Discretization Methods with embedded analytical Solutions for convection dominated Transport in Porous Media.

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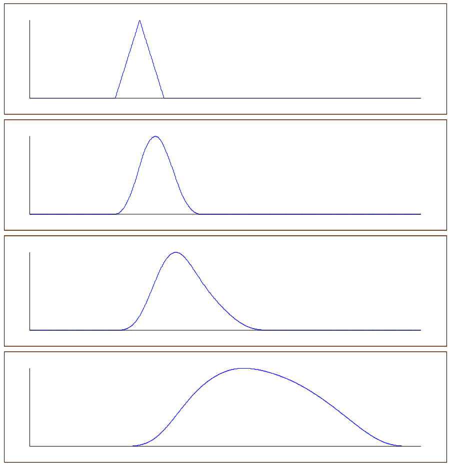


Analytical solution of one-dimensional convection-reaction-equations.

Introduction

Effective Discretization methods for convection-dominated transport equations.

- ▷ Task : Convection-dominated transport equation should be solved for large simulation-times.
- ▷ Problem: Stiff-systems and numerical diffusion, because of large scales in the reaction term and low order in the convection term. Standard discretization methods, e.g. implicit finite volume methods produce numerical artifacts.
- ▷ Solution: Modified discretization method based on finite volume methods with analytical solutions for the reaction-terms and higher order for the discretization-method to avoid the numerical artifacts.

Contents

1. Model-equations.

2. Analytical solutions for the one-dimensional convection-reaction-equations.

3. Spatial Discretization-method for the multi-dimensional convection-reaction-equation based on finite volume methods and explicit time Discretization.

4. Applications and verification of the methods with model-problems

5. New Design criterias for discretization methods based on finite Volume methods.

6. Future Works

Model-equations: Convection-Diffusion-Dispersion-Reaction-Equations

$$\phi\,\partial_t R_i(c_i) + \nabla \cdot \mathbf{v}\, c_i - \nabla \cdot D \nabla c_i = -\phi\, \lambda_i\, R_i(c_i) + \sum_{k=k(i)} \phi\, \lambda_k\, R_k(c_k)\ .$$

- ϕ : porosity .
- c_i : i-th concentration .
- R_i : i-th retardation-factor ,
  linear : $R_i = 1 + \frac{1-\phi}{\phi}\rho K_d^e$,
  nonlinear : $R_i = 1 + \frac{1-\phi}{\phi}\rho K(c_{e(i)})$,
  $c_{e(i)} = \sum_i c_i$ (summation over all isotopes for the element e) ,
  ρ : rock-density , K_d^e : constant factor (Henry-Isotherm) ,
  K : nonlinear function (Freundlich- or Langmuir-Isotherm) .
- λ_i : i-th decay-rate , $k(i)$: indices for the mother of the i-th isotopes .
- $\mathbf{v}$: velocity-vector , D : diffusions-dispersions-tensor .

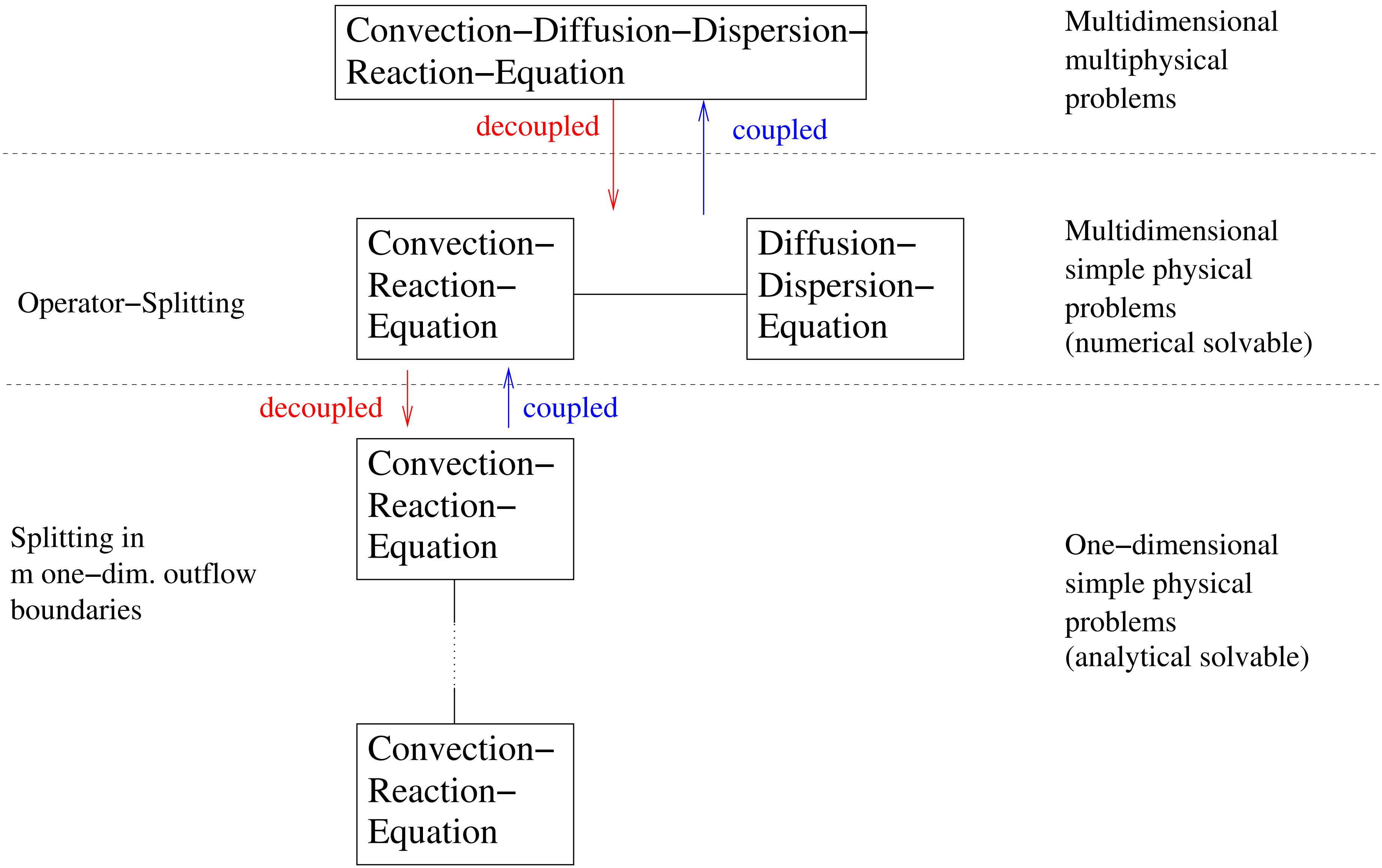
Design of Discretization-Methods and Operator-Splitting-Methods

Idea : Standard methods, e.g. Finite Volume Methods and improve them for the special equations.

