Theoretical and Numerical Analysis of Operator Splitting Procedures

Petra Csomós

Theses of Ph.D. Thesis

Eötvös Loránd University, Faculty of Science
Ph.D. School for Mathematics, Applied Mathematics Program

School Leader: Prof. Miklós Laczkovich, MHAS
Program Leader: Prof. András Prékopa, MHAS

Thesis advisor: Assoc. Prof. Dr. István Faragó,
candidate in mathematical science

Department of Applied Analysis
and Computational Mathematics

2007

Preliminaries

In my thesis I investigate the operator splitting procedures which are used to solve partial differential equations numerically. They can be considered as time-discretization methods which simplify or even make possible the numerical treatment of differential equations. They have been systematically studied first in Marchuk [17] and Strang [19], and since then they are widely applied to model various physical processes. The idea behind operator splitting procedures is that a certain physical phenomenon is the combined effect of several processes. The behaviour of a quantity (e.g. the concentration of chemical species) is formulated by a partial differential equation in which the local time derivative depends on the sum of the sub-operators describing the different processes. These sub-operators have different nature. Each sub-operator defines a sub-problem, for which usually there exists an efficient numerical method providing fast and accurate solution. For the whole (non-split) problem (being represented by the sum of the sub-operators) may not be found an adequate numerical method. Hence, application of the operator splitting procedures maens that instead of the whole problem, we treat the sub-problems and the corresponding sub-operators separately. The solution of the original problem is then obtained from the numerical solutions of the sub-problems. In my thesis I investigate the *sequential*, *Strang*, and *weighted splittings*. Let us consider an abstract Cauchy problem on the Banach space X with the linear operator G:

$$\begin{cases} \dfrac{\mathrm{d}u(t)}{\mathrm{d}t} = Gu(t), \qquad t \geq 0, \\ u(0) = x \in X. \end{cases} \tag{ACP}$$

The one-parameter family of linear operators $\big(U(t)\big)_{t\geq 0}$ is called *strongly continuous operator semigroup* on the Banach space X if

(i) $U(0) = I$,

(ii) $U(t+s) = U(t)U(s) \quad$ for all $t, s \geq 0$,

(iii) for every $x \in X$, the orbit maps $t \to U(t)x$ are continuous from $\mathbb{R}^+$ into X.

The operator G with the domain $D(G)$ is called the *generator* of the above operator semigroup if

$$Gx := \lim_{h\to 0} \frac{U(h)x - x}{h} \qquad \text{for all } x \in D(G) \quad \text{with}$$

$$D(G) := \left\{ x \in X : \lim_{h\to 0} \frac{U(h)x - x}{h} \quad \text{exists} \right\}.$$

It can be shown that the abstract Cauchy problem has a unique solution if $\big(G, D(G)\big)$ is a generator of a strongly continuous semigroup. Therefore, throughout my tesis I assume that the operators $\big(A, D(A)\big)$ and $\big(B, D(B)\big)$ generate the strongly continuous semigroups $\big(T(t)\big)_{t\geq 0}$ and $\big(S(t)\big)_{t\geq 0}$ on X, respectively, and the sum $G = A + B$ defined on $D(A+B) := \overline{D(A) \cap D(B)}$ generates the strongly continuous semigroup $\big(U(t)\big)_{t\geq 0}$ on X. The numerical solutions $u_n(t)$ of the problem (ACP) obtained by applying the different splitting procedures are defined as:

$$\begin{aligned} \text{sequential splitting:} \quad & u_n^{\mathrm{sq}}(t) := [S(t/n)T(t/n)]^n x, \\ \text{Strang splitting:} \quad & u_n^{\mathrm{St}}(t) := [T(t/2n)S(t/n)T(t/2n)]^n x, \\ \text{weighted splitting:} \quad & u_n^{\mathrm{w}}(t) := [\Theta S(t/n)T(t/n) + (1-\Theta)T(t/n)S(t/n)]^n x \end{aligned}$$

for all $t \geq 0$ and $n \in \mathbb{N}$ fixed, and $x \in D(A) \cap D(B)$, where $\Theta \in (0,1)$. Since operator splitting procedures can be regarded as certain time-discretization methods, their convergence is a crucial question in the applications. In my thesis I analyse the convergence of the operator splitting procedures by using the theoretical results of operator semigroup theory, and numerical experiments as well.

