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# Modified Discretization methods with embedded analytical solutions based on finite volume and discontinuous galerkin methods and applications in porous media.

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**Modified Discretization methods with embedded analytical solutions based on finite volume and discontinuous galerkin methods and applications in porous media**

Idea : Advanced standard discretisation methods with embedded onedimensional exact test-functions for different discretisations.

- Task : Multi-dimensional multi-physical problems in engineering-applications and mixing of parabolic and hyperbolic equations
- Model-Problem : Multi-physical and multi-dimensional processes
- Problems for the discretisation: Large scale problems (Stiff systems, artifical diffusion, oscillations)
- Solution: Discretization methods with smoother approximations (high resolution methods or analytical solutions).
- Methods: Domain-decomposition and Operator-Splitting methods.

## Contents

# 1 Motivation for the discretisation methods with embedded analytical solutions

1.) Characteristic methods (Transport and reaction exact):

Testfunctions (linear or constant) are exact transported.

Only approximation error for the initial condition and

splitting error in multi-dimensions.

2.) Locally improved test-functions

New improved test-space for the Finite Volume or DG-methods,

locally exact solutions.

# 2 Linear Operator-Splitting-Method

Idea: Decoupling of complex equations in simpler equations, solving simpler equations and re-coupling the results over the initial-conditions.

Equations: $\partial_t c = Ac + Bc$ ,
where the initial-conditions are $c(t^n) = c^n$.

Splitting-method of first order

$$\partial_t c^* = Ac^* \quad \text{with} \quad c^*(t^n) = c^n \ ,$$
$$\partial_t c^{**} = Bc^{**} \quad \text{with} \quad c^{**}(t^n) = c^*(t^{n+1}) \ ,$$

where the results of the methods are $c(t^{n+1}) = c^{**}(t^{n+1})$
and there are some splitting-errors for these methods,
Literature : [Strang 68], [Karlsen et al 2001].

# 3 Splitting-Errors of the Method

The error of the splitting-method of first order is

$$\partial_t c = (B + A)c$$
$$\tilde{c} = \exp(\tau(B + A))c(t^n) \ .$$

Local error for the decomposition and the full solution

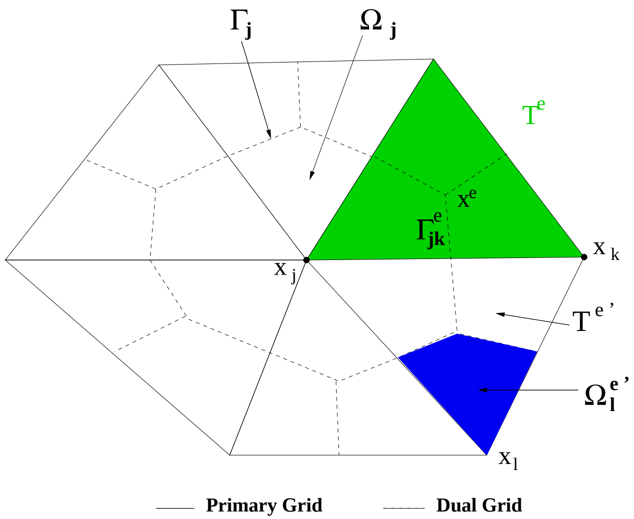
$$\begin{aligned} e(c) &= \tilde{c}(t^n + \tau) - \exp(\tau B)\exp(\tau A)c(t^n) \ , \\ &= \exp(\tau(B + A))c(t^n) - \exp(\tau B)\exp(\tau A)c(t^n) \ , \\ e(c)/\tau &= \frac{1}{2}\tau(BA - AB)c(t^n) + O(\tau^2) \ . \end{aligned}$$

$O(\tau)$ for A, B not commuting, otherwise one get exact results,

where $\tau = t^{n+1} - t^n$, [Strang 68].

# 4 Discretization-methods based on Voronoi-Boxes

- Local Mass-conservation, Simple test-functions (box-functions) .
- Un-structured Grids (adaptive grids), dual mesh.




