\partial t}\Big|_{\mathbf{x}(\mathbf{x}_o,t)\,t} + \lim_{\delta t \to 0} \mathcal{O}(\delta t)$$

$$= \left(\mathbf{v} \cdot \nabla\psi + \frac{\partial \psi}{\partial t} \right)_{\mathbf{x}(\mathbf{x}_o,t),\,t}, \quad \forall_{\mathbf{x}(\mathbf{x}_o,t),\,t}$$

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

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

physics (relating observations in the two reference frames)

Taylor , 1685-1731

ECMWF

More math:

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

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

Leibniz, 1646-1716

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

flow divergence, definition *flow Jacobian*

Euler, 1707-1783

Euler expansion formula,

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

Gauss, 1777-1855

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.

ECMWF

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

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

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

$$\frac{d\rho}{dt} = -\frac{\rho}{\mathcal{G}}\nabla\cdot\left(\mathcal{G}\mathbf{v}\right) \Leftrightarrow \frac{\partial \mathcal{G}\rho}{\partial t} + \nabla\cdot\left(\mathcal{G}\mathbf{v}\rho\right) = 0$$

key tools for deriving conservation laws

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

Lebesque1875-1941

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

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

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

$$= \int_{R^n} f(\Phi(x))\cdot|\det\Phi'(x)|\,d\lambda^n(x).$$

ECMWF

Elementary examples:

Shallow-water equations

$$\frac{\partial G\mathcal{D}}{\partial t} + \nabla \cdot (G\mathbf{v}^*\mathcal{D}) = 0,$$
$$\frac{\partial GQ_x}{\partial t} + \nabla \cdot (G\mathbf{v}^*Q_x) = G\left(-\frac{g}{h_x}\mathcal{D}\frac{\partial H}{\partial x} + fQ_y - \frac{1}{G\mathcal{D}}\frac{\partial h_x}{\partial y}Q_xQ_y\right),$$
$$\frac{\partial GQ_y}{\partial t} + \nabla \cdot (G\mathbf{v}^*Q_y) = G\left(-\frac{g}{h_y}\mathcal{D}\frac{\partial H}{\partial y} - fQ_x + \frac{1}{G\mathcal{D}}\frac{\partial h_x}{\partial y}Q_x^2\right),$$

(Szmelter & Smolarkiewicz, JCP, 2010)

anelastic system

$$\frac{d\mathbf{v}}{dt} = -\nabla\pi' - \mathrm{g}\frac{\theta'}{\overline{\theta}} - 2\mathbf{\Omega} \times \mathbf{v}' + \mathbf{M}' + F_{\mathbf{v}} \ ,$$
$$\nabla \cdot (\overline{\rho}\mathbf{v}) = 0 \ ,$$
$$\frac{d\theta'}{dt} = -\mathbf{v} \cdot \nabla\theta_e + F_\theta \ .$$

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

ECMWF

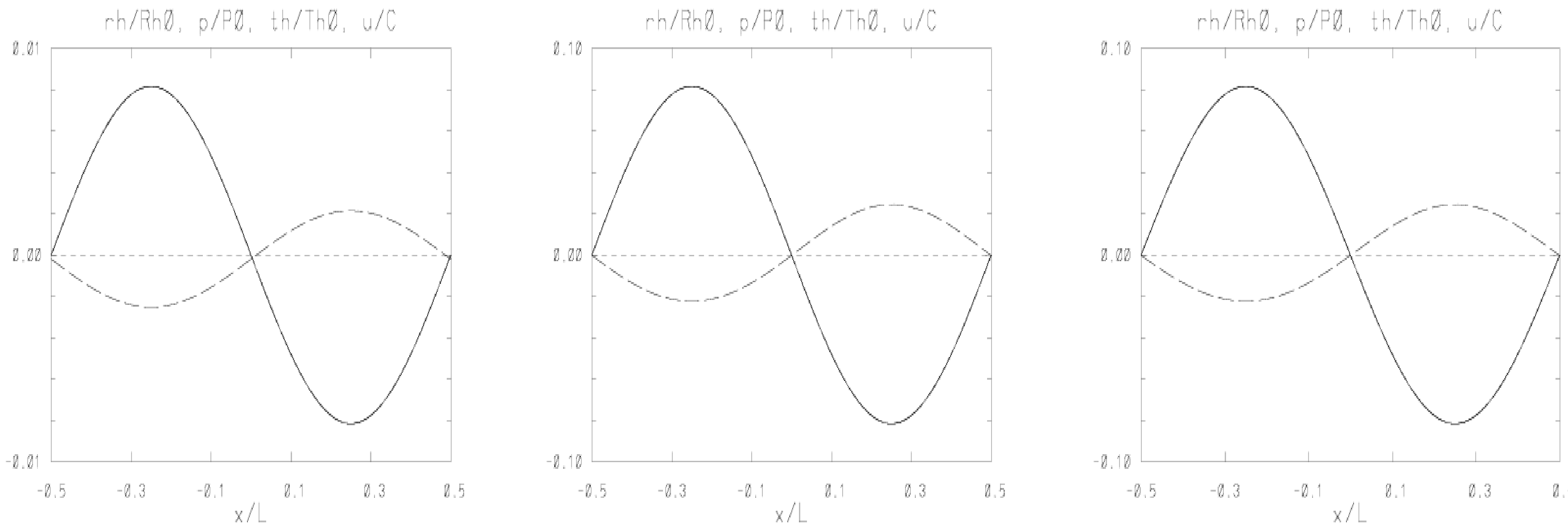
Why bother? Handling unresolved acoustic modes, while insisting on large time steps relative to speed of sound, makes numerics of non-hydrostatic atmospheric models based on the compressible Euler equations demanding

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

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

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

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 $ds = c_p d\ln\theta$

Helmholtz, 1821-1894

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:

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

for problems with small vertical scales and density perturbations:

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

incompressible Boussinesq equations

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

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

ECMWF

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 !

