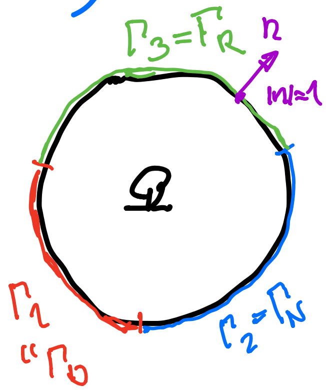
4.2.2.1. The Integral Balance Formulation of Second-Order Elliptic BVP

- Let $\Omega \subset \mathbb{R}^2$ (resp. $\mathbb{R}^d$) be some bounded (*) domain:
$\partial\Omega \in C^{(0,1)} \cap PC^{k}$, $k \geq 2$.

We consider the mixed BVP for the following

Diffusion – Convection – Reaction Eqn.:

$$(23) \quad Lu(x) := -\operatorname{div}(a(x)\nabla u(x)) + b^T(x)\nabla u(x) + c(x)u(x) = f(x)$$



$$a(x) = \begin{bmatrix} a_{11}(x) & a_{12}(x) \\ a_{21}(x) & a_{22}(x) \end{bmatrix} = a^T(x), \quad b(x) = \begin{bmatrix} b_1(x) \\ b_2(x) \end{bmatrix}^{*}, \quad c(x) \geq 0^{*}$$

uniformly p.d $\wedge$ * (i.e. elliptic !)

Special case: isotropic diffusion-reaction

$a(x) = a(x) I$, $b(x) = \mathbb{0}$, $c(x) \geq 0$

+ mixed Boundary Condition (BC):

$$\ell u(x) := \left\{ \begin{matrix} u(x) \\ \frac{\partial u}{\partial N}(x) := (a(x)\cdot\nabla u(x), n(x)) \\ \frac{\partial u}{\partial N}(x) + \varkappa(x)u(x) \end{matrix} \right\} = g(x) := \left\{ \begin{matrix} g_1(x), \ x \in \Gamma_1 \\ g_2(x), \ x \in \Gamma_2 \\ g_3(x), \ x \in \Gamma_3 \end{matrix} \right. \begin{matrix} \Gamma_e \\ \\ \Gamma_n \end{matrix}$$

(23)
$$\boxed{\begin{aligned} Lu(x) &= f(x), \ x \in \Omega \\ \ell u(x) &= g(x), \ x \in \Gamma \end{aligned}}$$

- For all $x \in \overline{\Omega}$, we now define the set

$$\mathcal{B}(x) := \{ B(x) : B \subset \Omega \text{ - open, simply connected, star-shaped domain} : x \in \overline{B},\ \partial B \in C^{0,1} \cap PC^2 \}$$

of all admissible boxes at the point $x \in \overline{\Omega}$, and integrate the PDE $Lu = f$ over $B(x) \in \mathcal{B}(x)$:

$$(24) \quad \int_{B(x)} Lu(y)\,dy = \int_{B(x)} f(y)\,dy \Leftrightarrow \int_{\Omega} Lu \cdot \chi_{B(x)}\,dy = \int_{\Omega} f(y)\,\chi_{B(x)}(y)\,dy$$

test function = characteristic function of the box $B(x)$, i.e.

$$\chi_{B(x)}(y) := \begin{cases} 1, & y \in \overline{B(x)} \\ 0, & \text{otherwise} \end{cases}$$

Partial integration in the main term yields:

$$-\int_{B(x)} \operatorname{div}(a(y)\nabla u(y))\,dy = -\int_{\partial B(x)} \underbrace{(a(y)\nabla u(y), n(y))}_{=: \frac{\partial u}{\partial N} = -\text{flux}}\,ds_y$$

Taking the natural BC on $\partial B_n(x) := \partial B(x) \cap \Gamma_n$, i.e.

$$\frac{\partial u}{\partial N}\Big|_{\partial B_2 := \partial B \cap \Gamma_2} = g_2 \quad \text{and} \quad \frac{\partial u}{\partial N}\Big|_{\partial B_3 := \partial B \cap \Gamma_3} = -\varkappa u + g_3,$$

into account, we immediately obtain the <u>Integral Bilance Form</u>:

