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Newton-Krylov Algorithm with Adaptive Error Correction For the Poisson-Boltzmann Equation

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Abstract: Discretization of the non-linear Poisson-Boltzmann Equation equation results in a system of non-linear algebraic equations with symmetric Jacobian. The Newton algorithm is the most useful tool for solving non-linear equations. It consists of solving a series of linear system of equations (Jacobian system). In this article, we are adaptively defining tolerance of the Jacobian system. We prove the convergence of our method. Numerical experiment shows that compared to the traditional method our approach can save a substantial amount of computational work. The presented algorithm can be easily incorporated into an existing molecular dynamics simulator.

1 Introduction

There has been work done on numerically solving nonlinear elliptic partial differential equations (PDEs). For example, Schwarz alternating methods [8, and references therein], multigrid methods [9; 12], pre-conditioned FFT [11]. Lets consider the following non-linear elliptic problem

$$-\operatorname{div}(\epsilon \operatorname{grad} p) + f(p, x, y) = b(x, y) \qquad \text{in} \quad \Omega, \tag{1}$$

$$p(x, y) = p^D \qquad \text{on} \quad \partial\Omega_D, \tag{2}$$

$$\mathbf{g}(x, y) = -\epsilon \operatorname{grad} p \qquad \text{on} \quad \partial\Omega_N. \tag{3}$$

The above problem is the Poisson-Boltzmann equation arising in molecular bio-physics. See the References [2; 10; 12; 13; 14; 15; 16; 20; 21]. Here Ω is a polyhedral domain in $\mathbb{R}^d$

(d = 2, 3), the source function b is assumed to be in $L^2(\Omega)$ and the medium property ϵ is uniformly positive. ϵ can be discontinuous in space. In the equations (2) and (3), $\partial\Omega_D$ and $\partial\Omega_N$ represents Dirichlet and Neumann part of the boundary. $f(p, x, y)$ represents nonlinear part of the equation. In biophysics literature the medium properties ϵ is referred as the permitivity [12; 13; 14; 15; 16; 20]. It takes the values of the appropriate dielectric constants in the different regions of the domain Ω. The equation (1), (2) and (3) models a wide variety of processes with practical applications. For example, pattern formation in biology, viscous fluid flow phenomena, chemical reactions, biomolecule electrostatics, crystal growth, etc. The Poisson-Boltzmann equation (PBE) one of the most popular continuum models for describing electrostatic interactions between molecular solutes in salty, aqueous media. The importance of the equation (1) for modelling biomolecules is well established (see [2; 10; 11; 12, and references therein]). The continuum electrostatics plays an important role in several areas of biomolecular simulation. For example, diffusional processes to determine ligand-protein and protein-protein binding kinetics, implicit solvent molecular dynamics of biomolecules, solvation and binding energy calculations to determine ligand-protein and protein-protein equilibrium binding constants, aid in rational drug design, and biomolecular titration studies. Equation (1) is solved by many molecular dynamics simulators [16; 21; 22; 23] for studying electorstatic interactions.

There are various methods for discretizing the nonlinear equation (1). For example, methods of Finite Elements, Finite Volumes and Finite Differences. Generally the equation (1) is discretized by the Finite Volume Method (see [16]). We are discretizing the equation (1) by the Finite Volume Method [1; 3; 7; 18] on quadrilateral mesh. For the convergence of the Finite Volume Method for non-linear partial differential equations, we refer to the References [3; 19, and references therein]. Discretization of the equation (1) results in a system of non-linear algebraic equations. In this research work, we are interested in computationally efficient solution of the formed non-linear system. A Finite Volume discretization of the nonlinear elliptic equation results in a system of non-linear equations

$$\mathbf{F}(\mathbf{p}) := \mathbf{A}_1\,\mathbf{p}_h + \mathbf{A}_2(\mathbf{p}_h) - \mathbf{b}_h = 0. \tag{4}$$

Here $\mathbf{F} = [F_1(\mathbf{p}), F_2(\mathbf{p}), \cdots, F_n(\mathbf{p})]^T$, $\mathbf{A}_1$ is the discrete representation of the symmetric continuous operator $-\mathrm{div}\,(\epsilon\,\mathrm{grad})$ and $\mathbf{A}_2$ is the discrete representation of the non-linear operator $f(p, x, y)$. For a Finite Volume Method, the degrees of freedom (DOF) are associated with the cell centers. Each degree of freedom or each cell in a mesh result in a discrete equation. Thus discretization of the equation (1) on a quadrilateral mesh consisting of n degrees of freedom results in $n \times 1$ nonlinear system of equations.