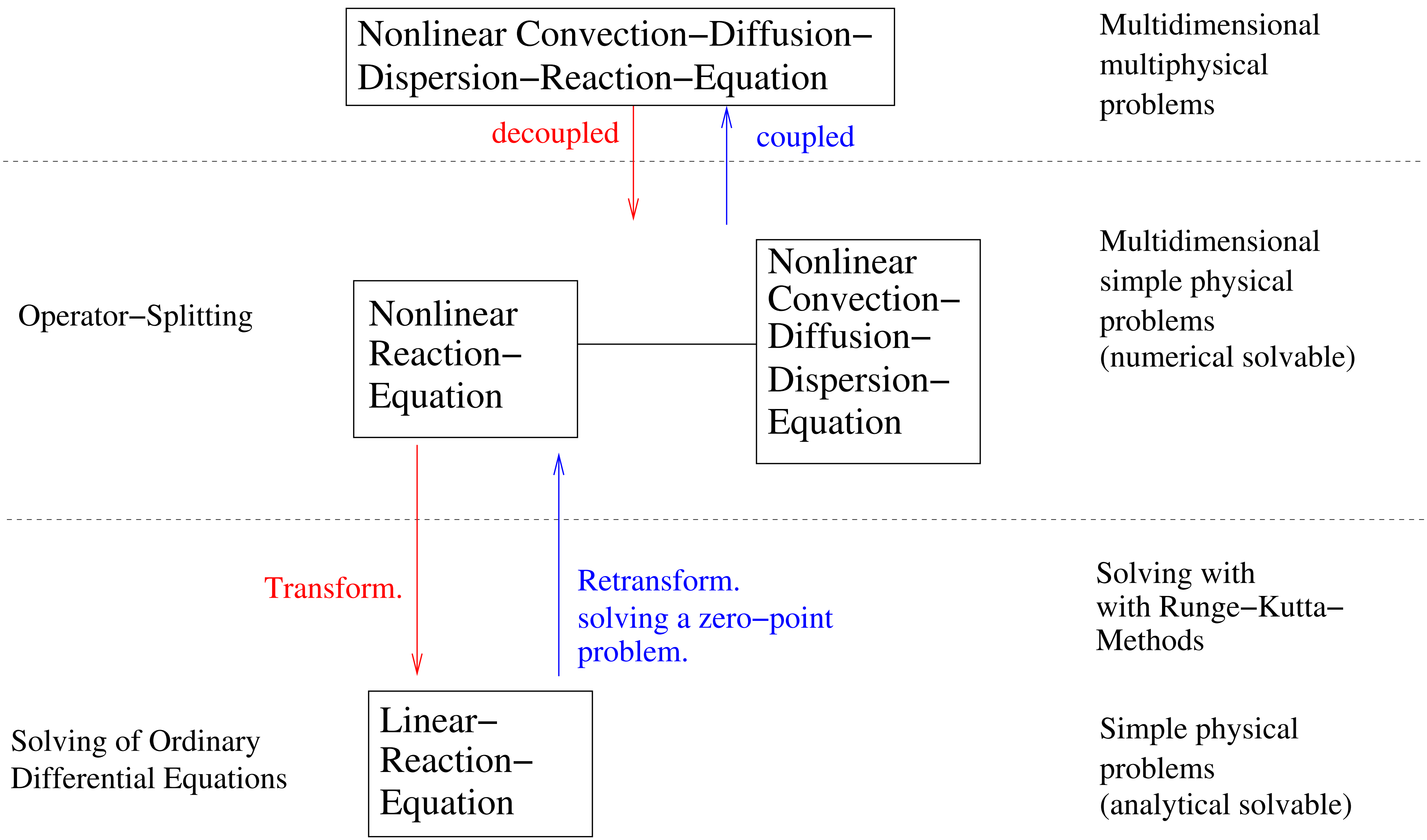
Multi-dimensional and Multi-physical problems decouple to one-dimensional and simple-physical problems.

- Operator-Splitting : Decoupling of equations with multi-physical processes in simpler equations with simple-physical processes (The terms of the equations are named operators).
- Dimensional-Splitting : Decoupling of multi-dimensional equations in one-dimensional equations, e.g. decoupling the m-dimensional convection-reaction-equation in m one-dimensional convection-reaction-equations, which are solved exact (m : number of the outflow-boundaries).

Decoupling of the equations (linear case)



Decoupling of the equations (nonlinear case)



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:

$$\partial_t c = Ac + Bc \ ,$$

whereby the initial-conditions are $c(t^n) = c^n$.

Splitting-method of first order:

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

whereby the result of the methods are $c(t^{n+1}) = c^{**}(t^{n+1})$.
And there are some splitting-errors for these methods.

Error of the Operator-Splitting-Method

The error of the splitting-method of first order :

$O(\tau)$ if A, B do not commute, otherwise it is exact,

whereby $\tau = t^{n+1} - t^n$.

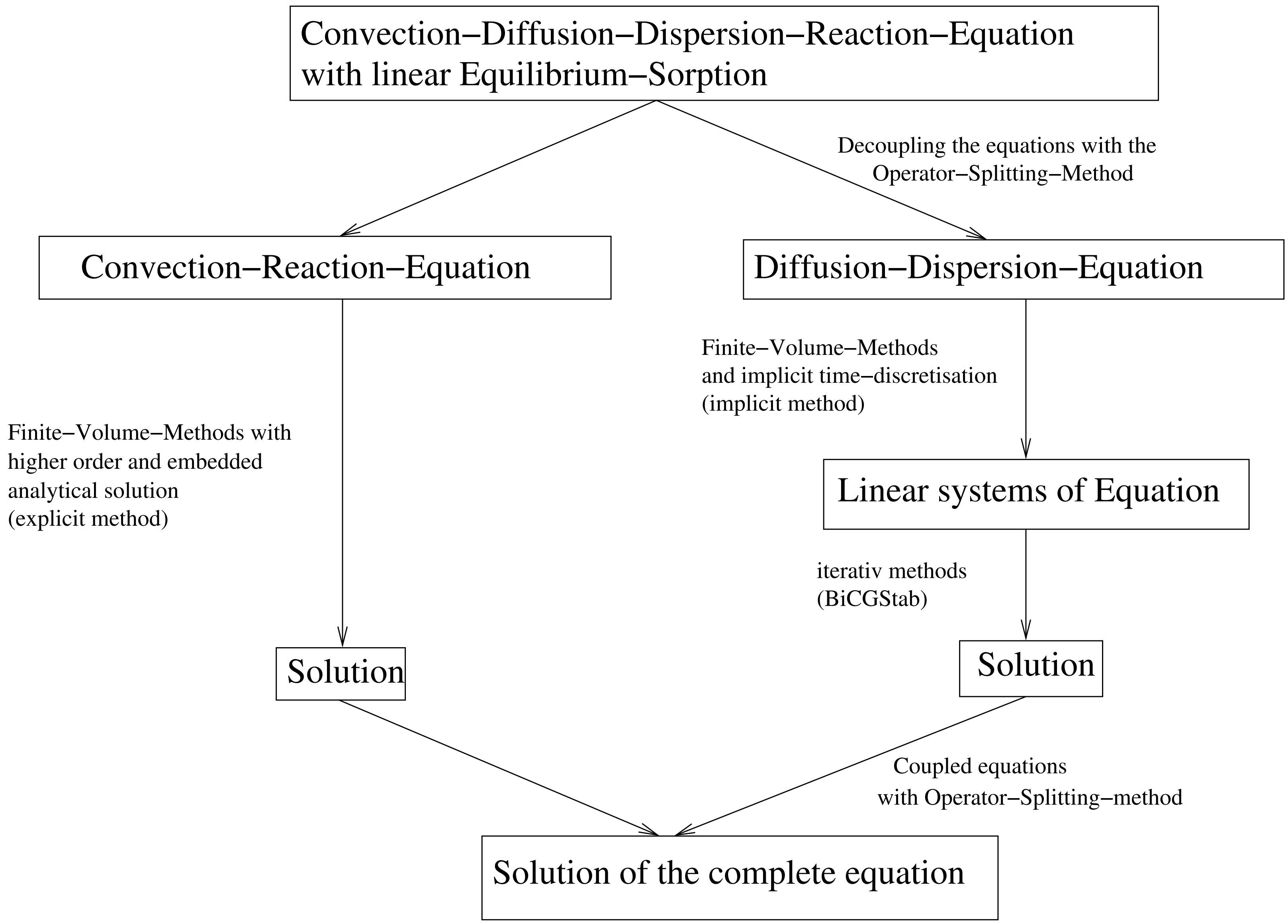
Proof: Solving the ODE's and subtracting the coupled and decoupled equations.

