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An L^1 refined projection approximate solution of the radiation transfer equation in stellar atmospheres

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Abstract

This paper deals with the numerical approximation of the solution of a weakly singular integral equation of the second kind which appears in Astrophysics. The reference space is the complex Banach space of Lebesgue integrable functions on a bounded interval whose amplitude represents the optical thickness of the atmosphere. The kernel of the integral operator is defined through the first exponential-integral function and depends on the albedo of the media. The numerical approximation is based on a sequence of piecewise constant projections along the common annihilator of the corresponding local means. In order to produce high precision solutions without solving large scale linear systems, we develop an iterative refinement technique of a low order approximation. For this scheme, parallelization of matrix computations is suitable. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Weakly singular kernel; Fredholm equation of the second kind; Projection approximation; Iterative refinement; Parallelization

1. Introduction

The system of equations dealing with radiative transfer in stellar atmospheres is strongly coupled and nonlinear. It can be stated by grouping the equations in three categories: transfer, structural and energy equations. For more specific details on the astrophysical model, see [5].

Here, we will consider the restricted problem which is obtained when the temperature and the pressure are given (or computed). Then the system of differential equations becomes linear and a linear integral formulation of the transfer problem is derived as follows:

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For each radiation frequency, the differential equation satisfied by the specific intensity of the radiation $I = I(\tau, \mu)$ in a plane parallel medium is

$$\mu \frac{\partial I}{\partial \tau}(\tau, \mu) = I(\tau, \mu) - \varphi(\tau), \quad \mu \in [-1, 1], \quad \tau \in]0, \tau_0[.$$

The variable $\tau \in]0, \tau_0[$ represents the optical depth, $\tau_0 \in]0, +\infty[$ is the optical thickness of the atmosphere, $\mu \in [-1, +1]$ is the cosine of the inclination angle from the outer normal to the plane $\tau = 0$. Depending on the frequency, typical values of τ_0 may be 0.001, 1, 1000 or 10^9 . The parameter τ_0 is adimensional but related to the spatial thickness of the medium.

The source function φ is given by

$$\varphi(\tau) = \varphi_*(\tau) + \varpi(\tau)J(\tau),$$

where φ_* describes the radiation due to internal (isotropic) sources, J is the mean intensity:

$$J(\tau) = \frac{1}{2} \int_{-1}^1 I(\tau, \mu) d\mu$$

and the albedo $\varpi(\tau) \in [0, 1]$ characterizes the scattering properties of the medium at τ .

If the boundary conditions are given by

$$I(0, \mu) = I^-(\mu) \quad \text{for } \mu \in [-1, 0[,$$

$$I(\tau_0, \mu) = I^+(\mu) \quad \text{for } \mu \in]0, 1],$$

then, for $\mu < 0$,

$$I(\tau, \mu) = I^-(\mu) \exp(\tau/\mu) - \frac{1}{\mu} \int_0^\tau \varphi(\tau') \exp[(\tau - \tau')/\mu] d\tau'$$

for $\mu > 0$,

$$I(\tau, \mu) = I^+(\mu) \exp[-(\tau_0 - \tau)/\mu] + \frac{1}{\mu} \int_\tau^{\tau_0} \varphi(\tau') \exp[(\tau - \tau')/\mu] d\tau'$$

and

$$I(\tau, 0) = \varphi(\tau).$$

Hence,

$$J(\tau) = J_\pm(\tau) + \frac{1}{2} \int_0^{\tau_0} E_1(|\tau - \tau'|) \varphi(\tau') d\tau',$$

where

$$J_\pm(\tau) = \frac{1}{2} \left(\int_{-1}^0 I^-(\mu) \exp(\tau/\mu) d\mu + \int_0^1 I^+(\mu) \exp[-(\tau_0 - \tau)/\mu] d\mu \right)$$

describes the radiation due to external sources, and E_1 is the first exponential-integral function. We recall that the exponential-integral functions are defined by

$$E_\nu(\tau) := \int_1^\infty \frac{\exp(-\tau\mu)}{\mu^\nu} d\mu, \quad \nu \geq 1,$$

and that, in a neighborhood of 0, $E_1(\tau)$ has a logarithmic behaviour:

$$\lim_{\tau \rightarrow 0^+} \frac{E_1(\tau)}{\ln \tau} = -1.$$

Also,

$$E'_{v+1} = -E_v \quad \text{and} \quad E_{v+1}(0) = \frac{1}{v} \quad \text{for } v \geq 1.$$

More details on these functions can be found in [1], where useful computational relationships are given.