An outline of the article is as follows. In the Section 2, Newton-Krylov and Quasi-Newton-Krylov algorithms are presented for solving non-linear system arising from the discretization of the nonlinear elliptic problems. Section 3 presents a convergence analysis of the Quasi-Newton algorithm. Section 4 reports numerical work and Finally Section 5 concludes the article.

2 Newton-Krylov Algorithm

Linearizing the non-linear operator (4) by the Taylor series around some initial guess $\mathbf{p}_0$

$$\mathbf{F}(\mathbf{p}) = \mathbf{F}(\mathbf{p}_0) + \boldsymbol{J}(\mathbf{p}_0)\,\Delta\mathbf{p}, \tag{5}$$

where $\boldsymbol{J}$ is the Jacobian matrix and $\boldsymbol{J}(\mathbf{p}_0)$ is the value of the Jacobian at the initial guess $\mathbf{p}_0$. $\Delta\mathbf{p}$ is the difference between the vectors $\mathbf{p}$ and $\mathbf{p}_0$; i.e., $\Delta\mathbf{p} = \mathbf{p} - \mathbf{p}_0$. $\boldsymbol{J}$ is a $n \times n$ (n is the degree of freedom) linear system and is given as

$$\boldsymbol{J} := \left(\frac{\partial F_i}{\partial p_j}\right) = \begin{pmatrix} \frac{\partial F_1}{\partial p_1} & \frac{\partial F_1}{\partial F_2} & \cdots & \frac{\partial F_1}{\partial p_n} \\ \frac{\partial F_2}{\partial p_1} & \frac{\partial F_2}{\partial F_2} & \cdots & \frac{\partial F_2}{\partial p_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial F_n}{\partial p_1} & \frac{\partial F_n}{\partial p_2} & \cdots & \frac{\partial F_n}{\partial p_n} \end{pmatrix},$$

Finite Volume discretization result in a symmetric Jacobian matrix. In the Section 3, we use the symmetric nature of the Jacobian for proving convergence of the Newton method. Setting equation (5) equal to zero reads

$$\boldsymbol{J}(\mathbf{p}_0)\,\Delta\mathbf{p} = -\mathbf{F}(\mathbf{p}_0), \tag{6}$$

The above linear system is the basis for the Newton's algorithm for finding the zeros of the non-linear vector function $\mathbf{F}(\mathbf{p})$. A Newton's iteration for solving non-linear system (4) is

$$\boldsymbol{J}(\mathbf{p}_k)\,\Delta\mathbf{p}_k = -\mathbf{F}(\mathbf{p}_k), \tag{7}$$

$$\mathbf{p}_{k+1} = \mathbf{p}_k + \Delta\mathbf{p}_k \quad k = 0, 1, 2, \ldots, m. \tag{8}$$

A Newton-Krylov Algorithm is given by the Algorithm 1. In the Quasi-Newton method,

Algorithm 1: Newton-Krylov Algorithm

Mesh the domain;
Form the non-linear system : $\mathbf{F}(\mathbf{p})$;
Set the iteration counter : $k = 0$;
while $k \leq \max_{iter}$ *or* $\|\Delta\mathbf{p}\|_{L_2} \leq tol$ *or* $\|\mathbf{F}(\mathbf{p})\|_{L_2} \leq tol$ **do**
  Solve the discrete system : $\boldsymbol{J}(\mathbf{p}_k)\,\Delta\mathbf{p} = -\mathbf{F}(\mathbf{p_k})$ with a fixed tolerance;
  $\mathbf{p_{k+1}} = \mathbf{p_k} + \Delta\mathbf{p}$;
  k^{++};
end

we are solving the Jacobian equation (7) approximately. We are solving the system $\boldsymbol{J}(\mathbf{p}_k)\,\Delta\mathbf{p}_k = -\mathbf{F}(\mathbf{p}_k) + \mathbf{r}_k$ with $\|\mathbf{r}_k\|$ is chosen adaptively. We have implemented the quasi-Newton iteration in the Algorithm 2. In the Algorithms 1 and 2, $\|\cdot\|_{L_2}$ denotes the discrete L_2 norm and $\max_{iter}$ is the maximum allowed Newton's iterations. It is

