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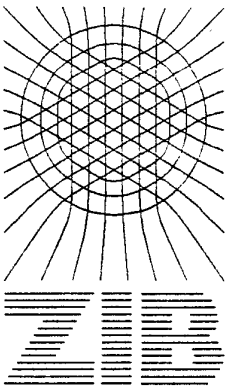

MICHAEL WULKOW

Adaptive Treatment of Polyreactions in Weighted Sequence Spaces

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MICHAEL WULKOW

Konrad–Zuse–Zentrum für Informationstechnik Berlin, Heilbronner Strasse 10, D-1000 Berlin 31, Federal Republic of Germany

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ABSTRACT

Countable systems of ordinary differential equations appear frequently in chemistry, physics, biology and statistics. They can be considered as ordinary differential equations in sequence spaces. In this work, a fully adaptive algorithm for the computational treatment of such systems is developed. The method is based on a time discretization of an abstract Cauchy problem in Hilbert space and a discrete Galerkin approach for the discretization of the arising stationary subproblems. The Galerkin method uses orthogonal functions of a discrete variable, which are generated by certain weight functions. A theory of countable systems in the associated weighted sequence spaces is developed as well as a theory of the Galerkin method. The Galerkin equations are solved adaptively either by use of analytical properties of the orthogonal functions or by an appropriate numerical summation. The resulting algorithm CODEX is applied to examples of technological interest, in particular from polymer chemistry.

INTRODUCTION

Polymers belong to the most important materials in our technology. In a *polymerization process* single molecules are linked together to long polymer chains. The mathematical modeling of a polymerization (see e.g. [35]) leads to as many single differential equations as polymer chains can arise during the reaction. In general this number is not known a priori (sometimes not even the scale), but must be assumed to be very large ($10^4 - 10^6$ in realistic examples) or even infinite. The resulting system is then called a *countable system of ordinary differential equations* (CODE). Countable systems appear also in other fields of chemistry, in physics [23], statistics and economics [20].

For the numerical treatment of CODE's there exist several methods, which have been originally developed for special problems in the applications. However, there is no comprehensive numerical approach up to now and "nearly nothing has been done concerning qualitative behavior of solutions" [13] in the theory.

As a new numerical approach, a *discrete Galerkin method* has been suggested by DEUFLHARD and the author [19]. Thereby orthogonal functions of a *discrete* variable are used to approximate the solution of a countable system. The method has been worked out and implemented for problems from polymer chemistry in the program package MACRON [1].

This paper presents the new algorithm CODEX, which extends the ideas of the discrete Galerkin method and avoids some drawbacks of MACRON, which arise from the fact, that it corresponds to the method of lines. A countable system is considered now as an evolution equation in a sequence space. Following ideas of BORNEMANN [6], [7], this equation is discretized in time first. The resulting stationary subproblem to perform a time step is then solved approximately by a Galerkin method in a scale of Hilbert spaces generated by a two-parameter family of weight functions. It turns out, that CODEX performs well for a wide class of problems with solutions having structural similarities to the suggested weight functions. The theoretical and numerical concepts can easily be applied to similar approaches in weighted sequence or function spaces.

After introducing some very common model problems, in Section 1 a basis independent theory of countable systems in the sequence spaces $H_{\rho,\alpha}$ is derived. Section 2 is concerned with the construction and examination of basis functions of $H_{\rho,\alpha}$, which are determined by the so–called *modified discrete Laguerre polynomials*. In Section 3 the algorithm is outlined very briefly, then the time discretization scheme and the Galerkin method in $H_{\rho,\alpha}$ are discussed. Section 4 illustrates the efficiency of CODEX on examples from polymer chemistry.

1 Countable Systems of Ordinary Differential Equations

1.1 Model Problems

We consider scalar initial value problems of the type (CODE)

$$u_s'(t) = f_s(t, u_1(t), u_2(t), \ldots)\ ,\ u_s(0) = \varphi_s\ ,\ s \in \mathbb{N}\ (s \geq 1)\ , \tag{1.1}$$

where the functions

$$f_s : [0, T_f] \times D \to \mathbb{R}\ ,\ D \subset \mathbb{R}^{\mathbb{N}}\ ,\ s \in \mathbb{N}\ ,$$

and the initial value

$$\varphi = (\varphi_s) \in \mathbb{R}^{\mathbb{N}}\ ,$$

are given. The actual sequence space will be specified later on. The prime denotes the derivative with respect to the time t. The index of the sequence will usually be called s. For ease of writing we will alternate between the notations $u_s(t)$ and $u(s,t)$ for the s–component of the sequence (grid function) u at time t. As far as the context is clear the time dependence will be omitted, such that $u(s)$ or u_s means $u(s,t)$.
A function

$$u\ :\ [0,T] \to D\ \ ,\ \ T \in (0\ , T_f]\ ,$$

is called a solution of (1.1), if $u_s(0) = \varphi_s$, $u_s \in C^1((0,T])$ and $u_s' = f_s(t,u)$ in $[0,T]$ for each $s \in \mathbb{N}$.

Example 1.1: Backward difference equation. Consider the equation

$$u'(t) = -\nabla u(t)\ ,\ u(0) = \varphi\ , \tag{1.2}$$

where the *backward difference operator* ∇ is defined by

$$(\nabla u)_1 = u_1\ ,\ (\nabla u)_s = u_s - u_{s-1}\ ,\ s = 2, 3, \ldots\ . \tag{1.3}$$

Equation (1.2) appears as a basic module in many problems (e.g. as *chain addition* $P_s + M \to P_{s+1}$ in polymerization models). For an initial sequence φ the solution of (1.2) can be written as

$$u_s(t) = (T(t)\,\varphi)(s)$$

in terms of a semigroup $T(t)$ given by

$$(T(t)\,\varphi)(s) = e^{-t} \sum_{r=1}^{s} \frac{t^{s-r}}{(s-r)!}\,\varphi(r)\ . \tag{1.4}$$

Specializing $\varphi_s = \delta_{s,1}$, $\delta_{s,r}$ the Kronecker symbol, the solution $u_s(t)$ is a *Poisson distribution* with parameter t:

$$u_s(t) = e^{-t}\,\frac{t^{s-1}}{(s-1)!}$$

Example 1.2: Summatory systems. Equations of this type have been studied by HILLE [28] and are related to mathematical models of *polymer degradation processes* [5], which have already been treated numerically by use of the discrete Galerkin method in [19] and [38] (see also Example 4.2). Let us consider the following system:

$$(1.5) \qquad u_s'(t) = -(s-1)\,u_s(t) + \sum_{r=s+1}^{\infty} u_r(t)\ ,\ u_s(0) = \varphi_s\ ,\ s \in \mathbb{N}\ .$$

The initial value problem (1.5) is *not uniquely* solvable, because its solution depends on an arbitrary (only integrable) function $f = f(t)$ [28]. However, with the definition of a family of Hilbert spaces

$$H_t := \left\{ u \in \mathbb{R}^{\mathbb{N}} \mid \|u\|_t^2 := \sum_{s=1}^{\infty} u_s^2\, e^{st} < \infty \right\}\ ,$$

the condition $u(t) \in H_t$ enforces the uniqueness of the solution and the boundedness of all statistical moments of u (Corollary 1.4). The latter property is a natural requirement in many problems. Finally, in H_t an efficient approximation of solutions of (1.5) is possible [19].

Example 1.3: Smolochowski model. In [19], the solution of the *Smolochowski model*

$$(1.6) \quad u_s'(t) = \frac{1}{2}\sum_{r=1}^{s-1} u_r(t)\,u_{s-r}(t) - u_s(t)\sum_{s=1}^{\infty} u_r(t)\ \ ,\ \ u_s(0) = \delta_{s,1}\ ,\ s \in \mathbb{N}\,,$$

could be approximated well in the scale of Hilbert spaces

$$(1.7) \qquad H_\rho := \left\{ u \in \mathbb{R}^{\mathbb{N}} \mid \|u\|_\rho^2 := \sum_{s=1}^{\infty} u_s^2\,(1-\rho)^{-1}\rho^{-(s-1)} < \infty \right\}$$

for $\rho > (\frac{t}{t+2})^2$. The condition on ρ is necessary and enforces the change of the space H_ρ with t. The reason is, that the operator describing this problem is not Lipschitz continuous as an operator on H_ρ for fixed ρ, but only as an operator on the scale H_ρ, $0 < \rho < 1$ (Example 1.6).

1.2 A Two-Parameter Scale of Hilbert Spaces

We construct weighted sequence spaces, which allow a theory of countable systems as well as an efficient numerical treatment of interesting problems.

Definition 1.1. *Define the weighted sequence spaces $H_{\rho,\alpha}$ by*

$$H_{\rho,\alpha} := \left\{ u \in \mathbb{R}^{\mathbb{N}} \mid \|u\|_{\rho,\alpha}^2 := \sum_{s=1}^{\infty} u_s^2 \, \Psi_{\rho,\alpha}(s)^{-1} < \infty \right\}, \tag{1.8}$$

where the weight function $\Psi_{\rho,\alpha}(s) > 0$ is given for $s \in \mathbb{N}$ by

$$\Psi_{\rho,\alpha}(s) = C^{\rho,\alpha} \binom{s-1+\alpha}{s-1} \rho^{s-1} \,, \; 0 < \rho < 1 \,, \; \alpha > -1 \,, \tag{1.9}$$

with the constant $C^{\rho,\alpha} = (1-\rho)^{1+\alpha}$ chosen such that $\|\Psi_{\rho,\alpha}\|_{\rho,\alpha} = 1$.

Remarks.

(i) Due to the normalization of the $\Psi_{\rho,\alpha}$, these weight functions can also be regarded as probability distributions. For $\alpha = 0$ the weight function $\Psi_{\rho,\alpha}$ reduces to the geometric distribution. For $\alpha \gg 1$, we obtain a narrow distribution; if we set $\alpha = \lambda/\rho$, $\Psi_{\rho,\lambda/\rho}$ converges pointwise to the Poisson distribution with parameter λ for $\rho \to 0$. A hyperbola of the form $1/s^{\alpha}$ is approximated well by choosing $\alpha < 0$ and ρ close to one.

(ii) For $0 < \rho < 1$ and $\alpha > -1$ the space $H_{\rho,\alpha}$ is equipped with the scalar product

$$(u \,, v)_{\rho,\alpha} := \sum_{s=1}^{\infty} u(s) \, v(s) \, \Psi_{\rho,\alpha}(s)^{-1} \,, \; u, v \in H_{\rho,\alpha} \,. \tag{1.10}$$

(iii) The embeddings

$$H_{\rho,\alpha} \hookrightarrow H_{\bar{\rho},\alpha} \;, \; 0 < \rho < \bar{\rho} < 1 \,, \tag{1.11}$$

and

$$H_{\rho,\alpha} \hookrightarrow H_{\rho,\beta} \;, \; -1 < \alpha < \beta \,, \tag{1.12}$$

are dense and continuous.

Lemma 1.2. *For $0 < \varepsilon < \rho < 1$ let $u \in H_{\rho-\varepsilon,0}$. Then for all polynomials p of degree j we have $p \cdot u \in H_{\rho,\alpha}$ for $\alpha > -1$.*

Proof. For $u \in H_{\rho-\varepsilon,0}$ we have by definition

$$\sum_{s=1}^{\infty} u(s)^2 \, e^{(\lambda+\bar{\varepsilon})s} \; < \infty \, ,$$

writing $\rho = e^{-\lambda}$, $\rho - \varepsilon = e^{-\lambda-\bar{\varepsilon}}$ in terms of $\lambda > 0$, $\bar{\varepsilon} > 0$. Then there is an $\bar{s} \geq 1$ with

$$e^{(\lambda+\bar{\varepsilon})s} > p(s)^2 \, e^{\lambda s}$$

for all $s > \bar{s}$. Thus $\|pu\|_{\rho,0}$ is bounded, if

$$\sum_{s=1}^{\infty} u(s)^2 \, p(s)^2 \, e^{\lambda s} \leq \sum_{s=1}^{\bar{s}} u(s)^2 \, p(s)^2 \, e^{\lambda s} + \sum_{s=\bar{s}+1}^{\infty} u(s)^2 \, e^{(\lambda+\bar{\varepsilon})s} \overset{!}{<} \infty \, ,$$

which is true for $u \in H_{\rho-\varepsilon,0}$. As

$$\binom{s-1+\alpha}{s-1}^{-1} \leq 1 \, , \; \alpha \geq 0 \text{ and } \binom{s-1+\alpha}{s-1}^{-1} \leq \frac{s}{1+\alpha} \, , \; -1 < \alpha < 0 \, ,$$

we get $u \in H_{\rho,\alpha}$ and $pu \in H_{\rho,\alpha}$ for all $\alpha > -1$. ∎

With Lemma 1.2 we can prove the important

COROLLARY 1.3. *If $u \in H_{\rho-\varepsilon,\alpha}$ for one $\alpha > -1$, then $u \in H_{\rho,\beta}$ for all $\beta > -1$.*

Proof. For $\beta \geq \alpha$ see (1.12). For $\beta < \alpha$ the inequality

$$\binom{s-1+\alpha}{s-1} \binom{s-1+\beta}{s-1}^{-1} \leq p(s)^2$$

holds by use of a polynomial p with degree $j \geq (\alpha - \beta)/2$. Application of Lemma 1.2 leads to the assertion. ∎

Remark. The condition $u \in H_{\rho-\varepsilon,\alpha}$ plays an important role in this work. Under numerical aspects it ensures, that we do not approximate an element at the 'edge' of the space $H_{\rho,\alpha}$. Corollary 1.3 implies, that on this condition the $\rho-$ scale is the crucial scale for the theory, whereas the α - scale gives some freedom for approximation purposes.

