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Finite Volume Discretization Techniques of Differential Operators

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"This material is based on *An introduction to Computational Fluid Dynamics using OpenFOAM with advanced topics* by Riccardo Rossi, Head and Founder of RED Fluid Dynamics, March/April 2021".

The scalar transport equation

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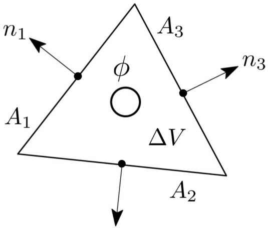
We use the **finite-volume method** (FVM) to solve the flow governing equations. The **integral form** of the scalar transport equation (STE) must be discretized and solved:

$$\int_V \frac{\partial \phi}{\partial t}\, dV + \int_A (u_j \phi) n_j \, dA = \int_A D \frac{\partial \phi}{\partial x_j} n_j \, dA + \int_V (S_\phi)\, dV$$

Discretization steps:

- Numerical integration
- Time-advancement schemes
- Differentiation schemes
- Interpolation schemes



Properties of numerical schemes

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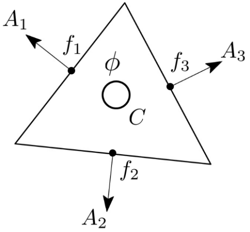
The important properties of a numerical schemes are:

- **Convergence/accuracy**: the numerical solution should converge to the exact solution of the PDE as the mesh size tends to zero
- **Conservation**: underlying conservation laws should be respected at the discrete level
- **Boundedness**: quantities like density, temperature and concentration should remain non-negative and free of spurious wiggles/spikes

And what about the **spectral-resolution**?

If we **integrate in time** the semi-discrete transport equation and we apply the unconditionally stable backward Euler scheme we get:

$$(\phi^{n+1} - \phi^n)\Delta V + \sum_f (u_j^n \phi^{n+1})_f A_{fj} = \sum_f D_f \frac{\partial \phi^{n+1}}{\partial x_j}\Big|_f A_{fj} + S_\phi^{n+1}\Delta V$$

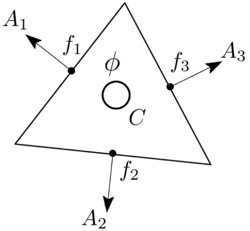


Note that the **midpoint rule** is **second-order accurate** only if variables are evaluated at the **cell/face centroid**.

$$(\phi^{n+1} - \phi^n)\Delta V + \sum_f (u_j^n \phi^{n+1})_f A_{fj} = \sum_f D_f \frac{\partial \phi^{n+1}}{\partial x_j}\Bigg|_f A_{fj} + S_\phi^{n+1} \Delta V$$

We need to define the **discretization method** for the following operators:

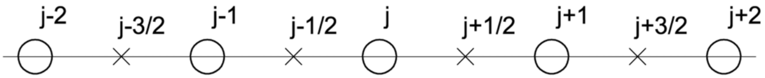
- Cell-centered gradient
- Diffusion operator
- Convection operator



The computation of **cell-centered gradients** is widely used in finite-volume schemes for **convection interpolation** and **diffusion discretization**.

On a uniform, one-dimensional stencil a **second-order accurate** formula based on **Taylor expansions** is the following:

$$\left.\frac{\partial \phi}{\partial x}\right|_j = \frac{\phi_{j+1} - \phi_{j-1}}{2\Delta x} - \frac{1}{6}\left.\frac{\partial^3 \phi}{\partial x^3}\right|_j \Delta x^2 + \mathcal{O}(\Delta x^3)$$



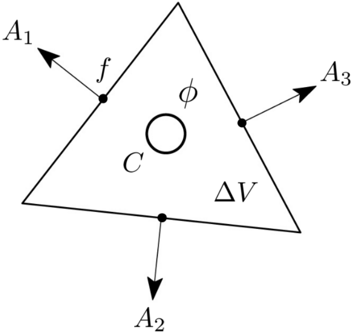
In the framework of **unstructured finite-volume schemes**, cell-centered gradients can be estimated via the **Gauss-Green theorem**:

$$\int_V \frac{\partial \phi}{\partial x_j}\, dV = \int_A \phi n_j\, dA$$

which, using the **midpoint rule** to evaluate the surface and volume integrals, gives:

$$\left.\frac{\partial \phi}{\partial x_j}\right|_c \approx \frac{1}{\Delta V} \sum_f \phi_f A_{fj}$$

where ϕ_f is the face-interpolated value.



