8th AIMS International Conference on Dynamical Systems,May 25 - 28, 2010, Technical University of Dresden, Germany, Lecture: Successive approximation methods for solving time-dependent problems,

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Outline of the talk

0) Motivation
1) Successive Approximation method
2) Analysis
3) Numerical Results

Introduction

We present a novel method to solve time-dependent differential equations.
The method is based on iterative splitting schemes and generally known as successive approximation methods.
Benefits:

- Iterative scheme can help to obtain higher order scheme
- Idea: Freasing timedependent case to a temporarily inhomogeneous equation (method of Tanabe and Sobolevski)

Drawback of standard methods, e.g. Expoential splitting, Magnus expansion schemes:

- Exponential character of the schemes and problem to acchieve algorithms beyond 6th order of accuracy.
- Magnus expansion is based on Bernoulli-series, so the convergence radius is also restricted in that direction (finite intervall).
- Computations for solving commutator exponentials are expensive.

Iterative Splitting Method

Methods of iterative operator splitting methods:

- Time-decomposition methods, one can splitt operators with respect to their time-scale (Waveform relaxation schemes, Successive approximation methods)
- Spatial-decomposition methods, one can splitt operators with respect to their spatial scale (Schwarz-Waveform relaxation schemes, Domain decomposition methods)

Aims and contribution with the decomposition methods

- Decoupling time-scales and spatial-scales (Reduce the stiffness in single operators).
- Decoupling the multi-physics (Reduce the unphysical behaviour with best choise of discretization and solver methods).
- Time-adaptivity, Space-adaptivity (Efficiency and local accurate computations).
- Parallelization in Time and Space (Speed up of computations)

Results : More efficient and fast algorithms with high accuracy and simple implementation.

Iterative Operator Splitting Methods (classical version)

$$\frac{\partial c_i(t)}{\partial t} = A c_i(t) \; + \; B c_{i-1}(t), \text{ with } \; c_i(t^n) = u^n, \tag{1}$$

$$\frac{\partial c_{i+1}(t)}{\partial t} = A c_i(t) \; + \; B c_{i+1}(t), \text{ with } \; c_{i+1}(t^n) = u^n, \tag{2}$$

where $c_0(t)$ is any fixed function for each iteration. (Here, as before, u^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 $c_{\mathrm{sp}}^{n+1} = c_{2m+1}(t^{n+1})$. (Clearly, 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.)

Approximation Methods to timedependent operators

We deal with the following timedependent linear evolution equations

$$\partial_t u = A(t)u, \; u(0) = u_0, \tag{3}$$

where A can be an unbounded and time-dependent operator. For solving Hamiltonian problems, it is often the case that $A(t) = T + V(t)$, where only the potential operator $V(t)$ is time-dependent.

The solution is given as

$$u(t) = \exp(\Omega(t)) u(0) \; . \tag{4}$$

This can be expressed as:

$$u(t) = \mathcal{T} \left(\exp(\int_0^t A(s) \, ds \right) u(0) \; , \tag{5}$$

where the time-ordering operator $\mathcal{T}$.

Magnus expansion to timedependent operators

The Magnus expansion is defined as:

$$\Omega(t) = \sum_{n=1}^{\infty} \Omega_n(t) \; , \tag{6}$$

where the first few terms are [Blanes and Casas 2008]

$$\begin{aligned} \Omega_1(t) &= \int_0^t dt_1 A_1, \; \Omega_2(t) = \frac{1}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 [A_1, A_2] \\ \Omega_3(t) &= \frac{1}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 ([A_1, [A_2, A_3] + [[A_1, A_2], A_3]) \\ &\cdots\cdots \qquad \text{etc.} \end{aligned} \tag{7}$$

where $A_n = A(t_n)$.

Successive Approximation Method to timedependent operators

Instead of the Magnus series (6) for solving explicit time-dependent problems, one can also directly implement successive approximation method.
The problem is given as:

$$\frac{\partial u}{\partial t} = A(t)u(t), \; a \leq t \leq b \tag{8}$$

We rewrite:

$$\frac{\partial u}{\partial t} = A(a)u(t) + (A(t) - A(a))u(t) \tag{9}$$

The abstract integral is given as, by the so called Duhamel Principle:

$$\begin{aligned} u(t) &= \exp((t-a)A(a))u_0 \\ &+ \int_a^t \exp((t-s)A(a))(A(s)-A(a))u(s)\,ds \end{aligned} \tag{10}$$

and $a \in [0, t]$ is a fixed time-point.