ECMWF

Perturbation forms in terms of potential temperature and Exner function

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

F.M. Exner, 1876-1930

compressible Euler equations

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

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

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

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

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

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

$\leftrightarrow$

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

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

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

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

ECMWF

- 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:

(Smolarkiewicz, Kühnlein & Wedi, JCP, 2014)

$$\frac{d\mathbf{u}}{dt} = -\Theta\nabla\varphi - \mathbf{g}\Upsilon_B\frac{\theta'}{\theta_b} - \mathbf{f}\times(\mathbf{u}-\Upsilon_C\mathbf{u}_e)\ ,$$

$$\frac{d\theta'}{dt} = -\mathbf{u}\cdot\nabla\theta_e\ ,$$

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

$$\Theta := \left[1,\ \frac{\theta(\mathbf{x},t)}{\theta_0},\ \frac{\theta(\mathbf{x},t)}{\theta_0}\right]\ ,$$

$$\Upsilon_B := \left[1,\ \frac{\theta_b(z)}{\theta_e(\mathbf{x})},\ \frac{\theta_b(z)}{\theta_e(\mathbf{x})}\right]\ ,$$

$$\Upsilon_C := \left[1,\ \frac{\theta(\mathbf{x},t)}{\theta_e(\mathbf{x})},\ \frac{\theta(\mathbf{x},t))}{\theta_e(\mathbf{x})}\right]\ ,$$

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

$$\varphi := \left[c_p\theta_b\pi',\ c_p\theta_0\pi',\ c_p\theta_0\pi'\right]\ ,$$

$$\varphi = c_p\theta_0\left[\left(\frac{R_d}{p_0}\varrho\theta\right)^{R_d/c_v} - \pi_e\right]$$ *gas law*

conservation-law forms ➔

Combined equations, conservation form:

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

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

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

$$d\psi/dt = R$$

$$\partial \varrho \psi / \partial t + \nabla \cdot (\varrho \mathbf{u} \psi) = \varrho R$$

specific vs. density variables

Accounting for curvilinear coordinates:

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

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

$\mathbf{v} = \dot{\mathbf{x}}$ not necessarily equal to $\mathbf{u}$

$\mathcal{G}(\mathbf{x}, t)$ denotes the Jacobian

$\mathcal{G}^2$ is the determinant of the metric tensor

Riemann, 1826-1863

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

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

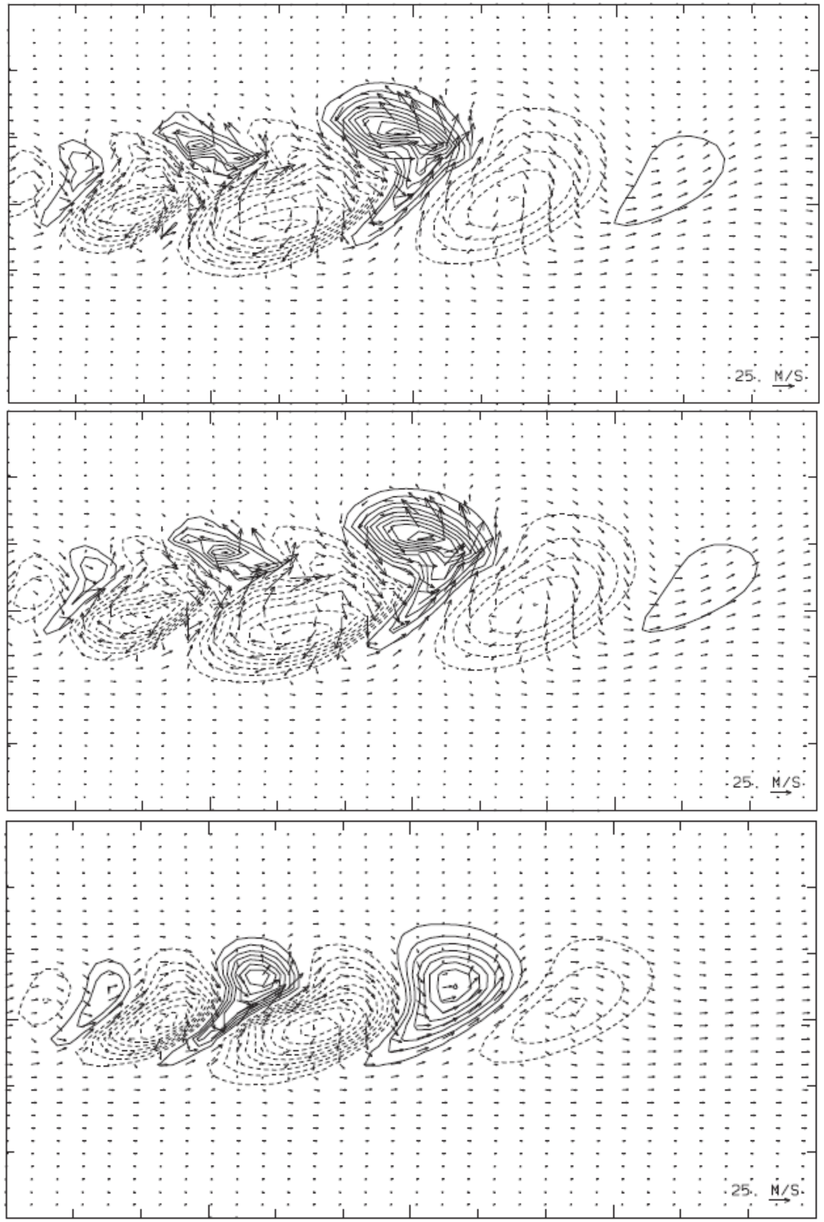
recall “the archetype problem, AP”

ECMWF

➔ *example* ➔ *integration schemes* ➔

Global baroclinic instability (Smolarkiewicz, Kühnlein & Wedi , JCP, 2014)