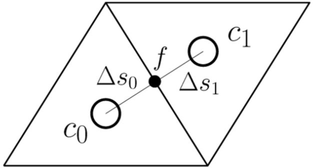
The **face interpolated value** as well can be estimated via **Taylor expansions**:

$$\phi_0 = \phi_f - \left.\frac{\partial \phi}{\partial s}\right|_f \Delta s_0 + \frac{\partial^2 \phi}{\partial s^2}\frac{\Delta s_0^2}{2} + \mathcal{O}(\Delta s_0^3)$$

$$\phi_1 = \phi_f + \left.\frac{\partial \phi}{\partial s}\right|_f \Delta s_1 + \frac{\partial^2 \phi}{\partial s^2}\frac{\Delta s_1^2}{2} + \mathcal{O}(\Delta s_1^3)$$

The **midPoint scheme** provides a simple **second-order** formula on **regular grids** ($\Delta s_0 = \Delta s_1$):

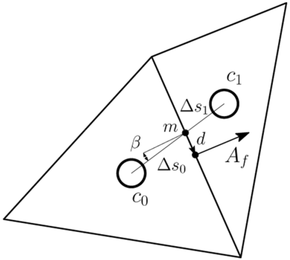
$$\phi_f^{MP} = \frac{\phi_1 + \phi_0}{2} + \mathcal{O}(\Delta s^2)$$



In complex geometries the computational grid usually deviates from regular elements and **quality parameters** are thus introduced.

Mesh quality:

- Aspect ratio ($\Delta s_1 / \Delta s_0$)
- Non-orthogonality (β)
- skewness (d)



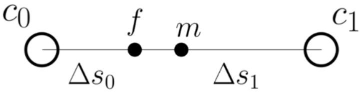
Mid-point rule:

$$\phi_f^M = \frac{\phi_1 + \phi_0}{2} + \mathcal{O}(\Delta s^2)$$

Linear interpolation:

$$\phi_f^L = \phi_0 \lambda_0 + \phi_1 (1 - \lambda_0) + \mathcal{O}(\Delta s^2)$$

$$\lambda_0 = \frac{\Delta s_0}{\Delta s}, \quad \Delta s = \Delta s_0 + \Delta s_1$$



Mid-point rule:

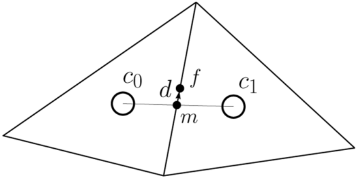
$$\phi_f^M = \frac{\phi_1 + \phi_0}{2} + \mathcal{O}(\Delta s^2)$$

Skew-corrected intepolation:

$$\phi_m^L = \phi_0\lambda_0 + \phi_1\lambda_1\,, \quad \lambda_1 = 1 - \lambda_0$$

$$(\nabla\phi)_m^L = (\nabla\phi)_0\lambda_0 + (\nabla\phi)_1\lambda_1$$

$$\phi_f^{SC} = \phi_m + (\nabla\phi)_m \cdot d$$

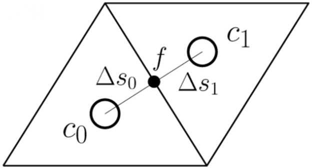


The discretization of the **diffusive flux** in the STE requires to evaluate the **scalar gradient** at the **face centroid**:

$$\int_A D\frac{\partial\phi}{\partial x_j}n_j \approx \sum_f D\frac{\partial\phi}{\partial x_j}\bigg|_f A_{fj}$$

On **regular grids**, the face gradient can be evaluated via the **central scheme**:

$$\frac{\partial\phi}{\partial x_j} \approx \frac{\phi_1 - \phi_0}{\Delta s} + \mathcal{O}(\Delta s^2)$$



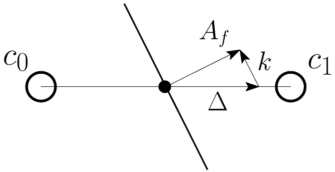
On **irregular** meshes, a **correction** for the **grid non-orthogonality**, when severe, might be needed to improve the accuracy of the numerical solution:

$$\left.\frac{\partial \phi}{\partial x_j}\right|_f A_{fj} = |\Delta| \frac{\phi_1 - \phi_0}{\Delta s} + k \cdot (\nabla \phi)_f$$

where

$$(\nabla \phi)_f = (\nabla \phi)_0 \lambda_0 + (\nabla \phi)_1 \lambda_1$$

is used to build up the **correction term**.



Convection interpolation operators I

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The discretization of the **convection operator** requires to evaluate the field at the **face centroid**.

A second-order accurate **central interpolation** on irregular meshes can be obtained using a **two-sided linear expansion** [1]:

$$\phi_f = \frac{1}{2}(\phi_0 + \phi_1) + \frac{1}{2}\left[\left.\frac{\partial \phi}{\partial x_i}\right|_0 R_{0i} + \left.\frac{\partial \phi}{\partial x_i}\right|_1 R_{1i} \right] + \mathcal{O}(\Delta s^2)$$

Alternatively, using a **one-sided linear expansion**, **upwind schemes** are obtained:

$$\phi_f = \phi_u + \left.\frac{\partial \phi}{\partial x_i}\right|_u R_{ui} + \mathcal{O}(\Delta s^2)$$

[1] P. Batten, C. Lambert, D.M. Causon, Positively conservative high-resolution convection schemes for unstructured elements, Int. J. Numer. Methods Eng. 39 (1996) 1821.

