Constructive Approximations of the Convection-Diffusion-Absoption Equation Based on the Cayley Transform Technique

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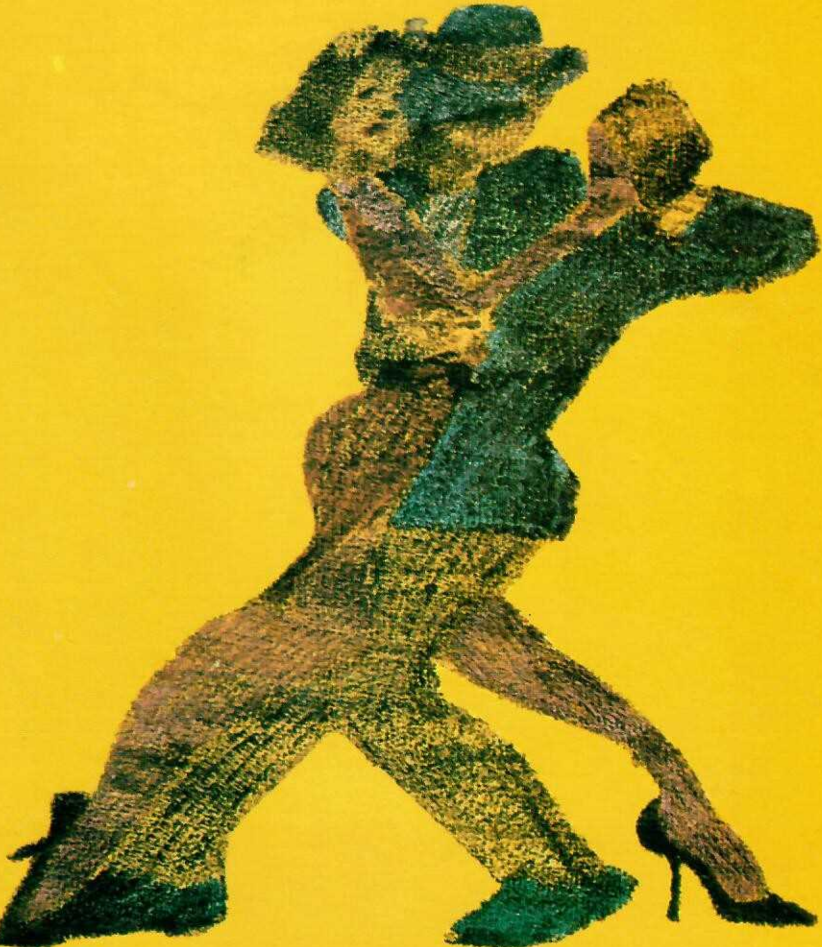

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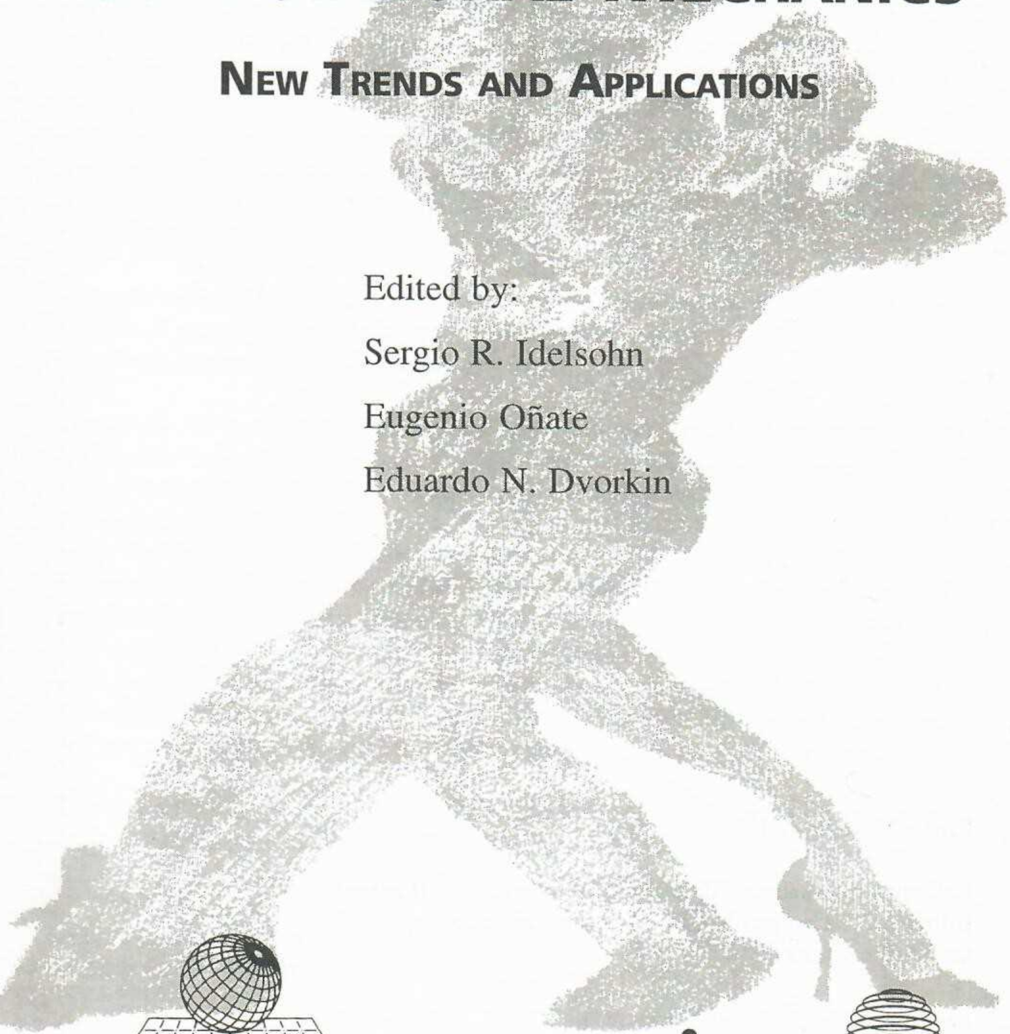

