

### **Recent developments in Numerical Methods**

- with a report from the ,PDEs on the sphere', April 2014, Boulder

30<sup>th</sup> WGNE-meeting 23-26 March 2015, NCEP, Washington

Michael Baldauf (DWD)



### ,Vertical' Grids and choice of vector components for well-balancing

- <u>covariant velocity components</u> (H. Weller)
   → avoids spurious vorticity production from pressure gradient term
   → fulfills one of the required ,mimetic' properties
   But what about conservation?
   (part of UK MO GungHo-project; finishes at end of 2015)
- <u>3D orthogonal grid</u> (J. Li)
- <u>cut cells</u> (A. Gadian) (personal opinion: needs 3D unstructured grids ← boundary layer!)
- vertical staggering: <u>Lorenz vs. Charney-Phillips grid</u> to avoid computational modes in the vertical (P. Ullrich)



## Representing Mountains



For numerous reasons in meteorology the cells should line up in columns

 $\therefore$  the mesh is non-orthogonal over orography

Usual approach: orthogonal prognostic velocity variables u, v, w in horizontal and vertical directions

: find  $\frac{\partial p}{\partial x}$  co-located with u without knowing p at this altitude (eg Klemp, Zangl)

 $\rightarrow$  pressure gradients not curl free

# Alternative: non-orthogonal prognostic variables (covariant)



Following horizontal discretisations on non-orthogonal grids:

Prognostic variables:  $\mathbf{u} \cdot \hat{\mathbf{d}}$ 

where  $\mathbf{d}_f = \mathbf{x}_i - \mathbf{x}_j$ 

 $\rightarrow$  curl free pressure gradients

 $\rightarrow$  no spurious generation of vorticity

### Cut cell structure

#### from Alan Gadian (NCAS)



FIG. 1. Illustration of the storage locations for the model variables on a staggered grid: at the center of each grid box is stored  $\Pi'$ , denoted by a filled circle; u, v, and w are stored on the gridbox faces perpendicular to their flow directions.

Following Steppeler et al. (2006), 3D lower boundary is represented with piecewise bilinear surfaces. To solve the flow through the irregular shaped cut cells, an approx finite-volume approach is used (Steppeler et al. (2002)).  $N = 3^4 - 2$  configurations.





FIG. 2. The orographic heights at the four corners of the grid column centered on (i, j)—marked ABCD—define a unique bilinear surface, which results in the grid box (i, j, k) being cut by the orography.

Pdes 2014-04-07 5

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#### Horizontal grids

several new global models use unstructured grids:

- MPAS (NCAR): icosahedron-hexagonal (J. Klemp)
- ICON (DWD-MPI): icosahedron-triangular (G. Zängl), see also ,WGNE DWD report'

#### cubed sphere grid:

McGregor: "A major issue for dynamical cores is how to stagger the winds to accurately balance the pressure gradients, whilst also accurately handling the Coriolis terms, i.e. obtain good geostrophic adjustment."

 $\rightarrow$  use "reversible staggering" of velocity components in VCAM, CCAM.

Horizontal grids are also necessary for spectral models, since non-linear terms (advection) are calculated in grid-space (B. Fornberg)

new proposal for IFS: octahedral reduced Gaussian grid (S. Malardel, N. Wedi)



## Alternative cubic grids

Original Sadourny (1972) C20 grid

Equi-angular C20 grid

Conformal-cubic C20 grid Used by VCAM

Used by CCAM

from John McGregor (CSIRO)

### Location of variables in grid cells



All variables are located at the centres of quadrilateral grid cells.

In CCAM, during semi-implicit/gravity-wave calculations, u and v are transformed reversibly to the indicated C-grid locations.

Produces same excellent dispersion properties as spectral method (see McGregor, MWR, 2006), but avoids any problems of Gibbs' phenomena.

2-grid waves preserved. Gives relatively lively winds, and good wind spectra.