In this paper we assume that the albedo ϖ is constant. Then the above transfer problem is described by the weakly singular integral equation of the second kind

$$\varphi = f + T\varphi,$$

where

$$f(\tau) := \varphi_*(\tau) + \varpi J_{\pm}(\tau),$$

$$(T\varphi)(\tau) := \frac{\varpi}{2} \int_0^{\tau_0} E_1(|\tau - \tau'|) \varphi(\tau') \, d\tau'.$$

This equation may be solved by iterative refinement methods together with projection discretization methods. In several applications f is a Lebesgue integrable function. The space $X := L^1([0, \tau_0])$ being invariant under T , we can settle the equation in this Banach space. We consider n linearly independent functions in X , $e_{n,j}$, spanning a subspace X_n of X where the integral operator will be projected thus yielding a finite rank approximation, T_n . The solution of the approximate equation $\varphi_n = f + T_n\varphi_n$, where 1 is in the resolvent set of T_n , leads to a system of n linear equations whose solution allows us to recover the approximate solution φ_n through a closed formula. The function φ_n is an approximation to φ that improves when n increases if the sequence of projections is pointwise convergent to the identity operator. Hence the required precision may lead to linear systems of considerable dimension whose condition number may increase with n . An iterative refinement scheme may overcome these problems by producing the approximate solution corresponding to a fine discretization T_m , where $m \gg n$, of T as the limit of a sequence of approximate solutions based on the solution of a linear system of low order n (n small but large enough to ensure convergence). This kind of refinement method is specially suited for parallelization, as blocks of the matrix representing T_m can be computed simultaneously, in different processors. The multiplications involving T_m can be executed in parallel also thus reducing the computing time.

2. Initial approximation

2.1. Convergence theory

We consider the complex Banach space $X := L^1([0, \tau_0])$ and the integral operator $T : X \rightarrow X$ defined by

$$(Tx)(\tau) := \int_0^{\tau_0} g(|\tau - \tau'|) x(\tau') \, d\tau', \quad x \in X, \quad \tau \in [0, \tau_0],$$

where the function g is defined by

$$g(\tau) := \frac{\varpi}{2} E_1(\tau), \quad 0 < \tau \leq \tau_0.$$

This function is weakly singular in the following sense:

$$\lim_{\tau \rightarrow 0^+} g(\tau) = +\infty, \tag{1}$$

$$g \in C^0(]0, \tau_0]) \cap X, \tag{2}$$

$$\sup_{\tau \in [0, \tau_0]} \int_0^{\tau_0} g(|\tau - \tau'|) d\tau' < +\infty \tag{3}$$

and also satisfies

$$g(\tau) > 0 \quad \text{for all } \tau \in]0, \tau_0], \tag{4}$$

$$g \text{ is a decreasing function on }]0, \tau_0]. \tag{5}$$

We have proved in [2] that these conditions imply that such an operator T is compact and that

$$\|T\|_1 = 2 \int_0^{\tau_0/2} g(\tau) d\tau = \varpi(1 - E_2(\tau_0/2)) < 1.$$

Hence the Fredholm equation of the second kind

$$\varphi = f + T\varphi \tag{6}$$

is uniquely solvable for each $f \in X$, and the solution φ depends continuously on f .