- $T^e$ Elements, $e = 1, \ldots, E$, number of elements .
- $\Omega_j$ dual cells, $j = 1, \ldots, N$, number of nodes .

# 5 Improved discretisation methods via exact transport and reaction on the Characteristics

The scalar equation is given by:

$$\partial_t R\, c + \nabla \cdot \mathbf{v}\, c = 0.0 \;,$$

where the initial-conditions are $c(x, t^0) = c^0(x)$ .

The spatial-integration plus the Theorem of Gauss for the derivatives:

$$\int_{\Omega_j} \partial_t (R\, c)\, dx = - \int_{\Omega_j} \nabla \cdot (\mathbf{v}\, c)\, dx \; = - \int_{\Gamma_j} \mathbf{n} \cdot (\mathbf{v}\, c)\, d\gamma,$$

where $\Omega_j$ is the j-th cell and $v_{jk} = \mathbf{n}_{jk} \cdot \int_{\Gamma_{jk}} \mathbf{v}(\gamma)\, d\gamma$ .

$$|\Omega_j|(R(c_j^{n+1}) - R(c_j^n)) = -\tau^n \sum_{k \in out(j)} v_{jk} \tilde{c}_{jk}^n + \tau^n \sum_{l \in in(j)} v_{lj} \tilde{c}_{lj}^n \;.$$

The discretization-scheme with the mass-notation is:

$$m_j^{n+1} - m_j^n = - \sum_{k \in out(j)} m_{jk}^n + \sum_{l \in in(j)} m_{lj}^n \ ,$$

where : $\qquad m_j^n = V_j \ R \ c_j(t^n) \ , \ m_{jk}^n = \tau \ \tilde{c}_{jk}^n v_{jk} \ ,$

with the limitation to fulfill the monotonicity (local min-max-property).

We use the reconstruction of the linear test-function :

$c_{jk}^n = c_j^n + \nabla c_j^n (x_{jk} - x_j)$ Limiters (Slope and Flux-Limiter) :

$$\min_{k \in in(i)} \{c_i^n, c_k^n\} \le c_{jk}^n \le \max_{k \in in(i)} \{c_i^n, c_k^n\} \ , \ j \in out(i) \ , \ \text{with limited value } \hat{c}_{jk}^n,$$

$$\tilde{c}_{jk}^n = \hat{c}_{jk}^n + \frac{\tau}{\tau_j} (c_j^n - \hat{c}_{jk}^n) \ , \ \tau_j = \frac{V_j}{\nu_j} \ ,$$

$$\nu_j = \sum_{k \in out(j)} v_{jk} \ , \ v_{jk} = \mathbf{n}_{jk} \cdot \int_{\Gamma_{jk}} \mathbf{v}(\gamma) \, d\gamma \ .$$

## Discretization of the Convection-Reaction-Equation

The equation is given by:

$$\partial_t R_i c_i = \underbrace{-\nabla \cdot \mathbf{v}\ c_i}_{transport}\ \underbrace{-R_i \lambda_i c_i}_{sink}\ \underbrace{+R_{i-1} \lambda_{i-1} c_{i-1}}_{source}\ ,$$

where the initial-conditions are $c_1(x, t^0) = c_1^0(x)$ otherwise $0.0$ .

The notation in mass-terms is given by:

$$m_{i,j}^{n+1} - m_{i,j}^{n} = - \sum_{k \in out(j)} m_{i,jk}^{n} + \sum_{l \in in(j)} m_{i,lj}^{n}\ ,$$

where $m_{i,jk}^n$ is the mass from cell $j$ to cell $k$ for the transport- and reaction-term.

