



Exterior Calculus in simulation of fluids

Juan Pablo Simarro Grande

simarro@inm.es

Instituto Nacional de Meteorología, Spain

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- Brief introduction to Exterior Calculus
- Exterior Calculus in physics, fluid mechanics
- A shallow water model on the sphere, using code and ideas from ICON prototype
- Exterior calculus applied to space discretization of the shallow water model on the sphere
- Some words about compressible atmospheric modelization

Some Exterior Calculus references

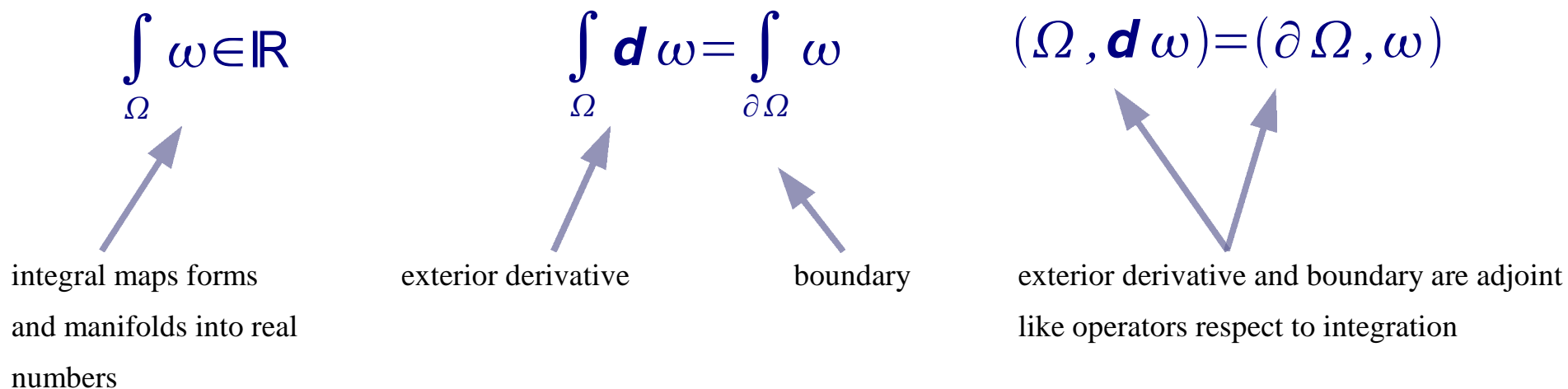
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Why Exterior Calculus?

- Most important Exterior Calculus objects are antisymmetric tensors fields or forms
- Forms are very suitable for integration, there is a generalization of the Stoke's Theorem
- It generalizes the gradient, curl and divergence operators of Vector Calculus
- Many theories of physics can be expressed in the Exterior Calculus nomenclature
- It has connections to other mathematical theories (vector calculus, integration, topology)
- In fluid dynamics vorticity theorems are simply expressed
- Integration operator provides a straightforward way to discretize differential forms
- Exterior derivative is a topological operator and is exactly discretized
- Conservative schemes can be constructed more or less straightforward
- The schemes presented here are near Finite Volume Method
- Is Exterior Calculus just a different language for the same discretization procedures?

Exterior Calculus objects

- **Differential forms are antisymmetric tensors** defined in a differentiable manifold
- A form can be integrated in a submanifold if its dimension is equal to the rank of the differential form. The boundary and exterior derivative operators are combined in the Stoke's classical theorems



- **Antisymmetry is important:** for instance, in integration theory there is the jacobian determinant, in vector calculus the cross product and curl of a vector field.

Forms

- Let be M a manifold and $\{x^i\}$ is a coordinate system. A **basis of the tangent space and its dual** are

$$\{e_1, \dots, e_n\} = \{dx^1, \dots, dx^n\} \quad \{e^1, \dots, e^n\} = \{\partial_{x^1}, \dots, \partial_{x^n}\}$$

- A **p-form** defined in a manifold is an antisymmetric tensor: at each point of the manifold it is defined a skew symmetric p-linear map from the tangent space to real numbers

$$\alpha(m): T_m M \times \dots \times T_m M \rightarrow \mathfrak{R}$$

- A function defined on a manifold is a **0-form**. The most simple **1-form** is the differential of a function, that is

$$df = \frac{\partial f}{\partial x^i} dx^i$$

- The **alternation** operator produces antisymmetric tensors, using the permutation group

$$\mathbf{A}(T)(v_1, \dots, v_p) = \frac{1}{p!} \sum_{\pi \in S_p} \sigma_\pi T(v_{\pi(1)}, \dots, v_{\pi(p)})$$

Forms and wedge product

- The **wedge product** or exterior product can be used to generate forms of higher rank. The wedge product is defined using alternation and tensor product operators. If α and β are forms of rank a and b respectively then

$$\alpha \wedge \beta = \frac{(a+b)!}{a!b!} A(\alpha \times \beta) \text{ where } \alpha \times \beta \text{ is the tensor product}$$

- Example: if α and β are 1-forms

$$\alpha \wedge \beta(v_1, v_2) = \alpha(v_1) \cdot \beta(v_2) - \alpha(v_2) \cdot \beta(v_1)$$

- The wedge product is **associative**, **bilinear** and **anticommutative**

$$\alpha \wedge \beta = (-1)^{a \cdot b} \beta \wedge \alpha$$

- **Coordinate representation** of a p -form is

$$\alpha = \alpha_{i_1, \dots, i_p} \cdot dx^{i_1} \wedge \dots \wedge dx^{i_p} \text{ where } i_1 < \dots < i_p$$

Forms and contraction or inner product

- If α is a p-form and \mathbf{v} a vector field, the **inner product** of \mathbf{v} and α is the (p-1)-form defined by

$$\mathbf{i}_{\mathbf{v}}\alpha(v_2, \dots, v_p) = \alpha(\mathbf{v}, v_2, \dots, v_p)$$

- It is linear and has the following **product rule like property**, for α being a p-form

$$\mathbf{i}_{\mathbf{v}}(\alpha \wedge \beta) = (\mathbf{i}_{\mathbf{v}}\alpha) \wedge \beta + (-1)^a \alpha \wedge (\mathbf{i}_{\mathbf{v}}\beta)$$

Forms and exterior derivative (I)

- Exterior derivative of a p-form is a (p+1)-form determined by the following properties

(i) The exterior derivative of a 0-form or a function is the differential

(ii) The exterior derivative is linear

(iii) Satisfies the product rule

$$d(\alpha \wedge \beta) = (d\alpha) \wedge \beta + (-1)^a \alpha \wedge (d\beta)$$

(iv) It is a local operator and applied twice gives zero

$$d^2 = 0$$

- This last property is related to vector calculus identities

$$\nabla \times \nabla f = 0$$

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

Forms and exterior derivative (II)

- The **coordinate expression** for the exterior derivative is

$$\alpha = \alpha_{i_1, \dots, i_p} \cdot dx^{i_1} \wedge \dots \wedge dx^{i_p} \text{ where } i_1 < \dots < i_p$$

$$d\alpha = \partial_{x^j} \alpha_{i_1, \dots, i_p} \cdot dx^j \wedge dx^{i_1} \wedge \dots \wedge dx^{i_p}$$

- A form is closed if its exterior derivative is zero. A form is exact if it is the exterior derivative of other form. A exact form is closed. **Poincaré Lemma** stands that a closed form is locally exact

if $d\alpha = 0$ then $\alpha = d\beta$ on a neighbourhood of each point

Vector Calculus (I)

- Following examples are in **3 dimensional euclidean space** and standard coordinates
- **Sharp** and **flat** operators maps from vector fields to 1-forms. Flat maps from vector fields to 1-forms and sharp do the inverse. In this case are simple because metric is the identity

$$v^b = v^1 dx^1 + v^2 dx^2 + v^3 dx^3$$

$$\# v = v^\# = v_1 \partial_{x^1} + v_2 \partial_{x^2} + v_3 \partial_{x^3}$$

- **Hodge operator** maps form p-forms to (n-p)-forms, where n is the dimension of the space (3 in this case) and p is an integer value from 0 to n

$$* 1 = dx^1 \wedge dx^2 \wedge dx^3$$

$$* dx^1 = dx^2 \wedge dx^3$$

$$* dx^2 = dx^3 \wedge dx^1$$

$$* dx^3 = dx^1 \wedge dx^2$$

- For 3 dimensions

$$** = 1$$

Vector Calculus (II)