$1+\delta$, $\delta > 1/2$

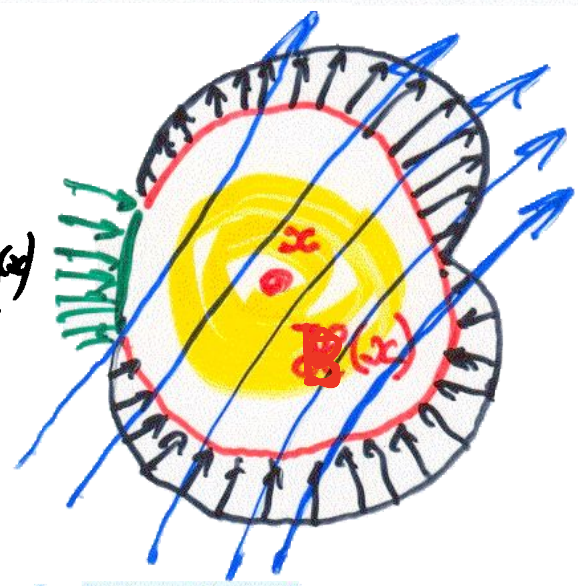
$$(25) \quad \boxed{\begin{array}{l} \text{Find } u \in V_g := \{ v \in V = H^1(\Omega) : v = g_1 \text{ on } \Gamma_1 \} \cap H^2(\Omega): \quad \text{Remark 4.13.1.} \\[1ex] -\int_{\partial B \setminus \partial B_n} (a\nabla u, n)\,ds + \int_B (b, \nabla u)\,dy + \int_B cu\,dy + \int_{\partial B_3} \varkappa u\,ds = \int_B f\,dy + \int_{\partial B_n} g\,ds \\[1ex] \forall \text{ admissible boxes } B = B(x) \in \mathcal{B}(x)\ \forall x \in \Omega \cup \Gamma_n, \\ \text{with given data } f, a, b, c \text{ in } \Omega \text{ and } g \text{ on } \Gamma. \end{array}}$$

Remark 4.13:

1. $u \in V_g \cap W_2^{1+\lambda}(\Omega)$ ensures an integrable trace of $\frac{\partial u}{\partial N} := (a\nabla u, n)$ on ∂B ($\frac{\partial u}{\partial N} \in L_1(\partial B)$!), if $\lambda > 1/2$ and if $a(\cdot)$ and $\partial\mathcal{H}$ are "sufficiently" smooth (Sobolev's embedding theorem on manifolds !).
2. Physical meaning of (25):
   The bilance equation (25) expresses the equilibrium (balance) of the following quantities:

$\mathcal{H} = B$

Total flux through $\partial\mathcal{H} \setminus \partial\mathcal{H}_N$ + input into $\mathcal{H}$ via convection + reaction by solution-dependent sources cu and $\varkappa u$ = total intensity of the sources given by the intensities of the volume sources f in $\mathcal{H}$ and the boundary sources g on $\partial\mathcal{H}_N$ (if $\neq \emptyset$)



→ see Modeling Lectures: Transport Theorem

3. In Section 4.2.2.3, we use the bilance equation (25) in discrete points $x \in \omega = \mathring{\omega} \cup \gamma_2 \cup \gamma_3$ (= primary grid) and special boxes $B(x)$ (= secondary grid) for constructing finite difference schemes on arbitrary triangular, rectangular and combined meshes
4. The generalization to 3D is trivial !

4.2.2.2. Primary and Secondary Grids

- Let us consider a regular triangulation $\mathcal{T}_h = \mathcal{T}_\Delta = \{\delta_r : r \in \mathcal{R}_h\}$ of a given, polygonally bounded domain $\Omega \subset \mathbb{R}^2$ (see also Chapter 3):

$$\Rightarrow \forall h \in \Theta : \quad \overline{\Omega} = \bigcup_{r \in \mathcal{R}_h} \overline{\delta}_r$$

