Numerical approximations of derivatives and integralls

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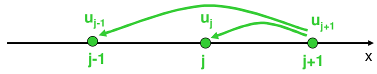
An implicit differencing scheme with second order accuracy



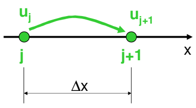
$$u_j = u_{j+1} + u'_{j+1}(-\Delta x) + u''_{j+1}\frac{\Delta x^2}{2} + o(\Delta x^2)$$

$$u_{j-1} = u_{j+1} + u'_{j+1}(-2\Delta x) + u''_{j+1}2\Delta x^2 + o(\Delta x^2)$$

$$u_j - \frac{u_{j-1}}{4} = \frac{3}{4}u_{j+1} + u'_{j+1}\left(-\frac{\Delta x}{2}\right) + o(\Delta x^2)$$

$$u'_{j+1} = \frac{\frac{3}{2}u_{j+1} - 2u_j + \frac{1}{2}u_{j-1}}{\Delta x} + o(\Delta x)$$

Euler method



Taylor polynomial of the solution from point j to point j+1:

$$u_{j+1} = u_j + u'_j\Delta x + o(\Delta x)$$

This is an integration scheme of first order accuracy.

A differencing scheme with first order accuracy:

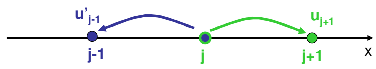
$$u'_j = \frac{u_{j+1} - u_j}{\Delta x} + o(1)$$

Another first order scheme:

$$u_j = u_{j+1} + u'_{j+1}(-\Delta x) + o(\Delta x)$$

u'_{j+1} usually is a given (but more complicated) function of x_{j+1} and u_{j+1}. Substitution of this function into the above formula leads to a more complicated expression for u_{j+1}. This kind of scheme is called implicit.

Adams-Basforth scheme



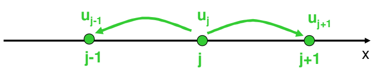
$$u_{j+1} = u_j + u'_j\Delta x + u''_j\frac{\Delta x^2}{2} + o(\Delta x^2)$$

$$u'_{j-1} = u'_j + u''_j(-\Delta x) + o(\Delta x) \quad / \; + \ldots \times \frac{\Delta x}{2}$$

$$u_{j+1} = u_j + \frac{3}{2}u'_j\Delta x - \frac{1}{2}u'_{j-1}\Delta x + o(\Delta x^2)$$

An explicit integrating scheme with second order accuracy
It is often used **for integrating the Navier-Stoket equations**.

CDS



$$u_{j+1} = u_j + u'_j\Delta x + u''_j\frac{\Delta x^2}{2} + o(\Delta x^2)$$

$$u_{j-1} = u_j + u'_j(-\Delta x) + u''_j\frac{\Delta x^2}{2} + o(\Delta x^2)$$

$$u'_j = \frac{u_{j+1} - u_{j-1}}{2\Delta x} + o(\Delta x)$$

Spatial derivatives in finite volume methods

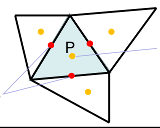
The generic transport equation in integral form:

$$\frac{\partial \rho\phi}{\partial t} + \nabla\cdot(\rho\phi\vec{v}) = \nabla\cdot\vec{S}_A + \nabla\cdot(\Gamma\nabla\phi) + S_v$$

In which Φ is the mass concentration of a conserved quantity (eg. in kg/kg).

Spatial derivatives are always in div(...), grad(...) or div(grad(...)) forms.
We only need to look for the discrete approximations of these operators, which is done - in the case of finite volume method - on the basis of surface and volume integrals along with some spatial interpolations.

The numerical mesh around the cell having its center in point P:



Face centroids.
Defined by surface vectors.

Cell centroid.
Here we store ϕ_P.

Anything can be interpolated from cells to surfaces...

Approximation of the divergence operator

From the volume integral the divergence operator we can obtain an average value for the numerical cell.
The Gauss-Ostrogradskij theorem for a vector quantity u:

$$\int_V \nabla \cdot \underline{u}\, dV = \oint_A \underline{u} \cdot d\,\underline{A}$$

For simplicity, we denote components of u vector by u_i. The cell-average of the divergence operator is now:

$$\tilde{\nabla} \cdot u_i = \frac{\sum_k \int_{A_k} u_\perp dA}{V_P}$$

in which ahol A_k a cella oldalfalainak indexe. The surface integral for one face is a scalar product:

$$\int_{A_k} u_\perp dA = \sum_{i=1}^{3} u_i dA_i$$

in which u_i is one component of u interpolated to the cell surface.

Gradient

A direct consequence of the Gauss-Ostrogradskij theorem:

$$\int_V \nabla \phi\, dV = \oint_A \phi \cdot d\,\underline{A}$$

The i-th component of the approximate gradient can be evaluated according to the following expression:

$$\tilde{\nabla}\Big|_i \phi = \frac{\sum_k \int_{A_k} \phi dA_i}{V_P}$$

A_i is the i-th component of the surface vector in Descartes system.

The approximate Laplacian

$$\Delta\phi = \nabla \cdot \nabla \phi$$

When calculating the discrete approximation of the operator the gradient must be interpolated onto the face centroids. This is denoted by < > in the following formula:

$$\tilde{\Delta}\phi = \tilde{\nabla} \cdot \left\langle \tilde{\nabla}\Big|_i \phi \right\rangle$$

For most field variables - excepting for the pressure field – the face normal component of the gradient vector can be calculated on a more simple way: from ϕ values stored in the centers of the adjacent cells.
In this case the discrete form of the Laplacian operator can be calculated as a linear combination of ϕ_P and the neighboring ϕ values:

$$\tilde{\Delta}\phi = A_P\, \phi_P + \sum A_\ell\, \phi_\ell$$