Methods

In my thesis I apply the results of the fields of operator splitting procedures, operator semigroup therory on Banach spaces (approximation and perturbation theory of operator semigroups), numerical analysis of finite difference methods applied for solving initial value problems (notions of convergence, consistency, and stability, and Lax's Theorem), operator semigroup approach to abstract delay equations (product Banach spaces, operator matrices), large-scale environmental modelling (air pollution transport models), and development of computer codes.

Theses of the thesis

In *Chapter 1* I give an overview on the analytical and numerical tools (operator semigroup theory, numerical analysis, delay equations, air pollution transport models) used in the thesis. In *Chapter 2* I define the operator splitting procedures, and present some results from the literature concerning their consistency analysis, and I introduce the results of Ito and Kappel [14] and Zagrebnov [21] about the convergence of the splitting procedures applied together with another time-discretization method. I show the following new result (see Csomós and Sikolya [12]).

1. **Thm. 2.4.5.** Zagrebnov shows in Theorem 10.18 of [21] that under certain conditions the estimates

$$\|f(\tfrac{t}{n}A)g(\tfrac{t}{n}B) - e^{t(A+B)}\| \leq C_1 \frac{\ln n}{n},$$
$$\|f^{1/2}(\tfrac{t}{n}A)g(\tfrac{t}{n}B)f^{1/2}(\tfrac{t}{n}A) - e^{t(A+B)}\| \leq C_2 \frac{\ln n}{n}$$

hold for all $t \geq 0$ and $n \in \mathrm{N}$ with some constants $C_1, C_2 > 0$. I show that the requirements for the functions f and g are fulfilled if they represent A–stable, consistent, and positivity preserving numerical methods. Hence, application of such methods together with sequential and Strangs splittings results in a norm-convergent numerical scheme.

In *Chapter 3* the convergence of the splitting procedures is analysed. In Section 3.1 I investigate the case when the split sub-problems are solved exactly (see Csomós and Nickel [10]), while in Section 3.2 the solutions of the sub-problems are obtained by applying spatial and temporal approximation schemes as well (see Bátkai, Csomós, and Nickel [2]).

2. **Prop. 3.1.6, Prop. 3.1.7.** I investigate the relationship between Lax's and Chernoff's Theorem (see Thm. 8 in Section 34.3 of Lax [16] and Cor. 5.3 in Chapter III. of Engel and Nagel [13]). I prove that the assumptions of the two theorems are equivalent if the step size of the numerical method varies in a compact interval, and the operator is the generator of the semigroup approximated by the investigated numerical method.

3. **Lemma 3.1.8.** I prove that the stability criterion of the sequential splitting implies the stabilitiy criteria of the Strang and weighted splittings. This result holds for the operators applied in reverse order as well. Hence, it suffices to control only one stability requirement for all investigated splitting procedures, that is, there exist constants $M \geq 1$, $\omega \in \mathbb{R}$ such that

$$\|[S(t/n)T(t/n)]^n\| \leq Me^{\omega t} \qquad \text{for all } t \geq 0,\ n \in \mathbb{N}. \tag{S}$$

   The result is valid also when spatial and temporal discretization methods are used as well (**Lemma 3.2.7.**, **Lemma 3.2.19.**).

4. **Prop. 3.1.10.** With the help of Chernoff's Theorem and the Trotter Product Formula (see Cor. 5.3 and Cor. 5.8 in Chapter III. of Engel and Nagel [13]), I show that the sequential, Strang, and weighted splittings are convergent at a fixed time level if the stability condition (S) is satisfied.