Example 1.4. Let ρ be given. Define $u(s) := \left(\sqrt{\rho}\right)^{s-1}/s$, $s \geq 1$. Then

$$\|u\|_{\rho,0}^2 = \frac{1}{1-\rho} \sum_{s=1}^{\infty} \frac{1}{s^2} < \infty \, ,$$

but $\sum_{s=1}^{\infty} u(s)^2 \, \Psi_{\bar{\rho},0}(s)^{-1}$ is not bounded for any $\bar{\rho} < \rho$. For $v(s) := s\,u(s)$ we see that $v \notin H_{\rho,0}$. This confirms, that the assumption of Lemma 1.2 and Corollary 1.3 concerning ρ is necessary.

COROLLARY 1.4. *Define for $k = 0, 1, \ldots$, the moments $\mu_k[u]$ of u by*

$$\mu_k[u] := \sum_{s=1}^{\infty} s^k \, u(s) \, . \tag{1.13}$$

Then for $u \in H_{\rho,\alpha}$ all moments of u are bounded.

Proof.

$$\sum_{s=1}^{\infty} s^k \, u(s) = \left(s^k \, \Psi_{\rho,\alpha} \, , \, u \right)_{\rho,\alpha} \leq \mu_{2k}[\Psi_{\rho,\alpha}] \, \|u\|_{\rho,\alpha} < \infty \, ,$$

using the Cauchy–Schwarz inequality and the fact that all moments of $\Psi_{\rho,\alpha}$ are bounded.

The following results are important for the treatment of certain nonlinear operators (e.g. the convolution operator in Example 1.6). We only consider the case $\alpha = 0$ here. For $\alpha \neq 0$ the constants become a little bit more complicated. The proofs are straightforward and can be found in [39].

LEMMA 1.5. *For $0 < \varepsilon < \rho$ it is $\Psi_{\frac{\rho-\varepsilon}{\sqrt{\rho}},0} \in H_{\rho-\varepsilon,0}$ and*

$$\|\Psi_{\frac{\rho-\varepsilon}{\sqrt{\rho}},0}\|_{\rho-\varepsilon,0} = \frac{1}{\sqrt{\varepsilon}} \, M_{\rho,\varepsilon} \, , \; M_{\rho,\varepsilon} := \frac{(\sqrt{\rho} - \rho + \varepsilon)}{\sqrt{(1 - \rho + \varepsilon)}}$$

COROLLARY 1.6. *For $u \in H_{\rho-\varepsilon,0}$, $0 < \varepsilon < \rho$, the following inequality holds:*

$$\sum_{s=1}^{\infty} u(s) \, \Psi_{\sqrt{\rho},0}(s)^{-1} \leq \frac{1}{\sqrt{\varepsilon}} \, \bar{M}_{\rho,\varepsilon} \, \|u\|_{\rho-\varepsilon,0} \, ,$$

with a constant

$$\bar{M}_{\rho,\varepsilon} := \frac{(\rho(1 - \rho + \varepsilon))^{1/2}}{1 - \sqrt{\rho}} \, .$$

1.3 THEORY OF COUNTABLE SYSTEMS

Mathematical theory concerning countable systems has been developed for many years, a survey is given in the monograph of DEIMLING [13]. In contrary to the most authors, which e.g. put conditions on linear countable systems, which are formulated as infinite matrix equations in an l^p-space, we will take a different view. The present approach is motivated by the *qualitative behavior* of the solutions and their efficient approximation. It turns out, that the operators studied here are Lipschitz continuous as operators on a fixed $H_{\rho,\alpha}$ - space or on the scale of these spaces.

Example 1.5. A degradation process in polymer chemistry (compare Example 4.2) can be written as ($s = 1, 2, \ldots$)

$$(1.14)\quad u'(t) = A_D\, u(t) := -(s-1)\, u(s) + 2\left(\sum_{r=1}^{\infty} (S_+)^r\, u\right)(s)\ ,\ u(0) = \varphi\ ,$$

in terms of the forward shift operator

$$(S_+\, u)(s) := u(s+1)\ .$$

The operator S_+ is bounded in $H_{\rho,\alpha}$ with the norm

$$(1.15)\qquad \|S_+\|_{\rho,\alpha} \le M_+ := \begin{cases} \sqrt{\rho(1+\alpha/2)} & ,\quad \alpha \ge 0\ , \\ \sqrt{\rho} & ,\quad -1 < \alpha < 0\ . \end{cases}$$

Thus the infinite sum of operators on the right-hand side of (1.14) converges uniformly to a bounded operator for

$$(1.16)\qquad \rho(1+\alpha/2) < 1$$

(a condition which plays a role in Example 4.2). However, the first term of A_D leads to difficulties. Let $\alpha = 0$ and define an operator A_1 by

$$(A_1\, u)_s := -(s-1)\, u_s\ ,\ s \in \mathbb{N}.$$

A_1 is not bounded in $H_{\rho,0}$, but a short calculation yields

$$(1.17)\qquad \|A_1\, u\|_{\rho,0} \le \frac{C}{\epsilon}\, \|u\|_{\rho-\varepsilon,0}\ ,\ \epsilon > 0\ ,$$

i.e. A_1 is Lipschitz continuous as a map from the 'smaller' space $H_{\rho-\varepsilon,0}$ to the 'larger' space $H_{\rho,0}$. The estimate (1.17) is the motivation for the following theorem, which follows Theorem 15.7 in the textbook [14] and has been converted from certain weighted l^1-spaces to the $H_{\rho,\alpha}$-spaces. Theorem 1.7 supplies existence and uniqueness of solutions of *nonlinear* ODE's in $H_{\rho,0}$ (for simplicity the α – scale is omitted and we write $\|\cdot\|_\rho$ instead of $\|\cdot\|_{\rho,\alpha}$).

THEOREM 1.7. *Consider a sub-scale of H_ρ – spaces for $\rho \in [\rho_0, 1)$, $0 < \rho_0 < 1$. Let $J = [0, T_f] \subset \mathbb{R}$ and assume:*

(a) The operator

$$F\ :\ J \times H_\rho \longrightarrow H_{\bar\rho}$$

is continuous for $\bar\rho > \rho$ and $F(t,0) \in H_{\rho_0}$ on J.

(b) There exists a constant M such that

$$\|F(t,u) - F(t,v)\|_{\bar\rho} \le \frac{M}{(\bar\rho - \rho)^\gamma} \|u - v\|_\rho \,, \; 0 < \gamma \le 1 \,, \tag{1.18}$$

for $t \in J$, $\bar\rho > \rho$ and $u, v \in H_\rho$.

Then for every $\rho \in (\rho_0, 1)$ the initial value problem

$$u'(t) = F(t, u(t)) \,, \; u(0) = \varphi \in H_{\rho_0} \,, \tag{1.19}$$

has a unique solution

$$u : [0, \delta(\bar\rho - \rho)^\gamma) \longrightarrow H_{\bar\rho} \,,$$

with $\delta = \min\{T_f \,, (M d_\gamma)^{-1}\}$. The constant $d_\gamma > 1$ can be computed in concrete cases, e.g. $d_1 = e$, $d_{1/2} = 2\sqrt{3}/3$.

Proof. The proof is based on a fixed point iteration in a scale of Hilbert spaces. We consider the successive approximations

$$u_k(t) = u_0 + \int_0^t F(s, u_{k-1}(s))\, \mathrm{d}s \,, \; k \ge 1 \,, \; u_0 = \varphi \,.$$

Due to the condition (a) and $\varphi \in H_{\rho_0}$, the iterate $u_k : J \to H_\rho$ is continuous for $\rho > \rho_0$. We will show by induction, that

$$\|u_k(t) - u_{k-1}(t)\|_{\bar\rho} \le C_{\rho_0}(t) \left(\frac{M t d_\gamma}{(\bar\rho - \rho_0)^\gamma} \right)^k \quad \text{for} \;\; \bar\rho > \rho_0 \,, \tag{1.20}$$

where $C_{\rho_0}(t) := \|\varphi\|_{\rho_0} + \dfrac{(1-\rho_0)}{M} \max\limits_{s \in [0,t]} \|F(s,0)\|_{\rho_0}$.
In a first step we obtain

$$\|u_1(t) - u_0\|_{\bar\rho} \le \frac{tM}{(\bar\rho - \rho_0)^\gamma} C_{\rho_0}(t) \,,$$

using $\|u\|_{\bar\rho} \le \|u\|_{\rho_0}$ for $\rho_0 \le \bar\rho$. The induction step yields

$$\|u_{k+1}(t) - u_k(t)\|_{\bar\rho} \le \frac{C_{\rho_0}(t)}{\varepsilon^\gamma} \frac{M^{k+1} t^{k+1} d_\gamma^k}{(\bar\rho - \varepsilon - \rho_0)^{\gamma k}} \frac{1}{k+1} \,,$$

where $\varepsilon > 0$ is chosen such that $\bar\rho - \varepsilon > \rho_0$. In order to get rid of the factor $1/(k+1)$ we set

$$\varepsilon = \frac{\bar\rho - \rho_0}{(k+1)^{1/\gamma}}$$

and end up with

$$\|u_{k+1}(t) - u_k(t)\|_{\bar\rho} \le C_{\rho_0}(t) \left(\frac{Mtd_\gamma}{(\bar\rho - \rho_0)^\gamma}\right)^{k+1} \frac{1}{d_\gamma} \left(\frac{k+1}{((k+1)^{1/\gamma} - 1)^\gamma}\right)^k .$$

The last factor on the right-hand side is bounded in k for $\gamma \le 1$. For $\gamma = 1/2$ the maximum is achieved at $k = 1$ with $d_{1/2}$. For $\gamma = 1$ we can see that $((k+1)/k)^k \le e$. Thus (1.20) holds for all k and as $Mtd_\gamma(\bar\rho - \rho)^{-\gamma} < 1$ for $t \in [0, \delta(\bar\rho - \rho_0)^\gamma)$ the sequence $u_k(t)$ is a Cauchy sequence and converges uniformly on every closed subinterval of $[0, \delta(\bar\rho - \rho_0)^\gamma)$ to a continuous $u(t)$ satisfying

$$u(t) = \varphi + \int_0^t F(s, u(s))\, \mathrm{d}s .$$

Moreover $u(t)$ is a solution of the initial value problem, since

$$F(\cdot, u(\cdot)) : [0, \delta(\bar\rho - \rho_0)^\gamma) \to H_{\bar\rho}$$

is continuous. In order to prove local uniqueness, we consider two solutions $u(t)$, $v(t) \in H_{\bar\rho}$, $\bar\rho > \rho_0$. For fixed t and $\rho_1 > \bar\rho$,

$$\|u(t) - v(t)\|_{\rho_1} \le \frac{Mtd_\gamma}{(\rho_1 - \bar\rho)^\gamma} C_1(t) \ , \ C_1(t) = \max_{s\in[0,t]} \|u(s) - v(s)\|_{\bar\rho} .$$

Now, similar to the considerations above, we 'fill in' estimates in k spaces between H_{ρ_1} and $H_{\bar\rho}$ - setting $\varepsilon = (\rho_1 - \bar\rho)/(k+1)^{1/\gamma}$ in the k-th step - and end up with

$$\|u(t) - v(t)\|_{\rho_1} \le C_1(t) \left(\frac{Mtd_\gamma}{(\rho_1 - \bar\rho)^\gamma}\right)^k .$$

Thus for $t < (\rho_1 - \bar\rho)^{-\gamma}(Md_\gamma)^{-1}$ we have $u(t) = v(t)$. The rest follows by continuation. ∎

Example 1.6. Consider the *convolution* operator A_C,

$$(A_C\, u)(s) = \sum_{r=1}^{s-1} u_r\, u_{s-r} ,$$

which is the first part of the Smolochowski model in Example 1.3. Using Lemma 1.5 and Corollary 1.6 it can be shown for the Frechét derivative DA_C of A_C, that

$$\|DA_C(u)\, v\|_\rho^2 \le \frac{1}{\varepsilon} 2(1 - \rho + \varepsilon)\, \|u\|_\rho^2\, \|v\|_{\rho-\varepsilon}^2 .$$

Application of the mean-value theorem gives (1.18) with $\gamma = 1/2$. Thus Theorem 1.7 explains, why the space H_ρ has to be changed with time for the Smolochowski model.

