Iterative Operator Splitting Method for Coupled Problems: Transport and Electric Fields

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Abstract

In this article a new approach is considered for implementing operator splitting methods for transport problems, influenced by eletric fields. Our motivation came to model PE-CVD (plasma-enhanced chemical vapor deposition) processes, means the flow of species to a gas-phase, which are influenced by an electric field. We consider a convection-diffusion equation and a Lorence force in the electrostatic case.

The iterative splitting schemes is given as an embedded coupling method and we apply such a scheme as a fast solver. The decomposition analysis is discussed for the nonlinear case. Numerical experiments are given with respect to explicit Adam-Bashforth schemes. We discuss the convergence behavior in time and space for the iterative schemes.

Key words: numerical analysis, iterative solver method, Adam-Bashforth methods, nonlinear convergence.
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1. Introduction

In the field of numerical modeling and simulation of transport problems, the influence of electrical fields are of interest.

We consider a coupled model of a convection-diffusion equation with a electrostatic field.

While the underlying equations are coupled nonlinear and linear equations, we propose iterative schemes to solve such schemes.

We deal with the following model equations:

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$$\frac{\partial u}{\partial t} = -\mathbf{v} \cdot \nabla u + \nabla \cdot D \nabla u, \quad (1)$$

$$\frac{\partial \mathbf{v}}{\partial t} = -\frac{\frac{\partial u}{\partial t}}{u} \mathbf{v} + \frac{\nu}{\mu} \mathbf{E}, \quad (2)$$

$$u(\mathbf{x}, \mathbf{t_0}) = u_0(\mathbf{x}), \quad (3)$$

$$\mathbf{v}(\mathbf{x}, \mathbf{t_0}) = \mathbf{v}_0(\mathbf{x}), \quad (4)$$

where u is the density of the ion concentrations, $\mathbf{v}$ is the velocity field, $\mathbf{E}$ is the electric field and ν, μ are parameters. We consider Neumann boundary conditions.

The iterative splitting scheme is considered after the spatial discretization and we obtain the following nonlinear ordinary differential equation system:

$$\frac{\partial u}{\partial t} = A_1(\mathbf{v}) u + B(\mathbf{v}) u, \quad (5)$$

$$\frac{\partial \mathbf{v}}{\partial t} = A_2(\frac{\partial u}{\partial t}, u) \mathbf{v} + \mathbf{f}, \quad (6)$$

where A_1, A_2, B are given of the spatial discretization. $\mathbf{f} = \frac{\nu}{\mu} \mathbf{E}$.

Here we deal with a iterative scheme to solve the nonlinear equation.

2. Mathematical Model

We motivate our study by simulating a growth rate of a deposition process that can be done by PE-CVD (plasma enhanced chemical vapor deposition) processes, see [1] and [2]. A gas exposed to an electric field in low pressure conditions (< 5 Torr) results in a non-equilibrium plasma, see [3] and [4]. Such ionized media, known as "cold" plasma or glow discharges, are powerful surface-modification tools in Material Science and Technology. Low-pressure plasmas allow to modify the surface chemistry and properties of materials compatible with low-medium vacuum, through a PE-CVD process, see applications [4]. Here a porous media model with permeable layers is an attractive simulation models. The transport, chemical and sorption processes in a homogeneous media can be used to simulate species transport in a plasma enhanced environment, controlled by pressure, by temperature and by additional electric fields.

We concentrate on a far-field model and assume a continuum flow, and that the transport equations can be treated with a convection-diffusion-reaction equation, due to a constant velocity field, see:

$$\frac{\partial u}{\partial t} + \nabla F u = 0, \text{ in } \Omega \times [0, t] \quad (7)$$

$$F = \mathbf{v} - D \nabla,$$

$$c(x, t) = c_0(x), \text{ on } \Omega, \quad (8)$$

$$\frac{\partial c(x, t)}{\partial n} = 0, \text{ on } \partial\Omega \times [0, t], \quad (9)$$

where c is the particle density of the ionized species. F the flux of the species. $\mathbf{v}$ is the flux velocity through the chamber and porous substrate which is influenced by the electric field. D is the diffusion matrix. The initial value is given as c_0 and we assume a Neumann boundary condition.

2.) Electric Field (Distribution)

To model the influence of the electric field on the concentration we use a pointwise approach that means we assume that the concentration in a point $\mathbf{x} \in \Omega$ behaves like a point-charge of mass $m = \mu u, \quad \mu \in \mathbb{R}^+$ and charge $q = \nu u \quad \nu \in \mathbb{R}$. We also assume that there is no interaction between these point-charges. (This interaction is already considered in the convection-diffusion equation). In general the Lorentz force in this case can be written as $\mathbf{F} = q(\mathbf{E} + v \times \mathbf{B})$. So that the Lorentz force in our electrostatic case is given as: $\mathbf{F} = \nu u \mathbf{E}$.

We can write the equation of motion as follows:

$$\begin{aligned} \frac{\partial \mathbf{p}}{\partial t} &= \mu u \mathbf{E} \\ \frac{\partial m}{\partial t}\mathbf{v} + m\frac{\partial \mathbf{v}}{\partial t} &= \nu u \mathbf{E} \\ \frac{\partial \mathbf{v}}{\partial t} + \frac{\frac{\partial u}{\partial t}}{u}\mathbf{v} &= \frac{\nu}{\mu}\mathbf{E} \end{aligned} \tag{10}$$

3. Discretization Methods

3.1. *Discretization methods of the Convection-Diffusion equation*

For the 3 dimensional convection-diffusion equation we apply a second order finite difference scheme in space and a higher order discretization scheme in time.

$$\begin{aligned} \frac{\partial u}{\partial t} &= -\mathbf{v}\nabla u + D\Delta u, \\ &= -v_x\frac{\partial u}{\partial x} - v_y\frac{\partial u}{\partial y} - v_z\frac{\partial u}{\partial z} + D\frac{\partial^2 u}{\partial x^2} + D\frac{\partial^2 u}{\partial y^2} + D\frac{\partial^2 u}{\partial z^2}, \\ u(\mathbf{x}, \mathbf{t_0}) &= u_0(\mathbf{x}), \end{aligned}$$

We apply dimensional splitting to our problem

$$\frac{\partial u}{\partial t} = A_x u + A_y u + A_z u$$

where

$$A_x = -v_x\frac{\partial u}{\partial x} + D\frac{\partial^2 u}{\partial x^2}.$$

We use a 1st order upwind scheme for $\frac{\partial}{\partial x}$ and a 2nd order central difference scheme for $\frac{\partial^2}{\partial x^2}$. By introducing the artificial diffusion constant $D_x = D - \frac{v_x \Delta x}{2}$ we achieve a 2nd order finite difference scheme

$$L_x u(x) = -v_x\frac{u(x) - u(x-\Delta x)}{\Delta x} + D_x\frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{\Delta x^2}.$$

because the new diffusion constant eliminates the first order error (i.e. the numerical viscosity) of the Taylor expansion of the upwind scheme. $L_y u$ and $L_z u$ are derived in the

same way.
For the discretization in time we use several explicit Runge-Kutta and Adam-Bashforth methods, this leads to restrictions of the step-size in time but on the other hand the cost of implicit methods is much to high in this 3-dimensional case.