$$\mathcal{T}_\Delta = \{\delta_r : r \in \mathcal{R}_h\} \ni \delta_r$$

$= \text{primary grid}$

$\hat{=}$ FE mesh

$x = x_{\delta_r}(\xi) \in P_1$, $\xi = \xi_{\delta_r}(x)$

$\boxed{\Delta = \Delta = \text{unit triangle}}$

Chapter 3: Def. 3.3

(3.8) $\underline{c}_1 h^2 \le |J_{\delta_r}| \le \overline{c}_1 h^2$

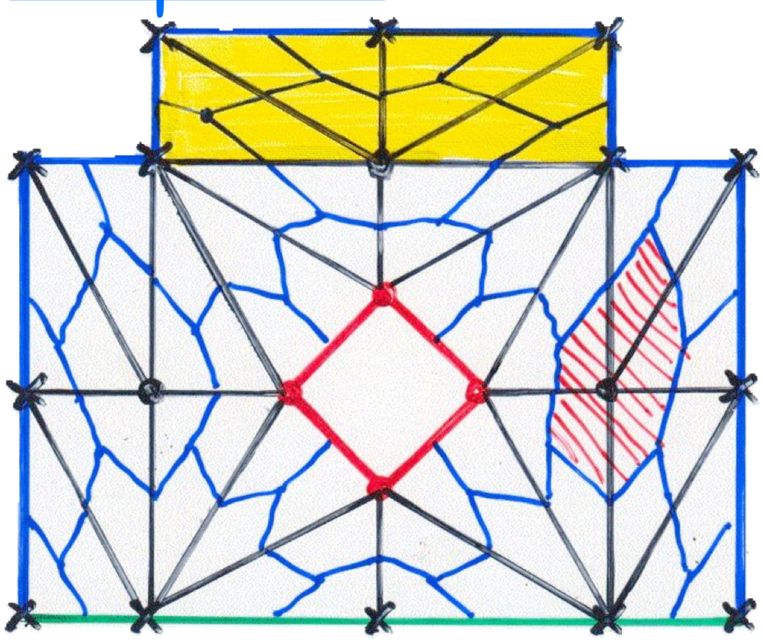
(3.9) $\| J_{\delta_r} \| \le c_2 h$

(3.10) $\| J_{\delta_r}^{-1} \| \le c_3 h^{-1}$

$x = x_{\delta_r}(\xi) \in Q_1$, $\xi = \xi_{\delta_r}(x)$

$\boxed{\Delta = \Box = \text{unit square}}$

- Example 4.14: CHIP



$\overline{\omega} = \omega \cup \gamma$

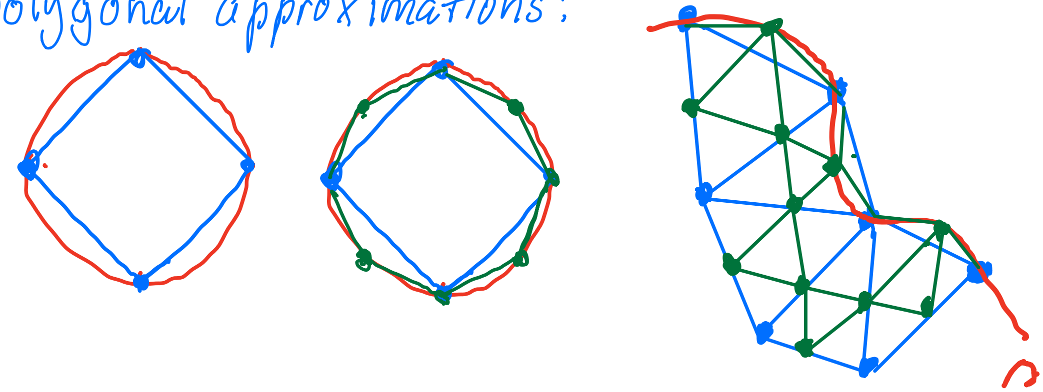
$\overline{\omega}_h = \omega_h \cup \gamma_h$

$x \in \omega := \overset{\circ}{\omega} = \{\bullet\} \cup \gamma_n = \{\times\} \;\hat{=}\; x^{(i)} : i \in \omega_h = \overset{\circ}{\omega}_h \cup \gamma_h$

$x \in \gamma = \gamma_1 = \{\bullet\} \;\hat{=}\; x^{(i)} : i \in \gamma_h = \gamma_{1h}$

Remark 4.15:

Curvilinear boundary parts are treated by polygonal approximations:



$$\overline{\Omega} = \bigcup_{r\in R_h} \overline{\tilde{\delta}_r}\,, \quad \mathcal{T}_\Delta = \{\tilde{\delta}_r : r\in R_h\} \ni \tilde{\delta}_r \xleftrightarrow[\text{map}]{\text{non-lin.}} \Delta = \quad \text{reference triangle}$$

$$h \to 0$$

$$\overline{\Omega}_h = \bigcup_{r\in R_h} \overline{\delta_r}\,, \quad \mathcal{T}_\Delta = \{\delta_r : r\in R_h\} \ni \delta_r \xleftrightarrow[\text{affine lin.}]{P_1\text{-map}} \Delta =$$

- In all grid points $x \in \overline{\omega}$, we define balance boxes $B(x) \in \mathcal{B}(X)$ such that

$$(26)\quad \begin{cases} H(x) = \operatorname{meas} B(x) = O(h^2) \quad \forall x\in\overline{\omega}, \\ \overline{\Omega} = \bigcup_{x\in\overline{\omega}} \overline{B(x)}, \\ \mathring{B}(x) \cap \mathring{B}(y) = \emptyset \quad \forall x,y\in\overline{\omega} : x\neq y \end{cases}$$

This yields a decomposition

$$\mathcal{T}_{\mathcal{K}} := \{ B(x) : x\in\overline{\omega} \} = \text{set of all boxes}$$

of Ω into boxes B (= control volume = finite volume) that is called <u>secondary grid</u>.