Where U is the unstaggered velocity component and u is the staggered value, define (Vandermonde formula)

$$\frac{u_{m-\frac{1}{2}} + 10u_{m+\frac{1}{2}} + 5u_{m+\frac{3}{2}}}{16} = \frac{5U_m + 10U_{m+1} + U_{m+2}}{16}$$

- accurate at the pivot points for up to 4<sup>th</sup> order polynomials
- solved iteratively, or by cyclic tridiagonal solver
- excellent dispersion properties for gravity waves, as shown for the linearized shallow-water equations

$$\begin{aligned} \frac{\partial u}{\partial t} - fv + g \frac{\partial h}{\partial x} &= 0, \\ \frac{\partial v}{\partial t} + fu + g \frac{\partial h}{\partial y} &= 0, \\ \frac{\partial h}{\partial t} + H \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) &= 0. \end{aligned}$$

from John McGregor (CSIRO)

### What is the octahedral grid?

It is a reduced Gaussian grid with the same number of latitude circles (*NDGL*) than the standard Gaussian grid ( $\leftrightarrow$  Gaussian weights) but with a new rule to compute the number of points per latitude circle.

Number of points per latitude NLOEN( $lat_N$ )=20  $\rightarrow$  Poles NLOEN( $lat_i$ )=NLOEN( $lat_{i-1}$ )+4

TL1279 :2.14 Mpoints TC1023 :5.45 Mpoints TC1279 :8.51 Mpoints TC01279 :6.59 Mpoints



Sylvie Malardel — NA@ECMWF

FD/RD

### Resolution the octahedral grid?



Sylvie Malardel — NA@ECMWF

13/03/2015

### TCo for Grid Point Only numerics in the IFS

- improve GP local derivative calculation on a reduced Gaussian grid
- available in Atlas library (enters the IFS from CY41R2)



### Baroclinic instability with PantaRhei (Christian Kühnlein)

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#### Time integration schemes

Standard schemes in NWP models:

- semi-implicit semi-Lagrange (SI-SL)
- horizontal explicit vertical implicit (HE-VI) (split-explicit (time-split) or non-split)

New proposals:

- Exponential (Rosenbrock) integrators (L. Bonaventura)
- parallel-in-time algorithms (B. Wyngate; Haut): implements what is known as a ,slow manifold' exponential integrators can be used for that, too. Certainly not mature, but see also: 4th workshop on Parallel-in-Time (PinT) 27-29 May 2015, Dresden



### Basic idea of exponential methods

Cauchy problem for nonhomogeneous linear ODE system:

$$\frac{d\mathbf{u}}{dt} = \mathbf{A}\mathbf{u} + \mathbf{g}(t) \qquad \mathbf{u}(0) = \mathbf{u}_0$$

Representation formula for the exact solution:

$$\mathbf{u}(t) = \exp{(\mathbf{A}t)\mathbf{u}_0} + \int_0^t \exp{(\mathbf{A}(t-s))\mathbf{g}(s)} \, ds$$

- Exponential methods: turn this into a numerical method with errors indepentent of  $\Delta t$  for linear problems
- Various extensions to nonlinear problems are available

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### **Conclusions and perspectives**

- Straightforward implementation of exponential methods leads to very accurate but very costly solutions
- For standard PDE problems, a local approximation of exp (∆tA)v is feasible
- Computation of exponential matrix becomes trivially parallel
- Computational overhead due to boundary buffer regions is limited in the case of anisotropic meshes and high order finite elements
- Next on the to do list: use Local Exponential Methods in a high order FE framework and with complex forcing terms (multiple ARD with chemistry)

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Boulder, 8.04.2014

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#### Characteristics of emerging computer architectures

- Unprecedented parallelism: Current High Performance computers can scale up to 250,000 processors. Efficient use of new architectures will require that we know how to scale up to 1 Billion parallel processors (more processors available that can be used by only spatial domaindecomposition?)
- Processors speeds will not be significantly faster than current • processors.
- Memory per processor limited. ۲
- We will have a greater need to have fault-tolerant algorithms.
- We will have to understand asynchronous computing.



Applying functions of a skew-Hermitian operator

### Asymptotic parallel-in-time method

- Take many big time steps  $n\Delta T$ , n = 1, 2, ..., N on an asymptotic approximation  $(\Delta T \gg \varepsilon)$
- Refine the solution in parallel on [nΔT, (n+1)ΔT] using small time steps Δt on the full equation

Figure 1 : Schematic of parallel-in-time algorithm



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from B. Wingate (Univ. Exeter)

The roots of the locally asymptotic slow/coarse solution

Slow Manifolds (nonlinear normal mode initialization, center manifolds, dynamical systems, etc) Machanauer (1977), Baer (1877), Tribbia (1979), etc Leith, Nonlinear Normal Mode Initialization and Quasi -Geostrophic Theory (1980) Lorenz, On the Existence of a Slow Manifold (1986)

Lorenz and Krishnamurthy, **On the non-Existence of the Slow** Manifold (1987)

Lorenz, The Slow Manifold - what is it? (1991)



(....so far the answer is 'it is a fuzzy manifold'.)