Algorithm 2: Quasi-Newton-Krylov Algorithm

Mesh the domain;
Form the non-linear system : $\mathbf{F}(\mathbf{p})$;
Set the iteration counter : $k = 0$;
while $k \leq \max_{iter}$ *or* $\|\Delta\mathbf{p}\|_{L_2} \leq tol$ *or* $\|\mathbf{F}(\mathbf{p})\|_{L_2} \leq tol$ **do**
  Solve the discrete system : $\boldsymbol{J}(\mathbf{p}_k)\,\Delta\mathbf{p} = -\mathbf{F}(\mathbf{p_k})$ with a tolerance $1.0 \times 10^{-(k+1)}$;
  $\mathbf{p_{k+1}} = \mathbf{p_k} + \Delta\mathbf{p}$;
  k^{++};
end

interesting to note the stopping criteria in the Algorithm 2. We are using three stopping criteria in the Algorithm. Apart from the maximum allowed iterations. We are using L_2 norm of residual vector ($\|\mathbf{F}(\mathbf{p})\|_{L_2}$) and also L_2 norm of difference in scalar potential vector ($\|\Delta\mathbf{p}\|_{L_2}$) as stopping criteria for the Algorithm. Generally in the literature, maximum allowed iterations and the residual vector are used as stopping criteria [12; 13; 14, and references therein]. If the Jacobian is singular than the residual vector alone cannot provide a robust stopping criteria.

In the next section we shows that both the L_2 norm of the difference vector $\|\Delta\mathbf{p}\|_{L_2}$ and L_2 norm of the residual vector $\|\mathbf{F}(\mathbf{p})\|_{L_2}$ converges quadratically.

3 Convergence of the Quasi-Newton method

Let the vector function $\mathbf{F}(\mathbf{p})$ is differentiable and its Jacobain $\boldsymbol{J}(\mathbf{p})$ satisfies the following

I: - Inverse of the Jacobian is bounded. Means, there exists a number $h > 0$ such that

$$\|\boldsymbol{J}(\mathbf{p}^*)^{-1}\| < \frac{1}{h}.$$

II: - The Jacobian is Lipschitz continuous. There exists a number $\beta > 0$ such that for all $\mathbf{p}$ in the interval $\|\mathbf{p} - \mathbf{p}^*\| \leq \beta$, the Jacobian satisfies

$$\|\boldsymbol{J}(\mathbf{p}) - \boldsymbol{J}(\mathbf{p}^*)\| \leq L\,\|\mathbf{p} - \mathbf{p}^*\|.$$

Here L is the Lipschitz constant.

III: - Solution of system of equations $\boldsymbol{J}(\mathbf{p}_k)\,\Delta\mathbf{p} = -\mathbf{F}(\mathbf{p}_k) + \mathbf{r}_k$ is more accurate near convergence such that

$$\|\mathbf{r}_k\| \leq C_1\,\|\mathbf{F}(\mathbf{p}_k)\|^2 \quad \text{and} \quad \|\mathbf{r}_k\| \leq C_2\,\|\Delta\mathbf{p}_k\|^2. \tag{9}$$

Then, the Quasi-Newton-Krylov method $\mathbf{p}_n := \mathbf{p} - \boldsymbol{J}(\mathbf{p})^{-1}\,[\mathbf{F}(\mathbf{p}) + \mathbf{r}_k]$ converge as

1: - $\|\mathbf{p}_n - \mathbf{p}^*\| \leq C_3\,\|\mathbf{p}^* - \mathbf{p}\|^2$.

