Finite volume discretization

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Discretization of the Navier-Stokes equation

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

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

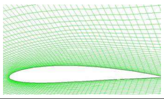
$$\frac{\partial \rho v}{\partial t}+\frac{\partial \rho vu}{\partial x}+\frac{\partial \rho v^2}{\partial y}+\frac{\partial \rho vw}{\partial y}=-\frac{\partial p}{\partial y}+\rho g_y+\frac{\partial}{\partial x}\left(\mu\frac{\partial v}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial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

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

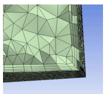
It might be discretized with finite differencing schemes on an equidistant Cartesian mesh, however...

sometimes, more complex meshes are necessary for efficient solution

Curvilinear, stretched

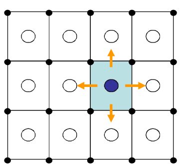


Unstructured, hybrid



The generic conservation law

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:

$$\Phi = \mathrm{U}/\rho$$

Convective and conductive fluxes:

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

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

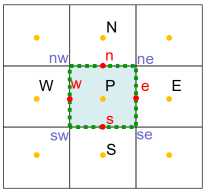
Fluxes are **evaluated** on the element faces.
Finite volume method is conservative: discretization errors do not produce or destroy conserved physical properties. Conservation equations are exactly fulfilled on the computational domain.

Approximation of surface integrals and volume integrals

$$\underbrace{\frac{\partial}{\partial t}\int_V \rho\Phi\, dV}_{\text{Volume integrals}} + \underbrace{\oint_A \rho\Phi\,\bar{v}\cdot d\bar{A}}_{\text{Surface integrals}} = \underbrace{\oint_A (\Gamma\nabla\Phi + \bar{S}_A)\cdot d\bar{A}}_{\text{Surface integrals}} + \underbrace{\int_V S_V\, dV}_{\text{Volume integrals}}$$

$$F_e = \int_A \vec{f}\cdot d\vec{A} = \langle f_\perp \rangle_e A_e \cong \frac{1}{2}\left(\vec{f}_P + \vec{f}_E\right)_\perp A_e$$ 2-nd order accurate

Compass notation:



Alternative surface integration schemes:

$$F_e \cong A_e \frac{1}{2}\left(\vec{f}_{ne} + \vec{f}_{se}\right)_\perp$$ 2-nd order accurate (trapeze method)

$$F_e \cong \frac{A_e}{6}\left(\vec{f}_{ne} + 4\vec{f}_e + \vec{f}_{se}\right)_\perp$$ 4-th order accurate (Simpson formula)

$$Q_P \cong \int_V q_\phi dV \cong q_{\phi,P} V_P$$ 2-nd order accurate

Interpolation of the fluxes must be at least as accurate as the integration scheme.

Finite volume approximation of spatial derivatives

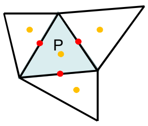
The generic transport equation can be also expressed in differential form:

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

Spatial derivatives are always in **div(...)**, **grad(...)** or **div(grad(...))** forms.

We only need to look for the discrete approximations of these operators.

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. Field variables are stored in this points.
- Face centroid. We need to interpolate here from the centroids.

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 an arbitrary vector quantity:

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

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.

Approximation of the gradient operator

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:

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

Approximation of the Laplacian operator

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

The same composition can be applied for discrete operators:

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

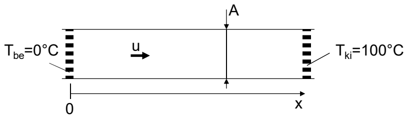
For most field variables - excepting for the pressure field – the face normal component of the gradient vector can be calculated on a more simple way: from ϕ values stored in the centers of the adjacent cells.
In this case the discrete form of the Laplacian operator can be calculated as a linear combination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

Application in 1D

Steady flow of a constant density fluid with heat conduction in a constant cross-section pipe

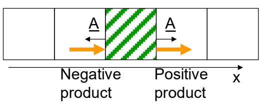


$$\underline{v} = \begin{pmatrix} u \\ v \\ w \end{pmatrix} \begin{matrix} \\ \leftarrow 0 \\ \leftarrow 0 \end{matrix}$$

Continuity: $\oint_A \rho\,\underline{v}\cdot d\underline{A} = 0 \longrightarrow \frac{\partial\,\rho u}{\partial x} = 0 \xrightarrow{\rho=\text{const.}}$ u = constant