2 Modified Discrete Laguerre Polynomials

In this section, an orthogonal basis of the spaces $H_{\rho,\alpha}$ is described in view of a Galerkin method in this spaces. The basis functions are given in terms of the *modified discrete Laguerre polynomials*. Important properties of these polynomials are presented in Section 2.2. The approximation of an element $u \in H_{\rho,\alpha}$ by the orthogonal basis is analyzed in Section 2.3. A Gauss summation in $H_{\rho,\alpha}$ is described in Section 2.4. As not stated otherwise, we always assume $0 < \rho < 1$ and $\alpha > -1$.

2.1 Construction of the Polynomials

First, we try to find polynomials $\{l_k\}$, which are orthogonal with respect to the scalar product

$$(u\,,\,v)^{\rho,\alpha} := \sum_{s=1}^{\infty} u(s)\,v(s)\,\Psi_{\rho,\alpha}(s)\ , \tag{2.1}$$

where $u\,,\,v : \mathbb{N} \to \mathbb{R}$ can be interpreted as sequences or as grid functions on $\mathbb{N}$. The isometric isomorphism

$$T_{\rho,\alpha}\ : H^{\rho,\alpha} := \left\{ u \in \mathbb{R}^{\mathbb{N}} \,|\, (u\,,\,u)^{\rho,\alpha} < \infty \right\} \longrightarrow H_{\rho,\alpha} \tag{2.2}$$

defined by

$$(T_{\rho,\alpha}\,u)(s) = u(s)\,\Psi_{\rho,\alpha}(s)$$

transforms the polynomial basis $\{l_k(\rho,\alpha)\}$ of $H^{\rho,\alpha}$ to the basis $\{\psi_k(\rho,\alpha)\} := \{\,\Psi_{\rho,\alpha}\,l_k(\rho,\alpha)\,\}$ of $H_{\rho,\alpha}$.

Fortunately the polynomials $l_k(\rho,\alpha)$ can be found in the literature, such that only special settings and properties have to be worked out here. We write the *forward product* as

$$(a)_n := a\,(a+1)\,\ldots\,(a+n-1)\ ,\ \ a \in \mathbb{R}\,,$$

and denote the *forward* difference operator by

$$(\Delta\,u)_s = u_{s+1} - u_s\ ,\ s = 1,\,2,\ldots\,. \tag{2.3}$$

Theorem 2.1.

(i) The Rodrigues formula

$$l_n(s;\rho,\alpha) = \frac{(1+\alpha)_n}{n!}\,\Psi_{\rho,\alpha}(s)^{-1}\,\Delta^n\left\{ C^{\rho,\alpha}\,\rho^{s-1}\binom{s-1+\alpha}{s-1-n}\right\}$$

generates polynomials $l_n(s) = l_n(s;\rho,\alpha)$ *which are orthogonal with respect to the scalar product (2.1) for* $0 < \rho < 1$ *and* $\alpha > -1$. *The orthogonality relation reads*

$$(2.4) \qquad (l_m\,,\, l_n)^{\rho,\alpha} = \delta_{nm}\,\gamma_n^{\rho,\alpha}\ ,\ \gamma_n^{\rho,\alpha} := \rho^n \binom{n+\alpha}{n}\,.$$

The polynomials $l_n(s;\rho,\alpha)$ *will be called modified discrete Laguerre polynomials.*

(ii) The polynomials $l_n(s;\rho,\alpha)$ *have a series representation*

$$(2.5) \qquad l_n(s;\rho,\alpha) = \sum_{k=0}^{n} \rho^{n-k}\,(\rho-1)^k \binom{n+\alpha}{n-k}\binom{s-1}{k}\,.$$

(iii) The three-term-recurrence for the modified discrete Laguerre polynomials is

$$\begin{aligned}(n+1)l_{n+1}(s;\rho,\alpha) \;=\; & [(n+\alpha+1)\rho + n - (1-\rho)(s-1)]l_n(s;\rho,\alpha) \\ & -(n+\alpha)\rho\, l_{n-1}(s;\rho,\alpha)\,,\end{aligned} \qquad (2.6)$$

started with $l_{-1} = 0$ *and* $l_0 = 1$.

(iv) The forward difference operator Δ *applied to* $l_n(s;\rho,\alpha)$ *induces a shift in the* α*-scale:*

$$(2.7)\Delta l_n(s;\rho,\alpha) = l_n(s+1;\rho,\alpha) - l_n(s;\rho,\alpha) = (\rho-1)\, l_{n-1}(s;\rho,\alpha+1)\,.$$

Proof. The only task is to find a formulation of results in the literature, which corresponds to the definition of $H^{\rho,\alpha}$ here. This is done in [39]. Basically, for part (i) results from [30] and [31] can be taken. The other parts are basing on [33], using that the modified discrete Laguerre polynomials are related to the *Meixner* polynomials $m_n(s;\rho,\gamma)$ as given in [24] by

$$l_n(s;\rho,\alpha) := \frac{\rho^n}{n!}\, m_n(s-1;\rho,1+\alpha)\,.$$

Remark. The classical *discrete Laguerre polynomials* associated to the geometric distribution (i.e. $\alpha = 0$) have been studied by GOTTLIEB [25] in 1938. For the *modified discrete Laguerre polynomials* we refer to LESKY [30], [31] and to the textbook of NIKIFOROV and UVAROV [33], which gives a modern survey on orthogonal polynomials. Properties of discrete orthogonal polynomials are proven e.g. by ASKEY and GASPER [2], [3], [24]. The modified discrete Laguerre polynomials with $\alpha = 0$ have been used for the solution of CODE's in [19] and [10]. In [38], the parameter α already has been introduced in order to realize a discrete Galerkin method for certain so–called *heterogeneous processes.*

2.2 Properties of the Polynomials

The approximation of solutions of countable systems in a most suited space requires the transformation of a given representation of $u \in H_{\rho,\alpha}$ to a basis expansion in a space $H_{\bar{\rho},\bar{\alpha}}$ (see also Section 3.3). We start with transformations with respect to the parameter ρ.

Lemma 2.2. *The transformation between the polynomial systems* $\{l_j(s;\rho,\alpha)\}$ *and* $\{l_j(s;\bar{\rho},\alpha)\}$ *can be expressed by*

$$
\begin{aligned}
l_j(s;\bar{\rho},\alpha) &= \sum_{k=0}^{j} d_\alpha^{j,k}(\rho,\bar{\rho})\, l_k(s;\rho,\alpha) \;,\quad 0<\bar{\rho}<1 \;, \\
d_\alpha^{j,k}(\rho,\bar{\rho}) &:= \frac{(\bar{\rho}-\rho)^{j-k}}{(1-\rho)^j}(1-\bar{\rho})^k \binom{j+\alpha}{j-k} \;,\quad j\geq k\geq 0 \;.
\end{aligned} \tag{2.8}
$$

Proof. After inserting the series representation (2.5) of the $l_k(s;\rho,\alpha)$ and the definition of the $d_\alpha^{j,k}(\rho,\bar{\rho})$ a reordering of the summations leads to

$$
\begin{aligned}
\sum_{k=0}^{j} d_\alpha^{j,k}(\rho,\bar{\rho})\, l_k(s;\rho,\alpha) = \left(\tfrac{\bar{\rho}-\rho}{1-\rho}\right)^j & \sum_{k=0}^{j}\left(\tfrac{\rho-1}{\rho}\right)^k \binom{s-1}{k}\binom{j+\alpha}{j-k} \times \\
& \times \sum_{\nu=k}^{j}\binom{j-k}{\nu-k}\left((\bar{\rho}-\rho)(1-\bar{\rho})\rho\right)^\nu \;.
\end{aligned}
$$

With the relation ([36],p. 3)

$$
\binom{j}{\nu}\binom{\nu}{k} = \binom{j}{k}\binom{j-k}{\nu-k}
$$

and the Binomial theorem we end up with

$$
\sum_{k=0}^{j} d_\alpha^{j,k}(\rho,\bar{\rho})\, l_k(s;\rho,\alpha) = \sum_{k=0}^{j}\binom{j+\alpha}{j-k}\binom{s-1}{k}(\bar{\rho}-1)^k\,\bar{\rho}^{j-k} = l_j(s;\bar{\rho},\alpha)
$$

■

As a consequence of this lemma we note that

$$
\frac{1}{\gamma_k^{\rho,\alpha}}\left(l_j(\bar{\rho},\alpha)\,,\, l_k(\rho,\alpha)\right)^{\rho,\alpha} = d_\alpha^{j,k}(\rho,\bar{\rho}) \tag{2.9}
$$

for $k \leq j$. For $k > j$ the scalar product is zero, of course.

COROLLARY 2.3. *An element* $u(s) \in H_{\rho,\alpha}$ *with basis expansion*

$$u(s) = \sum_{j=0}^{\infty} a_j(\rho,\alpha)\,\psi_j(s;\rho,\alpha) = \Psi_{\rho,\alpha} \sum_{j=0}^{\infty} a_j(\rho,\alpha)\,l_j(s;\rho,\alpha)\ ,$$

which is also in the space $H_{\bar{\rho},\alpha}$, *can be expressed in the* $H_{\bar{\rho},\alpha}$*- basis in terms of the coefficients*

$$a_j(\bar{\rho},\alpha) = \frac{1}{\bar{\rho}^j} \sum_{k=0}^{j} a_k(\rho,\alpha) \binom{j}{k} \frac{(\bar{\rho}-\rho)^{j-k}}{(1-\rho)^j} (1-\bar{\rho})^k \rho^k\ . \tag{2.10}$$

Note that this transformation is independent of α.

Proof. The projection of u to a basis element $\psi_j(\bar{\rho},\alpha) = \Psi_{\rho,\alpha}\, l_j(\bar{\rho},\alpha)$ can be written as

$$\frac{1}{\gamma_j^{\bar{\rho},\alpha}}\,(u\,,\,\psi_j(\bar{\rho},\alpha))_{\bar{\rho},\alpha} = \frac{1}{\gamma_j^{\bar{\rho},\alpha}} \sum_{k=0}^{\infty} a_k(\rho,\alpha)\ (l_k(\rho,\alpha)\,,\,l_j(\bar{\rho},\alpha))^{\rho,\alpha}$$

Insertion of Lemma 2.2 in the form (2.9) and remembering in the definition of the $\gamma_j^{\rho,\alpha}$ leads to (2.10). ∎

LEMMA 2.4. *The transformation between the* $\{l_j(s;\rho,\alpha)\}$ *and the* $\{l_j(s;\rho,\bar{\alpha})\}$ *is given by*

$$\begin{aligned} l_j(s;\rho,\bar{\alpha}) &= \sum_{k=0}^{j} d_\rho^{j,k}(\alpha,\bar{\alpha})\, l_k(s;\rho,\alpha)\ ,\ \bar{\alpha} > -1\ , \\ d_\rho^{j,k}(\alpha,\bar{\alpha}) &:= \rho^{j-k} \binom{\bar{\alpha}-\alpha+j-k-1}{j-k}\ ,\ j \geq k \geq 0\ . \end{aligned} \tag{2.11}$$

Proof. Following the lines of the proof of Lemma 2.2 we insert the series expansion of $l_j(s;\rho,\alpha)$ into the series on the right–hand side of (2.11) and reorder the summations:

$$\sum_{k=0}^{j} d_\rho^{j,k}(\alpha,\bar{\alpha})\, l_k(s;\rho,\alpha) = \rho^j \sum_{\nu=0}^{j} \binom{\rho-1}{\rho} \binom{s-1}{\nu} \sum_{k=\nu}^{j} \binom{k+\alpha}{k-\nu} \binom{\bar{\alpha}-\alpha+j-k-1}{j-k}\ .$$

In order to show, that the inner sum is equal to $\binom{j+\bar{\alpha}}{j-\nu}$, we set $m = j-\nu$, $n = \bar{\alpha}-\alpha+j-\nu$, $p = \nu+\alpha$, and use relation (3b), p. 8, [36]. ∎

The transformation of coefficients $a_j(\rho,\alpha)$ of an $H_{\rho,\alpha}$-basis expansion to coefficients $a_j(\rho,\bar{\alpha})$ of an $H_{\rho,\bar{\alpha}}$ - expansion works analogue to Corollary 2.3 and is independent of ρ in this case. This nice feature shows, how the two scales are separated.

