Numerical approximations of derivatives and integralls

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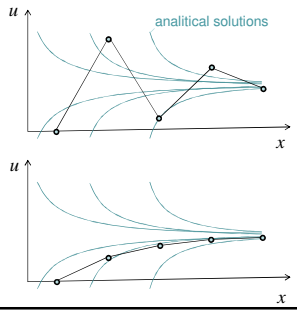
Different behavior…

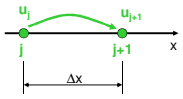
Physical processes lead to a temporal equilibrium in many cases.



Explicit Euler method:

Implicit Euler method:

Euler method



From the Taylor polynomial we can express a differencing scheme of first order accuracy:

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

Note that, the error term is one degree of magnitude higher.

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.

When the differencial equation is given in the explicit form:

$$u'_j = f(u_j, x_j)$$

we can integral step by step, by assuming:

$$u_{j+1} \cong u_j + f(u_j, x_j)\Delta x$$

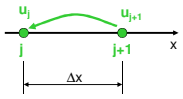
CDS

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

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

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

Bacward Euler method



When F is evaluated in j+1, we may end up with a more complicated expression for u_{j+1}. This kind of discretization is called implicit.

Another first order scheme:

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

from the backward Euler scheme we get:

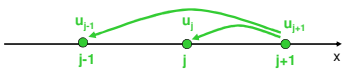
$$u'_{j+1} = \frac{u_{j+1} - u_j}{\Delta x} + o(1)$$

Now, we assume the differential equation in the form:

$$F(u'_{j+1}, u_{j+1}, x_{j+1}) = 0$$

$$F\left(\frac{u_{j+1} - u_j}{\Delta x}, u_{j+1}, x_{j+1}\right) \cong 0$$

An implicit differencing scheme with second order accuracy



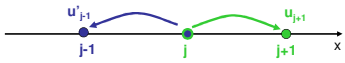
$$u_j = u_{j+1} + u'_{j+1}(-\Delta x) + u''_{j+1}\frac{\Delta x^2}{2} + o(\Delta x^2)$$

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

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

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

Adams-Basforth scheme



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

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

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

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

Approximation of the divergence operator

From the volume integral of the divergence operator we can obtain the cell average of the divergence term.
The Gauss-Ostrogradskij theorem for a vector quantity $\underline{u}$:

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

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

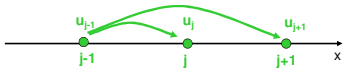
$$\tilde{\nabla} \cdot u_i = \frac{\sum_k \int_{A_k} u_\perp dA}{V_P}$$

in which A_k are the faces of the cell. The surface integral for each 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 $\underline{u}$ interpolated to the cell surface.

A 2 step 2nd order explicit Runge-Kutta type scheme



1st step: Use the Euler method for geting into point j:

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

Evaluate the derivative in point j:

$$d = f(u_j + o(\Delta x), x_j) = f(u_j, x_j) + o(\Delta x) = u'_j + o(\Delta x)$$

2nd step: Use CDS scheme around point j:

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

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.

Spatial derivatives in finite volume methods

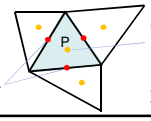
The generic transport equation in integral form:

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

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...

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:

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

In which A_P are constant values, depending only on the mesh parameters.