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SINGLE-RANK QUASI-NEWTON METHODS FOR THE SOLUTION OF NONLINEAR SEMICONDUCTOR EQUATIONS

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Abstract. This paper presents some of the author's experimental results in applying a family of iterative methods, the family of EN-like methods Eirola & Nevanlinna (1989), to equations obtained from the discretization of the nonlinear two dimentional Poisson equation occuring in semiconductor device modelling. It is shown that these iterative methods are efficient both in computation times and in storage requirements in comparison with other known methods.

Keywords: Semiconductor device, nonlinear Poisson equation, finite difference method, quasi-Newton methods, CG-like methods, GMRES, EN-method, preconditioner, numerical experiments.
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1 Introduction

Most semiconductor device models can be described by a nonlinear Poisson equation for the electrostatic potential, ψ, coupled with a system of convection-diffusion-reaction equations for the transport of charge and energy Lundstrom (1990). More specifically, ψ, satisfies an equation of the form

$$\nabla \cdot (\varepsilon \nabla \psi) = \exp(\psi - \phi_n) - \exp(\phi_p - \psi) - D,$$

The discretisation of this equation leads to a large nonlinear system of equations for the unknown potential.

The usual strategy for solving this nonlinear system is to linearise the system using, for example, Newton's method, then use efficient solvers for the obtained sparse linear systems. The most popular solvers are the conjugate gradient method CG, the generalized conjugate residual method GCR (Eisenstat et al., 1983) and the generalized minimal residual method GMRES (Saad & Schultz, 1986) which is very effective (cf. (Nachaoui, 1999)). The disadvantage of this method is that it requires substantial storage for the previous direction vectors.

Two methods that have not received much attention for solving this system are Broyden's method (Broyden, 1969) and the EN method (Eirola & Nevanlinna, 1989).The family of Broyden methods has suffered, for a long time, from a bad reputation for solving linear systems. But some efforts in Deuflhard et al. (1990) have shown that different line search strategies lead to versions that are competitive with GMRES. Since then, they have been widely used and adapted in the

resolution of non-linear systems stemming from different modeling, see for example Galperin (2017), Deuflhard (2011) and the references therein. The EN method can be related to GMRES (Vuik & Van Der Vorst, 1992).

Broyden's and EN methods, which are methods that have the remarkable merit of being both inversion-free and derivative-free methods and therefore suitable for solving non-differentiable operator equations.

In this paper we consider both families. We will see that the EN-like method often require less time than the Broyden methods, GCR and GMRES.

In the next section we present the physical model most commonly used to describe the electrostatic potentials in semiconductors. In the third section we illustrate the discretisation of the Poisson equation. In the fourth section we describe the Newton linearsition method employed to solve the discretised system of nonlinear equations. Section 5 is devoted to the iterative solvers mentioned above and their main characteristics. In the sixth section we present numerical results for a model test problem in the unit square with Dirichlet boundary conditions, on uniform grids. These results should give the reader some idea of the relative strength of the various methods. Finally in the seventh section we present numerical results and compare the methods for the solution of the system arising from the linearised Poisson equation for a specific device.

2 The Semiconductor Poisson Equation

The electric field $\mathbf{E}$ in a semiconductor device is related to the charge distribution ρ and the permittivity ε through the equation

$$\nabla \cdot (\varepsilon \mathbf{E}) = \rho. \tag{1}$$

The electric force field and the scalar potential ψ satisfy the equation

$$\mathbf{E} = -\nabla \psi. \tag{2}$$

Substituting (2) in (1) we get the Poisson equation

$$\nabla \cdot (\varepsilon \nabla \psi) = -\rho. \tag{3}$$

The total charge density is composed of the electron density n, the hole density p, and the nett concentration of impurity atoms, or the doping profile, D. Thus

$$\rho = q(p - n + D), \tag{4}$$

where q is the elementary electronic charge.

