Weierstrass Institute for Applied Analysis and Stochastics
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Jürgen Geiser

Operator Splitting Methods for Transport Equations with Nonlinear Reactions.

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Mohrenstrasse 39, 10117 Berlin, Germany ++49 (30) 2 03 72 541 http://www.wias-berlin.de/~geiser
geiser@wias-berlin.de

1 Introduction

Idea : Operator-splitting method for decoupling complex equations with mixed discretization methods.

- Task : Simulation of real life applications for complex problems, with mathematical background, e.g. time- and space processes.
- Models : Convection-diffusion models, heat-transfer models, Phase transitions
- Equations : Nonlinear Partial Differential equations with time-, space- variables.
- Solution: Adequate discretization methods for the convection-reaction equation with nonlinear reactions.
- Methods: Operator-Splitting, Characteristic- and Finite-Volume-methods, implicit-explicit-methods.

2 Contents

- Motivation for the Numerical Mathematics
- Introduction to the Methods for Discretisation and Operator-Splitting
- Operator-Splitting-Methods
- Discretization, Solvers and Implementation
- Analysis of the discretisation
- Real life applications (porous media, crystal-growth)
- Numerical Results
- Discussion and further works

3 Motivation for the Studying the Numerical Mathematics

- Approximate results in mathematics
- Application in Mathematics
- Paradigm Change in the mathematics with new computer technics
- efficiency of computations for real-life problems

Demand a new direction in the numerical mathematics done with simulation for realistic processes for the real-life-problem, based on time- and space dependent effects.

For this aspect the models based on partial differential equations are reseach topic in the numerical mathematics.

Example : Convection-diffusion-equation with nonlinear reactions

Model-equation for simulating the transport and decay of particles in a fluid, e.g. groundwater The mathematical equations are given as

$$u_t + \nabla \cdot (\mathbf{v}u - D\nabla u) = R(u) \ + \ f(\mathbf{x}, t), \ \mathbf{x} \in \Omega, \ t \in (0, T), \quad (1)$$

$$u|_{\partial\Omega} = 0, \ u(\mathbf{x}, 0) = u_0(\mathbf{x}). \quad (2)$$

The unknown density or concentration of the species $u = u(\mathbf{x}, t)$ is considered in $\Omega \times (0, T) \subset I\!R^d \times I\!R$, the space-dimension is denoted by d . The right-hand side $f(\mathbf{x}, t)$ is given in $\Omega \times (0, T)$. D is the Scheidegger diffusion-dispersion tensor and $\mathbf{v}$ is the divergence-free velocity.

We concentrate us to the following reaction-terms $R(u)$

$$R(u) = -au, \text{ radioactive decay}, \ a \geq 0, \tag{3}$$

$$R(u) = u^p, \text{ chemical-reaction}, \ p > 0, \tag{4}$$

$$R(u) = au - bu^2, \text{ logistic model}, \ a, b \geq 0, \tag{5}$$

$$R(u) = \frac{au}{u+b}, \text{ bio-remediation}, \ a, b \geq 0. \tag{6}$$

4 Operator-Splitting Methods

The operator-splitting methods are used to solve complex models in the geophysical and environmental physics. These ideas are applied to decouple in solving simpler equations and we use higher order discretization methods to improve order of the solution. Our operators are written as

$$u_t = A(u) + B(u), \tag{7}$$

with

$$A(u) = -\mathbf{v} \cdot \nabla u + R(u), \tag{8}$$

$$B(u) = \nabla \cdot (\mathbf{D} \nabla u) + f(\mathbf{x}, t). \tag{9}$$

Let N be a positive integer, $\Delta t := T/N$, $t_n = n\Delta t$ with $n = 0, 1, \ldots, N$ be a uniform partition of the time period $[0, T]$.

The operator-splitting method for the operators A, B can be used for a first order method as

$$u_t^{(1)} = A(u^{(1)}) \text{ with } t^n \leq t \leq t^{n+1} \text{ and } u^{(1)}(\mathbf{x}, t^n) = u(\mathbf{x}, t^n), \quad (10)$$

$$u_t^{(2)} = B(u^{(2)}) \text{ with } t^n \leq t \leq t^{n+1} \quad (11)$$

and the splitting-error can be written as

$$\rho_n = \frac{1}{2}\Delta t \; ((\frac{\partial A}{\partial u} B)(u) - (\frac{\partial B}{\partial u} A)(u)) + O(\Delta t^2) \; . \quad (12)$$

where we obtain a splitting-error $O(\Delta t)$, if the operators A, B did not commute otherwise we get an exact method.

