Modelling geophysical flows with nonoscillatory forward-in-time methods

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Outline:

Fundamentals;

Terminology & brief history;

Eulerian & Lagrangian reference frames;

Semi-implicit algorithms;

Nonhydrostatic (all-scale) PDEs;

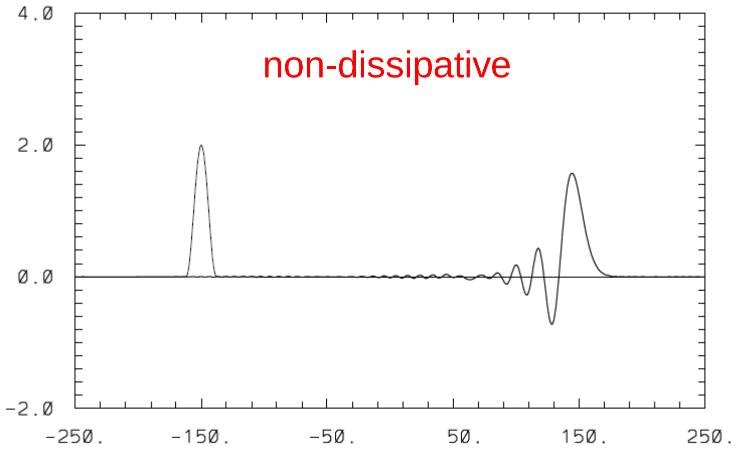
ILES

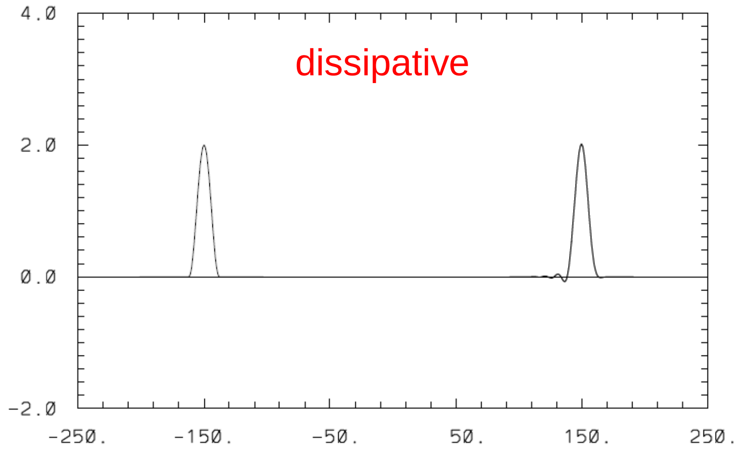
Examples

Fundamentals:

- Advection constitutes a key element of hydrodynamic (HD) description of nature.
- Axioms and PDEs of HD description imply that advection cannot change sign(s) of transported variables ➔ numerical L^2 integrability.
- These properties do not necessarily extend to discrete approximations.

1D advection with constant velocity $\frac{\partial \Psi}{\partial t} = -\frac{\partial}{\partial x}(u\Psi)$





2nd order leapfrog: centered in time and space (CTS);

solution at t^{n+1} ← solutions t^n & t^{n-1}

4th order “Lax-Wendroff’”: forward in time (FT);

solution at t^{n+1} ← solution t^n

Nonoscillatory forward in time (NFT)

