Numerical approximations of derivatives and integralls

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Finite difference method error and convergence

We shall calculate the change of exact solution U(x) by integrating the derivative on section x_{j+1}-x_j=Δx :

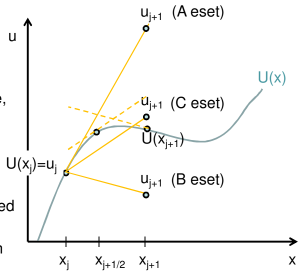
A) from the initial derivative,
B) from the terminal derivative,
C) from midpoint derivative.

The values of the approximate solution are: u_j, u_{j+1}…

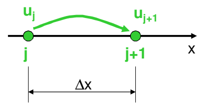
The approximation error $U(x_{j+1})$-u_{j+1} reduces with reduced intervalsize.

Some schemes are better than the other...

XLS demo



Forward Differencing Scheme (FDS)



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 exact solution from point j to point j+1:

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

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

This is an integration scheme of first order accuracy.

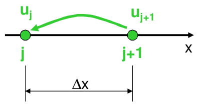
When the differencial equation is given in the explicit form:

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

we can integral step by step, by assuming:

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

Backward Differencing Scheme (BDS), implicit discretisation method



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 is given in the following form:

$$F(u', u, x) = 0$$

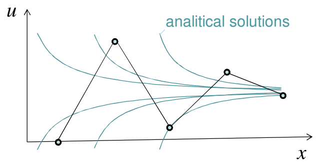
When F is evaluated in j+1, we may end up with a more complicated expression for u_{j+1}. This kind of discretization is called implicit:

unknown

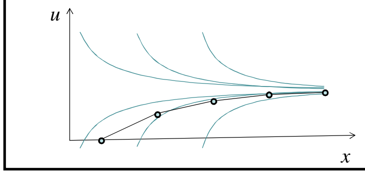
$$F(u'_{j+1}, u_{j+1}, x_{j+1}) = 0 \longrightarrow F\left(\frac{u_{j+1} - u_j}{\Delta x}, u_{j+1}, x_{j+1}\right) \cong 0$$

Different behavior…

Physical processes lead to a temporal equilibrium in many cases.

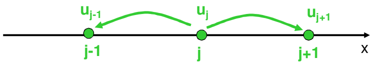


Explicit Euler method:



Implicit Euler method:

Central Differencing Scheme (CDS)



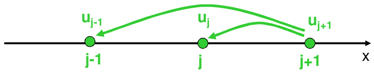
$$u_{j+1} = u_j + u'_j \Delta x + u''_j \frac{\Delta x^2}{2} + o(\Delta x^2)$$

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

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

Extensively used **in CFD for spatial discretization**.

An implicit differencing scheme with second order accuracy



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

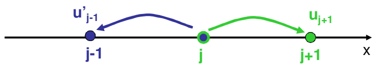
$$u_{j-1} = u_{j+1} + u'_{j+1}(-2\Delta x) + u''_{j+1}2\Delta x^2 + o(\Delta x^2)$$

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

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

Can be used for discretizing the **boundary layer equation**.

Adams-Basforth scheme



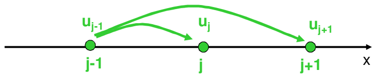
$$u_{j+1} = u_j + u'_j\Delta x + u''_j\frac{\Delta x^2}{2} + o(\Delta x^2)$$

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

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

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

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



1st step: Using the Euler method we can calculate approximate values: $\tilde{u}_j$ and $\tilde{u}'_j$

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

$$u'_j = f(u_j, x_j) = f(\tilde{u}_j + o(\Delta x), x_j) = f(\tilde{u}_j, x_j) + \left.\frac{\partial f}{\partial u}\right|_{u_j, x_j} \cdot o(\Delta x) = \tilde{u}'_j + o(\Delta x)$$

2nd step: Use CDS scheme around point j:

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

Can be used for calculating compressible flows (**eg. Lax-Wendroff method**).

Further important properties of numerical methods

1. **Consistency** The discretization of a PDE should become exact as the mesh size tends to zero (truncation error should vanish)
2. **Stability** Numerical errors which are generated during the solution of discretized equations should not be magnified
3. **Convergence** The numerical solution should approach the exact solution of the PDE and converge to it as the mesh size tends to zero
4. **Conservation** Underlying conservation laws should be respected at the discrete level (artificial sources/sinks are to be avoided)
5. **Boundedness** Physical quantities like densities, temperatures, concentrations etc. should remain nonnegative and free of spurious wiggles

These properties must be verified for each (component of the) numerical scheme.