For our nonlinear operators A and B given in equation (8) and (9) we apply the splitting-error and derive the following result

$$((\frac{\partial A}{\partial u} B)(u) - (\frac{\partial B}{\partial u} A)(u))$$
$$= ((-\mathbf{v} \cdot \nabla + \frac{\partial R}{\partial u})(\nabla \cdot \mathbf{D} \nabla))(u) - ((\nabla \cdot \mathbf{D} \nabla)(-\mathbf{v} \cdot \nabla + R))(u) \neq 0,$$

for nonlinear functions $R(u)$. We obtain an splitting-error of $O(\Delta t)$ for the nontrivial non-commuting case.

For the solution method of the coupled equation (1), we split into two equations for the small time period $[t_n, t_{n+1}]$

$$\frac{du}{dt} = u_t + \mathbf{v} \cdot \nabla u = R(u), \qquad (13)$$

$$u_t = \nabla \cdot (\mathbf{D} \nabla u) + f(\mathbf{x}, t). \qquad (14)$$

5 Discretisation and Solvers

a.) Convection-reaction-equation:

For the solution method of the coupled equation (1), we split into two equations for the small time period $[t_n, t_{n+1}]$

$$\frac{du}{dt} = u_t + \mathbf{v} \cdot \nabla u = R(u), \tag{15}$$

$$u_t = \nabla \cdot (\mathbf{D} \nabla u) + f(\mathbf{x}, t). \tag{16}$$

The convection-reaction equation is solved along the characteristics and becomes a nonlinear ODE

$$\left\{ \begin{array}{l} \dfrac{du^{(1)}}{dt} = R(u^{(1)}), \quad t \in (t_n^*, t_{n+1}), \\ u^{(1)}(\mathbf{x}^*, t_n^*) = u^{(2)}(\mathbf{x}^*, t_n^*), \end{array} \right. \tag{17}$$

where $(\mathbf{x}, t)$ is the exact backtracking of $(\mathbf{x}, t)$ and $u^{(2)}$ is the solution for the parabolic problem. For $n = 0$ or $\mathbf{x}^* \in \partial\Omega$, we replace $u^{(2)}(\mathbf{x}^*, t_n^*)$ by $u_0(\mathbf{x}^*)$ or the boundary condition. We solve our equation (17) numerically by explicit Euler or Runge-Kutta methods.

b.) Diffusion-Equation

The second part is an initial boundary value problem for a typical parabolic equation

$$\begin{cases} u_t^{(2)} = \nabla \cdot (\mathbf{D} \nabla u^{(2)}) + f(\mathbf{x}, t), \quad \mathbf{x} \in \Omega, \ t \in (t_n, t_{n+1}), \\ u^{(2)}|_{\partial\Omega} = 0, \\ u^{(2)}(\mathbf{x}, t_n) = u^{(1)}(\mathbf{x}, t_{n+1}). \end{cases} \tag{18}$$

It is solved by a standard finite difference, element, or volume methods. For explicit time-discretization methods of our equation (18), e.g. forward Euler-method, we restrict our time-step Δt for the stability condition $|\mathbf{D}| \Delta t / h^2 \leq 1/2$, with $|\mathbf{D}| << 1$. By using implicit time-discretization, e.g. backward Euler-method time-restriction is not necessary.

6 Implementation of Operator Splitting Methods

Strategies of the method based on software integration techniques such as dynamic link library(DLL) and component object model (COM).

A dynamic link library(DLL) is a collection of functions and data that are available for use by one or more applications running on the same computer system. Executable code modules in a DLL are loaded on demand and linked at run time, and then unloaded when they are no longer needed.

Nonlinear ODEs along characteristics are actually solved along approximate characteristics. Euler and Runge-Kutta methods can be applied.

Numerically solving an initial boundary value problem to a linear parabolic equation via the finite difference/element/volume method is now more or less a conventional task.

