Finite volumes to go

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Abstract

A minimalistic implementation of a cell centered finite volume method is presented. Upwind formulation of the convective term is applied to stabilize the algorithm in the case of convection dominance. The explicit one-step method is employed in the transient case. The discretization on unregular meshes is outlined.

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1 Convection-diffusion Model

The discretization of the general convection-diffusion model employing a cell-centered finite volume method is considered

$$\underbrace{\int_\Omega \frac{\partial}{\partial t}(\varrho\, u)\, dV}_{rate\ of\ change} = \int_\Gamma \vec{J}\cdot(-\hat{n})\, dA + \underbrace{\int_\Omega f\, dV}_{source} \tag{1}$$

where $\vec{J}$ is the general flux

$$\vec{J} = \underbrace{-\varepsilon \ \text{grad}\ u}_{diffusion} + \underbrace{\varrho\,\vec{v}\,u}_{convection} \tag{2}$$

V the volume, A the area, $\hat{n}$ the outwards pointing normal, t the temporal variable, ϱ the density, $u(x,t)$ the general dependent variable, x the spatial variable, ε the general diffusion coefficient and $\vec{v}$ the velocity.

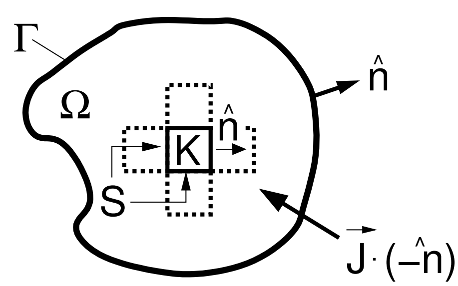


Figure 1: Integral balance

2 Structured meshes

2.1 Regular mesh, steady state

Concept

- rectilinear discretization (linear mesh spacing) of domain $\Omega = L_x \times L_y$ in a finite number of cells K with cell faces S

$$\begin{aligned} K_{i,j} &= \Delta x \times \Delta y \qquad i = 1\,..\,N_x,\ j = 1\,..\,N_y && (3)\\ \Delta x &= L_x \,/\, N_x && (4)\\ \Delta y &= L_y \,/\, N_y && (5)\end{aligned}$$

and of the time interval $[\,0,\, t_{max}\,]$ in time steps Δt

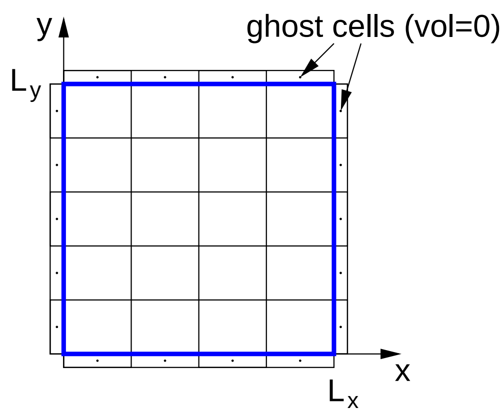


Figure 2: Spatial discretization

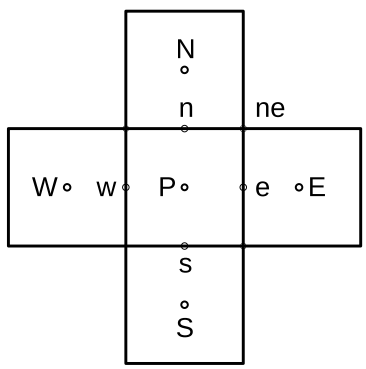


Figure 3: Mesh points of cell-molecule related to current cell

- constant material properties
- discretization of the fluxes trough interfaces between neighbor cells and trough boundary Γ
  - linear approximation of the gradient of u in the diffusion part
  - upwind formulation of the convective part
- mid point integration of all volume and surface integrals