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PREFACE

This CD ROM Proceedings contain the papers presented at the *Fourth World Congress on Computational Mechanics* (IV WCCM) held in the city of Buenos Aires (Argentina) on June 29-July 2, 1998. The first three congress in the series where held in Austin (1986), Stuttgart (1990) and Tokyo (1994). The 1998´Congress incorporated the XIX Ibero-Latin-American Conference on Computational Methods in Engineering (CILAMCE). This joint event was held under the auspices of the International Association for Computational Mechanics (IACM) and was jointly organized by the Argentinean Association for Computational Mechanics (AMCA) and the Spanish Association for Numerical Methods in Engineering (SEMNI).

The continuous importance of this research topic is demostrated by the fact that the number of papers has increased from 400 papers presented in the first congress to over 1000 papers in the Buenos Aires meeting.

The developments that have taken place in the different theoretical and engineering application fields of the broad area of Computational Mechanics are illustrated by the contents of these CD-ROM proceedings. The 700 papers included represent a Compendium of nearly 14.000 pages. The papers are clasified into the following main areas: (i) Mathematical Modelling and Numerical Methods, (ii) Solid and Structural Mechanics, (iii) Solid Materials Modeling, (IV) Fluid Mechanics (V) Heat Transfer and Fluid-Structure Interaction, (VI) Inverse Problems and Optimizations (VII) Software Development, Algorithms and Programming and (VIII) Applications Fields including problems in Biomechanics, Computational Physics, Electromagnetics, Environmental Sciences, Geomechanis, Forming Processes, Chemical Engineering, Robotics and Educational aspects of Computational Mechanics, among others.

The CD-ROM proceedings are printed directly from electronic versions of the manuscripts provided by the authors. The editors therefore can not accept responsability for any inaccuracies, comments or opinions contained in the papers.

Finally the editors wish to thank the authors for their participation and cooperation in making the IV WCCM a success.

S. Idelsohn, E. Oñate and E. Dvorkin,
Buenos Aires, June 1998

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PART I

MATHEMATICAL MODELING AND NUMERICAL METHODS

SECTION 1 - MATHEMATICAL MODELLING

The developments that have taken place in the different theoretical and engineering application fields of the broad area of Computational Mechanics are illustrated by the contents of these CD-ROM proceedings. The 700 papers included represent a Compendium of nearly 14.000 pages. The papers are clasified into the following main areas: (i) Mathematical Modelling and Numerical Methods, (ii) Solid and Structural Mechanics, (iii) Solid Materials Modeling, (IV) Fluid Mechanics (V) Heat Transfer and Fluid-Structure Interaction, (VI) Inverse Problems and Optimizations (VII) Software Development, Algorithms and Programming and (VIII) Applications Fields including problems in Biomechanics, Computational Physics, Electromagnetics, Environmental Sciences, Geomechanis, Forming Processes, Chemical Engineering, Robotics and Educational aspects of Computational Mechanics, among others.

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COMPUTATIONAL MECHANICS
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CONSTRUCTIVE APPROXIMATIONS OF THE CONVECTION-DIFFUSION-ABSORPTION EQUATION BASED ON THE CAYLEY TRANSFORM TECHNIQUE

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Key Words: CDA operators in Banach spaces, Cayley transform, non-selfadjointness.

Abstract. *In many practical problems the norm of the resolvent for the convection-diffusion-absorption (CDA) operator is large as a function of the Peclet number. As a result, conventional spectral analysis may be of limited usefulness for the solution of such problems. Even if the spatial operator is spectrally discretised, the solution of nonstationary problems requires a temporal discretisation that dictates a typically severe restriction on the method applicability in convection-dominated regions.*

To resolve these difficulties we develop a new method based on a combination of the Cayley transform technique and an effective iterated mapping. Error estimates for our numerical method are presented.

1 INTRODUCTION

The convection-diffusion-reaction equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} C(x,t,u) + \frac{\partial^2}{\partial x^2} D(x,t,u) + R(x,t,u) \tag{1.1}$$

with specified functional dependencies for C, D, R, and boundary and initial conditions provides an important example of models where challenges of modern mathematical theory and its application meet together.[1–3] On the one hand, there are a number of open questions in the field of the theoretical analysis of equation (1.1) that need to be addressed. On the other hand, since equation (1.1) arises in many areas of applications, efficient constructive procedures for its solution have to be developed in the real-time framework.

1.1 Statement of the Problem

In this paper we consider a special case of (1.1), known as the convection-diffusion-absorption (CDA) equation. Let us specify the functions C, D and R in (1.1) as follows

$$C = \beta(x,t)u, \; D = \mu(x,t)u, \; R = \alpha(x,t)u, \tag{1.2}$$

where β, μ, α in (1.2) denote the convection velocity and the diffusion and absorption coefficients respectively.

After simple transformations, the CDA operator,

$$\mathcal{L}u \equiv \frac{\partial}{\partial x}(\beta u) + \frac{\partial^2 (\mu u)}{\partial x^2} + \alpha u,$$

can be rewritten as

$$\mathcal{L}u = \tilde{\beta}\frac{\partial u}{\partial x} + \mu \frac{\partial^2 u}{\partial x^2} + \tilde{\alpha} u, \tag{1.3}$$

where

$$\tilde{\beta} = \beta + 2\frac{\partial \mu}{\partial x}, \; \tilde{\alpha} = \alpha + \frac{\partial \beta}{\partial x} + \frac{\partial^2 \mu}{\partial x^2}.$$

We assume that coefficient $\tilde{\beta}, \tilde{\alpha}$, and μ in (1.3) are time-independent.

