New Splitting Iterative Methods for Solving Multidimensional Neutron Transport Equations

Jacques Tagoudjeu

DISSERTATION.COM

Boca Raton

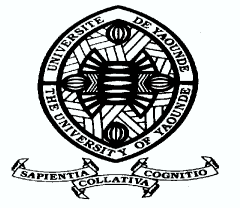
New Splitting Iterative Methods for Solving Multidimensional Neutron Transport Equations

Dissertation.com
Boca Raton, Florida
USA • 2011

ISBN-10: 1-59942-396-0
ISBN-13: 978-1-59942-396-8

UNIVERSITY OF YAOUNDE I
FACULTY OF SCIENCE

UNIVERSITE DE YAOUNDE I
FACULTE DES SCIENCES



DEPARTMENT OF MATHEMATICS
DEPARTEMENT DE MATHEMATIQUES

NEW SPLITTING ITERATIVE METHODS FOR SOLVING MULTIDIMENSIONAL NEUTRON TRANSPORT EQUATIONS

THESIS

Submitted and defended publicly in fulfilment of the requirements for the award of the Degree of Doctorat/Ph.D in Mathematics

Option: Numerical Analysis

by

Jacques TAGOUDJEU

D.E.A in Mathematics

In front of the Jury

PRESIDENT :

- **Pr. Gabriel NGUETSENG**, University of Yaoundé I, Cameroon,

ADVISOR :

- **Pr. AWONO ONANA**, University of Yaoundé I, Cameroon,

MEMBERS :

- **Pr. David BEKOLLE**, University of Yaoundé I, Cameroon,
- **Pr. Nicolas ANDJIGA**, University of Yaoundé I, Cameroon,
- **Pr. François TSOBNANG**, ISMANS, France,
- **Pr Abdelghani BELLOUQUID**, University Cadi Ayyad, Morocco.

Year 2010

Dedication

This work is dedicated to the late memory of my father ***TAMBANDUE Augustin****, and to my mother* ***NGONYIM Sarah****.*

Acknowledgement

Here I would like to express my sincere compliments to all who have contributed from far and close to the realization of this work.

I would like to express my sincere thanks to Professor Awono Onana, my supervisor, for his many suggestions during this research. I owe to him an enormous debt of gratitude for his tireless support throughout these last years. His guidance and broad perspective has always guided me to a right path. I am very fortunate, very proud, and very honored to be Awono's student.

I am thankful to Professor Gabriel Nguetseng who expressed his interest in my work in its early stages. He has always encouraged me and has accepted to review my work and chair the thesis committee. His careful reading of the manuscript and insightful comments and suggestions help me improve significantly this work. I am also thankful to Professor Abdelghani Bellouquid who has accepted to review my work and participate to my thesis committee. His helpful suggestions have improved this work enormously.

I am grateful to Professor David Bekollé, Professor Nicolas Andjiga and Professor François Tsopnang who have accepted to be members of my committee despite their extremely busy schedules.

I would like to acknowledge Professor Norman J. McCormick and Professor Edward W. Larsen for graciously providing me with some of their reprints which have been of great help in writing this thesis.

This research was carried out, at Ecole National Supérieure Polytechnique of the University of Yaoundé I. I wish to thank friends, school faculty and staff for making my time there a great experience. I also thank the faculty and staff of the Department of Mathematics of the Faculty of Science.

I wish to acknowledge partial support of this research by the African Millennium Mathematical Science Initiative (AMMSI) through a postgraduate scholarship award. I express my gratitude to Professor Bitjong Ndombol who made it possible.

My deepest gratitude goes to all my family for their love, constant support and encouragement during my studies. Special thanks go to my brothers Tchoupou Jean-Claude and Egoko Augustin for all what they have done for me. I extend my thanks to my friends from here and abroad who helped me in hard times and shared the good times with me.

Finally, I thank my wife Jane Yuego for her love, patience and encouragements. She has been very supportive through the difficult and enjoyable times during the last years of this thesis.

