Jürgen Geiser


Idea: Advanced standard discretisation methods with embedded onedimensional exact test-functions and decoupling in simpler operators.

- Task: Multi-dimensional multi-physical problems in engineering-applications and mixing of parabolic and hyperbolic equations in fluid- and gas-mechanics
- Model-Problem: Multi-physical, multi-scalar, multi-dimensional and multi-operator effects
- Problems for the discretisation: Embed all the different effects: e.g. stiff systems, artificial numerical effect, oscillations, unphysical behaviour
- Solution: Modified Discretisation methods with weighting factors, higher order functions, analytical support, decoupling in simpler parts.
- Methods: Reconstruction methods, DG-methods, operator splitting and Domain-decomposition methods.
Contents

1. Motivation for modified discretisation and solver methods

2. Solver methods: Operator-Splitting-methods and iterative methods

3. Discretisation methods: Finite-Volume-, Finite-Element-Methods (Flow cond. Based methods) and Discontinuous Galerkin methods

4. Modified discretisation methods: Reconstruction methods for higher order, improved testfunctions, enriched methods or near- far-field methods (bubble functions, multi-scaling).

5. Application in application in fluid- and gas-mechanics

6. Conclusions
1 Motivation for mixed discretisation methods

Standard methods are developed for continuous and smooth solutions, one-scales and isotrop domains.

Model in real-life application, climate models, material research request multi-physical solutions.

Modified methods are often specialised for one equation-part, e.g. Characteristic methods (Transport-reaction-equation).

Iterative results of equation-parts helps to initialise complexer methods.
(Local solutions as initial values for global solutions)
2 Discretisation-Methods

Based on Standard Methods we modify:

- Finite Volume Methods (Box-Methods with FBMC, Characteristic-Methods)
- Discontinuous Galerkin Methods (Embed of analytical local methods)
- Improved Finite-Element-Methods (near-field, finite-element-method and far-field, Greens-function-method)
3 Multi-physical, multi-dimensional, multi-operator, multi-scaling Problems

Discretisation and solver-methods for this problems are based on design of simplification of the complexity. So local discretisation-methods for all the different problem, e.g. adaptive and higher order methods or splitting-methods for decoupling into simpler problems and solve them effective and simpler.
Ideas for Coupling–Decoupling Multi–Structures (Multi–components, Multi–dimensions, Multi–physics, Multi–operators, Multi–scales)

- **Complicate Model with multi–structures (e.g. biological model)**
  - Decoupled (Question: Decomposable)
  - Coupled as a multi–structure general–methods to solve all the structures (intrinsic point of view)

**Decoupling in simpler structures**
Solve each simpler structure independent (extrinsic point of view)

- $u_1$, $u_2$, $u_3$, ......, $u_n$

**Coupled as a multi–structure**
Solve all the structures (intrinsic point of view)

- $u_1$, $u_2$, $u_3$, ......, $u_n$ -> $u$
4 Multi-Physical Methods

a.) General Discretisation methods for all physical operators, e.g. Finite Volume-Method for Convection-Diffusion-Reaction-Equation. Specialisation for this general methods via embedding correction methods, e.g. upwinding, exponential fitting, mixed methods for Convection-Diffusion-Term.

b.) Physical discretisation : Special Discretisation methods for each physical operator, e.g. Convection-Term is done with Characteristic-Methods. Idea of decoupling each physical operator and solve operator with adapted methods.
5 Multi-Scaling Methods

a.) General Solver-methods for all different scales, e.g. upscaling for an averaged scale and then a direct solver.

b.) Solver-methods for each different scale, e.g. solving on each different scale, decompose the problem into smaller scales.

Multi-Scaling-Problems

Problem exists on each scale

Decomposing in simpler scales
6 Decomposition Methods

a.) General Solver-methods for all different domain (unique domain).

b.) Solver-methods for each different domain, e.g. solving on each different domain (adaptivity, more effectivity).