Let E be a Banach space, and let us assume that the domain $D(\mathcal{L})$ of the CDA operator (1.3) is dense in E. For example, we may consider the space-time domain $Q = \Omega \times I$, with $\Omega = (d_0, d)$, $I = (0, T_0)$, $d > d_0$, $d > 0$, $T_0 \le +\infty$ and set $E \equiv L^\infty(d_0, d)$. Then $L^1(0, T_0; L^\infty(d_0, d))$ is the Banach space of Bochner integrable functions $u(t) \equiv u(\cdot, t)$ with the norm

$$\|u\|_{L^1} = \int_0^{T_0} \|u(s)\|_{L^\infty} ds.$$

Further let $u_0 \in L^\infty(d_0, d)$ and $f(t) \equiv f(\cdot, t) \in L^1(0, T_0; L^\infty)$.

In this paper we define the domain of the CDA operator (1.3) as follows

$$D(\mathcal{L}) = \{u : \ u \in C^2[d_0, d], \ u(d_0) = u(d) = 0\}$$

and assume that $E \equiv C[d_0, d]$. We are concerned with the following problem:

Find such a continuous function $u(\cdot, t) : \ [0, T_0) \to E \ \forall \ 0 \le t < T_0$ *which is continuously differentiable* $\forall \ 0 \le t < T_0$, $u(\cdot, t) \in D(\mathcal{L}) \ \forall \ 0 < t < T_0$, *and which satisfies the equation*

$$\frac{\partial u}{\partial t} = \mathcal{L}u + f \tag{1.4}$$

with the initial condition

$$u(x, 0) = u_0(x) \tag{1.5}$$

and boundary conditions

$$u(d_0, t) = u(d, t) = 0. \tag{1.6}$$

The assumption of homogeneous Dirichlet conditions (1.6) does not restrict generality of the problem since nonhomogeneous Dirichlet conditions can be homogenised by a simple linear transformation.

1.2 Applications

The model (1.3)–(1.6) describes rich dynamics subject to the topological structure of $\mathcal{L}$. This model provides an example of a multi-physics problem coupling several physical phenomena. In particular, the model (1.3)–(1.6) is used

- to describe the evolution of the concentration of a contaminant dropped into fluid running in a pipe,
- in the electro-magnetic theory,
- in fluid dynamics as a simplified model for fluid flow described by the Navier-Stokes system and
- in many other areas of applications.

To put it in a more general framework, we may say that many conservation laws of different physical quantities are well approximated by the model (1.3)–(1.6). However, when this model is applied to modelling real-world phenomena, the numerical solution of the problems arising involves serious difficulties. We explain this situation with a simple example. Changing variables x, t by $\xi = \tilde{\beta}/\mu x, \ \tau = t$ and setting $d_0 = 0$, the problem (1.3)–(1.6) is reducible to

$$\tilde{\mu}\frac{\partial U}{\partial \tau} = \frac{\partial U}{\partial \xi} + \frac{\partial^2 U}{\partial \xi^2} + \tilde{\alpha}_\mu U, \tag{1.7}$$

$$U(\xi, 0) = U_0(\xi), \;\; U(0, \tau) = U(\tilde{d}, \tau) = 0, \tag{1.8}$$

where U is the transplant of u, $\tilde{\mu} = \mu/\tilde{\beta}^2$, $\tilde{\alpha}_\mu = \tilde{\alpha}\tilde{\mu}$, $\tilde{d} = (\tilde{\beta}/\mu)d$.

In the setting (1.7)–(1.8) the quantity $\tilde{d}$ may be interpreted using the Peclet number.[1] For convection-dominated regions large Peclet numbers and small coefficients $\tilde{\mu}$ near the temporal derivative present principal difficulties for the solution of this type of problem. From the physical point of view, by using the model (1.7)–(1.8) we attempt to describe at least two physical processes that interact with each other on different space-time scales. More precisely, the equation (1.7) can be cast in the form of the Tichonov system for singular perturbations

$$\frac{\partial z}{\partial t} = f_1(x, t, y, z), \; \bar{\mu}\frac{\partial y}{\partial t} = f_2(x, t, y, z),$$

where

$$f_1 = \frac{\partial^2 y}{\partial t \partial x}, \;\; f_2 = z + \frac{\partial^2 y}{\partial x^2} + \tilde{\alpha}_\mu y.$$

Although there exist spatial regions with steep gradients, the long-time behaviour of the solution is expected to be sufficiently regular. Hence, in order to construct robust numerical procedures for the solution of the CDA problem we have to be able to adapt the approximation automatically with respect to the smoothness of the initial data. Such procedures for the solution of the problem (1.3)–(1.6) are developed in the next sections.

2 RESOLVENT BOUNDS FOR CDA OPERATORS

The qualitative features of the dynamics described by the model (1.3)–(1.6) are governed by the relative size of μ and $\tilde{\beta}$. For the limit (or reduced) problem with $\mu = 0$, solution discontinuities may not be excluded even for smooth initial data. It is the presence of diffusion in operator (1.3) that tends to make the solution continuous. Nevertheless, even in the case when $0 < \mu \ll 1$ and $|\tilde{\beta}|$ is relatively large, we often have to deal with narrow regions (called "layers") where the solution may change dramatically. In the general case of convection-diffusion-reaction equation (1.1) such layers may appear not only near the boundary but also in the interior of the region. A quite natural approach to the solution of such problems is to use domain decomposition methods (DDM).[2] When applied to nonstationary problems such a technique is often used in conjunction with an implicit-in-time discrete differentiation. Unfortunately, this leads to a gradual deterioration of accuracy due to the necessity of inverting certain operators associated with $\mathcal{L}$, at each time step. The same can be said about spectral and pseudospectral techniques when finite differences are used for temporal discretisation. In the latter case such methods can be interpreted as limiting cases of increasing-order-in-space finite difference methods.[4]

As an alternative, during recent years, attempts have been made to construct DDMs with no iterations for nonstationary problems.[2] Such methods employ the idea of a dynamic adaptation of the computed solution to the smoothness of initial data. The same idea, though from a different perspective, will be developed in this paper to the solution of problem (1.3)–(1.6).