To improve the error order one could use splitting-methods of higher order :

Strang-Splitting-method: $O(\tau^2)$ if A and B do not commute, otherwise the method is exact ($[A, B] = 0$).

Iterative Splitting-methods : They are exact, but have a higher complexity because of the multiple application of the iterative method.

Discretization of the method



Discretization of the convection-equation

The scalar equation is given by:

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

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

The integration over space and time are:

$$\int_{\Omega_j} \int_{t^n}^{t^{n+1}} \partial_t (R\, c)\ dt\ dx = - \int_{\Omega_j} \int_{t^n}^{t^{n+1}} \nabla \cdot (\mathbf{v}\ c)\ dt\ dx \ ,$$

where Ω_j is the j-th cell.

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

The discretization-scheme with the mass-notation is:

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

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

with the limitation to fulfill the monotonicity (local min-max-property)
1.) Slope limiter (limitation of the slope) :

$$2c_i^n - \max_{k \in in(i)} \{c_i^n, c_k^n\} \leq \ \ c_{jk}^n \ \ \leq 2c_i^n - \min_{k \in in(i)} \{c_i^n, c_k^n\} \ , \ j \in out(i) \ ,$$

$$\min_{k \in in(i)} \{c_i^n, c_k^n\} \leq \ \ c_{ki}^n \ \ \leq \max_{k \in in(i)} \{c_i^n, c_k^n\} \ , \ k \in in(i) \ .$$

We get the limited values : $\hat{c}_{jk}^n$.

2.) Flux limiter (limitation of the mass-flux) :

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

$$\tau_j = \frac{V_j}{\nu_j} \ , \text{(maximum time-step with Cour.-Numb. 1)} \ ,$$

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

Discretization of the Reaction-Equation

The linear reaction-equation is solved analytically.

$$\partial_t R_i \, c_i = -\lambda_i R_i c_i + \lambda_{i-1} R_{i-1} c_{i-1} \ ,$$

whereby the initial-cond. are $c_{01} = c_1(t^0)$ otherwise 0.0 and $\lambda_0 = 0$.
The solution of the equations are :

$$c_i = c_{01} \, \frac{R_1}{R_i} \, \Lambda_i \sum_{j=1}^{i} \Lambda_{j,i} \exp(-\lambda_j \, t) \ , \qquad (1)$$

whereby $i = 1, \ldots, M$ is and M is the number of equations and it is essential:

$$\Lambda_i = \prod_{j=1}^{i-1} \lambda_j \ , \ \Lambda_{j,i} = \prod_{\substack{j=1 \\ j \neq k}}^{i} \frac{1}{\lambda_k - \lambda_j} \ , \ \text{with } \lambda_k \neq \lambda_j \text{ for } k \neq j \ . \qquad (2)$$

Discretization of the Nonlinear-Reaction-Equation

The nonlinear reaction-equation is solved quasi-analytical.

$$\partial_t R(c_i) = -\lambda_i R(c_i) + \lambda_{i-1} R(c_{i-1}) \ ,$$

where the initial-cond. are $c_1^n = c_1(t^n)$ otherwise 0.0 and $\lambda_0 = 0$.
We transform the equations with $u_i = R(c_i)$.
The linear equation could be solved analytically

$$\partial_t u_i = -\lambda_i u_i + \lambda_{i-1} u_{i-1} \ ,$$

where the initial-cond. are $u_1^n = u_1(t^n) = R(c_1^n)$ otherwise 0.0 and $\lambda_0 = 0$. The solutions are u_i. We solve a fixed-point-problem:

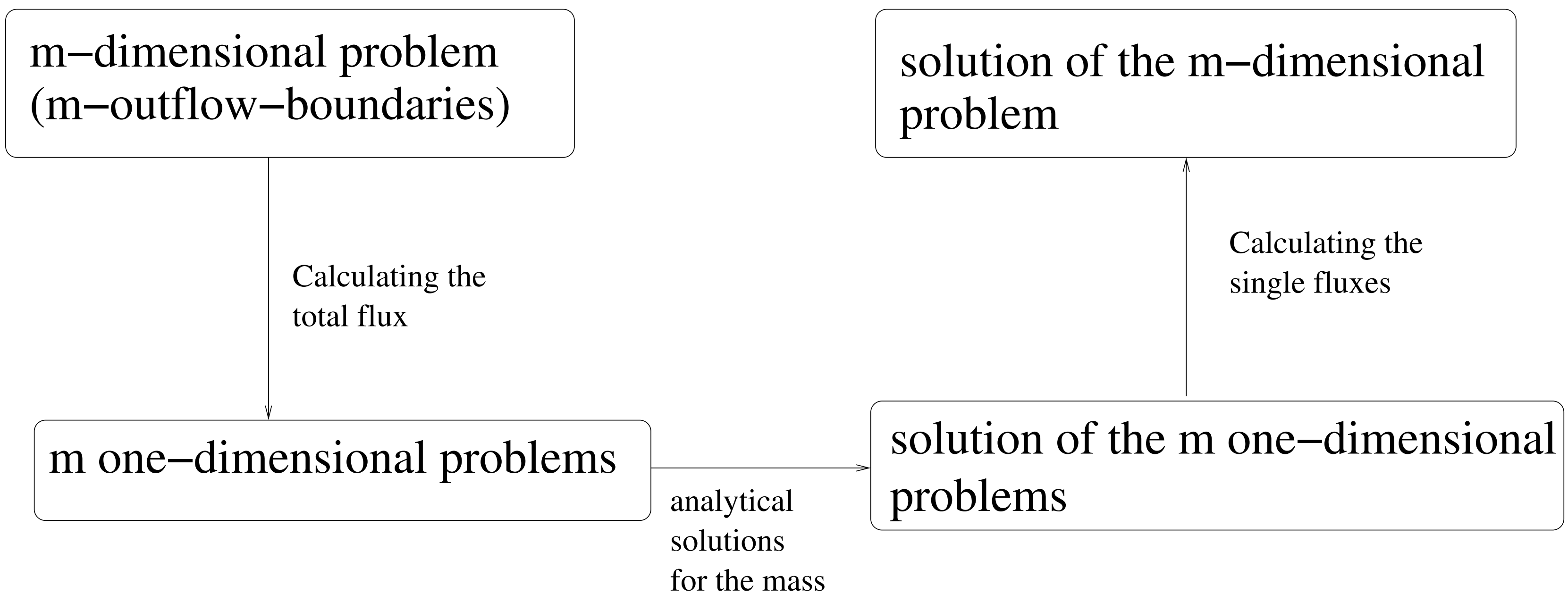
$$u_i^{n+1} - R(c_i^{n+1}) = 0 \ ,$$

where $u_i^{n+1} = u_i(t^{n+1})$ and $i = 1, \ldots, M$.

Discretization of the Convection-Reaction-Equation

Idea: Embedding of the analytical solution of the one-dimensional convection-reaction-equation in the finite-volume-method.

One could skip the operator-splitting-method between the convection- and reaction-equation and therefore the splitting-error.