Finally we prove two important shift properties of the discrete Laguerre polynomials.

COROLLARY 2.5. *The forward difference operator applied to* $l_j(s;\rho,\alpha)$ *can be expanded into*

$$\begin{aligned} \Delta\, l_j(s;\rho,\alpha) &= l_j(s+1;\rho,\alpha) - l_j(s;\rho,\alpha) \\ &= (\rho-1)\sum_{k=0}^{j-1} \rho^{j-1-k} l_k(s;\rho,\alpha)\ . \end{aligned} \tag{2.12}$$

Proof. Insertion of Lemma 2.4 into the fundamental difference relation (2.7) leads to transformation coefficients $d_\rho^{j,k}(\alpha,\alpha+1) = \rho^{j-1-k}$. ∎

COROLLARY 2.6. *The backward difference operator applied to* $l_j(s;\rho,\alpha)$ *can be expressed by*

$$\nabla\, l_j(s;\rho,\alpha) = l_j(s;\rho,\alpha) - l_j(s-1;\rho,\alpha) = (\rho-1)\sum_{k=0}^{j-1} l_k(s;\rho,\alpha)\ .$$

Proof. Backward shift of the difference relation (2.12) in the argument s yields

$$l_j(s-1;\rho,\alpha) + (\rho-1)\sum_{k=0}^{j-1} \rho^{j-1-k}\, l_k(s-1;\rho,\alpha) = l_j(s;\rho,\alpha)\ ,$$

which can be regarded as an infinite triangular system of linear equations in the variables $l_j(s-1;\rho,\alpha)$ for given $l_j(s;\rho,\alpha)$. This system can be solved recursively by induction for each index j. ∎

Further properties, which are related to degradation (Examples 1.2, 4.2) and combination processes (Example 1.3, 4.3) can be found in [39] and [38].

2.3 APPROXIMATION BY BASIS EXPANSIONS

Let $u \in H_{\rho,\alpha}$ be expanded in the orthogonal basis $\{\psi_k(\rho,\alpha)\} = \{\Psi_{\rho,\alpha} l_k(\rho,\alpha)\}$ of $H_{\rho,\alpha}$ by

$$u(s) = \Psi_{\rho,\alpha}(s) \sum_{k=0}^{\infty} a_k\, l_k(s;\rho,\alpha)\ . \tag{2.13}$$

The expansion coefficients a_k are given formally by

$$a_k = \frac{1}{\gamma_k^{\rho,\alpha}} \sum_{s=1}^{\infty} u(s)\, l_k(s;\rho,\alpha)\ , \tag{2.14}$$

and the Parseval equality yields

$$\|u\|^2_{\rho,\alpha} = \sum_{k=0}^{\infty} a_k^2 \, \gamma_k^{\rho,\alpha} \, . \tag{2.15}$$

The *orthogonal projection* to the n – dimensional subspace

$$H^n_{\rho,\alpha} = \text{span}\,\{\psi_0(\rho,\alpha), \ldots, \psi_n(\rho,\alpha)\} \subset H_{\rho,\alpha}$$

is defined by

$$\mathcal{P}_n^{\rho,\alpha} u(s) = \Psi_{\rho,\alpha}(s) \sum_{k=0}^{n} a_k \, l_k(s;\rho,\alpha) \, . \tag{2.16}$$

The associated *projection error* is

$$\mathcal{Q}_n^{\rho,\alpha} u(s) := u(s) - \mathcal{P}_n^{\rho,\alpha} u(s) = \Psi_{\rho,\alpha}(s) \sum_{k=n+1}^{\infty} a_k \, l_k(s;\rho,\alpha) \, . \tag{2.17}$$

Obviously we have $\|u - \mathcal{P}_n^{\rho,\alpha} u\|_{\rho,\alpha} \to 0$ for $n \to \infty$ for all $u \in H_{\rho,\alpha}$ and $\|\mathcal{P}_n^{\rho,\alpha}\|_{\rho,\alpha} \leq 1$. We want to estimate the norm of the projection error in terms of higher differences of u (analogue to the use of higher derivatives in the continuous case), which should be a measure of the smoothness of u in $H_{\rho,\alpha}$. In the polynomial spanned space $H^{\rho,\alpha}$ we could use the standard forward difference operator Δ. Because Δ applied to $l_k(\rho,\alpha)$ shifts the α-scale (2.7), the following definition seems to be natural in $H_{\rho,\alpha}$.

DEFINITION 2.7. *Let for $u \in H_{\rho,\alpha}$ the weighted difference operator*

$$\Delta_\alpha \, : \, H_{\rho,\alpha} \to H_{\rho,\alpha+1}$$

be defined by

$$\Delta_\alpha \, u = T_{\rho,\alpha+1} \, \Delta \, T^{-1}_{\rho,\alpha} \, u$$

in terms of the isomorphism (2.2). Higher weighted differences are inductively given by

$$\Delta^m_\alpha \, u := \Delta_{\alpha+m-1} \Delta_{\alpha+m-2} \cdots \Delta_\alpha \, u \, .$$

COROLLARY 2.8. *For $u \in H_{\rho,\alpha}$ with a representation (2.13) the m-th weighted higher difference can be written as*

$$\Delta^m_\alpha \, u(s) = \Psi_{\rho,\alpha+m}(s) \sum_{k=0}^{\infty} a_{k+m} \, (\rho-1)^m \, l_k(s;\rho,\alpha+m) \, .$$

Proof. Repeated application of the difference relation (2.7). ∎

As a consequence of Corollary 2.8 we can easily derive, that

$$\|\Delta_\alpha^m u\|^2_{\rho,\alpha+m} = \sum_{k=m}^{\infty} a_k^2 (1-\rho)^{2m} \gamma_{k-m}^{\rho,\alpha+m} < \infty \,. \tag{2.18}$$

DEFINITION 2.9. *For $u \in H_{\rho,\alpha}$, $m \geq 1$, define the m-th weighted difference norm $\|u\|_{\rho,\alpha,m}$ by*

$$\|u\|^2_{\rho,\alpha,m} := \|u\|^2_{\rho,\alpha} + \|\Delta_\alpha^m u\|^2_{\rho,\alpha+m} \,. \tag{2.19}$$

For $m = 0$ set

$$\|u\|_{\rho,\alpha,0} := \|u\|_{\rho,\alpha} \,.$$

Remark. This norms can be considered as discrete weighted Sobolev norms.

THEOREM 2.10. *For $u \in H_{\rho,\alpha}$ and $n+1 \geq m \geq 1$ the approximation error $\mathcal{Q}_n^{\rho,\alpha} u$ can be estimated by*

$$\|\mathcal{Q}_n^{\rho,\alpha} u\|_{\rho,\alpha} \leq C(\rho,\alpha,m)\, M(n,m)\, \|u\|_{\rho,\alpha,m} \,, \tag{2.20}$$

with a constant

$$C(\rho,\alpha,m)^2 = \frac{\rho^m}{(1-\rho)^{2m}} (1+\alpha)(2+\alpha)\dots(m+\alpha)$$

and the term

$$M(n,m)^2 = \frac{1}{(n+1)n\dots(n-m+2)} \,,$$

describing the asymptotic behavior.

Proof. Inserting (2.18) we start with

$$\begin{aligned} \|u\|^2_{\rho,\alpha,m} &= \sum_{k=0}^{\infty} a_k^2 \gamma_k^{\rho,\alpha} + \sum_{k=m}^{\infty} a_k^2 (1-\rho)^{2m} \gamma_{k-m}^{\rho,\alpha+m} \\ &\geq \sum_{k=n+1}^{\infty} a_k^2 \gamma_k^{\rho,\alpha} \left[1 + \tfrac{(1-\rho)^{2m}}{\rho^m} \tfrac{k(k-1)\dots(k-m+1)}{(1+\alpha)\dots(m+\alpha)}\right] \,, \end{aligned} \tag{2.21}$$

using

$$\gamma_{k-m}^{\rho,\alpha+m} = \rho^{k-m} \tbinom{k+\alpha}{k-m} = \gamma_k^{\rho,\alpha} \rho^{-m} \frac{k(k-1)\dots(k-m+1)}{(1+\alpha)\dots(m+\alpha)} \,.$$

The norm of the projection error can be written as

$$\|\mathcal{Q}_n^{\rho,\alpha} u\|_{\rho,\alpha}^2 = \sum_{k=n+1}^{\infty} a_k^2 \gamma_k^{\rho,\alpha}$$

and it can be seen that

$$(2.22) \qquad \begin{aligned} 1 \leq \; & \frac{\rho^m}{(1-\rho)^{2m}} \frac{(1+\alpha)(2+\alpha)\ldots(m+\alpha)}{(n+1)n\ldots(n+1-(m-1))} \times \\ \times \; & \left[1 + \frac{(1-\rho)^{2m}}{\rho^m} \frac{k(k-1)\ldots(k-m+1)}{(1+\alpha)\ldots(m+\alpha)}\right] \end{aligned}$$

for $n+1 \leq k$. Combining (2.21) and (2.22) gives the assertion (2.20). ∎

2.4 Summation of Gaussian Type

In the context of the discrete Galerkin method, the numerical evaluation of scalar products in $H_{\rho,\alpha}$ is necessary, which can be written in the form

$$(2.23) \qquad S = \sum_{s=1}^{\infty} u(s)\, v(s) \;, \quad \frac{u\; v}{\Psi_{\rho,\alpha}} \in H^{\rho,\alpha} \,.$$

Thus it is natural to construct a summation formula of Gaussian type [33], which uses the special structure of such sums. We replace a sum

$$S = \sum_{s=1}^{\infty} f(s)$$

by an approximation

$$\tilde{S} = \sum_{j=1}^{k+1} \omega_j\, f(s_j)$$

with *nodes* s_j and *weights* ω_j chosen, such that $S = \tilde{S}$ if $f \in H_{\rho,\alpha}^{2k+1}$, i.e. if it can be written as the product of a polynomial of degree $2k+1$ and $\Psi_{\rho,\alpha}$. It is well known from the theory of quadrature, that then the nodes are just the zeros of the modified discrete Laguerre polynomials. The nodes and weights can be computed easily for a given k by applying the QR-algorithm to a triangular eigenvalue problem, which contains terms from the three-term-recurrence formula of the modified discrete Laguerre polynomials (see the textbook [18], Chapter 9.3.). This makes a Gauss summation very efficient, even when the nodes have to be updated very often.
The Gauss summation captures exactly the structure of the approach and does not require any truncation of the $s-$axis. Moreover, in Example 4.2 and Example 4.3 double sums are evaluated by this technique very efficiently.

3 Approximation of Countable Systems

The numerical treatment of countable systems with the algorithm CODEX consists of two main parts:

(i) the time discretization and step-size control in $H_{\rho,\alpha}$

(ii) the solver for stationary problems in $H_{\rho,\alpha}$

The countable system is discretized in time first (i). The arising stationary problem is then solved by a Galerkin method (ii) within an accuracy supplied by the step-size control. The results of (ii) are also used to obtain a time error estimate of the approximation after a time step (ii). Finally, the solution is transformed to a space $H_{\bar{\rho},\bar{\alpha}}$ in order to minimize the number of degrees of freedom of the approximation (i).

The above order of the discretizations – first in time , then in 'space' – is called *Rothe's method* [37] and has been introduced by Bornemann [6] for the numerical solution of parabolic differential equations.

3.1 Discretization in Time

We discuss, how and under which conditions a countable system can be discretized in time by a given scheme and consider first an abstract (linear) Cauchy problem in $H_{\rho,\alpha}$:

$$u'(t) = A\,u(t) + f(t)\ ,\ u(0)\ \text{given.} \tag{3.1}$$

Theorem 3.1. *(Hersh/Kato [27], Brenner/Thomee [9]) Let the operator A be the generator of a C_0 - semigroup of contractions. For each A-acceptable rational approximation r of e^z of order p, there are constants C and κ, such that*

$$\|r^n(\tau A)v - e^{n\tau A}v\| \le C t\tau^p \|A^{p+1}v\|\ ,\ \ \textit{for } t = n\tau\ ,\ v \in D(A^{p+1})\,. \tag{3.2}$$

Proof. Theorem 3 in [9].