A finite rank approximation T_n of T will be constructed as follows:

Consider a family of grids \mathcal{G}_n such that

$$0 =: \tau_{n,0} < \tau_{n,1} < \dots < \tau_{n,n-1} < \tau_{n,n} := \tau_0.$$

We define

$$d_{n,i,j} := |\tau_{n,i} - \tau_{n,j}|,$$

$$h_{n,i} := d_{n,i,i-1},$$

$$h_n := \max\{h_{n,i} : i \in \llbracket 1, n \rrbracket\}.$$

For $x \in X$ we set

$$\langle x, e_{n,j}^* \rangle := \frac{1}{h_{n,j}} \int_{\tau_{n,j-1}}^{\tau_{n,j}} x(\tau') d\tau',$$

and, for $\tau \in [0, \tau_0]$,

$$e_{n,j}(\tau) := \begin{cases} 1 & \text{if } \tau \in]\tau_{n,j-1}, \tau_{n,j}], \\ 0 & \text{otherwise.} \end{cases}$$

It is clear that $\langle e_{n,j}, e_{n,i}^* \rangle = \delta_{i,j}$ for $i, j \in \llbracket 1, n \rrbracket$ and hence

$$\pi_n x := \sum_{j=1}^n \langle x, e_{n,j}^* \rangle e_{n,j}, \quad x \in X,$$

defines a bounded n -rank projection onto the subspace

$$X_n := \text{Span}\{e_{n,j} : j \in \llbracket 1, n \rrbracket\}$$

of piecewise constant functions defined a.e. in $[0, \tau_0]$. We define

$$T_n x := \pi_n T x = \sum_{j=1}^n \langle T x, e_{n,j}^* \rangle e_{n,j}.$$

Hence T_n is a bounded finite rank operator in X such that

$$T_n := \sum_{j=1}^n \langle \cdot, \ell_{n,j} \rangle e_{n,j},$$

where

$$\ell_{n,j} := T^* e_{n,j}^*.$$

In [2] we proved that,

$$\|\pi_n\|_1 = 1 \quad \text{for all } n,$$

and that

$$\lim_{n \rightarrow \infty} \|(I - \pi_n)x\|_1 = 0 \quad \text{for all } x \in X,$$

if $\lim_{n \rightarrow \infty} h_n = 0$.

Hence T_n is a uniform approximation of T if the grid is such that $\lim_{n \rightarrow \infty} h_n = 0$ and, in that case, 1 is not a spectral value of T_n for n large enough.

2.2. Numerics

The resolution for $\varphi_n \in X$ of the approximate equation

$$\varphi_n = f + T_n \varphi_n, \tag{7}$$

leads to an n -dimensional linear system. In fact, applying $\ell_{n,i}$ to each member we get the system with unknown x_n ,

$$x_n = b_n + A_n x_n, \tag{8}$$

where

$$A_n(i, j) := \langle e_{n,j}, \ell_{n,i} \rangle, \quad b_n(i) := \langle f, \ell_{n,i} \rangle, \quad x_n(j) := \langle \varphi_n, \ell_{n,j} \rangle.$$

Once this system is solved, the solution of (7) is recovered as

$$\varphi_n = f + \sum_{j=1}^n x_n(j) e_{n,j}.$$

In our case, the matrix A_n in (8) has the following entries:

For $i \neq j$,

$$A_n(i, j) = \frac{\varpi}{2h_{n,i}} [E_3(d_{n,i-1,j}) - E_3(d_{n,i-1,j-1}) + E_3(d_{n,i,j-1}) - E_3(d_{n,i,j})],$$

the diagonal coefficients of A_n being

$$A_n(j, j) = \varpi \left(1 + \frac{1}{h_{n,j}} \left[E_3(h_{n,j}) - \frac{1}{2} \right] \right).$$

As a free term f we shall consider the function

$$f(\tau) := \begin{cases} 1 & \text{if } 0 \leq \tau \leq \tau_0/2, \\ 0 & \text{if } \tau_0/2 < \tau \leq \tau_0, \end{cases}$$

which describes a sudden drop of the temperature on the $\tau = \tau_0/2$ layer of the atmosphere. Then the column b_n in (8) has entries

$$b_n(i) := \begin{cases} \frac{\varpi}{2h_{n,i}} [2h_{n,i} + E_3(\tau_0/2 - \tau_{n,i-1}) - E_3(\tau_0/2 - \tau_{n,i}) \\ \quad + E_3(\tau_{n,i-1}) - E_3(\tau_{n,i})] & \text{if } \tau_{n,i} \leq \tau_0/2, \\ \frac{\varpi}{2h_{n,i}} [E_3(\tau_{n,i} - \tau_0/2) - E_3(\tau_{n,i-1} - \tau_0/2) \\ \quad + E_3(\tau_{n,i}) - E_3(\tau_{n,i-1})] & \text{if } \tau_{n,i} > \tau_0/2. \end{cases}$$

