On new approaches and ideas useful in design of atmospheric models

J. Pudykiewicz

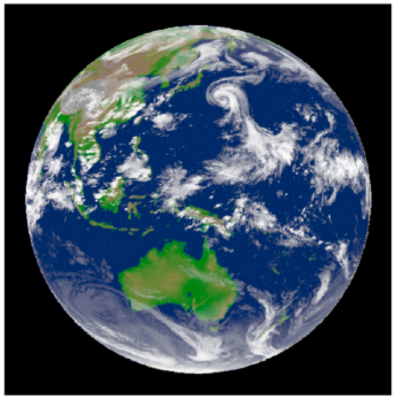
Atmosphere from the point of view of physics

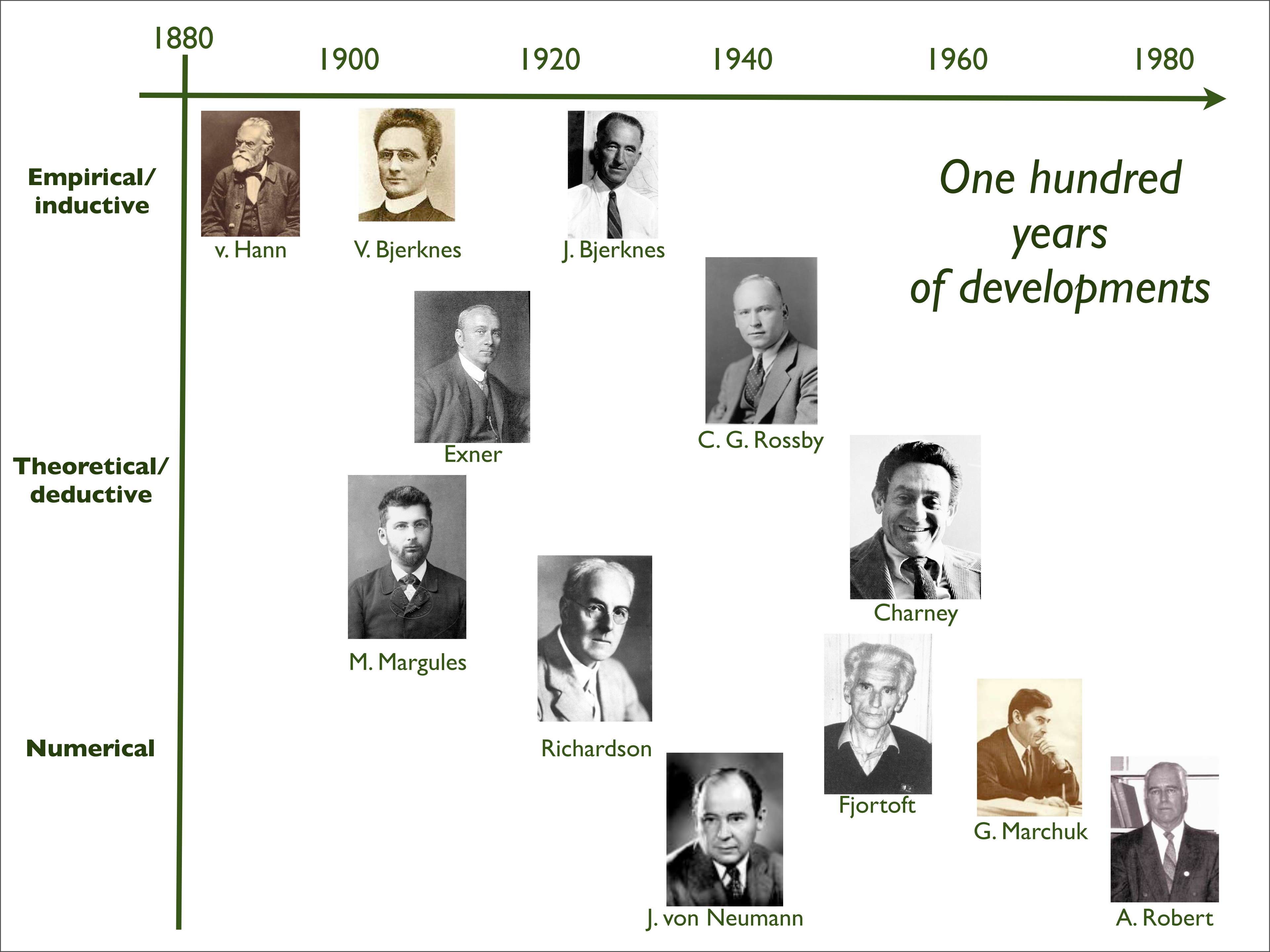
rotating stratified fluid exhibiting both barotropic and baroclinic instabilities

complex energy transfer between the scales

important interactions between waves and the mean flow;
turbulent and chaotic character

strong coupling between microphysical processes, fluid dynamics and electromagnetic phenomena...

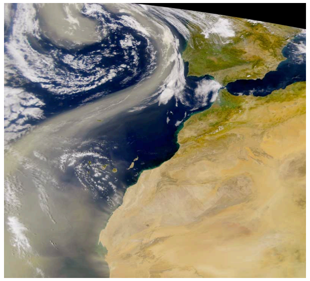



One hundred years of developments
1880
1900
1920
1940
1960
1980
Empirical/ inductive
Theoretical/ deductive
Numerical
v. Hann
V. Bjerknes
J. Bjerknes
Exner
C. G. Rossby
Charney
M. Margules
Richardson
Fjortoft
G. Marchuk
J. von Neumann
A. Robert

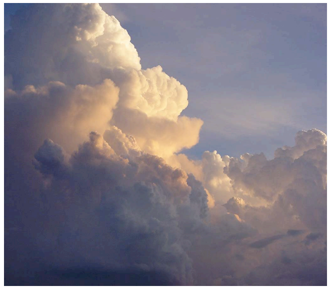
The developments in the dynamic meteorology, numerical methods and computer science led to the current highly developed models of the atmosphere

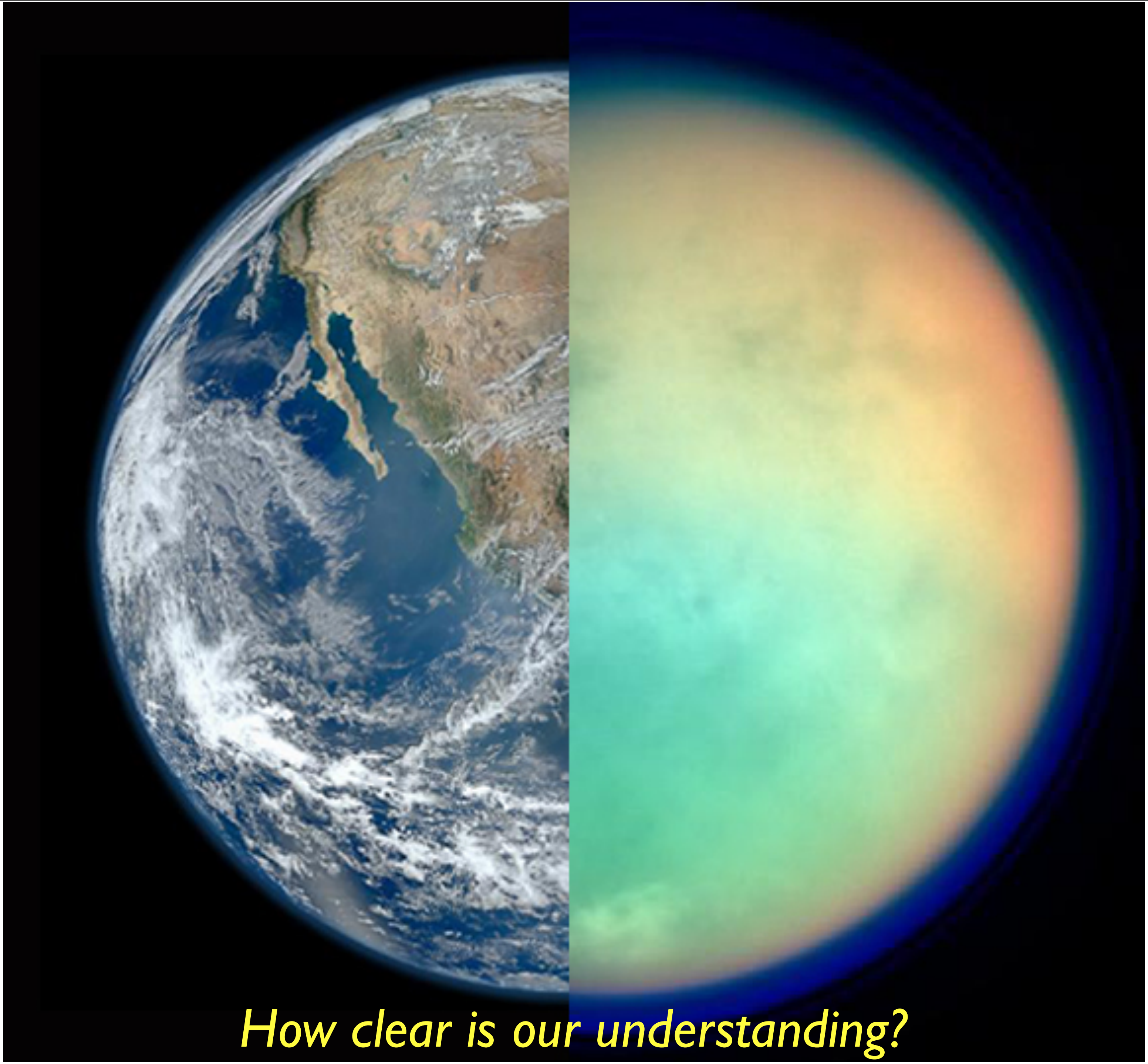
The ultimate weather prediction model is usually constructed upon the elastic system of equations and solved with semi - Lagrangian, semi-implicit method

Do we need to change this? Perhaps not, inevitable further mastering of the description of the unresolved scales should suffice to achieve the desired improvements of predictability...