- Cross product and dot product

$$\mathbf{u} \times \mathbf{v} = [* (u^b \wedge v^b)]^\#$$

$$\mathbf{u} \cdot \mathbf{v} = * (\mathbf{u}^b \wedge * (\mathbf{v}^b))$$

- Gradient, curl and divergence (f function, \mathbf{u} vector field)

$$\nabla f = (\mathbf{d} f)^\#$$

$$\nabla \times \mathbf{u} = (* \mathbf{d} \mathbf{u}^b)^\#$$

$$\nabla \cdot \mathbf{u} = * \mathbf{d} * (\mathbf{u}^b)$$

Generalized Stoke's Theorem

- In Exterior Calculus the Stoke's Theorem is a generalization of classical theorems

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

Fundamental Theorem of Calculus

$$\int_a^b f'(x) dx = f(b) - f(a)$$

Divergence Theorem

$$\int \int \int_{\Omega} \nabla \cdot \mathbf{F} dV = \int \int_{\partial\Omega} \mathbf{F} \cdot \mathbf{dA}$$

Green's Theorem

$$\int \int_{\Omega} \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} \right) dx dy = \int_{\partial\Omega} (P dx + Q dy)$$

Classical Stoke's Theorem

$$\int \int_{\Omega} \nabla \times \mathbf{F} \cdot \mathbf{dA} = \int_{\partial\Omega} \mathbf{F} \cdot \mathbf{dL}$$

- In each case there is a domain and its boundary, and a function and its derivative. A relation is established using the integration operator. The concept of **orientation** is important.

Lie derivative

- There are **dynamical** and **algebraic** definitions of the Lie derivative, and both are equivalents. For fluid dynamics, could be the dynamical approach is more intuitive. Let be \mathbf{u} a vector field with flow φ , and α a form, then

$$L_{\mathbf{u}}\alpha = \lim_{t \rightarrow 0} \frac{1}{t} [\varphi_t^* \alpha - \alpha] = \frac{d}{dt} [\varphi_t^* \alpha]_{t=0}$$

- Here the pull back operator φ^* is used to map vectors from the tangent space of one point to other upwind point (respect to vector field \mathbf{u}). This map is different from the parallel transport related to covariant derivatives: **Lie derivative and covariant derivatives are not equivalent** at all. Lie derivative is metric free.
- Lie derivatives of functions are directional derivatives (equivalent to covariant for 0-forms)

$$L_{\mathbf{u}}f = u^i \frac{\partial f}{\partial x^i}$$

Lie derivative and Jacobi-Lie bracket

- The commutator of Lie derivative of functions determines a vector field uniquely

$$[L_u L_v - L_v L_u] f = [\mathbf{u}, \mathbf{v}] f$$

- The vector field is the Jacobi-Lie bracket $[\mathbf{u}, \mathbf{v}]$ which is skew and verifies Jacobi identity

$$[\mathbf{u}, \mathbf{v}] \equiv \left(u^i \frac{\partial v^j}{\partial x^i} - v^i \frac{\partial u^j}{\partial x^i} \right) \partial_{x^j}$$

$$[\mathbf{u}, \mathbf{v}] = -[\mathbf{v}, \mathbf{u}]$$

$$[[\mathbf{u}, \mathbf{v}], \mathbf{w}] + [[\mathbf{v}, \mathbf{w}], \mathbf{u}] + [[\mathbf{w}, \mathbf{u}], \mathbf{v}] = 0$$

- The Lie derivative of a vector field \mathbf{v} along the vector field \mathbf{u} is

$$L_u \mathbf{v} = [\mathbf{u}, \mathbf{v}]$$

- It is possible to extend Lie derivatives to other tensors, in particular to forms. This is the **algebraic** approach. For example, in coordinates the Lie derivative of a 1-form α is

$$L_u \alpha = \left(u^i \frac{\partial \alpha_j}{\partial x^i} - \alpha_i \frac{\partial u^i}{\partial x^j} \right) dx^j$$

Lie derivative properties

- Lie derivative has many interesting properties. It **commutes with exterior derivative**

$$\mathbf{d} L_u \alpha = L_u \mathbf{d} \alpha$$

$$L_{f u} \alpha = f L_u \alpha + \mathbf{d} f \wedge i_u \alpha$$

$$L_{[u, v]} \alpha = L_u L_v \alpha - L_v L_u \alpha$$

$$i_{[u, v]} \alpha = L_u i_v \alpha - i_u L_v \alpha$$

Cartan's magic formula

- For differential forms the Lie derivative is

$$L_u = \mathbf{d} \circ i_u + i_u \circ \mathbf{d}$$

Other operators

- **Codifferential**, from Hodge and exterior derivative

$$\delta = * \circ \mathbf{d} \circ *$$

- **Laplace operator**

$$\Delta = \delta \mathbf{d} + \mathbf{d} \delta$$

Exterior Calculus in physics

- Some physics theories can be expressed in exterior calculus formulation, like **electrodynamics** and **fluid dynamics**. This formulation is **coordinate free**. The operators can be grouped in **topological** operators (exterior derivative, exterior product, contraction) and **metric** dependent operators (Hodge, sharp, flat)

Electromagnetism

- **Maxwell equations in differential form.** There are studies for the discretization of Maxwell equations using Exterior Calculus theory. Gradient, curl and divergence are exterior derivatives

Topological equations

$$dE = -\partial_t B$$

$$\nabla \times E = -\partial_t B$$

Faraday's Law of induction

$$dH = \partial_t D + J$$

$$\nabla \times H = \partial_t D + J$$

Ampère's Circuital Law

$$dB = 0$$

$$\nabla \cdot B = 0$$

Gauss's Law for magnetism

$$dD = \rho$$

$$\nabla \cdot D = \rho$$

Gauss's Law

Metric equations

$$D = *_{\epsilon} E$$

$$D = \epsilon E$$

$$B = *_{\mu} H$$

$$B = \mu H$$

E electric field, **B** magnetic flux density, **D** electric displacement field, **H** magnetic field, **J** current density, **ρ** electric charge density, **ϵ** electrical permittivity, **μ** magnetic permeability

Fluid dynamics

- The movement of the fluid is represented by a 1-form $\mathbf{u}(\mathbf{x},t)$. The integration of this 1-form along a curve is the circulation of the wind

$\int_E u$ is the circulation of u along the curve E

- This form corresponds to a vector field $\#u$ which is used for the Lie derivative. The fluid is represented also by its density ρ and entropy per unit mass χ . The dynamic of the fluid is determined by the **momentum, continuity and energy equations**.
- It is possible to describe the time variation of the fluid in terms of Lie derivative instead of the usual covariant derivative. For 0-forms both derivatives are the same, but it is not the case for 1-forms. The advection of momentum by itself is

$$\#u \cdot \nabla u = L_{\#u} u - \mathbf{d}\kappa \text{ where } \kappa \text{ is the kinetic energy}$$

- Lie derivative commutes with exterior derivative. This commutative property is interesting for describing vorticity properties of the fluid dynamics, also to derive the Ertel's Potential Vorticity equation.

Momentum equation

- The **momentum equation** of the fluid in an external gravitational field with diffusion and other sources is (in Vector Calculus notation)

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\alpha \cdot \nabla p - \nabla \phi - \lambda \Delta \mathbf{u} + \Lambda_u$$

where α is the specific volume, $p(\alpha, s)$ the pressure, ϕ the geopotential, λ the diffusion constant and Λ_u source terms. The advection term can be expressed in terms of Lie derivative and then

$$(\partial_t + L_{\#u})u - \mathbf{d}\kappa = -\alpha \mathbf{d}p - \mathbf{d}\phi - \lambda \Delta u + \Lambda_u$$

Continuity equation

- The continuity equation for mass is (in Vector Calculus notation)

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0$$

- These equation can be written in this form, where the Hodge operator is used

$$(\partial_t + L_{\#u}) * \rho = 0 \text{ where } * \rho = \rho \cdot dx^1 \wedge \dots \wedge dx^n$$

- It is equivalent to

$$\partial_t \rho + \delta(\rho u) = 0 \text{ where } \delta = * \mathbf{d} *$$

Entropy and tracers equations

- Entropy is conserved if flow is adiabatic, if it is not adiabatic there is a source term related to diabatic processes, like diffusion. The same scheme is used for any other magnitude, like water vapour or ozone content per unit mass of air. There are two possible equations, one called conservative form because leads to conservative schemes in a more straightforward way. These equations are (in Vector Calculus notation)

$$\partial_t \chi + \mathbf{u} \cdot \nabla \chi = \Lambda_\chi \qquad \partial_t(\rho \chi) + \nabla \cdot (\rho \chi \mathbf{u}) = \rho \Lambda_\chi$$

where χ is a tracer or entropy and Λ_χ source term.