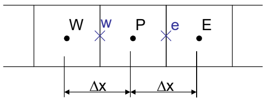
Energy equation: $\oint_A [\,c_v T + \cancel{\frac{u^2}{2}}\,]\,\rho\,\underline{v}\cdot d\underline{A} = \oint_A \lambda\nabla T\cdot d\underline{A}$

Applied for one cell:
by assuming fluxes in +x direction



Discretization

$$\oint_A \rho u T \cdot dA_x = \oint_A \frac{\lambda}{c_v}\frac{\partial T}{\partial x} \cdot dA_x$$



The numerical integral of fluxes:

$$(\rho u T)_e \cancel{A} - (\rho u T)_w \cancel{A} = \left(\frac{\lambda}{c_v}\frac{\partial T}{\partial x}\right)_e \cancel{A} - \left(\frac{\lambda}{c_v}\frac{\partial T}{\partial x}\right)_w \cancel{A}$$

Shorthand notations: $C_e = C_w = \rho u \qquad D_e = D_w = \dfrac{\lambda}{c_v \Delta x}$

$$C_e T_e - C_w T_w = D_e (T_E - T_P) - D_w (T_P - T_W)$$

... in a more simple form: $F_e - F_w = 0$,

in which: $F_e = C_e T_e - D_e (T_E - T_P)$ in the total flux.

In a 3D case we would have 4 more F values.

Application of the CDS scheme

$$C_e T_e - C_w T_w = D_e (T_E - T_P) - D_w (T_P - T_W)$$

Face temperatures (T_e and T_w) are obtained by a **linear interpolation**:

$$\left[\frac{C_e}{2}(T_P + T_E) - D_e (T_E - T_P)\right] - \left[\frac{C_w}{2}(T_W + T_P) - D_w (T_P - T_W)\right] = 0$$

The resultant linear equation for T_P:

$$A_P T_P = A_W T_W + A_E T_E$$

A_W	A_E	A_P
$D_w + C_w/2$	$D_e - C_e/2$	$A_W + A_E$

$$D_e + D_w + C_e/2 - C_w/2 = A_E + A_W + \underbrace{C_e - C_w}_{=0 \text{ continuity}}$$

Since $A_P = A_W + A_E$, the linear equation for A_P can be regarded as a weighted average of the neighboring T values. T_P cannot be an extreme value, if the „A" values are positive.

Solution of the system of linear algebraic equations

For 4 cells:

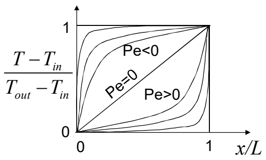
TC() TB() TA() TD()

$$\begin{bmatrix} -A_{1,P} & A_{1,E} & 0 & 0 \\ A_{2,W} & -A_{2,P} & A_{2,E} & 0 \\ 0 & A_{3,W} & -A_{3,P} & A_{3,P} \\ 0 & 0 & A_{4,W} & -A_{4,P} \end{bmatrix} \cdot \begin{bmatrix} T_{1,P} \\ T_{2,P} \\ T_{3,P} \\ T_{4,P} \end{bmatrix} = \begin{bmatrix} -A_{1,W} T_{be} \\ 0 \\ 0 \\ -A_{4,E} T_{ki} \end{bmatrix}$$

We can solve this system by Gauss elimination.
The matrix of the linear system is a tridiagonal matrix which requires only 2n operations in the case of n cells.
(This special case of the Gauss elimination is called the Thomas algorithm).

Unfortunately, such an efficient direct solution is not possible in 2D and 3D (iterative methods must be applied).

Analytical solution



$$\frac{T-T_{in}}{T_{out}-T_{in}}=\frac{e^{\rho u x c_v/\lambda}-1}{e^{\rho u L c_v/\lambda}-1}$$

Pe (Peclet number)

Depending on context, the same equation can be called the
- convection-diffusion equation,
- advection–diffusion equation,
- drift–diffusion equation,
- Smoluchowski equation, or
- (generic) scalar transport equation.

Implementation in Excel macro

1. Similar solution is obtained with different input parameters.
2. The error reduces with N^2. (Second order accuracy.)
3. Sometimes the solution oscillates. What is the condition for the onset of instabilities?

$$Pe=\frac{\rho u L}{\lambda/c_v}$$

$$Re=\frac{\rho u L}{\mu}$$

$$Pe_{\Delta x}=\frac{\rho u \Delta x}{\lambda/c_v}>2$$

Transportivity

By physical means:
T_E must have a decreasing affect on T_P for an increasing value of Pe, because the heat conduction is overridden by the adverse convective flux.
Does the numerical scheme behaves so?