Procedure for the 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 $c_1(x, t^n) = c_1^n(x)$ 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 $(0,1)$:

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

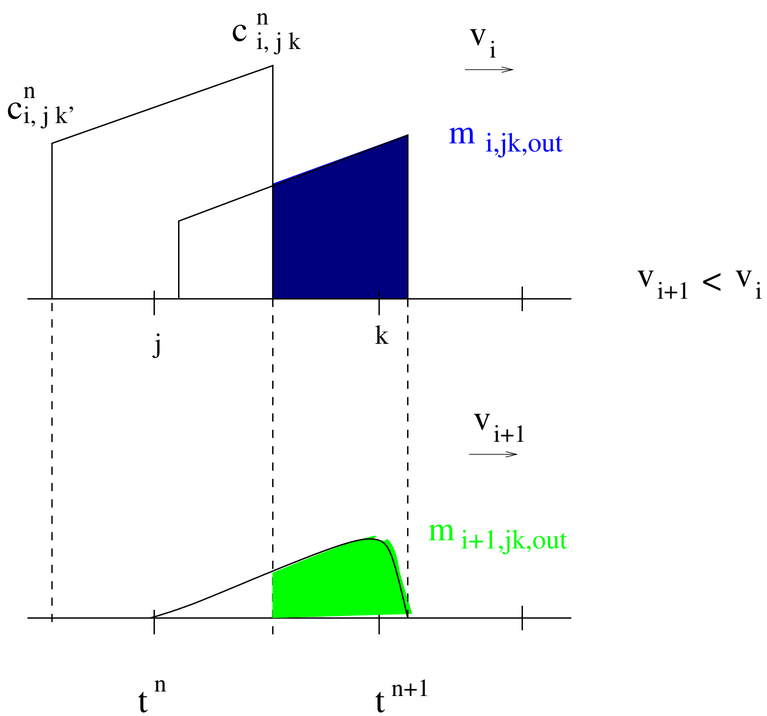
$$v_{i,j} = \frac{1}{\tau_{i,j}} \, , \quad \text{velocity in the cell j.}$$

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

and $a = V_j R_i (c^n_{i,jk} - c^n_{i,jk'})$, $b = V_j R_i c^n_{i,jk'}$ are the parameter for the linear initial-impulse for the finite-volume cell.



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

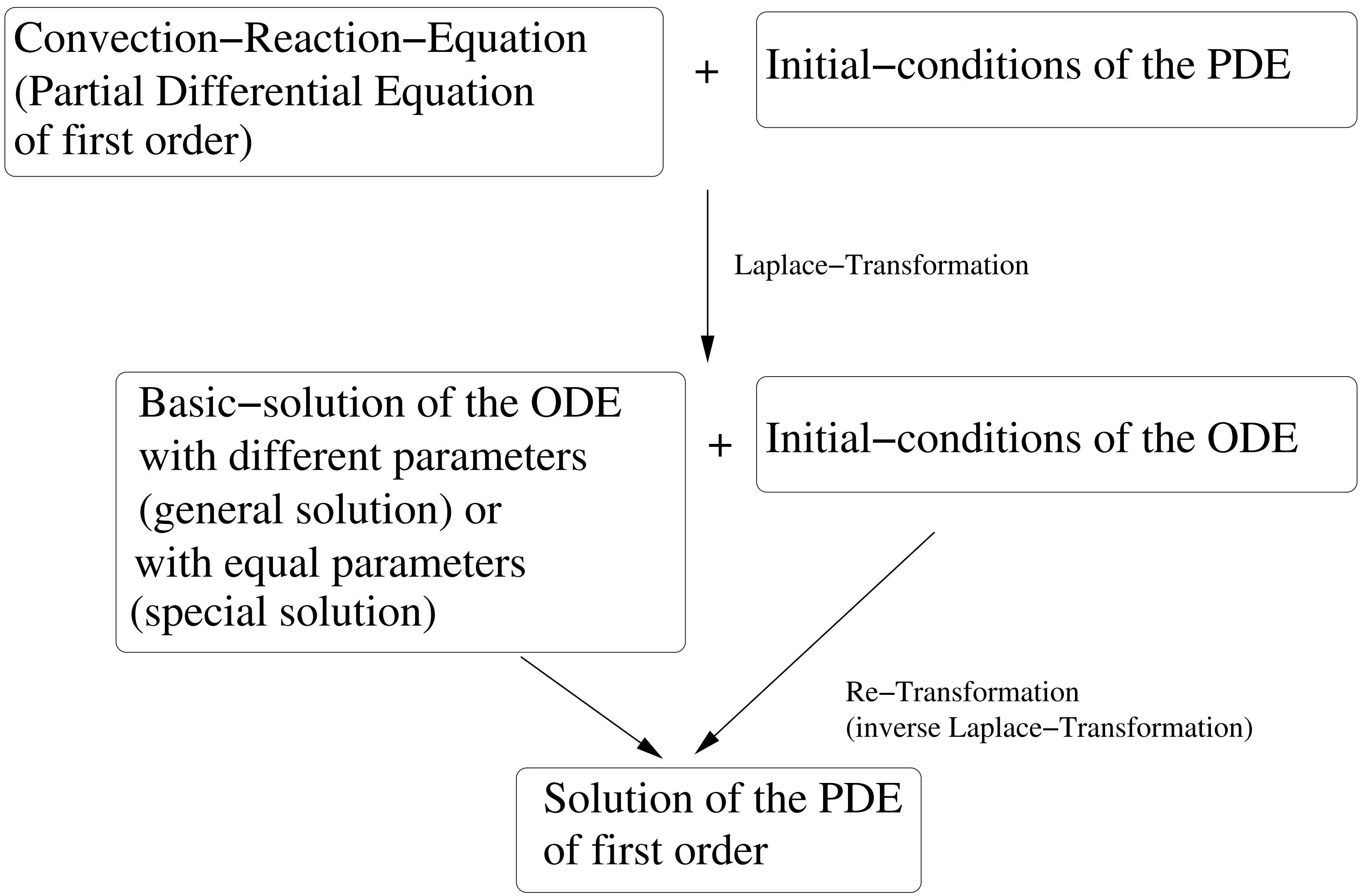
$$m_{i,jk}^n = \frac{v_{jk}}{\nu_j} \, m_{i,jk,out}^n \, .$$

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

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

Analytical solutions of the convection-reaction-equation

Laplace-transformation for the derivation of the solution:



Definition of the Laplace-Transformation

The Laplace-Transformation $\mathcal{L}$ is defined by:

$$\hat{f}(s) = \mathcal{L}(f(x)) := \int_0^\infty f(x) \exp(-sx) dx \; . \tag{3}$$

The Laplace-Transformation $\mathcal{L}$ assigns the function $f(x)$ the Laplace-Transformed $\hat{f}(s)$. The function $f(x)$ is defined in the codomain $0 \leq x < \infty$. The Laplace-transformed $\hat{f}(s)$ is defined in the codomain $0 < s < \infty$. Thereby x is the variable in the original-space and s is the variable in the Laplace-space.

Properties: Transformation from a PDE into an ODE.

The partial differential equation:

$$\frac{\partial u_i(x,t)}{\partial t} + v_i \frac{\partial u_i(x,t)}{\partial x} = -\lambda_i u_i(x,t) + \lambda_{i-1} u_{i-1}(x,t) \; , \quad (4)$$

with $i = 1, \ldots, M \; , \; \lambda_0 = 0.0 \; ,$

$$u_i(0,t) = 0.0 \; , \; \text{with} \quad i = 1, \ldots, M \; ,$$

$$u_1(x,0) = \begin{cases} ax + b & 0 \le x \le 1 \\ 0 & otherwise \end{cases} \; ,$$

$$u_i(x,0) = 0.0 \; , \; \text{with} \quad 0 \le x \text{ and } \quad i = 2, \ldots, M \; ,$$

is transformed into the ordinary differential equation:

$$\frac{\partial \hat{u}_i(s,t)}{\partial t} = -(s v_i + \lambda_i) \hat{u}_i(s,t) + \lambda_{i-1} \hat{u}_{i-1}(s,t) \; , \quad (5)$$

$$\hat{u}_1(s,0) = (\frac{a}{s^2} + \frac{b}{s})(1 - \exp(-s)) - \frac{a}{s} \exp(-s) \; ,$$

$$\hat{u}_i(s,0) = 0.0 \; , \quad \text{with} \quad i = 2, \ldots, M \; .$$

The solution of the ordinary differential equation is given as

$$\begin{aligned}
\hat{u}_1(s,t) &= \hat{u}_1(s,0)\ \exp(-(\lambda_1 + s v_1)t)\ , \\
\hat{u}_i(s,t) &= \hat{u}_1(s,0)\ \Lambda_i \\
&\quad \Big(\sum_{j=1}^{i} \exp(-(\lambda_j + s v_j)t) \Big(\prod_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{s(v_k - v_j) + (\lambda_k - \lambda_j)} \Big) \Big)\ .
\end{aligned}$$

where

$$\begin{array}{ll}
1. & \lambda_j \neq \lambda_k \quad \forall j,k = 1,\ldots,M, \quad \text{if} \quad j \neq k. \\
2. & v_j \neq v_k \quad \forall j,k = 1,\ldots,M, \quad \text{if} \quad j \neq k.
\end{array} \tag{6}$$

One could solve the ordinary differential equation with standard methods and the solution is re-transformed into the original-space.