Domain Decomposition

<table>
<thead>
<tr>
<th>Unique Domains</th>
<th>Overlapping domains</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Omega )</td>
<td>( \Omega_1 ) ( \Omega_2 ) ( \Omega_3 ) ( \Omega_4 ) ( \Omega_5 ) ( \Omega_6 )</td>
</tr>
</tbody>
</table>

Ω
7 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].
8 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

\[
e(c) = \tilde{c}(t^n + \tau) - \exp(\tau B) \exp(\tau A)c(t^n) = \exp(\tau(B + A))c(t^n) - \exp(\tau B) \exp(\tau A)c(t^n),
\]

\[
e(c)/\tau = \frac{1}{2}\tau(BA - AB)c(t^n) + O(\tau^2).
\]

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

where \(\tau = t^{n+1} - t^n\), [Strang 68].
9 Higher order splitting-methods

Strang or Strang-Marchuk-Splitting, cf. [Marchuk 68, Strang68]

\[ \frac{\partial c^*(t)}{\partial t} = Ac^*(t), \text{ with } t^n \leq t \leq t^{n+1/2} \text{ and } c^*(t^n) = c_{sp}^n, \]  
(1)

\[ \frac{\partial c^{**}(t)}{\partial t} = Bc^{**}(t), \text{ with } t^n \leq t \leq t^{n+1}, c^{**}(t^n) = c^*(t^{n+1/2}), \]

\[ \frac{\partial c^{***}(t)}{\partial t} = Ac^{***}(t), \text{ with } t^{n+1/2} \leq t \leq t^{n+1}, c^{***}(t^{n+1/2}) = c^{**}(t^{n+1}), \]

where \( t^{n+1/2} = t^n + 0.5\tau_n \) and the approximation on the next time level \( t^{n+1} \) is defined as \( c_{sp}^{n+1} = c^{***}(t^{n+1}) \).

The splitting error of the Strang splitting is

\[ \rho_n = \frac{1}{24} \tau_n^2 ([B, [B, A]] - 2[A, [A, B]]) c(t^n) + O(\tau_n^3). \]  
(2)

See, e.g. [Hundsdorfer, Verwer 2003].
10 Iterative splitting-Methods

\[
\frac{\partial c_i(t)}{\partial t} = A c_i(t) + B c_{i-1}(t), \text{ with } c_i(t^n) = c_{sp}^i, \quad (3)
\]

\[
\frac{\partial c_{i+1}(t)}{\partial t} = A c_i(t) + B c_{i+1}(t), \text{ with } c_{i+1}(t^n) = c_{sp}^i, \quad (4)
\]

where \( c_0(t) \) is any fixed function for each iteration. (Here, as before, \( c_{sp}^n \) denotes the known split approximation at the time level \( t = t^n \).) The split approximation at the time-level \( t = t^{n+1} \) is defined as

\[ c_{sp}^{n+1} = c_{2m+1}(t^{n+1}). \] (Clearly, the functions \( c_k(t) \) \( (k = i - 1, i, i + 1) \) depend on the interval \( [t^n, t^{n+1}] \), too, but, for the sake of simplicity, in our notation we omit the dependence on \( n \).)
11 Error for the Iterative splitting-method

For the local error function \( e_i(t) = c(t) - c_i(t) \) we have the relations

\[
\partial_t e_i(t) = A e_i(t) + B e_{i-1}(t), \quad t \in (t^n, t^{n+1}],
\]

\[
e_i(t^n) = 0,
\]

and

\[
\partial_t e_{i+1}(t) = A e_i(t) + B e_{i+1}(t), \quad t \in (t^n, t^{n+1}],
\]

\[
e_{i+1}(t^n) = 0,
\]

for \( m = 0, 2, 4, \ldots \), with \( e_0(0) = 0 \) and \( e_{-1}(t) = c(t) \).
\[ \mathcal{E}_i(t) = \begin{bmatrix} e_i(t) \\ e_{i+1}(t) \end{bmatrix}, \quad \mathcal{F}_i(t) = \begin{bmatrix} Be_{i-1}(t) \\ 0 \end{bmatrix}, \quad A = \begin{bmatrix} A & 0 \\ A & B \end{bmatrix}. \] (7)

Then, using the notations (7), the relations (5)–(6) can be written in the form

\[ \partial_t \mathcal{E}_i(t) = A \mathcal{E}_i(t) + \mathcal{F}_i(t), \quad t \in (t^n, t^{n+1}], \]

\[ \mathcal{E}_i(t^n) = 0. \] (8)