3.2. *Analytical solution of the Electrostatic field*

Equation (10) is a linear ODE. We have to solve it at every time-step with the initial condition $v(t^n) = v_n$. It has the following analytical solution:

$$v(t) = v_n \frac{u_n}{u(t)} + \frac{\nu}{\mu} E \frac{1}{u(t)} \int_{t_n}^{t} u(t) dt \tag{11}$$

Under the assumption of constant coefficients (that means it holds $u(t) = u(t_n) = u_n \quad \forall t \in [t_n, t_{n+1})$, $\dot{u}(t) = \dot{u}(t_n) = \dot{u}_n \quad \forall t \in [t_n, t_{n+1})$) we get a solution that is absolutely explicit:

$$v(t) = \left(v_n - \frac{\nu u_n}{\mu \dot{u}_n} E \right) \exp\left(- \frac{\dot{u}_n}{u_n} t \right) + \frac{\nu u_n}{\mu \dot{u}_n} E. \tag{12}$$

Remark 1 *The analytical solution is only given for theoretical analysis, for practical computations, we have to derive a numerical scheme. The schemes are discussed in the following parts.*

Iterative computation of the electrostatic field

We apply successive approximation to the computation of the electrostatic field:

$$v_i(t) = v_n \frac{u_n}{u_{i-1}(t)} + \frac{\nu}{\mu} E \frac{1}{u_{i-1}(t)} \int_{t_n}^{t} u_{i-1}(t) dt, \text{ for } i = 1, 2, 3, \ldots, \ t \in [t^n, t^{n+1}], \tag{13}$$

where we assume $u_{i-1}(t)$ is given from previous computations and $v_i(t^n) = v(t^n)$.

The stopping criterion is given as:

$$||v_i(t) - v_{i-1}(t)|| = err_1, ||u_i(t) - u_{i-1}(t)|| = err_2, \max\{err_1, err_2\} \leq err, \tag{14}$$

where err is a given error-bound.

The integral in (13) is computed as:

1.) Trapezoidal rule:

$$\int_{t_n}^{t} u_{i-1}(s) ds \approx \frac{1}{2}(t - t^n)(u_{i-1}(t) + u_{i-1}(t^n)) \ , \tag{15}$$

where we obtain a second order scheme.

2.) Taylor expansion around t^n

$$\int_{t_n}^{t} u_{i-1}(s) ds \approx (t - t_n) u_{i-1}(t^n) + \frac{1}{2} \ (t - t^n) \frac{du_{i-1}}{dt}(t^n) \ , \tag{16}$$

where we have a also a second order scheme and $\frac{du_{i-1}}{dt}(t^n)$ is given as:

$$\frac{du_{i-1}}{dt}(t^n) = A u_{i-1}(t^n) + B u_{i-1}(t^n) \ , \tag{17}$$

Remark 2 *We assume to have sufficient smoothness of the solution u_{i-1}. Further the computation of the derivation is given with the matrix operators.*

3.3. *Apriori error estimates: CFL Conditions*

In the following we describe the error estimates:

Lemma 1 *We assume to deal with finite difference discretization in space and Euler explicit time discretization. Then the time error estimate for the equation (1) is given as:*

$$\Delta t_{Adv} \leq \frac{\Delta x}{3v(\Delta t_{Adv})}, \tag{18}$$

$$v(t) = ||\mathbf{v}(t)|| = \left(v_n - \frac{\nu u_n}{\mu \dot{u}_n}||E||\right) \exp\left(-\frac{\dot{u}_n}{u_n}t\right) + \frac{\nu u_n}{\mu \dot{u}_n}||E|| \tag{19}$$

$$\Delta t_{Diff} \leq= \frac{\Delta x^2}{6D}, \tag{20}$$

$$\Delta t_{max} = \min(\Delta t_{Adv}, \Delta t_{Diff}); \tag{21}$$

where $||\cdot||$ *is the Euclidian norm for the vectors and equation (18) is a nonlinear equation solved with Newton's method.*

Proof 1

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = 3||\mathbf{v}||\frac{u_{i+1}^n - u_i^n}{\Delta x} + 3D\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \tag{22}$$

where i *are the spatial grid points and* $\mathbf{v}$ *is given analytically in equation (11).*

We obtain the stability criterion for a stable discretization scheme:

$$u_i^{n+1} \leq (1 - 3\frac{||\mathbf{v}||\Delta t}{\Delta x} - 6\frac{D\Delta t}{\Delta x^2})u_i^n + 3\frac{||\mathbf{v}||\Delta t}{\Delta x}u_{i+1}^n + 3\frac{D\Delta t}{\Delta x^2})(u_{i+1}^n + u_{i-1}^n) \tag{23}$$

where the CFL condition is given as:

$$(1 - 3\frac{||\mathbf{v}||\Delta t}{\Delta x} - 6\frac{D\Delta t}{\Delta x^2}) > 0 \tag{24}$$

we deal with the stronger restriction:

$$1 - 3\frac{||\mathbf{v}||\Delta t}{\Delta x} > 0 \tag{25}$$

$$1 - 6\frac{D\Delta t}{\Delta x^2}) > 0 \tag{26}$$

Then the CLF conditions are given as

$$\Delta t_{Adv} \leq \frac{\Delta x}{3v(\Delta t_{Adv})}, \tag{27}$$

$$v(t) = ||\mathbf{v}(t)|| = \left(v_n - \frac{\nu u_n}{\mu \dot{u}_n}||E||\right) \exp\left(-\frac{\dot{u}_n}{u_n}t\right) + \frac{\nu u_n}{\mu \dot{u}_n}||E|| \tag{28}$$

$$\Delta t_{Diff} \leq= \frac{\Delta x^2}{6D}, \tag{29}$$

$$\Delta t_{max} = \min(\Delta t_{Adv}, \Delta t_{Diff}); \tag{30}$$

where $||\cdot||$ *is the Euclidian norm for the vectors and the analytical solution of the velocity is given as:*

$$3\Delta t_{Adv}\left(v_n - \frac{\nu u_n}{\mu \dot{u}_n}||E||\right)\exp\left(-\frac{\dot{u}_n}{u_n}\Delta t_{Adv}\right) + 3\Delta t_{Adv}\frac{\nu u_n}{\mu \dot{u}_n}||E|| \leq \Delta x, \tag{31}$$

$$F(\Delta t_{Adv}) - \Delta x \leq 0 \tag{32}$$

and equation (32) is a real-valued function, where the roots are solved by Newton's method.