- These equations in exterior calculus nomenclature are

$$(\partial_t + L_{\#u}) \chi = \Lambda_\chi$$

- And in conservative form, that is, using mass continuity equation

$$(\partial_t + L_{\#u}) * (\rho \chi) = * (\rho \Lambda_\chi) \text{ where } * (\rho \chi) = (\rho \chi) \cdot dx^1 \wedge \dots \wedge dx^n$$

Vorticity equation and potential vorticity

- The fact that Lie derivative commutes with exterior derivative and that exterior derivative applied twice gives zero is important for deriving a vorticity equation. Applying exterior derivative to momentum equation

$$(\partial_t + L_{\#u}) \mathbf{d}u - \mathbf{d}^2 \kappa = -\mathbf{d} \alpha \wedge \mathbf{d} p - \mathbf{d}^2 \phi - \mathbf{d} (\lambda \Delta u + \Lambda_u)$$

it is obtained the following vorticity equation for adiabatic flow, where there is a source term for vorticity called solenoidal term, which is zero for barotropic flows

$$(\partial_t + L_{\#u}) \mathbf{d}u = -\mathbf{d} \alpha \wedge \mathbf{d} p$$

- **Potential vorticity** per unit mass is conserved following air parcel when the flow is adiabatic.

It is defined in 3 dimensional space as (here α is specific volume, s entropy, \mathbf{u} wind)

$$PV \equiv \alpha \cdot \nabla s \cdot \nabla \times \mathbf{u} \qquad \partial_t PV + \mathbf{u} \cdot \nabla PV = 0$$

- In exterior calculus nomenclature

$$PV \equiv * (\alpha \cdot \mathbf{d}s \wedge \mathbf{d}u)$$

- Using the trace equation in conservative form and a property of Hodge operator

$$(\partial_t + L_{\#u}) * (\rho \chi) = 0 \qquad * (\rho PV) \equiv ** (\rho \alpha \cdot \mathbf{d}s \wedge \mathbf{d}u) = \mathbf{d}s \wedge \mathbf{d}u$$

follows that Potential Vorticity conservation for adiabatic flow is equivalent to

$$(\partial_t + L_{\#u}) (\mathbf{d}s \wedge \mathbf{d}u) = 0$$

- This equation is demonstrated easily, using the vorticity equation, the conservation of entropy for adiabatic flow and the fact that pressure is function of entropy and specific volume

$$(\partial_t + L_{\#u}) (\mathbf{d}s \wedge \mathbf{d}u) = (\partial_t + L_{\#u}) \mathbf{d}s \wedge \mathbf{d}u + \mathbf{d}s \wedge (\partial_t + L_{\#u}) \mathbf{d}u = 0 \wedge \mathbf{d}u - \mathbf{d}s \wedge \mathbf{d}\alpha \wedge \mathbf{d}p = 0$$

Shallow water equations

- **Moment and mass continuity** equations are

$$(\partial_t + L_{\#u})u = \mathbf{d}k - \mathbf{d}(\phi + \phi_s)$$

$$(\partial_t + L_{\#u})*\phi = 0$$

- Because Lie derivative commute with exterior derivative, the vorticity conservation law is derived immediately from momentum equation

$$\mathbf{d}(\partial_t + L_{\#u})u = (\partial_t + L_{\#u})\mathbf{d}u = \mathbf{d}^2k - \mathbf{d}^2(\phi + \phi_s) = 0$$

- Enstrophy and total energy is also conserved, but more difficult to demonstrate.
- **Momentum equation** can be expressed in terms of the usual vorticity and kinetic energy advection terms

$$\partial_t u + \mathbf{i}_{\#u}\mathbf{d}u + \mathbf{d}k = -\mathbf{d}(\phi + \phi_s)$$

Vorticity term

Kinetic energy gradient

Geopotential gradient term including bottom height

- **Mass continuity** equation is also expressed in terms of divergence

$$\partial_t \phi = -\delta(u \phi)$$

Local variation in height is minus the divergence of wind dot height

$$\delta u = * \mathbf{d} * u$$

codifferential of wind is the divergence of the wind vector field

- An second order differential equation for the wind is obtained applying the exterior derivative to the continuity equation and the time derivative to the momentum equation

time derivative of momentum $\longrightarrow \partial_{tt} u + \partial_t(\mathbf{i}_{\#u} \mathbf{d} u + \mathbf{d} k) = -\partial_t \mathbf{d} \phi$

exterior derivative of continuity $\longrightarrow \partial_t \mathbf{d} \phi = -\mathbf{d} \delta(u \phi)$

- Reordering terms

$$\partial_{tt} u - \mathbf{d} \delta(u \phi) = -\partial_t(\mathbf{i}_{\#u} \mathbf{d} u + \mathbf{d} k)$$

- Same equation linearised around constant height and rest fluid

$$(\partial_{tt} - \phi_0 \mathbf{d} \delta) u = 0$$

Similar to wave equation

$$(\partial_{tt} - \phi_0 \Delta) u = 0$$

Shallow water model

- A shallow water model has been developed using **ICON prototype** subroutines related to **grid generation**, **RBF scheme** for wind reconstruction and **test cases**. Some of the operators are similar to those in ICON, like **vorticity**, **gradient**, **divergence** and **fluxes**. The linear system is completely different, based on momentum instead of geopotential, and implicit vorticity, divergence and diffusion are treated in other way. The model is conservative in total vorticity and mass.
- Including diffusion and Coriolis term, the model equations are

$$\partial_t u + \mathbf{i}_{\#u}(\mathbf{d}u + f) + \mathbf{d}k = -\mathbf{d}(\phi + \phi_s) + \lambda \Delta u$$

$$\partial_t \phi = -\delta(u \phi)$$

Time discretization

- Fully-implicit scheme obtained from iteration of semi-implicit
- Definitions at intermediate time level (similar for geopotential)

$$u^\alpha = (1 - \alpha)u^0 + \alpha u^+$$

$$u^\beta = (1 + \alpha)u^0 - \alpha u^-$$

extrapolation

- Semi-implicit system

$$\frac{u^+ - u^0}{\Delta t} = -\mathbf{i}_{\#u^\beta}(\mathbf{d}u^\alpha + f) - \mathbf{d}k^\beta - \mathbf{d}(\phi^{\alpha'} + \phi_s) + \lambda \Delta u^\alpha$$

$$\frac{\phi^+ - \phi^0}{\Delta t} = -\delta(\phi^\beta u^\alpha)$$

Semi-implicit terms include vorticity advection, geopotential gradient and diffusion terms. There is a different value for $\alpha' > \alpha$ in the geopotential gradient term for stability reasons as seen later.