Taking into account the discontinuity of f at $\tau_0/2$ and the possibility of a boundary layer at 0, we have built a family of quasi-uniform grids \mathcal{G}_n such that n is a multiple of 10 and

$$h_{n,i} = \begin{cases} \frac{\tau_0}{2n} & \text{if } i \in \llbracket 1, n/5 \rrbracket, \\ \frac{\tau_0}{n} & \text{if } i \in \llbracket n/5 + 1, n/2 \rrbracket, \\ \frac{\tau_0}{2n} & \text{if } i \in \llbracket n/2 + 1, 9n/10 \rrbracket, \\ \frac{4\tau_0}{n} & \text{if } i \in \llbracket 9n/10 + 1, n \rrbracket. \end{cases} \quad (9)$$

All the computations have been done with the physical parameters

$$\varpi = 0.75 \quad \text{and} \quad \tau_0 = 1000. \quad (10)$$

The relative error bound proved in [2] gives in the present case

$$\frac{\|\varphi - \varphi_n\|_1}{\|\varphi\|_1} \leq c(1 - E_2(h_n)) = O(-h_n \ln h_n). \quad (11)$$

For n large enough, the constant c in (11) is independent of n and can be estimated as follows:

$$c \leq \frac{10}{q} \left(1 + \frac{1}{q} \right) \|(T - I)^{-1}\|_1, \quad (12)$$

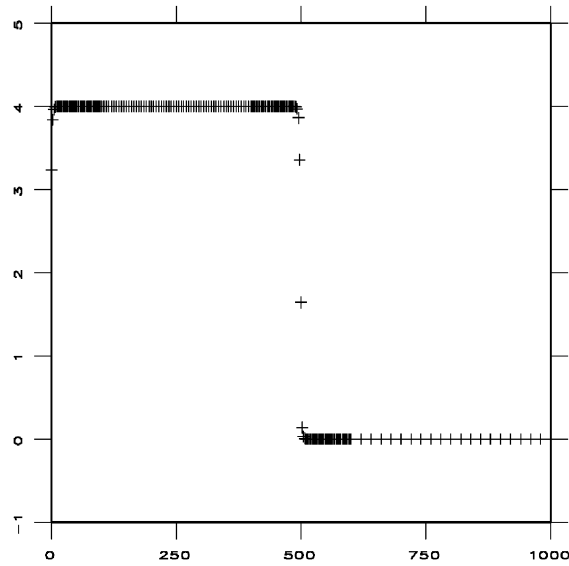


Fig. 1. φ_{200} corresponding to \mathcal{G}_{200} as in (9).

where

$$q := \inf_{\mathcal{G}_n} \frac{\min\{h_{n,i} : i \in \llbracket 1, n \rrbracket\}}{h_n} = 0.125$$

and hence

$$c \leq \frac{720}{1 - \varpi(1 - E_2(\tau_0/2))} < 2880.$$

The solution of (7) shown in Fig. 1 has been computed with the grid \mathcal{G}_{200} .