Due to our assumptions, \( A \) is a generator of the one-parameter \( C_0 \)-semigroup \( (\exp A t)_{t \geq 0} \), hence using the variations of constants formula, the solution of the abstract Cauchy problem (8) with homogeneous initial condition can be written as

\[ \mathcal{E}_i(t) = \int_{t^n}^{t} \exp(A(t - s)) \mathcal{F}_i(s) ds, \quad t \in [t^n, t^{n+1}]. \] (9)
By using the denotation we could derive

\[ \| \mathcal{E}_i \|_\infty = \sup_{t \in [t^n, t^{n+1}]} \| \mathcal{E}_i(t) \| \]  

we have

\[ \| \mathcal{E}_i \|_\infty (t) \leq \| \mathcal{F}_i \|_\infty \int_{t^n}^{t} \| \exp(\mathcal{A}(t - s)) \| ds = \]

\[ = \| B \| \| e_{i-1} \| \int_{t^n}^{t} \| \exp(\mathcal{A}(t - s)) \| ds, \quad t \in [t^n, t^{n+1}] . \]

Since \((\mathcal{A}(t))_{t \geq 0}\) is a semigroup, therefore the so called growth estimation

\[ \| \exp(\mathcal{A}t) \| \leq K \exp(\omega t); \quad t \geq 0 , \]  

holds with some numbers \( K \geq 0 \) and \( \omega \in \mathbb{R} \), cf. [Geiser,Farago 2005].
## Advanced Discretisation-Methods, integration of decomposing methods

<table>
<thead>
<tr>
<th>Discretisation Method</th>
<th>Modification for the method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Finite Volumes</td>
<td>Reconstruction Method</td>
</tr>
<tr>
<td>Finite Element</td>
<td>Enriched Methods</td>
</tr>
<tr>
<td></td>
<td>(e.g. Bubble Functions)</td>
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<tr>
<td>Discontinuous Galerkin</td>
<td>Embedded Testfunctions</td>
</tr>
<tr>
<td></td>
<td>(e.g. one-dimensional solutions)</td>
</tr>
</tbody>
</table>

Table 1: Modifications for the Standard Methods
13 Motivation for the discretisation methods for the Parabolic and Hyperbolic Differential-Equations

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.

3.) Locally improved trial-functions to improve the discretisation of critical terms. Idea skip the critical terms via analytical solutions.
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.
Improved discretisation methods via exact transport and reaction on the Characteristics

The scalar equation is given by:

$$\partial_t R c + \nabla \cdot v c = 0.0,$$

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

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

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

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

$$|\Omega_j|(R(c_{j}^{n+1}) - R(c_{j}^{n})) = -\tau^n \sum_{k \in \text{out}(j)} v_{jk} \tilde{c}_{jk}^{n} + \tau^n \sum_{l \in \text{in}(j)} v_{lj} \tilde{c}_{lj}^{n}.$$
The discretization-scheme with the mass-notation is:

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

where:

\[
m_{j}^{n} = V_{j} \ R \ c_{j}(t^{n}), \ m_{jk}^{n} = \tau \ \tilde{c}_{jk}^{n} v_{jk},
\]

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):

\[
\min_{k \in \text{in}(i)} \{c_{i}^{n}, c_{k}^{n}\} \leq c_{jk}^{n} \leq \max_{k \in \text{in}(i)} \{c_{i}^{n}, c_{k}^{n}\}, \ j \in \text{out}(i), \ 	ext{with limited value} \ \tilde{c}_{jk}^{n},
\]

\[
\tilde{c}_{jk}^{n} = \tilde{c}_{jk}^{n} + \frac{\tau}{\tau_{j}} (c_{j}^{n} - \tilde{c}_{jk}^{n}), \ \tau_{j} = \frac{V_{j}}{\nu_{j}},
\]

\[
\nu_{j} = \sum_{k \in \text{out}(j)} v_{jk}, \ v_{jk} = n_{jk} \cdot \int_{\Gamma_{jk}} \mathbf{v}(\gamma) \ d\gamma.
\]
**Discretization of the Convection-Reaction-Equation**

The equation is given by:

\[
\frac{\partial}{\partial t} R_i c_i = \underbrace{-\nabla \cdot \mathbf{v} c_i}_{\text{transport}} - \underbrace{R_i \lambda_i c_i}_{\text{sink}} + \underbrace{R_{i-1} \lambda_{i-1} c_{i-1}}_{\text{source}},
\]

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:

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

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:

\[ \nu_j = \sum_{k \in \text{out}(j)} v_{jk}. \]

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:

\[ m_{i,j,k,\text{out}}^n = m_{i2}(a, b, \tau^n, v_{1,j}, \ldots, v_{i,j}, R_1, \ldots, R_i, \lambda_1, \ldots, \lambda_i), \]