Geometric data

The volume V of cell $K_{i,j}$ is represented by $(\Delta x \times \Delta y \times 1)$ and its areas $A_w = A_e$ and $A_s = A_n$ by $(\Delta y \times 1)$ or $(\Delta x \times 1)$, respectively. The cell center coordinates (x_i, y_j) and the location of the cell vertices $(x_{e,i}\,,\, y_{n,j})$ are defined as

$$x_{e,i} = \Delta x \cdot i, \qquad i = 0..N_x + 1 \tag{6}$$

$$y_{n,j} = \Delta y \cdot j, \qquad j = 0..N_y + 1 \tag{7}$$

$$x_i = x_{e,i} - \Delta x\,/\,2, \qquad i = 0..N_x + 1 \tag{8}$$

$$y_j = y_{n,j} - \Delta y\,/\,2, \qquad j = 0..N_y + 1 \tag{9}$$

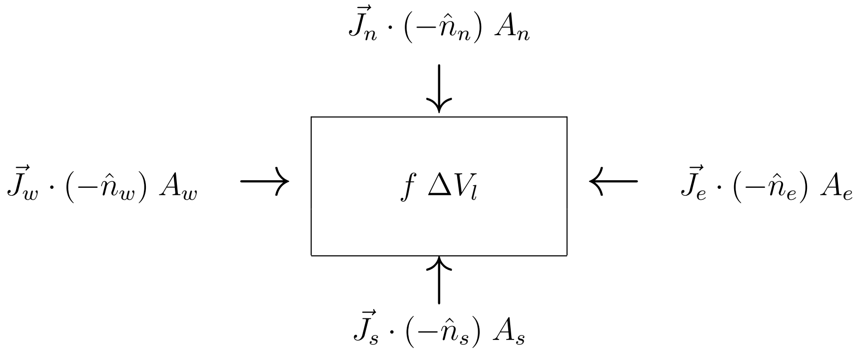


Figure 4: Balance over cell in steady state in 2D space

Balance over every cell K in compass coordinates

$$a_P\, u_P \;+\; a_W\, u_W \;+\; a_E\, u_E \;+\; a_S\, u_S \;+\; a_N\, u_N \;=\; b \tag{10}$$

with the following matrix and vector coefficients[1], c.f. Fig. 4 :

$$\dot{M}_w \;=\; \varrho\, v_w\, \Delta y \tag{11}$$

$$\dot{M}_e \;=\; \varrho\, v_e\, \Delta y \tag{12}$$

$$\dot{M}_s \;=\; \varrho\, v_s\, \Delta x \tag{13}$$

$$\dot{M}_n \;=\; \varrho\, v_n\, \Delta x \tag{14}$$

$$a_W \;=\; -\,\varepsilon_w\, \Delta y \,/\, (x_P - x_W) + \;\min\,(\,\dot{M}_w,\, 0\,) \tag{15}$$

$$a_E \;=\; -\,\varepsilon_e\, \Delta y \,/\, (x_E - x_P) + \;\min\,(\,\dot{M}_e,\, 0\,) \tag{16}$$

$$a_S \;=\; -\,\varepsilon_s\, \Delta x \,/\, (y_P - y_S) + \;\min\,(\,\dot{M}_s,\, 0\,) \tag{17}$$

$$a_N \;=\; -\,\varepsilon_n\, \Delta x \,/\, (y_N - y_P) + \;\min\,(\,\dot{M}_n,\, 0\,) \tag{18}$$

$$a_P \;=\; -\,(\,a_W \,+\, a_E \,+\, a_S \,+\, a_N\,) \,+\, \dot{M}_w \,+\, \dot{M}_e \,+\, \dot{M}_s \,+\, \dot{M}_n \tag{19}$$

$$b \;=\; f(x_P, y_P)\; \Delta x\, \Delta y \tag{20}$$

Solution of equation system employing successive overrelaxation

$u^{prev} \;=\; u^{init} +$ boundary conditions

repeat

    for $i = 1$ to N_x do

        for $j = 1$ to N_y do

            $u_P \;=\; (1-\omega)\, u_P^{prev} \;+\; \omega\; (-a_W u_W^{prev} - a_E u_E^{prev} - a_S u_S^{prev} - a_N u_N^{prev} + b) \;/\; a_P$

    $u^{prev} \;=\; u$

until $||\, u \,-\, u^{prev}\, || \,<\, \epsilon$

[1] $v_w,\, v_e,\, v_s,\, v_n$ are the velocities in direction of the outwards pointing normal. Consequently is $v_w = -v_x(x_w, y_P)$ and $v_e = +v_x(x_e, y_P)$

