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A new box iterative method for a class of nonlinear interface problems with application in solving Poisson–Boltzmann equation

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HIGHLIGHTS

- Present a new box iterative method for a class of nonlinear interface problems.
- Obtain a new hybrid solver of Poisson–Boltzmann Equation (PBE) as application.
- Develop a new Newton-PCG-MG scheme for nonlinear boundary value problems.
- Obtain a simple series solution for Poisson ball test model with multiple charges.
- Validate the new PBE hybrid software and demonstrate its high performance.

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ABSTRACT

In this paper, a new box iterative method for solving a class of nonlinear interface problems is proposed by intermixing linear and nonlinear boundary value problems based on a special seven-overlapped-boxes partition. It is then applied to the construction of a new finite element and finite difference hybrid scheme for solving the Poisson–Boltzmann equation (PBE) — a second order nonlinear elliptic interface problem for computing electrostatics of an ionic solvated protein. Furthermore, a modified Newton minimization algorithm accelerated by a multigrid preconditioned conjugate gradient method is presented to efficiently solve each involved nonlinear boundary value problem. In addition, the analytical solution of a Poisson dielectric test model with a spherical solute region containing multiple charges is expressed in a simple series of Legendre polynomials, resulting in a new PBE test model that works for a large number of point charges. The new PBE hybrid solver is programmed as a software package, and numerically validated on the new PBE test model with 892 point charges. It is also compared to a commonly used finite difference scheme in the accuracy of computing solution and electrostatic free energy for three proteins with up to 2124 atomic charges. Numerical results on six proteins demonstrate its high performance in comparison to the PBE finite element program package reported in Xie (2014).

1. Introduction

The classical alternating Schwarz method was introduced by Schwarz in [1] for the purpose of proving the solution existence and uniqueness of a Poisson boundary value problem in a domain that can be decomposed as the union of two

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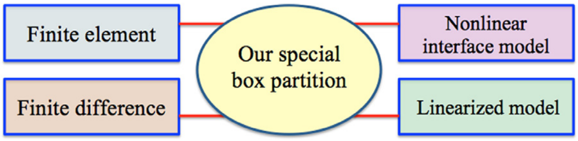

Fig. 1. Roles of our seven-overlapped-boxes partition in the development of hybrid nonlinear interface solvers.

"simpler" domains. With the development of parallel computer architectures in 1980s, it was extensively re-studied as one important numerical technique for solving various boundary value problems, known as domain decomposition methods and preconditioners [2–5]. Its essential idea is to divide a complicated problem into simple subproblems to conquer the problem. In this paper, we use this idea to construct a new box iterative method for solving a class of nonlinear interface boundary value problem, which arises frequently from steady state heat diffusion problems with two different diffusion parameters and electrostatic problems with two different permittivity parameters. As one important application, this new nonlinear iterative method is used to construct a new finite element and finite difference hybrid scheme to solve the Poisson–Boltzmann equation (PBE)—a second order nonlinear elliptic interface problem with singular source terms. PBE has been widely applied to the calculation of electrostatics for protein in ionic solvent [6–11].

The finite element method is a natural choice to deal with a flux interface condition on a complex interface (e.g., a molecular surface in the case of PBE) [12–16]. But, because of using an interface fitted unstructured mesh, its implementation requires a large amount of extra computer memory to store mesh data and the nonzero entries of coefficient matrices. A system of finite element equations defined on an unstructured mesh also becomes much less efficient to solve than a system of finite difference equations defined on a Cartesian grid mesh. In fact, a Cartesian grid mesh has simple data structures, can be generated cheaply, and can lead to standard finite difference stencils. As such, it has been widely used to develop fast linear and nonlinear iterative schemes including geometric multigrid iterative schemes [17], multigrid preconditioned Krylov subspace methods [18], Newton multigrid methods [19], and multigrid preconditioned Newton Krylov methods [20]. To take advantages of these fast iterative solvers and to reduce the cost of mesh generation, immersed boundary/interface methods in finite difference formulation [21–25], virtual node methods [26], and immersed finite element methods [27] have been developed to solve linear interface problems based on uniform Cartesian grid meshes.

We recently proposed a special seven-overlapped-boxes partition to hybridize finite element and finite difference methods in the numerical solution of a linear interface problem [28]. As illustrated in Fig. 1, we can also use this special box partition to intermix a nonlinear problem with its linearized problem in the case of solving a nonlinear interface problem. This observation motivated us to develop the new box iterative method for solving the nonlinear interface problem. That is, we can restrict the nonlinear interface problem to a much smaller subdomain, the central box, reduce it to a nonlinear boundary value problem on each neighboring box, and then approximate it as a linear boundary value problem when the solution is small enough. Moreover, different numerical techniques can be applied to different boxes to turn the box iterative method into an efficient hybrid nonlinear solver.

As one important application, in this paper, we use this box iterative method to develop a new PBE hybrid solver to reduce the computing cost of a finite element solution decomposition PBE solver, called SDPB, reported in [29]. In SDPB, the PBE solution u is constructed as a sum of three functions G, Ψ, and $\tilde{\Phi}$ with G being a given function that collects all the singularity points of u, Ψ a solution of a linear interface problem, and $\tilde{\Phi}$ a solution of a nonlinear interface problem (see (4.3)). Thus, we can apply the new box iterative method to the calculation of Ψ and $\tilde{\Phi}$ to yield the new PBE hybrid solver (see Algorithm 4.1). While SDPBS is adopted to solve each nonlinear interface problem on the central box, we construct an efficient modified Newton minimization algorithm to solve a nonlinear boundary value problem on each neighboring box based on the finite difference approach (see Section 5). In particular, the nonlinear boundary value problem is shown to be equivalent to a nonlinear variational problem with a unique minimizer (see Theorem 5.1), and each Newton equation of the modified Newton minimization algorithm is reformulated from a variational form into a linear boundary value problem (see (5.7)), making it possible to calculate each Newton search direction by a fast finite difference solver—a multigrid V-cycle preconditioned conjugate gradient method (PCG-MG) developed in [28]. Together with a line search scheme for determining the steplength of each search direction, this modified Newton method, which will be called Newton-PCG-MG for clarity, can become globally convergent in the calculation of $\tilde{\Phi}$ on each neighboring box.

To validate a PBE solver, we construct a new PBE test model (see (6.1)) by using the analytical solution of a Poisson dielectric test model with a spherical solute region D_p containing multiple charges (see (6.2)). So far, the Born ball model [30], which is a Poisson dielectric test model with one central charge only, was employed to construct a PBE test model [29,31]. The Kirkwood's dielectric sphere model [32], which is a linearized PBE test model with a spherical D_p containing multiple point charges, was used to validate the matched interface and boundary PBE solver (MIBPB) [33], but the tests were done by using only six point charges due to the expensive cost of computing the analytical solution of the Kirkwood's model, which is given as a double series of associated Legendre polynomial P_n^m (i.e., a sum from $n = 0$ to ∞ and $m = -n$ to n; see [33, (A6), (A8) and (A11)]). Although the analytical solution of the Poisson test model can be followed from the Kirkwood's model as a special case, to reduce the computing cost, we recalculate it using different techniques, such as superposition principle and rotational symmetry mapping, and express the analytical solution as a simple series of Legendre polynomials P_n (see