We note that the operator $\mathcal{L}$ from (1.3) is non-selfadjoint, and non-normal ($\mathcal{L}\mathcal{L}^* \neq \mathcal{L}^*\mathcal{L}$). This fact brings a major complexity in the theoretical analysis of the problem. As a result, the use of resolvent-based techniques for the solution of such problems is more appropriate than the spectrum-based technique.

Let $\Sigma(\mathcal{L})$ be a subset of the complex plane $\mathcal{C}$ that denotes the spectrum of the operator $\mathcal{L}$, and $\rho(\mathcal{L})$ be its resolvent set. Let also $\mathcal{L}^+ = -\mathcal{L}$. Then, if the operator $\mathcal{L}^+$ is strongly positive, $\mathcal{L}$ is the infinitesimal generator of an analytic semigroup $T(t)$.[5] Furthermore, for $u_0 \in D(\mathcal{L}^+)$, $T(t)u_0$ is the solution of the problem (1.4)–(1.6). In order to deal with more general problems we need to specify conditions under which the operator $\mathcal{L}^+$ is positive.

In the complex plane $\mathcal{C}$ we define a closed path for given positive numbers φ and γ as follows

$$\Gamma \equiv \Gamma(\varphi,\gamma) = \mathcal{R}(\varphi,\gamma) \cup \mathcal{A}(\varphi,\gamma), \tag{2.1}$$

where

$$\mathcal{R}(\varphi,\gamma) \equiv \mathcal{R}(\varphi,\gamma) \cup \{\rho \exp(\pm i\varphi), \gamma \leq \rho \leq \infty\},\ \mathcal{A}(\varphi,\gamma) = \{|z| = \gamma, |\arg z| \leq \varphi\}.$$

By (2.1) the complex plane is divided into two sets, Σ^+ and Ω_Γ, where

$$\Sigma^+ = \{z \in \mathcal{C} :\ 0 < \varphi \leq |\arg z| < \pi\} \cup \{z \in \mathcal{C} :\ |z| \leq \gamma\} \tag{2.2}$$

(for certain γ and φ), such that

$$\Sigma^+ \subset \rho(\mathcal{L}^+),\ \ \Sigma(\mathcal{L}^+) \subset \Omega_\Gamma. \tag{2.3}$$

We assume that there exists a constant $M > 0$ that

$$\|(zI - \mathcal{L}^+)^{-1}\| \leq \frac{M}{1+|z|}\ \ \forall\, z \in \Sigma^+. \tag{2.4}$$

Then operator $\mathcal{L}^+$ is positive if there exists $\varphi, \gamma, M > 0$ such that (2.2)–(2.4) are satisfied. The lower bound $\varphi(\mathcal{L}^+) \equiv \varphi(\mathcal{L}^+, E)$ of all φ for which $\mathcal{L}^+$ is positive is called the spectral angle of the operator $\mathcal{L}^+$.

Definition 2.1 *A positive operator $\mathcal{L}^+$ is called strongly positive if its spectral angle satisfies the inequality*

$$\varphi(\mathcal{L}^+) < \pi/2. \tag{2.5}$$

Further if $f(z)$ is an analytic function in Ω_Γ, bounded by Γ, and there exists $\epsilon > 0$ such that $|f(z)| \le c|z|^{-\epsilon}$, then the Cauchy-Riesz integral,

$$f(\mathcal{L}^+) = \frac{1}{2\pi i}\int_\Gamma f(z)(zI - \mathcal{L}^+)^{-1}dz, \tag{2.6}$$

converges in the operator norm and defines a bounded linear operator $f(\mathcal{L}^+)$. The orientation of Γ is chosen so that $\Sigma(\mathcal{L}^+) \subset \Omega_\Gamma$ is on the left. In this case, any positive power of the operator $\mathcal{L}^+$ may be defined by the substitution of $f(z) = z^{-\sigma}$, $\sigma > 0$, into (2.6) and using the identity $(\mathcal{L}^+)^\sigma = [(\mathcal{L}^+)^{-\sigma}]^{-1}$.

Then the domain $D^\sigma \equiv D((\mathcal{L}^+)^\sigma)$ of the operator $(\mathcal{L}^+)^\sigma$ becomes a Banach space with the norm

$$\|u\|_{D^\sigma} \equiv \|(\mathcal{L}^+)^\sigma u\|_E. \tag{2.7}$$

The adaptive property, built-in into computational algorithms, is a natural way of dealing with many applied problems. For CDA problems, the norm $\|\exp(t\mathcal{L})\|$ may exhibit a long, close-to-constant, transient period before eventually going down to exponential decay. From the practical point of view, it is this transient period, rather than an asymptotic behaviour of the solution, that often present a major interest in applications.

3 FUNDAMENTALS OF THE CAYLEY TRANSFORM FOR NON HOMOGENEOUS CDA PROBLEMS.

In a sequence of papers by Arov, Gavrilyuk and Makarov,[5–7] there was obtained an explicit-form solution for the homogeneous first order differential equation in a Hilbert space. Using the Cayley transform technique, they established a one-to-one correspondence between the continuous initial value problem and a discrete initial value problem. Such a correspondence allows us to construct approximations adapted to the smoothness of the initial data.

In the analysis of CDA problems, the natural spaces to deal with are Banach spaces. However, the Banach-space case requires a completely different methodology compared to the Hilbert case.[7] Without going into details, we note that Banach space constructions are essentially based on the notion of strong positivity of unbounded operators (see Definition 2.1) and require the technique based on the integrals of the form (2.6). We refer the reader to Gavrilyuk[6] for the detailed analysis of the general type of first order non-homogeneous linear differential equations.