The solution is given by:

$$u_1(x,t) = \exp(-\lambda_1 t) \begin{cases} 0 & 0 \leq x < v_1 t \\ a(x - v_1 t) + b & v_1 t \leq x < v_1 t + 1 \\ 0 & v_1 t + 1 \leq x \end{cases}, \quad (7)$$

$$u_i(x,t) = \Lambda_i \sum_{j=1}^{i} \left(L_{j,i} + \sum_{k>j}^{i} \begin{cases} M_{jk,i} & v_j < v_k \\ M_{kj,i} & v_k < v_j \\ 0 & otherwise \end{cases} \right), \quad (8)$$

with $i = 2, \ldots, M$,

whereby the factors $L_{j,i}$ and $M_{jk,i}$ are given by:

$$L_{j,i} \;:=\; \begin{cases} \exp(-\lambda_j t)\,\Lambda_{j,i}\,\Big(a(x-v_jt)+b & \\ -a\sum_{\substack{k=1\\k\neq j}}^{i}\frac{1}{\lambda_{jk}}\Big) & v_jt \le x \le v_jt+1 \\ 0 & otherwise \end{cases} ,$$

$$M_{jk,i} \;:=\; \begin{cases} \Lambda_{j,i}\,\Lambda_{jk,i}\,g_{jk} & v_jt \le x \le v_kt \\ \Lambda_{j,i}\,\Lambda_{jk,i}\,h_{jk} & v_jt+1 \le x \le v_kt+1 \\ 0 & otherwise \end{cases} , \text{ Couple-term },$$

and for the factors g_{jk} and h_{jk} are given by:

$$g_{jk} := -(b-\frac{a}{\lambda_{jk}})\exp(-\lambda_j t)\exp(-\lambda_{jk}(x-v_jt)) \;,$$

$$h_{jk} := (b-\frac{a}{\lambda_{jk}}+a)\exp(-\lambda_j t)\exp(-\lambda_{jk}(x-v_jt-1)) \;,$$

and the factors Λ_i , $\Lambda_{j,i}$ and $\Lambda_{jk,i}$ are :

$$\Lambda_i := \Big(\prod_{j=1}^{i-1} \lambda_j\Big) \; , \Lambda_{j,i} := \Big(\prod_{\substack{k=1 \\ k\neq j}}^{i} \frac{1}{\lambda_k - \lambda_j}\Big) \; ,$$

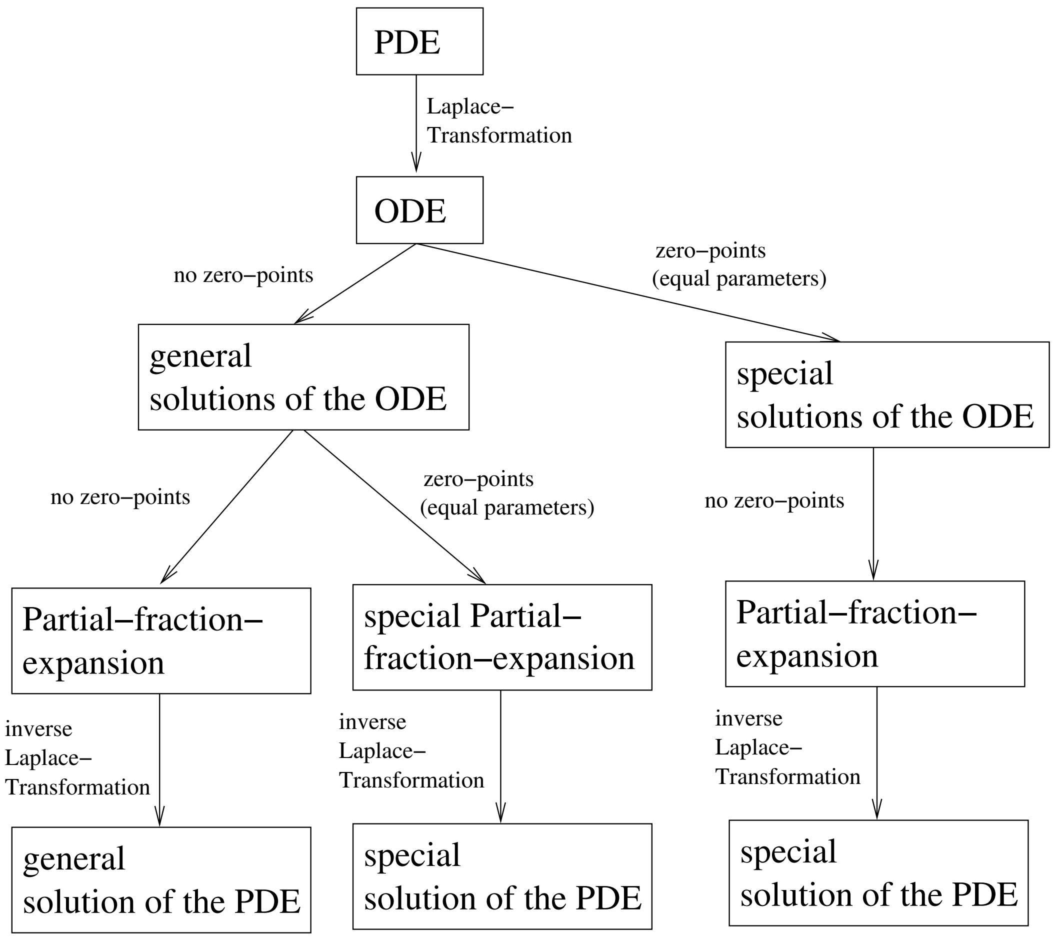
$$\Lambda_{jk,i} := \Big(\prod_{\substack{l=1 \\ l\neq k \\ l\neq j}}^{i} \frac{\lambda_{jl}}{\lambda_{jl} - \lambda_{jk}}\Big) \; , \; \lambda_{jk} := \frac{\lambda_j - \lambda_k}{v_j - v_k} = \lambda_{kj} \; .$$

The factors are given with the following parameters:

1. $\lambda_j \neq \lambda_k \quad \forall j, k = 1, \ldots, M,$ for $j \neq k.$
2. $v_j \neq v_k \quad \forall j, k = 1, \ldots, M,$ for $j \neq k.$
3. $\lambda_{jk} \neq \lambda_{jl} \quad \forall j, k, l = 1, \ldots, M,$ for $j \neq k \wedge j \neq l \wedge k \neq l.$

Calculating for the special solutions

For the special solutions one could eliminate the zero-points out of the equations. After the elimination one could transform the equations. The derivation is described in the thesis of J.Geiser Doktorarbeit 2003.