3. Iterative refinement scheme

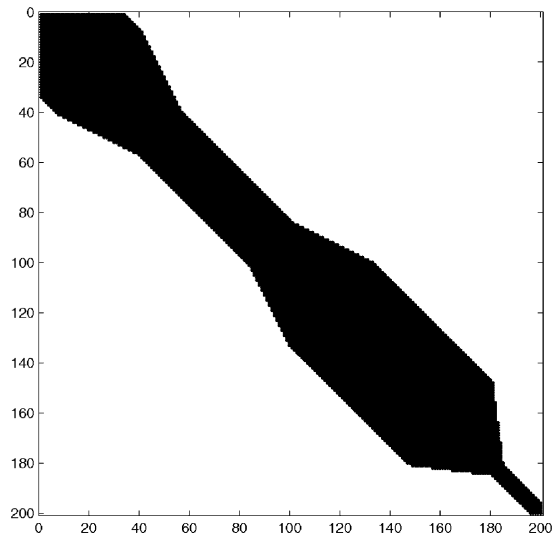
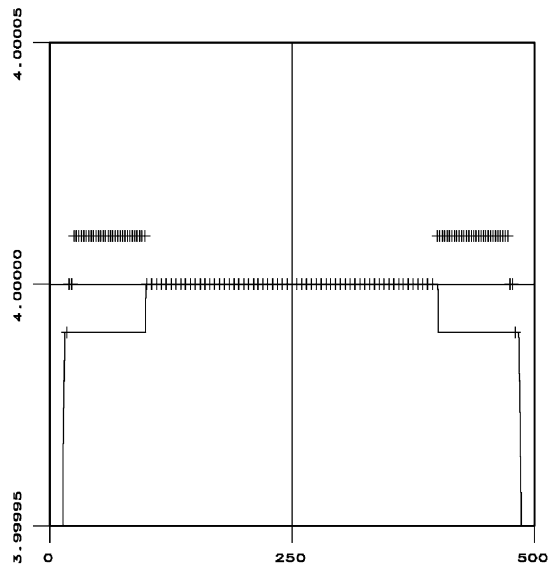
The bound (11) shows that φ_n is an approximation to φ that improves when n grows, and so the required precision may lead to linear systems of considerable dimension whose condition number may increase badly with n . The case illustrated in Fig. 1 is such that $h_n = 20$ and hence the estimate (11) indicates that

$$\frac{\|\varphi - \varphi_{200}\|_1}{\|\varphi\|_1} < 172\,800,$$

which is either a pessimistic bound or a useless one.

The profile of the matrix A_{200} is shown in Fig. 2 and the one of A_{1000} is quite similar: a non-symmetric band matrix of semi-bandwidth of about 20% of its order.

As the size of these matrices is not large we solved the problem by direct methods (LU factorization) and local differences between the solutions φ_{200} and φ_{1000} are shown in Figs. 3 and 4.

Fig. 2. Profile of matrix A_{200} .Fig. 3. Zoom of φ_{200} with crosses and φ_{1000} with a line.

Problems of this size can easily be solved by direct methods, nowadays, but for a growing size of the interval $[0, \tau_0]$, and consequently of the dimension of the matrix it will no longer be possible, either because it takes too long and/or because the matrix will not fit in the memory.

The iterative refinement methods may overcome these problems by getting the exact solution as the limit of a sequence of approximate solutions based on the solution of a linear system of dimension n (n small but large enough to ensure convergence). A simple iterative refinement formula can

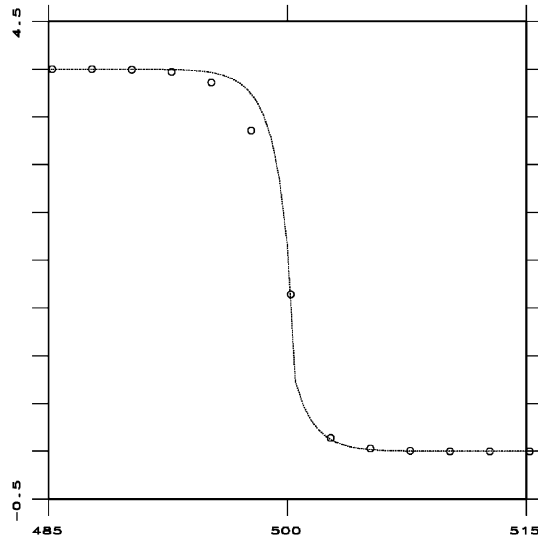


Fig. 4. Zoom of φ_{200} with circles and φ_{1000} with a dotted line.

be derived from the first iterative variant of Nyström method suggested by Atkinson [3, p. 139], properly adapted to the projection discretization we are dealing with:

$$\begin{aligned} \varphi^{(0)} &:= \varphi_n, \\ \rho^{(k)} &:= f + T\varphi^{(k)} - \varphi^{(k)}, \\ \varphi^{(k+1)} &:= \varphi^{(k)} - R_n \rho^{(k)}. \end{aligned}$$