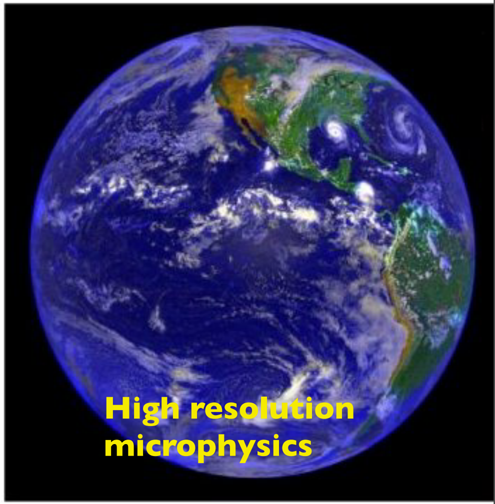


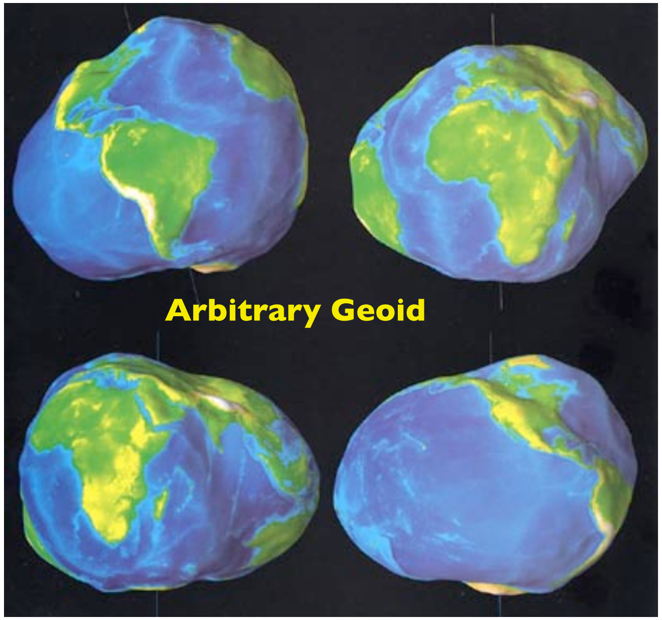



more resolution?

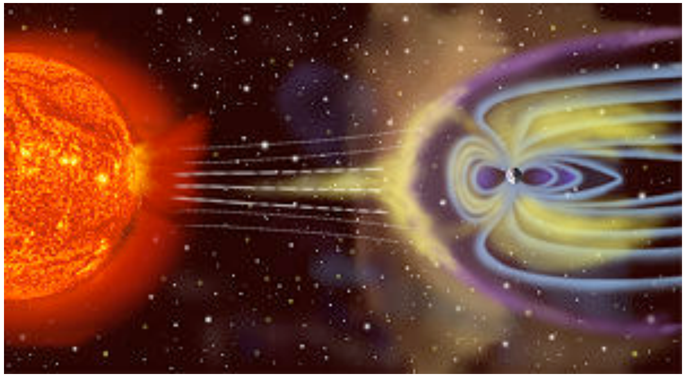
New Trends...

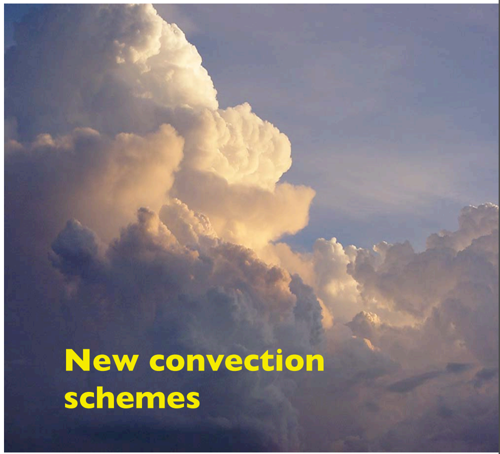
- *removal of shallow atmosphere approximation*
- *arbitrary geoid shape*
- *flexible spatial discretization*
- *new time integration schemes*
- *redefinition of the concept of parameterizations*
- *chemical and aerosol processes fully coupled with dynamics*
- *new forcings (electrodynamics, space weather data...)*

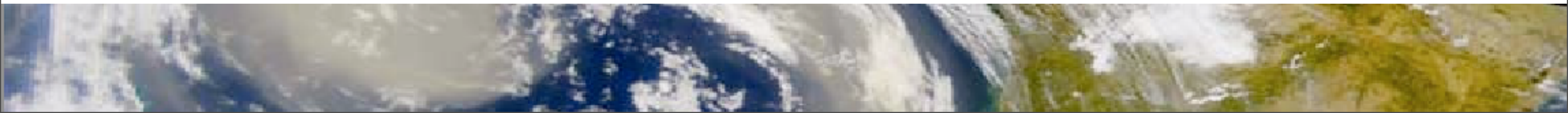


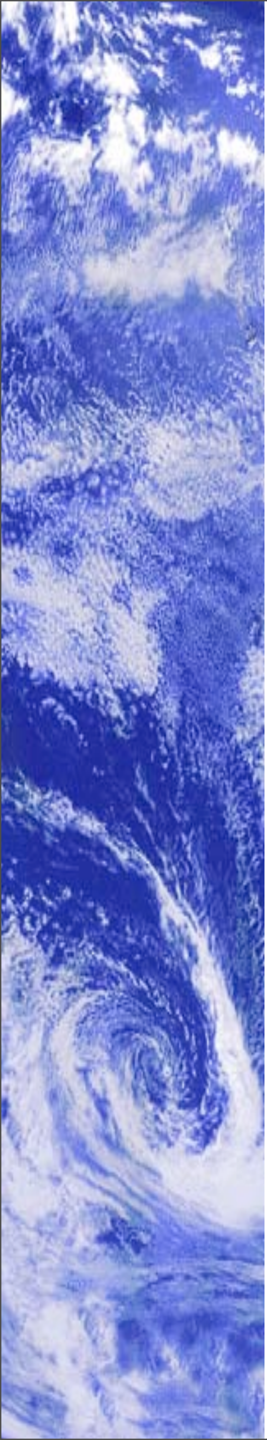


Solar-Terrestrial system and revision of the Bjerknes-Richardson paradigm or the end of a hydraulic analogy

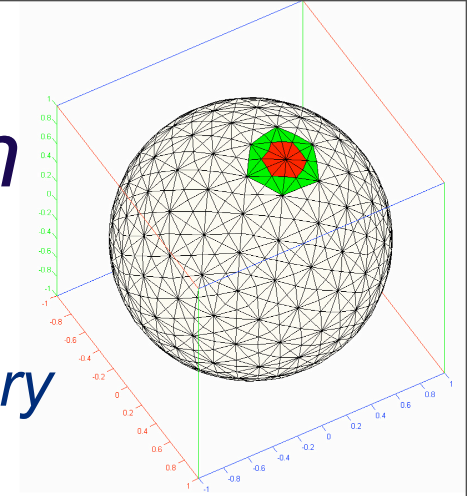








Flexible space discretization



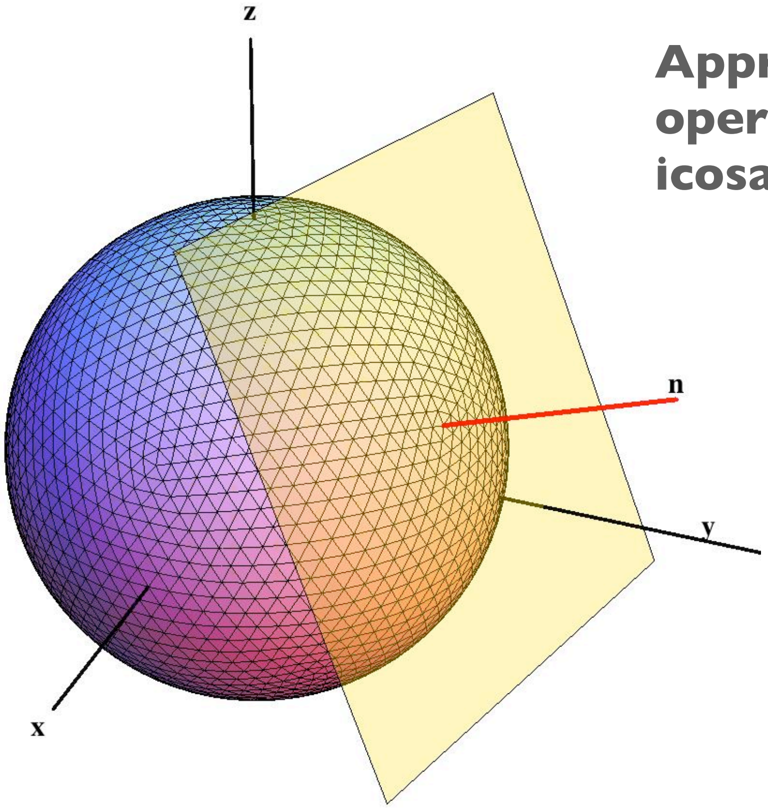
Formulation of the model on an arbitrary differentiable manifold

Strong theoretical background is provided by discrete differential geometry

Manifolds are represented via triangulation

Optimum triangulation could be established by the the minimization of the truncation error of the Laplace-Beltrami operator

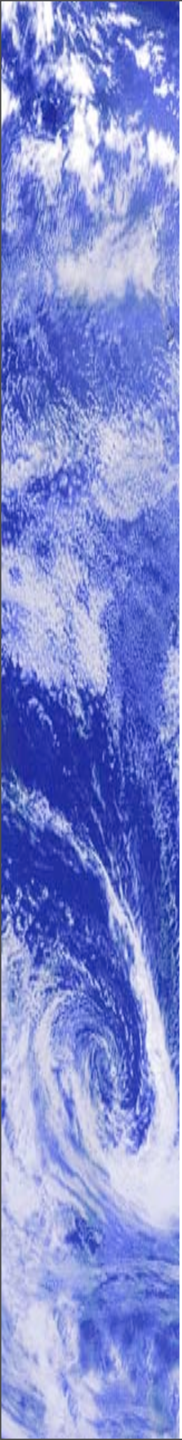
Discrete Differential-Geometry Operators for Triangulated 2-Manifolds by Mark Meyer, Mathieu Desbrun, Peter Schroder, and Alan H. Barr



Approximation of differential operators could be performed on icosahedral-geodesic grid

Poincare - Stokes-theorem:

$$\int_{\Omega} \mathbf{d}\omega = \int_{\partial\Omega} \omega$$



Semi-discretization...