Special solutions

We could eliminate the special-points $\lambda_l = \lambda_{a(l)}$ out of the equations and get the transformed equation.

$$\hat{u}_i(s,t) = \hat{u}_1(s,0)\, \Lambda_i \tag{9}$$

$$\cdot \Bigg(\frac{\exp(-(\lambda_l + s v_l) t)}{s(v_{a(l)} - v_l)} \prod_{\substack{k=1 \\ k \neq l \\ k \neq a(l)}}^{i} \frac{1}{s(v_k - v_l) + (\lambda_k - \lambda_l)}$$

$$+ \frac{\exp(-(\lambda_{a(l)} + s v_{a(l)}) t)}{s(v_l - v_{a(l)})} \prod_{\substack{k=1 \\ k \neq a(l) \\ k \neq l}}^{i} \frac{1}{s(v_k - v_{a(l)}) + (\lambda_k - \lambda_{a(l)})}$$

$$+ \sum_{\substack{j=1 \\ j \neq l \\ j \neq a(l)}}^{i} \exp(-(\lambda_j + s v_j) t) \prod_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{s(v_k - v_j) + (\lambda_k - \lambda_j)} \Bigg) .$$

Example for 2 equations for the special solutions

For the special solutions we use the same method of 2 components for $\lambda_1 = \lambda_2$, the further special solutions, confer [geiser-diss03].

The solution for $i = 2$ and $(l, a(l)) = (1, 2)$ are given as :

$$c_2 = \ \lambda_1 \ \exp(-\lambda_1 t) \left(\frac{1}{v_2 - v_1} \alpha_1 + \frac{1}{v_1 - v_2} \alpha_2 \right) , \tag{10}$$

$$\alpha_l = \begin{cases} 0 & 0 \leq x < v_l t \\ a \frac{(x - v_l t)^2}{2} + b(x - v_l t) & v_l t \leq x < v_l t + 1 \\ a \frac{1}{2} + b & v_l t + 1 \leq x \end{cases} . \tag{11}$$

The solutions are derived in the transformed Laplace-space and the term $\lambda_l - \lambda_{a(l)}$ is skipped because of the singular point.

Calculation of the analytical mass-solution

The mass is given by integrating over a norm-interval $(0, 1)$ and is given by:

1.) The mass, which is rested in the norm-interval:

$$m_{i1}(t) \;=\; \int_0^1 u_i(x,t)dx = \int_{\min_{k=1}^i \{v_k t\}}^1 u_i(x,t)dx \; . \tag{12}$$

2.) The mass, which is flowed out of the norm-interval:

$$m_{i2}(t) \;=\; \int_1^\infty u_i(x,t)dx = \int_1^{\max_{k=1}^i \{v_k t + 1\}} u_i(x,t)dx \; . \tag{13}$$

The analytical solution for the residual masses

After the integration and reduction we received the following mass, which retain in the cell.

$$
\begin{aligned}
m_{i1} \quad = \quad & \Lambda_i \sum_{j=1}^{i} \Lambda_{j,i} \\
& \cdot \exp(-\lambda_j t) \left(a \frac{(1 - v_j t)^2}{2} + b(1 - v_j t - \sum_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_{jk}}) \right. \\
& \left. - a(1 - v_j t)(\sum_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_{jk}}) + a \Big(\sum_{\substack{k=1 \\ k \neq j}}^{i} \frac{1}{\lambda_{jk}} (\sum_{\substack{l \geq k \\ l \neq j}}^{i} \frac{1}{\lambda_{jl}}) \Big) \right) \quad . \quad (14)
\end{aligned}
$$

The analytical solutions for the out flowing masses

The out flowing masses could derived form the total masses and the residual masses:

$$m_{i2} = m_{i,ges} - m_{i1} \; ,$$

whereby is:

$$\begin{aligned} m_{i,ges} &= m_{impuls} \, c_{i,GDGL} \\ &= (a\frac{1}{2} + b) \, \Lambda_i \sum_{j=1}^{i} \Lambda_{j,i} \exp(-\lambda_j t) \; . \end{aligned} \qquad (15)$$

The methods for the nonlinear equations

We have the nonlinearity in the time-discretization and in the reaction-term.

$$\partial_t f(u) + \nabla \cdot \mathbf{v}\, u - \nabla \cdot D \nabla\, u = -f(u)\;,$$

where the nonlinearity is given by the Freundlich- or Langmuir-Isotherm,

The first idea is a splitting method between the convection-diffusion and reaction-equation.

$$\begin{aligned} \partial_t f(u^*) &= -f(u^*)\;,\; u^* = u(0)\;, \\ \partial_t f(u^{**}) &= -\nabla \cdot \mathbf{v}\, u^{**} + \nabla \cdot D \nabla\, u^{**}\;,\; u^{**} = u^*(\Delta t)\;, \end{aligned} \quad (16)$$

where we could solve the nonlinear reaction analytical such that :

$$\begin{aligned} \partial_t w &= -w \; , \; w = f(u(0)) \; , \\ -w(\Delta t) + f(u) &= 0 \; , \; fixed - point - problem \; , \end{aligned}$$

The used Methods

Standard-Methods :

The convection-equation is explicit discretizised with finite volume methods of higher order.
The reaction-equation is exact solved (ordinary differential equation).
The partial solutions are coupled with Operator-Splitting methods.

Modified-Methods :

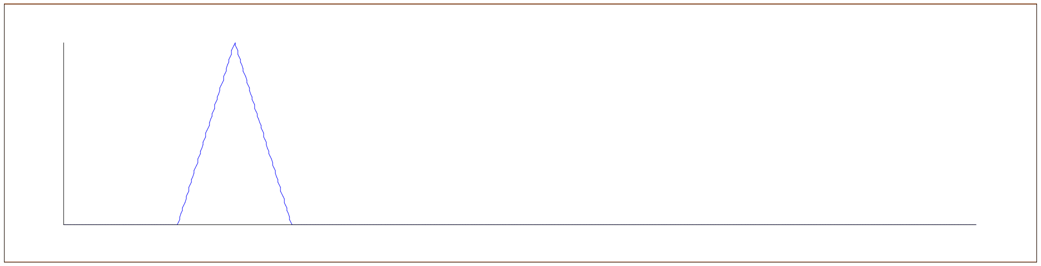
The convection-reaction-equation is explicit discretised with finite volume methods of higher order and embedded analytical solutions.
The operator-splitting-method is not used and therefore no operator-splitting error occur.

Application of the methods

One-dimensional example:
Decay chain : $c_1 \rightarrow c_2 \rightarrow c_3 \rightarrow c_4$
Decay rates : $\lambda_1 = 0.4, \lambda_2 = 0.3, \lambda_3 = 0.2, \lambda_4 = 0.0$ and the retardation-factors $R_1 = 1.0, R_2 = 2.0, R_3 = 4.0, R_4 = 8.0$.

Domain of the model: rectangle with 8×1 units,
Coarse grid : 8 elements ,
Refinement : uniform till level 7 $(131072$ elements) ,
Model time : $t = 0, \ldots, 6$.