This corresponds to a Newton-type method where the problem is stated in the form $f + T\varphi - \varphi = 0$ and the inverse of the Fréchet derivative of the left-hand side, which is nothing but the resolvent operator $R := (T - I)^{-1}$, is approximated by the approximate resolvent $R_n := (T_n - I)^{-1}$. This iteration formula converges linearly since the approximation T_n of a compact operator T obtained by a projection method yields the uniform norm convergence of R_n to R . Since the resolvent R_n satisfies

$$I + R_n = R_n T_n,$$

the Atkinson’s iteration can be rewritten as

$$\varphi^{(k+1)} := \varphi^{(0)} + R_n(T_n \varphi^{(k)} - T\varphi^{(k)}). \tag{13}$$

This formulation has the advantage of avoiding the computation of the residual $\rho^{(k)}$ which tends to zero as k tends to infinity in case of convergence. In practice the operator T is not used in this formula: a finer discretization of T , $T_m := \pi_m T \pi_m$, $m \gg n$ is used instead and its restriction to the subspace X_m is represented by an $m \times m$ matrix A_m , the coordinates of the projection of φ_m on X_m are denoted by x_m .

When the coarse grid is included in the finer one, n divides m and if we define $r := m/n$ we have

$$e_{n,i} = \sum_{k=r \times (i-1) + 1}^{r \times i} e_{m,k}.$$

Prolongation and restriction procedures are done through matrices C and D defined as follows:

$$D(i, j) = \langle e_{n,j}, \ell_{m,i} \rangle = \sum_{k=r \times (i-1)+1}^{r \times i} A_m(i, k) = \sum_{k=1}^m A_m(i, k) P(k, j)$$

for $i \in \llbracket 1, m \rrbracket$, $j \in \llbracket 1, n \rrbracket$, where

$$P(k, j) := \begin{cases} 1 & \text{if } r \times (j-1) + 1 \leq k \leq r \times j, \\ 0 & \text{otherwise.} \end{cases}$$

and so $D = A_m P$. Similarly,

$$C(i, j) := \langle e_{m,j}, \ell_{n,i} \rangle = \frac{1}{h_{n,i}} \sum_{k=r \times (i-1)+1}^{r \times i} \int_{\tau_{m,k-1}}^{\tau_{m,k}} (Te_{m,j})(\tau) d\tau$$

$$= \sum_{k=1}^m R(i, k) A_m(k, j)$$

for $i \in \llbracket 1, n \rrbracket$, $j \in \llbracket 1, m \rrbracket$, where

$$R(i, k) := \begin{cases} h_{m,k}/h_{n,i} & \text{if } r \times (i-1) + 1 \leq k \leq r \times i, \\ 0 & \text{otherwise} \end{cases}$$

and so $C = R A_m$. The numerical results obtained with this refinement formula are described in Section 5.

4. Parallel implementations

As the dimensions of the discretization matrices available until now are small and the LU factorization of the fine grid matrix is possible the first parallelizing option taken was the use of the ScaLAPACK library to parallelize that factorization. ScaLAPACK [4] is a library for parallel dense linear algebra computations over distributed memory MIMD machines. It is based on basic linear algebra subroutines (BLAS) and the LAPACK library for local computations, on PBLAS for the global addressing through call to BLAS and on basic linear algebra communication subroutines (BLACS) for the communications. Its implementation is adapted to the computation platform to be used, in our case, a cluster of 4 DEC ALPHA workstations connected by a Gigaswitch, and with parallel virtual machine (PVM) a software for communications in a distributed memory machine. ScaLAPACK has both general dense and band matrix storage structures. For dense matrices it uses a 2D block cyclic data distribution to guarantee a good load balance of the calculations. For narrow band matrices one-dimensional block column distribution is enough to achieve a good load balance and that is the distribution strategy that was used to parallelize Atkinson's algorithm (see Fig. 5). For this we assign to each of the P processors a block of NB contiguous columns of matrices A_m and C, and a block of NB contiguous rows of matrix D and vector x_m . For simplicity, in Fig. 5, $NB = n$ and matrix A_n and vector x_n can either be assigned to another processor or distributed in the same manner as A_m . Processors are supposed to be in a $1 \times P$ grid.