2: - $\|\mathbf{F}(\mathbf{p}_n)\| \leq C_4\,\|\mathbf{F}(\mathbf{p})\|^2$.

We bound inverse of the Jacobian matrix by using its symmetric nature. For a symmetric matrix $\mathbf{B}$, following are equivalent

inverse is bounded; i.e.,

$$\|\boldsymbol{B}^{-1}\| \leq \frac{1}{\Bbbk}, \tag{10}$$

and for any vector $\mathbf{v}$

$$\|\boldsymbol{B}\,\mathbf{v}\| \geq \Bbbk\,\|v\|. \tag{11}$$

Here the number $\Bbbk > 0$. In-equalities (10) and (11) are equivalent for a symmetric matrix $\boldsymbol{B}$. Now we use the Lipschitz continuity of the Jacobian, and also the equivalent expressions (10) and (11) for bounding inverse of the Jacobian.

For a vector $\mathbf{v}$, we can write

$$\|\boldsymbol{J}(\mathbf{p})\,\mathbf{v}\| = \|\boldsymbol{J}(\mathbf{p}^*) + (\boldsymbol{J}(\mathbf{p}) - \boldsymbol{J}(\mathbf{p}^*))\,\mathbf{v}\|, \tag{12}$$

by the in-equality $\|a+b\| \geq \|a\| - \|b\|$

$$\|\boldsymbol{J}(\mathbf{p})\,\mathbf{v}\| \geq \|\boldsymbol{J}(\mathbf{p}^*)\,\mathbf{v}\| - \|(\boldsymbol{J}(\mathbf{p}) - \boldsymbol{J}(\mathbf{p}^*))\,\mathbf{v}\|, \tag{13}$$

using in-equality (11) and also matrix norm in-equality $\|\boldsymbol{A}\mathbf{x}\| \leq \|\boldsymbol{A}\|\,\|\mathbf{x}\|$

$$\|\boldsymbol{J}(\mathbf{p})\,\mathbf{v}\| \geq \Bbbk\,\|\mathbf{v}\| - \|\boldsymbol{J}(\mathbf{p}) - \boldsymbol{J}(\mathbf{p}^*)\|\,\|\mathbf{v}\|, \tag{14}$$

by the Lipschitz continuity of the Jacobian

$$\begin{aligned} \|\boldsymbol{J}(\mathbf{p})\,\mathbf{v}\| &\geq \Bbbk\,\|\mathbf{v}\| - L\,\|\mathbf{p} - \mathbf{p}^*\|\,\|\mathbf{v}\| && (15)\\ &\geq [\Bbbk - L\,\|\mathbf{p} - \mathbf{p}^*\|]\;\|\mathbf{v}\|, && (16) \end{aligned}$$

now using the in-equality (10), inverse of the Jacobian is bounded as

$$\|\boldsymbol{J}(\mathbf{p})^{-1}\| \leq \left(\frac{1}{\Bbbk - L\,\|\mathbf{p} - \mathbf{p}^*\|}\right). \tag{17}$$

The fundamental theorem of calculus asserts that there is $t \in [0,1]$ such that

$$\mathbf{F}(\mathbf{z}) - \mathbf{F}(\mathbf{x}) = \int_0^1 \boldsymbol{J}[\mathbf{x} + t\,(\mathbf{z} - \mathbf{x})]\,(\mathbf{z} - \mathbf{x})\,dt. \tag{18}$$

By the definition of the Quasi-Newton iteration, we have

$$\mathbf{p}_n - \mathbf{p}^* = \mathbf{p} - \boldsymbol{J}(\mathbf{p})^{-1}\,[\mathbf{F}(\mathbf{p}) + \mathbf{r}] - \mathbf{p}^*, \tag{19}$$

$$= (\mathbf{p} - \mathbf{p}^*) + \boldsymbol{J}(\mathbf{p})^{-1}\,[\mathbf{F}(\mathbf{p}^*) - \mathbf{F}(\mathbf{p})] - \boldsymbol{J}(\mathbf{p})^{-1}\,\mathbf{r}, \tag{20}$$

using equation (18)