Transcription in m one-dimensional problems :

1.) Calculating the total-flux over all outflow-boundaries:

$$\nu_j = \sum_{k \in out(j)} v_{jk} \ .$$

2.) Calculating the velocity for every cell $j$ over the norm-interval $(0,1)$:

$$\tau_{i,j} = \frac{V_j R_i}{\nu_j} \ , \quad \text{maximal time-step with Courant-number } 1 \ ,$$

$$v_{i,j} = \frac{1}{\tau_{i,j}} \ , \quad \text{velocity in the cell j.}$$

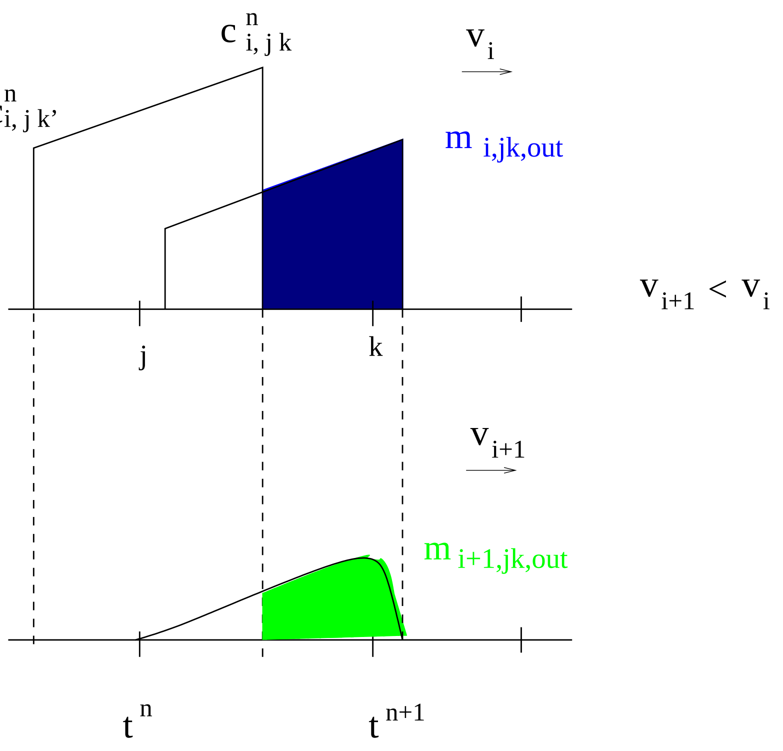
3.) Calculating of the analytical solution of the mass:

$$m^n_{i,jk,out} = m_{i2}(a, b, \tau^n, v_{1,j}, \ldots, v_{i,j}, R_1, \ldots, R_i, \lambda_1, \ldots, \lambda_i) \ ,$$

where $\tau^n \le \min_{\substack{i=1,\ldots,M \\ j=1,\ldots,I}} \tau_{i,j}$ (limitation of the time-step) ,

and $a = V_j R_i (c^n_{i,jk} - c^n_{i,jk'})$ , $b = V_j R_i c^n_{i,jk'}$ .

# Exact Tracking of Masses based on Convection and Reaction



4.) The partial masses are computed with the percentage of the total-mass with the outflow-boundaries:

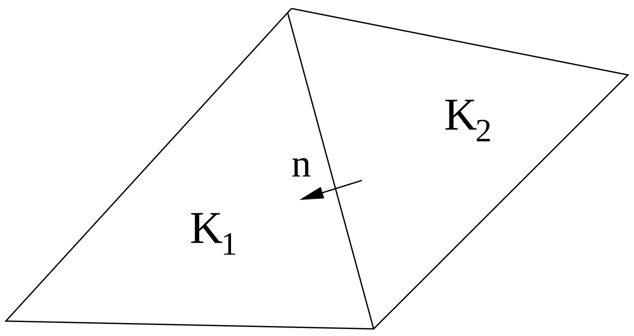
$$m_{i,jk}^n = \frac{v_{jk}}{\nu_j} \, m_{i,jk,out}^n \; .$$

Discretization in the mass-notation with embedded analytical one-dimensional solution:

$$m_{i,j}^{n+1} - m_{i,j}^n = - \sum_{k \in out(j)} \frac{v_{jk}}{\nu_j} \, m_{i,jk,out}^n + \sum_{l \in in(j)} \frac{v_{lj}}{\nu_l} \, m_{i,lj,out}^n \; .$$

# 6 Improved test-functions for Discontinuous Galerkin Methods

- Local Mass-conservation .
- Higher order methods (test-functions with higher polynoms .
- Application for Unstructured Grids (adaptive grids)
- One grid (Primary grid)




- Triangulation $\mathcal{K}_h$ for $h > 0$ for the domain $\Omega$.