5. **Thm. 3.2.14–16.** Based on Thm. 6.7 in Pazy [18] and the paper of Ito and Kappel [15], I prove a modified version of Chernoff's Theorem being valid also for approximate semigroups (**Thm. 3.2.11**). With its help I show that the convergence of the sequential, Strang, and weighted splittings follows from the stability condition similar to (S) as well as in the case when the semigroups are approximated by approximate semigroups $\big(T_n(t)\big)_{t\geq 0}$ and $\big(S_n(t)\big)_{t\geq 0}$, $n \in \mathrm{N}$ with generators A_n and B_n, respectively, satisfying the followings:

(i) *Consistency:*

(a) $\lim_{n\to\infty} J_n A_n P_n x = Ax$ for all $x \in D(A)$,

(b) $\lim_{n\to\infty} J_n B_n P_n x = Bx$ for all $x \in D(B)$.

(ii) *Convergence:*

(a) $\lim_{n\to\infty} J_n T_n(t) P_n x = T(t)x$ for all $x \in D(A)$ and for each arbitrary fixed $t \geq 0$,

(b) $\lim_{n\to\infty} J_n S_n(t) P_n x = S(t)x$ for all $x \in D(B)$ and for each arbitrary fixed $t \geq 0$.

In this case the convergence means that the solution $u(t)$ of the problem (ACP) for the different splitting procedures can be obtained as:

$$u(t) = \lim_{n\to\infty} J_n[S(t/n)T(t/n)]^n P_n x,$$
$$u(t) = \lim_{n\to\infty} J_n[T(t/2n)S(t/n)T(t/2n)]^n P_n x,$$
$$u(t) = \lim_{n\to\infty} J_n[\Theta S(t/n)T(t/n) + (1-\Theta)T(t/n)S(t/n)]^n P_n x \quad \text{with } \Theta \in (0,1)$$

for all $x \in X$, and uniformly for t in compact intervals, for the sequential, Strang, and weighted splitting, respectively. The operators J_n and P_n act between the Banach spaces X and X_n, where the latter is the space of the function defined on the spatial mesh. This case represents the convergence of the split solution when the split sub-problems are solved by using spatial approximations.

6. **Thm. 3.2.20–22.** I show that the convergence of the sequential, Strang, and weighted splittings remains valid also in the case when the semigroups are approximated using spatial and also temporal approximations. In this case the spatial discretization schemes need to be convergent at each time level, and the time-discretization methods should be stable and consistent:

(i) *Stability:*

(a) $\|[q_n(t)]^k\| \leq 1$ for all $t \in (0,T]$, $n, k \in \mathbb{N}$,

(b) $\|[r_n(t)]^k\| \leq 1$ for all $t \in (0,T]$, $n, k \in \mathbb{N}$,

and $q_n(0) = I$ and $r_n(0) = I$ for all $n \in \mathbb{N}$.

(ii) *Consistency:*

(a) $\lim_{t\to 0} \frac{1}{h}(J_n q_n(t) P_n x - x)$ exists for all $x \in D(A)$, $n \in \mathbb{N}$,

(b) $\lim_{t\to 0} \frac{1}{h}(J_n r_n(t) P_n x - x)$ exists for all $x \in D(B)$, $n \in \mathbb{N}$.

(iii) *Spatial convergence:*

(a) $\lim_{n\to\infty} J_n q_n(t) P_n x = T(t)x \qquad$ for all $x \in D(A)$
and for each arbitrary fixed $t \in (0, t_0]$,

(b) $\lim_{n\to\infty} J_n r_n(t) P_n x = S(t)x \qquad$ for all $x \in D(B)$
and for each arbitrary fixed $t \in (0, t_0]$.

Then the convergence of the splitting procedures together with the spatial and time-discretization methods means that the solution $u(t)$ of the problem (ACP) can be evaluated as the following limits:

$$
\begin{aligned}
u(t) &= \lim_{n\to\infty} J_n [r_n(t/n) q_n(t/n)]^n P_n x, \\
u(t) &= \lim_{n\to\infty} J_n [q_n(t/2n) r_n(t/n) q_n(t/2n)]^n P_n x, \\
u(t) &= \lim_{n\to\infty} P_n [\Theta r_n(t) q_n(t) + (1-\Theta) q_n(t) r_n(t)]^n P_n x, \qquad \Theta \in (0,1)
\end{aligned}
$$

for the sequential, Strang, and weighted splittings, respectively.

