Evaluation of Linear Solvers for Transfer Problems in Astrophysics*

Osni A. Marques[1] and Paulo B. Vasconcelos[2]

[1] Lawrence Berkeley National Laboratory,
1 Cyclotron Road, MS 50F-1650, Berkeley, CA 94720-8139, USA
oamarques@lbl.gov
[2] Faculdade de Economia da Universidade do Porto,
Rua Dr. Roberto Frias s/n, 4200-464 Porto, Portugal
pjv@fep.up.pt

Abstract. In this work we consider the numerical solution of a radiative transfer equation for modeling the emission of photons in stellar atmospheres. Mathematically, the problem is formulated in terms of a weakly singular Fredholm integral equation defined on a Banach space. Several computational approaches to solve the problem are discussed, using direct and iterative strategies that are implemented in open source packages.

1 Introduction

The emission of photons in stellar atmospheres can be modeled by a strongly coupled system of nonlinear equations. In this work we consider a restriction of the system by taking into account the temperature and pressure (see [2] and [9] for details on the corresponding model). The resulting integral equation, a radiative transfer problem, is then expressed as

$$T\varphi - z\varphi = f, \quad \varphi \in L^1(I), \quad I = [0, \tau^\star], \tag{1}$$

defined on a Banach space $L^1(I)$, where the integral operator T is defined as $(T\varphi)(\tau) = \frac{\varpi}{2}\int_0^{\tau^\star} E_1(|\tau - \tau'|)\,\varphi(\tau')\,d\tau'$. The variable τ represents the optical depth, $\tau^\star$ is the optical thickness of a stellar atmosphere, z is in the resolvent set of T and $\varpi \in \,]0,1[$ is the albedo (which is assumed to be constant in the present work). The free term f is taken to be $f(\tau) = -1$ if $0 \leq \tau \leq \tau^*/2$, and $f(\tau) = 0$ if $\tau^*/2 < \tau \leq \tau^*$. The first exponential-integral function E_1, defined by $E_1(\tau) = \int_1^\infty \frac{\exp(-\tau\mu)}{\mu} d\mu,\ \tau > 0$, has a logarithmic behavior in the neibhborhood of 0. This function is part of the exponential-integral functions, which are defined by $E_\nu(\tau) = \int_1^\infty \frac{\exp(-\tau\mu)}{\mu^\nu} d\mu,\ \nu \geq 1$. For computational purposes, these functions are evaluated according to [1].

* This work was partially supported by CMUP. CMUP is financed by FCT under programs POCTI and POSI from QCA III with FEDER and National funds.

The numerical approach used to solve this problem is based on the projection of the integral operator into a finite dimensional subspace. By evaluating the projected problem on a specific basis function we obtain a linear system of equations whose coefficient matrix is banded, sparse and nonsymmetric. In order to obtain a good accuracy it is necessary to use a large dimension for the space where the problem is projected into. One possible approach is to compute an approximate initial solution by projecting into a subspace of moderate (small) size and then iteratively refine the solution by a Newton-type method. This approach has been adopted with success in [12]. Alternatively, one can discretize the problem on a finer grid and then solve a large banded sparse algebraic linear system. In this case, depending on the dimension of the problem, we can employ either direct or iterative methods.

A large number of computational models and simulations that are carried out on nowadays high-end computers benefit from the use of advanced and promptly available software tools and libraries to achieve performance, scalability and portability. In these lines, we are interested in investigating the tradeoffs and capabilities implemented in several packages, in particular the ones that are available in the DOE Advanced CompuTational Software (ACTS) Collection [6], for the problem described above.

In the following sections, we outline the projection and matrix formulation that we use to tackle the integral operator. Next, we give a brief description of the ACTS Collection, and the tools that are pertinent to our problem. In our presentation, as well as in the final version of the paper, we will discuss numerical results and draw some conclusions.