- Godunov's predicament (1959) $\Rightarrow$ nonlinear schemes

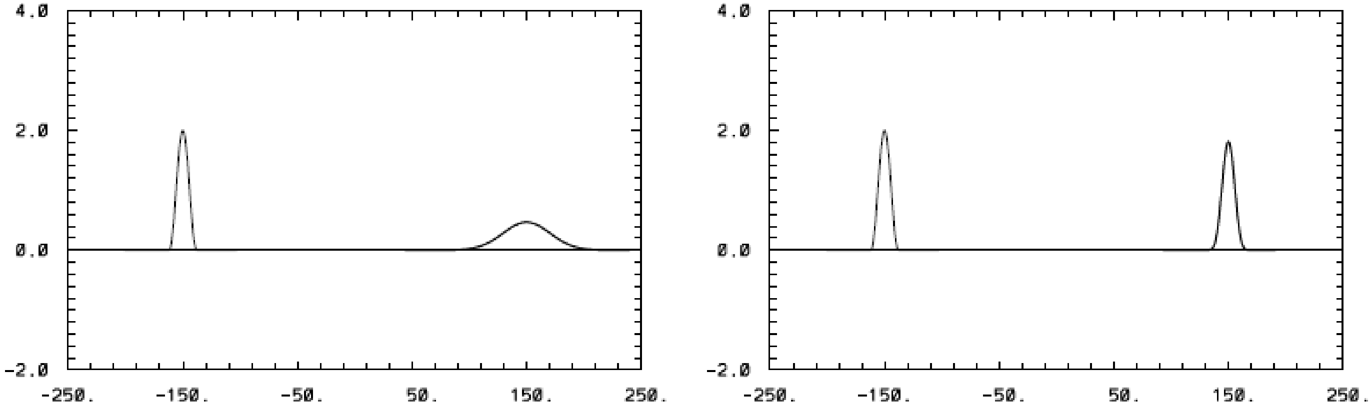


Figure 2: 1st-order upwind and 2nd-order MPDATA (a nonlinear Lax-Wendroff scheme)

Terminology & history (select papers; see introductions & references therein):

The Forward-in-Time Upstream Advection Scheme: Extension to Higher Orders

CRAIG J. TREMBACK, JAMES POWELL,* WILLIAM R. COTTON AND ROGER A. PIELKE
Colorado State University, Department of Atmospheric Science, Fort Collins, CO 80523

MWR, 1987, **115**, 540-551

Introduction to ''Computational Design for Long-Term Numerical Integration of the Equations of Fluid Motion: Two-Dimensional Incompressible Flow. Part I'' by DK Lilly

JCP, 1997, **135**, 101-102

A Class of Conservative Fourth-Order Advection Schemes and Impact of Enhanced Formal Accuracy on Extended-Range Forecasts

ZAVISA JANJIC
National Centers for Environmental Prediction, Camp Springs, Maryland

TIJANA JANJIC
Alfred Wegener Institute, Bremerhaven, Germany

RATKO VASIC
University Corporation for Atmospheric Research, Camp Springs, Maryland

MWR, 2011, **139**, 1556-1558

MPDATA: Third-order accuracy for variable flows

Maciej Waruszewski [a,*], Christian Kühnlein [b], Hanna Pawlowska [a], Piotr K. Smolarkiewicz [b]

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[b] *European Centre for Medium-Range Weather Forecasts, Shinfield Park, Reading, RG2 9AX, United Kingdom*

JCP, 2018, **359**, 361-379

Two reference frames

Eulerian ← → Lagrangian

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

archetype problem, AP

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

IFS-FVM

IFS-ST

- Generalised, 2nd order accurate, forward-in-time (FT), nonoscillatory (NFT) integrators for the archetype problem ➔ Eulerian/Lagrangian congruence

Eulerian

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

Lagrangian (semi)

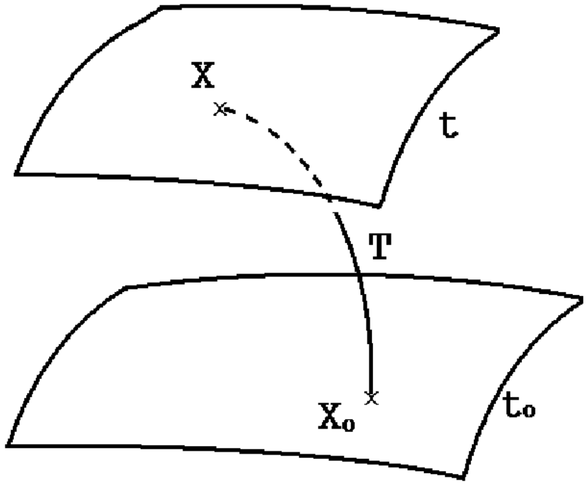
$$\frac{d\Psi}{dt} = R$$

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

Motivation for Lagrangian integrals

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

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



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

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

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

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

Semi-implicit formulations (solar MHD example)

