

secs1d

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Contents

I	Mathematical models	2
1	Full model	2
1.1	Conservation laws	2
2	Constitutive relations	2
2.1	Currents	2
2.2	Mobilities	2
2.3	Production terms	3
3	Simplified model used for Newton's method	4
3.1	Conservation laws	4
4	Constitutive relations	4
4.1	Currents	4
4.2	Production terms	4
5	Scaling factors/adimensional parameters	5
II	Function reference	5
6	Drift-Diffusion solvers	5
6.1	secs1d_dd_gummel_map	5
6.2	Demo 1 for uncton secs1d_dd_gummel_map	6
6.3	secs1d_dd_newton	10
6.4	Demo 1 for function secs1d_dd_newton	10
7	Non-linear Poisson solver	14
7.1	secs1d_nlpoisson_newton	14
7.2	Demo 1 for function secs1d_nlpoisson_newton	14
8	Physical constants and material properties	17
8.1	secs1d_physical_constants.m	17
8.2	secs1d_silicon_material_properties.m	18

Table 1: secs1d Package Description

Name:	secs1d
Description:	A Drift-Diffusion simulator for 1d semiconductor devices
Version:	0.0.9
Release Date:	2012-03-25
Author:	Carlo de Falco
Maintainer:	Carlo de Falco
License:	GPL version 2 or later
Depends on:	octave ($\geq 3.0.0$), bim ($\geq 0.0.0$),
Autoload:	No

A Licence

19

Part I

Mathematical models

1 Full model

1.1 Conservation laws

$$\begin{cases} -\lambda^2 \operatorname{div} (\varepsilon_r \operatorname{grad} \varphi) = p - n + N_D - N_A \\ -\operatorname{div} (J_n) + R_n n = G_n \\ \operatorname{div} (J_p) + R_p p = G_p \end{cases} \quad (1)$$

2 Constitutive relations

2.1 Currents

$$\begin{cases} J_n = \mu_n (\operatorname{grad} n - n \operatorname{grad} \varphi) \\ J_p = -\mu_p (\operatorname{grad} p + p \operatorname{grad} \varphi) \end{cases} \quad (2)$$

2.2 Mobilities

$$\begin{cases} \mu_n = \frac{2\bar{\mu}_n}{1 + \sqrt{1 + 4 \left(\frac{\bar{\mu}_n |E|}{v_{sat,n}} \right)^2}}; & \bar{\mu}_n = \mu_{min,n} + \frac{\mu_{0,n} - \mu_{min,n}}{1 + \left(\frac{N_D + N_A}{N_{ref,n}} \right)^{\beta_n}} \\ \mu_p = \frac{2\bar{\mu}_p}{1 + \sqrt{1 + 4 \left(\frac{\bar{\mu}_p |E|}{v_{sat,p}} \right)^2}}; & \bar{\mu}_p = \mu_{min,p} + \frac{\mu_{0,p} - \mu_{min,p}}{1 + \left(\frac{N_D + N_A}{N_{ref,p}} \right)^{\beta_p}} \end{cases} \quad (3)$$

2.3 Production terms

$$\begin{cases} R_n = \frac{p}{\tau_n(p+\theta) + \tau_p(n+\theta)} + p(C_n n + C_p p) \\ R_p = \frac{n}{\tau_n(p+\theta) + \tau_p(n+\theta)} + n(C_n n + C_p p) \end{cases} \quad (4)$$

$$G_n = G_p = \frac{\theta^2}{\tau_n(p+\theta) + \tau_p(n+\theta)} + \theta^2(C_n n + C_p p) + (\alpha_n |J_n| + \alpha_p |J_p|) \quad (5)$$

$$\begin{cases} \alpha_n = \alpha_n^\infty \exp\left(-\frac{E_{crit,n}}{|E|}\right) \\ \alpha_p = \alpha_p^\infty \exp\left(-\frac{E_{crit,p}}{|E|}\right) \end{cases} \quad (6)$$

3 Simplified model used for Newton's method

3.1 Conservation laws

$$\begin{cases} -\lambda^2 \operatorname{div} (\varepsilon_r \operatorname{grad} \varphi) = p - n + N_D - N_A \\ -\operatorname{div} (J_n) + R_n n = G_n \\ \operatorname{div} (J_p) + R_p p = G_p \end{cases} \quad (7)$$

4 Constitutive relations

4.1 Currents

$$\begin{cases} J_n = -\mu_n (\operatorname{grad} n - n \operatorname{grad} \varphi) \\ J_p = -\mu_p (\operatorname{grad} p + p \operatorname{grad} \varphi) \end{cases} \quad (8)$$

