Gradient, divergence, and laplacian discrete approximations for numerical ocean modelling

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Toulouse, France

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T-UGOm: the Toulouse Unstructured Grid Ocean model

T-UGOm: 2D version use in production, experimental 3D version (research tool).

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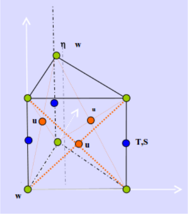

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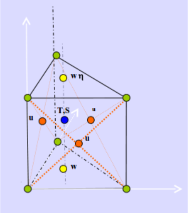

Finite volume

- Finite elements/volumes;
- time-splitting;
- 2D elements: triangles;
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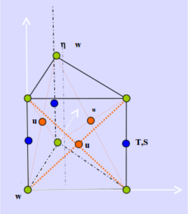

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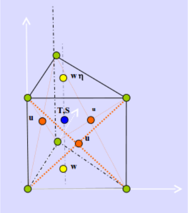

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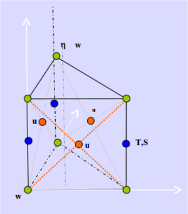

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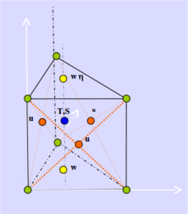

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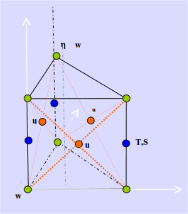

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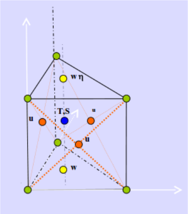

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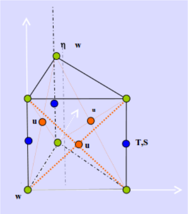

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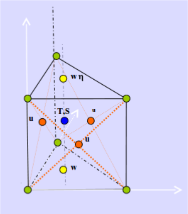

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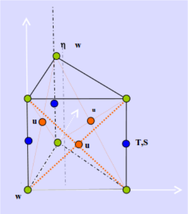

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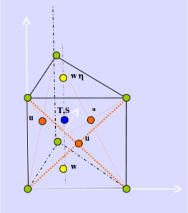

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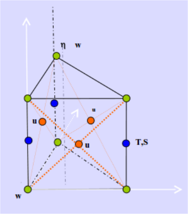

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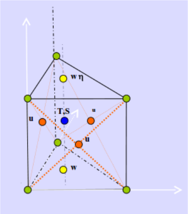

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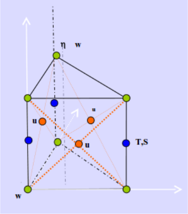

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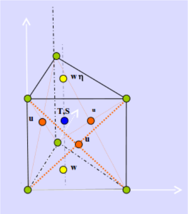

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Finite elements versus finites differences

Purpose:

1. Deeper understanding of similarities and differences between finite differences, finite elements and finite volumes;
2. make a rigorous generalised formalism, that can be used either in continuous and discontinuous case.

- Finite elements: explicit projection, derivation of interpolation functions (continuous interpolation);
- finite differences: implicit projection, rate of increase (discontinuous interpolation).

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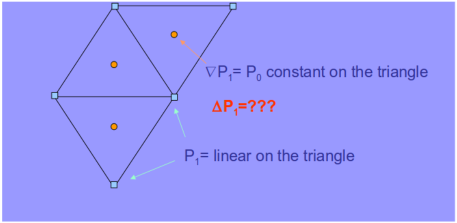

Generalised formalism

Finite elements "contain" finite differences

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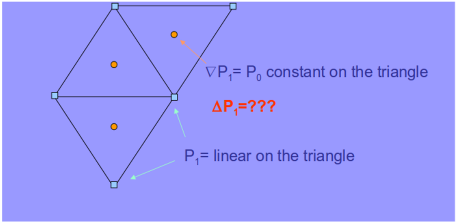

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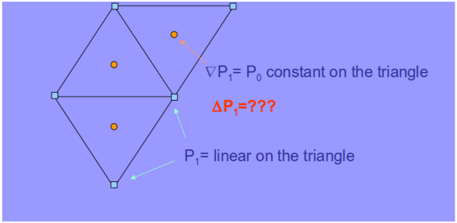