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

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

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

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

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

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

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

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

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

Unified framework, combined symbolic equations:

(Smolarkiewicz, Kühnlein & Wedi, JCP, 2014)

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

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

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

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

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

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

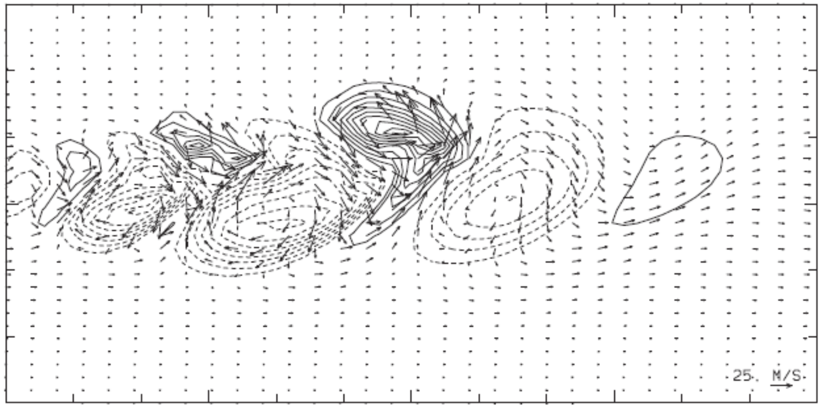
$$\varrho := \left[\rho_b(z),\ \rho_b\frac{\theta_b(z)}{\theta_0},\ \rho(\mathbf{x},t)\right] \ ,$$

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

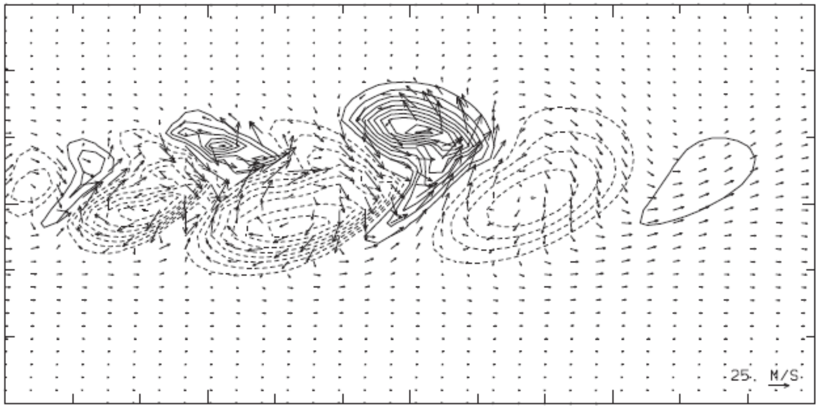
$$\varphi = c_p\theta_0\left[\left(\frac{R_d}{p_0}\varrho\theta\right)^{R_d/c_v} - \pi_e\right]$$ *gas law*

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

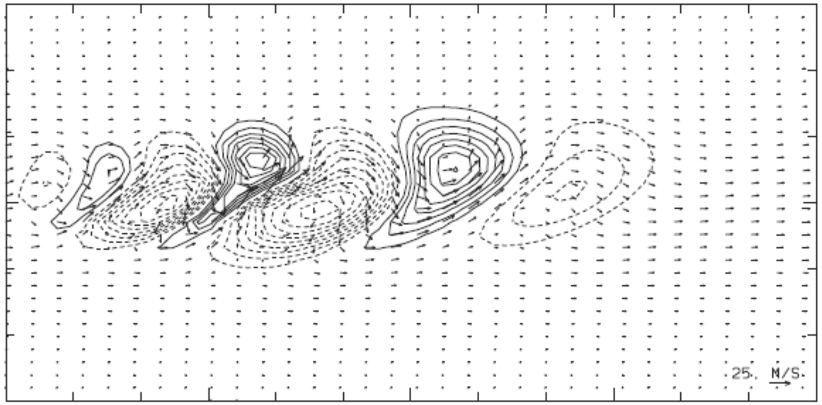
8 days, surface θ’,
128x64x48 lon-lat grid,
128 PE of Power7 IBM