In *Chapter 4* I analyse the convergence of the splitting procedures applied to the abstract delay equation:

$$
\begin{cases}
\dot{u}(t) = Cu(t) + \Phi u_t, \qquad t \geq 0, \\
u(0) = x \in X, \\
\quad u_0 = f \in \mathrm{L}^p\big([-1,0], X\big),
\end{cases}
\tag{DE}
$$

where the history function u_t is defined by $u_t(\sigma) := u(t+\sigma)$ for $\sigma \in [-1, 0]$. The equation (DE) can be written as an abstract Cauchy problem (ACP) by using the following operator G on the product Banach space $\mathcal{E}_p := X \times \mathrm{L}^p\big([-1,0], X\big)$, $1 \leq p < \infty$:

$$
G := \begin{pmatrix} C & \Phi \\ 0 & \frac{\mathrm{d}}{\mathrm{d}\sigma} \end{pmatrix}
$$

with the domain

$$
D(G) := \left\{ \tbinom{y}{g} \in D(C) \times \mathrm{W}^{1,p}\big([-1,0], X\big) :\ g(0) = y \right\}.
$$

Motivated by Section 3.3.2 in the book of Bátkai and Piazzera [1] and the results of Webb [20], I study two ways how to split the operator G in the abstract Cauchy problem (the two splittings of the operator correspond to the cases of bounded and unbounded delay operator Φ).

7. **Thm. 4.1.2, 4.1.8.** I prove that the sequential, Strang, and weighted splittings applied to the delay equation (DE) are convergent at a fixed time level for bounded and unbounded

delay operator Φ as well, since the stabilty criterion (S) is fulfilled under the assumptions that the operator $\big(C, D(C)\big)$ is a generator and dissipative, and the delay operator Φ has a special form. I illustrate my result with numerical examples as well (see Csomós and Nickel [10]).

8. **Thm. 4.2.5, 4.2.7.** I show that the sequential, Strang, and weighted splittings are convergent for the two ways of splitting of the operator appearing in the abstract Cauchy problem corresponding to the delay equation (DE), also in the case when consistent and convergent spatial approximation schemes are applied to solve the sub-problems (see Bátkai, Csomós, and Nickel [2]).

In *Chapter 5* the order of the total time-discretization error is investigated, i.e., when splitting procedures are applied together with other time-discretization methods (see Csomós and Faragó [9]).

9. **Table 5.5.** With the help of analytical and numerical computations, I show that an *interaction error* appears when splitting procedures are applied together with other time-discretization methods used to solve the split sub-problems numerically. I have found that the order of the total time-discretization method (splitting and numerical method together) is the minimum of the order of the splitting and that of the numerical method.

10. **Fig. 5.5–5.7.** I introduce another new kind of error notion for measuring the total error of the solution obtained by applying a splitting procedure together with time-discretization methods. Since the exact solution is generally not known, we need to estimate its total error by a *practical error* which can be computed from the numerical solutions. I show that this error behaves like the total error, therefore, it is a useful estimate for it.

In *Chapter 6* I present an idea how to shorten the computational time of the air pollution transport model (see Zlatev [22])

$$\frac{\partial c}{\partial t} = -\left(\frac{\partial\,(uc)}{\partial x} + \frac{\partial\,(vc)}{\partial y}\right) + K\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) + E - \sigma c \tag{APTM}$$

with some initial and boundary conditions, where $c(x, y, t)$ is the unknown concentration of a chemical species varying in space and time. Functions u, v, K, E, and σ represent the effects of the different physical processes: advection, diffusion, emission, and deposition.

11. **Fig. 6.10.** Implementing numerically the air pollution transport model (APTM), I demonstrate that the application of a splitting procedure can lead to shorten the computational time if different numerical methods with different time steps are chosen for each split sub-problem. As a comparison, I apply upwind and semi–Lagrangian scheme for the advection sub-problem in (APTM). Since the latter requires larger time step, it needs less computational step, i.e., shorter computational time (see Csomós [4]).