Convection interpolation operators II

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Several convection interpolation schemes have been proposed in the context of the FV framework. We report here the **low-order** and **high-order** upwind and central interpolation schemes:

Upwind (FOU) : $\phi_f = \phi_u + \mathcal{O}(\Delta s)$

linearUpwind (SOU) : $\phi_f = \phi_u + \left.\frac{\partial \phi}{\partial x_i}\right|_u R_{ui} + \mathcal{O}(\Delta s^2)$

midPoint (LOCD) : $\phi_f = \frac{1}{2}(\phi_0 + \phi_1) + \mathcal{O}(\Delta s^2)$

reconCentral (HOCD) : $\phi_f = \frac{1}{2}(\phi_0 + \phi_1) + \frac{1}{2}\left[\left.\frac{\partial \phi}{\partial x_i}\right|_0 R_{0i} + \left.\frac{\partial \phi}{\partial x_i}\right|_1 R_{1i}\right] + \mathcal{O}(\Delta s^2)$

Slope limiter

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In the framework of unstructured finite-volume schemes, **slope-limiting techniques** can be used to keep the **face-interpolation bounded**.

$$\phi_f = \phi_u + min(\alpha_f) \left.\frac{\partial \phi}{\partial x_j}\right|_u R_{uj}$$

For each cell, the **limiter** is given by:

$$\alpha_f = \begin{cases} min\left(1, \frac{\phi_{max} - \phi_u}{\phi_f - \phi_u}\right) & \text{if}(\phi_f - \phi_u) > 0 \\ min\left(1, \frac{\phi_{min} - \phi_u}{\phi_f - \phi_u}\right) & \text{if}(\phi_f - \phi_u) < 0 \\ 1 & \text{otherwise} \end{cases}$$

where ϕ_u is the cell-centroid value at the upwind side of the face.

In OpenFOAM, the schemes for **gradient** (cell-centered) computation and **diffusion/convection** discretization are specified in the **fvSchemes** dictionary file located in the **system** folder:

```
gradSchemes
{
    default linear;
    grad(u) cellLimited Gauss skewCorrected midPoint 1;
}
divSchemes
{
    div(phi, u) Gauss linearUpwind grad(u);
}
laplacianSchemes
{
    Laplacian(D, u) Gauss linear corrected;
}
```

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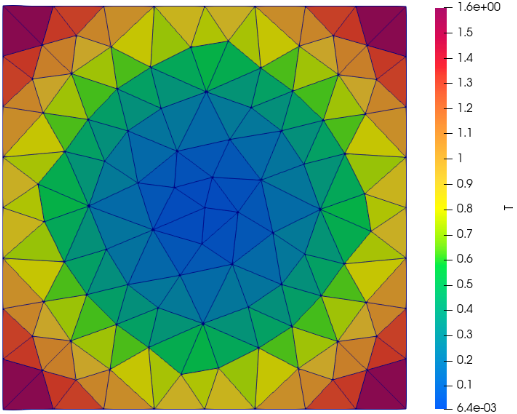

Test function:

$$T(x, y) = x^2 + y^2$$

$$\frac{\partial T}{\partial x} = 2x, \quad \frac{\partial T}{\partial y} = 2y$$

example I: computation of cell gradient

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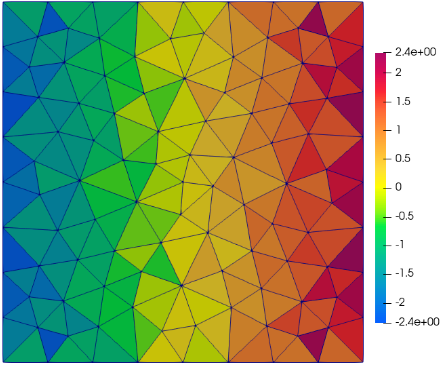
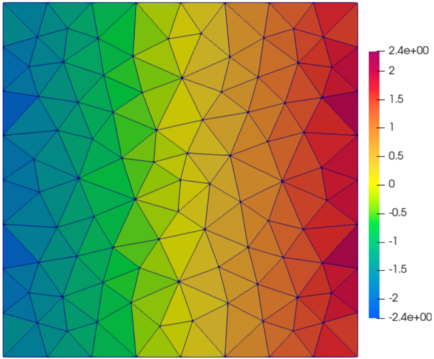
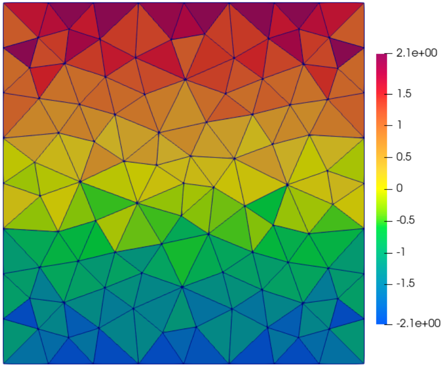