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

and \( a = V_j R_i (c_{i,j,k}^n - c_{i,j,k'}^n), \quad b = V_j R_i c_{i,j,k'}^n. \)
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:

\[ m_{i,jk}^n = \frac{v_{jk}}{v_j} \ m_{i,jk,\text{out}}^n \]

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

\[ m_{i,j}^{n+1} - m_{i,j}^n = - \sum_{k \in \text{out}(j)} \frac{v_{jk}}{v_j} \ m_{i,jk,\text{out}}^n + \sum_{l \in \text{in}(j)} \frac{v_{lj}}{v_l} \ m_{i,lj,\text{out}}^n \]
**Numerical results for the improved method** The results computed with the modified method is presented in the table 2.

<table>
<thead>
<tr>
<th>$l$</th>
<th>$E^2_{L_1}$</th>
<th>$\rho^2_{L_1}$</th>
<th>$E^3_{L_1}$</th>
<th>$\rho^3_{L_1}$</th>
<th>$E^4_{L_1}$</th>
<th>$\rho^4_{L_1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>3.06 $10^{-4}$</td>
<td>1.95</td>
<td>3.91 $10^{-5}$</td>
<td>1.986</td>
<td>7.79 $10^{-6}$</td>
<td>1.89</td>
</tr>
<tr>
<td>5</td>
<td>8.03 $10^{-5}$</td>
<td>2.007 $10^{-5}$</td>
<td>9.87 $10^{-6}$</td>
<td>1.93</td>
<td>5.81 $10^{-7}$</td>
<td>1.89</td>
</tr>
<tr>
<td>6</td>
<td>2.007 $10^{-5}$</td>
<td>2.01</td>
<td>2.60 $10^{-6}$</td>
<td>1.96</td>
<td>1.51 $10^{-7}$</td>
<td>1.94</td>
</tr>
<tr>
<td>7</td>
<td>4.36 $10^{-6}$</td>
<td>2.21</td>
<td>6.66 $10^{-7}$</td>
<td>1.96</td>
<td>1.51 $10^{-7}$</td>
<td>1.94</td>
</tr>
</tbody>
</table>

Table 2: Higher order methods for the components, $L_1$-error computed with the modified method.
16 Physical Discretisation-Methods, embedding of analytical solutions as test-functions

Idea: Define the critical numbers for each part of the equations (2 operators), compute the local analytical solutions. Embed the solutions in the test-functions. Based on the operators we derive an analytical methods.

\[ \partial_t c(x, t) = Ac(x, t) + Bc(x, t) \text{, with initial and boundary conditions} \]

1.) Local operator equation:
\[ Ac(x, \tilde{t}) + Bc(x, \tilde{t}) = 0 \text{, with initial and boundary conditions, fixed } \tilde{t} \] 
2.) Local analytical solution: Physical characteristic parameters
\[ \beta = \frac{\bar{B}}{\bar{A}} \text{, } \bar{A}, \bar{B} \text{ scalar values, analytical solution: } c = \exp(\beta)c_{init} \]
Example for Convection-Diffusion-Reaction-Equation

One-dimensional part:
\[ \partial_t c(x, t) = -v \partial_x c(x, t) + D \partial_{xx} c(x, t) + \lambda c(x, t) , \]

1.) Local solutions for Convection-Diffusion-equations:
\[-v \partial_x c(x, t) + D \partial_{xx} c(x, t) = 0 \text{, } t \text{ is fixed} .\]
Char. parameter : \( \beta = \frac{v}{D} \Delta x \), solutions : 
\[ c = \exp\left(-\frac{v}{D} (x_i - x)\right) c_{\text{init}} \]

2.) Local solutions for Diffusion-Reaction-equations:
\[ D \partial_{xx} c(x, t) - \lambda c = 0 \text{, } t \text{ is fixed} . \]
Char. para. : \( \beta_{1,2} = \pm \sqrt{\frac{\lambda}{D}} \Delta x \) solutions : 
\[ c = e^{-\sqrt{\frac{\lambda}{D}} (x_i - x)} c_{\text{init},1} + e^{\sqrt{\frac{\lambda}{D}} (x_i - x)} c_{\text{init},2} \]
Example for Convection-Diffusion-Reaction-Equation