On the same way that the electrostatic potential is related to the electric field, it is also possible to relate two quantities ϕ_n and ϕ_p. These two quantities are also called the Fermi levels associated to the electrons and the holes. They are measured in Volts and so they are homogeneous to the electrostatic potential. The concentration in electrons and holes are n and p. An example of model for n and p is

$$n = n_i f\left(\tfrac{q(\psi-\phi_n)}{kT}\right), \quad p = n_i f\left(\tfrac{q(\phi_p-\psi)}{kT}\right) \tag{5}$$

where k is Boltzmann's constant and T is the absolute temperature. The function f is the exponential function for the Boltzman statistics and is given by

$$f(x) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{t}}{1 + e^{t-x}} dt$$

for the Fermi statistics. Thus the complete Poisson equation for the electric potential is

$$\nabla \cdot (\varepsilon \nabla \psi) = q(n - p - D). \tag{6}$$

After a suitable scaling of the physical variables (cf. Mock (1983)) equation (6) in dimensionless form is

$$\nabla \cdot (\varepsilon \nabla \, \psi) = f(\psi - \phi_n) - f(\phi_p - \psi) - D, \tag{7}$$

subject to appropriate mixed boundary conditions as described in Hayeck et al. (1990). Thus the system to be solved is reduced to

$$\left\{ \begin{array}{rcl} \nabla \cdot (\varepsilon \nabla \, \psi) & = & f(\psi - \phi_n) - f(\phi_p - \psi) - D, \text{ in } \Omega \\ \psi & = & \psi_d \text{ on } \Gamma_D \\ \frac{\partial \psi}{\partial n} & = & g_n \text{ on } \Gamma_N, \end{array} \right. \tag{8}$$

where Γ_D and Γ_N are two disjoint portions of $\partial\Omega$, the boundary of Ω, such that $\partial\Omega = \Gamma_D \cup \Gamma_N$.

The main difculties in solving (7) come from the high nonlinearity and large amplitude variation of the functions n and p. In the next section, we only focus on the numerical solution of the problem. For more theoretical aspects, like existence and unicity of the solution in the appropriate space, we refer to Hayeck et al. (1990) and Nachaoui & Nassif (1992).

3 Discretisation

In this part, we present on a model problem the main numerical methods that are used to solve the static problem (8). This problem has a physical meaning, it is the equilibrium problem which is the particular case when no tension is applied on the contacts of the device. In this case there is no displacement of electric charges and we have $\phi_n = 0$ and $\phi_p = 0$. The system (8) reduces to

$$\left\{ \begin{array}{rcl} \nabla \cdot (\varepsilon \nabla \, \psi) & = & f(\psi) - f(-\psi) - D, \text{ in } \Omega \\ \psi & = & \psi_d \text{ on } \Gamma_D \\ \frac{\partial \psi}{\partial n} & = & g_n \text{ on } \Gamma_N, \end{array} \right. \tag{9}$$

In the following we assume that the geometrical structure of the device can be represented by a rectangular domain Ω in two space dimensions. We discretise (9) in two space dimensions using central finite-differences on an N by M quasi-uniform mesh. The mesh is defined by two sets of data, namely $\{x_i\}_{i=1}^N$ and $\{y_j\}_{j=1}^M$ which denote the cartesian coordinates of mesh points in the x-y plane. Using the mesh, the solution to the continuous problem in the region Ω is approximated in the region Ω by the solution to a discrete problem at the NM points (x_i, y_j), $1 \le i \le N$, $1 \le j \le M$. We adopt the following notation:

$$\begin{array}{rcll} h_i & = & x_{i+1} - x_i & i = 1, \ldots, N-1 \\ k_j & = & y_{j+1} - y_j & j = 1, \ldots, M-1 \\ \psi_{i,j} & = & \psi(x_i, y_j) & i = 1, \ldots, N, \quad j = 1, \ldots, M \end{array}$$

The finite difference discretisation relates the unknown potential $\psi_{i,j}$ at each mesh point (x_i, y_j) to the potential at its four nearest neighbour meshpoints. Thus for an internal meshpoint (x_i, y_j) the discrete equation is

$$\begin{aligned} &\varepsilon\left(\frac{\psi_{i+1,j} - \psi_{i,j}}{h_i} - \frac{\psi_{i,j} - \psi_{i-1,j}}{h_{i-1}}\right)\left(\frac{k_j + k_{j-1}}{2}\right) + \varepsilon\left(\frac{\psi_{i,j+1} - \psi_{i,j}}{k_j} - \frac{\psi_{i,j} - \psi_{i,j-1}}{k_{j-1}}\right)\left(\frac{h_i + h_{i-1}}{2}\right) \\ &-(n_{i,j} - p_{i,j} - D_{i,j})\left(\frac{h_{i-1} + h_i}{2}\right)\left(\frac{k_{j-1} + k_j}{2}\right) = 0, \end{aligned} \tag{10}$$

where $n_{i,j} = f(\psi_{i,j}),\ \ p_{i,j} = f(-\psi_{i,j})$. Writing out (10) for each i and j satisfying $1 \leq i \leq N$, $1 \leq j \leq M$, we obtain a large nonlinear system of equations for the unknown potential at each mesh point.