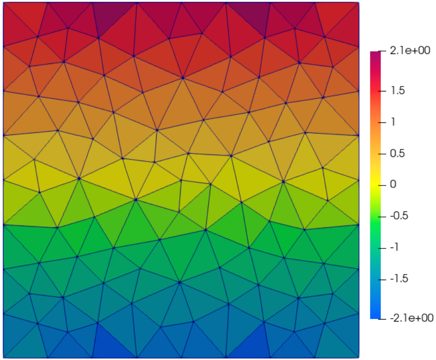
Sx - Gauss midPoint



Sx - Gauss skewCorrected linear

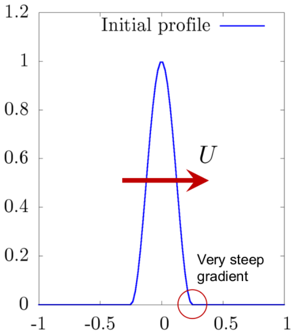


Sy - Gauss midPoint



Sy - Gauss skewCorrected linear

The (pure) **advection** of a scalar profile in uniform flow can be used to investigate the **conservation and spectral properties** of CIOs.



Flow parameters:

$$\frac{\partial \phi}{\partial t} + U\frac{\partial \phi}{\partial x} = 0\,,\, U = 1$$

$$\phi(x,0) = \begin{cases} cos^2(2\pi x) & \text{if} |x| \leq 0.25 \\ 0 & \text{if} |x| > 0.25 \end{cases}$$

example II: Advection of a scalar profile II

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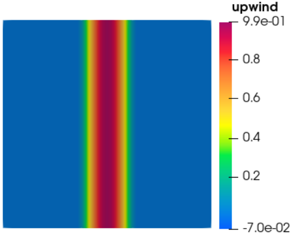

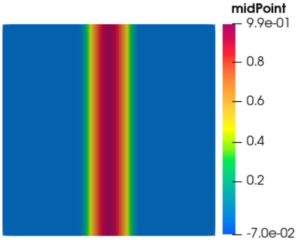

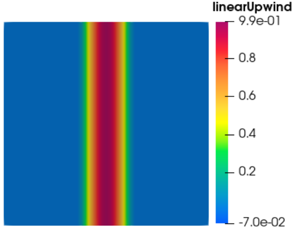

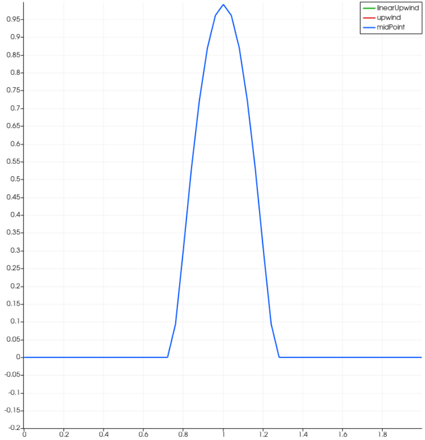

example II: Advection of a scalar profile II

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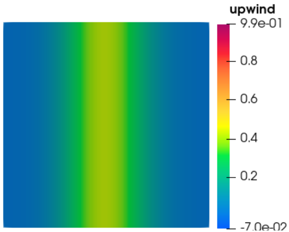

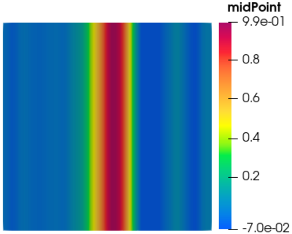

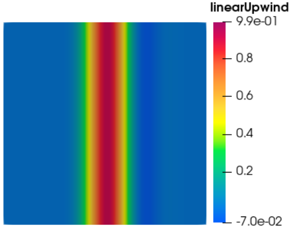

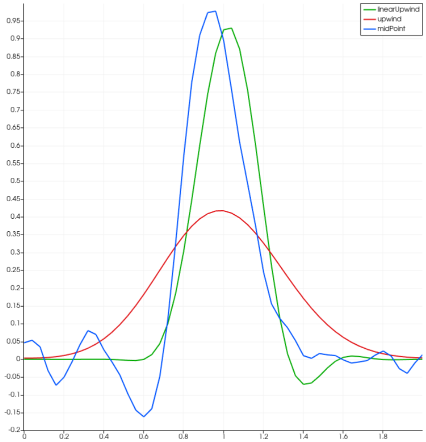

Thank you for your attention!