2 Projection Phase and Matrix Formulation

Integral equations as the one described in the previous section are usually solved by discretization; for instance by projection methods into a finite dimensional subspace. The operator T is thus approximated by T_n, its projection into the finite dimensional subspace $X_n = \mathrm{Span}\{e_{n,j},\ j = 1,\dots,n\}$ (spanned by n linearly independent functions in X). In this case, we consider in X_n the basis $e_n = [e_{n,1} \ \dots \ e_{n,n}]$ of piecewise constant functions on each subinterval of $[0,\tau^*]$ determined by a grid of $n+1$ points $0 = \tau_{n,0} < \tau_{n,1} < \dots < \tau_{n,n} = \tau^*$. For $x \in X$, let $\langle x, e^*_{n,j}\rangle = e^*_{n,j}(x) = \frac{1}{h_{n,j}} \int_{\tau_{n,j-1}}^{\tau_{n,j}} x(\tau)d\tau$, where $h_{n,j} = \tau_{n,j} - \tau_{n,j-1}$. We define $T_n x = \pi_n T x = \sum_{j=1}^{n} \langle Tx, e^*_{n,j}\rangle e_{n,j}$, where $\pi_n x = \sum_{j=1}^{n} \langle x, e^*_{n,j}\rangle e_{n,j} = e_n\langle x, e^*_n\rangle$. Therefore, T_n is a bounded finite rank operator in X such that for all $x \in X$, $T_n = \sum_{j=1}^{n} \langle \cdot, \ell_{n,j}\rangle e_{n,j} = e_n\langle \cdot, \ell_n\rangle$, where $\ell_n = T^* e^*_n \in X^*$ (the adjoint space of X).

The approximate problem $(T_n - zI)\varphi_n = f$ is then solved by means of an algebraic linear system of equations $(A_n - zI)x_n = b_n$, where A_n is a non singular matrix of order n, and $A_n(i,j) = \langle e_{n,j}, \ell_{n,i}\rangle,\ b_n(i) = \langle f, \ell_{n,i}\rangle,\ x_n(j) =$

$\langle \varphi_n, \ell_{n,j} \rangle$, (see [2]). Also, $\varphi_n = \dfrac{1}{z}\left(\sum_{j=1}^{n} x_n(j) e_{n,j} - f\right)$. In order to achieve an approximate solution φ_n with good accuracy by this method it may be necessary to use a very large n. To obtain the elements of the matrix A_n we compute

$$\begin{aligned} A_n(i,j) &= \frac{\varpi}{2h_{n,i}} \int_{\tau_{n,i-1}}^{\tau_{n,i}} \int_0^{\tau^*} E_1\left(|\tau - \tau'|\right) e_{n,j}\left(\tau'\right) d\tau' d\tau \\ &= \frac{\varpi}{2h_{n,i}} \int_{\tau_{n,i-1}}^{\tau_{n,i}} \int_{\tau_{n,j-1}}^{\tau_{n,j}} E_1\left(|\tau - \tau'|\right) d\tau' d\tau \end{aligned}$$

for $i, j = 1, ..., n$. Then, using the fact that $E_3(0) = 1/2$, we obtain:

$$A_n(i,j) = \begin{cases} \frac{\varpi}{2h_{n,i}}(-E_3\left(\tau_{n,i} - \tau_{n,j}\right) + E_3\left(\tau_{n,i-1} - \tau_{n,j}\right) + \\ \quad +E_3\left(\tau_{n,i} - \tau_{n,j-1}\right) + E_3\left(\tau_{n,i-1} - \tau_{n,j-1}\right)) & \text{if } i \neq j \\ \\ \varpi(1 + \frac{1}{h_{n,i}}(-E_3\left(h_{n,i}\right) - 1)) & \text{if } i = j \end{cases} .$$

3 ACTS: Tools of the Trade

The ACTS Collection consists of a set of computational tools for the solution of common and important computational problems. The tools were developed in various different laboratories and universities and have allowed a wide spectrum of important computational problems to be solved to content [7]. We refer the reader to the ACTS Information Center [8] for details about the tools available in the Collection.