Abstract

This thesis focuses on iterative methods for the treatment of the steady state neutron transport equation in slab geometry, bounded convex domain of $\mathbb{R}^n$ $(n = 2, 3)$ and in 1-D spherical geometry. We introduce a generic Alternate Direction Implicit (ADI)-like iterative method based on positive definite and m-accretive splitting (PAS) for linear operator equations with operators admitting such splitting. This method converges unconditionally and its SOR acceleration yields convergence results similar to those obtained in presence of finite dimensional systems with matrices possessing the *Young property A*. The proposed methods are illustrated by a numerical example in which an integro-differential problem of transport theory is considered. In the particular case where the positive definite part of the linear equation operator is self-adjoint, an upper bound for the contraction factor of the iterative method, which depends solely on the spectrum of the self-adjoint part is derived. As such, this method has been successfully applied to the neutron transport equation in slab and 2-D cartesian geometry and in 1-D spherical geometry. The self-adjoint and m-accretive splitting leads to a fixed point problem where the operator is a 2 by 2 matrix of operators. An infinite dimensional adaptation of minimal residual and preconditioned minimal residual algorithms using Gauss-Seidel, symmetric Gauss-Seidel and polynomial preconditioning are then applied to solve the matrix operator equation. Theoretical analysis shows that the methods converge unconditionally and upper bounds of the rate of residual decreasing which depend solely on the spectrum of the self-adjoint part of the operator are derived. The convergence of theses solvers is illustrated numerically on a sample neutron transport problem in 2-D geometry. Various test cases, including pure scattering and optically thick domains are considered.

Keywords: Neutron Transport, Iterative Methods, ADI, Self-Adjoint, $m-$Accretive, Operator Splitting, SOR, Minres, Preconditioning, Numerical Results.

Résumé

Cette thèse est consacrée aux méthodes itératives pour la résolution des équations monocinétiques du transport des neutrons. Nous introduisons une méthode itérative générique de type ADI (*Alternate Direction Implicit*) basée sur une décomposition définie positive et $m-$accretive, pour la résolution des équations linéaires dont les opérateurs admettent une telle décomposition. L'analyse théorique de cette méthode montre qu'elle converge inconditionnellement vers la solution de l'équation considérée et l'accélération de cette methode par la méthode des rélaxations successives donne des résultats similaires à ceux des systèmes d'équations linéaires dont les matrices possèdent la *propriété A de Young*. La méthode proposée est illustrée par des exemples numériques dans lesquels on considère une équation intégro-différentielle de la théorie du transport. Dans le cas particulier où la partie définie positive de l'opérateur de l'équation linéaire est de plus auto-adjointe, une majoration du facteur de contraction de la méthode itérative est obtenue. Une analyse de la version incomplète de la méthode est présentée. Ainsi, la méthode a été appliquée aux problèmes du transport des neutrons en géométrie plane, en dimension deux d'espace et en géométrie sphérique 1-D. Les résultats obtenus montrent l'efficacité de la méthode pour ces problèmes. La méthode de décomposition auto-adjointe et $m-$accretive mentionnée ci-dessus conduit à un problème équivalent du point fixe où l'opérateur est une matrice 2x2 d'opérateurs. La méthode du résidu minimal ainsi que ses versions préconditionnées par des préconditionneurs de type Gauss-Seidel et polynomial sont appliquées pour la résolution de ce problème. L'analyse théorique montre la convergence de ces méthodes. Une majoration du taux de décroissance du résidu dépendant uniquement du spectre de la partie auto-adjointe de l'opérateur du départ est obtenue pour chacune de ces méthodes. La convergence de ces méthodes est numériquement illustrée sur des exemples dans plusieurs types de domaines en dimension deux d'espace.

Mots Clés: Equation du Transport, Méthodes Itératives, Méthodes ADI , auto-adjoint, $m-$Accretive, Décomposition d'Opérateur, SOR, Minres, Preconditionnement, Results Numériques.

Contents

List of Tables

List of Figures

List of Publications

Parts of this thesis have been published as:

1. **Awono Onana** and **J. Tagoudjeu**: "A Preconditioned Minimal Residual Solver for a Class of Linear Operator Equations", *Computational Methods in Applied Mathematics, Vol. 10, No. 2, pp. 119–136 (2010)*

2. **Awono Onana** and **J. Tagoudjeu**: "A Minimal Residual Iterative Solver for Neutron Transport Equation", *Int. J. Contemp. Math. Sci., Vol. 4, No. 34, pp. 1671-1684 (2009).*

3. **Awono Onana** and **J. Tagoudjeu**: "A Splitting Iterative Method for Solving the Neutron Transport equation", *Mathematical Modelling and Analysis, Vol. 14, No. 3, pp. 271-289 (2009)*