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

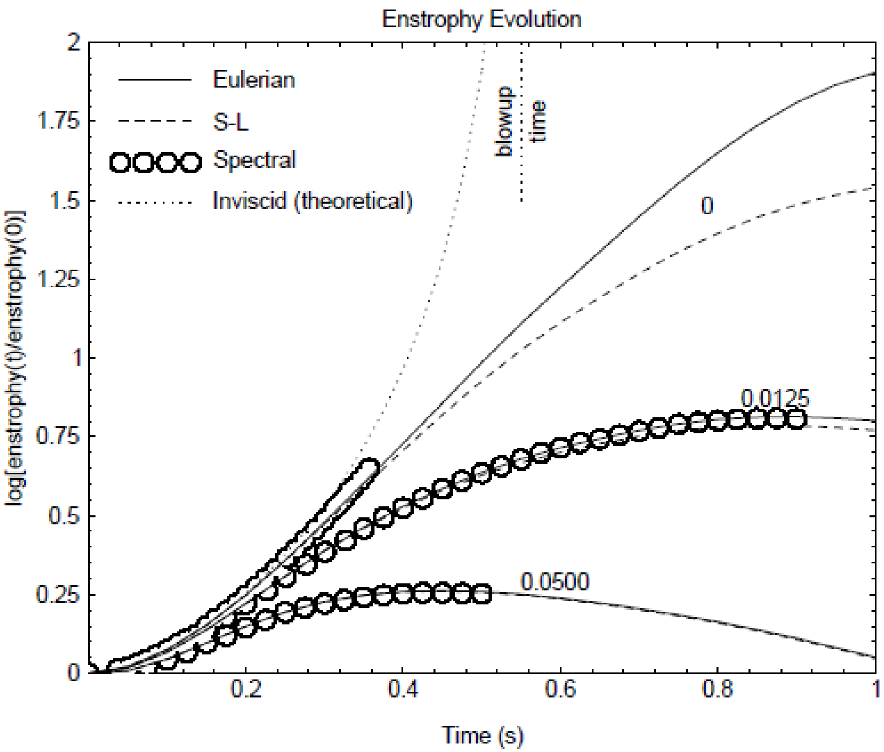


PSI, 2880 dt=300 s,
wallclock time=2.3 mns,



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

ILES---a beneficial byproduct of NFT methods



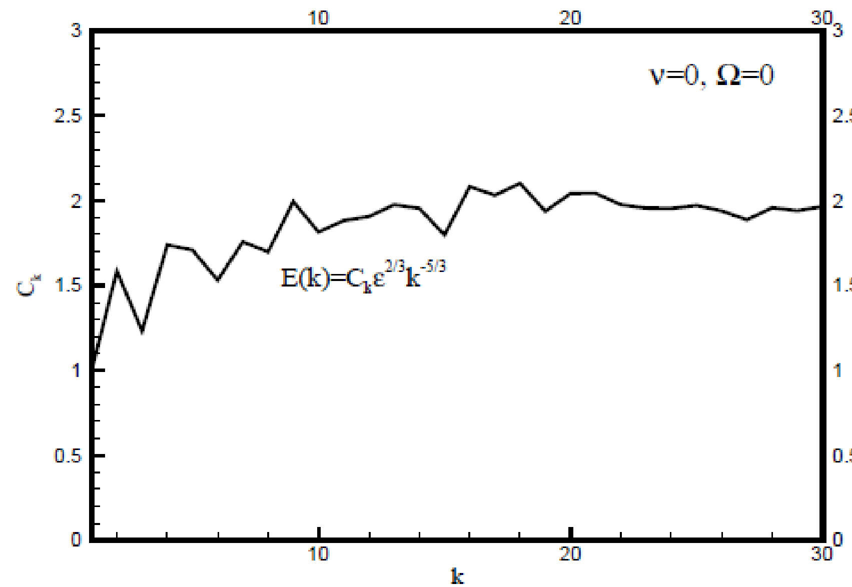


Figure 13: Left: Left: DNS/ILES of decaying turbulence, after Sm. & Prusa *IJNMF* 2002. Right: Kolmogoroff function $C_K(k) = \varepsilon^{-2/3}k^{5/3}E(k)$ for a flow with $\nu = 0.0$; after Domaradzki et al. *Phys. Fluids* 2003.

ILES vs. LES: convective PBL (Smolarkiewicz, Szmelter & Wyszogrodzki JCP 2013)