Multi-dimensional part (unique square)
\[
\partial_t c(x, y, t) = -v_1 \partial_x c(x, t) - v_2 \partial_y c(x, y, t) + \lambda c(x, y, t),
\]

Separation of the dimensions:
\[-v_1 \partial_x c - v_2 \partial_y c + \lambda c = 0, \ t \ \text{is fixed}.
\]

Char. parameter: \( \beta_1 = \frac{\lambda/2 \Delta x}{v_1}, \beta_2 = \frac{\lambda/2 \Delta y}{v_2}, \)

Multi-dim. Solutions for the test-functions:
\[
c = \exp\left(-\frac{\lambda/2}{v_1}(x_i - x)\right) \exp\left(-\frac{\lambda/2}{v_2}(y_j - y)\right) c_{init}
\]
17 Improved test-functions for Finite Element/Finite Volume Methods

Idea: Flow condition based interpolation finite elements, [Kohno, Bathe 02]

- Local Mass-conservation.
- Flow conditions over the elements (weight functions as exact functions).
- Stability for extrem Peclet-Numbers.
- Hybrid method between Finite element and finite Volume methods.
Embedding improved trial-functions for each terms.

Convection-Diffusion Equation (normed by the Peclet Number : $Pe$):

$$\nabla \cdot (\mathbf{v} c - \frac{1}{Pe} \nabla c) = 0 , \ c(x) \in \Phi, \ x \in \Omega$$

where we have Dirichlet-Boundary conditions : $c = c_0$ on $x \in \partial \Omega$,

We use the Petrov-Galerin variational formulation with subspace : $U_h, V_h$ and $W_h$ in $\Phi$ and find $u \in U_h, c \in V_h$ so that for all $w \in W_h$

$$\int_\Omega w \left( \nabla \cdot (\mathbf{v} u - \frac{1}{Pe} \nabla c) \right) d\Omega = 0$$
Adapted trial-functions for the operators:

1.) Trial function $V_h$ for the diffusion-operator:

We use the bilinear interpolation functions (e.g. diffusion-approximation with linear functions).

2.) Trial functions $U_h$ for the convection-operator:

We use the flow-conditions along each side of the elements:

(The solution of the one-dimensional equation $vu - \frac{1}{Pe} \partial_x u = 0$).

3.) Test-function $W_h$:

We use step-functions (i.d. box function) for each dual-element.
Trial- and Test-functions:

1.) Trial function $V_h$ for the diffusion-operator:

$$
\begin{bmatrix}
  h_1^V & h_4^V \\
  h_2^V & h_3^V
\end{bmatrix}
= h(\xi) h^t(\eta). \tag{13}
$$

where $h^t(y) = [y, 1-y]$ and $y = \xi, \eta$ with $0 \leq \xi, \eta \leq 1$.

2.) Trial function $U_h$ for the convection-operator:

$$
\begin{bmatrix}
  h_1^U & h_4^U \\
  h_2^U & h_3^U
\end{bmatrix}
= [h(x^1), h(x^2)] h(\eta) h^t(\eta). \tag{14}
$$

where $x^k = \frac{\exp(q^k \xi) - 1}{\exp(q^k) - 1}$ and $q^k = Pe(v^k \cdot \Delta x^k)$

$v^1 = 1/2(v_1 + v_2), v^2 = 1/2(v_3 + v_4)$

$\Delta x^1 = x_2 - x_1, \Delta x^2 = x_3 - x_4$
3.) Test-function $W_h$:

$$
W_h = \begin{cases} 
1 & (\xi, \eta) \in [0, 1/2] \times [0, 1/2] \\
0 & \text{else}
\end{cases}
$$

We get the nodal values with the trial-functions: $u = h_i^\phi c_i$, $c = h_i^\theta c_i$

The primary and dual mesh is given as
Stability and Consistence:

Idea: One could skip the convection-part by the analytical solution and reach smoother results.

Stability for the rectangular meshes (Transformation to a diffusion equation, via the skipping the convection-part, i.d. $\nu u - \frac{1}{Pe} \partial_x u = 0$):

$$\|c\|_{H^1(\Omega)} \leq C \|f_0\|_{L^2\Omega}$$

where $f_0$ is the right-hand side.