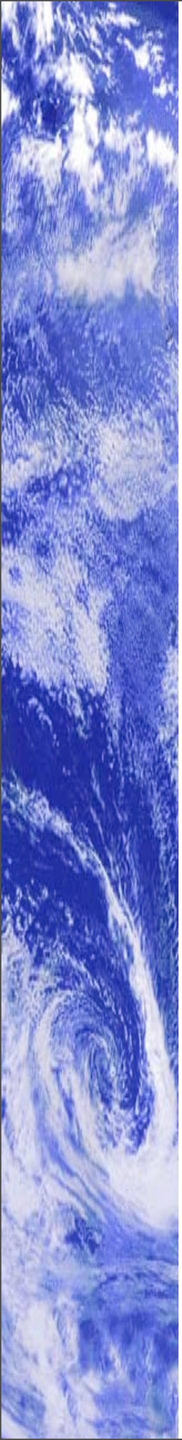
$$\frac{dU}{dt} = F(U)$$

$$U(t) = \{u_1(t), \ldots, u_m(t)\}^T$$

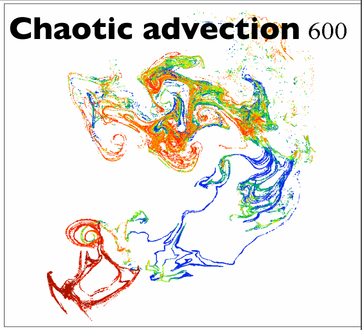
U {velocity, thermodynamic variables, concentrations of chemical species...}

Multiple time scales, homoclinic and heteroclinic points

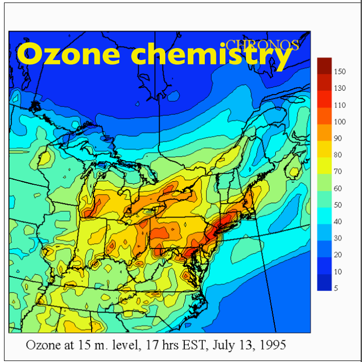
Chaotic behaviour of the system...



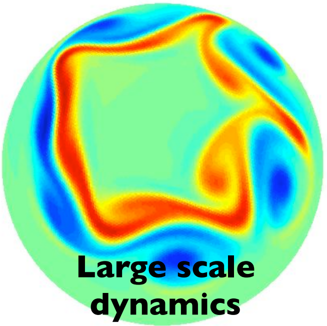
Unified approach to multiple problems in atmospheric models



$$\frac{dU}{dt} = F(U)$$

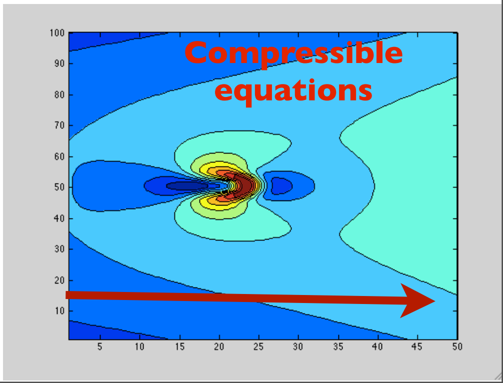


$$U(t) = \{u_1(t), \ldots, u_m(t)\}^T$$



On of the first ideas was to separate the linear (stiff) and nonlinear terms

$$\frac{dU}{dt} = \mathcal{L}U + N(U(t))$$



Use the implicit scheme for the linear term and the explicit for the nonlinear part

It is much better to use the dynamic linearization

$$\frac{dU}{dt} = F(U)$$

$$U(t) = \{u_1(t), \ldots, u_m(t)\}^T$$

$$\frac{dU}{dt}(t) = F_n + A_n(U(t) - U_n) + R(U(t))$$

$$R(U(t)) = F(U(t)) - F(U_n) - \frac{dF}{dU}(U_n)(U(t) - U_n)$$

$$A_n = \frac{dF}{dU}(U_n) \qquad U_n = U(t_n) \qquad F_n = F(U_n)$$

Jacobi operator

The use of the integrating factor $e^{-A_n t}$ yields

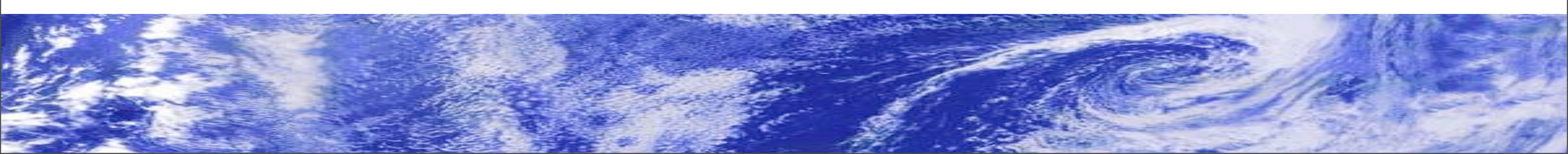
$$\frac{d}{dt}(e^{-A_n t}U(t)) = e^{-A_n t}(F_n - A_n U_n) + e^{-A_n t}R(U(t))$$

And integrating over $[t_n, t_n + h_n]$

followed by multiplication by $e^{A_n(t_n+h_n)}$

$$U(t_n + h_n) = U_n + (e^{A_n h_n} - I)A_n^{-1}F_n +$$

$$\int_{t_n}^{t_n+h_n} e^{A_n(t_n+h_n-t)}R(U(t))dt$$



Depending on the quadrature used we will obtain different versions of the exponential integration schemes. Their common property is that the desired solution could be expressed as weighted sum of "phi functions"

$$\phi_0 = e^A \qquad \phi_1 = \frac{e^A - I}{A} \qquad \phi_2 = \frac{e^A - (I + A)}{A^2}$$

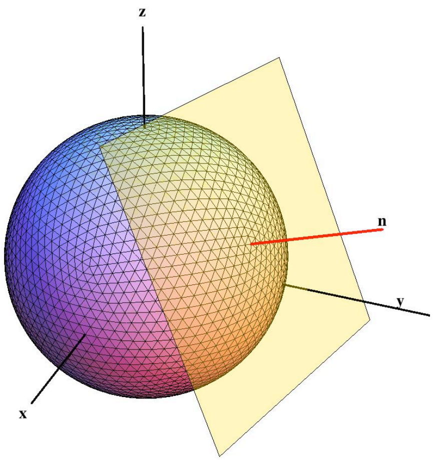
$$\phi_l(A) = A\phi_{l+1} + \frac{1}{l!}$$

"phi functions" are evaluated using the software available in the literature

Advection equation

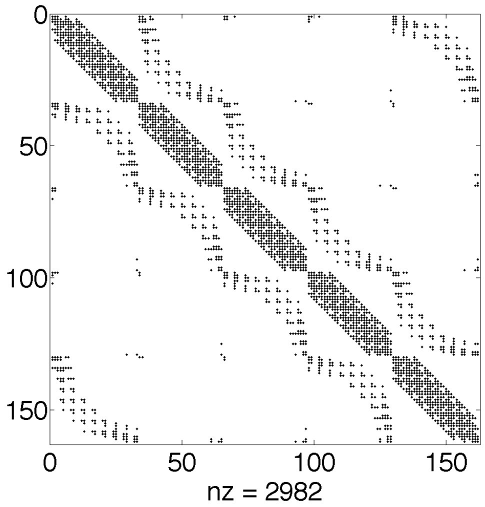
The simplest case for evaluation of the exponential propagation methods:

$$\frac{\partial U}{\partial t} + \nabla U \mathbf{v} = 0.$$



$$\frac{dU}{dt} = F(U)$$

$$U(t) = \{u_1(t), \ldots, u_m(t)\}^T$$



Jacobi operator structure is determined by the connectivity matrix

The scheme selected for the integration

$$U_{n+1} = U_n + \phi_1(A_n h) h F_n + \frac{2}{3}\phi_2(A_n h) h R_{n-1}$$

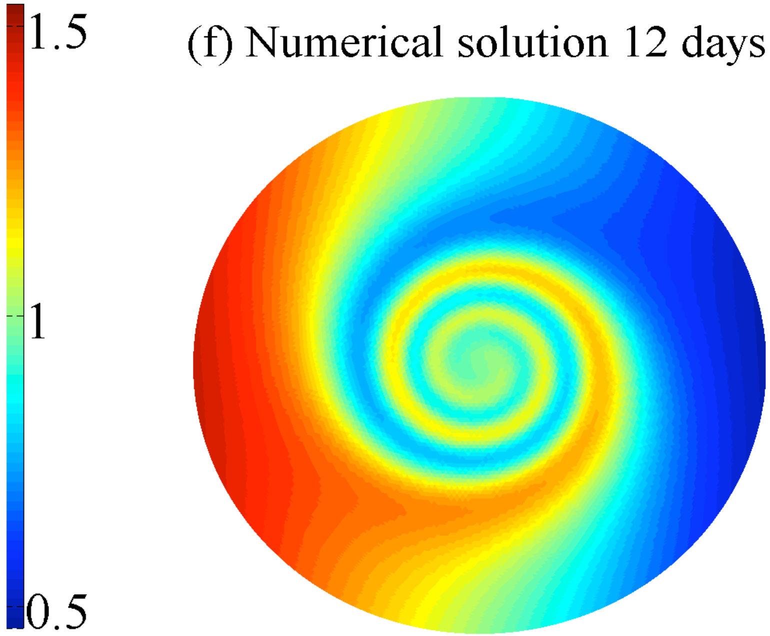
$$\phi_1(A_n h) = \frac{e^{A_n h} - I}{A_n h}$$