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



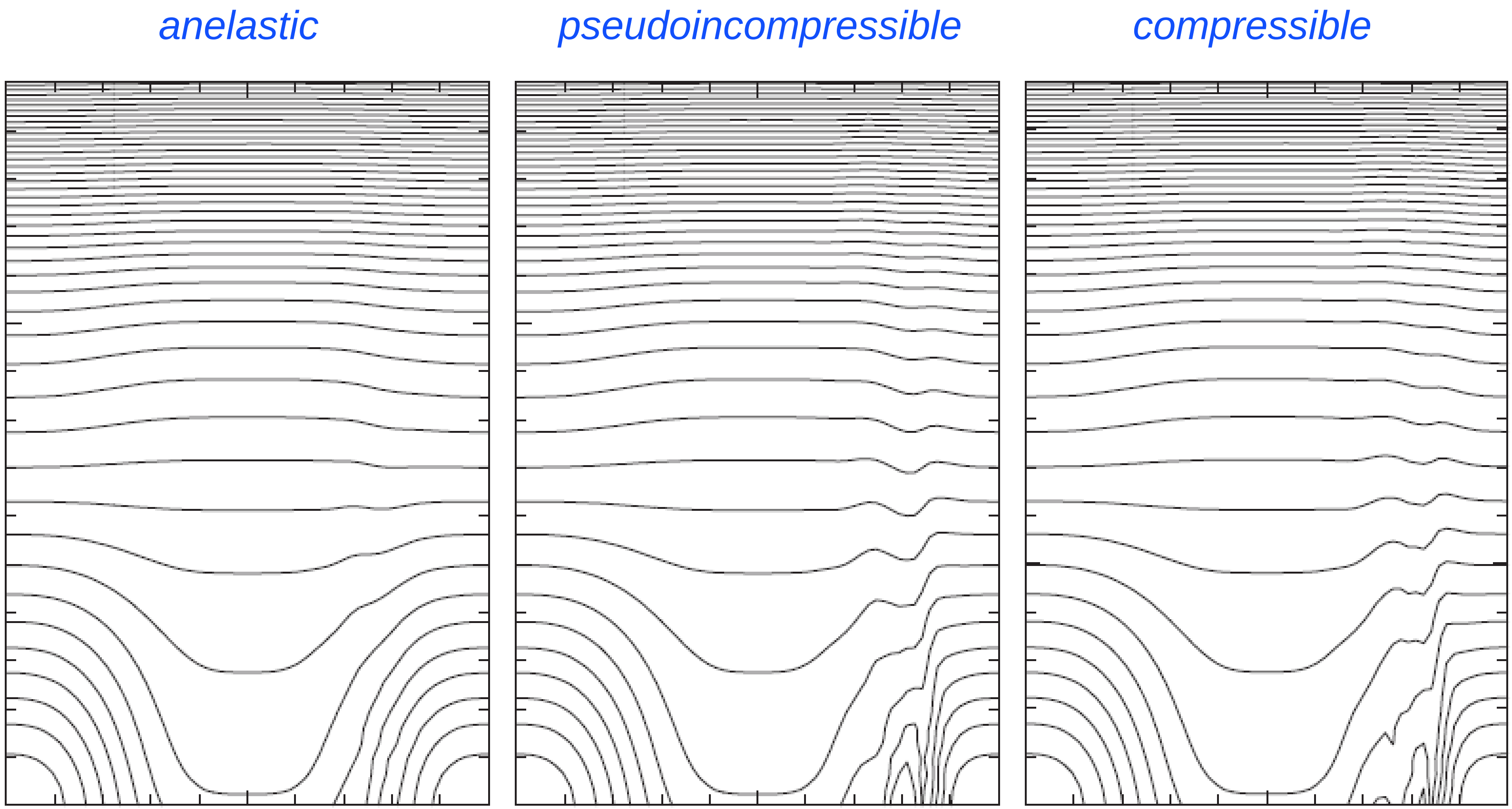
CMP, 2880 dt=300 s,
wallclock time=2.0 mns

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

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

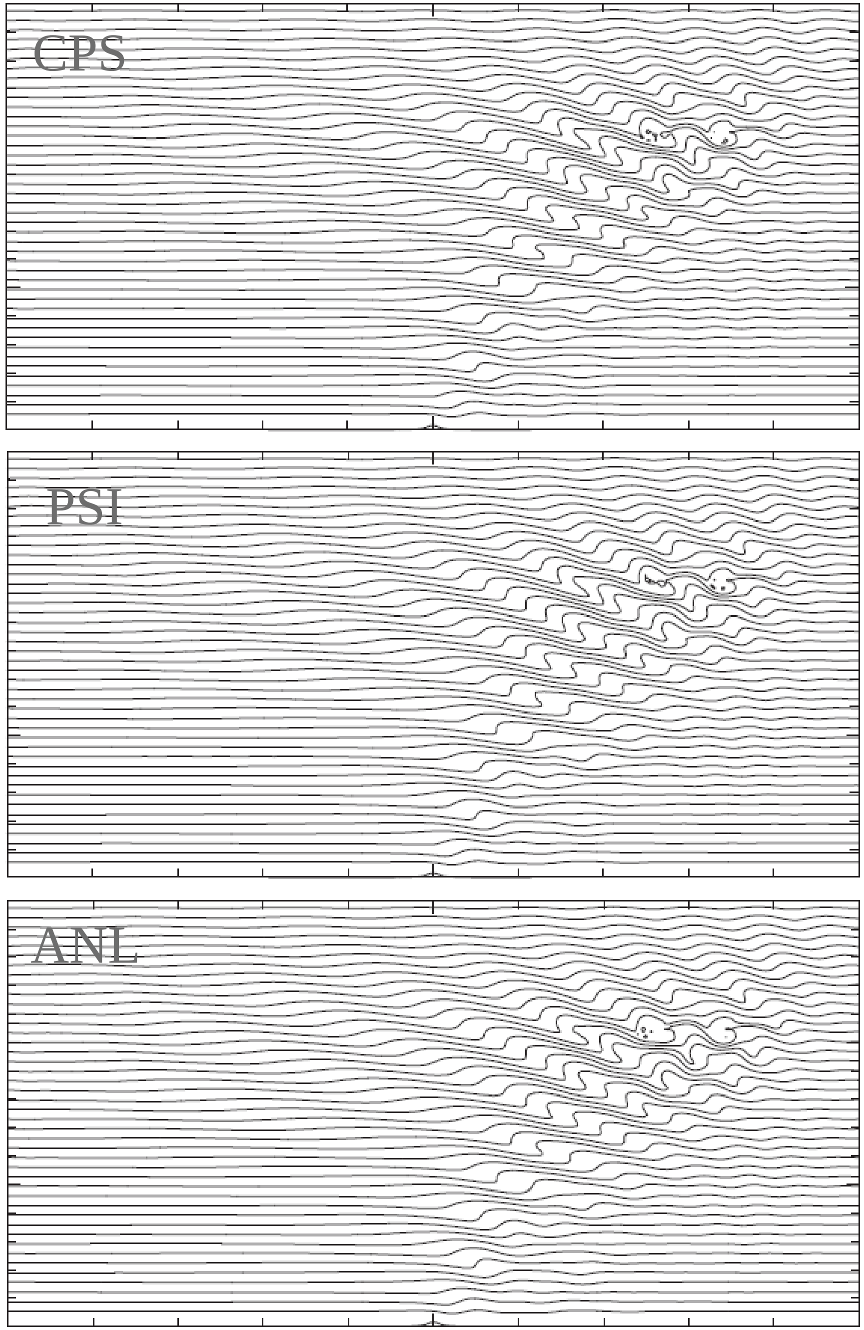
ECMWF

The role of baroclinicity



ECMWF

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



ECMWF

Part II: Integration Schemes

A) Forward-in-time (FT) non-oscillatory (NFT) integrators for all-scale flows,

Cauchy, 1789-1857

Kowalevski, 1850-1891

Lax, 1926-

Wendroff, 1930-

Robert, 1929-1993

ECMWF

- 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)