In this paper we are interested in solving equation (1) on a fine mesh. ACTS tools include the packages ScaLAPACK, SuperLU, PETSc and Trilinos. ScaLAPACK provides routines for distributed-memory message-passing MIMD architectures, in particular routines for solving systems of linear equations, least squares, eigenvalue problems and singular value problems. SuperLU is a library for the direct solution of large, sparse, nonsymmetric systems of linear equations, but that can also be applied efficiently to many symmetric systems. Working precision iterative refinement subroutines are provided for improved backward stability. PETSc provides a number of functionalities for the numerical solution of PDEs that require solving large-scale, sparse linear and nonlinear systems of equations. It includes nonlinear and linear equation solvers that employ a variety of Newton techniques and Krylov subspace methods. Trilinos is one the the last additions to ACTS. It targets the development of parallel solver algorithms and libraries within an object-oriented software framework. It contains self-contained packages, each one with its own set of requirements. One of this packages is AztecOO, which superseded the widely used package Aztec.

In Equation (1), the optical thickness of the atmosphere $\tau^\star$ depends on the frequency, typical values may be 0.001, 1, 1000 or 10^9. In [3], using an iterative refinement approach and a Beowulf class cluster computer with 20 processors, the problem was solved for $n = \tau^\star = 10^5$. To solve the local coarse grid linear system the software used was based on preconditioned Krylov subspace methods from SPARSKIT and on band block LU factorization from LAPACK. MPI was used for the global computations and communications.

In order to solve the problem for larger values of $\tau^\star$ we must use advanced software as well as high performance computers. Taking into account the characteristics of the coefficient matrix we will focus on SuperLU and PETSc, for the direct and iterative solution, respectively, of a large, sparse, nonsymmetric system of linear equations. In the final version of the paper we will present results obtained on a SUN cluster with 24 2.4 Ghz dual-processors AMD Opteron and on an IBM SP with 380 16-way computenotes.

References

1. M. Abramowitz and I.A. Stegun. *Handbook of Mathematical Functions.* Dover, New York, 1960.
2. M. Ahues, F.D. d'Almeida, A. Largillier, O. Titaud and P. Vasconcelos. An L^1 Refined Projection Approximate Solution of the Radiation Transfer Equation in Stellar Atmospheres. *J. Comput. Appl. Math.*, 140:13–26, 2002.
3. F.D. d'Almeida and P.B. Vasconcelos. A Parallel Implementation of the Atkinson Algorithm for Solving a Fredholm Equation. *Lecture Notes in Computer Science*, 2565:368–376, 2003.
4. L.S. Blackford, J. Choi, A. Cleary, E. D'Azevedo, J. Demmel, I. Dhillon, J. Dongarra, S. Hammarling, G. Henry, A. Petitet, K. Stanley, D. Walker, and R.C. Whaley. *ScaLAPACK Users' Guide.* Society for Industrial and Applied Mathematics, Philadelphia, PA, 1997.
5. J.J. Dongarra, I.S. Duff, D.C. Sorensen and H.A. van der Vorst. *Numerical Linear Algebra for High-Performance Computers.* Society for Industrial and Applied Mathematics, Philadelphia, 1998.
6. L.A. Drummond and O.A. Marques, An Overview of the Advanced CompuTational Software (ACTS) Collection. ACM TOMS, 31:282-301, 2005.
7. L.A. Drummond, V. Hernandez, O. Marques, J.E. Roman, and V. Vidal, A Survey of High-Quality Computational Libraries and their Impact in Science and Engineering Applications Collection. VECPAR 2004, *Lecture Notes in Computer Science*, Vol. 3402, Springer Verlag.
8. O.A. Marques and L.A. Drummond, The DOE ACTS Information Center. http://acts.nersc.gov.
9. B. Rutily. Multiple Scattering Theoretical and Integral Equations. *Integral Methods in Science and Engineering: Analytic and Numerical Techniques*, Birkhauser, 211-231, 2004.
10. Y. Saad. *Iterative Methods for Sparse Linear Systems.* PWS Publishing Company, 1996.
11. M. Snir, S. Otto, S. Huss-Lederman, D. Walker, J.J. Dongarra. *MPI: The Complete Reference.* The MIT Press, 1996.
12. P.B. Vasconcelos and F.D.d'Almeida, Performance evaluation of a parallel algorithm for a radiative transfer problem. to appear in *Lecture Notes in Computer Science*