Initialization for $t = 0.0$ with continuous triangle-impulse for the first component, for the other components 0.0:



Results for the calculations with standard- and modified-method

l	$E^1_{L_1}$	$\rho^1_{L_1}$	$E^2_{L_1}$	$\rho^2_{L_1}$	$E^3_{L_1}$	$\rho^3_{L_1}$	$E^4_{L_1}$	$\rho^4_{L_1}$
4	0.0		$1.71\ 10^{-3}$		$1.04\ 10^{-3}$		$2.407\ 10^{-4}$	
5	0.0	∞	$8.61\ 10^{-4}$	0.989	$5.28\ 10^{-4}$	0.978	$1.22\ 10^{-4}$	0.98
6	0.0	∞	$4.29\ 10^{-4}$	1.005	$2.65\ 10^{-4}$	0.995	$6.13\ 10^{-5}$	0.993
7	0.0	∞	$2.14\ 10^{-4}$	1.003	$1.31\ 10^{-4}$	1.016	$3.07\ 10^{-5}$	0.997

Table 1: L_1-error and convergence-order for the standard method

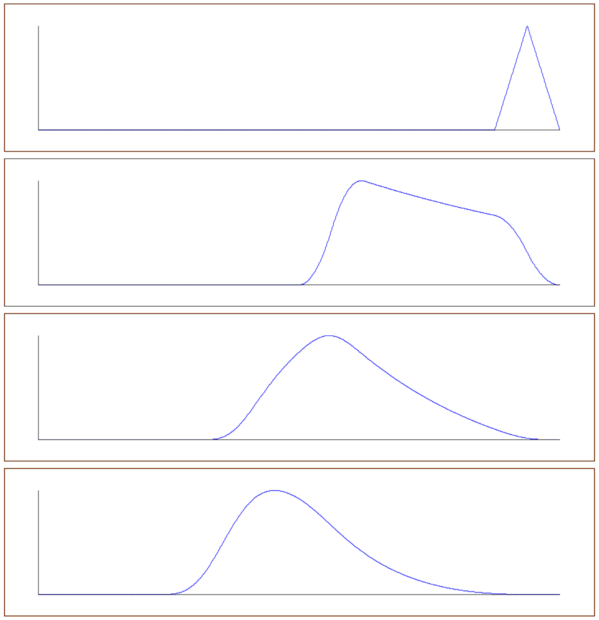
l	$E^1_{L_1}$	$\rho^1_{L_1}$	$E^2_{L_1}$	$\rho^2_{L_1}$	$E^3_{L_1}$	$\rho^3_{L_1}$	$E^4_{L_1}$	$\rho^4_{L_1}$
4	0.0		$3.06\ 10^{-4}$		$3.91\ 10^{-5}$		$7.79\ 10^{-6}$	
5	0.0	∞	$8.03\ 10^{-5}$	1.95	$9.87\ 10^{-6}$	1.986	$2.15\ 10^{-6}$	1.89
6	0.0	∞	$2.007\ 10^{-5}$	2.0	$2.60\ 10^{-6}$	1.93	$5.81\ 10^{-7}$	1.89
7	0.0	∞	$4.36\ 10^{-6}$	2.21	$6.66\ 10^{-7}$	1.96	$1.51\ 10^{-7}$	1.94

Table 2: L_1-error and convergence-order for the modified method

Modified method: First component is exact (Cour. $=1$), further components have second order, because of the analytical solutions.

Solutions of the one-dimensional test-examples

Solution with ascending retardation-factors in the time $t = 6$.



Example with ascending retardation-factors

Analogy results with descending retardation-factors $R_1 = 8.0, R_2 = 4.0, R_3 = 2.0, R_4 = 1.0$:

Example with descending retardation-factors

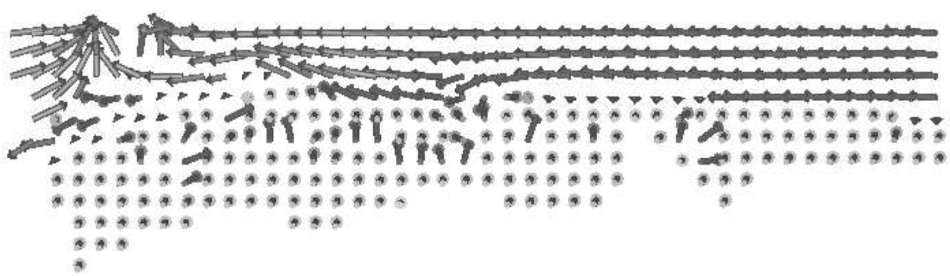
Results for the verifications

The standard method has an error with 1 order because of the used splitting method of 1 order.

The modified method has an error with 2 order because of the coupled equations. The splitting-error omits and the 2 order arise from the discretization method, which is of 2 order.

Simulations of a potential waste disposals

For the 3 dimensional damage event a sector of the domain is used with the size $6000[m] \times 1500[m]$. The flow of the groundwater and the transport with the contaminants are simulated. The parameters used for the examples are from the project-partner GRS (society of reactor security).



Computing of the velocity-field

The velocity-field done with $d^3 f$ (distributed density driven flow)

Flux-equation :

$$\partial_t(\phi\rho) \; + \nabla \cdot (\rho \mathbf{v}) = Q \; , \tag{17}$$

ρ : density of the fluid, ϕ : effective porosity, Q : source-term
$\mathbf{v}$ is given by the Darcy law :

$$\mathbf{v} = -\nabla p + \rho \; c \; \mathbf{g} \; , \tag{18}$$

p : fluid pressure , $\mathbf{g}$: gravity.

Transport-equation of the salt c is:

$$\partial_t(\phi\rho c) \; + \nabla \cdot (\rho \mathbf{v} c - \rho D \nabla c) = Q' \; , \tag{19}$$

The decay chain of a realistic potential damage events

$$Pu-244 \rightarrow Pu-240 \rightarrow U-236 \rightarrow Th-232 \rightarrow Ra-228$$

$$Cm-244 \rightarrow Pu-240$$

$$U-232$$

$$Pu-241 \rightarrow Am-241 \rightarrow Np-237 \rightarrow U-233 \rightarrow Th-229$$

$$Cm-246 \rightarrow Pu-242 \rightarrow U-238 \rightarrow U-234 \rightarrow Th-230 \rightarrow$$

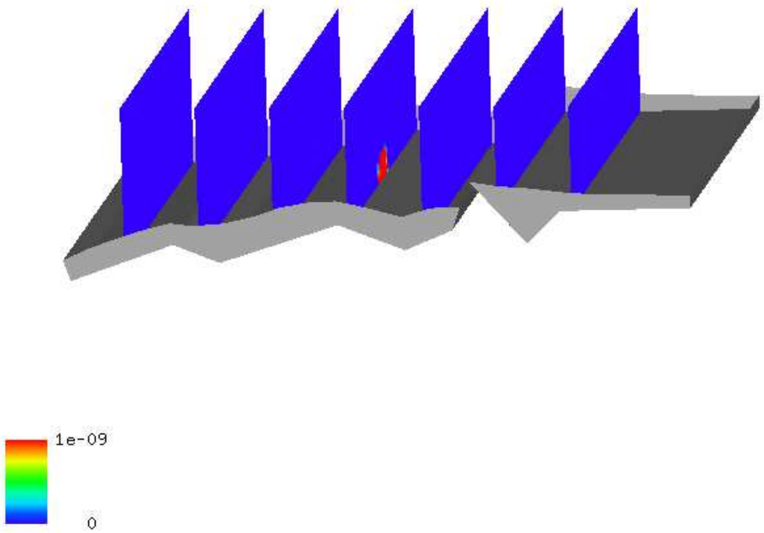
$$Ra-226 \rightarrow Pb-210$$

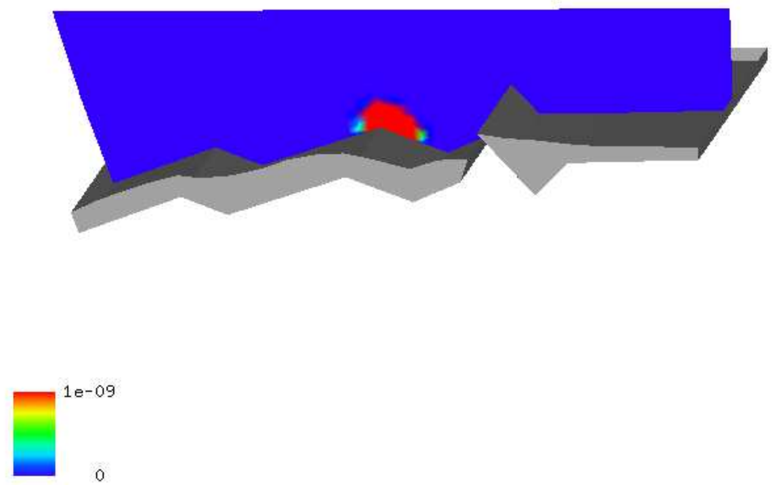
$$Am-242 \rightarrow Pu-238 \rightarrow U-234$$

$$Am-243 \rightarrow Pu-239 \rightarrow U-235 \rightarrow Pa-231 \rightarrow Ac-227$$

Uranium is few retarded and decayed slow, e.g. Uranium is transported very wide and the contamination in the porous media is high.