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

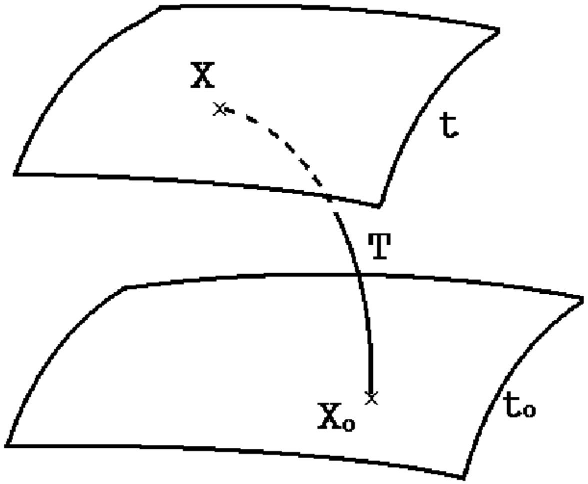
$$\Psi_i^{n+1} = \mathcal{A}_i\left(\Psi^n + 0.5\delta t R^n\right) + 0.5\delta t R_i^{n+1}$$

ECMWF

Motivation for Lagrangian integrals

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

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



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

$$\Psi_{\mathbf{i}}^{n+1} = \Psi_o + 0.5\delta t (R_{\mathbf{i}}^{n+1} + R_o) + \delta t \mathcal{O}(\delta t^2)$$

$$\Psi_{\mathbf{i}}^{n+1} = (\Psi + 0.5\delta t R)_o + 0.5\delta t R_{\mathbf{i}}^{n+1} + \mathcal{HOT}$$

ECMWF

Motivation for Eulerian integrals

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

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

forward-in-time temporal discretization:

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

Second order Taylor expansion about t=nδt & 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≡0), a 2nd order-accurate solution for an inhomogeneous problem with "arbitrary" R is:

$$\Psi_{\mathbf{i}}^{n+1} = \mathcal{A}_{\mathbf{i}}\left(\widetilde{\Psi}^n, \mathbf{V}^{n+1/2}, G^n, G^{n+1}\right) + 0.5\delta t \mathcal{R}_{\mathbf{i}}^{n+1} \ ,$$

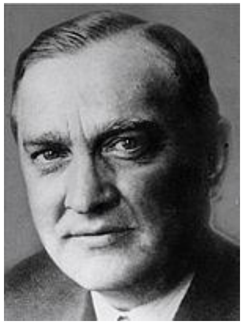
where

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

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

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

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



1892-1945

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

Eulerian semi-implicit compressible algorithms → → →

Semi-implicit formulations (solar MHD example)

$$\frac{\partial \rho^* \mathbf{\Psi}}{\partial \bar{t}} + \overline{\nabla} \cdot (\mathbf{V}^* \mathbf{\Psi}) = \rho^* \mathbf{R} \ ,$$

$$\mathbf{\Psi} = \{\mathbf{u}, \Theta', \mathbf{B}\}^T$$

$$\mathbf{R} = \{\mathbf{R_u}, R_{\Theta'}, \mathbf{R_B}\}^T$$

$$\mathbf{\Psi}_\mathrm{i}^n = \mathcal{A}_\mathrm{i}\left(\widetilde{\mathbf{\Psi}}, \widetilde{\mathbf{V}}^*, \rho^*\right) + 0.5\delta t \mathbf{R}_\mathrm{i}^n \equiv \widehat{\mathbf{\Psi}}_\mathrm{i} + 0.5\delta t \mathbf{R}_\mathrm{i}^n$$

$$\mathbf{\Psi}_\mathrm{i}^{n,\nu} = \widehat{\mathbf{\Psi}}_\mathrm{i} + 0.5\delta t \ \mathbf{L\Psi}\big|_\mathrm{i}^{n,\nu} + 0.5\delta t \ \mathbf{N}(\mathbf{\Psi})\big|_\mathrm{i}^{n,\nu-1} - 0.5\delta t \ \widetilde{\mathbf{G}}\overline{\nabla}\mathbf{\Phi}\big|_\mathrm{i}^{n,\nu}$$

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

$$\mathbf{\Psi}_\mathrm{i}^{n,\nu} = [\mathbf{I} - 0.5\delta t \mathbf{L}]^{-1} \left(\widehat{\widehat{\mathbf{\Psi}}} - 0.5\delta t \widetilde{\mathbf{G}}\overline{\nabla}\mathbf{\Phi}^{n,\nu}\right)\Big|_\mathrm{i}$$

$$\widehat{\widehat{\mathbf{\Psi}}} \equiv \widehat{\mathbf{\Psi}} + 0.5\delta t \mathbf{N\Psi}\big|^{n,\nu-1}$$

➔ thermodynamic/elliptic problems for “pressures” **Φ**

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

in some detail for compressible Euler PDEs of all-scale atmospheric dynamics

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

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

semi-implicit ``acoustic" scheme:

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

$$\widehat{\theta}'_{\mathrm{i}} = \mathcal{A}_{\mathrm{i}}\left(\widetilde{\theta}', \mathbf{V}^{n+1/2}, \varrho^{*\,n}, \varrho^{*\,n+1}\right)$$

$$\widehat{\mathbf{u}}_{\mathrm{i}} = \mathcal{A}_{\mathrm{i}}\left(\widetilde{\mathbf{u}}, \mathbf{V}^{n+1/2}, \varrho^{*\,n}, \varrho^{*\,n+1}\right)$$

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

$$\nu = 1, .., N_\nu$$

(RE: Banach principle)

$$\theta'|_{\mathrm{i}}^{\nu} = \widehat{\theta}'_{\mathrm{i}} - 0.5\delta t\left(\widetilde{\mathbf{G}}^T\mathbf{u}^\nu\cdot\nabla\theta_e\right)_{\mathrm{i}}$$

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

$$\varphi_{\mathrm{i}}^{\nu} = c_p\theta_0\left[\left(\frac{R_d}{p_0}\varrho^{n+1}\theta^{\nu-1}\right)^{R_d/c_v} - \pi_e\right]_{\mathrm{i}}$$