## Notation for Discontinuous Galerkin-Methods

- Broken Sobolev-space by:

$$H^l(\mathcal{K}_h) = \{v \ \in \ L^2(\Omega) \ : \ v|_K \in H^l(K) \ \ \forall K \in \mathcal{K}_h\} \ . \qquad (1)$$

- Triangulation $\mathcal{K}_h$ for $h > 0$ for the domain $\Omega$.
- Sub-domain $K \in \mathcal{K}_h$ is a Lipschitz boundary
- $\mathcal{E}_h^i$ of all interior boundaries $e$ of $\mathcal{K}_h$.
- $\mathcal{E}_h^b$ of all exterior boundaries $e$ of $\Gamma = \partial\Omega$.

We have then the jumps across the edge $e = \partial K_1 \cap \partial K_2$ :

$$[v] = (v|_{K_2})|_e - (v|_{K_1})|_e \ . \qquad (2)$$

We also have the averages on the interfaces

$$\{v\} = \frac{(v|_{K_2})|_e + (v|_{K_1})|_e}{2} \ . \qquad (3)$$

## Mixed Formulation for the Convection-diffusion-reaction-equation

The solution is given by $u(x,t) \in C^2(\Omega) \times C^1([0,T])$ and $\underline{p}(x,t) \in (C^2(\Omega) \times C^1([0,T]))^d$ for the classical formulation [Geiser,Lazarov04]

$$\partial_t R u + \nabla \cdot \underline{v}\, u - \nabla \cdot a^{1/2}\, \underline{p} + R\lambda\, c = f \;, \text{ in } \Omega \tag{4}$$

$$-a^{1/2}\, \nabla u + \underline{p} = 0 \;, \tag{5}$$

$$u = g_1 \;, \text{ on } \Gamma_1 \;,$$

$$(\underline{v}\, u - a^{1/2}\, \nabla u) \cdot \underline{n} = g_2 \;, \text{ on } \Gamma_2 \;,$$

$$u(0) = u_0 \;, \text{ in } \Omega$$

The inner product $L^2(S)$ is denoted as $(\cdot,\cdot)_S$, and for $S = \Omega$ we skip the $S$.

## Variational Formulation for the mixed equations

For the mixed methods we have to find the unknowns $\underline{p} \in L_2((H^1(\mathcal{K}_h))^d, [0,T])$ and $u \in L_2(H^1(\mathcal{K}_h), [0,T])$ as follows :

$$(R\,\partial_t u, \phi) - \sum_{K \in \mathcal{K}_h} (u, \underline{v} \cdot \nabla\phi)_K + \sum_{e \in \mathcal{E}_h} (h_{conv}(u), [\phi])_e$$

$$+ \sum_{K \in \mathcal{K}_h} < a^{1/2}\,\underline{p}, \nabla\phi >_K + \sum_{e \in \mathcal{E}_h} (h_{diff}(u_h), [\phi])_e + (R\,\lambda u, \phi)$$

$$= \sum_{e \in \mathcal{E}_h^D} (g_2, \phi)_e \; + \; (f, \phi) \; , \;\; \phi \in H^1(\mathcal{K}_h) \; ,$$

$$< \underline{p}, \underline{\chi} > + \sum_{K \in \mathcal{K}_h} (u, \nabla \cdot a^{1/2}\,\underline{\chi})_K + \sum_{e \in \mathcal{E}_h} (h_{diff}(\underline{p}_h), [a^{1/2}\,\underline{\chi} \cdot \underline{n}])_e$$

$$= \sum_{e \in \mathcal{E}_h^D} (g_1, \underline{\chi} \cdot \underline{n})_e \; , \;\; \underline{\chi} \in (H^1(\mathcal{K}_h))^d \; .$$