In Fig. 6 we describe the parallel algorithm in a Master/Slave paradigm for simplicity of the description but it can easily be programmed in a single program multiple data (SPMD) fashion too.

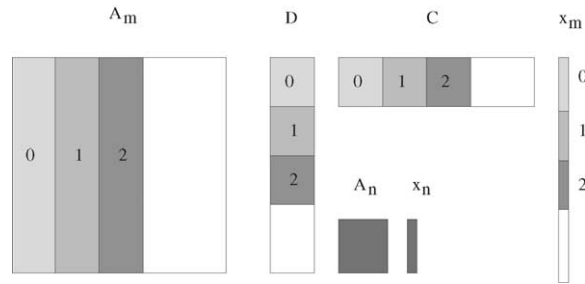


Fig. 5. One-dimensional block column distribution for band matrices.

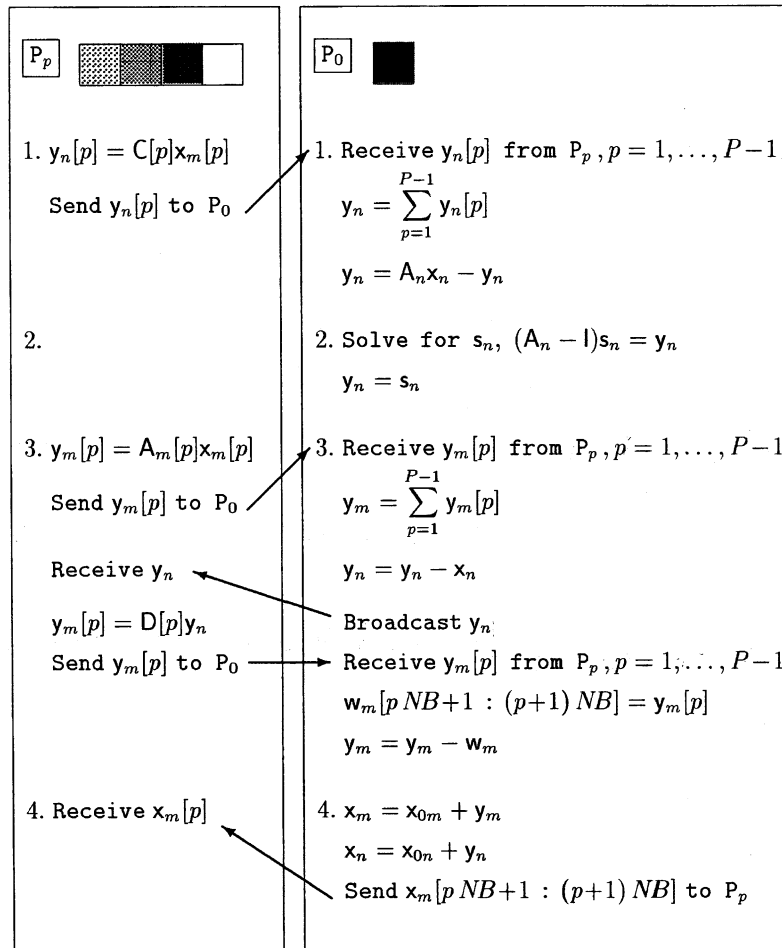


Fig. 6. Parallel algorithm for the Atkinson's method.

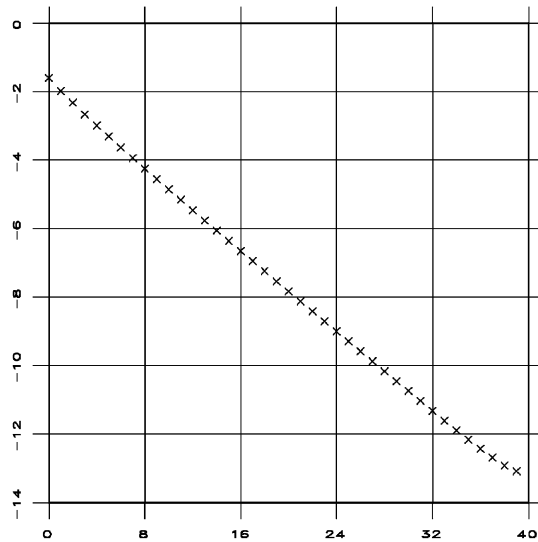


Fig. 7. Graph of $k \mapsto \log_{10} \left(\frac{\|x_m^{(k)} - b_m - A_m x_m^{(k)}\|_1}{\|x_m^{(k)}\|_1} \right)$.