4 Newton and Modified Newton Methods

We consider the solution of the nonlinear system of equations (10) rising from the discretisation of the Poisson equation. We can write this system of equations as $F(\mathbf{\Psi}) = \mathbf{0}$. Newton's method for nonlinear equations may be derived by assuming that an approximation $\mathbf{\Psi}^{(k)}$ to the solution $\mathbf{\Psi}^*$ is available. We put $\delta^{(k)} = \mathbf{\Psi}^* - \mathbf{\Psi}^{(k)}$, then we can write

$$F'(\mathbf{\Psi}^{(k)})\delta^{(k)} = -F(\mathbf{\Psi}^{(k)}), \qquad k = 0, 1, 2, \ldots \tag{11}$$

$F'(\mathbf{\Psi})$ denotes the Jacobian matrix. Hence presumably a better approximation to $\mathbf{\Psi}^*$ is $\mathbf{\Psi}^{(k+1)} = \mathbf{\Psi}^{(k)} + \delta^{(k)}$, where $\delta^{(k)}$ is obtained by solving the linear system of equations (11). In order to circumvent the phenomenon of Newton *overshoot* we can use an improved Newton method based on the introduction of a parameter t_k in the evaluation $\mathbf{\Psi}^{(k+1)}$, the new estimate becomes $\mathbf{\Psi}^{(k+1)} = \mathbf{\Psi}^{(k)} + t_k\delta^{(k)},\ k = 0, 1, 2, \ldots$ where the damping parameter t_k may be chosen in such a way that the iterative method reduces the norm of the nonlinear equations at each step, thus we require that $\|F(\mathbf{\Psi}^{(k+1)})\| < \|F(\mathbf{\Psi}^{(k)})\|,\ k = 0, 1, 2, \ldots$

5 A comparison of the EN- and the B-methods

In this section we consider two family of rank-one updates quasi-Newton methods for the solution of problems governed by the equation $F(u) = 0$. These methods gradually build up an approximate Jacobian matrix of F by using gradient information from the previous iterate visited by the algorithm. F is defined here by $F(u) = Au - b$, and its Jacobian equals A.

5.1 Broyden methods

The B-methods is mostly used to solve nonlinear systems but it can used to solve a linear system.

Algorithm 1 B-method
u_0, H_0 arbitrary, $r_0 = b - Au_0$

For $k = 0, 1, 2, ...$
$p_k = H_k r_k, q_k = Ap_k,$
$u_{k+1} = u_k + \alpha_k p_k, r_{k+1} = r_k - \alpha_k q_k$
Stop if $\|r_{k+1}\|$ is small enough
$H_{k+1} = H_k + \frac{(p_k - H_k q_k)}{f_k^t q_k} f_k^t$
end

where f_k needs to be chosen in such a way, that $f_k^t q_k \neq 0$. One obtains for the choice $f_k = q_k$, the so-called Broyden's bad method BBM. Obviously from the name, this variant often does not perform as well as the original Broyden's method, $f_k = H_k p_k$, which is also often called Broyden's "good" method GBM. These are the best known choices for f_k. There are, however, a few other interesting choices. For the special case of a hermitian matrix A , a hermitian update for H_k is needed, which yields the choice $f_k = p_k - H_k q_k$. The interesting aspect of this method is that it

finds an approximation H_k of the inverse of A, which is corrected during each iteration by a rank-one update in such a way that $H_{k+1}q_i = p_i, i \leq k$ for $k+1$ points $q_i = Ap_i;\ i = 0, ..., k$. Then, Broyden's method will terminate within at most n step, since the algorithm constructs a better approximation H_k to A^{-1} on each iteration, until finally $H_n = A^{-1}$, if $f_i^t q_i \neq 0,\ i = 0, ..., n_1$ (see also Luenberger (1984)). Let us now turn our attention to the second undetermined parameter, α_k. The most obvious choice for α_k is 1. One can show that for this case Broyden's method terminates within at most $2n$ steps (Gay (1979)). An other choice that produces Broyden's methods that are competitive with GMRES is (see Deuflhard et al. (1990)) $\alpha_k = \frac{f_k^t r_k}{f_k^t q_k}$.

