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Data-sparse approximation on the computation of a weakly singular Fredholm equation: A stellar radiative transfer application

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ABSTRACT

Data-sparse representation techniques are emerging on computing approximate solutions for large scale problems involving matrices with low numerical rank. This representation provides both low memory requirements and cheap computational costs.
In this work we consider the numerical solution of a large dimensional problem resulting from a finite rank discretization of an integral radiative transfer equation in stellar atmospheres. The integral operator, defined through the first exponential-integral function, is of convolution type and weakly singular.
Hierarchically semiseparable representation of the matrix operator with low-rank blocks is built and data-sparse matrix computations can be performed with almost linear complexity. This representation of the original fully populated matrix is an algebraic multilevel structure built from a specific hierarchy of partitions of the matrix indices.
Numerical tests illustrate the benefits of this matrix technique compared to standard storage schemes, dense and sparse, in terms of computational cost as well as memory requirements.
This approach is particularly useful when a fine discretization of the integral equation is required and the resulting linear system of equations is of large dimension and numerically difficult to solve.

1. Introduction

For the solution of large dimensional linear systems direct methods, such as LU factorization followed by triangular solvers, are prohibitive requiring $\mathcal{O}(n^2)$ to store and $\mathcal{O}(n^3)$ floating point operations, where n is the order of the matrix. It is noteworthy to state that the performance of direct solver methods is largely that of the factorization. On the other hand, in the case of iterative methods, the solution of linear systems of equations scales with $\mathcal{O}(n^2)$, and the most expensive operation in terms of CPU are matrix-vector products.

To reduce storage complexity, sparsity of the problem is a desirable property. Sparse matrices store only its nonzero entries and can be represented efficiently by $\mathcal{O}(n)$ units of storage. Direct methods with these structures are complex and LU factorization reveals fill-in, which may lead to a full factored matrix. In turn, iterative methods can be competitive

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by benefiting from the cheap linear-cost matrix-vector products. However, efficient iterative procedures also require the computation of preconditioners, often obtained by direct methods such as incomplete LU factorization. Nevertheless, there are cases where the discretization of the problem, as for integral equations, does not produce sparse matrices, so dense (full) storage must be used, with the consequent blow-up in computational cost.

Data-sparse representation applies to a matrix that may be dense but allows for computations to be carried out accurately and performed in less than $\mathcal{O}(n^2)$ operations. Indeed, large scale computations require linear complexity algorithm. Data-sparse representations require only $\mathcal{O}(nk\log(n))$ units of storage, where k, the rank, is proportional to $\log(n)$, and the operations are of order $\mathcal{O}(nk^q\log(n)^q)$ for $1 \leq q \leq 3$ [11]. For instance, hierarchical matrices, $\mathcal{H}$-matrices, [10,12], build a hierarchical decomposition of the matrix in blocks, where most of the off-diagonal blocks are represented as the product of two low-rank matrices. In order to treat even larger problems, the structure of $\mathcal{H}$-matrices [11,3] can be improved to build $\mathcal{H}^2$-matrices and HSS matrices, reducing the storage complexity to $\mathcal{O}(nk)$, by replacing the low-rank structure by a hierarchical representation. They are build using hierarchical partitioning and nested bases. Furthermore these data-sparse storage schemes allow for inexpensive computation of some operations that would otherwise be prohibitive, such as LU factorization.

1.1. Previous work

Past recent work on a companion eigenvalue problem related with the integral operator of the light propagation in stellar atmospheres was conducted with the use of $\mathcal{H}$-matrices. Analytical expressions for the approximate degenerate kernels and error upper bounds for these approximations were developed in [15].

1.2. Contribution

Actual petascale (10^{15} floating point operations per second – flops) and future exascale (10^{18} flops) machines require new mathematical algorithms and codes with low arithmetic complexity and low communication complexity. The present contribution deals with the numerical approximation of an integral formulation of a radiative transfer problem in stellar atmospheres and explores the use of data-sparse structures to provide almost linear complexity both to storage and computations. Its aim is to show that the combined use of efficient numerical methods and the clever data storage provides fast answers, enabling large dimensional problems to be solved. Furthermore, the way in which the discretization process for the integral operator handles the singularity enables the use of the HSS matrix technique.

1.3. Outline

The remaining sections are organized as follows. Section 2 presents a radiative transfer problem in stellar atmospheres, formulated by a weakly singular integral operator, whose discretization leads to large matrices. Section 3 briefly presents data-sparse representations, particularly $\mathcal{H}$-matrices and HSS structures. Computational experiments are illustrated in section 4. Finally, section 5 concludes.

2. The integral radiative transfer problem

The integral equation describing the radiative transfer of energy in a static and stationary plane-parallel stellar atmosphere has the form [5]

$$S(\tau) := S_0(\tau) + \varpi(\tau)\int_0^{\tau^\star} g(|\tau-\tau'|)S(\tau)d\tau', \tag{1}$$

where S is the source function of the radiation field, S_0 represents the contribution of the internal and external sources and g is the kernel. The parameters involved are $\tau^\star < \infty$, the optical thickness of the atmosphere, $\tau \in [0, \tau^\star]$, the optical depth, and $\varpi(\tau) \in [0, 1]$, the albedo. The latter characterizes the scattering properties of the stellar plasma.

In a monochromatic and isotropic scattering process the kernel of the integral equation

$$g(\tau,\sigma) := \frac{1}{2}E_1(|\tau-\sigma|), \tag{2}$$

depends on the first exponential-integral function E_1, the first of a family functions E_ν [16] defined by

$$E_\nu(\tau) := \int_1^\infty \frac{\exp(-\tau\mu)}{\mu^\nu}d\mu, \quad \tau > 0, \nu \geq 0, \tag{3}$$

and is weakly singular in the sense given in [1].

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