It remains to check here, when $v \in D(A^{p+1})$ is valid for a given p.

Corollary 3.2. *Let A additionally satisfy the conditions of Theorem 1.7 in $H_{\rho,\alpha}$ and let $v \in H_{\rho-\varepsilon,\alpha}$. Then $v \in D(A^p)$ for all fixed $p \in \mathbb{N}$.*

Proof. Define $\varepsilon_k := \varepsilon/k$, $1 \le k \le p$. Then A is bounded from $H_{\rho-\varepsilon_k,\alpha}$ to $H_{\rho-\varepsilon_{k+1},\alpha}$. ∎

As noted in Section 1.2, the condition $v \in H_{\rho-\varepsilon,\alpha}$ is crucial for guaranteeing senseful numerical approximations anyway.

Discretization scheme for the linear case. Starting at time t, we use the implicit Euler scheme leading to an approximation u^1 of $u(t+\tau)$. The task is then to get an estimation of the time error $\|u^1 - u(t+\tau)\|$ for predicting a new reasonable step-size $\bar{\tau}$. This is usually be done by computing a 'better' approximation u^2 and then taking the difference $\|u^2 - u^1\|$ as an estimate of the time error. However, in the case of partial differential equations or countable systems, u^1 and u^2 can only be *approximated.* It turned out [6], that their approximation error has to be comparatively small for not perturbing the time error estimation. In order to avoid this disadvantage, BORNEMANN developed a so-called *multiplicative error correction scheme* [7], which allows the *direct* estimation of the time error. The accuracy requirements for the u^1 and u^2 are then less restrictive than in the case described above. For linear problems (3.1) the discretization scheme looks as follows (for details see [7]):
Let $\varphi = \bar{u}(t)$ the exact solution of (3.1) at time t. In order to perform a time step τ we compute:

$$
\begin{aligned}
u^1 &= (I - \tau A)^{-1}(\varphi + \tau f(t)) \quad \text{(implicit Euler step)}, \\
\eta^1 &= \frac{1}{2}\tau(I - \tau A)^{-1}(A(\varphi - u^1) - (f(\tau) - f(0))), \\
u^2 &= u^1 + \eta^1
\end{aligned}
\tag{3.3}
$$

The approximation u^2 is of order $p = 2$ and the rational function of the scheme is A-acceptable. Note, that only *one* type of stationary subproblem has to be solved in a global time step (in contrary to the application of extrapolation ([6], [39]), where problems with different τ appear).

In [7] it is pointed out, that u^1 has to be computed with an accuracy

$$
\mathsf{eps} = \frac{1}{8}\,\mathsf{TOL} \ , \tag{3.4}
$$

TOL the required global tolerance for $u(t)$, to ensure the reliable working of the time step control.

Remark. Due to the multiplicative error correction this requirement is much weaker than in the case of extrapolation used in [6] and [39].

Discretization scheme for nonlinear problems. For the nonlinear case (see Example 4.3)

$$u'(t) = f(u(t)) \ , \ u(0) \ \text{given},$$

the *semi-implicit* Euler scheme [16] is used as basic discretization:

$$\begin{aligned} (I - \tau A)\ \Delta u^1 &= \tau\, f(\varphi)\ , \\ u^1 &= \varphi + \Delta u^1\ . \end{aligned} \tag{3.5}$$

with A now the Frechét derivative $f_u(\varphi)$ of the right-hand side $f(u)$. Obviously the implicit Euler discretization is identical with the semi–implicit Euler scheme in the linear case. A correction formula, which fulfills the two requirements (direct computation of the error, only one type of stationary problem) is given by:

$$\begin{aligned} \eta^1 &= -\frac{1}{2}\tau^2\,(I - \tau A)^{-1}\, A\, f(\varphi)\ , \\ u^2 &= u^1 + \eta^1\ . \end{aligned} \tag{3.6}$$

As will be demonstrated in Example 4.3, the scheme (3.6) works very well for nonlinear countable systems. A theory comparable to Theorem 3.1 does not yet exist.

The numerical implementation of the above formulas requires an adaptive Galerkin method for the solution of the linear systems in (3.3) and (3.6). The correction terms η^1 are then computed with the same accuracy using the results of the Euler step. When a time step τ has been performed, a new step size $\bar{\tau}$ can be computed by

$$\bar{\tau} = \tau \sqrt{\frac{\mathrm{TOL}}{\|\eta^1\|}}\ .$$

3.2 Galerkin Approximations in $H_{\rho,\alpha}$

Before we discuss the details of the Galerkin method, we restrict to the following types of linear operators:

(i) τA is contractive, i.e. $\tau \|A\|_{\rho,\alpha} < 1$.

(ii) A is the generator of a C_0 - semigroup of contractions.

Some of the considerations below can be extended by assuming e.g. a V-ellipticity of A (in Theorem 3.3 and Theorem 3.7), but such an assumption does not really fit to CODE's and a general classification of the appearing operators is still missing. Consequently the following results have to be understand as exemplary.

As seen in Section 3.1, the computational realization of (semi-) implicit Euler steps requires the solution of equations of the type

$$(I - \tau A)\, u = \varphi \ . \tag{3.7}$$

Assuming that the solution of (3.7) has a basis expansion in $H_{\rho,\alpha}$ and inserting it into the equation, we can derive (by analytical or numerical manipulations) a linear (also infinite) system, which defines the expansion coefficients. Truncation of this system at dimension $n+1$, then called the *Galerkin equations*, leads to a Galerkin approximation

$$\tilde{u}^{n,l} = \sum_{k=0}^{n} \tilde{a}_k^l \, \psi_k(s;\rho,\alpha) \in H_{\rho,\alpha}^n \ , \ n \geq 0 \, , \tag{3.8}$$

of u, where the $\tilde{a}_k^l$ are not necessarily the expansion coefficients a_k of u, because:

(i) the Galerkin equations may be not self-closing, i.e. the entries of the linear system are depending on coefficients a_k , $k > n$ implying a dependency of the solution a_k on the truncation index. This effect is denoted by a *tilde*

(ii) in many problems the matrix entries and the right-hand side have to be approximated numerically. The superscript l characterizes the accuracy of the associated algorithm.

For fixed n the Galerkin equations can be written as

$$\left(\mathcal{P}_n^{\rho,\alpha}(\tilde{u}^{n,l} - \tau A \tilde{u}^{n,l}) \, , \, \psi_j \right)_{\rho,\alpha} = \left(\mathcal{P}_n^{\rho,\alpha}\varphi \, , \, \psi_j \right)_{\rho,\alpha} \ , \ \tilde{u}^{n,l} \in H_{\rho,\alpha}^n \ , \tag{3.9}$$

for $j = 0, \ldots, n$. After insertion of the basis expansion we obtain an $n+1$-dimensional linear system

$$(I - \tau B)\, a = b \, , \tag{3.10}$$

with the matrix $B := (b_{jk})$,

$$b_{jk} := (A\psi_k \, , \, \psi_j)_{\rho,\alpha}^l \ ,$$

and the right-hand side $b = (b_0^l, \ldots, b_n^l)^T$,

$$b_j = (\varphi \, , \, \psi_j)_{\rho,\alpha}^l \ .$$

The vector $a = (\tilde{a}_0^l, \ldots, \tilde{a}_n^l)^T$ contains the coefficients of $\tilde{u}^{n,l}$. As said before, the superscript l indicates, that the scalar products may be not evaluated exactly. For given coefficients a, the approximation $\tilde{u}^{n,l}$ is pointwise computed in the program by a fast algorithm [15].

In the following we have to deal with three errors:

(i) The pure projection error

$$\bar{\varepsilon}_n = \|u - \mathcal{P}_n^{\rho,\alpha} u\|, \tag{3.11}$$

where u denotes the solution of (3.7).

(ii) The error $\|u - \tilde{u}^n\|$, where $\tilde{u}^n$ is the solution of a Galerkin equation, which may not be self-closing.

(iii) The general error $\|u - \tilde{u}^{n,l}\|$, which includes all effects.

We will discuss later in this section, how the error is estimated in general and we will illustrate, that the error introduced by numerical summations can be controlled. First we examine the case, that the Galerkin equations are not perturbed.

The case of unperturbed Galerkin equations. We ask for existence of solutions $\tilde{u}^n$ of the Galerkin equations (3.9) and for estimates $\|u - \tilde{u}^n\|_{\rho,\alpha}$. The following theorem, essentially taken from [40], Theorem 21.G, is a standard result for Galerkin methods in Hilbert spaces – adapted to our case.

THEOREM 3.3. *Let $A : D(A) \subset H_{\rho,\alpha} \to H_{\rho,\alpha}$ be a linear operator. For the following cases the problem (3.7) has a unique solution in $H_{\rho,\alpha}$ and the Galerkin method converges, i.e. $\|\tilde{u}^n - u\| \to 0$ for $n \to \infty$.*

(i) τA is contractive. Then the estimate

$$\|u - \tilde{u}^n\| \leq (1 - \tau \|A\|_{\rho,\alpha})^{-1} \|u - \mathcal{P}_n^{\rho,\alpha} u\| \tag{3.12}$$

holds.

(ii) A is generator of a C_0 - semigroup of contractions and fulfills the invariance condition

$$\mathcal{P}_n^{\rho,\alpha} A = \mathcal{P}_n^{\rho,\alpha} A \, \mathcal{P}_n^{\rho,\alpha} \ , \quad \text{for all } \ n \in \mathbb{N} \, . \tag{3.13}$$

Then we have convergence for $\tau > 0$ and for the Galerkin solution $\tilde{u}^n$ holds

$$\tilde{u}^n = \mathcal{P}_n^{\rho,\alpha} u.$$

Proof. (i) This can easily be proven by use of the Banach fixed-point theorem and the Neumann series.
(ii) The infinitesimal generator A of a C_0 - semigroup of contractions is characterized by the Lumer-Phillips theorem ([34], Theorem 4.3):
A is dissipative, i.e. $(Au\,,\,u) \leq 0$ and for a $\lambda_0 > 0$ the range of $\lambda_0 I - A$ is $H_{\rho,\alpha}$.
For $\tilde{u}^n \in H^n_{\rho,\alpha}$ it follows from

$$(\mathcal{P}_n^{\rho,\alpha} A\tilde{u}^n\,,\,\tilde{u}^n)_{\rho,\alpha} = (A\tilde{u}^n\,,\,\tilde{u}^n)_{\rho,\alpha}$$

that $\mathcal{P}_n^{\rho,\alpha} A$ is also dissipative and the range condition is fulfilled in $H^n_{\rho,\alpha}$ because of (3.13). Hence $\mathcal{P}_n^{\rho,\alpha} A$ generates a contractive C_0 - semigroup too. ∎

Error estimation. In view of Theorem 3.3 the numerical implementation of the discrete Galerkin method requires an estimate of the projection error at least.

LEMMA 3.4. *Define an error estimate ε_n of the projection error (3.11) by*

$$\varepsilon_n^2 := \|u^{n+1} - u^n\|^2 = a_{n+1}^2\,\gamma_{n+1}^{\rho,\alpha}\,, \tag{3.14}$$

and assume that there exist $C < 1$ and $n_0 \geq 1$ such that for $n > n_0$ the relation

$$\varepsilon_{n+1} \leq C\,\varepsilon_n \tag{3.15}$$

holds. Then

$$\varepsilon_n \leq \bar{\varepsilon}_n \leq \left(\frac{1}{1-C^2}\right)^{1/2} \varepsilon_n\,,\ n \geq n_0\,.$$

Proof. Obviously

$$\varepsilon_n^2 \leq \bar{\varepsilon}_n^2 = \sum_{k=n+1}^{\infty} a_k^2\,\gamma_k^{\rho,\alpha}$$

since $\gamma_k^{\rho,\alpha} > 0$. On the other hand it follows from (3.15) for $n \geq n_0$ that

$$\bar{\varepsilon}_n^2 = \sum_{k=n+1}^{\infty} \varepsilon_{k-1}^2 \leq \varepsilon_n^2 \sum_{k=0}^{\infty} C^{2k} = \frac{1}{1-C^2}\,. \quad ∎$$

The actual value of C can be estimated in the algorithm by considering successive error estimates for increasing n. Whenever C turns out to be near or larger than one, a warning is given by the program. In applications the projection error has to be measured in a scaled norm, of course.