EPI3

$$\phi_2(A_n h) = \frac{e^{A_n h} - (I + A_n h)}{A_n^2 h^2}$$

$$R_{n-1} = F(U_{n-1}) - F(U_n) - A_n(U_{n-1} - U_n)$$

Tokman (2006) Efficient integration of large stiff systems of ODEs with exponential propagation iterative methods, J. Comp. Phys. (213), 748-776



Deformation flow

Advection algorithm is mass conserving and stable for very large Courant numbers (much larger than SL methods)

Reaction-diffusion waves and pattern formation

When reacting species can diffuse on the sphere the system can be described by a coupled set of reaction-diffusion equations

$$\frac{\partial \phi}{\partial t} = f(\phi, \psi) + D_1 \nabla^2 \phi$$

$$\frac{\partial \psi}{\partial t} = g(\phi, \psi) + D_2 \nabla^2 \psi$$

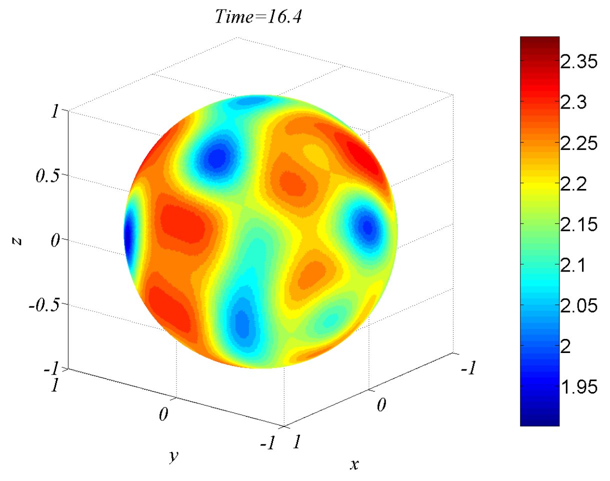
One of the possible solutions of these system are so called reaction-diffusion waves first suggested by A. Turing in his seminal paper on morphogenesis (the concept is used also as an explanation for self-organization processes in physical, biological and economical systems).

In geophysics reaction-diffusion waves can be used to explain the distribution of chemical species in the environment, distribution of ice in the polar caps, surface properties important in the simulation of climatic system. The results could be obtained without an excessive calculations....

The method is often illustrated with so called bruselator system

Oscillations (reactions-diffusion waves)

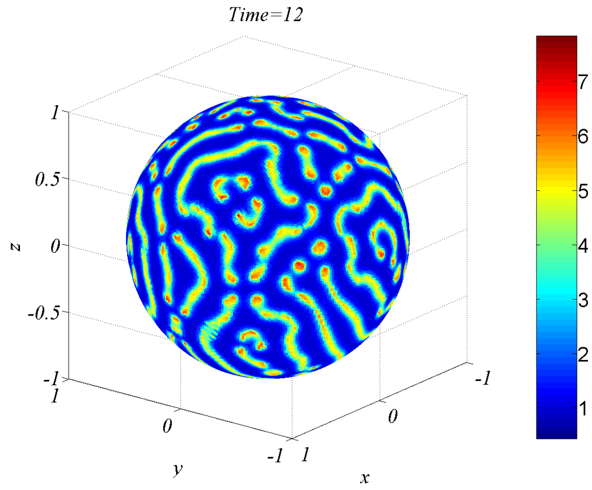
Complex eigenvalues of the Jacobian



Pattern formation

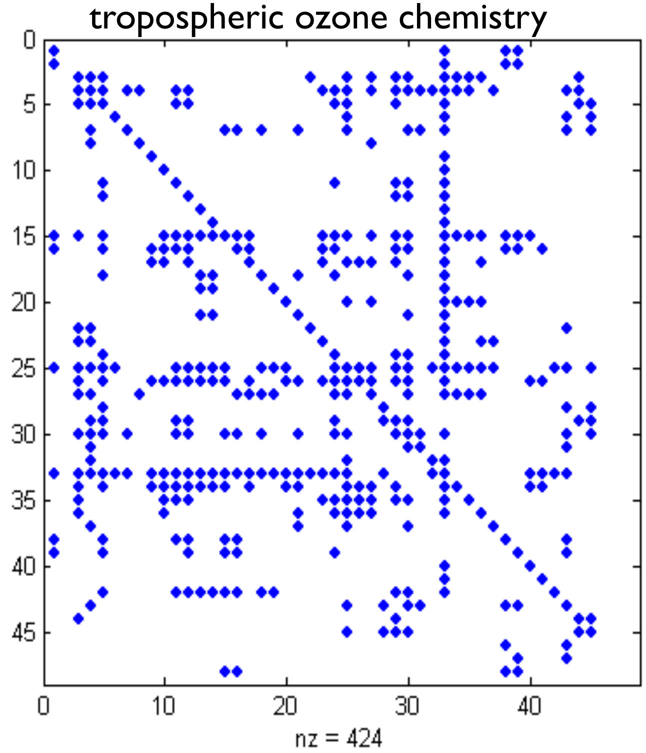
Diffusion combined with reactive terms leads to the evident sharpening of the patterns

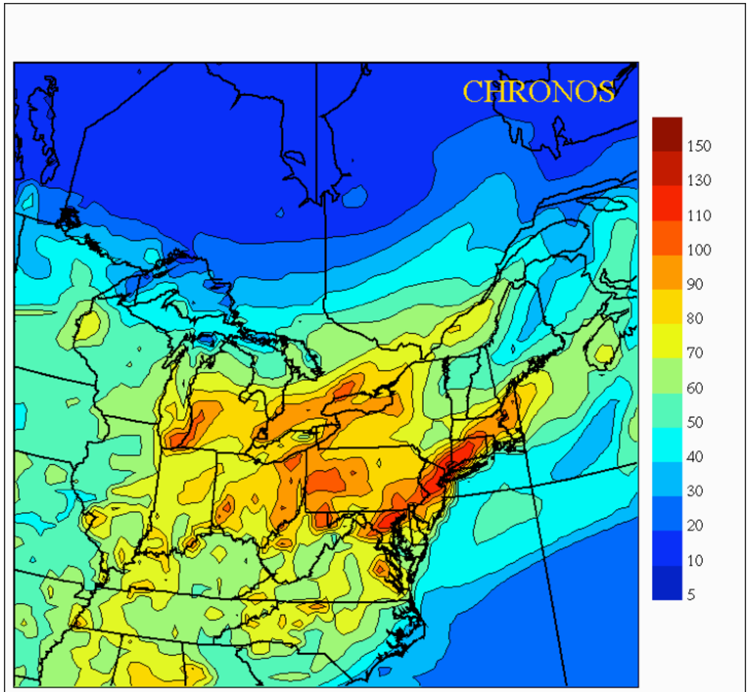
negative eigenvalues of the Jacobian



CHemical Reactions of an Ozone and NOx System

$$\partial_t \varphi^k = -\nabla \mathbf{u} \varphi^k + \nabla \mathbf{K} \nabla \varphi^k + F_c^k(\varphi^1, \ldots, \varphi^{N_s})$$

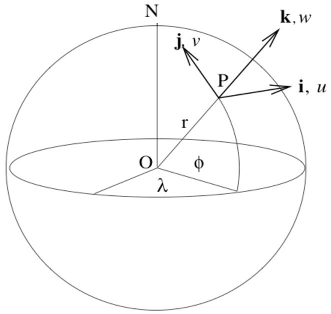




Ozone at 15 m. level, 17 hrs EST, July 13, 1995

The same method of solution could be used for an arbitrary system of chemical reactions after evaluation of the Jacobi operator (single routine for transport, mixing and chemistry)

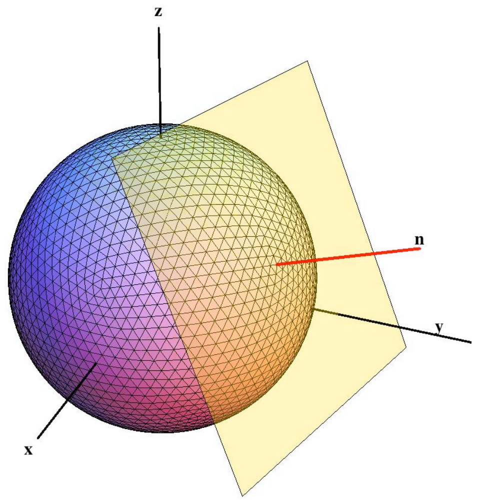
Shallow water system



The shallow water equations in vector invariant form

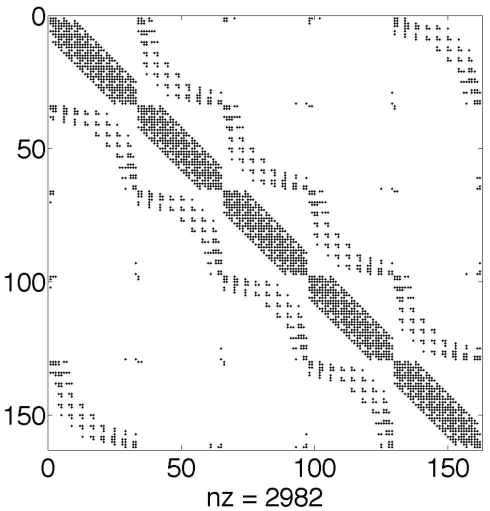
$$\frac{\partial \mathbf{v}}{\partial t} + (\zeta + f)(\mathbf{k} \times \mathbf{v}) = -\nabla(gh + \frac{\mathbf{v}\mathbf{v}}{2})$$