Discretization of the Navier-Stokes equation is rather difficult on this way…

$$\frac{\partial\rho}{\partial t}+\frac{\partial\rho u}{\partial x}+\frac{\partial\rho v}{\partial y}+\frac{\partial\rho w}{\partial x}=0$$

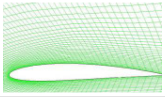
$$\frac{\partial\rho u}{\partial t}+\frac{\partial\rho u^2}{\partial x}+\frac{\partial\rho uv}{\partial y}+\frac{\partial\rho uw}{\partial y}=-\frac{\partial p}{\partial x}+\rho g_x+\frac{\partial}{\partial x}\left(\mu\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial u}{\partial z}\right)$$

$$\frac{\partial\rho v}{\partial t}+\frac{\partial\rho vu}{\partial x}+\frac{\partial\rho v^2}{\partial y}+\frac{\partial\rho vw}{\partial y}=-\frac{\partial p}{\partial y}+\rho g_y+\frac{\partial}{\partial x}\left(\mu\frac{\partial v}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial v}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial v}{\partial z}\right)$$

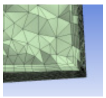
$$\frac{\partial\rho w}{\partial t}+\frac{\partial\rho wu}{\partial x}+\frac{\partial\rho wv}{\partial y}+\frac{\partial\rho w^2}{\partial y}=-\frac{\partial p}{\partial z}+\rho g_z+\frac{\partial}{\partial x}\left(\mu\frac{\partial w}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial w}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial w}{\partial z}\right)$$

In some cases more complex meshes are necessary for efficient solution

Curvilinear, stretched

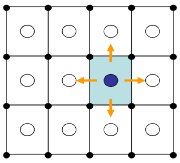


Unstructured, hybrid



Finite volume method

Discrete solution



U: volume intensity of an arbitrary conserved quantity.

$$\frac{\partial}{\partial t}\int_V U\,dV+\oint_A \vec{F}\cdot d\vec{A}=\int_V S_V\ dV+\oint_A \vec{S}_A\cdot d\vec{A}$$

The conserved quantity per init mass of fluid:

$$\Phi=U/\rho$$

Convective and conductive fluxes:

$$\vec{F}_C=\rho\Phi\vec{v} \qquad \vec{F}_D=-\Gamma\nabla\Phi$$

$$\frac{\partial}{\partial t}\int_V \rho\Phi\,dV+\oint_A \rho\Phi\,\vec{v}\cdot d\vec{A}=\oint_A(\Gamma\nabla\Phi+\vec{S}_A)\cdot d\vec{A}+\int_V S_V\ dV$$

Fluxes are evaluated on the element faces.
Finite volume method is conservative: discretization errors do not produce or destroy conserved physical properties. Conservation equations are exactly fulfilled on the computational domain.

Spatial derivatives in finite volume methods

The generic transport equation in integral form:

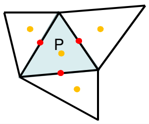
$$\frac{\partial \rho\phi}{\partial t} + \nabla \cdot (\rho \phi \vec{v}) = \nabla \cdot \vec{S}_A + \nabla \cdot (\Gamma \nabla \phi) + S_v$$

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:

Coordinates of face vector separating the ℓ^{th} neighbor are represented by $dA_{\ell,i}$, in which i=1,2,3 (for x,y,z).



● Cell centroid.
Here we store ϕ_P.

● Face centroid.
We need to interpolate here from the centers.

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 u:

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

The discrete representation of the divergence term is defined as a volume average over element P:

$$\tilde{\nabla} \cdot u_i = \frac{\sum_{\ell} \sum_{i=1}^{3} u_{\ell,i} dA_{\ell,i}}{V_P}$$

$u_{\ell,i}$ are Descartes coordinates of vector u being **interpolated** to face centroids. This expression is a linear combination of u values stored in P and in neighboring cells.

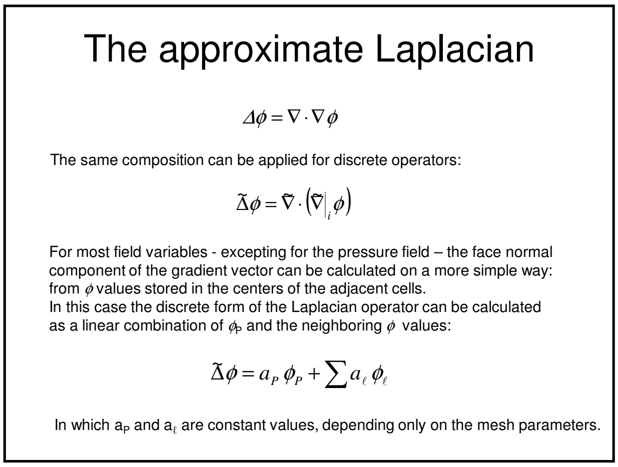
Gradient

A direct consequence of the Gauss-Ostrogradskij theorem:

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

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

$$\tilde{\nabla}\Big|_i \phi = \frac{\sum_{\ell} \phi_\ell\, dA_{\ell,i}}{V_P}$$



The approximate Laplacian

$$\mathit{\Delta}\phi = \nabla \cdot \nabla \phi$$

The same composition can be applied for discrete operators:

$$\tilde{\Delta}\phi = \tilde{\nabla} \cdot \left(\tilde{\nabla}\big|_i \phi\right)$$

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 and a_ℓ are constant values, depending only on the mesh parameters.