$$\mathbf{p}_n - \mathbf{p}^* = (\mathbf{p} - \mathbf{p}^*) + \boldsymbol{J}(\mathbf{p})^{-1}\left(\int_0^1 [\boldsymbol{J}(\mathbf{p} + t\,(\mathbf{p} - \mathbf{p}^*))]\,(\mathbf{p}^* - \mathbf{p})\,dt\right) - \boldsymbol{J}(\mathbf{p})^{-1}\,\mathbf{r}, \tag{21}$$

$$= (\mathbf{p} - \mathbf{p}^*)\,\boldsymbol{J}(\mathbf{p})\,\boldsymbol{J}\,(\mathbf{p})^{-1} + \boldsymbol{J}(\mathbf{p})^{-1}\left(\int_0^1 [\boldsymbol{J}(\mathbf{p} + t\,(\mathbf{p} - \mathbf{p}^*))]\,(\mathbf{p}^* - \mathbf{p})\,dt\right) - \boldsymbol{J}(\mathbf{p})^{-1}\,\mathbf{r}, \tag{22}$$

$$= \boldsymbol{J}(\mathbf{p})^{-1}\int_0^1 [\boldsymbol{J}(\mathbf{p} + t\,(\mathbf{p}^* - \mathbf{p})) - \boldsymbol{J}(\mathbf{p})]\,(\mathbf{p}^* - \mathbf{p})\,dt - \boldsymbol{J}(\mathbf{p})^{-1}\,\mathbf{r}, \tag{23}$$

taking norm of both the sides of the above equation and using $\|x - y\| \le \|x\| + \|y\|$, $\|x\,y\| \le \|x\|\,\|y\|$, $\|\int x\| \le \int \|x\|$

$$\|\mathbf{p}_n - \mathbf{p}^*\| \le \|\boldsymbol{J}(\mathbf{p})^{-1}\|\int_0^1 \|\boldsymbol{J}(\mathbf{p} + t\,(\mathbf{p}^* - \mathbf{p})) - \boldsymbol{J}(\mathbf{p})\|\,\|\mathbf{p}^* - \mathbf{p}\|\,dt + \|\boldsymbol{J}(\mathbf{p})^{-1}\|\,\|\mathbf{r}\|, \tag{24}$$

by the Lipschitz continuity of the Jacobian; i.e., $\|\boldsymbol{J}(\mathbf{p} + t\,(\mathbf{p}^* - \mathbf{p})) - \boldsymbol{J}(\mathbf{p})\| \le L\,t\,\|\mathbf{p}^* - \mathbf{p}\|$. We get

$$\|\mathbf{p}_n - \mathbf{p}^*\| \le \|\mathbf{p}^* - \mathbf{p}\|\;\|\boldsymbol{J}(\mathbf{p})^{-1}\|\int_0^1 L\,t\,\|\mathbf{p}^* - \mathbf{p}\|\,dt + \|\boldsymbol{J}(\mathbf{p})^{-1}\|\,\|\mathbf{r}\|, \tag{25}$$

$$\le \|\mathbf{p}^* - \mathbf{p}\|^2\,\|\boldsymbol{J}(\mathbf{p})^{-1}\|\,\frac{L}{2} + \|\boldsymbol{J}(\mathbf{p})^{-1}\|\,\|\mathbf{r}\|, \tag{26}$$

since $\|\mathbf{r}\| \le C_2\,\|\mathbf{p}^* - \mathbf{p}\|^2$

$$\|\mathbf{p}_n - \mathbf{p}^*\| \le \|\mathbf{p}^* - \mathbf{p}\|^2\,\|\boldsymbol{J}(\mathbf{p})^{-1}\|\,\frac{L}{2} + C_2\,\|\boldsymbol{J}(\mathbf{p})^{-1}\|\,\|\mathbf{p}^* - \mathbf{p}\|^2, \tag{27}$$

combining above in-equality and in-equality (17)

$$\|\mathbf{p}_n - \mathbf{p}^*\| \le \|(\mathbf{p}^* - \mathbf{p})\|^2\left(\frac{L}{2.0\,[\mathbb{k} - L\,\|\mathbf{p} - \mathbf{p}^*\|]} + \frac{2.0\,C_2}{2.0\,[\mathbb{k} - L\,\|\mathbf{p} - \mathbf{p}^*\|]}\right), \tag{28}$$

or

$$\|\mathbf{p}_n - \mathbf{p}^*\| \le \|(\mathbf{p}^* - \mathbf{p})\|^2\left(\frac{L + 2.0\,C_2}{2.0\,[\mathbb{k} - L\,\|\mathbf{p} - \mathbf{p}^*\|]}\right). \tag{29}$$