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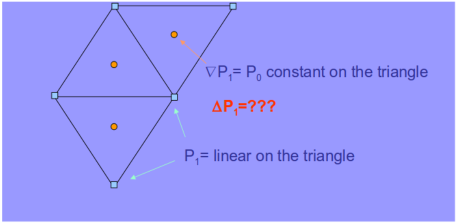

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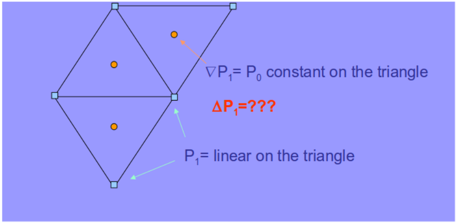

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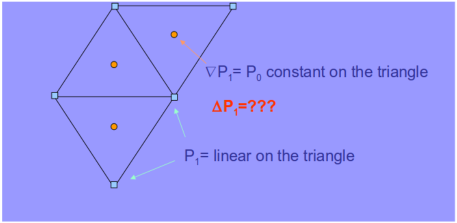

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Some difficulties

- Shallow water and generalised wave equations: $\boldsymbol{\nabla} \cdot \overline{\boldsymbol{u}}$ and $\boldsymbol{\nabla}\eta$
  $\Rightarrow$ need to compute discrete divergences and gradients;
- advection-diffusion equation: $\nabla \cdot \nabla c$ (laplacian can be also use for kinetic momentum equation)
  $\Rightarrow$ need to compute laplacians of discontinuous functions (non-measurable);
- σ-layers modelling: discontinuous elevation
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Outlook

1. Divergence and gradient
2. Looking for an optimal reformulation of laplacian in discontinuous case
3. σ-layers modelling

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Definitions

Measures

Definition

$\forall E$ *measurable space,* $\forall m \in \mathbb{N}^\star$ *and* $p \in [1;+\infty[$*,* $W^{m,p}(E)$*: Sobolev's space.*

Definition

$d\boldsymbol{x}$*: Lebesgue's measure.*

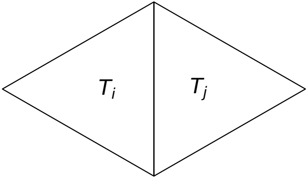
Definition

$d\sigma(\boldsymbol{x})$*: frontier measure (e.g. 2D: path length).*

Definitions

Notations

Let T_i and T_j be two neighbouring elements and $\Gamma_{i,j}$ their common edge.



$\forall \psi \in W^{m,p}(E)$ and, $\forall n \in \mathbb{N}^{\star}$, $\forall \boldsymbol{f} \in \left[W^{m,p}(E)\right]^n$, let:

$$\overline{\overline{\psi}}_{i,j} = \frac{1}{2}\left(\psi|_{T_i} + \psi|_{T_j}\right), \qquad (1)$$

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$\forall \beta_{i,j} \in [0;1]$ such as $\beta_{j,i} = 1 - \beta_{i,j}$, let:

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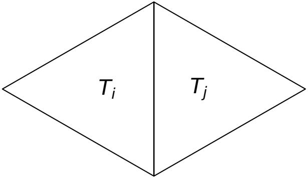

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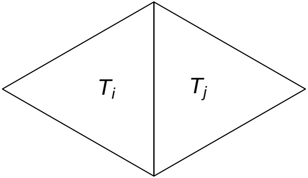

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Proposed approximations

Basics

Analogy with Dirac's measure

$$\int_{\Gamma_{i,j}} \boldsymbol{\nabla} \psi d\sigma\left(\boldsymbol{x}\right) \approx \int_{\Gamma_{i,j}} \underline{\underline{\psi}}_{i,j} \cdot \boldsymbol{n}_{i,j} d\sigma\left(\boldsymbol{x}\right), \quad (5)$$

$$\int_{\Gamma_{i,j}} \boldsymbol{\nabla} \cdot \boldsymbol{f} d\sigma\left(\boldsymbol{x}\right) \approx \int_{\Gamma_{i,j}} \underline{\underline{\boldsymbol{f}}}_{i,j} \cdot \boldsymbol{n}_{i,j} d\sigma\left(\boldsymbol{x}\right), \quad (6)$$

$\boldsymbol{n}_{i,j}$: the unit vector normal to $\Gamma_{i,j}$ and orientated from T_i to T_j.