4. **Awono Onana** and **J. Tagoudjeu**: "Iterative Methods for a Class of Linear Operator Equations", *Int. J. Contemp. Math. Sci., Vol. 4, No. 12, pp. 549-564 (2009).*

5. **Awono Onana** and **J. Tagoudjeu**: "A SOR acceleration of Self-Adjoint and m-Accretive Splitting Iterative Solver for 2-D Neutron Transport Equation", *Math. Model. Nat. Phenom., Vol. 5, No. 7, pp. 60-66 (2010)*

6. **Awono Onana** and **J. Tagoudjeu**: " A self-adjoint m-accretive splitting iterative method for the solution of neutron transport equation in 1-D spherical geometry", *Proceeding of 9th African Conference on Research in Computer Science and Applied Mathematics - CARI-09 (Eds. E. Badouel, A. Sbihi, M.K. Assogba), pp 331-338, (2008)*;

7. **Awono Onana** and **J. Tagoudjeu**: "A SOR acceleration of Self-Adjoint and m-Accretive Splitting Iterative Solver for 2-D Neutron Transport Equation", *Proceeding of the 9th International Conference JANO'9, Mohammedia-Morocco, (2008), pp 318-321.*

General Introduction

Overview and Motivation

Transport equations are mathematical models describing the transport of particles, energy, momentum or any transportable quantity. Initially Established by Ludwig Boltzmann more than a century ago in a study in connection with the kinetic theory of gas, the transport equations are ubiquitous in physics and in engineering. They model various phenomena in various domains such as nuclear reactor design, radiation transfer, meteorology, biology, radiotherapy, tomography, particle transport, stellar and planetary radiation, epidemiology, vehicular traffic and many others. The Boltzmann transport equations are nonlinear integro-differential equations that describe the behavior of the statistical distribution of particles in a given media, using seven independent variables: 3 in space, 2 in angle, 1 in energy or frequency and 1 in time. In the case of neutral particles, these equations become linear. The neutron transport equation is a particular generic case. In many situations, the solution of the neutron transport equation is a rapidly changing function of the spatial, angular and energy variables. Moreover, the neutron transport equation behaves like totaly different equation types from a physical situation to another. It behaves like a hyperbolic wave equation in void-like regions, in scattering dominant optically thick regions it behaves like elliptic equation for steady state case and parabolic equation for time-dependent case.

Due to their multidimensionality, the asymmetry of their operators, the lack of smoothness of their solutions and many other singularities, transport equations are very arduous to solve. Therefore, their mathematical and numerical complexities continue to be subject of intense scientific attention. In this connection, there is need of original ideas and methods on the techniques to be implemented for the solution of the transport equations. Considerable efforts have been devoted this last years on the computational techniques for the numerical approximation of the solution of the transport equations.

There are in general two classes of computational methods for the numerical treatment of the neutron transport equation (see [47] and the references therein): the stochastic Monte Carlo methods and the deterministic methods. Additionally, hybrid methods coupling stochastic and deterministic approaches can be applied. Each approach has its strengths and weaknesses.

The principle underlying the Monte Carlo methods is to ignore the mathematical description of the transport problem, and to directly simulate a large number of particle histories [47]. The Monte Carlo methods use the basic concept of following the paths of particle packages by randomly selecting the new directions and energies of the particles, to estimate average behavior of particle in phase-space. They work in principle for any problem. They are suitable for solving transport equations in media where the mean free paths are not very small [74]. There are no discretization errors in Monte carlo simulation, but statistical errors occur, due to the fact that the simulation ends after N histories have been processed [47]. Unfortunately this method is very time-consuming, especially in three dimensions, because the error of the results decreases very slowly [69].