2.2 Regular mesh, transient

Modification of coefficients

$$a_P^* = a_P + \frac{\varrho}{\Delta t}\,\Delta x\,\Delta y \tag{21}$$

$$b^* = b + \frac{u_P^{past}\,\varrho}{\Delta t}\,\Delta x\,\Delta y \tag{22}$$

Explicit solution of equation system

$u^{past} = u(\,t = 0\,) +$ boundary conditions

$t = 0$

repeat

  $t = t + \Delta t$

  for $i = 1$ to N_x do

    for $j = 1$ to N_y do

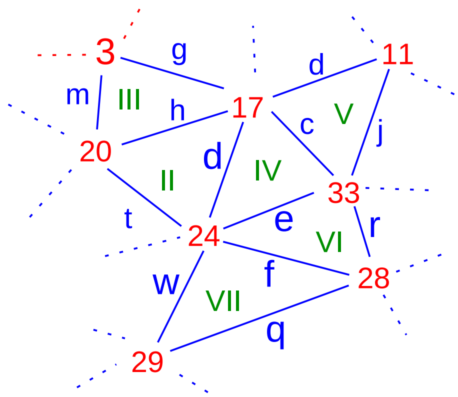
      $u_P = \left(-a_W\,u_W^{past} - a_E\,u_E^{past} - a_S\,u_S^{past} - a_N\,u_N^{past} + b^*\right) / a_P^*$

  $u^{past} = u$

until $t \geq t_{end}$

Note: The explicit Θ-one-step method is unstable if the time step size exceeds a critical size. For instance, for a pure diffusion problem is the theoretical limit

$$\Delta t_{min} = \frac{\min\left(\Delta x^2,\ \Delta y^2\right)}{2\,\max\varepsilon} \tag{23}$$



cell list

⋮	⋮	⋮	⋮
III	20	17	3
IV	24	33	17
V	11	17	33
VI	28	33	24
VII	28	24	29
⋮	⋮	⋮	⋮

face list

⋮	⋮	⋮
c	V	IV
d	II	IV
e	VI	IV
f	VI	VII
⋮	⋮	⋮

Figure 5: Cell list vs. face list

3 Unstructured Meshes

Connectivity

This section deals with an extension of Sec. 2 for unstructured meshes. Because of the irregular connectivity

$$\text{vertices} \iff \text{cells},$$

two additional pointer arrays

- cell list
- face list

have to be generated (c.f. Fig. 5) to describe the spatial discretization of the domain

$$\Omega = \bigcup_{l=0}^{N_K-1} K_l \tag{24}$$

where N_K is the number of cells. Every cell K_l can have the shape of any polygon or polyhedra with a number of faces $N_{l,S} > 2$ in 2D or $N_{l,S} > 3$ in 3D space). Consequently, the integration of the cell surface $\partial K_l = S_l$ reads as

$$S_l = \sum_{m=0}^{N_{l,S}-1} S_{l,m} \tag{25}$$

Mid point integration of surface and volume integrals

$$\sum_l \left(\frac{\partial}{\partial t} (\varrho u) \, \Delta V_l \right) = \sum_l \left(\sum_m \vec{J}_{l,m} \cdot (-\hat{n}_{l,m}) \, A_{l,m} \right) + \sum_l \left(f_l \, \Delta V_l \right) \tag{26}$$

Splitting of volume-specific source

$$f = f^C + f^P \, u \tag{27}$$

Linear approximation of the diffusion part of $\vec{J}$ and upwind discretization of the convective part

$$\vec{J}_{l,m} \cdot (-\hat{n}_{l,m}) = +\varepsilon_{l,m} \left.\frac{\partial u}{\partial n}\right|_{l,m} - \varrho_{l,m}\, v_{l,m}\, u_{l,m} \tag{28}$$

$$\begin{aligned} \vec{J}_{l,m} \cdot (-\hat{n}_{l,m}) &= +\varepsilon_{l,m}\,(Pe_{l,m})\, \frac{u_{l,M} - u_l}{|\vec{L}_{l,m}|} \\ &\quad - \varrho_{l,m}\, v_{l,m}\, \langle v_{l,m} < 0 \rangle\, u_{l,M} + \varrho_{l,m}\, v_{l,m}\, \langle v_{l,m} > 0 \rangle\, u_l \end{aligned} \tag{29}$$

where $\langle \cdot \rangle$ is a boolean expression

$$\langle \text{ condition } \rangle = \begin{cases} 1 & : \text{ if condition is true} \\ 0 & : \text{ otherwise} \end{cases} \tag{30}$$

and[2]