4. Splitting methods to couple Electrostatic and Convection Diffusion equation

We concentrate on the splitting methods, which can be classified as classical and iterative splitting methods.

We propose iterative splitting methods by discussing the additive iterative splitting methods, see [5] and [6].

We consider the following the nonlinear problem

$$\frac{\partial u}{\partial t} = A_1(\mathbf{v})u + B(\mathbf{v})u, \tag{33}$$

$$\frac{\partial \mathbf{v}}{\partial t} = A_2(\frac{\partial u}{\partial t}, u)\mathbf{v} + \mathbf{f}, \tag{34}$$

where the initial conditions are $u^n = u(t^n), \mathbf{v}^n = \mathbf{v}(t^n)$. The operators A_1 and A_2 are spatially discretized operators, e.g. they correspond in space to the discretized convection and diffusion operators (matrices). Hence, they can be considered as bounded operators with a sufficient large spatial step $\Delta x > 0$.

4.1. *Iterative splitting methods*

The following algorithm is based on the iteration with fixed splitting discretization step size τ. On the time interval $[t^n, t^{n+1}]$ we solve the following subproblems consecutively for $i = 1, 3, \ldots 2m + 1$, cf. [5] and [6].

$$\frac{\partial u_i(t)}{\partial t} = A_1(\alpha \mathbf{v}_{i-1}(t) + (1-\alpha)\mathbf{v}_{i-1}(t^n))u_i(t) \tag{35}$$

$$+ B(\alpha \mathbf{v}_{i-1}(t) + (1-\alpha)\mathbf{v}_{i-1}(t^n))u_{i-1}(t),$$

$$\text{with } u_i(t^n) = u^n, \mathbf{v}_{i-1}(t^n) = \mathbf{v}^n,$$

$$\frac{\partial \mathbf{v}_i(t)}{\partial t} = A_2(\alpha(\frac{\partial u_i}{\partial t}, u_i) + (1-\alpha)(\frac{\partial u}{\partial t}(t^n), u(t^n)))\mathbf{v}_i(t) \ + \ \mathbf{f}, \tag{36}$$

$$\text{with } u_i(t^n) = u^n, \mathbf{v}_i(t^n) = \mathbf{v}^n,$$

where $u_0 \equiv u^n, \mathbf{v}_0 \equiv \mathbf{v}^n$ are the known split approximation at time level $t = t^n$. The split approximation at time level $t = t^{n+1}$ is defined as $u^{n+1} = u_i(t^{n+1}), \mathbf{v}^{n+1} \equiv \mathbf{v}_i(t^{n+1})$.

While $\alpha \in [0, 1]$ is the weighting factor and $\alpha = 0$ is purely explicit and we are done in $i = 1$, $\alpha = 1$ is pure implicit and we have approximate the last solutions.

Remark 3 *The stop criterion of the iterative splitting scheme is given as:*
– *We stop after a fixed number of iterative steps, e.g. $i = 3$*
– *or we stop after an error bound is reached, we assume that there exists an i with:*

$$\max\{||u_i(t) - u_{i-1}(t)||,\ ||v_i(t) - v_{i-1}(t)||\} \leq err, \tag{37}$$

where $||\cdot||$ i a given vector norm, e.g. Euklidian norm and $err \in I\!R^+$ is a given error bound, e.g. $err = 10^{-4}$.

5. Error Analysis: Coupling Methods

For a simpler notation, we define $c = (u, \mathbf{v})^t$ as a new variable, including the concentration and velocity field.

Based on this, we deal with nonlinear differential equations of the following type:

$$\frac{dc}{dt} = A(c(t))c(t) + B(c(t))c(t), \text{with } c(t^n) = c^n, \tag{38}$$

where $c = (u, \mathbf{v})^t$, with $\mathbf{v}$ is the velocity field (including the electrostatic field in a analytical version) and u is the concentration of the species.

The main idea is to bound the operators $A(c(t))$ and $B(c(t))$ in the discretized equation to satisfy a stable method.

A first idea is the fix-point scheme, that is discussed in the following subsection.

5.1. *Consistency and stability analysis*

In the sequel we demonstrate the error analysis for the linear and nonlinear decomposition methods. In this section we designate as $e_i(t) := c(t) - c_i(t)$ the error between the exact solution and the approximated solution after i iterations.

Here we discuss the linearization techniques and their approximations.

Theorem 1 *Let us consider the following problem*

$$\partial_t c(t) = A(c(t))c(t) + B(c(t))c(t), \quad 0 < t \leq T \ ,$$

$$c(0) = c_0 \ ,$$

where A, B are nonlinear differentiable bounded operators A, B in a Banach space $\mathbf{X}$. Linearizing the nonlinear operators yields the linearized equation

$$\begin{aligned} &\partial_t c(t) = \tilde{A}c(t) + \tilde{B}c(t) + R(c_{\tilde{i}})c_{\tilde{i}}, \quad 0 < t \leq T \ , \\ &\tilde{A} = A(c_{\tilde{i}}) + \tfrac{\partial A(c_{\tilde{i}})}{\partial c} c_{\tilde{i}} \ , \tilde{B} = B(c_{\tilde{i}}) + \tfrac{\partial B(c_{\tilde{i}})}{\partial c} c_{\tilde{i}} \ , \\ &R(c_{\tilde{i}}) = \tfrac{\partial A(c_{\tilde{i}})}{\partial c} c_{\tilde{i}} + \tfrac{\partial B(c_{\tilde{i}})}{\partial c} c_{\tilde{i}} \ , \\ &c(0) = c_0 \ , \end{aligned} \tag{39}$$

where $\tilde{A}, \tilde{B}, \tilde{A} + \tilde{B} : \mathbf{X} \to \mathbf{X}$ are given, linear bounded operators being generators of the C_0-semigroup and $c_0 \in \mathbf{X}$ is a given element. The linearization is of the form $A(c)c \approx A(c_{\tilde{i}})c_{\tilde{i}} + (\frac{\partial A(c_{\tilde{i}})}{\partial c} c_{\tilde{i}})(c - c_{\tilde{i}})$ where $c_{\tilde{i}} \in \mathbf{X}$ is a linearized solution, we further assume

$(\frac{\partial A(c_{\tilde{i}})}{\partial c})c_{\tilde{i}}$ *is a constant Jacobian matrix.*
We assume that the iteration process (??)–(??) is convergent and the convergence is of second order.
It holds

$$\|e_i\| = K\tau_n \|e_{i-1}\| + \mathcal{O}(\tau_n^2), \tag{40}$$

where K *is an estimation of the residual* $||R(\tilde{c})|| \leq R_{\max} \in I\!R^+$ *for all* $\tilde{c} \in \mathbf{X}$ *and* $||\tilde{B}|| \leq \tilde{K}$.