(RE: thermodynamic pressure)

$$\theta_{\mathrm{i}}^{\nu} = \left(\widehat{\theta}' - 0.5\delta t\widetilde{\mathbf{G}}^T\mathbf{u}^\nu\cdot\nabla\theta_e + \theta_e\right)_{\mathrm{i}} \qquad \theta_{\mathrm{i}}^{0} = \mathcal{A}_{\mathrm{i}}\left(\theta^n, \mathbf{V}^{n+1/2}, \varrho^{*\,n}, \varrho^{*\,n+1}\right)$$

simple but computationally unaffordable; example ➔

(RE: elliptic pressure)

$$\overbrace{\mathbf{u}^\nu + 0.5\delta t\mathbf{f}\times\mathbf{u}^\nu - (0.5\delta t)^2\mathbf{g}\Upsilon_B\frac{1}{\theta_b}\widetilde{\mathbf{G}}^T\mathbf{u}^\nu\cdot\nabla\theta_e}^{\mathbf{L}\mathbf{u}^\nu} =$$

$$\hat{\mathbf{u}} - 0.5\delta t\left(\mathbf{g}\Upsilon_B\frac{\widehat{\theta'}}{\theta_b} - \mathbf{f}\times\Upsilon_C^{\nu-1}\mathbf{u}_e - \mathcal{M}'(\mathbf{u},\mathbf{u},\Upsilon_C)^{\nu-1}\right)$$

$$-0.5\delta t\Theta^{\nu-1}\widetilde{\mathbf{G}}\nabla\varphi^\nu \quad\equiv\quad \boxed{\widehat{\hat{\mathbf{u}}} - 0.5\delta t\Theta^{\nu-1}\widetilde{\mathbf{G}}\nabla\varphi^\nu} \quad \rightarrow$$

$$\boxed{\mathbf{u}^\nu = \check{\hat{\mathbf{u}}} - \mathbf{C}\nabla\varphi^\nu} \quad \text{where } \check{\hat{\mathbf{u}}} = \mathbf{L}^{-1}\widehat{\hat{\mathbf{u}}} \text{ and } \mathbf{C} = \mathbf{L}^{-1}0.5\delta t\Theta^{\nu-1}\widetilde{\mathbf{G}}$$

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 $\mathbf{u}^\nu = \check{\hat{\mathbf{u}}} - \mathbf{C}\nabla\varphi^\nu$ and … →

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

diagonally preconditioned Poisson problem for pressure perturbation

ECMWF

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 $\gamma \equiv R_d/c_v$

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

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

$$\check{\check{\mathbf{v}}} - \widetilde{\mathbf{G}}^T\mathbf{C}\nabla\varphi^\nu$$

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

*And how does one solve this "thing" **?***

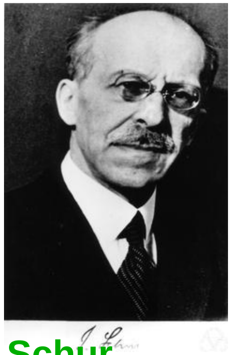
Part II: Integration Schemes

B) Elliptic solvers for boundary value problems (BVP) in atmospheric models

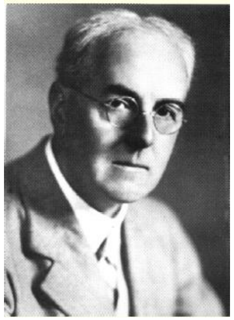
Poisson, 1781-1840

Helmholtz, 1821-1894

Krylov, 1863-1945



Schur, 1875-1941



Richardson, 1881-1953

Taxonomy:

Direct methods (e.g., spectral, Gaussian elimination, conjugate-gradients (CG))
vs. Iterative methods (e.g., Gauss-Seidel, Richardson, multigrid, CG)

Matrix inversion vs. matrix-free methods

Approximate vs. Exact projection ➔ user-friendly libraries vs. bespoke solvers

Multiple terminologies & classifications; common grounds; the state-of-the-art

Basic tools and concepts:

Banach principle, Neumann series, Gaussian elimination, Thomas 3-diagonal algorithm, Fourier transformation, calculus of variations, multigrid

Physical analogies:

Heat equation, damped oscillation equation, energy minimisation

Notion of variational Krylov-subspace solvers: i) basic concepts and definitions

symbolism: $0 = -\sum_{\ell=1}^{3}\left(\frac{A_\ell^\star}{\zeta_\ell}\nabla\cdot\zeta_\ell(\check{\check{\mathbf{v}}} - \widetilde{\mathbf{G}}^T\mathbf{C}\nabla\varphi)\right) - B^\star(\varphi - \widehat{\varphi})$ $\equiv$ $\boxed{\mathcal{L}(\varphi) - R = 0}$

linear BVP

pseudo-time augmentation $\boxed{\frac{\partial\varphi}{\partial\tau} = \mathcal{L}(\varphi) - R}$ $\rightarrow$

Richardson 1910, Frankel 1952; Birkhoff and Lynch 1984

$\frac{\partial e}{\partial\tau} = \mathcal{L}(e)$ *where* $e \equiv \varphi - \overline{\varphi}$ *is the solution error, so* $R = \mathcal{L}(\overline{\varphi})$ $\rightarrow$

$\frac{\partial\langle e^2\rangle}{\partial\tau} = 2\langle e\mathcal{L}(e)\rangle$ *where* $\langle\ldots\rangle$ *is the domain integral* $\rightarrow$

as $\tau \to \infty$ [red box] *gives the exact solution to* [green box] *provided*

$$\forall e \neq 0 \;\; \langle e\mathcal{L}(e)\rangle < 0$$

:= negative definiteness *(comments on dissipativity, semi-definiteness and null spaces)*

ECMWF

i) basic concepts and definitions, cnt.

Next, the "energy" functional

$$\mathcal{J}(\varphi) \equiv -\frac{1}{2}\langle\varphi\boldsymbol{\mathcal{L}}(\varphi)\rangle + \langle\varphi R\rangle \quad \rightarrow$$

$$\boxed{\mathcal{J}(\varphi) = -\frac{1}{2}\langle e\boldsymbol{\mathcal{L}}(e)\rangle + \mathcal{J}(\overline{\varphi}) + \frac{1}{2}[\langle\varphi\boldsymbol{\mathcal{L}}(\overline{\varphi})\rangle - \langle\overline{\varphi}\boldsymbol{\mathcal{L}}(\varphi)\rangle]} \quad \rightarrow$$

$$\mathcal{J}(\varphi) > \mathcal{J}(\overline{\varphi}) \quad \forall\varphi$$ *given*

$$\langle\xi\boldsymbol{\mathcal{L}}(\varphi)\rangle = \langle\varphi\boldsymbol{\mathcal{L}}(\xi)\rangle \ \forall\varphi,\xi$$