Theorem 3.1 *Let all requirements formulated in Section 2 for problem (1.3)–(1.6) be satisfied. Then $\forall\ u_0 \in E$ problem (1.3)–(1.6) has at most one solution and such a solution can be represented in the following form*

$$u(\cdot,t) = T(t)u_0(\cdot) + \int_0^t T(t-s)f(\cdot,s)ds, \tag{3.1}$$

where $\{T(t)\}_{t\ge 0}$ is the analytic semigroup with the generator $\mathcal{L}$.

It appears (see details in[5,7]) that the continuous semigroup $\{T(t)\}_{t\geq 0}$ and a discrete semigroup $\{T_\gamma^n\}_{n\geq 0}$ are intrinsically connected by the solution of the following discrete initial value problem

$$y_\gamma^{n+1} = T_\gamma^n y_\gamma^n,\ n = 0, 1, ...,\ y_\gamma^0 = u_0, \tag{3.2}$$

where $\{y_\gamma^n\}_{n\geq 0}$ is a transplant of $u(\cdot, t)$. A one-to-one correspondence between the operators T and T_γ^n are expressed by the following relationships

$$T(t) = \sum_{k=0}^{\infty}(-1)^k \varphi_k(2\gamma t) T_\gamma^k,\ \ T_\gamma^k = (-1)^k \left[\int_0^\infty \psi_k(t) T\left(\frac{t}{2\gamma}\right) dt + I\right], \tag{3.3}$$

where

$$\varphi_k(t) = -\frac{t}{k}\exp(-t/2) L_{k-1}^{(1)}(t),\ \ \psi_k(t) = -\exp(-t/2) L_{k-1}^{(1)}(t) \tag{3.4}$$

and $L_k^{(\alpha)}$ are Laguerre polynomials defined by recurrence formulae

$$nL_n^{(\alpha)}(\xi) = (-\xi + 2n + \alpha - 1) L_{n-1}^{(\alpha)}(\xi) - (n + \alpha - 1) L_{n-2}^{(\alpha)}(\xi),\ n = 1, 2, ... \tag{3.5}$$

$$L_{-1}^{(\alpha)}(\xi) = 0,\ L_0^{(\alpha)}(\xi) = 1. \tag{3.6}$$

In particular, relationships (3.3)–(3.6) allow us to establish useful identities for the solution of the homogeneous problem (1.3)–(1.6):

$$u(\cdot, t) = \sum_{k=0}^{\infty}(-1)^k \varphi_k(2\gamma t) y_\gamma^k,\ \ y_\gamma^k = (-1)^{k+1} \left[\int_0^\infty \psi_k(t) u\left(\cdot, \frac{t}{2\gamma}\right) dt + u_0\right]. \tag{3.7}$$

In the general case, the homogeneous problem (1.3)–(1.6) and (3.2) are connected by the following identity

$$\begin{aligned} T(t)u_0 = \exp(-\gamma t) \sum_{k=0}^{\infty}(-1)^k L_k^{(0)}(2\gamma t)(y_\gamma^k + y_\gamma^{k+1}) = \\ \exp(-\gamma t) \sum_{k=0}^{\infty}(-1)^k \left[L_k^{(0)}(2\gamma t) - L_{k-1}^{(0)}(2\gamma t)\right] y_\gamma^k. \end{aligned} \tag{3.8}$$

The operator $T(t)$ can be defined using the Cayley transform of the operator $\mathcal{L}^+$,

$$T_\gamma = (\gamma I - \mathcal{L}^+)(\gamma I + \mathcal{L}^+),\ \ \gamma > 0, \tag{3.9}$$

as follows

$$T(t) = \exp(-\gamma t) \sum_{k=0}^{\infty}(-1)^k L_k^{(0)}(2\gamma t) T_\gamma^k (I + T_\gamma). \tag{3.10}$$

Then the following result follows from Theorem 6 in Gavrilyuk.[6]

Theorem 3.2 *If*

$$f(\cdot,t) \in D((\mathcal{L}^+)^\sigma), u_0 \in D((\mathcal{L}^+)^\sigma), (\mathcal{L}^+)^\sigma f(\cdot,t) \in L^1(0,T_0;E) \tag{3.11}$$

for a real number $\sigma > 3/4$, then the function $u(\cdot,t)$ given by (3.1) with the operator $T(t)$ defined by (3.10) is a solution of the CDA problem (1.3)–(1.6).

If, in addition to (3.11), the function $f(\cdot,t)$ is locally Holder continuous on $(0,T_0)$, then this solution is unique.

Remark 3.1 *The solution of the homogeneous problem (1.3)–(1.6) is unique if there exists $\sigma > 3/4$ such that $u_0 \in D((\mathcal{L}^+)^\sigma)$.*

Using (3.1) and (3.10), we are now in a position to define an approximate solution of the CDA problem (1.3)–(1.6) as follows

$$u^N(\cdot,t) = T^N(t)u_0 + \int_0^t T^N(t-s)f(\cdot,s)ds, \tag{3.12}$$

where the operator $T^N(t)$ is determined as the truncated series (3.10), and

$$T^N(t)u_0 = \exp(-\gamma t)\sum_{k=0}^{N}(-1)^k L_k^{(0)}(2\gamma t)(y_\gamma^k + y_\gamma^{k+1}), \tag{3.13}$$

$$\int_0^t T^N(t-s)f(\cdot,s)ds = \sum_{k=0}^{N}(-1)^k T_\gamma^k (I+T_\gamma) \times$$
$$\int_0^t \exp(-\gamma(t-s))L_k^{(0)}\left(2\gamma(t-s)\right) f(\cdot,s)ds. \tag{3.14}$$

The accuracy result for the approximation (3.12)–(3.14) of the CDA problem (1.3)–(1.6) is given by the following theorem (see Gavrilyuk[6]).