One could also obtain the result with Lipschitz-constants.

We now prove the argument using the semi-group theory.

Proof 2 *Let us consider the iteration (??)–(??) in the sub-interval* $[t^n, t^{n+1}]$.
The linearized splitting method is given as :

$$\frac{\partial c_i(t)}{\partial t} = \tilde{A} c_i(t) + \tilde{B} c_{i-1}(t) + R(c_{i-1}) c_{i-1}(t), \tag{41}$$

$$\text{with } c_i(t^n) = c^n \tag{42}$$

$$c_0(t^n) = c^n \ , \ c_{-1} = 0,$$

$$\frac{\partial c_{i+1}(t)}{\partial t} = \tilde{A} c_i(t) + \tilde{B} c_{i+1}(t) + R(c_{i-1}) c_{i-1}(t), \tag{43}$$

$$\text{with } c_{i+1}(t^n) = c^n \ ,$$

where c^n *is the known split approximation at the time level* $t = t^n$. *We solve the subproblems consecutively for* $i = 0, 2, \ldots, 2m$.

For the error function $e_i(t) = c(t) - c_i(t)$ *we have the relations*

$$\begin{aligned} \partial_t e_i(t) &= \tilde{A}(e_i(t)) + \tilde{B}(e_{i-1}(t)) + R(e_{i-1}) e_{i-1}(t), \quad t \in (t^n, t^{n+1}], \\ e_i(t^n) &= 0 \ , \end{aligned} \tag{44}$$

and

$$\begin{aligned} \partial_t e_{i+1}(t) &= \tilde{A}(e_i(t)) + \tilde{B}(e_{i+1}(t)) + R(e_{i-1}) e_{i-1}(t), \quad t \in (t^n, t^{n+1}], \\ e_{i+1}(t^n) &= 0 \ , \end{aligned} \tag{45}$$

for $m = 0, 2, 4, \ldots,$ *with* $e_0(0) = 0$ *and* $e_{-1}(t) = c(t)$ *and*
$\tilde{A} = A(e_{i-1}) + \frac{\partial A(e_{i-1})}{\partial c} e_{i-1}$, $\tilde{B} = B(e_{i-1}) + \frac{\partial B(e_{i-1})}{\partial c} e_{i-1}$,
$R(e_{i-1}) = \frac{\partial A(e_{i-1})}{\partial c} e_{i-1} + \frac{\partial B(e_{i-1})}{\partial c} e_{i-1}$.

In the following we derive the linearized equations. We use the notation $\mathbf{X}^2$ *for the product space* $\mathbf{X} \times \mathbf{X}$ *enabled with the norm* $\|(u, v)\| = \max\{\|u\|, \|v\|\}$ $(u, v \in \mathbf{X})$. *The elements* $\mathcal{E}_i(t)$, $\mathcal{F}_i(t) \in \mathbf{X}^2$ *and the linear operator* $\mathcal{A} : \mathbf{X}^2 \to \mathbf{X}^2$ *are defined as follows*

$$\mathcal{E}_i(t) = \begin{bmatrix} e_i(t) \\ e_{i+1}(t) \end{bmatrix}; \quad \mathcal{A} = \begin{bmatrix} \tilde{A} & 0 \\ \tilde{A} & \tilde{B} \end{bmatrix}, \tag{46}$$

$$\mathcal{F}_i(t) = \begin{bmatrix} R(e_{i-1})e_{i-1} + \tilde{B}e_{i-1} \\ R(e_{i-1})e_{i-1} \end{bmatrix} . \tag{47}$$

where have the bounded and linearized operators $\tilde{A}$, $\tilde{B}$ and $R(e_{i-1}$.

Using notation (18) and (46), the relations (44)–(45) can be written in the form

$$\begin{aligned} \partial_t \mathcal{E}_i(t) &= \mathcal{A}\mathcal{E}_i(t) + \mathcal{F}_i(t), \quad t \in (t^n, t^{n+1}], \\ \mathcal{E}_i(t^n) &= 0. \end{aligned} \tag{48}$$

Due to our assumptions that A and B are bounded and differentiable and that we have a Lipschitzian domain, $\mathcal{A}$ is a generator of the one-parameter C_0 semigroup $(\mathcal{A}(t))_{t\geq 0}$. We also assume the estimate of our term $\mathcal{F}_i(t)$ with the growth conditions.

We can estimate the right hand side $\mathcal{F}_i(t)$ with help of Lemma 1 presented after this proof. Hence, using the variations of constants formula, the solution of the abstract Cauchy problem (48) with homogeneous initial condition can be written as (cf. e.g. [7])

$$\mathcal{E}_i(t) = \int_{t^n}^{t} \exp(\mathcal{A}(t-s))\mathcal{F}_i(s)ds, \quad t \in [t^n, t^{n+1}]. \tag{49}$$

Hence, using the denotation

$$\|\mathcal{E}_i\|_\infty = \sup_{t\in[t^n,t^{n+1}]} \|\mathcal{E}_i(t)\| \ , \tag{50}$$

and taking into account Lemma 1, we have

$$\begin{aligned} \|\mathcal{E}_i(t)\|_\infty &\leq \|\mathcal{F}_i\|_\infty \int_{t^n}^{t} \|\exp(\mathcal{A}(t-s))\|ds \\ &\leq C\ \|e_{i-1}(t)\| \int_{t^n}^{t} \|\exp(\mathcal{A}(t-s))\|ds, \quad t \in [t^n, t^{n+1}]. \end{aligned} \tag{51}$$

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

$$\|\exp(\mathcal{A}t)\| \leq K\exp(\omega t)\ , \quad t \geq 0\ , \tag{52}$$

with some numbers $K \geq 0$ and $\omega \in I\!R$ (see [7]).