We have the convective-fluxes:

$$\hat{h}_{conv}(u_h) = \begin{cases} \{u_h \, \underline{v} \, \underline{n}\} & \text{central differences} \\ \{u_h \, \underline{v} \, \underline{n}\} - \frac{|\underline{v} \, \underline{n}|}{2}[u_h] & \text{upwind} \end{cases} ,$$

$$\hat{h}_{diff}(\underline{w}_h) = (a^{1/2} \, \underline{n} \, \{u_h\}, \{a^{1/2} \, \underline{p}_h \cdot \underline{n}\})^t + C_{diff}[(u_h, \underline{p}_h)^t] \, ,$$

where the flux-matrix $C_{diff}$ is given as

$$C_{diff} = \begin{pmatrix} 0 & -c_{1,2} & \dots & -c_{1,d+1} \\ c_{1,2} & 0 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ c_{1,d+1} & 0 & \dots & 0 \end{pmatrix} = \begin{pmatrix} 0 & -\underline{c}^T \\ \underline{c} & 0 \end{pmatrix} ,$$

where $\underline{c} = (c_{1,2}, \dots, c_{1,d+1})^T$ , and $c_{1,i} = c_{1,i}((\underline{w}_h|_{K_2})|_e, (\underline{w}_h|_{K_1})|_e)$ is locally Lipschitz.

## Stability of the mixed form

We have the stability for the full-discrete form with the solutions $u_h \in V$ and $\underline{p}_h \in W$ such that

$$R \, \frac{1}{2} ||u_h(T)||^2_{L^2(\Omega)} + \int_0^T \; \Theta_C(\underline{w}_h, \underline{w}_h) \; dt + \int_0^T \; ||\underline{p}_h||^2_{(L^2(\Omega))^d} \; dt$$

$$+ \int_0^T \frac{R \, \lambda}{2} \; ||u_h||^2_{L^2(\Omega)} \; dt \le \frac{1}{2} ||u_h(0)||^2_{L^2(\Omega)}$$

$$+ \int_0^T \; \frac{1}{2 \; R \; \lambda} \; ||f||^2_{L^2(\Omega)} \; dt \; ,$$

where $\Theta_C(\underline{w}_h, \underline{w}_h) = \sum_{e \in \mathcal{E}_h} < [\underline{w}_h] \; , \; C \; [\underline{w}_h] >_e$,

and $C = \begin{pmatrix} c_{1,1} & -\underline{c}^T \\ & \\ \underline{c} & 0 \end{pmatrix}$ is the flux-matrix.

**Design of new test-functions with local analytical solutions**

For the adjoint-problem of the convection-reaction-terms we get

$$- \sum_{K \in \mathcal{K}_h} (u_h, \underline{v} \cdot \nabla \phi)_K + (u_h, R\, \lambda \phi) \tag{6}$$

$$= \sum_{K \in \mathcal{K}_h} (u_h, -\underline{v} \cdot \nabla \phi + R\, \lambda\, \phi) = 0\ ,$$

where $u_h, \phi \in V_h$ and solve the adjoint local equation for the convection-reaction in space

$$-\underline{v} \cdot \nabla \phi + R\, \lambda\, \phi = 0\ , \tag{7}$$

where the initial condition is $\phi(0) = \phi_0$.

## New Test-function with local analytical solutions in 1 dimension

We derive the one-dimensional solutions for the local convection-reaction equation, given as adjoint problem [Geiser 04], [Farhat 02]

$$-v \, \partial_x \phi + R \, \lambda \, \phi = 0 \, , \tag{8}$$

where we derive the local solution

$$\phi_{anal,i}(x) = a_0 \begin{cases} \exp(-\beta \, (x_{i+1/2} - x)) & v > 0 \\ \\ \exp(-\beta \, (x - x_{i-1/2})) & v < 0 \end{cases} \, , \tag{9}$$

where $\beta = \frac{R \, \lambda}{|v|}$ ,

$$\phi_{new,i} = \phi_{anal,i}(x) \, , \tag{10}$$

where $x_{i-1/2} < x < x_{i+1/2}$.