In deterministic approaches, the principle is to ignore the random aspects of individual particle histories and solve the transport problems, by converting these problems into large system of algebraic equations and solving the resulting system of algebraic equations [47]. The first step of deterministic methods consists in discretizing the transport equation with respect to each of its variables : The energy variable is often discretized by multigroup approximation, in which the energy range is divided into energy groups and the interaction cross sections are approximated by histograms in energy, each histogram having one value within each energy group [49, 34]. This yields the multigroup time-dependent or time-independent according to the equation initially considered. The treatment of the time-dependent transport equation can be done by using varieties of methods such as finite difference and variational methods [2]. Finite-differencing the derivative in time is the widely used approach. The energy and time discretization lead to a coupled system of steady state single energy equations which only depend on the spatial and the angular variables. The angular discretization is often accomplished by the integral method, discrete ordinates method (S_N) and the expansion of the angular flux in terms of angular basis functions such as spherical harmonics method (P_N), Walsh functions, wavelet functions and others (see [49, 34, 27, 26, 28, 78] and the references therein). The finite difference methods, finite element methods, nodal methods and the method of characteristics are

usually used for the spatial discretization (see [2, 3, 4, 18, 19, 49, 48, 29, 34, 23, 61, 60]). The second step in deterministic approaches consists in solving the algebraic system of equations resulting from the discretization of the transport problem. Due to the number of independent variables of the transport problem, this system is very large and thus difficult to invert directly. The solution strategy for solving the resulting system of equations have then focussed on iterative methods [47].

Literature Review on Iterative Methods

Iterative methods are widely used for solving linear operator equations (see [1, 10, 72, 43, 45, 68, 39, 54, 65] and the reference therein). The GMRES algorithm for linear equations with bounded operators in separable Hilbert space has been study in [39]. It was shown that the results of the finite dimensional case can be generalized in the continuous case if the operator is algebraic [39]. Recently, some new iterative methods for solving linear operator equations with bounded [54] and unbounded [68] operators have been introduced and analyzed. These methods make use of the adjoint operator in the transformation of the initial equation. For the particular case of neutron transport equation, there is extensive use of iterative methods for the continuous and the discrete problems (see [5, 6, 7, 34, 30, 56, 58, 66, 67, 77, 79, 85, 84] and the references therein). The standard method is the source iteration method based on a decoupling between the differential and integral parts of the transport operator. This method becomes extremely slow in the critical case (optically thick and scattering dominant regions). Several acceleration techniques of the convergence of the source iteration method such as Diffusion Synthetic Acceleration (DSA) [5, 84], Transport Synthetic Acceleration (TSA) [5], Coarse Mesh Rebalance (CMR) [88], Quasi-Diffusion acceleration [87] and multigrid algorithms have been introduced and studied [30, 56, 5, 46, 63]. Alternative methods to the source iteration approach are the Krylov subspace iteration methods such as Conjugate Gradirnt (CG), Generalized Minimal Residual (GMRES), Bi-conjugate Gradient Stabilized (BiCGSTAB) and their preconditioned versions [5, 47, 66]. The Distribution Iteration (DI) methods based on reducing the global transport equation into coupled-cell partial current that can be solved directly [36], have been applied. The angle space distribution iteration method which combines a non-linear, high angular-resolution flux approximation within individual spatial cells with a coarse angular-resolution flux approximation that couples all cells in a

spatial mesh, has proved its efficiency for slab geometry problems [83]. In [62], a new iterative method based on the idea of dividing the transport solution into its particular and homogeneous components was successfully implemented in slab geometry with isotropic scattering and one energy group. Based on the natural splitting of the integral part of transport operator, other methods such as Jacobi, Gauss-Seidel [79] and Successive over-relaxation (SOR) iteration have been successfully applied to transport problem by solving a fixed point problem derived from the source iteration method. Using the same splitting, an adaptation to the infinite dimensional case of the minimal residual iteration method (see [6, 7]) has been proposed for the solution of the transport in slab geometry, in 2-D cartesian geometry and in 1-D spherical geometry. This method has been proved to be efficient and it competes with the SOR method. Further, its preconditioned versions have been analyzed (see [80]).

Thesis Objectives and Results

In this thesis, focus is given on iterative methods for the numerical treatment of the single group steady state neutron transport equation in slab geometry, bounded convex domain of $\mathbb{R}^n$ $(n = 2, 3)$ and in 1-D spherical geometry.

We introduce a generic ADI-like iterative method (see [59]) based on positive definite and m-accretive splitting (PAS) for linear operator equations with operators admitting such splitting. As mentioned above, theoretical results show the convergence of the method and its SOR acceleration yields convergence results similar to those obtained in presence of finite dimensional systems with matrices possessing the *Young property A* (see [50, 89]). The proposed methods are illustrated by a numerical example in which an integro-differential problem of transport theory is considered. In the particular case where the positive definite part of the linear equation operator is self-adjoint, an upper bound for the contraction factor of the iterative method which depends solely on the spectrum of the self-adjoint part is derived . As such, this method has been successfully applied to the neutron transport equation in slab and 2-D cartesian geometry and in 1-D spherical geometry.