Theorem 3.3 *Let assumption (3.11) and all assumptions of Section 2 be satisfied. Then the following accuracy estimates*

$$\sup_{t\in[0,T_0)} \|u^N(\cdot,t) - u(\cdot,t)\|_{D^\Theta} \le cN^{-(\sigma-\Theta-\delta)}\left(\|(\mathcal{L}^+)^\sigma u_0\| + \|(\mathcal{L}^+)^\sigma f(\cdot,t)\|_{L^1}\right)$$

$\forall\, \delta \in (0, \sigma-\Theta)$, *where* $\sigma > \Theta \ge 0$; *and*

$$\sup_{t\in[t_0,t_1]} \|u^N(\cdot,t) - u(\cdot,t)\|_{D^\Theta} \le cN^{-(\sigma-\Theta-\delta+1/4)}\left(\|(\mathcal{L}^+)^\sigma u_0\| + \|(\mathcal{L}^+)^\sigma f(\cdot,t)\|_{L^1}\right)$$

$\forall\, \delta \in (0, \sigma-\Theta+1/4)$, *where* $\sigma \ge \Theta \ge 0$ *and* $[t_0,t_1] \subset (0,\infty)$
hold for the approximate solution (3.12)–(3.14) of the problem (1.3)–(1.6).

Remark 3.2 *From the computational point of view, it is reasonable to use an interpolation of $f(\cdot,t)$ unless the integrals in (3.14) can be computed analytically. A technique based on such an interpolation (with the accuracy rate automatically depending on the smoothness of the initial data u_0 and $f(\cdot,t)$) can be found in Gavrilyuk and Makarov.*[7]

The approximate solution $u^N(\cdot,t)$ defined by (3.12)–(3.14) is a semidiscrete solution of the problem (1.3)–(1.6). Computational procedures for fully discrete approximations are developed in Sections 4 and 5. The major difficulty in the construction of such procedures consists of the fact that the solution of (1.3)–(1.6) changes its qualitative behaviour as $\mu/|\tilde{\beta}|$ decreases. Loosely speaking, the problem "switches" from parabolic to hyperbolic nature. In the next section we start from the consideration of the diffusion-dominated case when the ratio $\mu/|\tilde{\beta}|$ is relatively large. The latter feature of the problem allows us to construct an effective numerical method.

4 DISCRETISATION PROCEDURES FOR DIFFUSION-DOMINATED CDA PROBLEMS.

In order to use approximation (3.12)–(3.14), one has to find $y^k_\gamma, k=0,1,...,N$. The latter problem is reducible to the solution of the following operator equations[6]

$$(\gamma I + \mathcal{L}^+)y^{k+1}_\gamma = \bar{y}^k_\gamma,\ k=0,1,... \tag{4.1}$$

$$\bar{y}^k_\gamma = (\gamma I - \mathcal{L}^+)y^k_\gamma,\ y^0_\gamma = u_0. \tag{4.2}$$

For the nonstationary CDA problems (1.3)–(1.6) these equations can be reduced to a sequence of boundary value problems for second order ODEs. An effective method of such a reduction was recently developed in Gavrilyuk.[6] The basic idea behind this approach, known as the projection method, consists of the construction of two sequences, $V_n^{'}$ and V_n, and a projection operator P_n such that

$$V_n \subset V_n^{'} \cap D(\mathcal{L}^+);\ P_n:\ E \to V_n^{'};\ D(\mathcal{L}^+) \to V_n,$$

where $\{V_n^{'}\}_{n\ge 0}$ defines a sequence of $(n+1)$-dimensional subspaces of E. Then, in analogy with (4.1)–(4.2) we define the following projection operator equations

$$(\gamma I + \mathcal{L}^+_n)\tilde{y}^{k+1}_\gamma = (\gamma I - \mathcal{L}^+_n)\tilde{y}^k_\gamma,\ k=0,1,...,\ \tilde{y}^0_\gamma = P_n u_0, \tag{4.3}$$

where

$$\tilde{y}^k_\gamma \in V_n; \mathcal{L}^+_n y = P_n \mathcal{L} y\ \forall\ y \in V_n.$$

If the values of $\tilde{y}^k_\gamma, k=0,1,...$ are found from (4.3), we are in the position to define the fully discrete approximation for the solution of the problem (1.3)–(1.6) as follows

$$u^N_n(\cdot,t) = \exp(-\gamma t)\sum_{k=0}^{N}(-1)^k L^{(0)}_k(2\gamma t)(\tilde{y}^k_\gamma + \tilde{y}^{k+1}_\gamma) +$$

$$\sum_{k=0}^{N}(-1)^k \int_0^t \exp(-\gamma(t-s))L^{(0)}_k\left(2\gamma(t-s)\right)T^k_\gamma(I+T_\gamma)f(\cdot,s)ds. \tag{4.4}$$

The theoretical analysis of the accuracy of (4.4) was developed in.[6]

Theorem 4.1 *Let $\mathcal{L}_n^+$ be a densely defined operator in E and the assumptions on the operator $\mathcal{L}^+$ from Section 2 be satisfied. We assume that there exist $\sigma > 0$ and a function $r(n,\sigma)$ such that*

$$u_0 \in D\left((\mathcal{L}^+)^\sigma\right) \text{ and } \|P_n v - v\| \le cr(n,\sigma)\|(\mathcal{L}^+)^\sigma v\| \ \forall\, v \in D\left((\mathcal{L}^+)^\sigma\right)$$

with constant c independent of u_0, n and N. Then the following estimates

$$\sup_{t\in[0,\infty)} \|u_n^N(\cdot,t) - u(\cdot,t)\| \le c(N^{-\sigma+\delta} + r(n,\sigma)N^{\delta_1}\|(\mathcal{L}^+)^\sigma u_0\|,$$

and

$$\sup_{t\in[t_0,t_1]} \|u_n^N(\cdot,t) - u(\cdot,t)\| \le c(N^{-\sigma-1/4+\delta} + r(n,\sigma)\|(\mathcal{L}^+)^\sigma u_0\|$$

hold for any arbitrarily small δ, δ_1 ($[t_0,t_1] \subset (0,\infty)$).