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**Chuck Leith** 

Ed Lorenz

### Alternative discretization schemes

Finite-element (FE)-like Schemes ( $\rightarrow$  see 'WGNE numerics report 2014')

- <u>Discontinuous Galerkin</u> (DG) for Tsunami modelling (S. Vater)
- Hybridized DG (T. Bui-Thanh) Cockburn, Gopalakrisnan et al. (für Poisson-eq)
- ,non-conservative' DG (P. Ullrich)
- HE-VI approach for DG (L. Bao)
- use of mixed FE to avoid spurious modes (C. Cotter)
- ADER schemes (M. Norman)



### NEPTUNE

### Navy Environmental Prediction sysTem Using the NUMA corE

### **Scalability**



~15-km global mesh, ERDC Garnet (Cray-XE6)

### from Carolyn Reynolds NRL)

- The NEPTUNE SE solver (dynamics, no I/O) has nearly ideal scaling.
- Does not loose efficiency for as few as 80 points per task.

### **Baroclinic Wave Test**

Northern Hemisphere 850-hPa Vorticity Day 9







 NEPTUNE
 NMMB (low diff)
 NMMB (high diff)

 Image: Neptune
 Image: Neptune

Spurious waves in some models associated with frontal collapse.
Differences in cyclone positions due to set un/resolution

Differences in cyclone positions due to set up/resolution

From Jeff Whitaker's presentation "Results from a global non-hydrostatic dynamical core comparison using idealized tests", AMS Annual Meeting, Phoenix, AZ, January 2015



From Jeff Whitaker's presentation "Results from a global non-hydrostatic dynamical core comparison using idealized tests", AMS Annual Meeting, Phoenix, AZ, January 2015

### What Is ADER-DT?

- ADER-DT = <u>Abritrary DER</u>ivatives with <u>Differential Transforms</u>
- ADER: (Spatial derivatives)+(the PDE itself)  $\rightarrow$  (time derivatives)  $\frac{\partial q}{\partial t} + \frac{\partial f(q)}{\partial x} = 0 \implies \frac{\partial q}{\partial t} = -\frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$  $\frac{\partial^2 q}{\partial x \partial t} = -\frac{\partial^2 f}{\partial q^2} \left(\frac{\partial q}{\partial x}\right)^2 - \frac{\partial f}{\partial q} \frac{\partial^2 q}{\partial x^2} \implies \frac{\partial^2 q}{\partial t^2} = -\frac{\partial^2 f}{\partial q^2} \frac{\partial q}{\partial t} \frac{\partial q}{\partial x} - \frac{\partial f}{\partial q} \frac{\partial^2 q}{\partial t \partial x}$
- Temporal order of accuracy matches the spatial order
- A Differential Transform (DT) is just a Taylor Series coefficient  $Q(k_x, k_t) = \frac{1}{k_x!k_t!} \frac{\partial^{k_x+k_y}q(x,t)}{\partial x^{k_x}\partial t^{k_t}} \qquad q(x,t) = \sum_{k_x=0}^{N-1} \sum_{k_t=0}^{N-1} Q(k_x, k_t) x^{k_x} t^{k_t}$

from Matthew R. Norman (Oak Ridge NL)



### ADER-DT versus Runge-Kutta

- Multi-stage time discretizations most common (Runge-Kutta)
  - Multiple copies of the fluid state (taxing on memory)
  - Multiple data transfers per time step / small effective time step (?)
  - Higher than 4th-order is difficult and expensive to obtain
  - Maintaining non-oscillatory properties reduces time step even further
  - WENO limiting typically applied at each stage
- ADER-DT improves upon this
  - Only one copy of the fluid state is needed, more work per byte
  - Only one data transfer per time step / much larger effective time step
  - Any order of accuracy is as easy as changing one line of code
  - Non-oscillatory properties automatically maintained, same time step
  - Only one WENO procedure per large time step

from Matthew R. Norman (Oak Ridge NL)