In general we obtain a perturbed approximation (3.8). The error $\|\tilde{u}^{n,l} - u\|_{\rho,\alpha}$ can be written in terms of the projection error and a so-called *truncation error*:

$$\begin{aligned} \|\tilde{u}^{n,l} - u\|^2_{\rho,\alpha} &= \|u - \mathcal{P}^{\rho,\alpha}_n u\|^2_{\rho,\alpha} + \|\tilde{u}^{n,l} - u^n\|^2_{\rho,\alpha} \\ &= \sum_{k=n+1}^{\infty} a_k^2 \gamma_k^{\rho,\alpha} + \sum_{k=0}^{n} (\tilde{a}_k^l - a_k)^2 \gamma_k^{\rho,\alpha} . \end{aligned} \tag{3.16}$$

Let now an algorithm produce successive approximations $\tilde{a}_k^l$ of a_k - e.g by increasing the truncation index n or by Gauss summations in (3.10) with an increasing number of nodes. Assuming that

$$\tilde{a}_k^l \to a_k \quad \text{for } l \to \infty\,,\ k \text{ fixed}\,,$$

the following error estimation can be applied ($\varepsilon_{P,n,l} = \varepsilon_n$ in Lemma 3.4):

$$\varepsilon^2_{n,l} := \varepsilon^2_{T,n,l} + \varepsilon^2_{P,n,l} := \sum_{k=0}^{n} (\tilde{a}_k^l - \tilde{a}_k^{l+1})^2 \gamma_k^{\rho,\alpha} + \left(\tilde{a}_{n+1}^{l+1}\right)^2 \gamma_{n+1}^{\rho,\alpha} . \tag{3.17}$$

We are only interested in a truncation error (respectively its estimate) $\varepsilon_{T,n,l}$ being just a little smaller than the projection error $\varepsilon_{P,n,l}$ for that the estimate of the projection error is reliable. Thus we require l to be chosen such that

$$\|\tilde{u}^{n+1,l} - u^{n+1}\|_{\rho,\alpha} < \kappa \, \|\tilde{u}^{n,l} - u\|_{\rho,\alpha} \tag{3.18}$$

with some safety factor $0 < \kappa < 1$ (see also [17], (1.26)). In actual computations, the terms on both sides are replaced by the estimates suggested in (3.17), κ is set to $1/4$.

The Effect of Numerical Summation. Finally we examine, whether a numerical summation algorithm as presented in Section 2.4 can be applied to construct the Galerkin equations. The scalar products in (3.10) are replaced by approximations $(u\,,\,v)^l_{\rho,\alpha}$, where the index l denotes now, that

$$(u\,,\,v)^l_{\rho,\alpha} = (u\,,\,v)_{\rho,\alpha} \quad \text{for } \frac{u\,v}{\Psi_{\rho,\alpha}} \in H^l_{\rho,\alpha} . \tag{3.19}$$

The question is, how l must be chosen for not perturbing the Galerkin method essentially. As the discussion of the general problem requires additional assumptions on the operator A again, in this paper we treat only the case of a projection

$$u^{n,l} = \mathcal{P}^{\rho,\alpha}_n u\ ,\ \mathcal{P}^{\rho,\alpha}_n \text{ numerically evaluated,}$$

as an example and ask how u^n is perturbed. We use techniques described in the textbook by CIARLET [11] for the case of finite elements.

The solution $u^n \in H^n_{\rho,\alpha}$ of the equation

$$(u^n, v^n)_{\rho,\alpha} = (u, v^n)_{\rho,\alpha} \ , \ \forall v^n \in H_{\rho,\alpha} \ , \ u \in H_{\rho,\alpha} \ \text{ given,} \tag{3.20}$$

is just the projection $u^n = \mathcal{P}^{\rho,\alpha}_n u$. Let the perturbed projection $u^{n,l}$ be the solution of

$$(u^{n,l}, v^n)^l_{\rho,\alpha} = (u, v^n)^l_{\rho,\alpha} \ \ \forall v^n \in H_{\rho,\alpha} \ , \tag{3.21}$$

where the index l characterizes a summation formula. Following estimates in the proof of the STRANG lemma ([11], Theorem 4.1.1), we can show that

$$\|u - u^{n,l}\| \leq M \, \|u - u^n\| + \sup_{w^n \in H^n_{\rho,\alpha}} \frac{|(u, w^n)_{\rho,\alpha} - (u, w^n)^l_{\rho,\alpha}|}{\|w^n\|} \ . \tag{3.22}$$

The error $E^l(f)$ of a numerical summation in $H_{\rho,\alpha}$ is given by

$$E^l(f) = \sum_{s=1}^{\infty} f(s) - \sum_{j=1}^{\bar{l}} \omega_j \, f(s_j) \tag{3.23}$$

where $\bar{l}$, the s_j and the ω_j are chosen such that $E^l(f) = 0$ for $f \in H^l_{\rho,\alpha}$. Thus the missing term in (3.22) is

$$|(u, w^n)_{\rho,\alpha} - (u, w^n)^l_{\rho,\alpha}| = | \, E^l(\frac{u \, w^n}{\Psi_{\rho,\alpha}}) \, | \ . \tag{3.24}$$

In order to get an estimate of this error, we prove an analogue to the Bramble-Hilbert lemma [8].

LEMMA 3.5. *Let f be a continuous linear form on the space $H_{\rho,\alpha}$ with the property*

$$\forall p \in H^l_{\rho,\alpha} \ , \ \ f(p) = 0 \ . \tag{3.25}$$

Then with the expressions $C(\rho, \alpha, m)$ and $M(l, m)$ from Theorem 2.10 the following estimate holds:

$$\forall v \in H_{\rho,\alpha} \ , \ \ |f(v)| \leq \|f\| \, C(\rho, \alpha, m) \, M(l, m) \, \|v\|_{\rho,\alpha,m} \tag{3.26}$$

for $l + 1 \geq m \geq 1$.

Proof. For all $v \in H_{\rho,\alpha}$ and $p \in H^l_{\rho,\alpha}$ we may write

$$|f(v)| = |f(v+p)| \leq \|f\|_{\rho,\alpha} \|v+p\|_{\rho,\alpha}$$

and thus

$$|f(v)| \leq \|f\|_{\rho,\alpha} \inf_{p \in H^l_{\rho,\alpha}} \|v+p\|_{\rho,\alpha} .$$

The expression on the right-hand side can be estimated by

$$\inf_{p \in H^l_{\rho,\alpha}} \|v+p\|_{\rho,\alpha} = \|v - \mathcal{P}^{\rho,\alpha}_l v\|_{\rho,\alpha} \leq C(\rho,\alpha,m)\, M(l,m)\, \|v\|_{\rho,\alpha,m}$$

for $l+1 \geq m \geq 1$ using Theorem 2.10. ∎

LEMMA 3.6. *For $w^n \in H^n_{\rho,\alpha}$ the summation error $E^l(u\, w^n \Psi^{-1}_{\rho,\alpha})$, $l \geq n$, can be estimated by*

$$|E^l(u\, w^n \Psi^{-1}_{\rho,\alpha})\| \leq C_S \|w^n\|\, C(\rho,\alpha,m)\, M(l-n,m)\, \|u\|_{\rho,\alpha,m} , \tag{3.27}$$

where C_S is a constant depending on the summation rule.

Proof. For fixed $w^n \in H^n_{\rho,\alpha}$ we define a linear form

$$\begin{aligned} f : \; & H_{\rho,\alpha} \to \mathbb{R} , \\ & u \mapsto E^l(u\, w^n \Psi^{-1}_{\rho,\alpha}) , \end{aligned}$$

which is continuous in u and has the norm $C_S \|w^n\|$. Moreover we have $f(u) = 0$ for $u \in H^{l-n}_{\rho,\alpha}$. Then application of Lemma 3.5 gives the assertion. ∎

Finally we insert Theorem 2.10 and Lemma 3.6 into (3.22) and obtain

THEOREM 3.7. *If equation (3.21) is solved by applying a summation rule, which is exact in $H^l_{\rho,\alpha}$, $l \geq n$, the error of $u^{n,l}$ can be estimated by*

$$\|u - u^{n,l}\| \leq C(\rho,\alpha,m)\, \|u\|_{\rho,\alpha,m}\, (M(n,m) + C_S\, M(l-n,m)) . \tag{3.28}$$

Theorem 3.7 shows, that the summation formula has to be of order $l = 2n$, such that the pure and perturbed projection have the same asymptotic behavior. Thus we use a Gauss summation with $n+1$ nodes in $H^n_{\rho,\alpha}$ leading to

$$l = 2n+1 .$$

Theorem 3.7 also shows, that for fixed n

$$\|u^n - u^{n,l}\| \to 0 \quad \text{for} \quad l \to \infty .$$

3.3 Weight Function Fitting

In order to minimize the computational effort of the discrete Galerkin method, a good choice of the parameters ρ and α is crucial. In this work, we choose an *heuristic* approach which is an extension of the *moving weight function* concept suggested in [19]. After each step, an actual approximation $u^n \in H_{\rho,\alpha}$ is transformed to $\bar{u}^{\bar{n}} \in H_{\bar{\rho},\bar{\alpha}}$ (using the formulas derived in Section 2.2), where $\bar{n} < n$ is expected.
The main idea is the fitting of the first moments of $u^n \in H_{\rho,\alpha}$ to those of the weight function $\Psi_{\bar{\rho},\bar{\alpha}}$, a procedure which is possible by Corollary 1.4. Due to the normalization of the family $\Psi_{\rho,\alpha}$ this leads to an implicit definition of the parameters $\bar{\rho}, \bar{\alpha}$ by

$$
\begin{aligned}
\frac{\mu_1[u]}{\mu_0[u]} &\stackrel{!}{=} \mu_1[\Psi_{\bar{\rho},\bar{\alpha}}] &&= \frac{1+\bar{\alpha}\,\bar{\rho}}{1-\bar{\rho}}\,, \\
\frac{\mu_2[u]}{\mu_0[u]} &\stackrel{!}{=} \mu_2[\Psi_{\bar{\rho},\bar{\alpha}}] &&= \frac{\bar{\alpha}^2\bar{\rho}^2+3\bar{\alpha}\bar{\rho}+\bar{\rho}+1}{(1-\bar{\rho})^2}\,.
\end{aligned}
\tag{3.29}
$$

From (3.29) it follows, that ($\mu_k = \mu_k[u]$):

$$
\begin{aligned}
\bar{\rho}(u) = \bar{\rho} &= \frac{\mu_0\mu_2 - \mu_1^2 - \mu_1\mu_0 + \mu_0^2}{\mu_0\mu_2 - \mu_1^2}\,, \\
\bar{\alpha}(u) = \bar{\alpha} &= \frac{2\mu_1^2 - \mu_1\mu_0 - \mu_2\mu_0}{\mu_0\mu_2 - \mu_1^2 - \mu_1\mu_0 + \mu_0^2}
\end{aligned}
\tag{3.30}
$$

The requirements $0 < \bar{\rho} < 1$ and $\bar{\alpha} > -1$ are fulfilled, whenever the denominators of the expressions in (3.30) are positive. Whenever only the parameter ρ has to be adapted (i.e. $\alpha = 0$), (3.29) leads to (consistent with [19], (3.15))

$$
\bar{\rho}(u) = 1 - \frac{\mu_0[u]}{\mu_1[u]}\,. \tag{3.31}
$$

In order to compute the moments $\mu_0[u]$, $\mu_1[u]$, $\mu_2[u]$ for $u \in H_{\rho,\alpha}$ given in the basis expansion, we use the fact, that the monomials s^k can be represented in terms of the polynomials $l_k(\rho,\alpha)$ by

$$
s^k = \sum_{m=0}^{k} b_{km}\, l_m(s)\ ,\ k = 0, 1, \dots\ , \tag{3.32}
$$

with coefficients $b_{km} = b_{km}(\rho,\alpha)$, $b_{kk} \neq 0$. Then $\mu_k[\Psi_{\rho,\alpha}] = b_{k0}$ and insertion of u into the definition of the moments yields

$$
\mu_k[u] = \sum_{m=0}^{k} b_{km}\, a_m\, \gamma_m^{\rho,\alpha}\,. \tag{3.33}
$$

For $k \leq 2$ the coefficients b_{km} can be calculated to be

$$b_{10} = \nu_1(\rho, \alpha) \ , \ b_{11} = -\frac{1}{1-\rho}$$

and

$$b_{20} = \nu_2(\rho, \alpha) \ , \ b_{21} = -\frac{2\alpha\rho + \rho + 3}{(1-\rho)^2} \ , \ b_{22} = \frac{2}{(1-\rho)^2} \ .$$

In general, the condition (3.29) has the nice characterization for weight functions Ψ with p parameters $c_1, \ldots, c_p$, and associated orthogonal polynomials, that for the coefficients of the respective expansion in $H_{c_1,\ldots,c_p}$ the relation

$$a_1 = a_2 = \ldots = a_p = 0 \tag{3.34}$$

is valid. This property has been used in [19] for $p = 1$ ($c_1 = \rho$) to derive a differential equation for the parameter of the Galerkin method.