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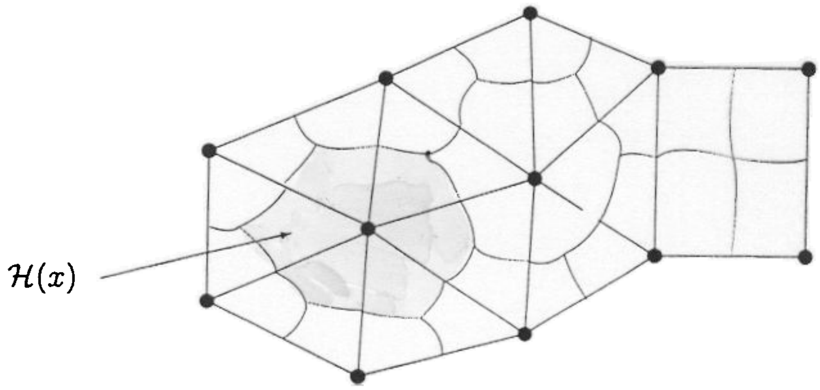
On the construction of secondary grids for primary triangular grids

- Zur Konstruktion der Sekundärvernetzung zu einer primären Dreiecks- (Vierecks-) Vernetzung gibt es verschiedene Möglichkeiten:

1) Beliebige Sekundärvernetzung, z.B. der Art: Arbitrary seondary grid

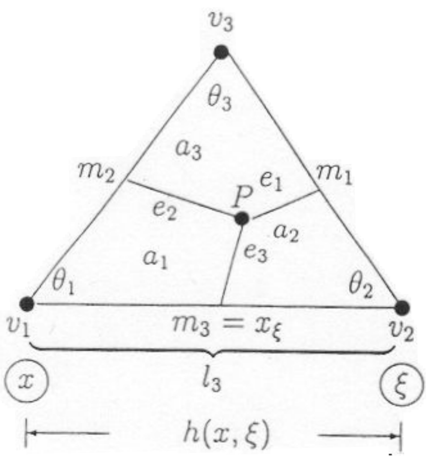


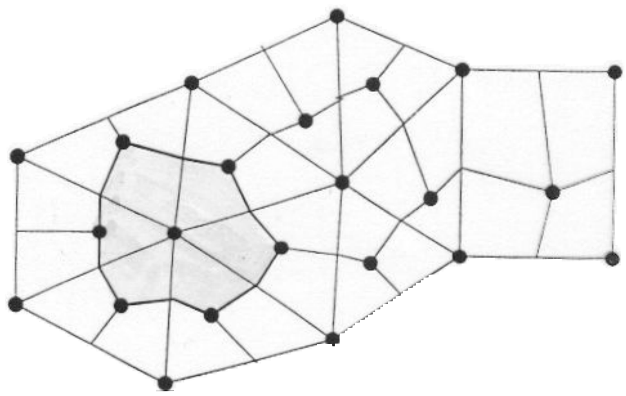
2) Polygonal berandete Boxen: Polygonally bounded boxes

2a) Seitenmittelpunkt ⟷ allgemein Punkt $P_r \in \delta_r$ bzw. $\in \bar{\delta}_r$:

Mid points m_i ⟷ general point $P_r \in \delta_r$ resp. $\in \bar{\delta}_r$

$\delta = \delta_r \in \mathcal{T}$



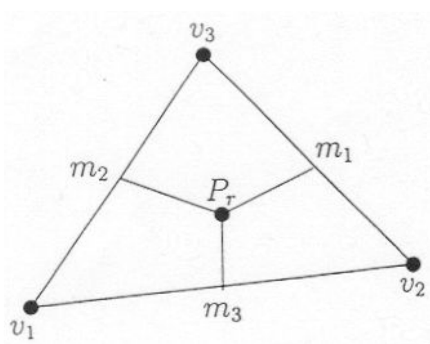


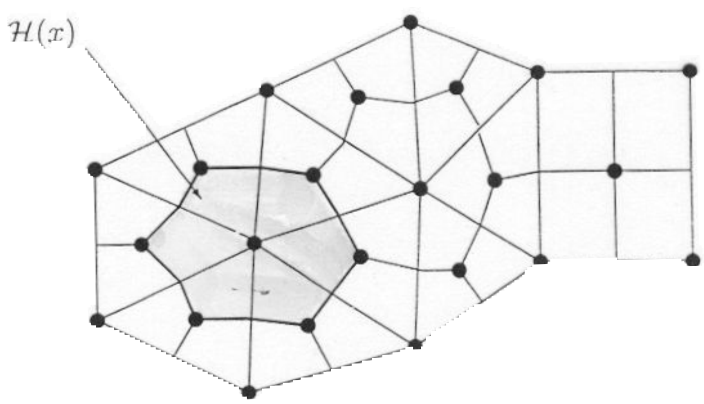
Mid points m_i ⟷ Barycenter of δ_r

2b) Seitenmittelpunkt ⟷ Schwerpunktmethode: P_r = Schwerpunkt von δ_r:

Methode MD (Medians):

$P_r = \frac{1}{3}(v_1 + v_2 + v_3), a_1 = a_2 = a_3 = \frac{1}{3}|\delta_r|$



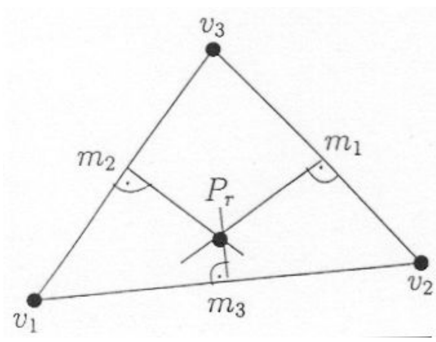


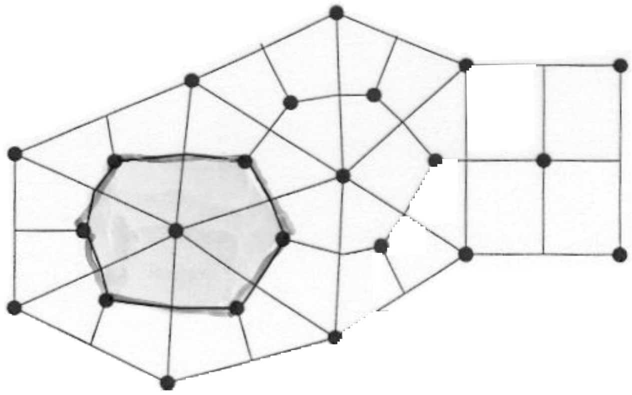
(⟶ Siehe Modellbeispiel !)

→ see our model problem CHIP

Method of Perpendicular Bisectors

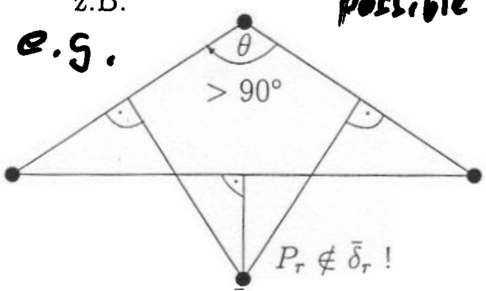
2c) Mittelsenkrechtenmethode: P_r = Schnittpunkt der Mittelsenkrechten:
Methode PB (Perpendicular Bisectors) = Voroni-Netz:





Attention:

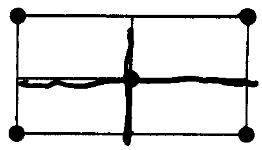
Vorsichtig $P_r \notin \bar{\delta}_r$ möglich ! possible
z.B. e.g.



Vor: für $P_r \in \bar{\delta}_r$: $\Theta \leq \pi/2$
$\forall$ Innenwinkel Θ.
! $\Theta > \frac{\pi}{2}$ für einen Innenwinkel
$\curvearrowright P_r \notin \bar{\delta}_r$ for some interior angle

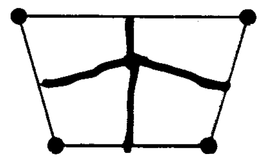
Assumption which ensures that $P_r \in \bar{\delta}_r$:
$\forall$ interior angles $\Theta \leq \pi/2$

rectangle
- Rechteck:

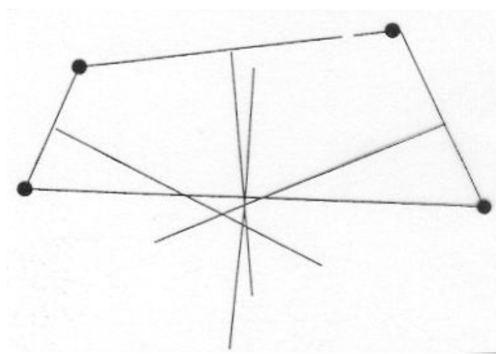


- gl. Trapez:

trapezoid



- kein allgemeines Viereck zulässig !



general quadrilaterals are not admissible !