5. Numerical results and conclusions

The application of the Atkinson's refinement formula to the equation (6) with a coarse grid of $n=200$ subintervals and a fine grid of $m=1000$ subintervals, in the four discretization zones described in (9) leads to a solution that coincides, within the machine precision, with the solution given by the projection method when $m=1000$, as expected.

Fig. 7 shows the evolution of the 1-norm of the relative residual of the iterative solution vector obtained by the Atkinson's formula when T is replaced by T_m . The iteration stopped when this relative residual is less than or equal to 10^{-13} . This last residual, obtained in iteration number 39 is shown in Fig. 8.

The elapsed and CPU times for the sequential computation of the solution of the problem of dimension $m=1000$, by LU factorization plus solutions of the triangular systems (LU+Triang.solve) and Atkinson's method up to a 1-norm residual less than or equal to 10^{-7} are given in Table 1. This table also includes the time for these computations with the preconditioned GMRES method (see [6]) with sparse structures. GMRES is an iterative method based on Krylov subspaces. The preconditioners used were the incomplete LU factorization of level 0 (ILU0) and the incomplete LU factorization with threshold criteria for dropping fill-ins in the factorization (ILUT).

As we can see, apart from the PGMRES+ILUT, the three options take similar times, and these are small enough to make parallelization avoidable.

PGMRES + ILU0 benefits from the fact that the band matrix is not very sparse and so the preconditioner is actually almost the solution of the linear system. ILUT gives an approximation to LU factors by dropping fill-in's smaller than 10^{-4} and so the factors are much more sparse than the matrices involved in the other iterative methods. The matrix multiplications are then faster than in the others.

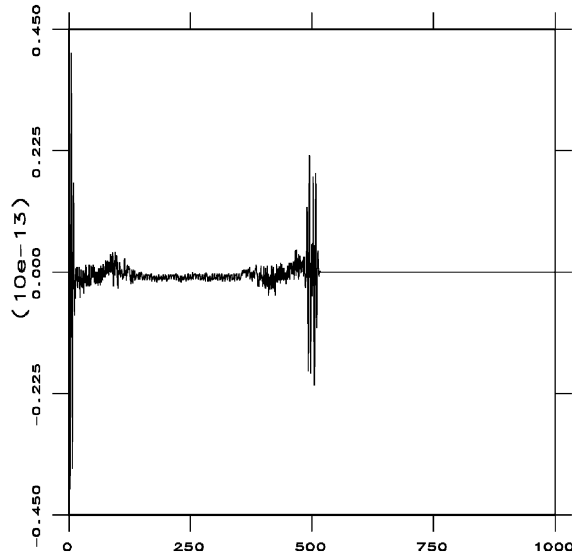


Fig. 8. Last iteration relative residual.

Table 1
Sequential results in seconds for $m = 1000$

	Elapsed time	CPU time
LU + Triang.solve	4.39	3.41
PGMRES + ILU0	3.10	2.92
PGMRES + ILUT	0.95	0.70
Atkinson's method	4.75	3.16

Table 2
Times in seconds for $m = 1000$

	Elapsed time	CPU time
LU sequential	4.39	3.41
LU parallel	12.87	1.60

The computing times are so small that the parallelization only augments the computation time since it reduces the CPU time but adds communication and synchronization time. If the ratio arithmetic computation to communication time is not large enough it is preferable not to parallelize. Table 2 shows this with the results of the parallelization of the LU factorization plus the solution of triangular systems in seconds on a cluster of four workstations DEC ALPHA when $m = 1000$.

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