- *Assume that $(\mathcal{A}(t))_{t\geq 0}$ is a bounded or exponentially stable semigroup, i.e. that (52) holds with some $\omega \leq 0$. Then obviously the inequality*

$$\|\exp(\mathcal{A}t)\| \leq K; \quad t \geq 0\ , \tag{53}$$

  holds, and hence from (51), we have

$$\|\mathcal{E}_i(t)\|_\infty \leq K\tau_n \|e_{i-1}(t)\|, \quad t \in (0, \tau_n). \tag{54}$$

- *Assume that $(\mathcal{A}(t))_{t\geq 0}$ has exponential growth with some $\omega > 0$. From (52) we have*

$$\int_{t^n}^{t^{n+1}} \|\exp(\mathcal{A}(t-s))\|ds \leq K_\omega(t), \quad t \in [t^n, t^{n+1}], \tag{55}$$

where

$$K_\omega(t) = \frac{K}{\omega}\left(\exp(\omega(t-t^n)) - 1\right), \quad t \in [t^n, t^{n+1}] , \tag{56}$$

and hence

$$K_\omega(t) \leq \frac{K}{\omega}\left(\exp(\omega\tau_n) - 1\right) = K\tau_n + \mathcal{O}(\tau_n^2) , \tag{57}$$

where $\tau_n = t^{n+1} - t^n$*. The estimations (54) and (57) result in*

$$\|\mathcal{E}_i\|_\infty = K\tau_n\|e_{i-1}\| + \mathcal{O}(\tau_n^2). \tag{58}$$

Taking into the account the definition of $\mathcal{E}_i$ *and the norm* $\|\cdot\|_\infty$*, that results to have the estimation* $||e_{i+1}|| \leq ||e_i||$*, we obtain*

$$\|e_i\| = K\tau_n\|e_{i-1}\| + \mathcal{O}(\tau_n^2),$$

which proves our statement. □

Lemma 2 *The term* $\mathcal{F}_i(t)$ *given by (47) can be estimated as*

$$||\mathcal{F}_i(t)|| \leq C||e_{i-1}|| . \tag{59}$$

where we assume the boundedness of $R(e_{i-1})$ *and* $\tilde{B}$*, see Theorem 1.*
Proof 3 *We have the norm* $||\mathcal{F}_i(t)|| = \max\{\mathcal{F}_{i_1}(t), \mathcal{F}_{i_2}(t)\}$*.*
Each term can be bounded as follows.

$$\begin{aligned} ||\mathcal{F}_{i_1}(t)|| &\leq ||(R(e_{i-1}(t)) + \tilde{B})e_{i-1}(t)|| \\ &\leq (R_{max} + \tilde{K})||e_{i-1}(t)|| , \end{aligned} \tag{60}$$

$$\begin{aligned} ||\mathcal{F}_{i_2}(t)|| &\leq ||R(e_{i-1}(t))e_{i-1}(t)|| \\ &\leq R_{max}||e_{i-1}(t)|| . \end{aligned} \tag{61}$$

where R_{max} *and* $\tilde{K}$ *are constants and defined in Theorem 1.*
So we obtain the estimate

$$||\mathcal{F}_i(t)|| \leq C||e_{i-1}(t)||,$$

where $C = R_{max} + \tilde{K}$*.* □

5.2. *Iterative operator-splitting method as a fix-point scheme*

The iterative operator-splitting method is used as a fix-point scheme to linearize the nonlinear operators, see [8] and [6].

We restrict our attention to time-dependent partial differential equations of the form:

$$\frac{du}{dt} = A(u(t))u(t) + B(u(t))u(t), \text{with } u(t^n) = c^n, \tag{62}$$

where $A(u), B(u) : \mathbf{X} \to \mathbf{X}$ are linear and densely defined in the real Banach space $\mathbf{X}$, involving only spatial derivatives of c, see [9]. In the following we discuss the standard iterative operator-splitting methods as a fix-point iteration method to linearize the operators.

We split our nonlinear differential equation (62) by applying:

$$\frac{du_i(t)}{dt} = A(u_{i-1}(t))u_i(t) \ + \ B(u_{i-1}(t))u_{i-1}(t), \text{ with } \ u_i(t^n) = c^n, \tag{63}$$

$$\frac{du_{i+1}(t)}{dt} = A(u_{i-1}(t))u_i(t) \ + \ B(u_{i-1}(t))u_{i+1}, \text{ with } \ u_{i+1}(t^n) = c^n, \tag{64}$$

where the time step is $\tau = t^{n+1} - t^n$. The iterations are $i = 1, 3, \ldots, 2m+1$. $u_0(t) = c_n$ is the starting solution, where we assume the solution c^{n+1} is near c^n, or $u_0(t) = 0$. So we have to solve the local fix-point problem. c^n is the known split approximation at the time level $t = t^n$.
The split approximation at time level $t = t^{n+1}$ is defined as $c^{n+1} = u_{2m+2}(t^{n+1})$. We assume the operators $A(u_{i-1}), B(u_{i-1}) : \mathbf{X} \to \mathbf{X}$ to be linear and densely defined on the real Banach space $\mathbf{X}$, for $i = 1, 3, \ldots, 2m+1$.
Here the linearization is done with respect to the iterations, such that $A(u_{i-1}), B(u_{i-1})$ are at least non-dependent operators in the iterative equations, and we can apply the linear theory.
The linearization is at least in the first equation $A(u_{i-1}) \approx A(u_i)$, and in the second equation $B(u_{i-1}) \approx B(u_{i+1})$
We have

$$||A(u_{i-1}(t^{n+1}))u_i(t^{n+1}) - A(u^{n+1})u(t^{n+1})|| \leq \epsilon,$$

with sufficient iterations $i = \{1, 3, \ldots, 2m+1\}$.
Remark 4 *The linearization with the fix-point scheme can be used for smooth or weak nonlinear operators, otherwise we loose the convergence behavior, while we did not converge to the local fix-point, see [6].*

6. Experiments

We deal with the following coupled transport and flow-field equations:

$$\frac{\partial u}{\partial t} = -\mathbf{v} \cdot \nabla u + \nabla \cdot D \nabla u, \tag{65}$$

$$\frac{\partial \mathbf{v}}{\partial t} = -\frac{\frac{\partial u}{\partial t}}{u}\mathbf{v} + \frac{\nu}{\mu}\mathbf{E}, \tag{66}$$

$$u(\mathbf{x}, \mathbf{t_0}) = u_0(\mathbf{x}), \tag{67}$$

$$\mathbf{v}(\mathbf{x}, \mathbf{t_0}) = \mathbf{v}_0(\mathbf{x}), \tag{68}$$

where we have Neumann boundary conditions.
We deal with several methods and have the following general setting. Let $\Omega = [0,1] \times [0,1] \times [0,1]$, the unit cube. There we set up the initial concentration

$$u_{t_0}(\mathbf{x}) = 2 \exp\left(\frac{-(\mathbf{x} - \mathbf{a})^2)}{0.02}\right) \quad \forall \mathbf{x} \in \Omega \tag{69}$$

$$\text{with } \mathbf{a} = (0.5, 0.5, 0.5)^T \tag{70}$$

which is just the analytical solution

$$u_a(\mathbf{x}, t) = \frac{1}{t} \exp\left(\frac{-(\mathbf{x} - \mathbf{v}t)^2}{4Dt}\right) \tag{71}$$

with $\mathbf{v} = \mathbf{1}$ and $D = 0.01$ at $t = t_0 = 0.5$ on Ω.
During the following experiments we will set $\mathbf{v} = \mathbf{0}$ and consider an equidistant lattice of N^3 points ($\Delta x = \Delta y = \Delta z = \Delta = \frac{1}{N-1}$). We set $\Delta_0 = \frac{1}{60}$, $\Delta t_0 = \frac{1}{4}\Delta_0$ and $t_{end} = 1.5041\bar{6}$ ($t_{end} = t_0 + 241 \cdot \Delta t_0$).