Time discretization, linear system

- Substituting from continuity equation into momentum

$$u^\alpha + (\alpha \Delta t) \cdot \mathbf{A} u^\alpha - (\alpha \alpha' \Delta t^2) \cdot \mathbf{B} u^\alpha = \mathbf{R}$$

$$\mathbf{A} u^\alpha = \mathbf{i}_{\#u^\beta} \mathbf{d} u^\alpha - \lambda \Delta u^\alpha$$

$$\mathbf{B} u^\alpha = \mathbf{d} \delta(\phi^\beta u^\alpha)$$

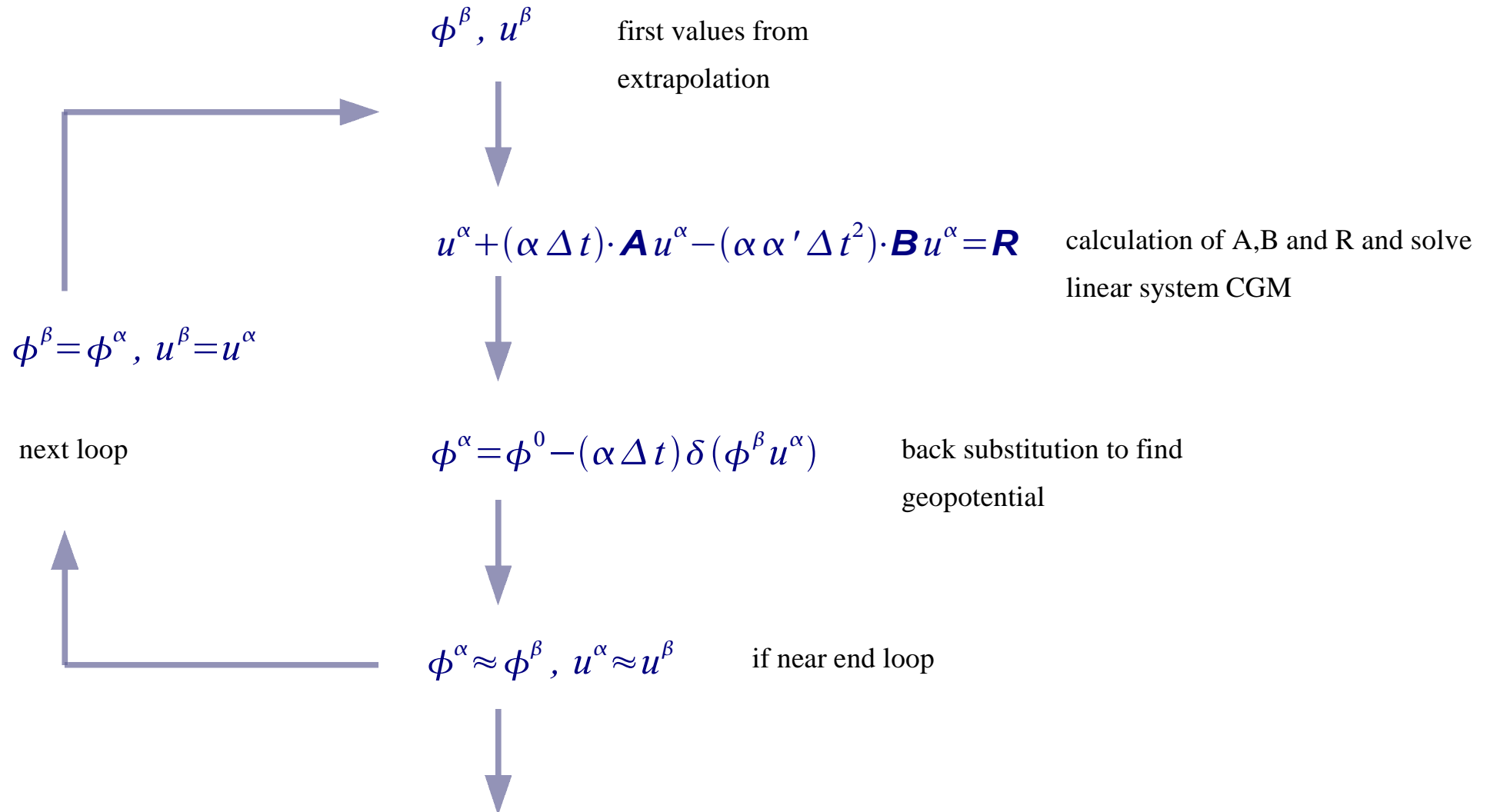
$$\mathbf{R} = u^0 - (\alpha \Delta t)(\mathbf{d} k^\beta + \mathbf{i}_{\#u^\beta} f) - (\alpha \Delta t) \mathbf{d}(\phi^0 + \phi_s)$$

- Operators **A** and **B** are linear, and the equation can be solved using a linear solver. **Conjugate Gradient Method** is used in the model
- Back substitution in continuity equation provides geopotential

$$\phi^\alpha = \phi^0 - (\alpha \Delta t) \delta(\phi^\beta u^\alpha)$$

Fully-implicit loop

- Fully-implicit scheme



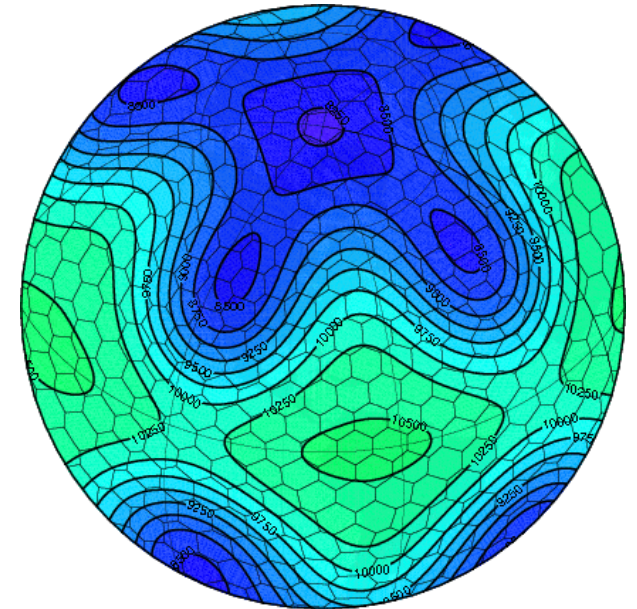
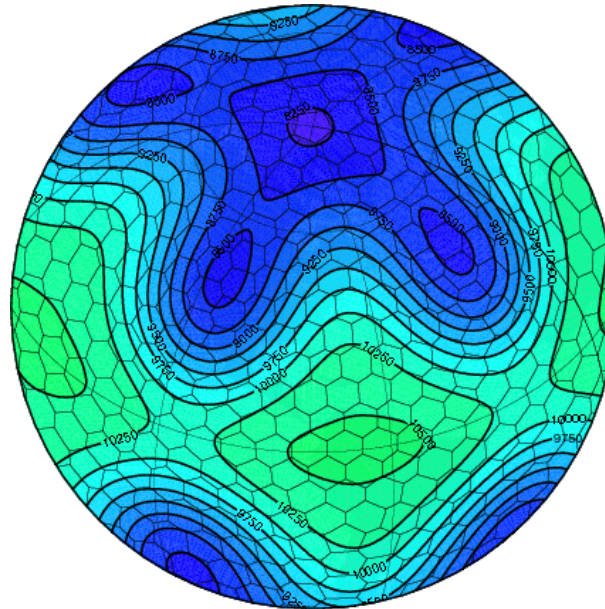
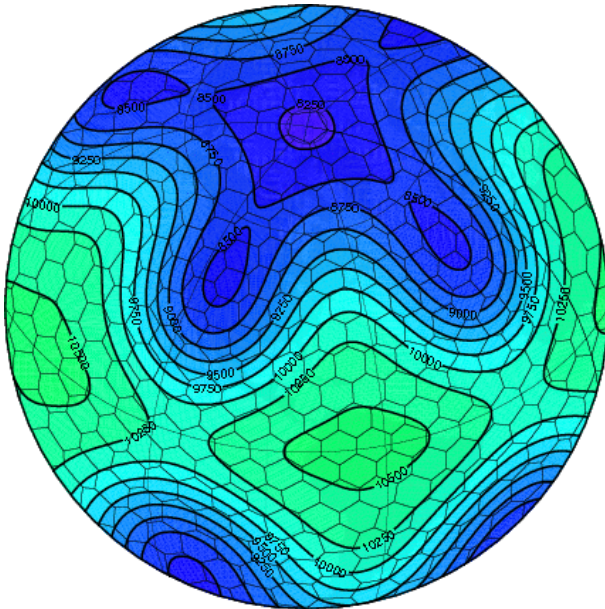
A comparison between fully-implicit and semi-implicit

- Comparison between fully-implicit and semi-implicit for test 6

High resolution spectral reference solution. Test 6, 10 days forecast, geopotential

Fully implicit, 2 loops. It is stable with $\alpha=0.5$. Test with optimized grid level 7, time step 1200 s and no numerical diffusion

Semi implicit, only 1 loop. To be stable must be $\alpha>0.5$ Test with $\alpha=0.7$, time step 1200 s and no numerical diffusion



Spatial discretization

- It is defined a **primary and secondary or dual grid**
- Each grid have **points, edges and cells**
- Any **operator** maps values from on grid to other
- **A p-form is integrated in a p-dimensional cell**