:= self-adjointness *or symmetry in matrix representation,*

a common property of Laplacian, since $\xi\triangle\varphi \equiv \nabla\cdot(\xi\nabla\varphi - \varphi\nabla\xi) + \varphi\triangle\xi$

(comment on suitable boundary conditions)

ECMWF

i) basic concepts and definitions, cnt. 2

$\boxed{\mathcal{L}(\varphi) - R = 0}$ *only for exact solution, otherwise it defines the **residual error***

$$r \equiv \mathcal{L}(\varphi) - R \quad \left(\Longrightarrow \quad r = \mathcal{L}(e) \right) \rightarrow$$

$\square$ *can be rewritten as* $\boxed{\dfrac{\partial \varphi}{\partial \tau} = r} \rightarrow \boxed{\dfrac{\partial r}{\partial \tau} = \mathcal{L}(r)} \rightarrow$

$$\frac{\partial \langle r^2 \rangle}{\partial \tau} = 2\langle r \mathcal{L}(r) \rangle \rightarrow r \to 0 \text{ as } \tau \to \infty, \text{ for negative definite } \mathcal{L}$$

Richardson iteration *($\Delta\tau = \beta$)*

$$\varphi^{n+1} = \varphi^n + \beta(\mathcal{L}(\varphi^n) - R)$$

(comments on stability vs convergence, and spectral implications)

ECMWF

Notion of variational Krylov-subspace solvers: ii) canonical schemes

Steepest descent and minimum residual

By the same arguments like applied to continuous equations , Richardson iteration implies

$$e^{n+1} = e^n + \beta\mathcal{L}(e^n) \quad \textit{and} \quad r^{n+1} = r^n + \beta\mathcal{L}(r^n)$$

For self adjoint operators □ *implies* $\mathcal{J}(e) = -\frac{1}{2}\langle e\mathcal{L}(e)\rangle = -\frac{1}{2}\langle er\rangle$

Because the exact solution minimises the energy functional, one way to assure the optimal convergence is to minimise $-\langle e^{n+1}r^{n+1}\rangle$ ➔

$$\langle r^n r^n\rangle + \langle e^n\mathcal{L}(r^n)\rangle + 2\beta\langle r^n\mathcal{L}(r^n)\rangle = 0$$

And from self adjointness $\beta = -\dfrac{\langle r^n r^n\rangle}{\langle r^n\mathcal{L}(r^n)\rangle}$

Steepest descent For any initial guess φ^0, set $r^0 = \mathcal{L}(\varphi^0) - R$; then iterate :

For $n = 0, 1, 2, \ldots$until convergence do

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

$$\varphi^{n+1} = \varphi^n + \beta r^n \ ,$$

$$r^{n+1} = r^n + \beta\mathcal{L}(r^n) \ ,$$

$$\text{exit if} \quad \| r^{n+1} \| \leq \varepsilon \ .$$

Digression, orthogonality of subsequent iterates $\langle r^n r^{n+1}\rangle = 0$

$$\frac{\partial}{\partial\beta}\langle e^{n+1} r^{n+1}\rangle = 0 \implies \langle \frac{\partial e^{n+1}}{\partial\beta} r^{n+1}\rangle + \langle e^{n+1}\frac{\partial r^{n+1}}{\partial\beta}\rangle = 0 \rightarrow$$

$$\langle r^n r^{n+1}\rangle + \langle e^{n+1}\mathcal{L}(r^n)\rangle = 2\langle r^n r^{n+1}\rangle = 0$$

Minimum residual: *Self adjointness can be difficult to achieve in practical models, the minimum residual circumvents this by minimising* $\langle r^{n+1} r^{n+1}\rangle$ *instead* →

$$\langle r^n \mathcal{L}(r^n)\rangle + \beta\langle \mathcal{L}(r^n)\mathcal{L}(r^n)\rangle = 0 \rightarrow$$

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

Steepest descent and minimum residual are important for understanding, but otherwise uncompetitive. The true foundation is provided by conjugate gradients and residuals

$$\frac{\partial^2\varphi}{\partial\tau^2} + \frac{1}{T}\frac{\partial\varphi}{\partial\tau} = \mathcal{L}(\varphi) - R \rightarrow$$ *3 term recurrence formula*

$$\varphi^{n+1} = \gamma\varphi^n + (1-\gamma)\varphi^{n-1} + \beta(\mathcal{L}(\varphi^n) - R)$$

a.k.a 2nd order Richardson, due to Frankel 1950

ECMWF

Conjugte gradient (CG) and conjugate residual (CR):

$$\varphi^{n+1} = \gamma\varphi^n + (1-\gamma)\varphi^{n-1} + \beta(\mathcal{L}(\varphi^n) - R)$$
$$e^{n+1} = \gamma e^n + (1-\gamma)e^{n-1} + \beta\mathcal{L}(e^n)$$
$$r^{n+1} = \gamma r^n + (1-\gamma)r^{n-1} + \beta\mathcal{L}(r^n)$$

the coefficients of which could be determined via norms' minimisation, analogous to steepest descent and minimum residual, or instead ➔

$$\varphi^{n+1} = \varphi^n + \beta^n\left(\frac{(\gamma^n-1)\beta^{n-1}}{\beta^n}\cdot\frac{(\varphi^n-\varphi^{n-1})}{\beta^{n-1}} + r^n\right) \equiv \varphi^n + \beta^n(\alpha^n p^{n-1} + r^n)$$

➔ For any initial guess φ^0, set $p^0 = r^0 = \mathcal{L}(\varphi^0) - R$;

For $n = 0, 1, 2, \ldots$until convergence do

$$\beta^n = \ldots.. \ ,$$

$$\varphi^{n+1} = \varphi^n + \beta^n p^n \ ,$$

$$r^{n+1} = r^n + \beta^n \mathcal{L}(p^n) \ ,$$

$$\alpha^{n+1} = \ldots.. \ ,$$

$$p^{n+1} = \alpha^{n+1}p^n + r^{n+1}$$

exit if $\| r^{n+1} \| \leq \varepsilon$,

CG

$$\beta^n = -\frac{< r^n r^n >}{< p^n\mathcal{L}(p^n) >}$$

$$\alpha^{n+1} = \frac{< r^{n+1} r^{n+1} >}{< r^n r^n >}$$

CR

$$\beta^n = -\frac{< r^n\mathcal{L}(p^n) >}{< \mathcal{L}(p^n)\mathcal{L}(p^n) >}$$

$$\alpha^{n+1} = -\frac{< \mathcal{L}(r^{n+1})\mathcal{L}(p^n) >}{< \mathcal{L}(p^n)\mathcal{L}(p^n) >}$$

$$\mathcal{L}(p^{n+1}) = \mathcal{L}(r^{n+1}) + \alpha^{n+1}\mathcal{L}(p^n)$$

… variational Krylov-subspace solvers: iii) operator 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

$$\frac{\partial \mathcal{P}(\varphi)}{\partial \tau} = \mathcal{L}(\varphi) - R$$