To calculate the error we will use a reference solution which is generated with Kutta's fourth order method where $N = 241$ so that $\Delta = \frac{1}{240}$ and $\Delta t = \frac{1}{48}\Delta$.
In the following tabular (Kutta fourth order) all values have the dimension $1 \cdot 10^{-3}$.

	Δt_0	$\frac{1}{2}\Delta t_0$	$\frac{1}{3}\Delta t_0$	$\frac{1}{4}\Delta t_0$	$\frac{1}{5}\Delta t_0$	$\frac{1}{6}\Delta t_0$	$\frac{1}{7}\Delta t_0$	$\frac{1}{8}\Delta t_0$	$\frac{1}{9}\Delta t_0$	$\frac{1}{10}\Delta t_0$	$\frac{1}{11}\Delta t_0$	$\frac{1}{12}\Delta t_0$
Δ_0	0.9195	0.9600	0.9735	0.9803	0.9843	0.9870	0.9889	0.9904	0.9915	0.9924	0.9931	0.9938
$\frac{1}{2}\Delta_0$	∞	∞	0.3427	0.3498	0.3540	0.3568	0.3589	0.3604	0.3615	0.3625	0.3633	0.3639
$\frac{1}{3}\Delta_0$	∞	∞	∞	∞	∞	0.1179	0.1200	0.1215	0.1227	0.1236	0.1244	0.1251
$\frac{1}{4}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	0

The last value is zero because this was the reference solution. The result is graphically shown in figure 1.

In the following tabular (Heun third order) all values have the dimension $1 \cdot 10^{-3}$.

	Δt_0	$\frac{1}{2}\Delta t_0$	$\frac{1}{3}\Delta t_0$	$\frac{1}{4}\Delta t_0$	$\frac{1}{5}\Delta t_0$	$\frac{1}{6}\Delta t_0$	$\frac{1}{7}\Delta t_0$	$\frac{1}{8}\Delta t_0$	$\frac{1}{9}\Delta t_0$	$\frac{1}{10}\Delta t_0$	$\frac{1}{11}\Delta t_0$	$\frac{1}{12}\Delta t_0$
Δ_0	0.9195	0.9600	0.9735	0.9803	0.9843	0.9870	0.9889	0.9904	0.9915	0.9924	0.9931	0.9938
$\frac{1}{2}\Delta_0$	∞	∞	0.3427	0.3498	0.3540	0.3568	0.3589	0.3604	0.3615	0.3625	0.3633	0.3639
$\frac{1}{3}\Delta_0$	∞	∞	∞	∞	∞	∞	0.1200	0.1215	0.1227	0.1236	0.1244	0.1251
$\frac{1}{4}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	$8 \cdot 10^{-9}$

The result is graphically shown in figure 2.

In the following tabular (Adam-Bashforth second order) all values have the dimension $1 \cdot 10^{-3}$.

	Δt_0	$\frac{1}{2}\Delta t_0$	$\frac{1}{3}\Delta t_0$	$\frac{1}{4}\Delta t_0$	$\frac{1}{5}\Delta t_0$	$\frac{1}{6}\Delta t_0$	$\frac{1}{7}\Delta t_0$	$\frac{1}{8}\Delta t_0$	$\frac{1}{9}\Delta t_0$	$\frac{1}{10}\Delta t_0$	$\frac{1}{11}\Delta t_0$	$\frac{1}{12}\Delta t_0$
Δ_0	∞	0.9599	0.9735	0.9802	0.9843	0.9870	0.9889	0.9904	0.9915	0.9924	0.9931	0.9938
$\frac{1}{2}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	0.3604	0.3615	0.3625	0.3632	0.3639
$\frac{1}{3}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞
$\frac{1}{4}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞

The result is graphically shown in figure 3.

In the following tabular (Adam-Bashforth third order) all values have the dimension $1 \cdot 10^{-3}$.

	Δt_0	$\frac{1}{2}\Delta t_0$	$\frac{1}{3}\Delta t_0$	$\frac{1}{4}\Delta t_0$	$\frac{1}{5}\Delta t_0$	$\frac{1}{6}\Delta t_0$	$\frac{1}{7}\Delta t_0$	$\frac{1}{8}\Delta t_0$	$\frac{1}{9}\Delta t_0$	$\frac{1}{10}\Delta t_0$	$\frac{1}{11}\Delta t_0$	$\frac{1}{12}\Delta t_0$
Δ_0	∞	∞	∞	0.9803	0.9843	0.9870	0.9889	0.9904	0.9915	0.9924	0.9931	0.9938
$\frac{1}{2}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞
$\frac{1}{3}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞
$\frac{1}{4}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞

The result is graphically shown in figure 4.

In the following tabular (Adam-Bashforth fourth order) all values have the dimension $1 \cdot 10^{-3}$.

	Δt_0	$\frac{1}{2}\Delta t_0$	$\frac{1}{3}\Delta t_0$	$\frac{1}{4}\Delta t_0$	$\frac{1}{5}\Delta t_0$	$\frac{1}{6}\Delta t_0$	$\frac{1}{7}\Delta t_0$	$\frac{1}{8}\Delta t_0$	$\frac{1}{9}\Delta t_0$	$\frac{1}{10}\Delta t_0$	$\frac{1}{11}\Delta t_0$	$\frac{1}{12}\Delta t_0$
Δ_0	∞	∞	∞	∞	∞	0.9870	0.9889	0.9904	0.9915	0.9924	0.9931	0.9938
$\frac{1}{2}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞
$\frac{1}{3}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞
$\frac{1}{4}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞

The result is graphically shown in figure 5.

In the following tabular (Adam-Bashforth fifth order) all values have the dimension $1 \cdot 10^{-3}$.