### Adaptive mesh refinement (AMR)

- Parallel, adaptive framework for mapped, multi-block domains (D. Calhoun) ٠
- Comparison of Adaptive and Uniform 2D Galerkin Simulations (A. Müller)
- Assessments of the Chombo AMR Model in Shallow Water Mode (J. Ferguson)
- Adaptive Mesh Refinement for Tropical Cyclone Prediction (E. Hendricks)
- Mass conservation properties of CG/DG Methods on non-conforming dynamically adaptive meshes (M. Kopera)
- Tsunami simulation (S. Vater)



**AMR codes are difficult to write** (data structures, time integration, load balancing, ...) ... and hard to use (physics, visualization, ...)!

### Beyond ... AMR Skeptics?

- Coarse/fine boundaries with abrupt resolution changes are regarded with suspicion,
- Lack of good refinement criteria dampens enthusiasm for trying out AMR,
- Not obvious how to extend sophisticated numerical algorithms and applications to the adaptive setting,
- Physics parameterizations! When multi-resolution grids are used ...
- Multi-rate time stepping is not often used (it seems)
- The goals are often modest : "Do no harm!"
- One way coupling of regional, static grids

from Donna Calhoun (Boise State University)



## 2. Barotropic Instability of the ITCZ

#### NO AMR HIGH

#### <u>AMR</u>



CPU time: 12.3 h

CPU time: 3.3 h

AMR useful for resolving ITCZ-like PV strip and its barotropic instability and break down Instability happens faster in AMR simulation, higher most unstable mode (WN 6) Factor of 4 speedup

from E. Hendricks (NRL)

### NEPTUNE: Navy Environmental Prediction sysTem Using the NUMA corE NUMA Adaptive Mesh Refinement



- Non-conforming adaptive mesh refinement (AMR) capability increases efficiency (potential game changer – resolution where its needed).
- Applications: tropical cyclones, dispersion, urban, coastal, cyclones...



### **Derivation and use of approximated/filtered equation sets**

Derivation of a <u>'semi-hydrostatic' equation</u> system by a variational principle (Dubos, Tort)

Comparison between anelastic and compressible solvers in the same numerical environment (P. Smolarkiewicz)  $\rightarrow$  'Panta Rhei' -project at ECMWF



### 1.Global baroclinic instability; large-time-step solutions for various PDEs

the compressible solver is even faster than the anelastic!

2014 Slide 4





New dyn. core developments (1)



### Met Office

UK MO newly developed dynamical core: ,ENDGame' shows several beneficial aspects (less off-centring, more accurate cubic Lagrange interpolation in the vertical, ...)

however, one problem identified:

temperature bias in 20 year AMIP run is stronger than for older ,New dynamics'



© Crown copyright Met Office (ND=New Dynamics; EG=ENDGame; ERA=ERA-Interim)

from Nigel Wood (UK MetOffice)



Use continuous first derivative in vertical  $\Rightarrow$  cubic Hermite

$$d_k^+ = d_k^-$$

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Difference from Exact Solution



![](_page_32_Picture_1.jpeg)

#### Summary

A more accurate scheme can produce significantly worse results! Need to capture wave like aspects of advection of  $\theta$ Key feature of scheme is reversibility Recover this by ensuring continuity of derivative

Pros Bias in tropical tropopause bias reduced by ~2°C Derivatives estimated using quadratics: no change to stencil Hermite interpolation offers new options for monotonicity

Cons

Order of accuracy reduced by cubic Hermite – Perhaps use quartic polynomials for derivatives and extend stencil

from Nigel Wood (UK MetOffice)

#### New dyn. core developments at JMA

The Japan Meteorological Agency (JMA) has been exploring nextgeneration global numerical weather prediction (NWP) model, namely non-hydrostatic global NWP model. The effort was initiated in 2009. The current candidates are:

- a finite volume method yin-yang grid model using a regional dynamical core developed at Numerical Prediction Division of JMA (ASUCA GLOBAL)
- a finite volume method icosahedral-grid model developed by JAMSTEC, Tokyo-Univ., and RIKEN (NICAM)
- a semi-implicit semi-Lagrangian spectral model using Double Fourier series developed by Meteorological Research Institute of JMA
- a non-hydrostatic expansion of the current semi-implicit semi-Lagrangian spherical harmonics spectral model of JMA