Results:

We could combine the good characteristics of finite element methods (flexibility in $h^p$ methods) and the conservation of finite volume (e.g. mass conservation)
18 Improved test-functions for Discontinuous Galerkin Methods

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

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

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Notation for Discontinuous Galerkin-Methods

- Broken Sobolev-space by:

\[ H^l(K_h) = \{ v \in L^2(\Omega) : v|_K \in H^l(K) \ \forall K \in K_h \} . \quad (17) \]

- Triangulation \( K_h \) for \( h > 0 \) for the domain \( \Omega \).

- Sub-domain \( K \in K_h \) is a Lipschitz boundary

- \( E^i_h \) of all interior boundaries \( e \) of \( K_h \).

- \( E^b_h \) of all exterior boundaries \( e \) of \( \Gamma = \partial \Omega \).

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

\[ [v] = (v|_{K_2})|_e - (v|_{K_1})|_e . \quad (18) \]

We also have the averages on the interfaces

\[ \{v\} = \frac{(v|_{K_2})|_e + (v|_{K_1})|_e}{2} . \quad (19) \]
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 \( p(x, t) \in (C^2(\Omega) \times C^1([0, T]))^d \) for the classical formulation [Geiser05]

\[
\partial_t Ru + \nabla \cdot v u - \nabla \cdot a^{1/2} p + R\lambda c = f, \text{ in } \Omega, \quad (20)
\]

\[
-a^{1/2} \nabla u + p = 0, \quad (21)
\]

\[
u u - a^{1/2} \nabla u \cdot n = g_2, \text{ on } \Gamma_2,
\]

\[
u u = g_1, \text{ on } \Gamma_1,
\]

\[
u u(0) = u_0, \text{ in } \Omega.
\]

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

\( p \in L_2((H^1(K_h))^d, [0, T]) \) and \( u \in L_2(H^1(K_h), [0, T]) \) as follows:

\[
\begin{align*}
(R \partial_t u, \phi) &- \sum_{K \in K_h} (u, \nu \cdot \nabla \phi)_K + \sum_{e \in E_h} (h_{conv}(u), [\phi])_e \\
&+ \sum_{K \in K_h} \langle a^{1/2} p, \nabla \phi \rangle_K + \sum_{e \in E_h} (h_{diff}(u_h), [\phi])_e + (R \lambda u, \phi) \\
&= \sum_{e \in E_h^D} (g_2, \phi)_e + (f, \phi), \quad \phi \in H^1(K_h),
\end{align*}
\]

\[
\langle p, \chi \rangle + \sum_{K \in K_h} (u, \nabla \cdot a^{1/2} \chi)_K + \sum_{e \in E_h} (h_{diff}(p_h), [a^{1/2} \chi \cdot n])_e \\
= \sum_{e \in E_h^D} (g_1, \chi \cdot n)_e, \quad \chi \in (H^1(K_h))^d.
\]
We have the convective-fluxes

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

\[
\hat{h}_{\text{diff}}(w_h) = \left( a^{1/2} n \{u_h\}, \{a^{1/2} p_h \cdot n\} \right)^t + C_{\text{diff}} [(u_h, p_h)^t],
\]

where the flux-matrix \( C_{\text{diff}} \) is given as

\[
C_{\text{diff}} = \begin{pmatrix}
0 & -c_{1,2} & \ldots & -c_{1,d+1} \\
-1 & 0 & \ldots & 0 \\
0 & -1 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & 0
\end{pmatrix} = \begin{pmatrix}
0 & -c^T \\
c & 0
\end{pmatrix},
\]

where \( c = (c_{1,2}, \ldots, c_{1,d+1})^T \), and \( c_{1,i} = c_{1,i}((w_h | K_2)|_e, (w_h | K_1)|_e) \) 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 \( p_h \in W \) such that

\[
R \frac{1}{2} \| u_h(T) \|^2_{L^2(\Omega)} + \int_0^T \Theta_C (\underline{w}_h, \underline{w}_h) \, dt + \int_0^T \| p_h \|^2_{(L^2(\Omega))^d} \, dt \\
+ \int_0^T \frac{R \lambda}{2} \| u_h \|^2_{L^2(\Omega)} \, dt \leq \frac{1}{2} \| u_h(0) \|^2_{L^2(\Omega)} \\
+ \int_0^T \frac{1}{2R \lambda} \| f \|^2_{L^2(\Omega)} \, dt ,
\]

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

\[
C = \begin{pmatrix}
c_{1,1} & -c^T \\
c & 0
\end{pmatrix}
\]
is the flux-matrix.
Design of new test-functions with local analytical solutions