The self-adjoint and m-accretive splitting leads to a fixed point problem where the operator is a 2 by 2 matrix of operators. An infinite dimensional adaptation of minimal residual and preconditioned minimal residual algorithms using Gauss-Seidel, symmetric

Gauss-Seidel and polynomial preconditioning is then applied to solve the matrix operator equation. Theoretically, the methods are shown to be unconditionally convergent and upper bounds of the rate of residual decreasing which depend solely on the spectrum of the self-adjoint part of the operator are derived. The convergence of theses solvers is numerically illustrated on a sample neutron transport problem in 2-D geometry. Various test cases, including pure scattering and optically thick domains are considered.

Thesis Organization

The remaining of this thesis is structured as follows.

In Chapter 1, the presentation and the properties of the neutron transport equation are given. After a physical derivation of the neutron transport equation, existence and uniqueness results are presented for the time-dependent and the time-independent equations. Additionally, some alternative forms of this equation such as integral form, second order forms and the diffusion approximation, which can reduce the complexity of the initial first order integro-differential transport equations in certain circumstances are presented.

In Chapter 2, usual ways for the discretization of the transport equation in energy, time, space and direction are are briefly discussed. Some iterative approaches for solving the transport equations are presented.

In Chapter 3, focus is given on iterative methods for the numerical treatment of the single group steady state neutron transport equation in slab geometry, bounded convex domain of $\mathbb{R}^n$ $(n = 2, 3)$ and in 1-D spherical geometry. These methods are ADI-like iterative method based on positive definite and m-accretive splitting (PAS) for linear operator equations with operators admitting such splitting. we present the PAS iterative method. The convergence analysis of the method and its SOR acceleration is provided. The convergence of the proposed methods are illustrated by a numerical example in which an integro-differential problem of transport theory is considered. Next, the convergence analysis of the Self-Adjoint and m-Accretive (SAS) iterative method and its incomplete version are presented and the convergence of the method is numerically illustrated and compared with the standard Source Iteration method and multigrid method on sample problems in slab geometry and in two dimensional space. Further, we introduce and analyze an infinite dimensional adaptation of a minimal residual algorithm linked to the self-adjoint and m-Accretive Splitting. Comparative numerical results are presented for

a sample neutron transport problem in 2-D geometry. Finally the convergence of the previous minimal residual algorithm with Symmetric Gauss-Seidel and polynomial preconditioning is established and comparative numerical results are presented.

Chapter 1

The Neutron Transport Equation

This chapter is devoted to the presentation and the properties of the neutron transport equation. After a physical derivation of the neutron transport equation, existence and uniqueness results are presented for the time-dependent and the time-independent equations. Additionally, some alternative forms of this equation such as integral form, second order forms and the diffusion approximation, which can reduce the complexity of the initial first order integro-differential transport equations in certain circumstances are presented.

1.1 Introduction

The evolution of a system of particles in a given domain is characterized by the particle distribution function f, which is a positive function depending on time t, the position $\mathbf{x} \in \mathbb{R}^d$ and the velocity $\mathbf{v} \in \mathbb{R}^d$ of particles. This distribution function describes the statistical evolution of the system of particles. It must satisfy :

$$f(t, \cdot, \cdot) \in L^1_{loc}(\mathbb{R}^d \times \mathbb{R}^d), \tag{1}$$

where $L^1_{loc}(\mathbb{R}^d \times \mathbb{R}^d)$ denotes the space of functions $u : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ such that the restriction of u to any compact subset of $(\mathbb{R}^d \times \mathbb{R}^d)$ is an integrable function [25]. Therefore, the quantity $f(t, \mathbf{x}, \mathbf{v})d\mathbf{x}d\mathbf{v}$ represents the probability of finding particles in an element of volume $d\mathbf{x}d\mathbf{v}$, around the point $(\mathbf{x}, \mathbf{v})$ at time t.

The distribution function f is governed by a particle transport equation or kinetic equation. For each system of particles there exists particular types of kinetic equations. The specific form of these equations is determined by the nature of the considered system