## New Test-function with local analytical solutions in 2 dimension

Assumption of a 2 dim. and decoupable velocity and regular quadratic cells :

$$-v_x \; \partial_x \phi - v_y \; \partial_y \phi + R \, \lambda \, \phi = 0 \; , \tag{11}$$

where we derive the local solution

$$\phi_{anal,i}(x) = a_0 \; \begin{cases} \exp(-\beta_x \; (x_{i+1/2} - x)) & v_x > 0 \\ \\ \exp(-\beta_x \; (x - x_{i-1/2})) & v_x < 0 \end{cases} \; , \tag{12}$$

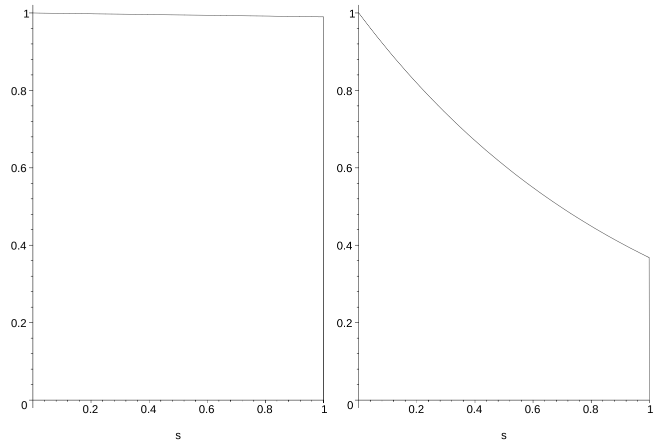
where $\beta_x = \frac{R \, \lambda}{2|v_x|}$ and $\beta_y = \frac{R \, \lambda}{2|v_y|}$ ,

$$\phi_{new,i,j} = \phi_{anal,i}(x) \; \phi_{anal,j}(y) \; , \tag{13}$$

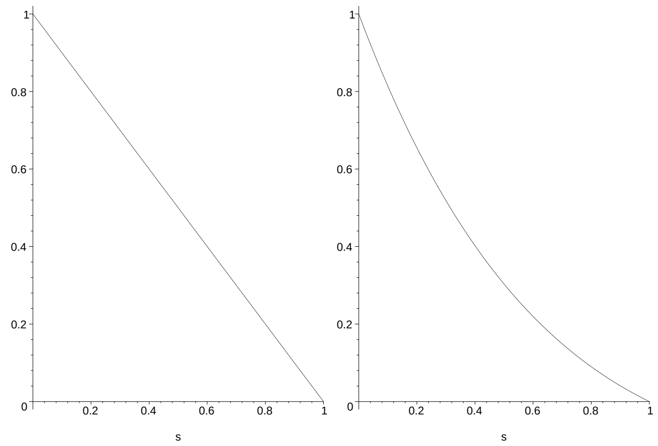
where $x_{i-1/2} < x < x_{i+1/2}$ and $y_{j-1/2} < y < y_{j+1/2}$.

## Test-functions : constant and linear

Constant test-functions: Standard and new functions




Linear test-functions: Standard and new functions



## Applications

We applied for a 2d with standard test-functions for the convection-reaction-equation :

Rotating Gaussian-impulse calculated with the convection-reaction-equation :

| Level | $h^{-1}$ | Elements | $E_{L_1}$ | Conv. order for $E_{L_1}$ | Time-Steps |
|---|---|---|---|---|---|
| 4 | 8 | 1024 | $4.37\ 10^{-2}$ | | 10 |
| 5 | 16 | 4096 | $2.59\ 10^{-2}$ | $0.75$ | 20 |
| 6 | 32 | 16384 | $1.04\ 10^{-2}$ | $1.31$ | 40 |
| 7 | 64 | 65536 | $2.92\ 10^{-3}$ | $1.83$ | 80 |

Table 1: Convergence-Results for the DG-method for different levels and time-steps

## 7 Conclusions and future works

- Mixed discretisation methods.
- Improved methods with analytical test-functions in 2 dimensions.
- Error-estimates for embedded methods.
- Applications to complex models, e.g. transport-reaction-, bio-remediation- and chemical-models.
- Multi-scaling-problems with improved analytical solutions on different scales.