For proving the second convergence result. We use multi-dimensional mean-value lemma; i.e.,

$$\|\mathbf{F}(\mathbf{x}) - \mathbf{F}(\mathbf{y}) - \boldsymbol{J}(\mathbf{y})\,(\mathbf{x}-\mathbf{y})\| \le \frac{l}{2}\,\|\mathbf{x}-\mathbf{y}\|^2. \tag{30}$$

Combining mean value lemma with the definition of the Quasi-Newton iteration $\mathbf{p_{k+1}} = \mathbf{p_k} - \boldsymbol{J}(\mathbf{p}_k)^{-1}\,(\mathbf{F}(\mathbf{p}_k) + \mathbf{r})$ reads

$$\left\|\mathbf{F}(\mathbf{p}_{k+1}) - \mathbf{F}(\mathbf{p}_k) + \boldsymbol{J}(\mathbf{p}_k)\,\left[\boldsymbol{J}(\mathbf{p}_k)^{-1}\,(\mathbf{F}(\mathbf{p}_k) + \mathbf{r})\right]\right\| \le \frac{l}{2}\,\left\|\boldsymbol{J}(p_k)^{-1}\,(\mathbf{F}(\mathbf{p}_k) + \mathbf{r})\right\|^2,$$

since $\boldsymbol{J}\,\boldsymbol{J}^{-1} = \mathbf{I}$

$$\|\mathbf{F}(\mathbf{p}_{k+1}) - \mathbf{F}(\mathbf{p}_k) + \mathbf{F}(\mathbf{p_k}) + \mathbf{r}\| \le \frac{l}{2}\,\left\|\boldsymbol{J}(p_k)^{-1}\,(\mathbf{F}(\mathbf{p}_k) + \mathbf{r})\right\|^2,$$

using $\|x+y\| \le \|x\| - \|y\|$

$$\begin{aligned}
\|\mathbf{F}(p_{k+1})\| &\le \frac{l}{2}\,\left\|\boldsymbol{J}(p_k)^{-1}\,(\mathbf{F}(\mathbf{p}_k) + \mathbf{r})\right\|^2 + \|\mathbf{r}\|, && (31)\\
&\le \frac{l}{2}\,\left[\|\boldsymbol{J}(\mathbf{p}_k)^{-1}\|^2\,\|\mathbf{F}(\mathbf{p}_k) + \mathbf{r}\|^2\right], && (32)\\
&\le \frac{l}{2}\,\left[\|\boldsymbol{J}(\mathbf{p}_k)^{-1}\|^2\,\left(\|\mathbf{F}(\mathbf{p}_k)\| + \|\mathbf{r}\|\right)^2\right], && (33)\\
&\le \frac{l}{2}\,\left[\|\boldsymbol{J}(\mathbf{p}_k)^{-1}\|^2\,\left(\|\mathbf{F}(\mathbf{p}_k)\|^2 + \|\mathbf{r}\|^2 + 2.0\,\|\mathbf{F}(\mathbf{p}_k)\|\,\mathbf{r}\right)\right], && (34)\\
&\le \frac{l}{2}\,\left[\|\boldsymbol{J}(\mathbf{p}_k)^{-1}\|^2\,\left(\|\mathbf{F}(\mathbf{p}_k)\|^2 + C_1\|\mathbf{F}(\mathbf{p}_k)\|^2 + 2.0\,C_1\,\|\mathbf{F}(\mathbf{p}_k)\|^3\right)\right], && (35)\\
&\le \frac{l}{2}\|\mathbf{F}(\mathbf{p}_k)\|^2\,\left[\|\boldsymbol{J}(\mathbf{p}_k)^{-1}\|^2\,\left(1.0 + C_1 + 2.0\,C_1\,\|\mathbf{F}(\mathbf{p}_k)\|\right)\right], && (36)
\end{aligned}$$