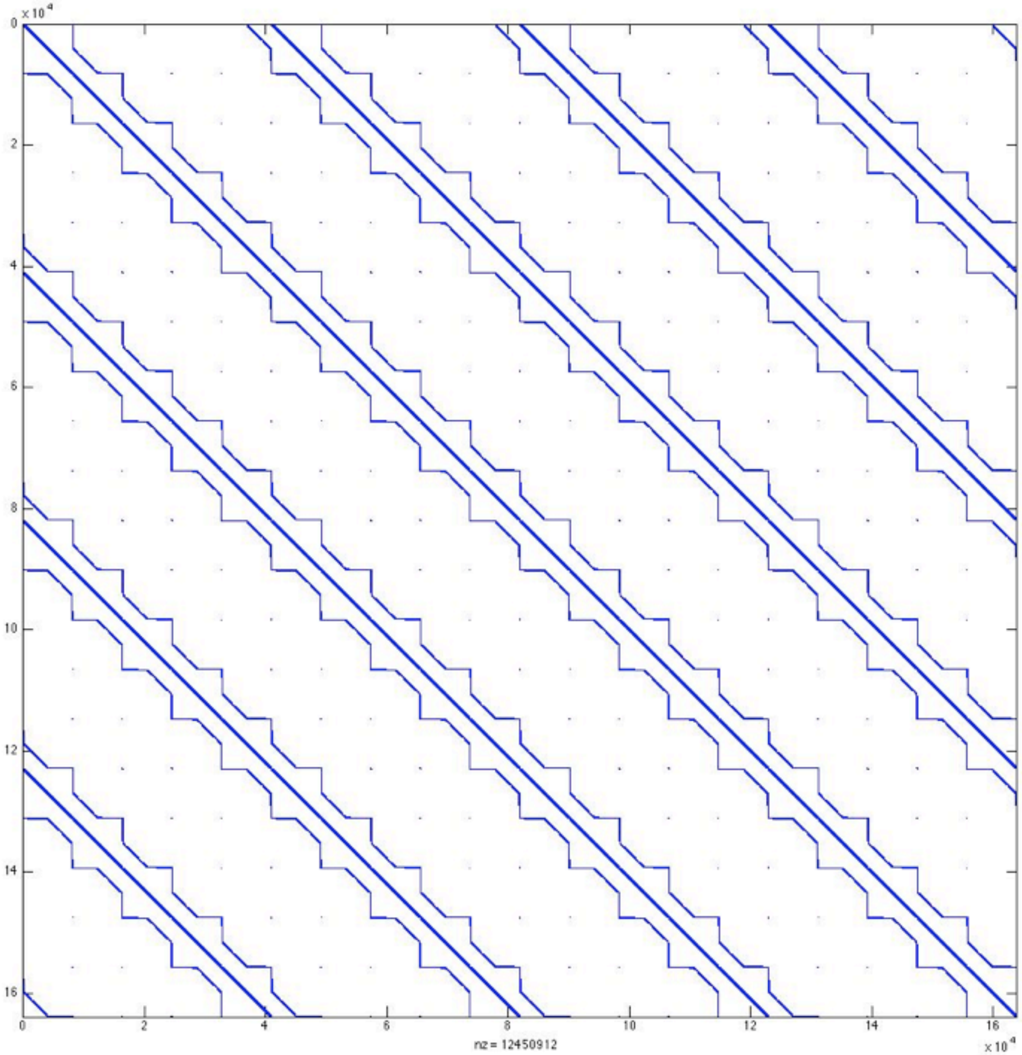
$$\frac{\partial h^\star}{\partial t} + \nabla(h^\star \mathbf{v}) = 0,$$



Semidiscrete autonomous system

$$\begin{cases} \frac{d}{dt}\{u^x\} = -\mathbf{W}^x - \mathbf{GS}_x\{f\} \\ \frac{d}{dt}\{u^y\} = -\mathbf{W}^y - \mathbf{GS}_y\{f\} \\ \frac{d}{dt}\{u^z\} = -\mathbf{W}^z - \mathbf{GS}_z\{f\} \\ \frac{d}{dt}\{h^\star\} = -\mathbf{D}_x\{u^x h^\star\} - \mathbf{D}_y\{u^y h^\star\} - \mathbf{D}_z\{u^z h^\star\}, \end{cases}$$





sparse matrix (4n)x(4n)

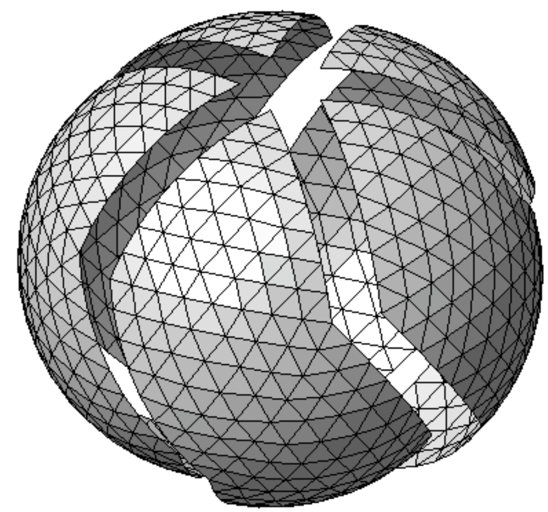
Jacobian for the shallow water system

The Jacobi operator:

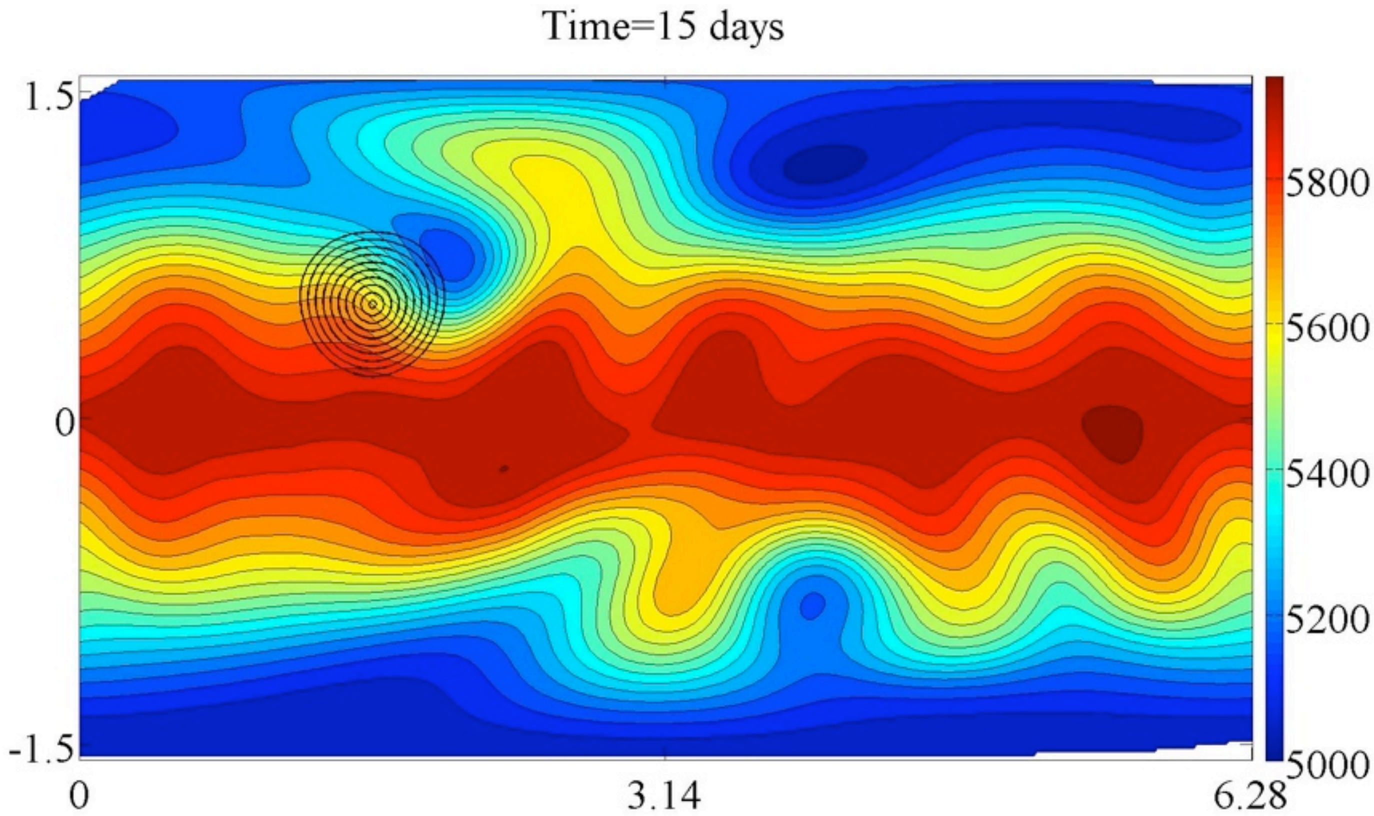
$$\frac{\partial(F_x,\, F_y,\, F_z,\, G)^T}{\partial(u_x,\, u_y,\, u_z,\, h)}$$

$$F_x^i = -(AGt_\gamma^{ij}\, u_\gamma^j + f^i).*(N_y^i\, u_z^i - N_z^i\, u_y^i) - GS_x^{ij}(\frac{1}{2}({u_x^j}^2 + {u_y^j}^2 + {u_z^j}^2) + g(h^j + h_s^j)$$

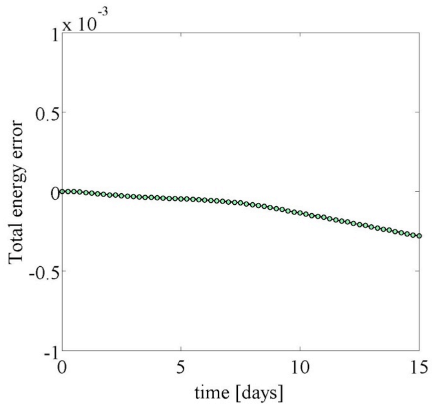
$$G^i = -(D_x^{ij}\, h^j\, u_x^j + D_y^{ij}\, h^j\, u_y^j + D_z^{ij}\, h^j\, u_z^j)$$

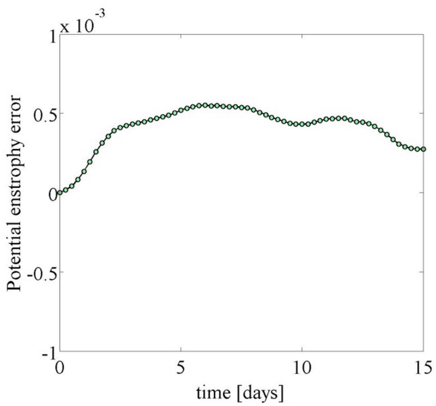


Zonal flow perturbed by mountain, grid number 6, dt=7200 sec.