5.2 EN-like methods

Algorithm 2 EN–method
u_0, H_0 arbitrary, $r_0 = b - Au_0$, $E_0 = I - AH_0$

For $k = 0, 1, 2, ...$
$\tilde{u}_k = H_k E_k r_k, v_k = \frac{E_k^t A\tilde{u}_k}{\|A\tilde{u}_k\|^2}$
$H_{k+1} = H_k + \tilde{u}_k v_k^t$, $E_{k+1} = I - AH_{k+1}$
$u_{k+1} = u_k + H_{k+1}r_k$, $r_{k+1} = E_{k+1}r_k$
Stop if $\|r_{k+1}\|$ is small enough
end

The EN method was first proposed by Eirola and Nevanlinna in Eirola & Nevanlinna (1989). The main idea is to improve an approximation H_k to A^{-1} via a rank-one update $\tilde{u}_k v_k^t$ on each iteration of the method while simultaneously improving an approximation u_k to the solution of the linear system. The rank-one update is chosen in such a way that the matrix $E_k = I - AH_k$, which is an indicator of the quality of H_k, is obtained by premultiplying E_{k-1} by a projector $I - cc^t$, in order to guarantee that the new approximation will not be worse than the old one. This can be achieved by choosing $v_k = E_k^t A\tilde{u}_k / \|A\tilde{u}_k\|^2$. The best choice for $\tilde{u}_k$ is $A^{-1}E_k r_k$ (where the residual r_k is defined by $r_k = b - Au_k$), which would lead to $r_{k+1} = 0$. Such a choice clearly begs the question of solving the system of linear equations, so the best available approximation of A^{-1} is used to yield $\tilde{u} = H_k E_k r_k$. The resulting algorithm is: Algorithm 2.

Recalling the definition of p_k and q_k in Algorithm 1 and taking $f_k = E_k^t A H_k E_k r_k$, we can rewrite the evaluation of H_{k+1} as in Algorithm 1. This gives arise to a scheme that more closely resembles Broyden's methods :

Algorithm 3 EN-method
u_0, H_0 arbitrary, $r_0 = b - Au_0$

For $k = 0, 1, 2, ...$
$p_k = H_k r_k, q_k = Ap_k,$
$H_{k+1} = H_k + \frac{(p_k - H_k q_k)}{f_k^t q_k} f_k^t$
$\tilde{p}_k = H_{k+1} r_k$, $\tilde{q}_k = A\tilde{p}_k,$
$u_{k+1} = u_k + \tilde{p}_k, r_{k+1} = r_k - \tilde{q}_k$
Stop if $\|r_{k+1}\|$ small enough
end

where f_k needs to be chosen in such a way, that $f_k^t q_k \neq 0$. To obtain a corresponding EN-like

method to BBM, called BEN, one only needs to replace f_k with q_k. The choice of $f_k = H_k^t p_k$ gives the corresponding EN-like method to GBM, denoted by GEN. We note that, for the EN-method the new approximation H_{k+1} to A^{-1} is used to evaluate the direction vector, while for the B-method H_k is used. This can lead to a faster convergence as it is shown in figure 1 and figure 2. To avoid the expansive explicit computation of the matrices H_k, which are generally dense, one can replace H_{k+1} by its definition to get $H_{k+1}u = H_0u + \sum_{i=0}^{k} \frac{f_i^t u}{f_i^t q_i}(p_i - H_i q_i)$. This approach has been used in Deuflhard et al. (1990) and Engleman et al. (1981) for B-method and in Eirola & Nevanlinna (1989) for the EN-method. The resulting algorithms are:

Algorithm 4 B-method
u_0, H_0 arbitrary, $r_0 = b - Au_0$,
$p_0 = H_0 r_0$, $q_0 = Ap_0$,

For $k = 0, 1, 2, ...$
$\zeta_k = f_k^t q_k$
$t_k = H_0 q_k + \sum_{i=0}^{k-1} \frac{f_i^t q_k}{\zeta_i} z_i$
$z_k = p_k - t_k$, $u_{k+1} = u_k + \alpha_k p_k$,
$r_{k+1} = r_k - \alpha_k q_k$
Stop if $\|r_{k+1}\|$ is small enough
$p_{k+1} = (1 - \alpha_k)p_k + \frac{f_k^t r_k}{\zeta_k} z_k, q_{k+1} = Ap_{k+1}$
end

Algorithm 5 EN–method
u_0, H_0 arbitrary, $r_0 = b - Au_0$,

For $k = 0, 1, 2, ...$
$p_k = H_0 r_k + \sum_{i=0}^{k-1} \frac{f_i^t r_k}{\zeta_i} z_i$
$q_k = Ap_k$, $\zeta_k = f_k^t q_k$, $t_k = r_k - q_k$
$z_k = H_0 t_k + \sum_{i=0}^{k-1} f_i^t t_k z_i$
$s_k = p_k + \frac{f_k^t r_k}{\zeta_k} z_k, u_{k+1} = u_k + s_k$,
$r_{k+1} = r_k - As_k$
Stop if $\|r_{k+1}\|$ is small enough
end