In order to construct $Y(t)$ we use Tanabe-Solevski's method with successive approximation we obtain:

$$u_1(t) = \exp((t-a)A(a))u_0, \tag{11}$$

$$\ldots$$

$$u_{n+1}(t) = \exp((t-a)A(a))u_0 + \int_a^t \exp((t-s)A(a))(A(s)-A(a))u_n(s)\, ds \tag{12}$$

and formally we have:

$$u(t) = \exp((t-a)A(a))u_0 + \int_a^t \exp((t-s)A(a))R(s,a)u_0\, ds \tag{13}$$

The recursive operators are given as:

$$R(t,s) = \sum_{m=1}^{\infty} R_m(t,s), \tag{14}$$

$$R_1(t,s) = \begin{cases} (A(t) - A(s)) \exp((t-s)A(a)) ds & , s < t \\ 0 & , s \geq t \end{cases} \tag{15}$$

$$R_m(t,s) = \int_s^t R_1(t,\sigma) R_{m-1}(\sigma,t) \, d\sigma. \tag{16}$$

Analysis

We consider the following time dependent problem,

$$\frac{\partial u}{\partial t} = Au(t) + B(t)u(t), \;\; u(0) = u_0 \tag{17}$$

Our intension is to solve this problem by iterative scheme explained as follows, since this might balance the dominant terms in the equations (9),

$$\begin{aligned} \frac{\partial u_i}{\partial t} &= Au_i + B(t)u_{i-1}, \; i = 1, 2, \ldots, m, & (18) \\ \frac{\partial u_{j+1}}{\partial t} &= Au_j + B(t)u_{j+1}, \; j = m, m+1, \ldots M, & (19) \end{aligned}$$

where $m < M$ are integers. We apply only the one-side iteration to operator A.

The exact solutions of this system of equation then can be written by using the integration constant formula as follows:

$$\begin{aligned} \frac{\partial u_i}{\partial t} &= \exp(At)u_0 + \int_0^t \exp((t-s)A)B(s)u_{i-1}(s)\,ds \\ \frac{\partial u_{i+1}}{\partial t} &= \phi(t)u_0 + \int_0^t \phi(t)\phi^{-1}(s)Au_i(s)\,ds \end{aligned}$$

where $\phi(t)$ is the fundamental set of solution of the second equation in the system (18).

The function $\phi(t)$ can be written in terms of the Magnus series, we then have

$$\phi(t) = \exp(\Omega(t)) \tag{20}$$

$$= \exp(\sum_{j=1}^{\infty} \Omega_j(t)) \tag{21}$$

where

$$\Omega_1(t) = \int_0^t dt_1 B_1, \; \Omega_2(t) = \frac{1}{2}\int_0^t dt_1 \int_0^{t_1} dt_2 [B_1, B_2]$$
$$\Omega_3(t) = \frac{1}{6}\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 ([B_1, [B_2, B_3] + [[B_1, B_2], B_3])$$
$$\cdots\cdots \quad \text{etc.} \tag{22}$$

where $B_j = B(t_j)$.

In the following Lemma is used to bound the perturbation:

Lemma

If A generates an analytical semigroup $\exp(At)$ *and* $B(t)$ *is a bounded function. We have dom*$(A) \subset \mathbf{X}$, *dom*$(B(t)) \subset \mathbf{X}$ *and dom*$(A) =$ *dom*$(B) =$ *dom*$(A + B)$*, where* $\mathbf{X}$ *is a Banach space with the operator norm* $|| \cdot ||$*.*

With the assumption: $||B(s+\tau)u_{i-1}(s+\tau) - B(s)u_{i-1}(s)|| \leq \gamma||u_{i-1}(s+\tau) - u_{i-1}(s)||, \forall s, s+\tau \in [0, t]$, and γ is a positive constant independent of t.
We obtain:
a.) $A + B(t)$
b.) and the perturbed semigroup $y(t) = exp(At + \Omega(t))$ can be given as

$$u_i(t) = \exp(tA)u(0) + \int_0^t \exp((t-s)A)B(s)u_{i-1}(s)ds. \quad (23)$$

Proof.

The proof idea is perturbation in semigroups, see [Engel and Nagel 2000]. The operator B can be estimated with A-boundedness ($|| \cdot ||_A$ norm).

$\square$

Timedependent Case:
We deal with the perturbation theory [Engel, Nagel 2000]. The same proof methods are used for the time-dependent case. The variation of constants can be extended to a time-dependent case, see [Pazy 1983].