4 Numerical Examples

The considerations of this paper led to the program CODEX written in the language C. Details of the implementation can be found in [39] for the case of extrapolation in time. The use of the multiplicative correction formula as time discretization lets the structure of the program in principle unchanged.

In this chapter some numerical results are presented featuring:

- the time discretization (linear and nonlinear)
- the adaptivity of the method with respect to the parameters ρ, α
- the adaptivity with respect to the truncation index n
- the numerical preprocessing with Gauss summation.

All computations have been performed on a SPARC–station 1+ using double precision. The computing times (CPU) are given in seconds.

4.1 Chain Addition Polymerization

We consider the backward difference equation from Example 1.1:

$$u'(t) = -\nabla u(t)\ ,\ u(0) = \varphi\ ,$$

which is the (normalized) CODE of the reaction step $P_s + M \xrightarrow{k_p} P_{s+1}$. The Galerkin equations can be derived analytically by applying Corollary 2.5. The process is started with the geometric distribution $\varphi = \Psi_{\rho_0,0} \in H_{\rho_0,0}$ and has been integrated here up to $t_{end} = 50$ sec. The choice $\rho_0 = 0.3$ is made to illustrate the parameter control of the algorithm. From (1.4) the solution $u(t)$ is expected to be similar to a Poisson distribution with parameter $\lambda = t$. As the weight function $\Psi_{\rho,\alpha}$ tends to such a Poisson distribution for $\rho \to 0$ and $\alpha = t/\rho$, we can expect to obtain Galerkin approximations in spaces $H_{\rho,\alpha}$ with $\rho \ll \rho_0$ and α large. It turns out actually, that the parameter ρ decreases to $\rho(t_{end}) = 3.6{\cdot}10^{-3}$, whereas the parameter α increases from zero to $\alpha(t_{end}) = 13844.4$ – this is presented in Figure 1 (logarithmic scale). Table 1 reflects the behavior of the time-step control, where it can be seen, that the maximum true error (computed in $H_{\rho,\alpha} = H_{\rho(t),\alpha(t)}$, using (1.4)) over all time steps fits to the required accuracy TOL. Throughout this chapter $n_{\max}$ may denote the maximum of the number of expansion coefficients in $H_{\rho(t),\alpha(t)}$ required to represent the solution after a global time step. Figure 2 shows the time layers chosen by the algorithm. The

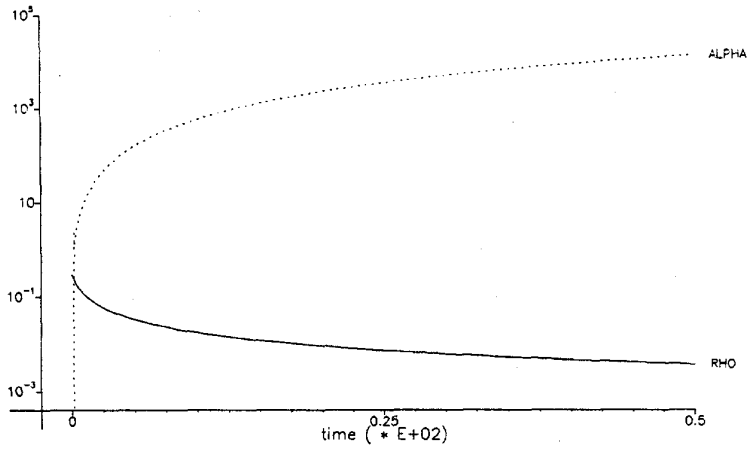

Figure 1: Time evolution of ρ and α

TOL	Time steps	n_{max}	norm of true error in $H_{\rho,\alpha}$	CPU
10^{-1}	59	4	$5 \cdot 10^{-2}$	0.5
10^{-2}	157	5	$9 \cdot 10^{-3}$	1.5
10^{-3}	482	7	$1 \cdot 10^{-3}$	5.0

Table 1:
CODEX: performance for different tolerances

initial step size is 10^{-3} and increases in time to a scale of 1. It can be shown, that

$$\|\nabla\|_{\rho,\alpha} \to \infty \ , \ \alpha \text{ fixed}, \ \rho \to 0 \ .$$

This would result in time steps tending to zero in general cases, but insertion of $\rho\alpha = t$ (the parameter of the Poisson distribution) shows, that the step sizes may tend to one. The behavior of the error estimation compared to the true error for TOL=0.1 is presented in Figure 3.

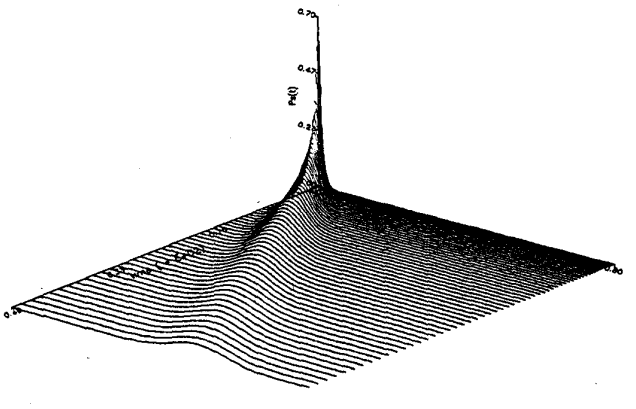

Figure 2: Moving Poisson distribution emerging from an initial geometric distribution

Remark. Due to the properties of the Gauss summation, it does not matter to replace the analytical properties (here: Corollary 2.5) of the discrete Laguerre polynomials applied to the difference operator by a numerical summation. Then the example can be extended to a *reversible process* with *s-dependent* reaction probabilities. In [26], p. 292, a *master equation* describing a *birth-death*-process from chemistry is given by

$$u_s(t) = w(s-1,s-2)u_{s-1}(t)+w(s-1,s)u_{s+1}(t)-(w(s,s-1)+w(s-2,s-1))u_s(t) \tag{4.1}$$

with transition probabilities

$$\begin{aligned} w(s,s-1) &= ak_1(s-1)+k_2'c \ , \\ w(s,s+1) &= k_1'(s+1)s+k_2b(s+1) \end{aligned} \tag{4.2}$$

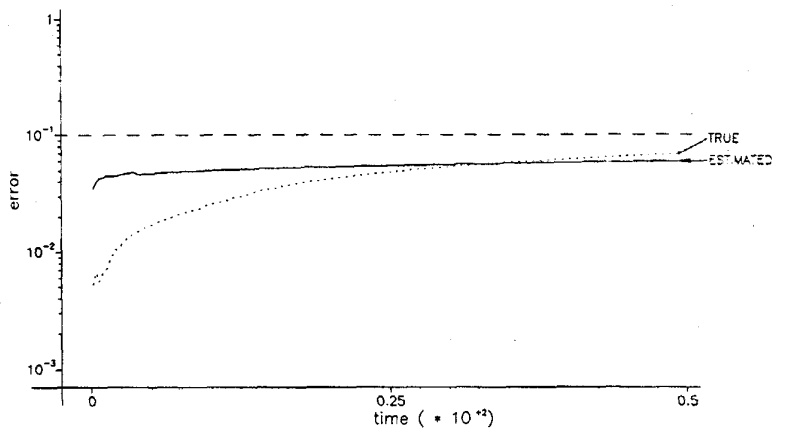

Figure 3: Behavior of the error–estimator

and a, b, k_1, k_1', k_2, k_2' constants. This problem can be solved by CODEX, leading to a traveling Poisson distribution comparable to Figure 2.

4.2 Polymer Degradation

In a degradation reaction of the type

$$P_s \xrightarrow{k_{sr}} P_r + P_{s-r} \ , \quad s > r \geq 1 \ , \tag{4.3}$$

a polymer P_s of chain length s breaks at position r into two polymers of length r and length $s-r$. In general (see e.g. [5]) the reaction rate coefficients k_{sr} depend on the degree of the polymer s and the location r of the breaking bond in the polymer chain. Mathematical modeling of a degradation leads to the following CODE, with $u_s(t)$ the *number* of polymers of chain length s at time t:

$$u_s'(t) = (A_D u)(s) := -\left(\sum_{r=1}^{s-1} k_{sr}\right) u_s(t) + 2 \sum_{r=s+1}^{\infty} k_{rs}\, u_r(t) \ , \tag{4.4}$$

re-defining the degradation operator (1.14). A realistic initial distribution $u_s(0)$ from [5] can be described qualitatively by

$$u_s(0) = \frac{s}{r_{\max}} \bar{\rho}^s \ , \quad \bar{\rho} = e^{-1/r_{\max}} \ , \tag{4.5}$$

such that the maximum of the distribution $u_s(0)$ roughly occurs at chain length $s = r_{\max}$ (e.g. $r_{\max} \approx 60000$ in [5]). We mentioned in Section 1.3, that the $H_{\rho,\alpha}$ - theory is valid for the degradation operator only if $\rho(1+\alpha/2) < 1$. Therefore we cannot use the exact representation

$$u_s(0) = \frac{\bar{\rho}}{(1-\bar{\rho})^2 r_{\max}} \Psi_{\bar{\rho},1}(s) \ , \ s \geq 1 \ ,$$

if $\bar{\rho} > 2/3$. This implies, that distributions of the type (4.5) can only be represented in $H_{\bar{\rho},1}$ for $r_{\max} = 1$ – the case of a geometric distribution. Hence we use the representation of $u_s(0)$ in $H_{\rho,0}$ with $\rho = 2\bar{\rho}/(1+\bar{\rho})$ (due to (3.31)) and the expansion coefficients

$$a_k = \frac{\bar{\rho}}{(1-\bar{\rho})^2 \, r_{\max}} 2^{-k}(1-k) \ , \ k \geq 0 \ ,$$

and have to control the moving weight function fitting additionally by $\bar{\rho}(1+\bar{\alpha}/2) < c$, $c < 1$ a safety factor.

The degradation problem will be attacked here for the reaction coefficients

$$k_{sr} = k_s = k_p \, s^{\beta} \ , \ k_p = 2.11 \cdot 10^{-7} \ , \ \beta = -1/3 \, . \tag{4.6}$$

This modeling of a *heterogeneous* polymerization is suggested in [5] and has been treated in [38] by replacing the fractional power s^{β} by a so-called *factorial* power. Introducing a (small and analyzed) modeling error, the problem could be solved there using product linerization formulas of discrete Laguerre polynomials. In order to solve the original problem, we have to evaluate (respectively approximate) the scalar products

$$\begin{aligned} &\left(A_D \, \psi_k(\rho,\alpha) \, , \, \psi_j(\rho,\alpha)\right)_{\rho,\alpha} = \\ &\sum_{s=1}^{\infty} l_j(s) \left((1-s) \, k_s l_k(s) \Psi_{\rho,\alpha}(s) + 2 \sum_{r=1}^{\infty} l_k(r+s) \, \Psi_{\rho,\alpha}(r+s) \, k_{r+s} \right) \end{aligned} \tag{4.7}$$

by applying a double Gauss summation. Before discussing the realistic setting ($r_{\max} = 60000$), we show that the problem is reliably approximated by CODEX. For that we choose $r_{\max} = 50$ in (4.5), $k_p = 1.0$ in (4.6) and $t_{end} = 0.01$, such that a reference solution can be obtained by a direct integration of system (4.4) truncated at $s_{\max} = 1000$ and treated as an ODE. Table 2 shows the nice behavior of the Galerkin approximations for different tolerances. The original case with $r = 60000$ in (4.5) and $t_{end} = 3600$ sec. implies that the interesting maximum chain length $s_{\max}$ is larger than 400000. Obviously it is no longer possible to compute a direct solution of the problem in this case. but a comparison of

TOL	$n_{\max}$	norm of true error in $H_{\rho,\alpha}$	CPU
10^{-1}	6	$6 \cdot 10^{-2}$	5
$5 \cdot 10^{-2}$	7	$4 \cdot 10^{-2}$	12
10^{-2}	10	$6 \cdot 10^{-3}$	39
$5 \cdot 10^{-3}$	11	$3 \cdot 10^{-3}$	72

Table 2:
CODEX: performance for heterogeneous degradation.