Replacing f_k with q_k in Algorithm 4, resp. in algorithm 5, yields BBM, resp. BEN. For GBM we need to determine the vectors $t_k^{(i)} = H_i q_k$ and for the GEN we need to evaluate, in addition to $t_k^{(i)}$, the vectors $p_k^{(i)} = H_i r_k$, the new efficient versions are given by

Algorithm 6 GBM
u_0, H_0 arbitrary, $r_0 = b - Au_0$,
$p_0 = H_0 r_0$, $q_0 = Ap_0, t_0 = H_0 q_0$
For $k = 0, 1, 2, ...$
$t_k^{(0)} = H_0 q_k$
$t_k^{(i)} = t_k^{(i-1)} + \frac{p_{i-1}^t t_k^{(i-1)}}{\zeta_i} z_{i-1}$, $i = 1, \cdots, k$
$\zeta_k = p_k^t t_k^{(k)}$, $z_k = p_k - t_k^{(k)}$
$u_{k+1} = u_k + \alpha_k p_k$,
$r_{k+1} = r_k - \alpha_k q_k$
Stop if $\|r_{k+1}\|$ is small enough
$p_{k+1} = (1 - \alpha_k) p_k + \frac{p_k^t p_k}{\zeta_k} z_k$,
$q_{k+1} = Ap_{k+1}$
end

Algorithm 7 GEN
u_0, H_0 arbitrary, $r_0 = b - Au_0$,

For $k = 0, 1, 2, ...$
$p_k^{(0)} = H_0 r_k$
$p_k^{(i)} = p_k^{(i-1)} + \frac{(p_{i-1}^{(i-1)})^t p_k^{(i-1)}}{\zeta_i} z_{i-1}$, $i = 1, \cdots, k$
$q_k = Ap_k^{(k)}$, $t_k^{(0)} = H_0 q_k$
$t_k^{(i)} = t_k^{(i-1)} + \frac{(p_{i-1}^{(i-1)})^t t_k^{(i-1)}}{\zeta_i} z_{i-1}$, $i = 1, \cdots, k$
$\zeta_k = (p_k^{(k)})^t t_k^{(k)}$, $z_k = p_k^{(k)} - t_k^{(k)}$
$s_k = p_k^{(k)} + \frac{(p_k^{(k)})^t p^{(k)}}{\zeta_k} z_k$,
$u_{k+1} = u_k + s_k$, $r_{k+1} = r_k - As_k$
Stop if $\|r_{k+1}\|$ is small enough
end

Taking $f_k = E_k^t E_k q_k$ and setting $\tilde{c} = E_k q_k, \tilde{u} = H_k E_k r_k$ leads to a scaling invariant version of the EN method, denoted by SEN (see Eirola & Nevanlinna (1989),Vuik & Van Der Vorst (1992)). Replacing the evaluation of $\tilde{u}$ in the EN methods with $\tilde{u} = H_k r_k$ leads to the General Conjugate Residual algorithm GCR Eisenstat et al. (1983), see Vuik & Van Der Vorst (1992) for the proof.

5.3 Preconditioning

The performance of iterative methods depends heavily on the spectral properties of the matrix A. For this reason one usually uses a so-called preconditioning matrix M such that $M^{-1}A$ has a more favorable spectrum than A. An important class of preconditioning methods is that based on incomplete LU factorisations of the matrix A, where L is a sparse lower triangular matrix. A way of obtaining this situation is to restrict the usual Gaussian elimination process to a prescribed subset J of the entries of A. The idea is that the computational and storage requirements of the factorization process will be largely reduced and solving system $LUP = Q$ will be a cheap operation typically of the order of one or a few matrix-vector multiplications. A detailed discussion can be found in Nachaoui (1999).

6 Numerical results for the model

We have applied the methods described above to solve the system $Ax = b$ where A is obtained through a standard five point finite difference discretisation of $\Delta u = f$ in $\Omega = [0,1][0,1]$ with Dirichlet boundary conditions which satisfy the solution $u(x,y) = xy + exp(xy)$. We chose two step sizes $h = 1/5$ and $h = 1/20$.