We note that the operator $\mathcal{L}^+$ defined on an appropriate domain as the mapping $L^p(d_0,d) \to L^p(d_0,d)$, $1 \le p \le \infty$, is strongly positive.

Hence, the Cayley transform technique described above can also be applied in this case. If we set $d_0 = -1, d = 1$ then it is easy to see that equations (4.1)–(4.2) are equivalent to the following problem

$$\mu(y_\gamma^k)''(\xi) + \tilde{\beta}(y_\gamma^k)'(\xi) + [\tilde{\alpha} - \gamma]y_\gamma^k(\xi) = F,\ y_\gamma^k(-1) = y_\gamma^k(1) = 0, \tag{4.5}$$

where

$$F \equiv F(\xi, y_\gamma^{k-1}) \equiv -\mu(y_\gamma^{k-1})'' - \tilde{\beta}(y_\gamma^{k-1})' - [\tilde{\alpha} + \gamma]y_\gamma^{k-1},\ y_\gamma^0(\xi) = u_0(\xi).$$

The problem (4.5) is approximated by (4.3) with $V_n' = \mathcal{P}_n,\ V_n = \{(1-\xi^2)p_{n-2}(\xi)\}$, where $\tilde{y}_\gamma^{k+1}$ is sought in the form

$$\tilde{y}_\gamma^{k+1} = (1-\xi^2)\sum_{s=0}^{n-2} a_s^{(s)}\xi^s \tag{4.6}$$

and $\mathcal{P}_n$ denotes the set of all algebraic polynomials of degree not exceeding n. Following the technique developed in[6] we include the endpoints $\xi_0 = -1, \xi_n = 1$ in the set of collocation points. Then the boundary conditions will be satisfied automatically. Other collocation points are chosen as the roots of the Gegenbauer ultraspherical polynomials C_{n-1}^λ for $\alpha = 3/2$ (then $C_{n-1}^{3/2}(\xi) = L_n'(\xi)$, where $L_n(\xi)$ are Legendre polynomials). Having $\xi_j, j = 0,1,...,n$ (note that the collocation points coincide with the nodes of the

Gauss-Lobatto quadrature formula), we determine coefficients $a_s^{(n)}$ in (4.6) by equating the residual to zero at these points

$$\mu(\tilde{y}_\gamma^k)''(\xi_j) + \tilde{\beta}(\tilde{y}_\gamma^k)'(\xi_j) + [\tilde{\alpha} - \gamma]\tilde{y}_\gamma^k(\xi_j) - F(\xi_j, \tilde{y}_\gamma^{k-1}) = 0, \; j = 1, ..., n-1 \tag{4.7}$$

with $\tilde{y}_\gamma^0 = \tilde{y}_\gamma^n = 0$.

We note that with the decreasing μ the number of collocation points has to be increased significantly in order to get appropriate accuracy. When $\mu \to 0^+$ the number of collocation points eventually becomes unreasonable for practical computations. This can be expected from the estimates given in Theorem 4.1 because the solution in these cases is highly non-smooth. One has to deal with regions where the solution changes significantly. Although the discontinuities are smoothed out due to the presence of diffusion and the physical quantities remain continuous, an increasing number of terms are necessary in their numerical representations.

5 ITERATED MAPPING FOR CONVECTION-DOMINATED CDA PROBLEMS.

When $\mu \to 0^+$ serious computational difficulties arise in solving boundary value problems (4.5). Due to the presence of boundary layers in many applied CDA problems, collocation points should be clustered near the boundary. In such cases we propose to combine the method described in the previous sections with an iterated mapping technique.

For the solution of the problem (4.7) in the convection dominated case we use the Chebyshev-Gauss-Lobatto collocation points

$$\xi_j = \cos(\pi j/n), \; j = 0, 1, ..., n. \tag{5.1}$$

Of course, such a choice can not be a guarantee against ill-conditioning of matrices arising from discretisation procedures when n increases. This problem may become a serious limitation when non-stationary problems are solved using explicit time-stepping.[2] In contrast to such methods, we use a decomposition of evolution problems into a sequence of stationary problems by "elimination" of the temporal variable. Hence, the conditioning issues are essentially less severe in our approach compared to the conventional methodologies.

The spacing between the collocation points chosen according to (5.1) is $\mathcal{O}(n^{-2})$ near the boundary. If the CDA problem exhibits a boundary layer of the width $\mathcal{O}(\mu)$, then in order to obtain good numerical solutions, at least 1 point should be placed in such a layer. The result of such a placement is that the number of collocation points has to be at least $n = \mathcal{O}(1/\sqrt{\mu})$. From the computational point of view this means that in order to get a reasonable accuracy for $\epsilon = 10^{-10}$ we need an "unreasonable" number of collocation points (at least 10^5).

The situation described above is typical when one deals with non-normal linear operators.[1] It is clear that we have to transform the original set of collocation points in such a way that the operator considered on the new set would be a near normal.[8] Such a transformation will automatically place more points into boundary layers.

Several "stretching" techniques were recently reported in the literature.[8,9] The performance of the majority of them depends on the choice of a parameter (or parameters), the optimal value(s) of which is far from obvious. For example, we may use the transformation

$$z_i = g(\xi_i, \zeta),\ g(\xi, \zeta) = \frac{\sin^{-1}(\zeta\xi)}{\sin^{-1}(\zeta)},\ \xi_i \in [-1, 1],\ i = 0, 1, ..., n,\ \zeta \in [-1, 1], \tag{5.2}$$

where the extent of the stretching depends on α. The extreme stretching corresponds to $\zeta = \cos(\pi/n)$ (see[8]). The optimal choice of ζ depends on specific features of the problem under consideration and requires certain heuristic procedures.