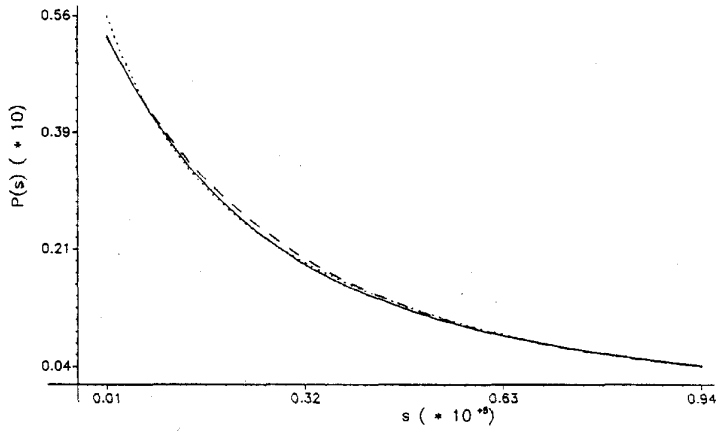

Figure 4: Comparison of the results for a heterogeneous degradation, $t_{end} = 3600$ sec., obtained by different methods.

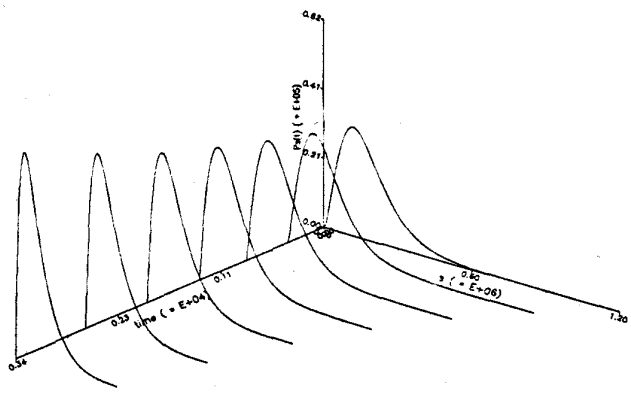

Figure 5: Time evolution of the weight distribution in a degradation process

a result in [38] ($\cdots$), of the new (—) and of the old (- $\cdot$) version of CODEX [39] shows, that the solution seems to be very reasonable (Figure 4). The computing times are comparable to Table 2. Figure 5 presents the time evolution of the weight distribution $s \cdot u_s(t)$ (chosen for ease of representation) of this process, where each line represents one time step.

4.3 Soot Formation

In the last example we show, that very general types of reactions can be treated by using the techniques derived in this paper.

Coagulation (combination) processes are described in the chemical notation by

$$P_r + P_s \xrightarrow{k_{rs}} P_{r+s} ,$$

where P_s may denote a polymer molecule or a soot (smog) particle of size s. This reaction module appears frequently in applications - distinguished by different modelings of the reaction rate coefficients $k_{rs} = k_{sr}$. It can also be considered as the reverse process of a degradation (4.3). In polymer chemistry often moment dependent rate coefficients are in use, whereas the modeling of surface effects of the combination of *smog particles* leads to coefficients dependent on the size of the reacting molecules. The CODE of a coagulation process reads in general

($u_s(t)$ defined as in Example 4.2)

$$(4.8)\quad u_s'(t) = F(u(t))(s) := \frac{1}{2}\sum_{r=1}^{s-1} k_{r,s-r}\, u_r(t)\, u_{s-r}(t) - u_s(t)\sum_{r=1}^{\infty} k_{sr}\, u_r(t)\ .$$

Concerning the k_{sr}, we refer to a model by FRENKLACH [21], where the following reaction coefficients are suggested:

$$(4.9)\qquad k_{rs} := k_p \left(\frac{1}{r}+\frac{1}{s}\right)^{1/2} \left(r^{1/3}+s^{1/3}\right)^2\ ,\ k_p \text{ constant.}$$

Note, that the algorithm CODEX works for arbitrary coefficients k_{sr} (as far as the $H_{\rho,\alpha}$ - theory is valid).

The problem (4.8) has been attacked by different authors. In [21], a special approximation of the moments is tried just for the coefficients (4.9). In [32], a discrete Fourier transform is applied, but this requires a certain separation of r and s in the expression for the k_{rs}. A continuous modeling as in [22] leads to theoretical difficulties.

In order to obtain a reference solution of (4.8), we perform again a direct time integration of a truncated system as an ODE (replace ∞ by $s_{\max}$ in (4.8), $s_{\max}$ large enough).
Such an integration up to an interesting t_{end} took more than 14000 sec. (CPU) on a Cray-YMP. This value would be even larger, if the truncation index $s_{\max}$ was not known from the simulations with CODEX a priori ! A realistic number of size-classes is given in [21] to be about $s_{\max} = 10000$, thus we used $k_p = 1$ and t_{end} large enough to obtain comparable results. By the way we note, that the whole simulation with CODEX is independent of the parameter $s_{\max}$.

The application of the semi-implicit Euler scheme (3.5) in CODEX requires the Frechét derivative $DF(\varphi)(u)$ of F with respect to u at φ, which can be computed pointwise (the time dependency is omitted) by

$$(4.10)\quad DF(\varphi)(u)(s) = \sum_{r=1}^{s-1} k_{r,s-r}\,\varphi_{s-r}\,u_r - \varphi_s\sum_{r=1}^{\infty} k_{sr}\,u_r - u_s\sum_{r=1}^{\infty} k_{sr}\,\varphi_r\ .$$

As in Example 4.2, the entries of the Galerkin equations are computed by a double Gauss summation with two infinite sums of the structure described in Section 2.4. This can be done after an appropriate re-ordering of the appearing sums.

It turns out, that the solution $u_s(t)$ (number distribution) at $t = 100$ sec. has a narrow peak for small chain lengths ($s < 100$). This peak is obviously hard to approximate (i.e. time consuming) by a polynomial expansion as used herein

(see Figure 6). Nevertheless, a relative accuracy of 8-10% can be obtained in moderate computing times (about 50 sec. CPU on a SPARC 1+), which increase strongly for higher accuracies. This is an effect of properties of the basis functions, not a consequence of the used time and operator discretization. For

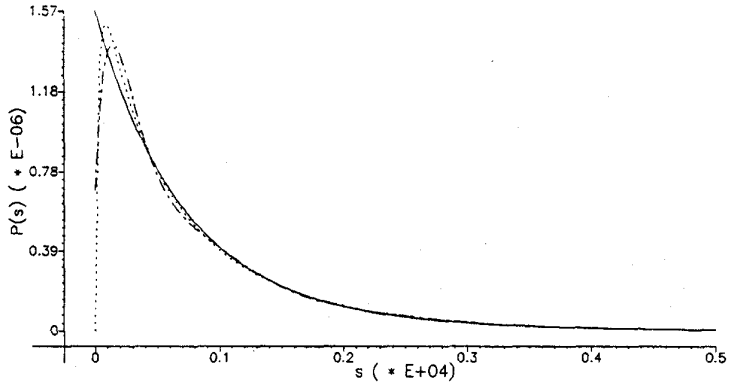

Figure 6: Comparison between direct solution ($\cdots$) and Galerkin approximations with $n = 4$ (–) and $n = 20$ (--) of a heterogeneous coagulation process at t=100.

a better study of the algorithm for higher accuracies, we compute directly the weight distribution $u_s(t) \cdot s$ from a transformed equation (4.8). Table 3 shows the performance of CODEX for a simulation up to $t = 100$ sec. in this case. If

TOL	time-steps	$n_{\max}$	true error in $H_{\rho,\alpha}$	CPU
10^{-1}	50	5	$1.4 \cdot 10^{-1}$	16
$5 \cdot 10^{-2}$	67	7	$8.5 \cdot 10^{-2}$	49
10^{-2}	135	14	$3.1 \cdot 10^{-2}$	1386

Table 3:
CODEX: performance for several tolerances.

the direct solution at $t = 100$ sec. is directly represented by a basis expansion with the parameters obtained by CODEX (i.e. ρ, α and n), the behavior of the time error estimation can be studied. In Table 4 it can be seen, that this device works very accurate. Figure 7 shows the time evolution (in logarithmic scale) of the weight distribution up to $t = 100$ sec., showing how fast the mean value increases with time. Table 5 compares the computing times of CODEX and

TOL	time-error (true)	time-error (estimation)
10^{-1}	$4 \cdot 10^{-2}$	$5 \cdot 10^{-2}$
$5 \cdot 10^{-2}$	$2.5 \cdot 10^{-2}$	$2.5 \cdot 10^{-2}$
10^{-2}	$9 \cdot 10^{-3}$	$5 \cdot 10^{-3}$

Table 4:
CODEX: Comparison of the time error and its estimation.

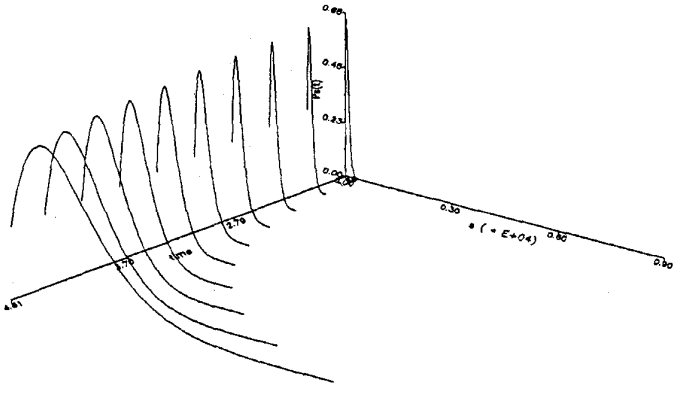

Figure 7: Time evolution of the weight distribution in a soot formation

a direct integration with the non-stiff ODE-solver DIFEX1 [16] on SPARC 1+ and CRAY-YMP. As can be seen, the time for the direct integration increases quadratically with the value of $s_{\max}$. Therefore it is in principle only possible on a supercomputer – with tremendous effort and preventing a treatment of a CODE as a large ODE in general. The computing time of CODEX increases for tolerances up to $5 \cdot 10^{-2}$ in principle with the number of time steps – independent of $s_{\max}$. Figure 8 illustrates the adaptivity of the discrete Galerkin method with

t	$s_{\max}$	CPU CODEX	CPU DIFEX1	CPU (DIFEX1) Cray-YMP
1.0	50	13	18	5
2.0	90	19	36	10
5.0	250	27	365	25
10.0	600	34	–	92
50.0	1200	51	–	441
100.0	8500	59	–	> 14000

Table 5:
Computing times (sec.) for direct (non-stiff) integration (DIFEX1) on SPARC and CRAY and CODEX (TOL $= 5 \cdot 10^{-2}$).

respect to the truncation index n for the tolerances 10^{-1}, $5 \cdot 10^{-2}$, 10^{-2}. Because the coagulation process roughens the distribution with time (as an element of $H_{\rho,\alpha}$), an increasing number of expansion coefficients is necessary, in particular at the beginning.

We conclude the presentation of the examples with the remark, that the techniques implemented in CODEX can be extended obviously to problems with combinations of operators as well as to systems of CODE's. The restrictions given by the class of basis functions used herein can be overcome by choosing other weight functions or combinations of them.

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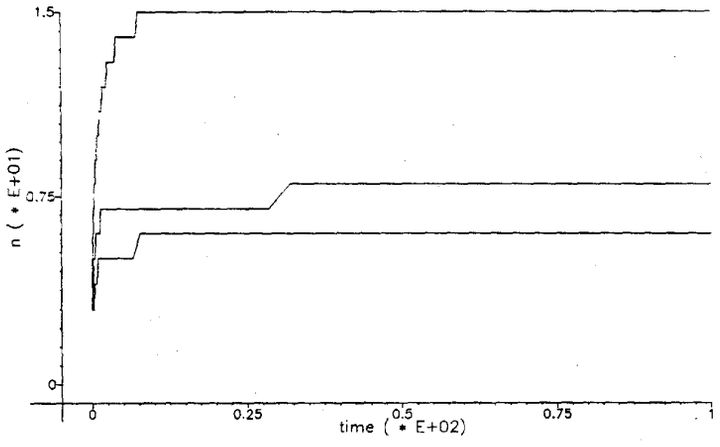

Figure 8: Time evolution of number of expansion coefficients for different tolerances.

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