F primary faces, oriented hexagons or pentagons

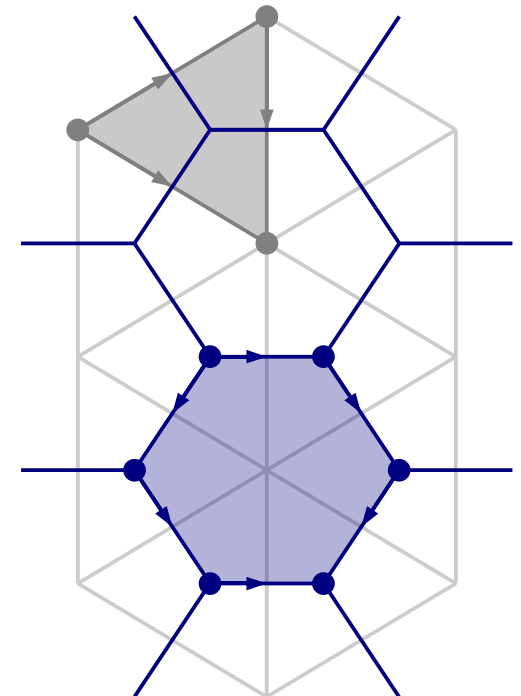
E primary edges, lines with orientation

V primary vertex, centre of triangles

F secondary faces, oriented triangles

E secondary edges, lines with orientation

V secondary vertex, centre of hexagons



Spatial discretization (II)

- A p -form is integrated in a p -dimensional cell
- Discrete wind and geopotential are

$$u_E = \int_E u$$

circulation of wind along a primary edge,
is a discrete 1-form

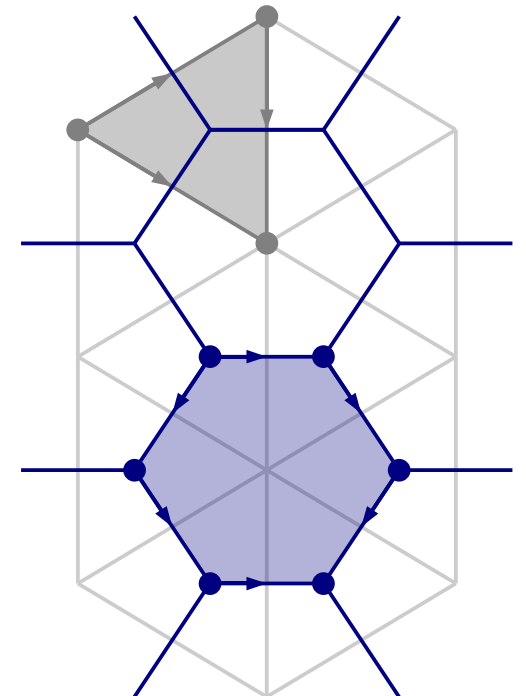
$$*\phi_F = \int_F *\phi$$

geopotential integrated in a secondary
face, is a discrete 2-form

- For example, discrete vorticity is a 2-form

$$\zeta_F = \int_F \mathbf{d}u$$

vorticity integrated in a primary face, is a
2-form. Exterior derivative maps from 1
forms to 2 forms in this case



Spatial discretization (III)

- Notation: a **discrete linear operator** from one grid to other is

$$c_G = (\mathbf{A}b)_G = \sum_{G'} [\mathbf{A}]_{GG'} b_{G'}$$

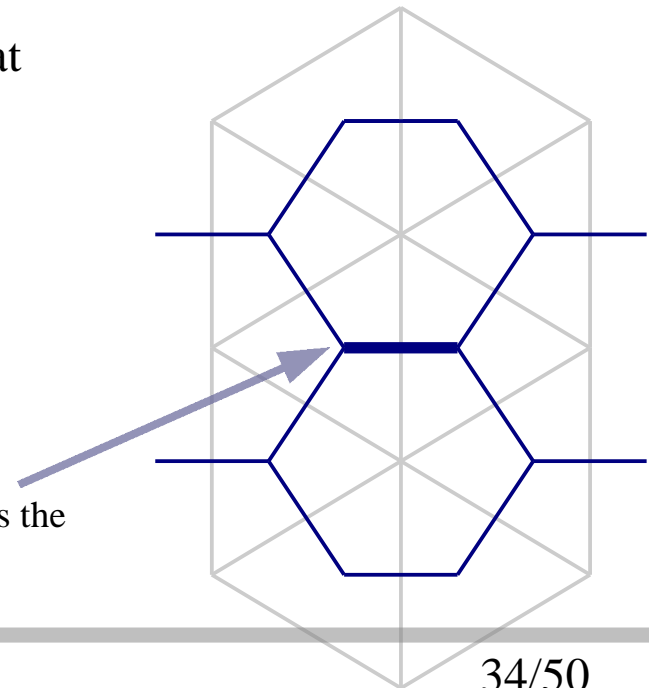
Discrete field defined at grid G is the result of operator A applied to b

Matrix from grid G' to G

Discrete field defined at grid G'

- The **stencil** of an operator is the number of non zero values at each line of its matrix. In the shallow water model described here the stencil is 15.

An edge and the 15 edges which forms the stencil in the SW model




Discrete exterior derivative (I)

- Discrete exterior derivative for 1-forms in primary grid is

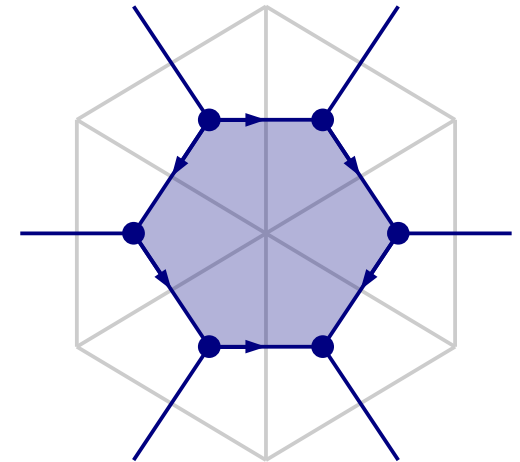
$$(\mathbf{d}u)_F \stackrel{(1)}{=} \int_F \mathbf{d}u \stackrel{(2)}{=} \int_{\partial F} u \stackrel{(3)}{=} \sum_{E \in \partial F} \sigma_{FE} \int_E u \stackrel{(4)}{=} \sum_{E \in \partial F} \sigma_{FE} u_E$$

(1) Definition of discrete 2 rank form (2) Stoke's Theorem (3) The boundary of a primary face is composed by primary edges plus a sign due to relative orientation (4) Discrete 1 rank form definition. It is a topological operator, no interpolations are needed at this point

- Discrete exterior derivative is a sparse matrix

$$(\mathbf{d}u)_F = \sum_{E \in \partial F} \sigma_{FE} u_E \equiv \sum_E [\mathbf{d}]_{FE} u_E$$


0, 1 and -1 are the values that appear in this matrix and in any discrete exterior derivative matrix



Discrete exterior derivative (II)

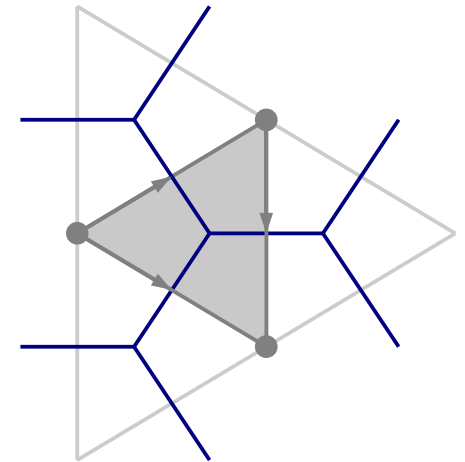
- Discrete exterior derivative for 1-forms in **secondary grid** is

$$(\mathbf{d}a)_F \stackrel{(1)}{=} \int_F \mathbf{d}a \stackrel{(2)}{=} \int_{\partial F} a \stackrel{(3)}{=} \sum_{E \in \partial F} \sigma_{FE} \int_E a \stackrel{(4)}{=} \sum_{E \in \partial F} \sigma_{FE} a_E$$

- (1) Definition of discrete 2 rank form (2) Stoke's Theorem (3) The boundary of a secondary face is composed by secondary edges plus a sign due to relative orientation (4) Discrete 1 rank form definition