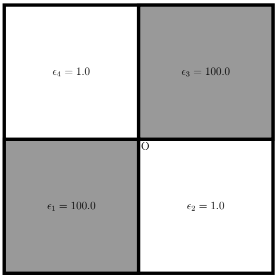
using the in-equality (17) for bounding inverse of the Jacobian

$$\|\mathbf{F}(\mathbf{p}_{k+1})\| \le \|\mathbf{F}(\mathbf{p}_k)\|^2\,\left[\frac{l}{2}\left(\frac{L}{[\![\mathbb{k} - L\,\|\mathbf{p}-\mathbf{p}^*\|]\!]}\right)^2\,\left(1.0 + C_1 + 2.0\,C_1\,\|\mathbf{F}(\mathbf{p}_k)\|\right)\right]. \tag{37}$$

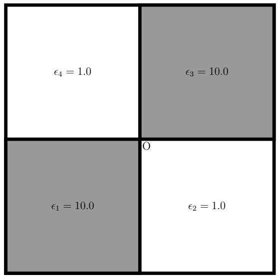
4 Numerical Experiments

We are solving the simplified Poisson Boltzmann equation (38) on $\Omega = (-1,1)\times(-1,1)$ with $k = 1.0$ [2; 10; 11; 12]. Problems with discontinuity in ϵ are of practical applications [10]. The domain Ω is divided into four equal sub-domains as shown in the Figure 1 based on the medium properties ϵ. It should be noted that elliptic problems with discontinuous coefficients can produces very ill conditioned linear systems.

$$\begin{aligned}
-\nabla\cdot(\epsilon\nabla p) + k\,\sinh(p) &= f \qquad \text{in} \quad \Omega, && (38)\\
p(x,y) &= x^3 + y^3 \qquad \text{on} \quad \partial\Omega_D. && (39)
\end{aligned}$$



(a) In the sub-domain Ω_i, $\epsilon = \epsilon_i$, $i = 1, \dots, 4$.



(b) In the sub-domain Ω_i, $\epsilon = \epsilon_i$, $i = 1, \dots, 4$.

Figure 1: Distribution of medium property ϵ in the domain $\Omega = [-1, 1] \times [-1, 1]$. Domain Ω is divided into four equal sub-domains Ω_i.

Here source function f is

$$f = 2.0\, y\, (y - 1) + 2.0\, x\, (x - 1) - 100.0\, (x - 1)\, y\, (y - 1)\, \exp\, [x\, (x - 1)\, y\, (y - 1)]$$

For solving the linear systems, we are using ILU-preconditioned the Conjugate-Gradient (CG) method. For the Newton algorithm the tolerance of the CG method is 1.0×10^{-15}. For the quasi-Newton method the tolerance of the CG method varies with the iterations k of the Algorithm 2 as follows: $1.0 \times 10^{-(k+1)}$, $k = 0, 2, \dots, 14$.

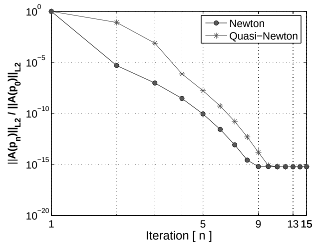
In the first computation, we assume the distribution of ϵ is given by the Figure 1(a). Thus in the first and third quadrants of the domain $\epsilon = 100.00$ and in the second and fourth quadrant of the domain $\epsilon = 1.0$. Figures 2(a), 2(b) and 4 reports the outcome of our numerical work. The Figure 2(a) presents convergence of the quasi-Newton and Newton methods. The Figure 2(b) compares convergence of the quasi-Newton and Newton methods. The Figure 4 is showing the computational complexity of the quasi-Newton and the Newton methods. It can be seen from the Figures. Even if initial iterations of the Newton-Krylov algorithm are solved approximately, the convergence rate of the algorithm remains unaffected. As was found through theoretical analysis. The Figure 4 shows that such an approximation saves a substantial amount of computational effort.

