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Fast linear solver for radiative transport equation with multiple right hand sides in diffuse optical tomography

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ABSTRACT

It is well known that radiative transfer equation (RTE) provides more accurate tomographic results than its diffusion approximation (DA). However, RTE-based tomographic reconstruction codes have limited applicability in practice due to their high computational cost. In this article, we propose a new efficient method for solving the RTE forward problem with multiple light sources in an all-at-once manner instead of solving it for each source separately. To this end, we introduce here a novel linear solver called block biconjugate gradient stabilized method (block BiCGStab) that makes full use of the shared information between different right hand sides to accelerate solution convergence. Two parallelized block BiCGStab methods are proposed for additional acceleration under limited threads situation. We evaluate the performance of this algorithm with numerical simulation studies involving the Delta–Eddington approximation to the scattering phase function. The results show that the single threading block RTE solver proposed here reduces computation time by a factor of 1.5–3 as compared to the traditional sequential solution method and the parallel block solver by a factor of 1.5 as compared to the traditional parallel sequential method. This block linear solver is, moreover, independent of discretization schemes and preconditioners used; thus further acceleration and higher accuracy can be expected when combined with other existing discretization schemes or preconditioners. Published by Elsevier Ltd.

1. Introduction

Diffuse optical tomography (DOT) has become a popular area of research that attracts significant and increasing attentions [\[1](#page--1-0),[2\]](#page--1-0). In DOT, low-energy near-infrared (NIR) light is used to probe biological tissue. Measurements of transmitted and reflected light intensities are used to recover a spatial

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distribution of various optical properties, for instance, absorption and scattering coefficients inside the medium under investigation. Tissues optical properties vary depending on the type and location of tissue $[3]$; thus reconstructed optical properties can provide physiologically important information such as oxy-hemoglobin $(HbO₂)$ and deoxy-hemoglobin (Hb) in tissue. DOT has applied mainly to brain imaging [\[4,5\],](#page--1-0) breast imaging [6–[9\],](#page--1-0) vascular imaging [\[10\],](#page--1-0) small animal imaging [\[11](#page--1-0),[12\]](#page--1-0) and imaging of finger joints [\[13,14\]](#page--1-0).

The DOT problem can be described in general terms as an inverse problem that is defined to find an optimal set of optical properties that minimizes a mismatch between

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predictions and measurements of light intensities. Predictions and measurements are made on the tissue surface with a known distribution of light sources. Multiple forward problems need to be solved in each inverse iteration to generate an updating direction for the target variables from the current estimate of optical properties in tissue. Traditional unconstrained approach formulates the DOT problem as [\[15\]:](#page--1-0)

$$
\min_{\mu} f(\mu) = \frac{1}{2} \sum_{k=1}^{N_S} ||QF_{\mu}^{-1}(b^{(k)}) - M^{(k)}||^2 + R(\mu)
$$
 (1)

where μ is the optical property of the imaging object and F_{μ} is the forward model of light intensity distribution defined as a function of μ , N_s is the number of sources used, $M^{(k)}$ is the measurement and $b^{(k)}$ represents the right hand side of the discretized forward model given by $A_{\Psi}(\vec{k}) = b^{(k)}$ with the kth light source, where A is the linear operator generated by the discretization of the forward light propagation model and $\psi^{(k)}$ is the vector that contains light intensities of all discretized directions and locations in the medium for the kth light source, Q denotes the measurement operator that models the light propagation from the object surface to the detectors and $R(\mu)$ is the regularization term on the optical property. The PDE-constrained approach that does not require an explicit solution of the forward model of light intensities can be formulated as follows [\[16,17\]:](#page--1-0)

$$
\min f(\mu, \psi^{(1)}, ..., \psi^{(N_S)}) = \frac{1}{2} \sum_{k=1}^{N_S} ||Q\psi^{(k)} - M^{(k)}||^2 + R(\mu)
$$

s.t. $F_{\mu}(\psi^{(k)}) = b^{(k)}$ for $k = 1, ..., N_S$ (2)

where $\psi^{(k)}$ denotes the light intensity distribution of the forward model, $R(\mu)$ is the regularization term.