P ("left" preconditioner) approximates L but is easier to invert.

$$\varphi^{n+1} = \varphi^n + \beta \mathcal{P}^{-1}(\mathcal{L}(\varphi^n) - R) = \varphi^n + \beta \mathcal{P}^{-1}(r)$$

Preconditioned conjugate residual:

$$\frac{\partial^2 \mathcal{P}(\varphi)}{\partial \tau^2} + \frac{1}{T}\frac{\partial \mathcal{P}(\varphi)}{\partial \tau} = \mathcal{L}(\varphi) - R$$

$$\varphi^{n+1} = \varphi^n + \beta^n \mathcal{P}^{-1}(p^n) \ ,$$

$$r^{n+1} = r^n + \beta^n \mathcal{L}\mathcal{P}^{-1}(p^n) \ ,$$

$$\mathcal{P}^{-1}(p^{n+1}) = \alpha^{n+1}\mathcal{P}^{-1}(p^n) + \mathcal{P}^{-1}(r^{n+1})$$

replacing $p_{new} = \mathcal{P}^{-1}(p_{old})$ →

For any initial guess φ^0, set $r^0 = \mathcal{L}(\varphi^0) - R$, $p^0 = \mathcal{P}^{-1}(r^0)$

For $n = 0, 1, 2, \ldots$until convergence do

$$\beta^n = -\frac{< r^n \mathcal{L}(p^n) >}{< \mathcal{L}(p^n)\mathcal{L}(p^n) >} \ ,$$

$$\varphi^{n+1} = \varphi^n + \beta^n p^n \ ,$$

$$r^{n+1} = r^n + \beta^n \mathcal{L}(p^n) \ ,$$

$$\text{exit if} \quad \| r^{n+1} \| \leq \varepsilon \ ,$$

$$q^{n+1} = \mathcal{P}^{-1}(r^{n+1}) \ ,$$

$$\alpha^{n+1} = -\frac{< \mathcal{L}(q^{n+1})\mathcal{L}(p^n) >}{< \mathcal{L}(p^n)\mathcal{L}(p^n) >} \ ,$$

$$p^{n+1} = \alpha^{n+1} p^n + q^{n+1} \ ,$$

$$\mathcal{L}(p^{n+1}) = \mathcal{L}(q^{n+1}) + \alpha^{n+1}\mathcal{L}(p^n) \ .$$

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

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

2)
$$\frac{\mathcal{D}e^{\mu+1} - \mathcal{D}e^{\mu}}{\Delta\tilde{\tau}} = \mathcal{P}^h(e^{\mu}) - \mathcal{D}(e^{\mu+1} - e^{\mu}) + \mathcal{P}^z(e^{\mu+1}) - r^{\nu+1}$$
$$\Delta\tilde{\tau} \rightarrow \infty, \qquad \text{block Jacobi}$$

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

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

$$e^{\nu+1} = \sum_{k,l} \hat{e}_{k,l}(z) \exp[i(k \cdot x + l \cdot y)]$$
$$r^{\nu+1} = \sum_{k,l} \hat{r}_{k,l}(z) \exp[i(k \cdot x + l \cdot y)]$$
$$\sum_{k,l} \left\{ \mathcal{C}_{k,l}(z)\hat{e}_{k,l} + \mathcal{B}_{k,l}(z)\frac{d^2\hat{e}_{k,l}}{dz^2} - \hat{r}_{k,l} \right\} \exp[i(k \cdot x + l \cdot y)] \equiv 0$$
$$\forall_{k,l} \quad \left(\mathcal{C}_{k,l}(z) + \mathcal{B}_{k,l}(z)\frac{\delta^2}{\delta z^2} \right) \hat{e}_{k,l}(z) = \hat{r}_{k,l}(z)$$

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

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

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 $n = 1, 2, \ldots$ until convergence do

for $\nu = 0, .., k-1$ do

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

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

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

exit if $\| r^{\nu+1} \| \leq \varepsilon^*$,

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

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

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

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

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

end do,

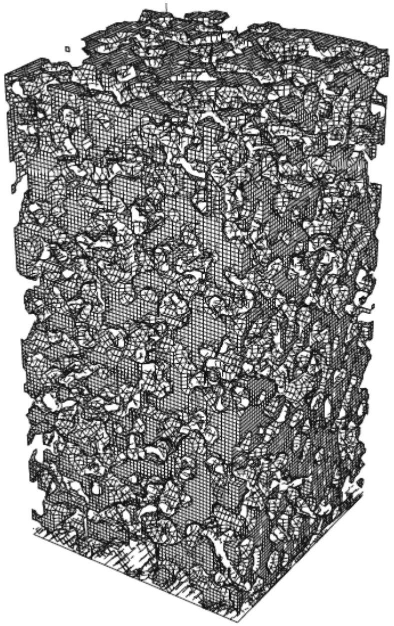
reset $[\Psi, r, q, \mathcal{L}(q)]_i^k$ to $[\Psi, r, q, \mathcal{L}(q)]_i^0$,

end do.

$$\nabla \cdot \mathbf{v} = 0,$$

$$d\mathbf{v}/dt = -\nabla\pi' + \mathbf{g}' + \nu\Delta\mathbf{v} - \alpha\mathbf{v}$$

$$\left\{\nabla \cdot \left[\hat{\mathbf{v}} - 0.5\Delta t(1+\Delta t\alpha)^{-1}\nabla\pi'\right]\right\}_i = 0.$$