Theorem

Let us consider the abstract Cauchy problem in a Banach space $\mathbf{X}$

$$\begin{aligned} \partial_t c(t) &= Ac(t) + B(t)c(t), \quad 0 < t \leq T \text{ and } x \in \Omega, \\ c(0) &= c_0, \; t \in [0, T], \end{aligned} \tag{24}$$

where $A, B(t) : D(A) \subset \mathbf{X} \to \mathbf{X}$, $B(t) : D(B(t)) \subset \mathbf{X} \to \mathbf{X}$ *are given linear bounded operators which are generators of the* C_0*-semigroup and* $c_0 \in \mathbf{X}$ *is a given element.*

Further, we assume the estimations of the bounded timedependent operator:

$$||B(t)\exp(At)x|| \leq \beta||x||, \tag{25}$$

$\tau_n = (t^{n+1} - t^n)$.
The error of the first time-step is of accuracy $\mathcal{O}(\tau_n^m)$, where $\tau_n = t^{n+1} - t^n$ and we have equidistant time-steps, with $n = 1, \ldots, N$. Then the iteration process (18) for $i = 1, 2, \ldots, m$ is consistent with the order of the consistency $\mathcal{O}(\tau_n^m)$.

Proof.

For $i = 1$, we have:

$$c_1(t^{n+1}) = \exp(A\tau_n)c(t^n), \tag{26}$$

and the solution is given as

$$\begin{aligned} c(t^{n+1}) &= \exp(A\tau_n)c(t^n) \\ &+ \int_{t^n}^{t^{n+1}} \exp(A(t^{n+1} - s))B(s)\exp(sA + \int_0^s B(\tilde{(}s))d\tilde{s})c(t^n)\, ds, \end{aligned}$$

□

We obtain:

$$||e_1|| \leq || \exp((A\tau + \int_{t^n}^{t^{n+1}} B(s)ds))c(t^n) - c_1|| \quad (27)$$

$$= || \int_{t^n}^{t^{n+1}} \exp(A(t^{n+1} - s))B(s) \exp(sA + \int_0^s B(\tilde{s})d\tilde{s})c(t^n) \, ds||$$

$$\leq C\tau ||B(\xi)|| ||c(t^n)|| \quad (28)$$

where $\xi \in [t^n, t^{n+1}]$ and the exp functions can be estimated by C.

The same argumentation is used for $i = 2$:

$$||e_2|| \leq \tag{29}$$

$$= \int_{t^n}^{t^{n+1}} || \exp(A(t-s))B(s)|| \tag{30}$$

$$\int_{t^n}^{s} || \exp(A(s-\rho))B(\rho) \exp((\rho - t^n)(A+B))c(t^n) \, d\rho|| ds$$

$$= \tilde{C}\tau^2 ||B(\xi)||^2 \; ||c(t^n)||$$

where $\xi \in [t^n . t^{n+1}]$
Based on the bounded operators we can apply the recursive argument.

For the iterations till $i = m$, we obtain for c_i and c:

By shifting $0 \rightarrow t^n$ and $\tau_n \rightarrow t^{n+1}$, we obtain our result:

$$||e_i|| \leq \tilde{C} ||B(\xi)||^m \tau_n^m ||c(t^n)||,$$

where $\xi \in [t^n, t^{n+1}]$ and $\tilde{C}$ is a non-timedependent constant. The same proof idea can be applied to the even iterative scheme.

Algorithm

The algorithm is given as, for one time step, h, in the interval $[t_n, t_n + h]$,

$$\begin{aligned} u(t_n + h) &= e^{hA_a} u(t_n) \\ &\quad + \int_{t_n}^{t_n+h} e^{(t_n+h-s)A_a} (A(s) - A_a) u(s) \, ds \end{aligned} \tag{31}$$

where $A_a = A(a)$ is $n \times n$ constant matrix.

Successive approximation steps then can be read as

$$\begin{aligned}
u_1(t_n+h) &= e^{hA_a} u(t_n), \\
u_2(t_n+h) &= e^{hA_a} u(t_n) + \int_{t_n}^{t_n+h} e^{(t_n+h-s)A_a} (A(s)-A_a) u_1(s)\, ds \\
\ldots\ldots & \\
u_k(t_n+h) &= e^{hA_a} y(t_n) + \int_{t_n}^{t_n+h} e^{(t_n+h-s)A_a} (A(s)-A_a) u_{k-1}(s)\, ds.
\end{aligned}$$

After approximating the integrals in each iterations by quadrature formulas, we rewrite the solutions as

$$u_k(t_n + h) \;\; = \;\; e^{hA_a} u(t_n) + \sum_{j=1}^{s} w_j F(u_j^*), \;\; k = 2, ...m \quad (32)$$

where $F(s) = e^{(t_n + h - s)A_a}$, w_j are weights and $u_j^* \in [t_n, t_n + h]$ are nodes.

We simply use the trapezoidal rule for approximating the integrals, we then have following iterative solving scheme,

$$\begin{aligned} u_k(t_n + h) &= e^{hA_a}(I + \frac{h}{2}(A(t_n) - A_a)u(t_n) \\ &\quad + \frac{h}{2}(A(t_n + h) - A_a)u_{k-1}(t_n + h) \end{aligned} \qquad (33)$$

for $k = 2, ...m$. Here $u(t_0) = u_0$ (initial condition), $u(t_n) = u_k(t_{n-1} + h), n = 1, ..N$ and $N = \frac{b-a}{h}$. The algorithm will continue until the following condition is fulfilled,

$$|u_k - u_{k-1}| \leq Tol.$$

It can be easily seen in Equation (34), the scheme involves only one approximation of exponential of a constant matrix.