EP13



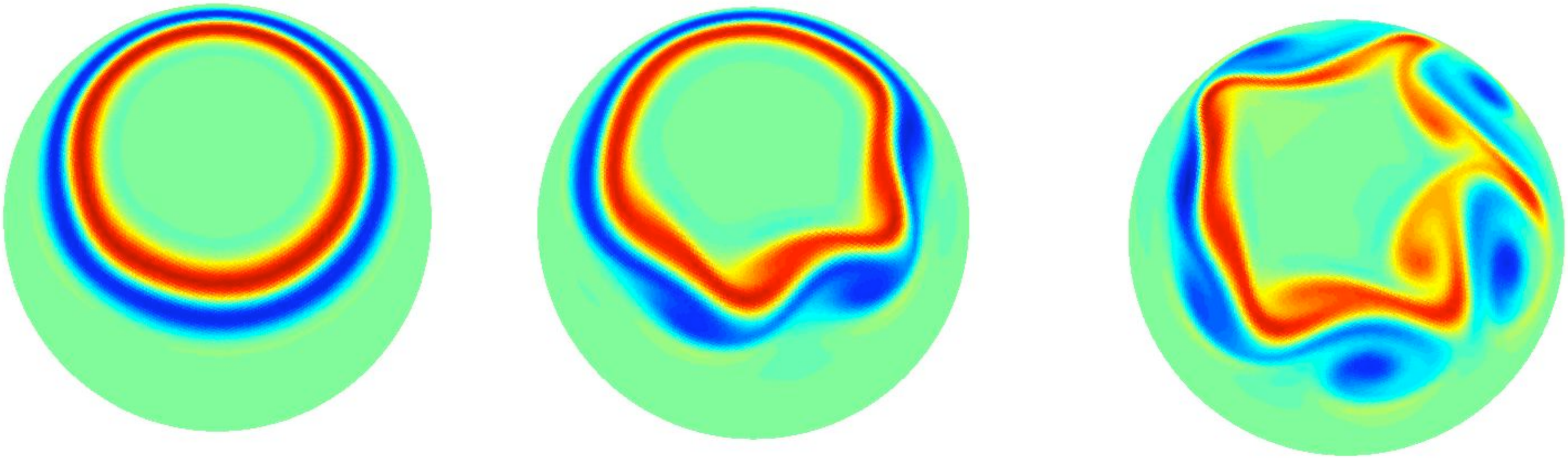


Advantages of the exponential integration method

The exponential methods are able to resolve high frequencies to the required level of tolerance without severe time step restriction of the explicit numerical schemes

The good resolution of the high frequencies with exponential methods is in contrast to usual implicit integration used with large time steps, which either damp high frequencies or map them to one and the same frequency (or nearly so) in the discretization

Unstable jet, grid number 6, dt=7200 sec



The main conclusion from the research performed with barotropic model was that although it is accurate the overall efficiency is not satisfactory...

Clancy C., Pudykiewicz J. (2013) On the use of exponential time integration methods in atmospheric models, Tellus A, vol. 65

Speed-up factor

$$\eta = \frac{T_{explicit}}{T_{exponential}} = \frac{4\,T_d\,(\frac{\tau s}{\Delta t})}{T_d^e\,(\frac{\tau s}{\Delta t_e})} = 4\,\frac{T_d}{T_d^e}\,\frac{\Delta t_e}{\Delta t}$$

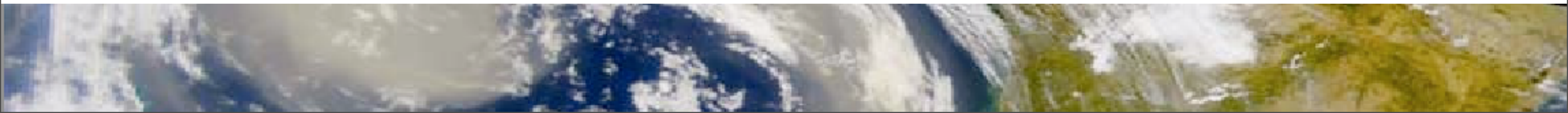
Time for evaluation of the:

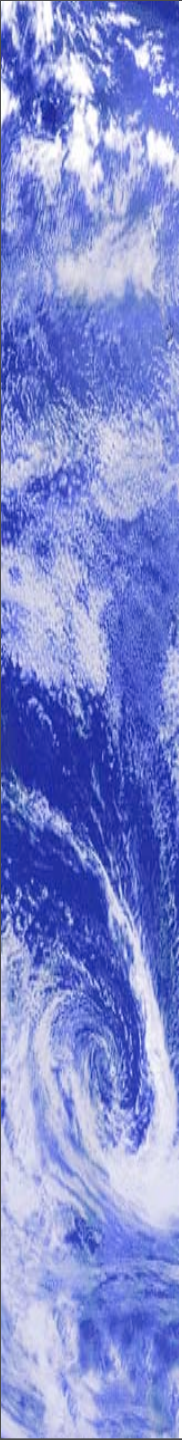
T_d - **Right hand side**

T_d^e **"- phi functions" (EPI3)**

Time steps

Δt - **Runge-Kutta scheme,** Δt_e - **EPI3 scheme**





$$\eta = 4\,\alpha\,\beta, \;\; \alpha = \frac{T_d}{T_d^e}, \;\; \beta = \frac{\Delta t_e}{\Delta t}$$

Original runs from October 2012:

$$T_d = 0.3, \;\; T_d^e = 20, \;\; \Delta t = 240, \;\; \Delta t_e = 7200, \;\; \eta = 1.8$$

Optimized version of the solver with phipm:

$$T_d = 0.3, \;\; T_d^e = 8, \;\; \Delta t = 240, \;\; \Delta t_e = 7200, \;\; \eta = 4.5$$

New version with phipmv will probably permit $\eta = 7$

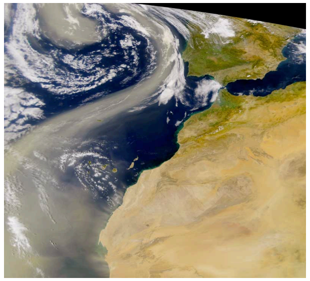
Icosahedral grid number 6 with 41000 nodes (MATLAB 2007); these numbers are smaller with new editions of MATLAB and much smaller when the code is converted to Fortran. Big gains are achieved with the fast sparse matrix vector multiplication procedures...Further work in multilevel model

Euler equations

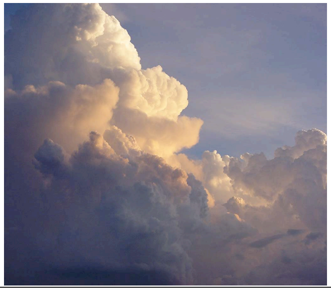
$$\frac{\partial \rho}{\partial t} + \nabla \rho \mathbf{v} = 0$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \rho \mathbf{v} \otimes \mathbf{v} = -\nabla p - \rho g \mathbf{k} + 2\rho\Omega \times \mathbf{v}$$

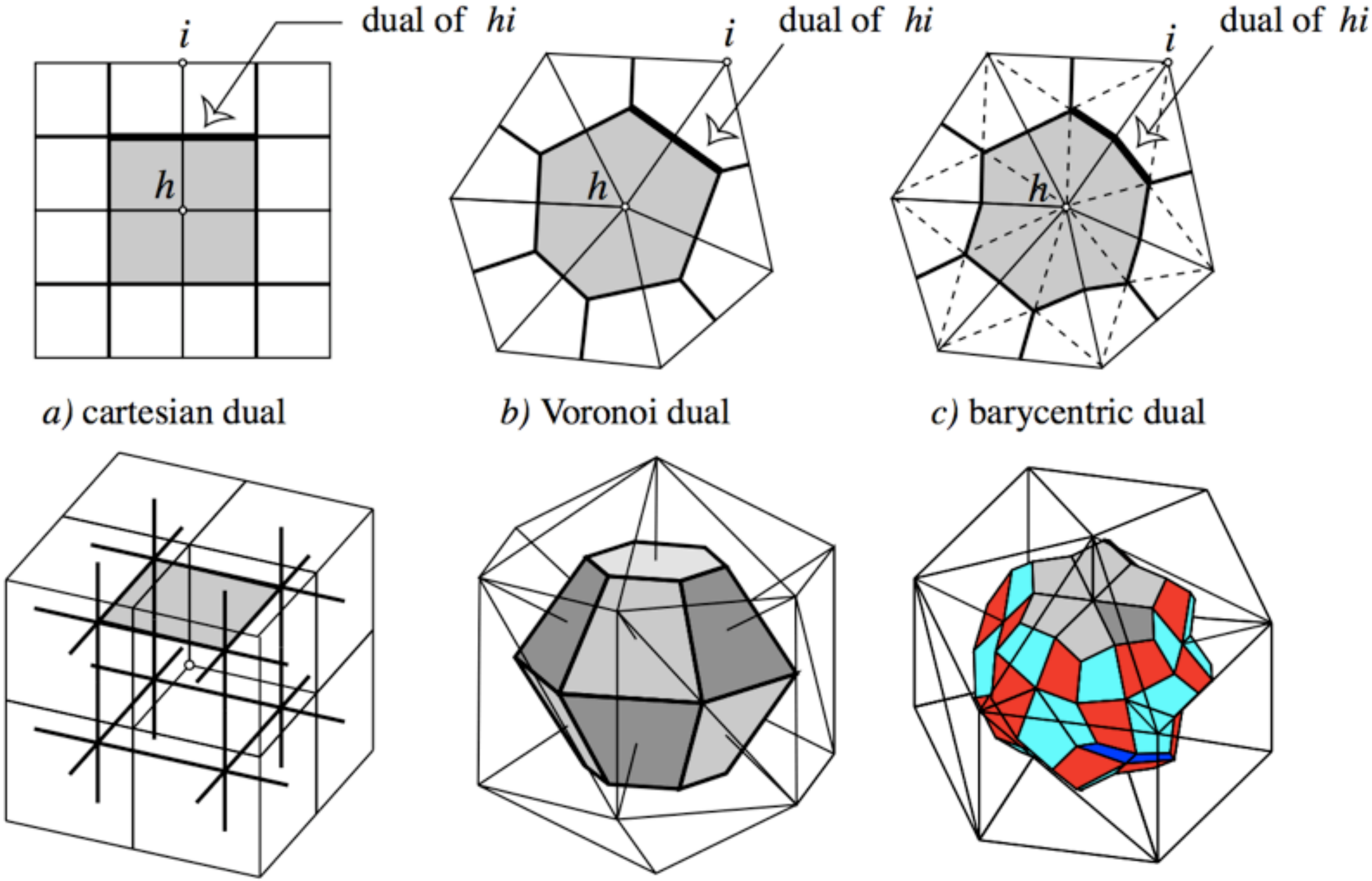
$$\frac{\partial \rho e}{\partial t} + \nabla h \rho \mathbf{v} = \mathbf{v} \nabla p + q_{heat}$$