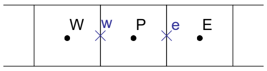
$$A_E=D_e-C_e/2$$

$$C_e=\rho u \qquad D_e=\frac{\lambda}{c_v\,\Delta x} \qquad Pe=\frac{\rho u L}{\lambda/c_v}$$

$$A_E=\frac{D_e}{2}\left(2-\frac{C_e}{D_e}\right)=\frac{D_e}{2}\left(2-\frac{\rho u \Delta x}{\lambda/c_v}\right)=\frac{D_e}{2}\left(2-Pe_{\Delta x}\right)$$

The cell Peclet number is the ratio of convective and conductive heat fluxes.
In the case of $Pe_{\Delta x}>>2$ the value of A_E can be a very large negative value.
This is not sensible from physical point of view.
This case is also numerically unstable.

Upwind Differencing Scheme (UDS)



for u>=0: $T_w = T_W,\quad T_e = T_P$

for u<0: $T_w = T_P,\quad T_e = T_E$

$$A_W T_W + A_E T_E = A_P T_P$$

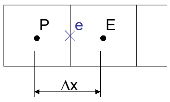
A_W	A_E	A_P
$Max(C_w,0)+D_w$	$Max(-C_e,0)+D_e$	$A_W + A_E$

Further numerical experiments...

Accuracy reduced to 1-st order.

Artificial diffusion

An important source of numerical errors. It came from the inaccurate interpolation:



$$T_e = T_P + \frac{\Delta x}{2}\frac{dT}{dx} + o(\Delta x)$$

we neglect these

$$F_e = C_e T_P + C_e \frac{\Delta x}{2}\frac{dT}{dx} - D_e (T_E - T_P)$$

It is like if the heat conductivity grew.
Let's substitute the numerical approximation of the temperature gradient:

$$\frac{dT}{dx} = \frac{T_E - T_P}{\Delta x}$$

$$F_e = C_e T_P + \frac{C_e}{2}(T_E - T_P) - D_e (T_E - T_P)$$

$$D_e = \frac{\lambda}{c_v \Delta x} \longrightarrow \frac{\lambda_{artif.}}{c_v \Delta x} = \frac{\rho u}{2} \longrightarrow \lambda_{artif.} = \frac{\rho u c_v \Delta x}{2}$$

Hybrid Differencing Scheme (HDS)

by Spalding (1972)
The positivity of the "A"s must be ensured.
We need to apply unwinding only if the absolute value of $Pe_{\Delta x}$ is too high.:

$Pe_{\Delta x} \le -2$ $\quad F_e = C_e T_E$

$-2 < Pe_{\Delta x} \le 2$ $\quad F_e = C_e \left[\frac{1}{2}\left(1 + \frac{2}{Pe_{\Delta x}}\right) T_P + \frac{1}{2}\left(1 - \frac{2}{Pe_{\Delta x}}\right) T_E \right]$

$2 < Pe_{\Delta x}$ $\quad F_e = C_e T_P$

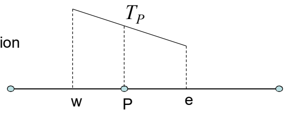
It is of second order accuracy for conduction dominated problems. (For small $Pe_{\Delta x}$ cases.)

$$A_W T_W + A_E T_E = A_P T_P$$

A_W	A_E	A_P
$Max\left(C_w, \left[D_w + \frac{C_w}{2}\right], 0\right)$	$Max\left(-C_e, \left[D_e - \frac{C_e}{2}\right], 0\right)$	$A_W + A_E$

Second Order Upwinding (SOU)

We can interpolate T within the simulation cell by using its gradient:



Wall fluxes than can be than evaluated like: $$T_e = T_P + \left.\frac{dT}{dx}\right|_P \frac{\Delta x}{2}$$

Gradients are calculated in 2 steps:

Firstly: $$\left.\frac{dT}{dx}\right|_P = \frac{T_e' - T_w'}{\Delta x} \qquad T_e' = \frac{T_P + T_E}{2}, \qquad T_w' = \frac{T_W + T_P}{2}$$

Secondly: $\left.\frac{dT}{dx}\right|_P$ gradients are limited on such a way that they shouldn't introduce oscillations. For details on the gradient limiters please refer: C Hirsch, Numerical computation of internal and external flows.

The numerical diffusion in practice

2D heat transport with zero heat conductivity (λ=0).