In the second comptation, we assume the distribution of ϵ is given by the Figure 1(b). Figures 4(a), 4(b) and 4 are the outcome of our numerical work. These results again suggest that initial iterates can be solved approximately without sacrificing convergence. Such an approximation saves a great amount of computational effort.

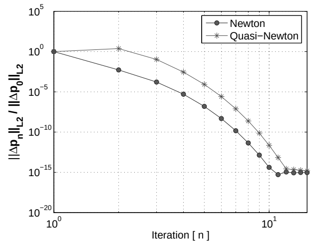
It can be noticed in the Figures 2(a), 2(b), 4(a) and 4(b), that accuracy of the solution through both approaches is same after 9 or 10 iterations.

5 Conclusions

We have presented a Quasi-Newton method for solving non-linear system of equation with symmetric Jacobian matrix. A convergence analysis of the method is also presented.



(a) Convergence of the L_2 norm of residual vector $\mathbf{A}(\mathbf{p})$.



(b) Convergence of the L_2 norm of difference vector $\Delta\mathbf{p}$.

Figure 2: Distribution of medium property ϵ is given in the Figure 1(a).

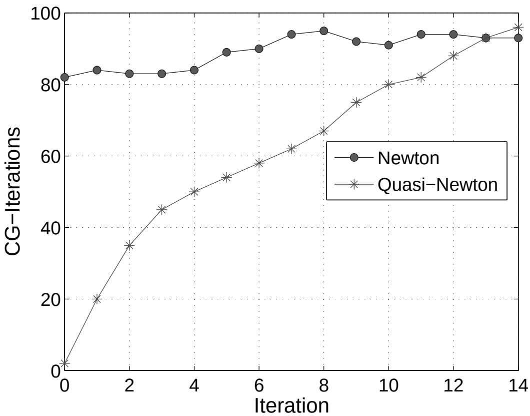
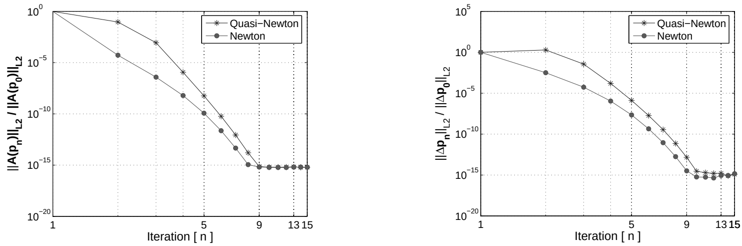


Figure 3: Distribution of medium property ϵ is given in the Figure 1(a). Computational work required by the Quasi-Newton and Newton methods.



(a) Convergence of the L_2 norm of residual vector $\mathbf{A}(\mathbf{p})$.

(b) Convergence of the L_2 norm of difference vector $\Delta\mathbf{p}$.

Figure 4: Distribution of medium property ϵ is given in the Figure 1(b).

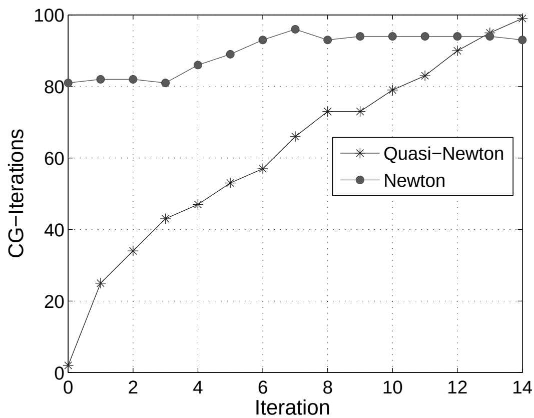


Figure 5: Distribution of medium property ϵ is given in the Figure 1(b). Computational work required by the Quasi-Newton and Newton methods.

Discretization of the non-linear Poisson-Botzmann equation results in a non-linear system with symmetric Jacobian matrix. Numerical work shows that the presented technique is computationally efficient compared to the traditional method. An efficient solution technique for Poisson-Boltzmann equation is interest to the researchers in computational chemistry, bio-physics, molecular dynamics, etc. The presented algorithm can be easily implemented in an existing simulator.

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