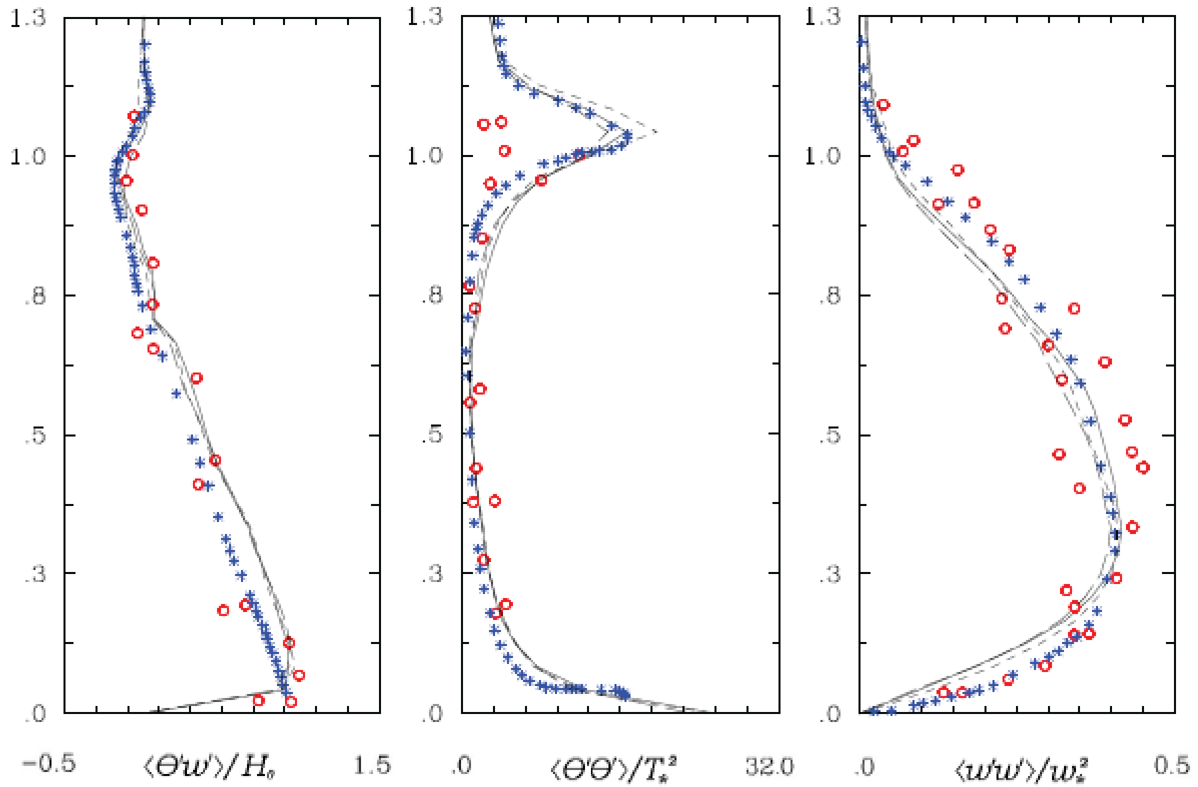
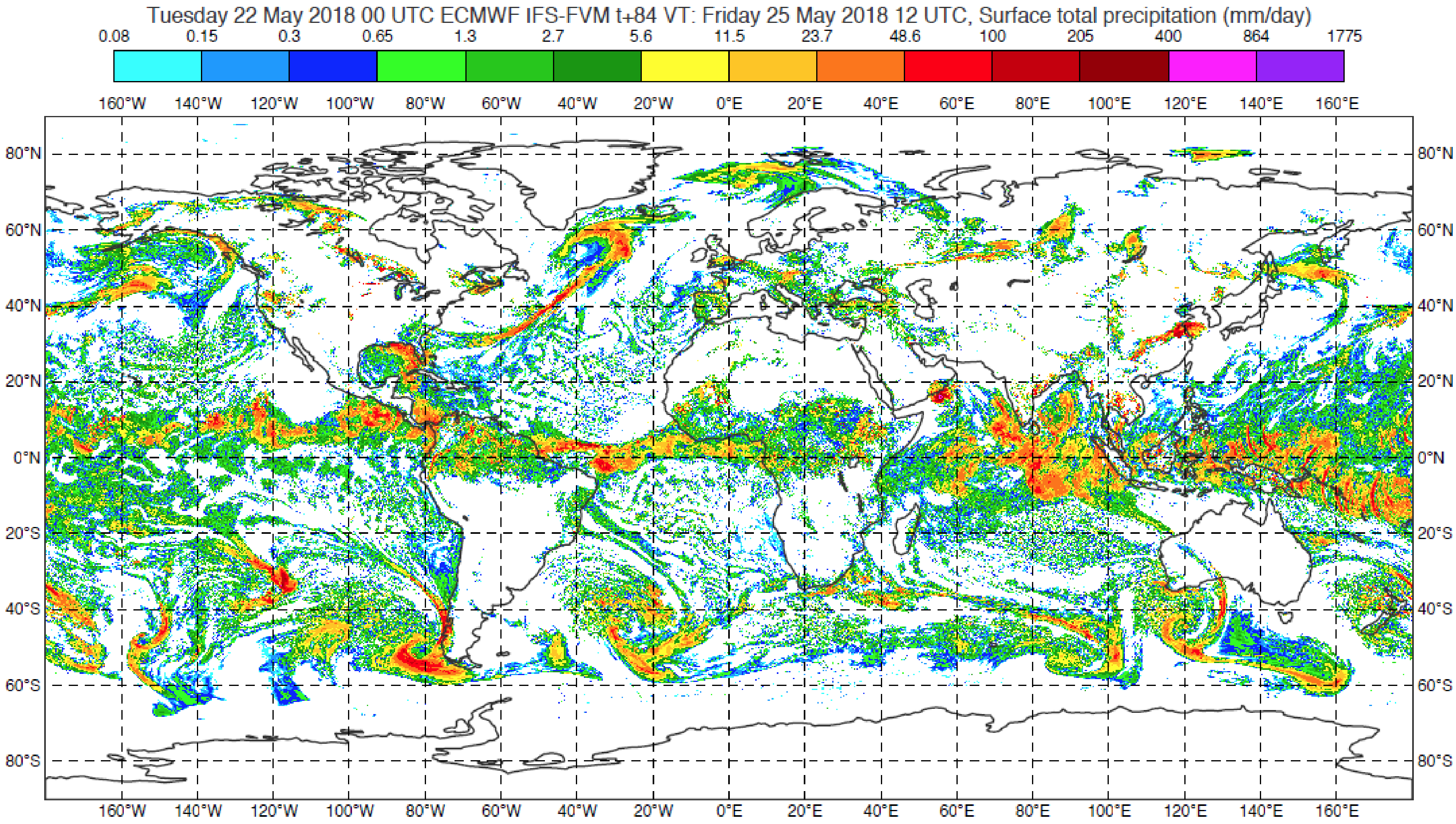


Fig. 4. Vertical profile of dimensionless resolved heat flux, and variances of temperature as well as vertical velocity in Runs **T** (solid), **G** (long dashes), and **R** (short dashes), with dimensionless height z/z_i on the ordinates; blue crosses denote LES result of [25], and red circles represent field and laboratory data.