- Discrete exterior derivative is a sparse matrix

$$(\mathbf{d}a)_F = \sum_{E \in \partial F} \sigma_{FE} a_E \equiv \sum_E [\mathbf{d}]_{FE} a_E$$

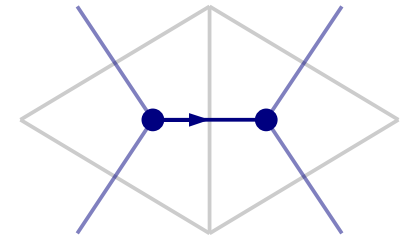


Discrete exterior derivative (III)

- Discrete exterior derivative of discrete 0-forms

$$(\mathbf{d}\phi)_E \stackrel{(1)}{=} \int_E \mathbf{d}\phi \stackrel{(2)}{=} \int_{\partial E} \phi \stackrel{(3)}{=} \sum_{V \in \partial E} \sigma_{EV} \int_V \phi \stackrel{(4)}{=} \sum_{V \in \partial E} \sigma_{EV} \phi_V$$

- (1) Definition of discrete 1 rank form (2) Stoke's Theorem (3) The boundary of a primary edge is composed by primary vertex plus a sign due to relative orientation (4) Discrete 0 rank form definition



- Discrete exterior derivative is

$$(\mathbf{d}\phi)_E = \sum_{V \in \partial E} \sigma_{EV} \phi_V \equiv \sum_V [\mathbf{d}]_{EV} \phi_V$$

Hodge operators (I)

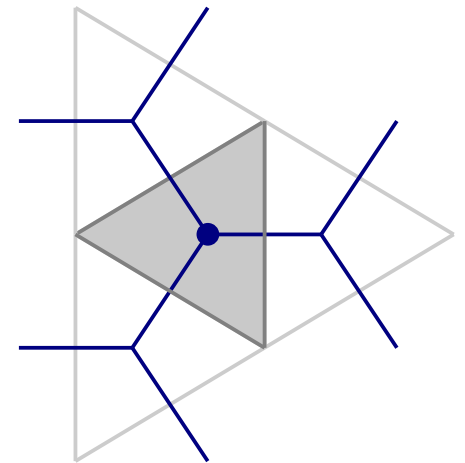
- The **discrete Hodge operator for a 0-form** or function is the integrated value of this function over a face. For the primary grid

$$(* \phi)_F \underset{(1)}{=} \int_F * \phi \underset{(2)}{=} \int_F \phi \upsilon \underset{(3)}{\approx} \phi_{\mathbf{v}} \int_F \upsilon \underset{(4)}{=} \phi_{\mathbf{v}} \upsilon_F$$

- (1) Definition of discrete 2 rank form (2) Continuous Hodge operator, use of volume form υ
 (3) Approximation of the integral, use of function value at one vertex (4) Definition of discrete volume 2 rank form. **This is a metric operator, interpolation and approximations are used in the discrete formulation.**

- This discrete version is **diagonal**, one value of the function is used in each face

$$(* \phi)_F = \upsilon_F \phi_{\mathbf{v}} \equiv \sum_{\mathbf{v}} [*]_{F\mathbf{v}} \phi_{\mathbf{v}}$$

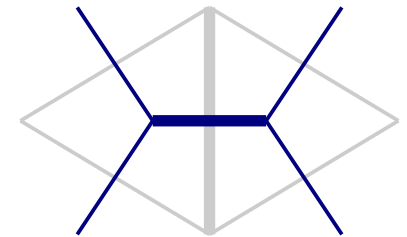


Hodge operators (II)

- The **discrete Hodge operator for a 1-form** is related to the flux of a vector field. Metric is needed. In 2 dimensional grids it maps from primary edges to secondary edges

$$(*u)_E \stackrel{(1)}{=} \int_E *u \stackrel{(2)}{\approx} u_E (v_E/v_E)$$

(1) Definition of discrete 1 rank form (2) Approximation to the flux when **primary and secondary grids are orthogonal** with the use of length of the edges v



- This discrete version is **diagonal**

$$(*u)_E = (v_E/v_E) u_E \equiv \sum_E [*]_{EE} u_E$$

- Same discrete operator from secondary to primary edges

Divergence term (I)

- The linear system to be solved has a **second order in time term B** related to divergence of geopotential multiplied by wind

$$\mathbf{B} u^\alpha = \mathbf{d} \delta(\phi^\beta u^\alpha) \qquad u^\alpha + (\alpha \Delta t) \cdot \mathbf{A} u^\alpha - (\alpha \alpha' \Delta t^2) \cdot \mathbf{B} u^\alpha = \mathbf{R}$$

- Using the expression for the codifferential (divergence in this case)

$$\mathbf{B} u^\alpha = \mathbf{d} * \mathbf{d} * (\phi^\beta u^\alpha)$$

- The discretization of this expression is a composition of linear operators (matrix multiplication). The operators involved are the exterior derivative and Hodge

$$[\mathbf{B}]_{EE} u_E^\alpha = [\mathbf{d}]_{EV} [*]_{VF} [\mathbf{d}]_{FE} [*]_{EE} (\phi^\beta u^\alpha)_E$$

Divergence term (II)

- In detail, the B matrix is the composition of the following linear operations

$$(\phi^\beta u^\alpha)_E \quad \text{Wind dot geopotential at each primary edge (needed geopotential interpolation)}$$

$$[*]_{EE}(\phi^\beta u^\alpha)_E \quad \text{Flux of geopotential at each secondary edge (triangle edge)}$$

$$[d]_{FE}[*]_{EE}(\phi^\beta u^\alpha)_E \quad \text{Sum of fluxes at each triangle (related to averaged divergence)}$$

$$[*]_{VF}[d]_{FE}[*]_{EE}(\phi^\beta u^\alpha)_E \quad \text{Divergence at triangle centre or primary vertex}$$

$$[d]_{EV}[*]_{VF}[d]_{FE}[*]_{EE}(\phi^\beta u^\alpha)_E \quad \text{Gradient of divergence at each primary edge}$$

- Finally B matrix maps from primary edge to primary edge grid

$$[B]_{EE}u_E^\alpha = [d]_{EV}[*]_{VF}[d]_{FE}[*]_{EE}(\phi^\beta u^\alpha)_E$$

Divergence term (III)

- Because some stability problems there was tested this term with a **non diagonal Hodge operator**. Test done so far indicates **stability is improved when increasing the order of the Hodge operator** in the divergence term.

$$[\mathbf{B}]_{EE} u_E^\alpha = [\mathbf{d}]_{EV} [*]_{VF} [\mathbf{d}]_{FE} [*]_{EE} (\phi^\beta u^\alpha)_E$$

Hodge operator from secondary faces to primal vertex modified to obtain more stable scheme

- The modified Hodge operator is

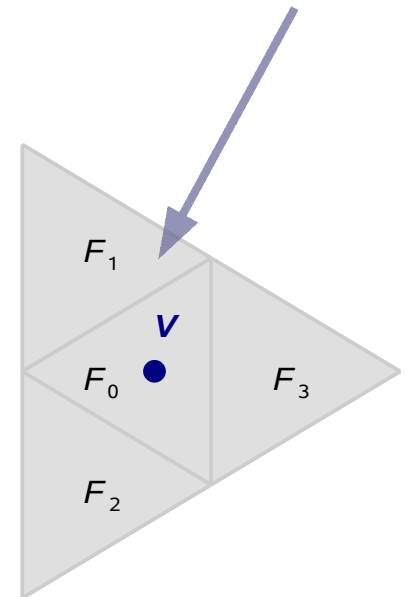
$$[(*)' \varphi]_{\mathbf{v}} = \sum_{i=0}^3 \gamma_i (\varphi_{F_i} / U_{F_i}) \text{ where } \sum_{i=0}^3 \gamma_i = 1$$

- Diagonal Hodge operator

$$[* \varphi]_{\mathbf{v}} = \sum_F [*]_{\mathbf{v}F} \varphi_F = \varphi_{F_0} / U_{F_0}$$

Both diagonal and non diagonal discrete Hodge operator tends to the continuous operator when increasing spatial resolution