Proposed approximations

Actual approximation

$$\int_{\Omega_k} \psi \boldsymbol{\nabla} \cdot \boldsymbol{f} d\boldsymbol{x} = \sum_{i=1}^{N_k} \int_{\mathring{T}_i} \psi \boldsymbol{\nabla} \cdot \boldsymbol{f} d\boldsymbol{x} + \sum_{i=1}^{N_k} \sum_{j : T_j \in \{\text{neighbours of } T_i\}} \int_{\Gamma_{i,j}} \psi \boldsymbol{\nabla} \cdot \boldsymbol{f} d\sigma(\boldsymbol{x}), \quad (7)$$

Ω_k: discretised problem space,

N_k: number of elements,

$\mathring{T}_i$: interior of T_i.

Analogy with finite differences

$$\int_{\Gamma_{i,j}} \psi \boldsymbol{\nabla} \cdot \boldsymbol{f} d\sigma(\boldsymbol{x}) \approx \int_{\Gamma_{i,j}} \overline{\overline{\psi}}_{i,j} \underline{\underline{\boldsymbol{f}}}_{i,j} \cdot \boldsymbol{n}_{i,j} d\sigma(\boldsymbol{x}). \quad (8)$$

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Proposed approximations

Actual approximation

$$\int_{\Omega_k} \psi \boldsymbol{\nabla}\cdot\boldsymbol{f} d\boldsymbol{x} = \sum_{i=1}^{N_k} \int_{\mathring{T}_i} \psi \boldsymbol{\nabla}\cdot\boldsymbol{f} d\boldsymbol{x} + \underbrace{\sum_{i=1}^{N_k} \sum_{j:T_j \in \{\text{neighbours of } T_i\}} \int_{\Gamma_{i,j}} \psi \boldsymbol{\nabla}\cdot\boldsymbol{f} d\sigma(\boldsymbol{x})}_{\text{discontinuity}}, \quad (7)$$

Ω_k: discretised problem space,

N_k: number of elements,

$\mathring{T}_i$: interior of T_i.

Analogy with finite differences

$$\int_{\Gamma_{i,j}} \psi \boldsymbol{\nabla}\cdot\boldsymbol{f} d\sigma(\boldsymbol{x}) \approx \int_{\Gamma_{i,j}} \overline{\overline{\psi}}_{i,j} \underline{\underline{\boldsymbol{f}}}_{i,j}\cdot\boldsymbol{n}_{i,j} d\sigma(\boldsymbol{x}). \quad (8)$$

Standard integration properties

Proposition (Leibniz's formula)

$\forall E$ measurable space, either continuous or discrete, with the proposed approximations, the following Leibniz's formula is verified:

$$\int_E \boldsymbol{\nabla} \cdot \psi \boldsymbol{f} d\boldsymbol{x} = \int_E \psi \boldsymbol{\nabla} \cdot \boldsymbol{f} d\boldsymbol{x} + \int_E \boldsymbol{\nabla} \psi \cdot \boldsymbol{f} d\boldsymbol{x}.$$

Proposition (Stokes' formula)

Let Γ_E be E fronter and $\boldsymbol{n}_{\Gamma_E}(\boldsymbol{x})$ be the unit vector normal to Γ_E on point $\boldsymbol{x}$, directed to the outside. Then, with the proposed approximations,
$\forall E$ measurable space, either continuous or discrete, Stokes' formula is verified:

$$\int_E \boldsymbol{\nabla} \cdot \boldsymbol{f} d\boldsymbol{x} = \int_{\Gamma_E} \boldsymbol{f} \cdot \boldsymbol{n}_{\Gamma_E} d\sigma(\boldsymbol{x}).$$

(Le Bars 2010; Lyard and Le Bars in prep.)