(R reference EULAG; G & T, EULAG-EB on R's grid and an unstructured mesh)

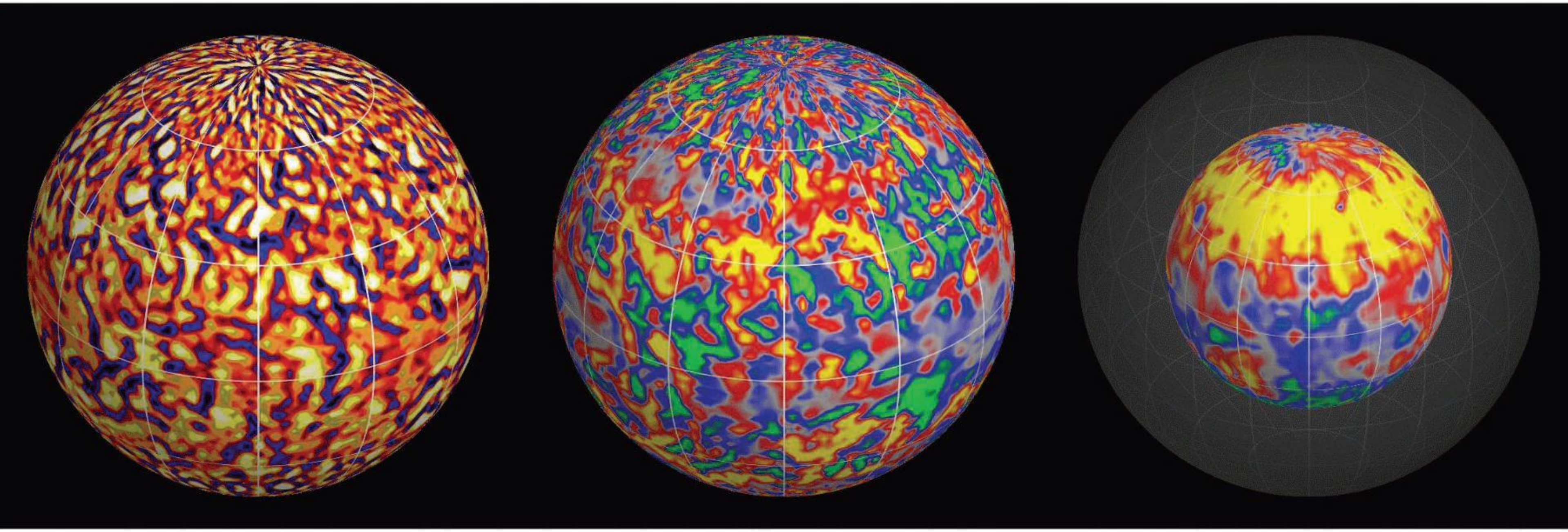
IFS-FVM



84h forecast, O1280 (9km) resolution

Solar Dynamo

www.sciencemag.org SCIENCE VOL 340, 5 APRIL 2013



Radial velocity & zonal magnetic field on the scale of O(10) weeks

Zonal magnetic field on the scale of O(10) years

Digression on boundary conditions in elliptic solvers:

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

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

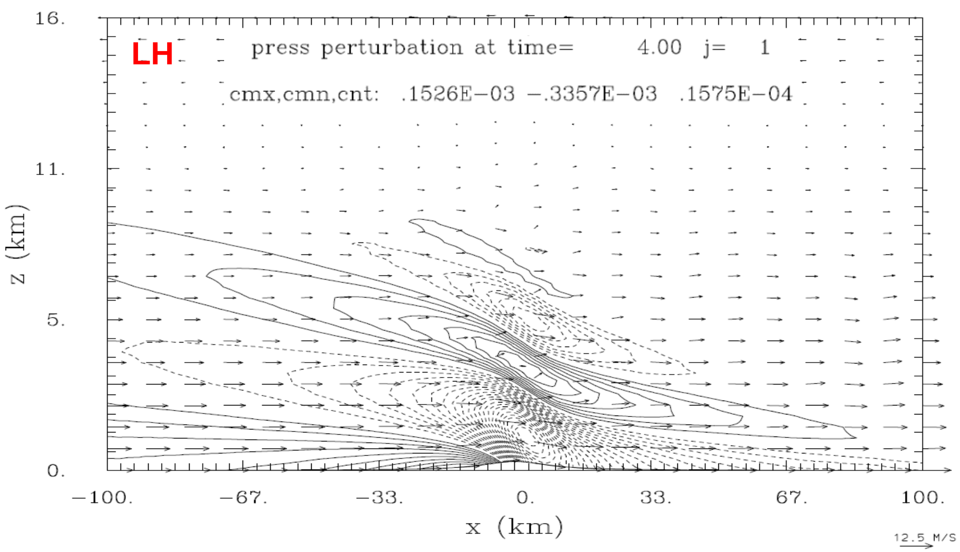
$$n\cdot\nabla\phi^{\nu+1}\big|_B = n\cdot\nabla\phi^{\nu}\big|_B + \beta^{\nu}\, n\cdot\nabla r^{\nu}\big|_B$$

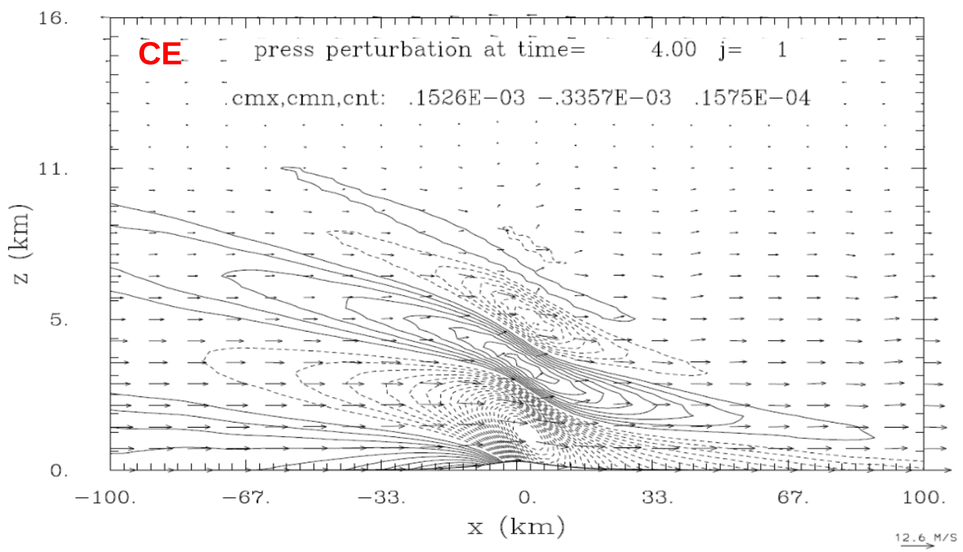
bc satisfied $\forall\nu$ if satisfied for $\nu=0$ given $\forall\nu$ $n\cdot\nabla r^{\nu}\big|_B = 0$

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

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

arbitrary constant is zero





Conclusions:

1. *Since their origin in 1960s, elementary FT advection schemes evolved into powerful NFT methods for modelling fluid flows across a wide range of scales and physical scenarios.*
2. *The resulting flow solvers can be available in compatible Eulerian and semi-Lagrangian variants.*
3. *The flux-form NFT flow solvers readily extend to unstructured-meshes and generalised forms of the governing PDEs (Smolarkiewicz, Kühnlein & Wedi , JCP, 2019).*
4. *Semi-implicit NFT methods enable simulation of all-scale soundproof and compressible PDEs using essentially the same numerics, thus enabling consistent advancements of blended theoretical formulations*

Further reading:

P. Charbonneau, P.K. Smolarkiewicz, Modeling the Solar Dynamo, Science 340 (2013), 42;

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.