![](_page_33_Picture_6.jpeg)

![](_page_33_Picture_7.jpeg)

from M. Sakamoto et al. (JMA)

### ASUCA GLOBAL

A non-hydrostatic model with the finite volume method: ASUCA

- Horizontally explicit and vertically implicit treatment for acoustic waves (HEVI)
- the 3-step Runge-Kutta time integration method by Wicker and Skamarock (2002)
- a flux limiter proposed by Koren (1993)
   → without any numerical diffusion and viscosity to stabilize the calculation
- general coordinate transformations, which allows us to use the Lambert conformal conic projection and the latitude longitude projection
- ASUCA will provide 9 hour forecasts around Japan every hour, with a horizontal resolution of 2 km in the near future.

![](_page_34_Picture_7.jpeg)

JMA-

from M. Sakamoto et al. (JMA)

### Dynamical core model intercomparison project (DCMIP)

- The 2-week summer school and model intercomparison project DCMIP-2012 highlighted the newest modeling techniques for global climate and weather models
- Took place at NCAR from July/30-August/10/2012
- Brought together over 26 modeling mentors and organizers, 37 students, and 19 speakers
- DCMIP-2012 paid special attention to emerging non-hydrostatic dynamical cores
- Hosted18 participating dynamical cores (3 remote groups)
- Our vision: establish DCMIP as a long-term virtual community via the cyberinfrastructure-supported workspace
- Gateway to the virtual community, and open invitation to become a member and participate: http://earthsystemcog.org/projects/dcmip-2012/

from Christiane Jablonowski

![](_page_35_Picture_9.jpeg)

Christiane Jablonowski, James Kent, Paul Ullrich, Kevin Reed, Peter Lauritzen, Ram Nair, Mark Taylor

## The Architecture of the DCMIP Test Suite

The tests are hierarchical and increase in complexity

http://earthsystemcog.org/projects/dcmip-2012/test\_cases

### • 3D Advection

- Pure 3D advection without orography
- Pure 3D advection in the presence of orography
- Dry dynamical core without rotation
  - Stability of a steady-state at rest in presence of a mountain
  - Mountain-induced gravity waves on small planets
  - Thermally induced gravity waves on small planets
- Dry dynamical core with the Earth's rotation
  - From large (hydrostatic) to small (nonhydrostatic) scales, nonlinear baroclinic waves on a shrinking planet with dynamic tracers PV and  $\theta$
- Simple moisture feedbacks
  - Moist baroclinic waves with large-scale condensation
  - Moist baroclinic waves with simplified physics (simple-physics)
  - Idealized tropical cyclones

from Christiane Jablonowsky

![](_page_36_Picture_17.jpeg)

![](_page_36_Picture_18.jpeg)

#### **DCMIP–Going Forward**

- Should there be another DCMIP, e.g. in June 2016?
- If there is interest, what are the scientific frontiers that we want to explore?
- What are the adequate test cases to answer our open model design questions? We need to address all scales (micro, meso, synoptic, planetary)!
- Open invitation to participate in the planning process
- Should we change the format of DCMIP (e.g. fewer test scenarios run during DCMIP and submission of additional results ahead of time)? Longer? Shorter?
- Do we need stricter rules to determine the 'readiness' of model? The readiness of the DCMIP-2012 models and their mentors varied widely.

from Christiane Jablonowsky

#### A possible new DCMIP-16?

Ideas additionaly to the existing tests (see slide before)

- variable resolution / grid transition tests
- New equation sets? (Arakawa, Konor (2009), non-spherical earth (White, Wood, 2012, ...)
- deep atmosphere; high model tops
- more (linear) analytic solutions used
  - Analytical sol. for gravity-/sound wave expansion on sphere (M. Baldauf)
- consistent tracer transport
  - transport with toy-chemistry  $(Cl_2 \rightarrow Cl + Cl, Cl + Cl \rightarrow Cl_2)$
  - consistency of Ertel PV
- Physics-dynamics coupling: (simple) moist interactions
  - non-hydrostatic supercell simulations on a small planet (J. Klemp)
  - shallow-water test with a simple dissipative force physics-dynamics coupling test (J. Thuburn)
- Long-term ,climate like': Held-Suarez
  - Moist variant of the Held-Suarez test (D. Thatcher)

summary from Christiane Jablonowsky

Nicht benutzte Folien

![](_page_40_Picture_1.jpeg)