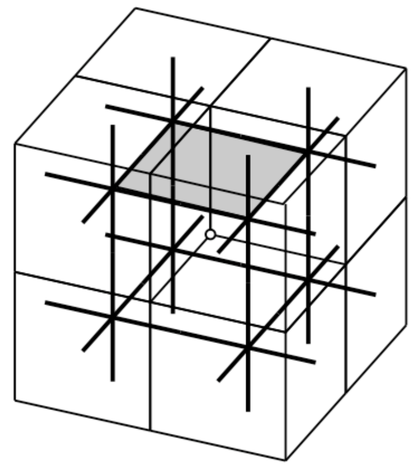

When generalizing the method to the compressible system in 3-D we consider multiple grid options



Equations used are from Robert (1993)

$$\frac{d\mathbf{C}}{dt} = \mathbf{B}$$

$$\mathbf{C} = (u, v, w, q', T')$$



Cartesian grid is used...

$$B_1 = -R\,T\frac{\partial q'}{\partial x}$$

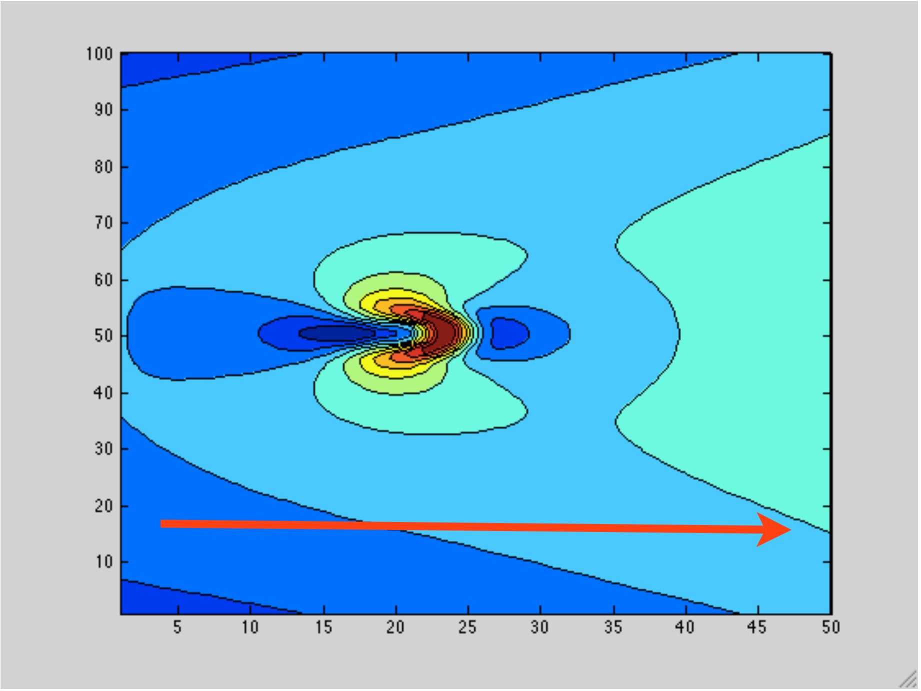
$$B_2 = -R\,T\frac{\partial q'}{\partial y}$$

$$B_3 = -R\,T\frac{\partial q'}{\partial z} + \frac{gT'}{T^*}$$

$$B_4 = -\frac{D}{1-\kappa} + \frac{g\,w}{R\,T^*}$$

$$B_5 = -\frac{\kappa\,T}{1-\kappa}D$$

Notation is standard and it is same as in Robert (1993)



$$U_{n+1} = U_n + \phi_1(A_n h) h F_n$$

EPI2

Courant number 150

Boundary conditions enforced by relaxation

Finite differences or finite volumes

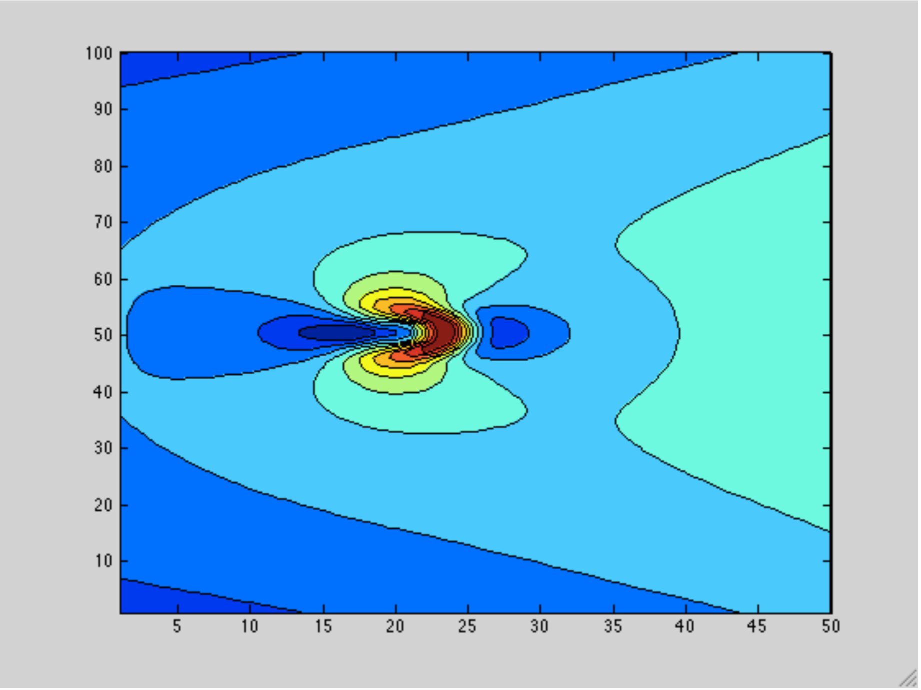
Major findings

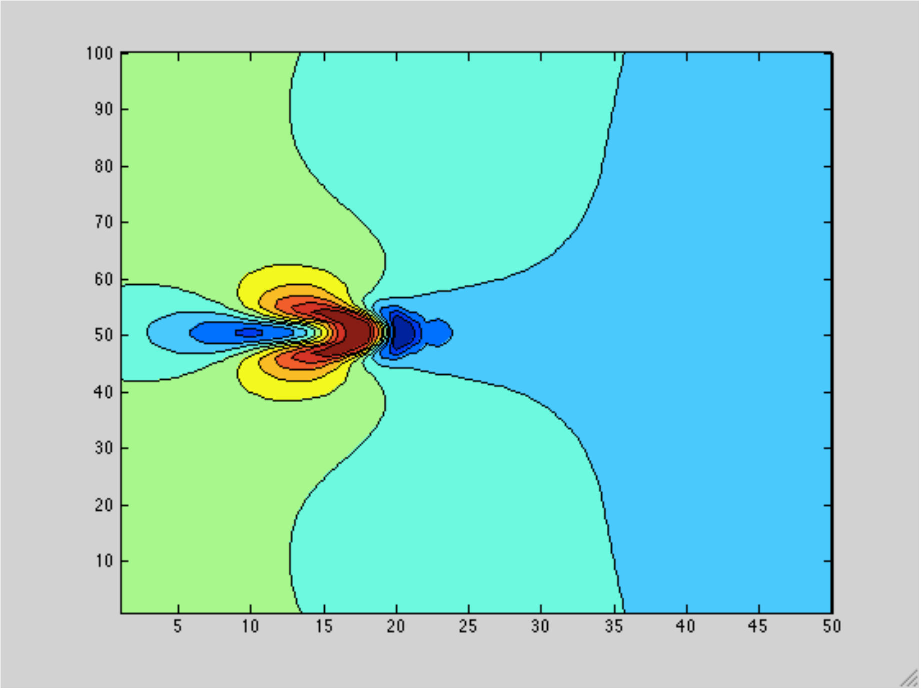
The scheme is free of noise even when the low order spatial discretization is combined with the exponential integration scheme

The method works very well on A-grid

Efficiency ratio with respect to the explicit solver is the same as in the barotropic model

The system is very sensitive to the relaxation procedure used to impose the boundary conditions

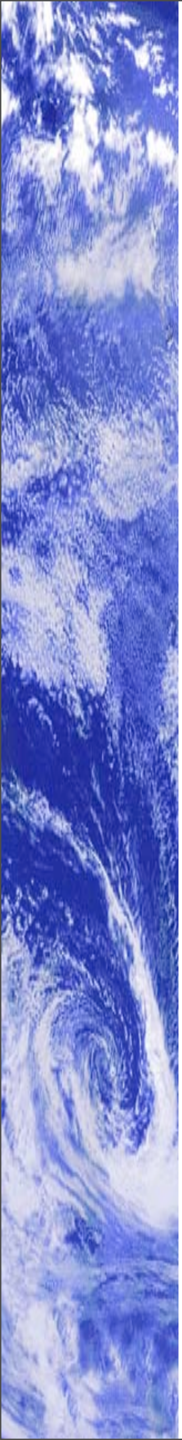




$$U_{n+1} = U_n + \phi_1(A_n h) h F_n$$

EPI2

relaxation applied at the top whereas on the left side was
no relaxation for w at the top