In the general case both the standard collocation method without transformations and the method with one iteration of mapping may fail to resolve the problem (4.7) satisfactorily for small μ and computationally reasonable n. Instead of these methods, we propose to use a sequence of variable transformations in the spirit of the technique described in.[9] More precisely, as a stretching technique we use the iterated map $\xi \equiv g_m(\bar{\xi})$ applied to the equations (4.5) where

$$g_0(\bar{\xi}) \equiv \bar{\xi},\ g_m = \sin\left(\frac{\pi}{2} g_{m-1}(\bar{\xi})\right),\ m \geq 1. \tag{5.3}$$

Such a map possesses the following properties (see proof in[9])

- the sequence (5.3) defines a one-to-one mapping and $g_m([-1, 1]) \to [-1, 1]$;
- if $\bar{\xi}_j, j = 0, 1, ..., n$ are chosen according to (5.1), then

$$g_m(\bar{\xi}_0) - g_m(\bar{\xi}_1) = g_m(\bar{\xi}_{n-1}) - g_m(\bar{\xi}_n) = \frac{8}{\pi^2}\left(\frac{\pi^2}{4n}\right)^{2^{m+1}} [1 + \mathcal{O}(n^{-2})]. \tag{5.4}$$

By procedure (5.3), we can control both the number of collocation points n, and the number of iterations in the stretching technique m when $\mu \to 0^+$. This allows us to keep the number of collocation points reasonable even in those numerical experiments that require boundary layer resolution.

Let us transform the problem (4.5) using the change of variables

$$\xi \to \bar{\xi}(\xi),\ \text{where}\ \xi = \xi(\bar{\xi}) = g_m(\bar{\xi}). \tag{5.5}$$

We obtain

$$\mu z''(\bar{\xi}) + \left[\mu \frac{\bar{\xi}''}{(\bar{\xi}')^2} + \frac{\tilde{\beta}}{\bar{\xi}'}\right] z'(\bar{\xi}) + \frac{\tilde{\alpha} - \gamma}{(\bar{\xi}')^2} z(\bar{\xi}) = \frac{F}{(\bar{\xi}')^2}. \tag{5.6}$$

As in,[9] let

$$\bar{\xi} = h_m\left(g_m(\bar{\xi})\right) = h_m(\xi), h_m = g_m^{-1},\ m = 0, 1, ... \tag{5.7}$$

where the function $h_m(\xi)$ is defined as a mapping $[-1,1] \to [-1,1]$ by the following formulae

$$h_0(\xi) = \xi,\ h_m(\xi) = \frac{2}{\pi} \arcsin\left(h_{m-1}(\xi)\right),\ m \geq 1. \tag{5.8}$$

If we notice that

$$h_0'(\xi) = 1,\ h_0''(x) = 0, \tag{5.9}$$

then after transformations using (5.7)–(5.9) we can find recursive computational formulae for the term $1/\bar{\xi}'$ and $\bar{\xi}''/(\bar{\xi}')^2$ in (5.6). In fact we get the following result

$$1/\bar{\xi}' = \prod_{k=0}^{m-1} \left[\frac{\pi}{2} \cos\left(\frac{\pi}{2} g_k(\bar{\xi})\right)\right],\ m \geq 1, \tag{5.10}$$

$$\begin{aligned}
&\bar{\xi}''/(\bar{\xi}')^2 = \frac{\pi}{2} \tan\left(\frac{\pi}{2} h_m\right) + \left(\frac{\pi}{2}\right)^2 \cos\left(\frac{\pi}{2} h_m\right) \tan\left(\frac{\pi}{2} h_{m-1}\right) + \\
&\left(\frac{\pi}{2}\right)^3 \cos\left(\frac{\pi}{2} h_m\right) \cos\left(\frac{\pi}{2} h_{m-1}\right) \tan\left(\frac{\pi}{2} h_{m-2}\right) + ... \\
&... + \left(\frac{\pi}{2}\right)^{m+1} \left[\prod_{j=1}^{m} \cos\left(\frac{\pi}{2} h_j\right)\right] \tan\left(\frac{\pi}{2} h_1\right) = \\
&\frac{\pi}{2} \sum_{i=1}^{m} \left(\frac{\pi}{2}\right)^{i-1} \tan\left(\frac{\pi}{2} h_{m-i+1}\right) \prod_{j=1}^{i-1} \cos\left(\frac{\pi}{2} h_{i-j+1}\right).
\end{aligned} \tag{5.11}$$

In (5.11) we set $\prod_{j=1}^{i-1} \cos\left(\frac{\pi}{2} h_{i-j+1}\right) = 1$ when $i = 1$.

Hence, we finally come to the following system of linear equations

$$\mu z''(\bar{\xi}_j) + \left[\mu \frac{\bar{\xi}_j''}{(\bar{\xi}_j')^2} + \frac{\beta}{\bar{\xi}_j'}\right] z'(\bar{\xi}_j) + \frac{\tilde{\alpha} - \gamma}{(\bar{\xi}_j')^2} z(\bar{\xi}_j) - \frac{F}{(\bar{\xi}_j')^2} = 0, \tag{5.12}$$

where $1/\bar{\xi}_j'$ and $\bar{\xi}_j''/(\bar{\xi}_j')^2$ are computed by (5.10), (5.11).

As a final remark, we notice that the condition number of matrices obtained as a result of iterated mapping (5.3) has the same growth rate in n as for the original problem.[9] On the other hand, the Cayley transform technique allows us to avoid explicit time stepping. Hence, our methodology is largely unaffected by the problem of ill-conditioning compared to classical finite differences and pseudospectral methods for nonstationary problems.

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