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

\[- \sum_{K \in \mathcal{K}_h} (u_h, v \cdot \nabla \phi)_K + (u_h, R \lambda \phi) = 0\]  \hspace{1cm} (22)

\[- \sum_{K \in \mathcal{K}_h} (u_h, -\nu \cdot \nabla \phi + R \lambda \phi) = 0,\]

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

\[- \nu \cdot \nabla \phi + R \lambda \phi = 0,\]  \hspace{1cm} (23)

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]

\[-v \partial_x \phi + R \lambda \phi = 0\]  \hspace{1cm} (24)

where we derive the local solution

\[\phi_{anal,i}(x) = a_0 \begin{cases} \exp(-\beta (x_{i+1/2} - x)) & v > 0 \\ \exp(-\beta (x - x_{i-1/2})) & v < 0 \end{cases}, \hspace{1cm} (25)\]

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

\[\phi_{new,i} = \phi_{anal,i}(x), \hspace{1cm} (26)\]

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:

\[-v_x \partial_x \phi - v_y \partial_y \phi + R \lambda \phi = 0, \quad (27)\]

where we derive the local solution

\[
\phi_{\text{anal},i}(x) = a_0 \begin{cases} 
\exp(-\beta_x (x_{i+1/2} - x)) & v_x > 0 \\
\exp(-\beta_x (x - x_{i-1/2})) & v_x < 0
\end{cases}, \quad (28)
\]

where \( \beta_x = \frac{R \lambda}{2 |v_x|} \) and \( \beta_y = \frac{R \lambda}{2 |v_y|} \).

\[
\phi_{\text{new},i,j} = \phi_{\text{anal},i}(x) \phi_{\text{anal},j}(y), \quad (29)
\]

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:

<table>
<thead>
<tr>
<th>Level</th>
<th>$h^{-1}$</th>
<th>Elements</th>
<th>$E_{L_1}$</th>
<th>Conv. order for $E_{L_1}$</th>
<th>Time-Steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>8</td>
<td>1024</td>
<td>$4.37 \times 10^{-2}$</td>
<td></td>
<td>10</td>
</tr>
<tr>
<td>5</td>
<td>16</td>
<td>4096</td>
<td>$2.59 \times 10^{-2}$</td>
<td>0.75</td>
<td>20</td>
</tr>
<tr>
<td>6</td>
<td>32</td>
<td>16384</td>
<td>$1.04 \times 10^{-2}$</td>
<td>1.31</td>
<td>40</td>
</tr>
<tr>
<td>7</td>
<td>64</td>
<td>65536</td>
<td>$2.92 \times 10^{-3}$</td>
<td>1.83</td>
<td>80</td>
</tr>
</tbody>
</table>

Table 3: Convergence-Results for the DG-method for different levels and time-steps.
Advantages of the flexible DG-Methods

The DG-Methods are flexible in choosing the test-functions and we have more freedom-degrees in choosing the local characters of the function. We could therefore approximate the discontinuity (shocks, jumps) with respect to the functions.
19 Applications in Fluid-Mechanics

1.) Waste-Disposal (Transport reaction-Equation)
2.) Flow-Field of the groundwater and Transport-Field for the nuclids
1.) Sublimation Growth for SiC single Crystal (Heat-equation)

Stationary Temperature Field

- Height: 25 cm
- $T_{\text{min}} = 537.517$ K
- $T_{\text{max}} = 3312.53$ K
- $\Delta T_{\text{max}} = 0$ K
- Heating power in crucible: 7811.89 W
- Heating power in coil: 2188.11 W
- Prescribed power: 10000 W
- Frequency: 10000 Hz
- Coil: 5 rings
- Top: 0.18 m
- Bottom: 0.02 m
2.) Heat-flow-field with heat-transfer and radiation

Heat Source Field

height = 25 cm

PowDens_min=0 W/m^3
PowDens_max=7.70727e+06 W/m^3

heating power in crucible=7546.33 W
heating power in coil=2453.67 W

prescribed power = 10000 W
frequency = 10000 Hz

coil:
5 rings
top = 0.18 m
bottom = 0.02 m

t=100000 s
tstep=1e-05 s

delta powDens[W/m^3] between isolines

0 3e+07 powDens[W/m^3]
21 Conclusions and future works

- Mixed discretisation methods as idea decomposing into simpler problems.
- Detecting the physical change between hyperbolic and parabolic equations and using the adequate discretisation methods for each part problem.
- 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.