The forward light propagation model plays a very important role in DOT since an improper light propagation model will lead to inaccurate reconstruction results. One frequent used approach to model photon propagation is the Monte Carlo (MC) method $[18]$. In this approach photons are considered as individual particles. Launching millions of them into a medium and tracking each one individually, one obtains a statistical approximation of the real distribution of photons in the medium. One can show that for an infinite number of photons, the so-calculated distribution of photons converges to the correct results. However, because of the substantial computational cost this approach is not very practical when used in combination with large-scale inverse solvers. Less computationally demanding are deterministic light propagation models that are based on the radiative transfer equation (RTE) and its diffusion approximation (DA). Of these two the DA model is most commonly used in tissue optics, because it is easy to implement and provides solutions very fast. However, DA-based results are often not accurate enough when considering small-tissue geometries, high-absorbing and low-scattering tissues, and void-like region. In these cases the diffusion approximation is not valid and RTE-based codes need to be employed [\[19\]](#page--1-0).

The RTE is a partial differential-integro equation in which a dependent variable (i.e., radiance in units of W/cm^2 /sr) is defined as a function of two independent variables (i.e., spatial position and angular direction). Due to strong coupling in directions, analytic solutions of RTE are not available for most cases and numerical solvers need to be implemented. Recently, several efficient RTE solvers have been developed (see [20–[23\]](#page--1-0) and their references). However, to our best knowledge, all existing algorithms are designed to solve a single right hand side. Therefore, only one source is considered. On the other hand, RTE-based DOT codes are based on multiple right hand sides, which correspond to multiple light sources illumination. Traditional methods to solve multiple right hand sides are to solve each right hand side separately or solve multiple right hand sides simultaneously in parallel [\[24,25\]](#page--1-0). However, the extensive computational power those parallel solvers required are not always available; hence we focus here on the numerical method for solving multiple right hand sides simultaneously on a single thread or limited threads (thread number is less than source number).

In order to solve multiple right hand sides efficiently, we make full use of the fact that the same coefficient matrix is shared among multiple right hand sides in the linear system resulting from multiple sources illumination:

$$
F_{\mu}(\Psi) = B \tag{3}
$$

where Ψ is the matrix of solution vectors $\psi^{(1)}$, $\psi^{(2)}$, ..., $\psi^{(N_S)}$ and *B* of right hand sides $b^{(1)}$, $b^{(2)}$, ..., $b^{(N_S)}$ pertaining to the ith light source illumination. Methods for solving such linear systems with multiple right hand sides have been extensively studied in other areas [26–[31\].](#page--1-0) The block Krylov subspace methods have been shown to be effective compared to other solvers designed for multiple right hand sides [\[32,33\].](#page--1-0) In our work, we introduce the Krylov subspace block BiCGStab algorithm [\[34\].](#page--1-0) Compared to other methods, it has the advantages of low memory requirement, simple structure and stable convergence. Besides these, it can be readily combined with other numerical techniques such as high order differencing schemes or acceleration schemes to obtain additional speedup or increased accuracy with little effort.

The remainder of the paper is organized as follows. We first review Krylov subspace and block Krylov subspace methods and introduce the block BiCGStab algorithm in Section 2. A second order finite volume scheme combined with discrete ordinates for discretization of RTE in frequency-domain is introduced in [Section 3.](#page--1-0) Then two parallelization methods of the block BiCGStab are proposed in [Section 4.](#page--1-0) Numerical results are presented in [Section 5](#page--1-0) that address the performance evaluation of the block BiCGStab algorithm. Finally our conclusions are summarized in [Section 6](#page--1-0).

2. Preconditioned block linear solver for RTE with multiple sources

2.1. Krylov subspace method and preconditioned BiCGStab algorithm

To understand the block Krylov subspace algorithm, we begin with a brief introduction of traditional Krylov subspace algorithms. Krylov subspace methods are the most widely used iterative methods so far for large-scale sparse linear systems $Ax = b$. In Krylov subspace methods, we

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