Conclusions

From the results of my thesis I conclude the followings. The investigated splitting procedures are convergent when the exact split solutions are known, and also in the case when stable, consistent, and convergent spatial and temporal discretization methods are used to approximate them. In the latter case the order of the total error is always the minimum of the order of the splitting and the order of the numerical method. This means that the order of the total time-discretization can be less than the order of the applied splitting procedure, if some lower order numerical method with improper chosen time step is used together with it.

Application of the previous results implies the convergence of the investigated splitting procedures for abstract delay equations in case of bounded and unbounded delay operators. One can also conclude that the computational time of an air pollution transport model can be shortened by applying splitting procedures, since each sub-problem can be solved using different numerical methods with different time steps.

References

[1] A. Bátkai, S. Piazzera, *Semigroups for Delay Equations*, A K Peters, Wellesley, Massachusetts. (2005)

[2] A. Bátkai, P. Csomós, and G. Nickel, Splitting and approximations for delay equations (in preparation).

[3] P. Csomós, Operator splitting procedures for air pollution transport models, *Lecture Notes in Computational Sciences* **3743**, Springer-Verlag, 331–338. (2006)

[4] P. Csomós, Analysis of a transport model applying operator splitting and semi-Lagrangian method, *International Journal of Computational Science and Engineering* (to appear).

[5] P. Csomós, Analytical solutions and numerical experiments for optimizing operator splitting procedures, *Időjárás, Quarterly Journal of the Hungarian Meteorological Service* **110** 3-4., 379–415. (2006)

[6] P. Csomós, Some aspects of interaction between splitting procedures and numerical methods, in K. Georgiev et al. (Eds.), NATO ARW Advances in Air Pollution Modelling for Environmental Security, *NATO Science Series*, Springer-Verlag, 77–91. (2005)

[7] P. Csomós, I. Faragó, and Á. Havasi, Weighted sequential splittings and their analysis, *Computers and Mathematics with Applications* **50**, 1017–1031. (2005)

[8] P. Csomós, I. Dimov, I. Faragó, Á. Havasi, and Tz. Ostromsky, Computational complexity of weighted splitting scheme on parallel computers, *International Journal of Parallel, Emergent and Distributed Systems* **223**, 137–147. (2007)

[9] P. Csomós, I. Faragó, Error analysis of the numerical solution of split differential equations, *Mathematical and Computer Modelling* (to appear).

[10] P. Csomós, G. Nickel, Operator splittings for delay equations, *Computers and Mathematics with Applications* (to appear).

[11] P. Csomós, I. Faragó, Á. Havasi, Operator splitting and global error analysis, in D. Melas and D. Syrakov (Eds.), NATO ARW Air Pollution Processes in Regional Scale, *Kluwer Academic Publishers*, 37–44. (2002)

[12] P. Csomós, E. Sikolya, Numerical methods for split differential equations (in preparation).

[13] K. – J. Engel, R. Nagel, *One-Parameter Semigroups for Linear Evolution Equations*, Springer-Verlag, Berlin. (2000)

[14] K. Ito, F. Kappel, *Evolution Equations and Approximations*, World Scientific, River Edge, N. J. (2002)

[15] K. Ito, F. Kappel, The Trotter – Kato theorem and approximation of PDE's, *Mathematics of Computation* **67** No. 221, 21–44. (1998)

[16] P. D. Lax, *Functional Analysis*, John Wiley & Sons, New York. (2002)

[17] G. I. Marchuk, Some application of splitting-up methods to the solution of mathematical physics problems, *Applik. Mat.* **13** (2), 103–132. (1968)

[18] A. Pazy, *Semigroups of Linear Operators and Applications to Partial Differential Equations*, Springer-Verlag, New York. (1983)

[19] G. Strang, On the construction and comparison of difference schemes, *SIAM J. Numer. Anal.*, September, Vol. 5, No. 3, 506–517. (1968)

[20] G. F. Webb, Functional differential equations and nonlinear semigroups in L^p-spaces, *Journal of Differential Equations*, **20**, 71–89. (1976)

[21] V. A. Zagrebnov, *Topics in the Theory of Gibbs Semigroups*, Leuven University Press. (2003)

[22] Z. Zlatev, *Computer Treatment of Large Scale Air Pollution Models*, Kluwer Academic Publishers, Dordrecht. (1995)