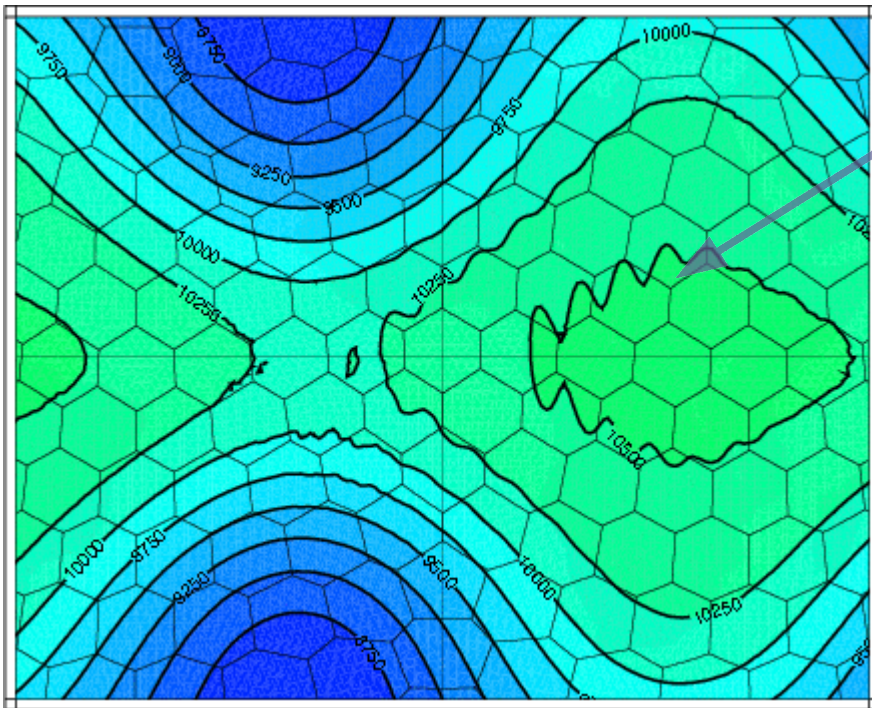
In the modified Hodge operator value at primal vertex (blue dot) calculated from 4 secondary faces values



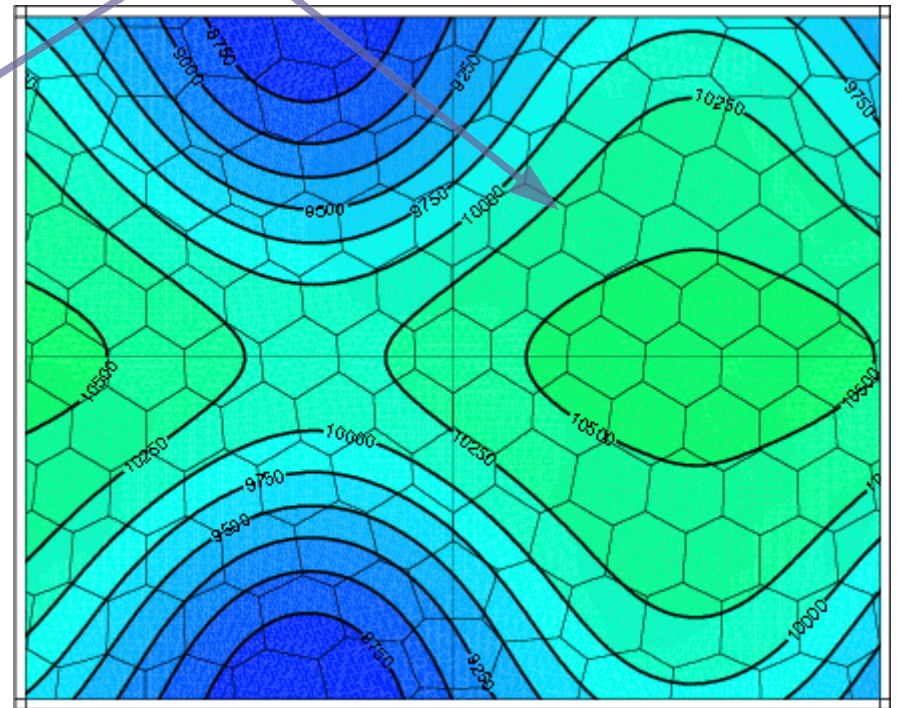
Divergence term (IV)

- This non diagonal Hodge operator combined with $\alpha' > \alpha$ in the the geopotential gradient term has great impact on stability, as seen in the tests performed for grid levels 7 and 8.

Diagonal Hodge operator for test 6, grid level 7 optimized,
time step 1200 seconds, $\alpha=0.5$, $\alpha'=0.5$, 2.5 days



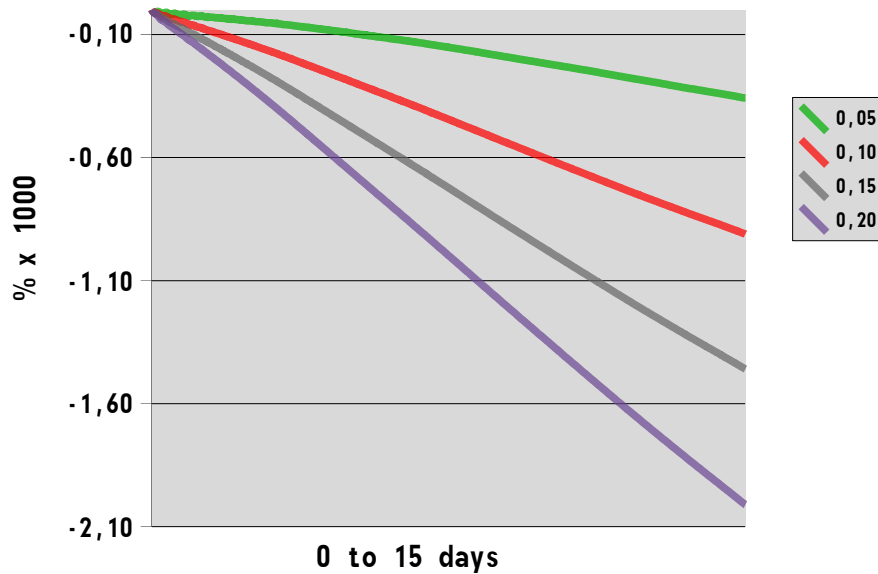
The same using non diagonal Hodge operator, $\alpha=0.5$ and
 $\alpha'=0.8$. Much more stability near equator



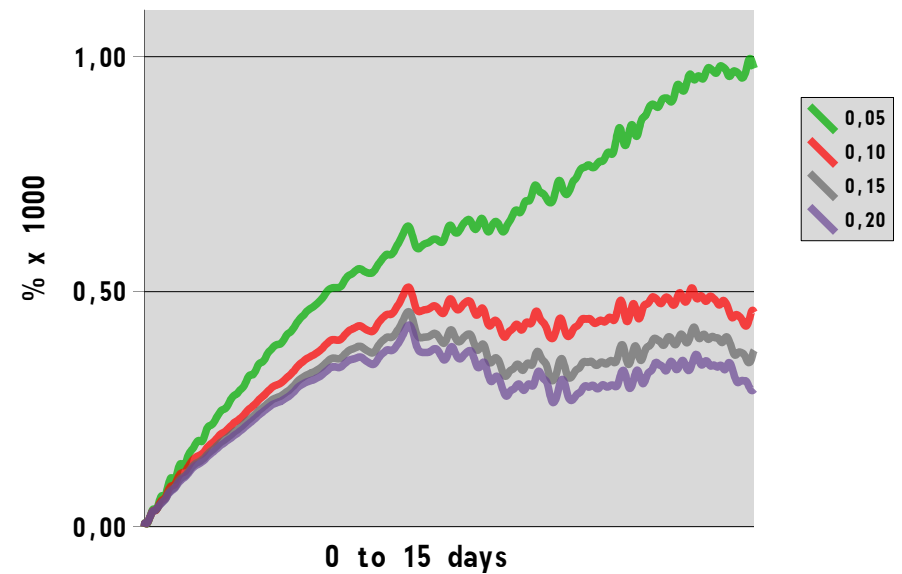
Divergence term (V)

- The value of α' has also impact in energy and enstrophy conservation.

Total energy for test 6, level 7 optimized grid, time step 1200 seconds, conserved up to 0.002% of initial value



Same test for enstrophy. Enstrophy increases a little, as one expect due to vorticity noise.