Outlook

1 Divergence and gradient

2 Looking for an optimal reformulation of laplacian in discontinuous case

3 σ-layers modelling

Objectives

1. $\forall \xi \in W^{m,p}(\Omega_k)$, to determine values of $\int_{\Omega_k} \boldsymbol{\nabla} \cdot \psi \boldsymbol{\nabla} \xi d\boldsymbol{x}$ and $\int_{\Omega_k} \boldsymbol{\nabla} \psi \cdot \boldsymbol{\nabla} \xi d\boldsymbol{x}$:
   - two derivations, then one integration;
   - only one derivation in previous gradient and divergence definitions;
2. to verify the following two Leibniz's formulas:

$$\int_{\Omega_k} \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} (\psi \xi) d\boldsymbol{x} = \int_{\Omega_k} \psi \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} \xi d\boldsymbol{x} + 2 \int_{\Omega_k} \boldsymbol{\nabla} \xi \cdot \boldsymbol{\nabla} \psi d\boldsymbol{x} + \int_{\Omega_k} \xi \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} \psi d\boldsymbol{x}, \quad (9)$$

$$\int_{\Omega_k} \boldsymbol{\nabla} \cdot \xi \boldsymbol{\nabla} \psi d\boldsymbol{x} = \int_{\Omega_k} \xi \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} \psi d\boldsymbol{x} + \int_{\Omega_k} \boldsymbol{\nabla} \xi \cdot \boldsymbol{\nabla} \psi d\boldsymbol{x}; \quad (10)$$

3. with Λ an arbitrary discontinuity repartition factor, to verify Stokes' formula:

$$\int_{\Omega_k} \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} \psi = \sum_{i=1}^{N_k} \sum_{j:T_j \in \{\text{neighbours of } T_i\}} \left(\int_{\Gamma_{i,j}} \boldsymbol{n}_{i,j} \cdot \boldsymbol{\nabla} \psi d\sigma(\boldsymbol{x}) + \int_{\Gamma_{i,j}} \Lambda \boldsymbol{n}_{i,j} \cdot \underline{\underline{\boldsymbol{\nabla} \psi}}_{i,j} d\sigma(\boldsymbol{x}) \right) \quad (11)$$

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Methodology

For now on, we see three possibilities:

1. to define a bounded discontinuous gradient, then use previous divergence definition;
2. to determine continuous field approximation and then compute laplacian;
3. use a filter to convolute the discontinuous field, then the gradient and so the laplacian can be controlled with filter slope (not detailed here).

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Using previous developments

Bounded discontinuous gradient, then use previous divergence definition

$$
\begin{aligned}
\int_{\Omega_k} \xi \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} \psi d\boldsymbol{x} = \sum_{i=1}^{N_k} \Bigg[\int_{\overset{\circ}{T_i}} \xi \boldsymbol{\nabla} \cdot \boldsymbol{\nabla} \psi d\boldsymbol{x} + & \sum_{j:T_j \in \{\text{neighbours of } T_i\}} \left(\int_{\Gamma_{i,j}} \Lambda \overline{\overline{\xi}}_{i,j} \underline{\underline{\boldsymbol{\nabla} \psi}}_{i,j} \cdot \boldsymbol{n}_{i,j} d\sigma(\boldsymbol{x}) \right. \\
& - \int_{\Gamma_{i,j}} \Lambda \boldsymbol{n}_{i,j} \cdot \underline{\underline{\psi}}_{i,j} \overline{\overline{\boldsymbol{\nabla} \xi}}_{i,j} d\sigma(\boldsymbol{x}) + \frac{L_e}{A_e} \int_{\Gamma_{i,j}} \Lambda \overline{\overline{\xi}}_{i,j} \underline{\underline{\psi}}_{i,j} d\sigma(\boldsymbol{x}) \\
& \left. - \frac{L_e}{A_e} \int_{\Gamma_{i,j}} \Lambda^2 \underline{\underline{\xi}}_{i,j} \times \underline{\underline{\psi}}_{i,j} d\sigma(\boldsymbol{x}) \right) \Bigg],
\end{aligned}
\tag{12}
$$

$$
\begin{aligned}
\int_{\Omega_k} \boldsymbol{\nabla} \cdot \xi \boldsymbol{\nabla} \psi d\boldsymbol{x} = \sum_{i=1}^{N_k} \Bigg[\int_{\overset{\circ}{T_i}} \boldsymbol{\nabla} \cdot \xi \boldsymbol{\nabla} \psi d\boldsymbol{x} + & \sum_{j:T_j \in \{\text{neighbours of } T_i\}} \left(\int_{\Gamma_{i,j}} \Lambda \underline{\underline{\xi \boldsymbol{\nabla} \psi}}_{i,j} \cdot \boldsymbol{n}_{i,j} d\sigma(\boldsymbol{x}) \right. \\
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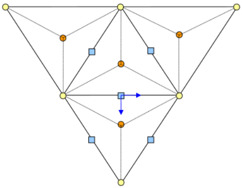
\end{aligned}
\tag{13}
$$

L_e: edge measurement (e.g 2D: segment length),
A_e: element measurement (e.g. 2D: element area).