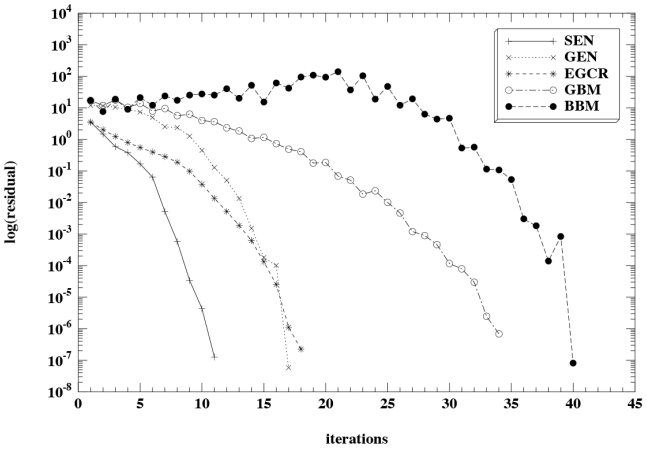

Figure 1: Residuals for the model problem with $h = 0.2$

We note from figure 1 and figure 2 that all the EN-methods are much faster than the B-methods. The SEN method gives the best performance in terms of CPU. For $h = 0.2$ the difference between GEN and EGCR is negligable; SEN is 3.6 times faster than the BBM and the slowest EN-method EGCR is about, 50% faster than GBM. For $h = 0.05$, the SEN is usually superior; the GEN is 1.44 times slower than EGCR and when we ran the problem with the BBM, the norm of the residual vector increased without bound. The slowest EN method, GEN, is about 26% faster than GBM.

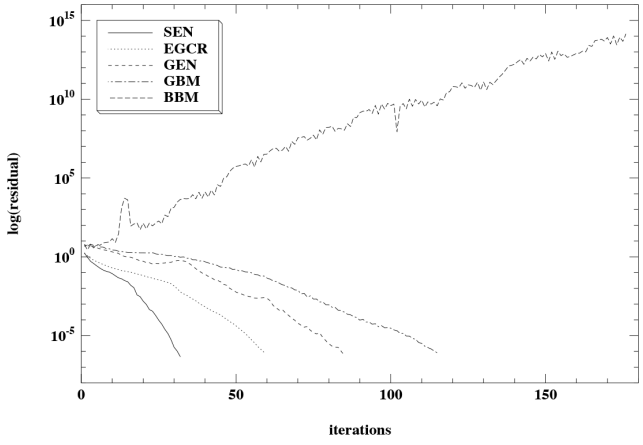

Figure 2: Residuals for the model problem with $h = 0.05$

7 Numerical Results for the Linearised Poisson Equation

We now present the results obtained for the solution of the linearised systems (3.1) arising from the nonlinear Poisson equation. We present results for the forward biased diode with

Dirichlet conditions on Ohmic contacts, i.e. source, drain and homogeneous Neumann boundary conditions elsewhere. The doping densities per cm^3 are $n = 5.5 \times 10^{17}$, $p = -5.5 \times 10^{17}$. We solve the Poisson equation for this device, on an uniform rectangular grid with step size $h = 0.05$

Table 1: Counts for B- and En-methods

	Newton_iter	Total_iter	Residual_norm
Newton-SEN	3	88	3.148E-007
Newton-GEN	3	256	7.779E-007
Newton EGCR	3	180	4.812E-008
Newton-GBM	3	345	6.587E-007
Newton-BBM	–	–	–

The iteration counts for the various B- and En-methods for this problem are given in Table 1. A convergent solution was obtained after three Newton iterations except for BBM. Again, all the EN-methods are much faster than the B-methods. The results show that the best performances were obtained by Newton-SEN; it is almost 4 times faster than Newton-GBM, about 51% faster than Newton-EGCR and about 65% faster than Newton-GEN. Due to space limitation, we have not presented results with preconditioned versions, but a more detailed discussion, including more sophisticated restarted EN-like methods and a comparison of EN-like and Broyden methods, used as nonlinear solvers will be presented in a future work.

8 Conclusion

In this paper we considered the equilibrium problem associated to semiconductor. This is the case where no tension is applied on the contacts of the device. The problem is discretized using finite difference Methods. In order to solve the resultiong discret problem, a single rank quasi-Newton method is introduced to make the solution of the original nonlinear problem easier. We compared this method with other classical methods. We have shown that the traditional iterative B-methods for solving linear equations are not competitive with the new family EN-like methods when applied to the solution of the linearised Poisson equation describing the potential in a semiconductor device.

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