Experiments

Consider the following scalar equation,

$$u'(t) = 2u + tu, \quad u(0) = 1, \tag{34}$$

the exact solution is

$$u(t) = e^{-2} e^{\frac{(t+2)^2}{2}}. \tag{35}$$

The comparison of the numerical solution obtained by successive approximation and the exact solution of the scalar equation is shown in Figures (1) and (2) for different time intervals.

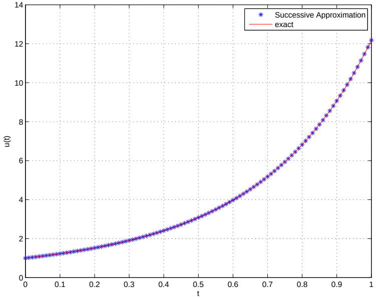

Figure: Comparison of approximate solution by successive approximation and exact solution of scalar equation for shorter time scale.

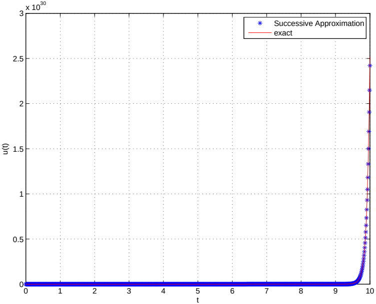

Figure: Comparison of approximate solution by successive approximation and exact solution of scalar equation for longer time scale.

Second example: Radial Schrödinger equation

We first consider the radial Schrödinger equation

$$\frac{\partial^2 u}{\partial r^2} = f(r,e)u(r) \tag{36}$$

where

$$f(r,E) = 2V(r) - 2E + \frac{l(l+1)}{r^2} \tag{37}$$

The equation (37) can be transformed as a harmonic oscillator with a time dependent spring constant after relabeling $r \rightarrow t$ and $u(r) \rightarrow q(t)$ and defining

$$k(t, E) \quad = \quad -f(t, E). \tag{38}$$

By redefining the variables as $u(t) = q(t)$ and $\dot{u}(t) = p(t)$, and $Y(t) = (q(t), p(t))$, the Equation (37) can be put into the system of equation as

$$\dot{Y}(t) \quad = \quad A(t) Y(t) \tag{39}$$

and Hamiltonian of the system is written by

$$H \quad = \quad \frac{1}{2} p^2 + \frac{1}{2} k(t, E) q^2. \tag{40}$$

For specific example, the ground state of hydrogen atom can be modeled as Schrodinger equation with the parameters $l = 0, E = -1/2, V(t) = -1/(t-a), a$ is arbitary constant. Now the time dependent oscillator corresponds to

$$\mathrm{A(t)} \;=\; \begin{pmatrix} 0 & 1 \\ f(t) & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ f(t) & 0 \end{pmatrix} \equiv T + V(t),$$

with

$$f(t) \;=\; (1 - \frac{2}{t-a}). \tag{41}$$

The exact solution for this model with the initial conditions $q(0) = -a, p(0) = 1 + a, a = -0.001$ is

$$q(t) \;=\; (t-a)e^{-t}. \tag{42}$$

The comparison of exact and approximation of the hydrogen

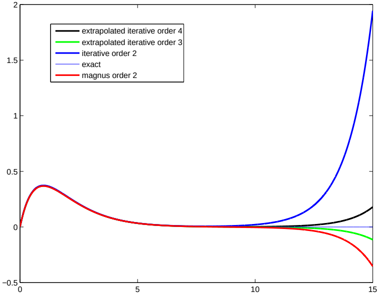

Figure: Comparison of exact and approximation of the hydrogen ground state wave function for various schemes in shorter time scale.

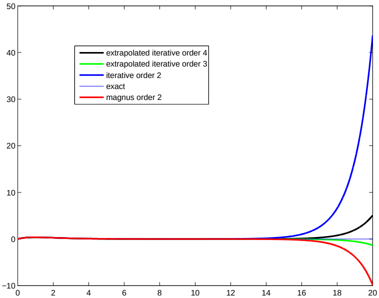

Figure: Comparison of exact and approximation of the hydrogen ground state wave function for various schemes in longer time scale.

Remark

The numerical results show that our higher order treatment gives a better long time behavior than the standard magnus expansion.

Future Works

Outview

1) Convergence Analysis.
2) Nonlinear Problems.
3) Application to real-life problems, e.g. Monte Carlo schemes.