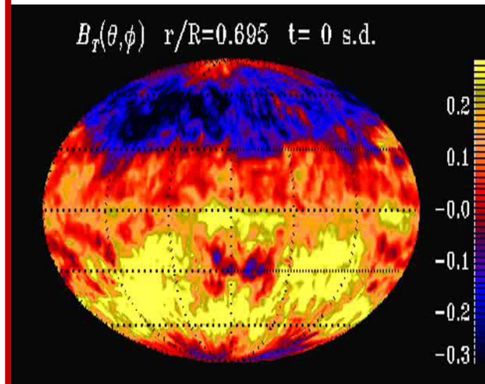


$$\frac{D\mathbf{v}}{Dt} = -\nabla\pi - \mathbf{g}\frac{\theta'}{\theta_o} + 2\mathbf{v}' \times \boldsymbol{\Omega} + \frac{1}{\mu\rho_o}(\mathbf{B}\cdot\nabla)\mathbf{B} + \mathcal{D}_{\mathbf{v}},$$

$$\frac{D\theta'}{Dt} = -\mathbf{v}\cdot\nabla\theta_e + \mathcal{H} - \alpha\theta',$$

$$\frac{D\mathbf{B}}{Dt} = -\nabla\pi^* + (\mathbf{B}\cdot\nabla)\mathbf{v} - \mathbf{B}(\nabla\cdot\mathbf{v}) + \mathcal{D}_{\mathbf{B}},$$

$$\nabla\cdot(\rho_o\mathbf{v}) = 0, \nabla\cdot\mathbf{B} = 0,$$



ECMWF

A few remarks on boundary conditions:

$$r = \mathcal{L}(\phi) - R = \frac{1}{\rho^*}\nabla\cdot\rho^*(\hat{\mathbf{v}} - \mathbf{C}\nabla\phi)$$

$$\phi^{\nu+1} = \phi^{\nu} + \beta^{\nu} r^{\nu}$$

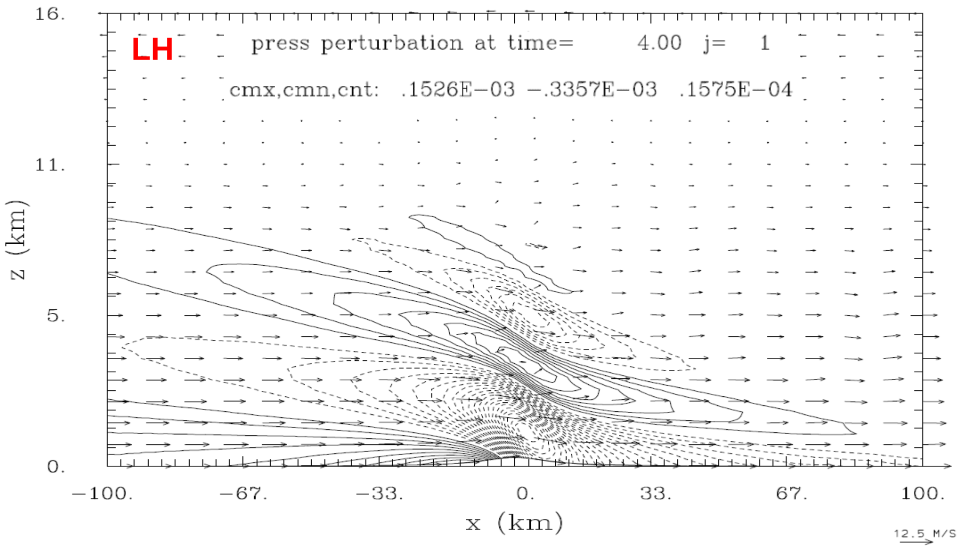
$$\mathbf{n}\cdot\nabla\phi^{\nu+1}\big|_B = \mathbf{n}\cdot\nabla\phi^{\nu}\big|_B + \beta^{\nu}\,\mathbf{n}\cdot\nabla r^{\nu}\big|_B$$

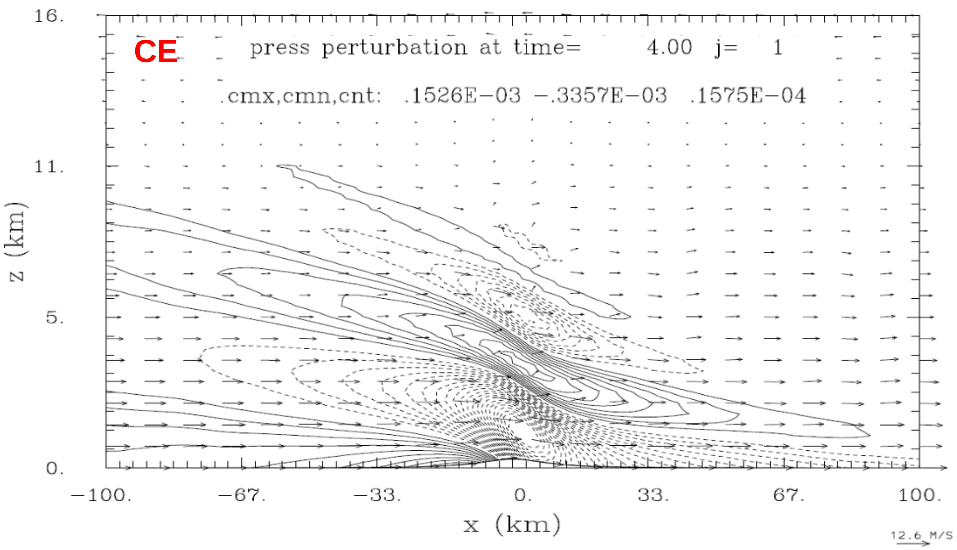
bc satisfied $\forall\nu$ if satisfied for $\nu=0$ given $\forall\nu\ \mathbf{n}\cdot\nabla r^{\nu}\big|_B = 0$

$$\int\phi^{\nu+1}\rho^* d^3x = \int\phi^{\nu}\rho^* d^3x$$

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

arbitrary constant is zero





Principal conclusions

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

2. The respective PDEs are integrated using essentially the same numerics.

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

4. The flux-form flow solvers readily extend to unstructured-meshes and generalised forms of the governing PDEs (Smolarkiewicz, Kühnlein & Wedi , JCP, 2019)

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

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

C. Kühnlein, P.K. Smolarkiewicz, An unstructured-mesh finite-volume MPDATA for compressible atmospheric dynamics, J. Comput. Phys. 334 (2017) 16-3.

P.K. Smolarkiewicz, C. Kühnlein, N.P. Wedi, Semi-implicit integrations of perturbation equations for all-scale atmospheric dynamics, *J. Comput. Phys*. 376 (2019) 145-159.

C. Kühnlein, W. Deconinck, R. Klein, S. Malardel, Z. Piotrowski, P.K. Smolarkiewicz, J. Szmelter, N.P. Wedi, FVM 1.0: a nonhydrostatic finite-volume dynamical core for the IFS, Geosci. Model Dev. (2019) 12, 651–676.

P.K. Smolarkiewicz, L. Margolin, Variational methods for elliptic problems in fluid models, in: ECMWF Proceedings, Workshop on Developments in Numerical Methods for Very High Resolution Global Models, 2000, pp.137–159, Reading, UK.