	Δt_0	$\frac{1}{2}\Delta t_0$	$\frac{1}{3}\Delta t_0$	$\frac{1}{4}\Delta t_0$	$\frac{1}{5}\Delta t_0$	$\frac{1}{6}\Delta t_0$	$\frac{1}{7}\Delta t_0$	$\frac{1}{8}\Delta t_0$	$\frac{1}{9}\Delta t_0$	$\frac{1}{10}\Delta t_0$	$\frac{1}{11}\Delta t_0$	$\frac{1}{12}\Delta t_0$
Δ_0	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	0.9931	0.9938
$\frac{1}{2}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞
$\frac{1}{3}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞
$\frac{1}{4}\Delta_0$	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞	∞

The result is graphically shown in figure 6.

This results show that the quality of all four methods is much more restricted by the accuracy in space than in time.

Remark 5 *We receive convergent results in time and space for the Adam-Bashforth and iterative splitting solver. The results can be improved by using higher order Adam-Bashforth methods and more refined grids.*

7. Conclusion

We discussed iterative splitting schemes for nonlinear coupled partial differential equations. The numerical analysis is presented for nonlinear and spatial discretised equations and we obtain higher order results with more iterative steps. With explicit discretization schemes as Adam-Bashforth methods, we can accelerate our solver schemes, while we skip costly implicit methods. A priori error estimates allow to optimize the time steps. In future we are taken into account a framework to couple partial differential equations based on fix-point and iterative schemes.

8. Appendix

8.1. *Explicit Time-Integration Methods*

To have fast methods, we consider explicit time-integration methods for the coupled equations.

We consider Adam-Bashforth (AB) and Runge-Kutta (RK) methods.

While the time steps $AB1$ is $\Delta t \approx \frac{1}{\sqrt{50}}\Delta x$ and $AB2$ is $\Delta t \approx \frac{1}{\sqrt{200}}\Delta x$, we apply the RK schemes with $\Delta t \approx \frac{1}{\sqrt{7}}\Delta x$.

8.1.1. *Adam-Bashforth methods*

$$y_{n+1} = y_n + h \sum_{j=0}^{s} b_j \, f(t_{n-j}, y_{n-j}) \tag{72}$$

$$b_j = \frac{(-1)^j}{j!(s-j)!} \int_0^1 \prod_{i=0, i\neq j}^{s} (u+i)\, du, \quad j = 0, \ldots, s. \tag{73}$$

We consider here
$s = 2$ (second order)

$$y_{n+1} = y_n + h \left(\frac{3}{2} f(t_n, y_n) - \frac{1}{2} f(t_{n-1}, y_{n-1}) \right) \tag{74}$$

and $s = 3$ (third order)

$$y_{n+1} = y_n + h \left(\frac{23}{12} f(t_n, y_n) - \frac{16}{12} f(t_{n-1}, y_{n-1}) + \frac{5}{12} f(t_{n-2}, y_{n-2}) \right) \tag{75}$$

and $s = 4$ (fourth order)

$$y_{n+1} = y_n + h \left(\tfrac{55}{24} f(t_n, y_n) - \tfrac{59}{24} f(t_{n-1}, y_{n-1}) + \tfrac{37}{24} f(t_{n-2}, y_{n-2}) - \tfrac{3}{8} f(t_n - 3, y_n - 3) \right), \tag{76}$$

and $s = 5$ (fifth order)

$$\begin{aligned} y_{n+1} &= y_n + h\big(\tfrac{1901}{720} f(t_n, y_n) - \tfrac{1387}{360} f(t_{n-1}, y_{n-1}) \\ &\quad + \tfrac{109}{30} f(t_{n-2}, y_{n-2}) - \tfrac{637}{360} f(t_{n-3}, y_{n-3}) + \tfrac{251}{720} f(t_n - 4, y_n - 4)\big). \end{aligned} \tag{77}$$

8.1.2. *Explicit Runge-Kutta methods*

In general a s-stage Runge-Kutta method can be written in the following way:

$$y_{n+1} = y_n + h \sum_{j=1}^{s} b_j k_j \tag{78}$$

where

$$k_j = f\left(t_n + hc_j, y_n + h\sum_{l=1}^{s} a_{jl}k_l\right) \tag{79}$$

We will take into account the following two:
Heun's third-order

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{2}{3} & 0 & \frac{2}{3} & 0 \\ \hline & \frac{1}{4} & 0 & \frac{3}{4} \end{array} = \begin{array}{c|c} c & A \\ \hline & b^T \end{array} \tag{80}$$

and
Kutta's classical fourth-order

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{array} = \begin{array}{c|c} c & A \\ \hline & b^T \end{array} \tag{81}$$

8.2. *Matrix Exponential Methods*

Another way of computing fast explicit schemes of ODE systems of first order are matrix exponentials.

We deal with:

$$\frac{dy}{dt} = Ay,\ y(0) = y_0, \tag{82}$$

where we assume $A = D + N$, D is the diagonal part and N is the nilpotent part of the matrix A.

We assume also $[D, N] = 0$ and we have the solution:

$$y(t) = \exp(Dt)\exp(Nt)y_0, \tag{83}$$

where $\exp(Dt)$ can be computed just exponentiating every entry on the main diagonal and

$$\exp(Nt) \approx I + N\,t + N^2\,\frac{t^2}{2} + N^3\,\frac{t^3}{3}, \tag{84}$$

where N is the nilpotent matrix and $N \cdot N$ is only a shift of the to the next higher upper or lower diagonal.

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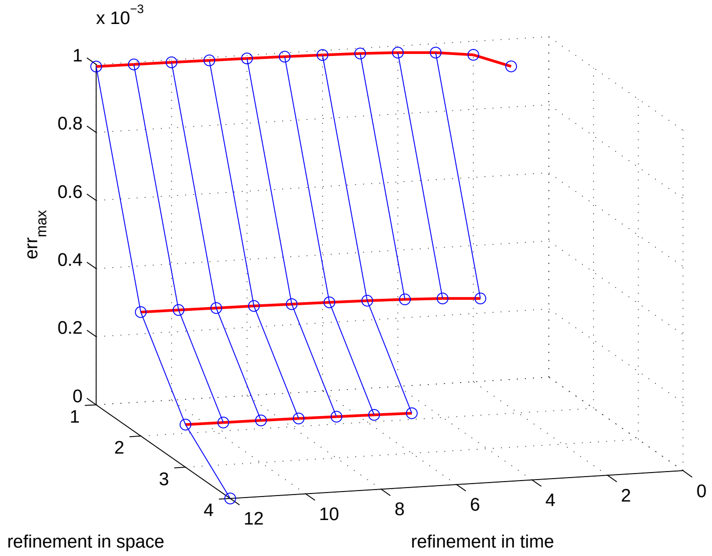