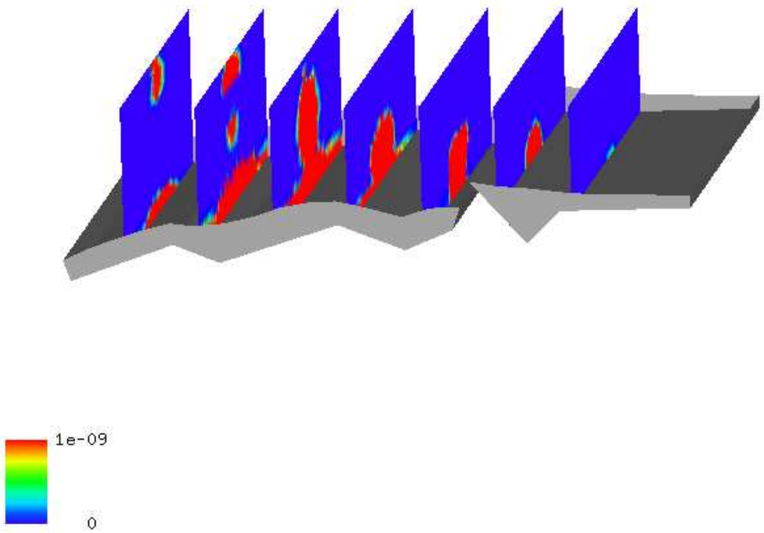
Concentration of U-236 in the time $t = 100\ [a]$.

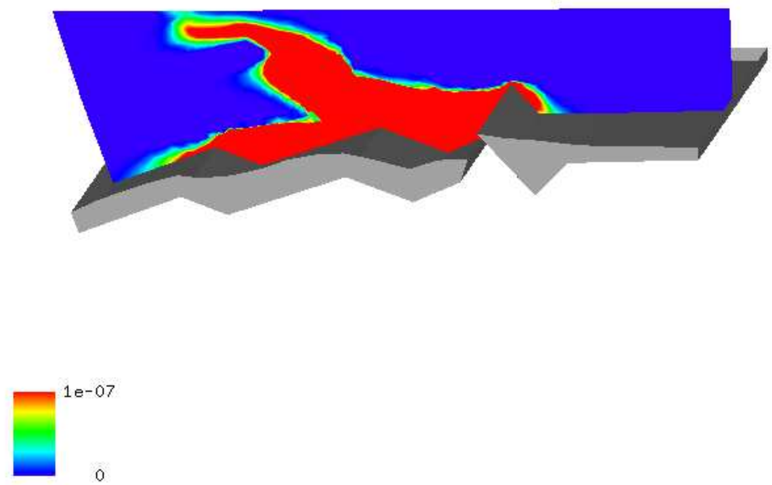




(visualised with the program Grape (University Freiburg, Germany))

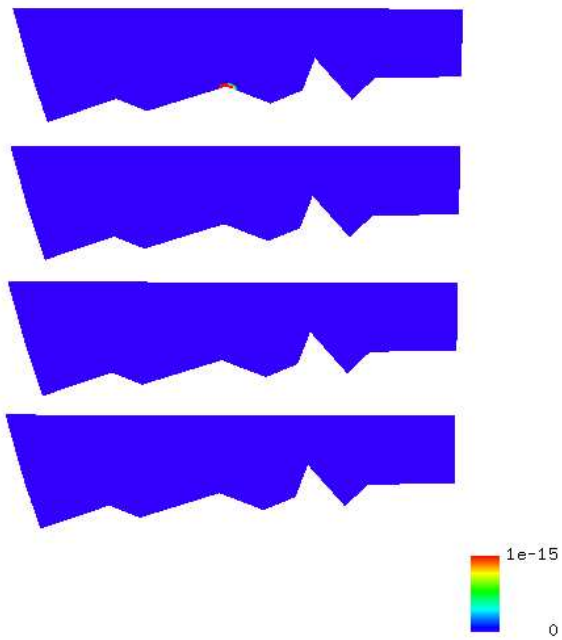
Concentration of von U-236 in the time $t = 10000\ [a]$.

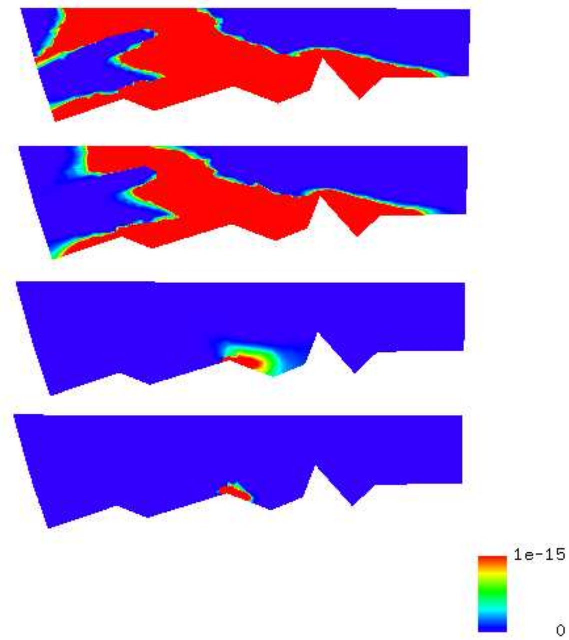




Decay chain : U-238 $\rightarrow$ U-234 $\rightarrow$ Th-230 $\rightarrow$ Ra-226

Solutions in the time-point $t = 50\ [a]$ and $t = 10000\ [a]$.





Computing times of a realistic potential damage event in 3d

Done with a Linux-PC-Cluster with Athlon-computers $1.6\,GHz$,
time step-width : $0.11 - 3.0\ [a]$,
Coarse grid: 8301 elements ,
uniform calculation : 2 times uniform refined
adaptive calculation : 2 times uniform refined, till level 5 adaptive refined

Processors	Refinement	Number of elements	Number of time-steps	time for one time step	total time
16	uniform	531264	3600	13.0 sec.	13.0 h
72	adaptive	580000	3600	18.5 sec.	18.5 h

Table 3: Three dimensional calculations of a realistic potential damage event.

Visualisation of the calculations (films)

3d-Calculations

Velocity field and calculation with 3 components

2d-Calculations:

Calculation with 3 components in 2d

Conclusions and future works

- ▷ Embedding of analytical solutions in discretization-methods to get higher order methods.
- ▷ Decouple multidimensional and multi-physics problems into one-dimensional and simpler-physical problems.
- ▷ Derivation of further analytical solutions for the diffusion-reaction-equation and also for the nonlinear equation-parts and embedding the results in explicit discretization methods.
- ▷ General higher order methods for the discretization for convection-diffusion-reaction-equations with analytical improvements (DG-Methods, ELLAM-methods)