(Lyard and Le Bars in prep.)

Continuous field approximation

$$\forall i \in \{1,2,\dots,N_k\}\,,\ \boldsymbol{\nabla}\psi|_{T_i} = \boldsymbol{\nabla}\psi|_{\overset{\circ}{T_i}} + \sum_{j:T_j\in\{\text{neighbours of } T_i\}} \underline{\underline{\psi}}_{i,j}\,\delta_{i,j}\boldsymbol{n}_{i,j}$$



Analogy with least squares method: determine $\boldsymbol{u}$ constant on T_i such as

$$\int_{T_i} \left\| \boldsymbol{\nabla}\psi - \boldsymbol{\nabla}\psi|_{\overset{\circ}{T_i}} - \boldsymbol{u} \right\|^2 d\boldsymbol{x} =$$

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Laplacian of the continuous approximation

$$\int_{\Omega_k} \boldsymbol{\nabla}\cdot\xi\boldsymbol{\nabla}\psi d\boldsymbol{x} = \sum_{i=1}^{N_k}\int_{\overset{\circ}{T_i}} \boldsymbol{\nabla}\cdot\xi\boldsymbol{\nabla}\psi d\boldsymbol{x} + \sum_{i=1}^{N_k}\sum_{j:T_j\in\{\text{neighbours of } T_i\}}\int_{\Gamma_{i,j}} \underline{\underline{\xi\boldsymbol{\nabla}\psi}}_{i,j}\cdot\boldsymbol{n}_{i,j}d\sigma(\boldsymbol{x}) \quad (14)$$

According to Stokes' formula:

$$\int_{\Omega_k} \xi\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\psi d\boldsymbol{x} = \sum_{i=1}^{N_k}\Bigg[\int_{\overset{\circ}{T_i}} \xi\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\psi d\boldsymbol{x} + \sum_{j:T_j\in\{\text{neighbours of } T_i\}}\Bigg(\int_{\Gamma_{i,j}}\Lambda\overline{\overline{\xi}}_{i,j}\underline{\underline{\boldsymbol{\nabla}\psi}}_{i,j}\cdot n_{i,j}d\sigma(\boldsymbol{x}) \quad (15)$$

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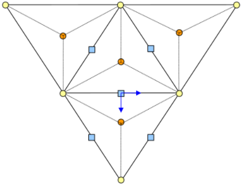

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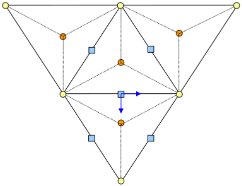

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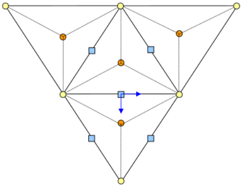

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(Lyard and Le Bars in prep.)

Outlook

3D σ-layers, finite volumes formulation

Finite differences equations (change of vertical coordinates) can be seen as layer-integrated equations, with application of Leibniz's formula

Volume conservation: $0 = \int_{s_0}^{s_1} \nabla \cdot \boldsymbol{u} ds = \int_{s_0}^{s_1} \nabla_H \cdot \boldsymbol{v} dz + [w]_{s_0}^{s_1}$

According to Leibniz's formula: $\int_{s_0}^{s_1} \nabla \cdot \boldsymbol{u} ds = \nabla_H \cdot \int_{s_0}^{s_1} \boldsymbol{v} dz - [\boldsymbol{v} \cdot \nabla_H s]$

$\boldsymbol{u}$: 3D velocity;
$\boldsymbol{v}$: horizontal velocity;
w: vertical velocity;
ω: omega velocity.