Fig. 1. Maximum error Kutta's fourth

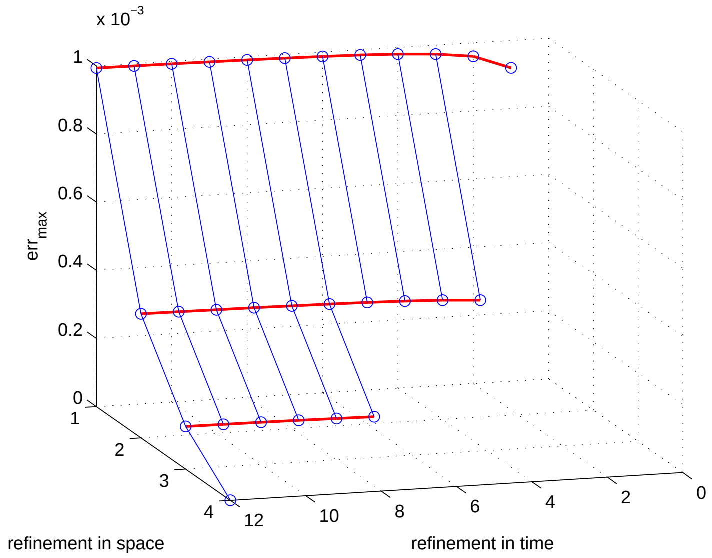

Fig. 2. Maximum error Heun's third

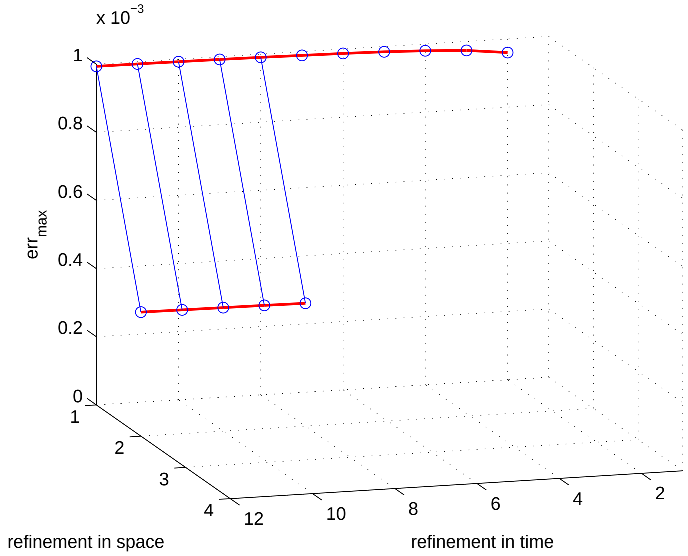

Fig. 3. Maximum error Adam-Bashforth second

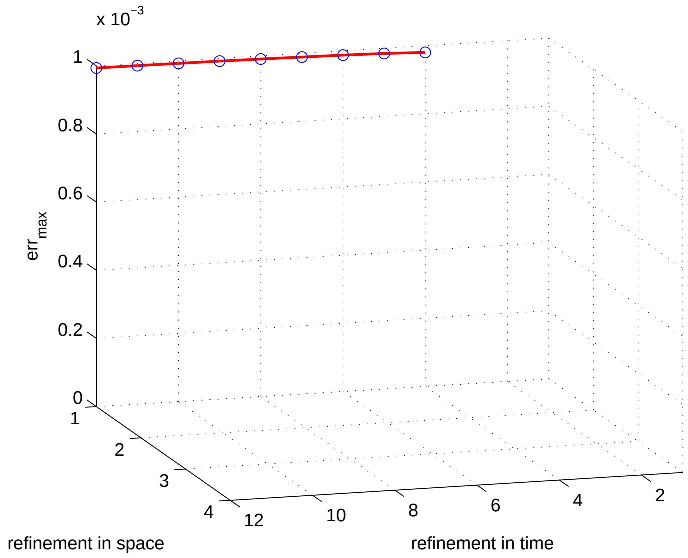

Fig. 4. Maximum error Adam-Bashforth third

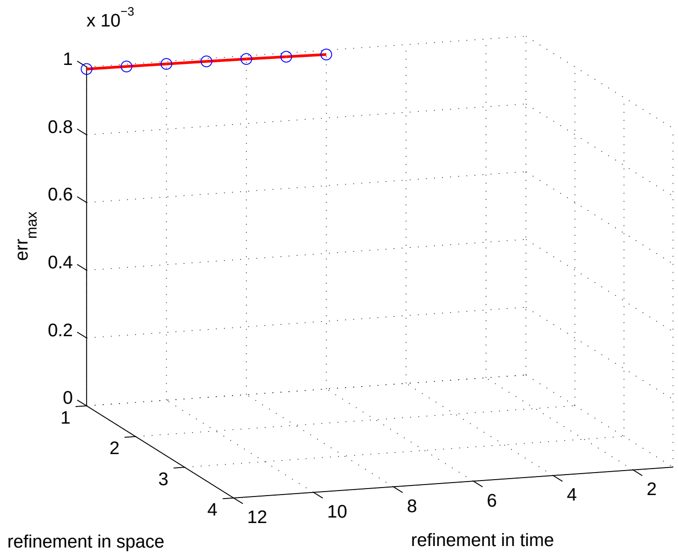

Fig. 5. Maximum error Adam-Bashforth fourth

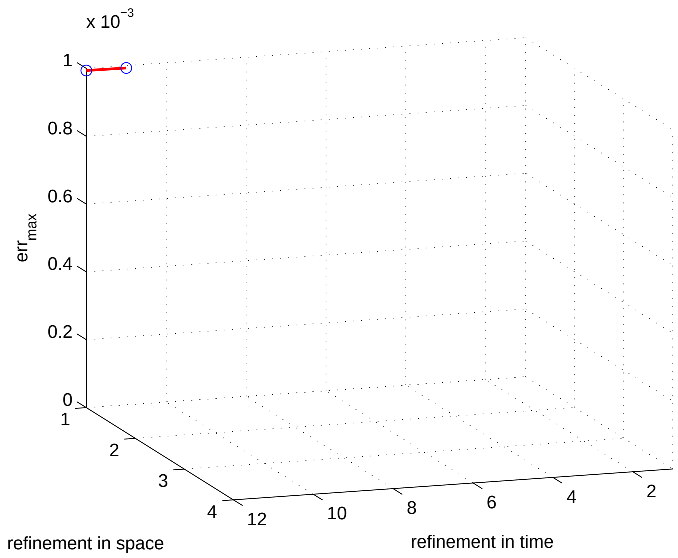

Fig. 6. Maximum error Adam-Bashforth fifth