#### from B. Wingate (Univ. Exeter)

### Summary for parallel-in-time (Haut & Wingate, SIAM J. Sci Comp 2014)

- Proposed Locally Asymptotic slow integrator for the parareal algorithm. Has it's theoretical roots in the 'slow manifold'.
- Separation of time scales not required for it to work, but it means you'll get a parallel-speed-up-in-time, allowing you to use things like asynchronous computing, fault tolerance, and large time steps.
- Initial results from the shallow water equations are promising. A factor of 10 • over the best parareal methods available and a factor of 100 over standard methods for epsilon=10<sup>-2</sup>
- We can double the resolution and keep the same coarse time step.
- We haven't even tried exploiting this parallelism on GPUs or getting more • speed out of an asynchronous algorithm.
- There is a crucial step to introducing even more parallelism is the representation of the linear propagators.

![](_page_40_Picture_10.jpeg)

### **DTs Make ADER Cheaper & Simpler**

![](_page_41_Figure_1.jpeg)

- All PDE terms are space-time polynomials (no quadrature)
- Non-linearly coupled, high-order accuracy w/ no stages (scalable)
- Any order of accuracy by changing just one line of code
- Automatically preserves non-oscillatory properties
- Easily adapted to any grid, spatial operator, or PDE set
- When using WENO, only one limiting applied per time step
- *p*-refinement happens in time as well, not only in space

from Matthew R. Norman (Oak Ridge NL)

![](_page_42_Picture_1.jpeg)

### Why are AMR codes difficult to write?

- Heterogeneous data structures for storing hierarchy of grids •
- Dynamically creating and destroying grids
- Need a "factory" paradigm to create user defined auxiliary dataarrays (material properties, metric terms, bathymetry, etc)needed for each new grid
- Communication between patches
- Parallel load balancing and IO ٠
- Efficient implementation of multi-rate time stepping schemes ٠
- User interface for mixed type equations and solvers
- Error estimation, tuning for efficient use of grids
- . . . . . . . . .

from Donna Calhoun (Boise State University)

![](_page_42_Picture_13.jpeg)

![](_page_43_Picture_1.jpeg)

#### ...and hard to use

- Time stepping methods beyond one-step, single stage methods, including ۲ multi-stage Runge-Kutta, IMEX, SSP, parallel-in-time, exponential integrators, HEVI, spectral deferred correction, ...
- Accuracy of multi-rate schemes for PDEs with mixed ۲ elliptic/parabolic/hyperbolic terms
- Elliptic and parabolic solvers (iterative? direct? Explicit? Implicit?) ۲
- **Refinement criteria?** •
- Higher order accuracy •
- Complex physics
- Visualization
- Debugging and post-processing

from Donna Calhoun (Boise State University)

![](_page_43_Picture_12.jpeg)

![](_page_44_Picture_0.jpeg)

![](_page_44_Picture_1.jpeg)

- ENDGame uses less off-centring (EG=0.55 cf. ND=0.7/1.0)
- More accurate cubic Lagrange interpolation for θ (cf. second-order scheme in New Dynamics)
- Symptoms of the problem:
  - Sharp change in gradient□
  - Small amplitude wave motion
  - Semi-Lagrangian advection of potential temperature is part of problem

from Nigel Wood (UK MetOffice)

#### **DCMIP Test Cases: Goals and Wish-List**

Test cases should

- be designed for hydrostatic and non-hydrostatic dynamical cores on the sphere, ideally: for both shallow and deep atmosphere models
- be easy to apply: analytic initial data (if possible) suitable for all grids formulated for different vertical coordinates
- be as easy as possible, but as complex as necessary
- be cheap and easy to evaluate: small Earth, standard diagnostics
- be relevant to atmospheric phenomena
- reveal important characteristics of the numerical scheme
- have an analytic solution or converged reference solutions
- deal with moisture in a simple way
- find broad acceptance in the modeling community

from Christiane Jablonowsky