Then:

$$\int_{s_0}^{s_1} \nabla \cdot \boldsymbol{u} ds = \nabla_H \cdot \int_{s_0}^{s_1} \boldsymbol{v} dz + [\omega]_{s_0}^{s_1} + \left[\frac{\partial s}{\partial t}\right]_{s_0}^{s_1} \qquad (16)$$

In case of element-wise constant elevation/layer position:

- spatial derivations require correction terms due to discontinuities;
- Leibniz's formula does not hold (i.e. requires additional correction terms) if layers are not face to face from one column to another;
- *most known models do not care properly about those two issues, may it be because it would significantly increase computation time?*

3D σ-layers, finite volumes formulation

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Then: $$\int_{s_0}^{s_1} \boldsymbol{\nabla} \cdot \boldsymbol{u} ds = \boldsymbol{\nabla}_H \cdot \int_{s_0}^{s_1} \boldsymbol{v} dz + [\omega]_{s_0}^{s_1} + \left[\frac{\partial s}{\partial t}\right]_{s_0}^{s_1} \tag{16}$$

$\boldsymbol{u}$: 3D velocity;
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In case of element-wise constant elevation/layer position:

- spatial derivations require correction terms due to discontinuities;
- Leibniz's formula does not hold (i.e. requires additional correction terms) if layers are not face to face from one column to another;
- *most known models do not care properly about those two issues, may it be because it would significantly increase computation time?*

3D σ-layers, finite volumes formulation

Finite differences equations (change of vertical coordinates) can be seen as layer-integrated equations, with application of Leibniz's formula

Volume conservation: $0 = \int_{s_0}^{s_1} \boldsymbol{\nabla} \cdot \boldsymbol{u} ds = \int_{s_0}^{s_1} \boldsymbol{\nabla}_H \cdot \boldsymbol{v} dz + [w]_{s_0}^{s_1}$

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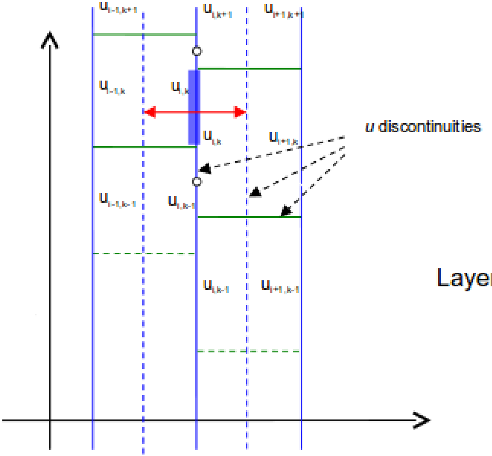
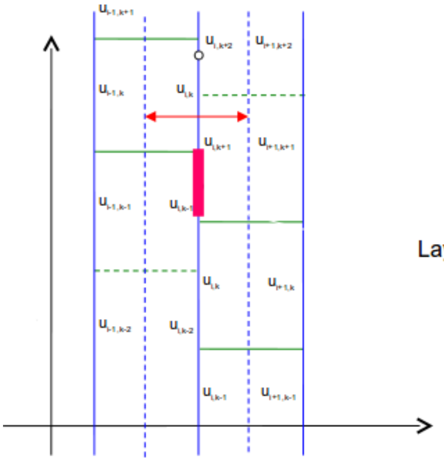
Leibniz's formula holds in this case



Layers have a partial continuity

Leibniz's formula does not hold in this case



Layers are disjoint

Some partial conclusions 1/2

- Most of FD, FV and FE dynamical and tracers discrete equations are identical if discontinuities are properly treated;
- laplacian operator (for piece-wise constant fields) needs further investigation:
  - simple extension from 1D to 2D does not work in general;
  - FD and FE may differ significantly;
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Some partial conclusions 2/2

- Discontinuous elevation/layer positions are a real issue:
  - if treated properly, suppress computational interest of FV;
  - if not treated properly, lead to inconsistencies (such as the hydrostatic one). In most FV formulation, elevation is piece-wise constant in mass conservation computation, continuous in pressure gradient computation (thus inconsistent);
- structured and unstructured models suffer the same issue, except that variable resolution can help in large bathymetry gradient regions (such as the continental shelf slopes);
- we have started to investigate a new 3D discretisation that allows to keep FV schemes with continuous elevation/layers (to be continued).

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References

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Thank you