7 Numerical experiments

Example 1: Linear Reaction

We consider a 2-dimensional problem with a linear reaction. Our rotating velocity is $\mathbf{v} = (-4y, 4x)$ and we have constant scalar diffusion $D > 0$. A linear reaction $R(u) = Ku$ with K being a constant. A null source/sink, i.e., $f \equiv 0$. The initial condition is specified as a Gaussian hill

$$u_0(x,y) = \exp\left(-\frac{(x-x_c)^2 + (y-y_c)^2}{2\sigma^2}\right).$$

Then the exact solution is given by

$$u(x,y,t) = \frac{2\sigma^2}{2\sigma^2 + 4Dt}\exp\left(Kt - \frac{(x^*-x_c)^2 + (y^*-y_c)^2)}{2\sigma^2 + 4Dt}\right),$$

where $(x^*, y^*, 0)$ is the backtrack of the characteristic from (x, y, t).

For simplicity, we use a uniform triangular mesh. The 2nd order Runge-Kutta (or Heun) method is used for characteristic tracking. The finite element solver for the parabolic part (as a DLL) is derived from the source code in OFELI.

For numerical runs, we choose $T = \pi/2$, $\Omega = [-1, 1] \times [-1, 1]$, $D = 10^{-4}$, $K = 0.1$, $(x_c, y_c) = (-0.5, -0.5)$, and $\sigma^2 = 0.01$. For the parabolic solver, we use 20 micro steps within each global time step $[t_n, t_{n+1}]$. Accordingly, we set the maximal number of time steps in characteristic tracking to 20 also. Table 1 lists some results for the numerical solution at the final time. We still obtain very good numerical solutions, even though large global time steps are used.

Numerical results for the first example

Mesh size h	L^∞-error	L^1-error	ρ_{L_1}	L^2-error
1/20	1.266×10^{-2}	1.247×10^{-4}		3.138×10^{-4}
1/40	1.031×10^{-2}	5.061×10^{-5}	1.301	2.085×10^{-4}
1/50	9.984×10^{-3}	4.153×10^{-5}	1.127	1.923×10^{-4}
1/60	9.796×10^{-3}	3.613×10^{-5}	1.308	1.825×10^{-4}

Table 1: Numerical results of example 1 with $\Delta t = \pi/8$.

We get a first order convergence result with the first order splitting.

We deal with the numerical convergence-rate :

$$\rho_{L_1} = \ln\left(\frac{err^l_{L_1}}{err^{l-1}_{L_1}}\right) / \ln\left(\frac{h^l}{h^{l-1}}\right)$$

Example 2: Nonlinear Reaction

The second example is a simplified model for single-species biodegradation: $R(u) = au/(u+b)$. We consider a 2-dimensional problem with a constant velocity filed (V_1, V_2), a scalar diffusion $D > 0$, and no source. The initial condition is a Gaussian hill.

For numerical runs, we choose $T = 1$, $\Omega = [-1,1] \times [-1,1]$, $(V_1, V_2) = (1,1)$, $D = 10^{-4}$, $a = b = 1$, $(x_c, y_c) = (-0.5, -0.5)$, and $\sigma^2 = 0.01$. Table 2 lists some results of the numerical solution at the final time.

No exact solution is known for this problem. But from Table 2, we can observe that the operator splitting method is stable, and keeps positivity of the solution.

Numerical results for the second example

Δt	h	U_{min}	U_{max}	Δt	h	U_{min}	U_{max}
0.25	1/20	0.0	1.5159	0.125	1/40	0.0	1.5251
0.25	1/40	0.0	1.5176	0.10	1/20	0.0	1.5248
0.25	1/60	0.0	1.5179	0.10	1/50	0.0	1.5268

Table 2: Numerical results of example 2.

We get a decreasing of the errors and convergence to the exact result. The time-space table show the decreasing in time is higher than in space.

Improvement : Higher order methods for the Splitting-method.

8 Conclusions and future works

- Higher order operator-splitting methods.
- Theory for accurate decoupling Multi-physical and Multi-scaling problems.
- Mixed methods for operato-splitting methods and iterative methods.
- Physical splitting methods