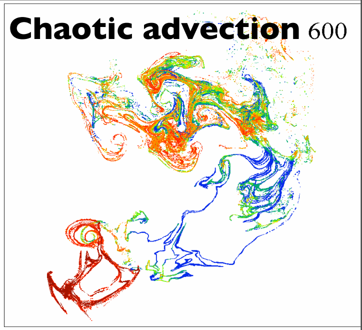
Conclusions

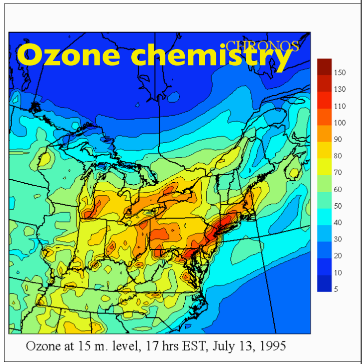
Combining the **Poincare-Stokes** theorem (on arbitrary polyhedral grid) with **exponential** integrators leads to the effective technique for solution of multiple problems including:

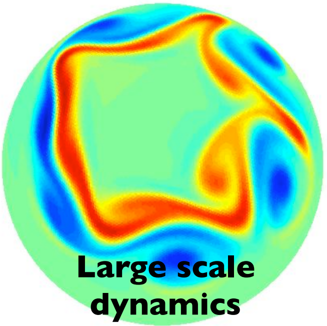
- advection
- chemical kinetics and transport
- shallow water equations on the sphere
- multilayer hydrostatic models on the sphere
- Euler equations

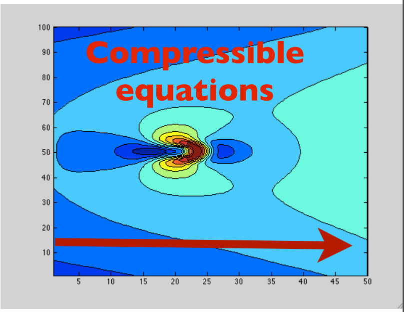
Theoretically all these problem are solved with one universal method

All codes have very good potential for parallel processing

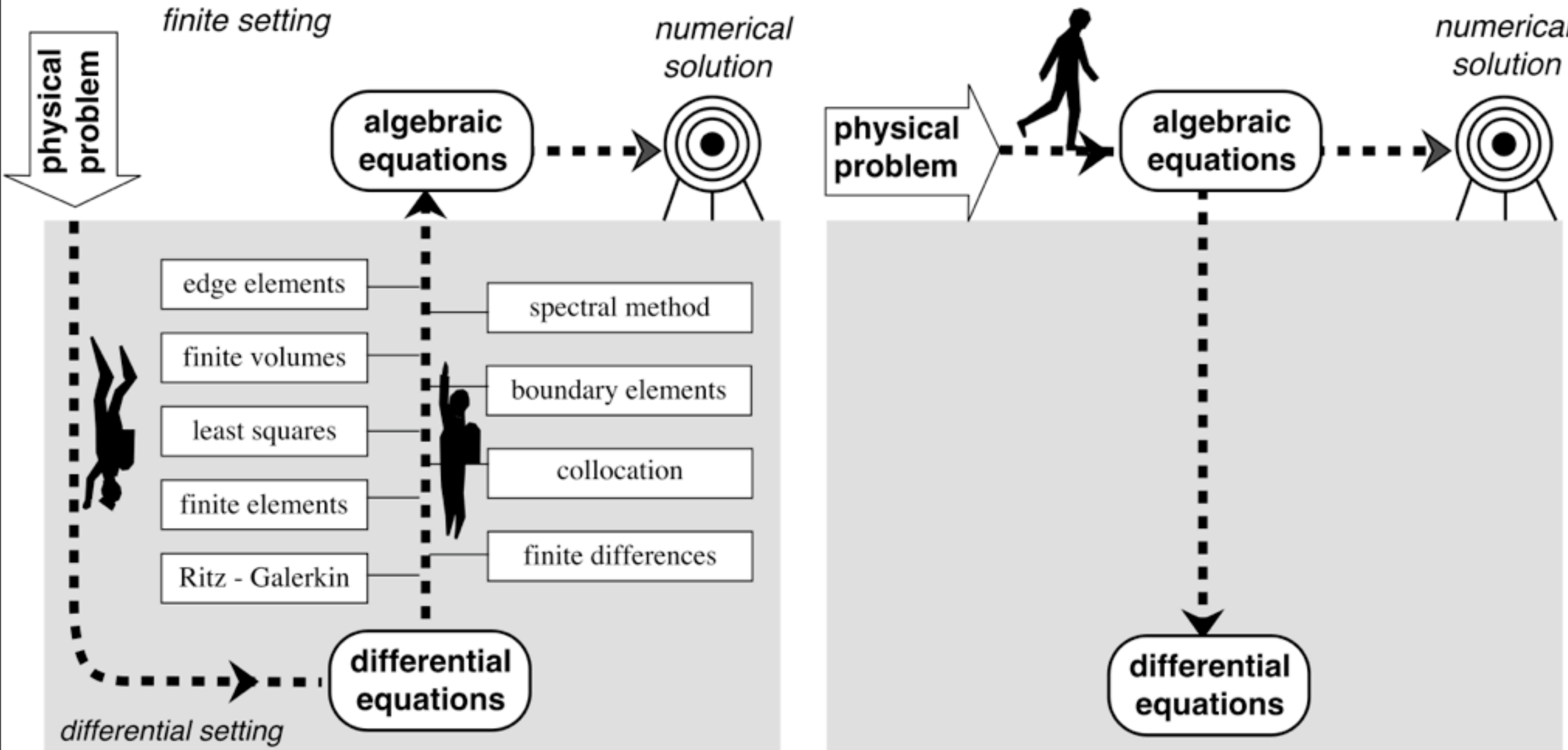








After extensive use of Poincare Stokes theorem to discretize continuous problems one can ask: Are we really using partial differential equations in our models?



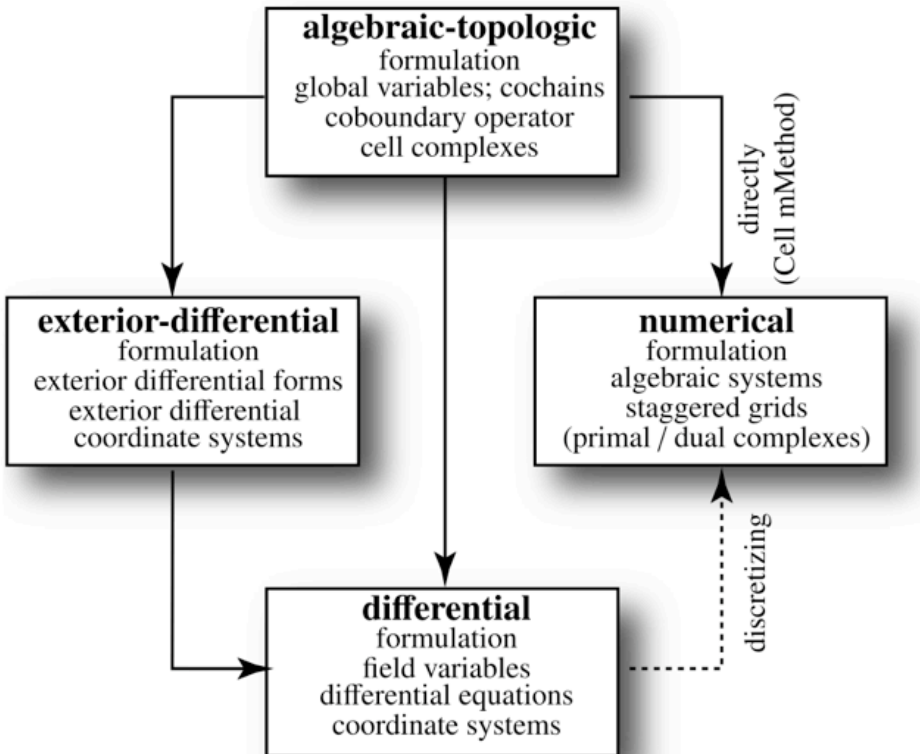
from E. Tonti (2014) Why starting from differential equations for computational physics?

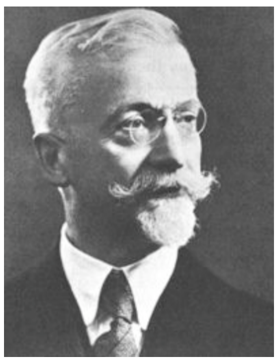
The issue of discretization in more general context

from E. Tonti (2014) Why starting from differential equations for computational physics?

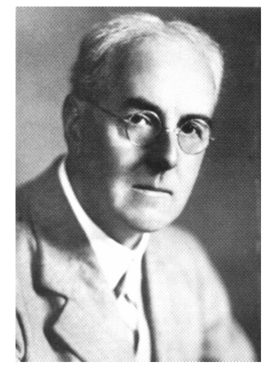
(I have selected names of scientist who I believe are most representative for the problem)

Poincare





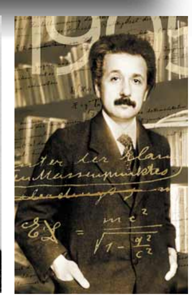
Cartan



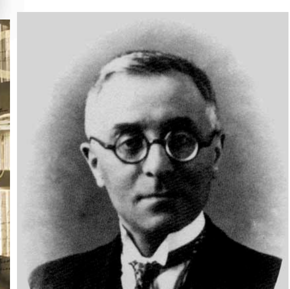
Richardson

Lagrange

Riemann



Einstein



Levi Civitta

Thank you for your attention

Richardson's forecast factory, drawing by F. Shuiten