$$l = \text{index of cell}$$

$$m = \text{indices of faces of cell}$$

$$M = \text{indices of cell neighbors corresponding to } m$$

$$\vec{P}_l = (x_l, y_l, z_l)^T \tag{31}$$

$$\vec{P}_{l,m} = (x_{l,m}, y_{l,m}, z_{l,m})^T \tag{32}$$

$$\vec{L}_{l,m} = \vec{P}_{l,M} - \vec{P}_l \tag{33}$$

$$\vec{l}_{l,m} = \vec{P}_{l,m} - \vec{P}_l \tag{34}$$

$$\bar{A}_{l,m} = \vec{A}_{l,m} \cdot \hat{L}_{l,m} = A_{l,m}\, \hat{n}_{l,m} \cdot \hat{L}_{l,m} \tag{35}$$

$$u_{l,m} = u_l + (u_{l,M} - u_l)\, \frac{|\vec{l}_{l,m}|}{|\vec{L}_{l,m}|} \tag{36}$$

$$\dot{M}_{l,m} = \varrho_{l,m}\,(\vec{P}_{l,m}, u_{l,m}, t)\; v_{l,m}\,(\vec{P}_{l,m}, u_{l,m}, t)\; \bar{A}_{l,m} \tag{37}$$

$$D^0_{l,m} = \frac{\varepsilon_{l,m}\,(\vec{P}_{l,m}, u_{l,m}, t)}{|\vec{L}_{l,m}|}\, \bar{A}_{l,m} \tag{38}$$

$$Pe_{l,m} = \left| \frac{\dot{M}_{l,m}}{D^0_{l,m}} \right| \tag{39}$$

$$\delta^*(Pe) = \begin{cases} 1 & : \text{ if upwind} \\ \max\,\{1 - 0.5\,Pe,\, 0\} & : \text{ if hybrid} \\ \max\,\{1 - 0.1\,Pe^5,\, 0\} & : \text{ if power law} \end{cases} \tag{40}$$

$$D_{l,m} = D^0_{l,m}\, \delta^*(\,Pe_{l,m}\,) \tag{41}$$

[2]The velocity $v_{l,m}$ is the component of $\vec{v}$ in the direction of the outwards pointing normal of the cell face: $v_{l,m} = \vec{v}\,(\vec{P}_{l,m}) \cdot (-\hat{n}_{l,m})$

$$\tau \;=\; \begin{cases} \varrho\,(\vec{P}_l, u_l, t)\,/\,\Delta t & : \text{ if transient} \\ 0 & : \text{ otherwise} \end{cases} \tag{42}$$

One-step time integration (fully implicit)

$$\sum_l \varrho_l\,(u_l \,-\, u_l^{past})\,\Delta V_l \;=\; \sum_l \Bigg[\;\; \textstyle\sum_m \left\{ \begin{array}{l} \varepsilon_{l,m}(Pe_{l,m})\,(u_M \,-\, u_l)\,/\,|\vec{L}_{l,m}| \\ -\,\varrho_{l,m}\,v_{l,m}\,\langle v_{l,m} > 0\rangle\,u_l \\ -\,\varrho_{l,m}\,v_{l,m}\,\langle v_{l,m} < 0\rangle\,u_{l,M} \end{array} \right\} (\vec{A}_{l,m}\cdot\hat{L}_{l,m})$$
$$+ \quad (f_l^C \,+\, f_l^P\,u_l)\,\Delta V_l \;\Bigg]\,\Delta t \tag{43}$$

Re-arrangement in matrix form

$$u_l\,\left\{(-f^P(\vec{P}_l, u_l, t) \,+\, \tau)\,V_l \,+\, \sum_{l,m}(D_{l,m} \,+\, \langle v_{l,m} > 0\rangle\,\dot{M}_{l,m})\right\}$$
$$+\,\sum_{l,m} u_M\,\left\{-D_{l,m} \,+\, \langle v_{l,m} < 0\rangle\,\dot{M}_{l,m}\right\} \;=\; \left\{(f^C(\vec{P}, u_l, t) \,+\, \tau\,u_l^{past})\,V_l\right\} \tag{44}$$

Location of non-zero elements for a tetrahedron cell matrix with $M = 0..3$

	l	$M=0$	$M=1$	$M=2$	$M=3$
l	•	•	•	•	•
$M=0$	•	•			
$M=1$	•		•		
$M=2$	•			•	
$M=3$	•				•