Vorticity and diffusion terms (I)

- The other term in the linear system is **first order in time matrix A** that includes **vorticity advection** and wind **diffusion**

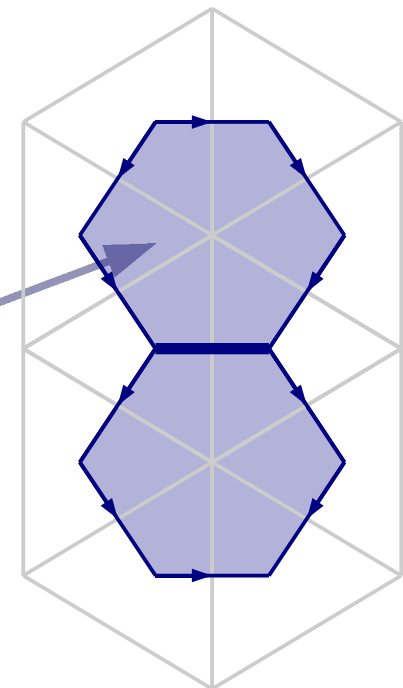
$$\mathbf{A} u^\alpha = \mathbf{i}_{\#u^\beta} \mathbf{d} u^\alpha - \lambda \Delta u^\alpha \qquad u^\alpha + (\alpha \Delta t) \cdot \mathbf{A} u^\alpha - (\alpha \Delta t)^2 \cdot \mathbf{B} u^\alpha = \mathbf{R}$$

- Vorticity** term is the composition of contraction and exterior derivative operators

$$[\mathbf{i}_{\#u^\beta} \mathbf{d} u^\alpha]_{\mathbf{E}} = [\mathbf{i}_{\#u^\beta}]_{\mathbf{EF}} [\mathbf{d}]_{\mathbf{FE}} u_{\mathbf{E}}^\alpha$$

Contraction to find vorticity flux over primary edge: **RBF** reconstruction to find the wind perpendicular to edge is used. Vorticity is interpolated at edge

Exterior derivative to find vorticity at two primary faces



Vorticity and diffusion terms (II)

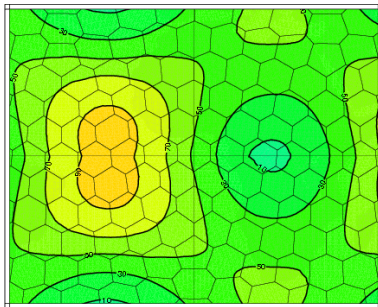
- **Diffusion** is linear and its matrix is calculated from codifferential and exterior derivatives

$$[\Delta u^\alpha]_E = ([\mathbf{d}]_{EV} [\delta]_{VE} + [\delta]_{EF} [\mathbf{d}]_{FE}) u_E^\alpha$$

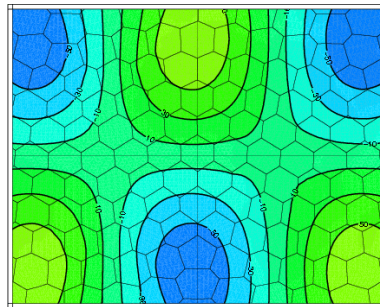
Continuous Laplace operator

$$\Delta = \mathbf{d} \delta + \delta \mathbf{d}$$

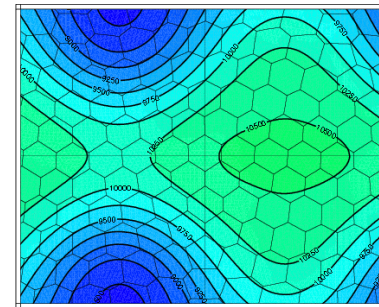
Diffusion reduces vorticity noise, but total energy and enstrophy is not conserved. Results for test 6, 10 days forecast near equator, no diffusion above.



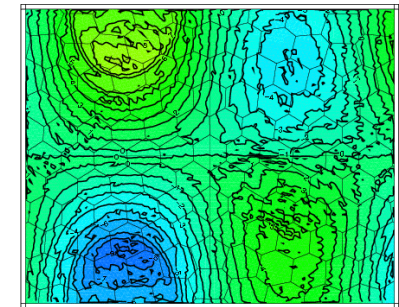
u component



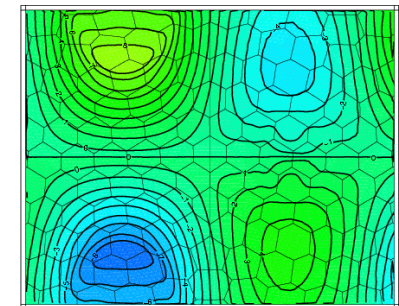
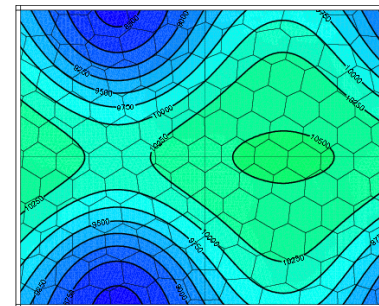
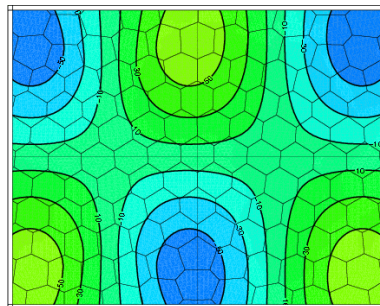
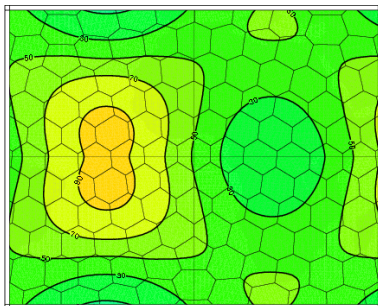
v component



Geopotential



Vorticity



Compressible fluid (I)

- In the case of atmospheric simulation the equations are, momentum equation (including Coriolis, gravitational force, wind diffusion and source terms from physics) and mass and thermodynamic equations

$$\partial_t u + \mathbf{i}_{\#u}(\mathbf{d}u + f) + \mathbf{d}k = -\alpha \mathbf{d}p - \mathbf{d}\phi + \lambda \Delta u + \Lambda_u$$

$$\partial_t \rho + \delta(u \rho) = 0$$

$$\partial_t s + \delta(us) = \Lambda_s$$

u is wind, f Coriolis vorticity, k kinetic energy, α specific volume, p pressure, ϕ geopotential, λ diffusion coefficient, ρ mass per volume unit, s entropy per volume unit, and Λ source terms

- Equivalent to

$$(\partial_t + L_{\#u})u = \mathbf{d}k - \alpha \mathbf{d}p - \mathbf{d}\phi + \lambda \Delta u + \Lambda_u$$

$$(\partial_t + L_{\#u}) * \rho = 0$$

$$(\partial_t + L_{\#u}) * (\rho s) = * \Lambda_s$$

Compressible fluid (II)

- Again, applying the exterior derivative to momentum equation, and because Lie derivative commute with exterior derivative

$$\partial_t \mathbf{d}u + \mathbf{d}i_{\#u}(\mathbf{d}u + f) = -\mathbf{d}\alpha \wedge \mathbf{d}p - \mathbf{d}(\lambda \Delta u + \Lambda_u)$$

- For adiabatic flow, the vorticity equation

$$\partial_t \mathbf{d}u + \mathbf{d}i_{\#u}(\mathbf{d}u + f) = -\mathbf{d}\alpha \wedge \mathbf{d}p$$

$$\partial_t \int_{\Omega} \mathbf{d}u + 0 = -\int_{\Omega} \mathbf{d}\alpha \wedge \mathbf{d}p$$

Local time derivative of vorticity

Advection of vorticity including rotation

Solenoidal term, is zero for barotropic fluid

- **Theoretically** it is possible to construct a discrete scheme which verifies a **vorticity** equation like this. Also conservative in **mass** and **entropy**.

Conclusions

- Exterior Calculus is an interesting mathematical tool to fluid dynamics, specially in conservative properties, topological and vorticity aspects.
- A shallow water model on the sphere in an icosahedral grid has been developed using ICON grid generation, operators and test. It has different linear system and different implicit treatment of vorticity and diffusion terms.
- The schemes proposed shows that a non diagonal Hodge operator in the gravity wave term as great impact on stability in this model.
- Finally some ideas about compressible fluids, in particular to find schemes conservative in mass, entropy and vorticity.

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