4.2 Production terms

$$\begin{cases} R_n = \frac{p}{\tau_n(p + \theta) + \tau_p(n + \theta)} + p (C_n n + C_p p) \\ R_p = \frac{n}{\tau_n(p + \theta) + \tau_p(n + \theta)} + n (C_n n + C_p p) \end{cases} \quad (9)$$

$$G_n = G_p = \frac{\theta^2}{\tau_n(p + \theta) + \tau_p(n + \theta)} + \theta^2 (C_n n + C_p p) \quad (10)$$

5 Scaling factors/adimensional parameters

Given any generic quantity u having units U , we define the *scaled* quantity \hat{u} as

$$\hat{u} := \frac{u}{\bar{u}}$$

where \bar{u} is the scaling factor associated with u and having the same units as u .

Scaling factor	Value	Units
\bar{x}	L	m
\bar{n}	$\ N_D^+ - N_A^-\ _{L^\infty(0,L)}$	m ⁻³
$\bar{\varphi}$	$K_B T / q \simeq 26 \cdot 10^{-3}$	V
$\bar{\mu}$	$\max\{\mu_{0,n}, \mu_{0,p}\}$	m ² V ⁻¹ s ⁻¹
\bar{t}	$\bar{x}^2 / (\bar{\mu} \bar{\varphi})$	s
\bar{R}	\bar{n} / \bar{t}	m ⁻³ s ⁻¹
\bar{E}	$\bar{\varphi} / \bar{x}$	V m ⁻¹
\bar{J}	$q \bar{\mu} \bar{n} \bar{E}$	A m ⁻²
$\bar{\alpha}$	\bar{x}^{-1}	m ⁻¹
\bar{C}_{Au}	\bar{R} / \bar{n}^3	m ⁶ s ⁻¹

Table 2: Scaling factors for the Drift-Diffusion model equations.

We also introduce the following adimensional numbers

$$\lambda^2 := \frac{\varepsilon_0 \bar{\varphi}}{q \bar{n} \bar{x}^2}, \quad \theta := \frac{n_i}{\bar{n}}$$

having the meaning of squared normalized Debye length and normalized intrinsic concentration, respectively.

Part II

Function reference

6 Drift-Diffusion solvers

6.1 secs1d_dd_gummel_map

```
[n, p, V, Fn, Fp, Jn, Jp, it, res] = secs1d_dd_gummel_map (x, D, Na, Nd,
                                                         pin, nin, Vin, Fnin,
                                                         Fpin, l2, er, u0n,
                                                         uminn, vsatn, betan,
                                                         Nrefn, u0p, uminp, vsatp,
                                                         betap, Nrefp, theta, tn, tp,
```

Cn, Cp, an, ap, Ecritnin, Ecritpin,
toll, maxit, ptoll, pmaxit)

This function solves the scaled stationary bipolar DD
equation system using Gummel algorithm

```
input:
    x                spatial grid
    D, Na, Nd        doping profile
    pin              initial guess for hole concentration
    nin              initial guess for electron concentration
    Vin              initial guess for electrostatic potential
    Fnin             initial guess for electron Fermi potential
    Fpin             initial guess for hole Fermi potential
    l2               scaled Debye length squared
    er               relative electric permittivity
    uOn, uminn, vsatn, Nrefn electron mobility model coefficients
    uOp, uminp, vsatp, Nrefp hole mobility model coefficients
    theta           intrinsic carrier density
    tn, tp, Cn, Cp, an, ap, Ecritnin, Ecritpin generation recombination model parameters
    toll            tolerance for Gummel iterarion convergence test
    maxit           maximum number of Gummel iterarions
    ptoll           convergence test tolerance for the non linear Poisson solver
    pmaxit          maximum number of Newton iterarions

output:
    n               electron concentration
    p               hole concentration
    V               electrostatic potential
    Fn              electron Fermi potential
    Fp              hole Fermi potential
    Jn              electron current density
    Jp              hole current density
    it              number of Gummel iterations performed
    res             total potential increment at each step
```

6.2 Demo 1 for uncton secs1d_dd_gummel_map

```
% physical constants and parameters
secs1d_physical_constants;
secs1d_silicon_material_properties;

% geometry
```

```

L = 10e-6;          % [m]
xm = L/2;

Nelements = 1000;
x = linspace (0, L, Nelements+1)';
sinodes = [1:length(x)];

% dielectric constant (silicon)
er = esir * ones (Nelements, 1);

% doping profile [m-3]
Na = 1e23 * (x <= xm);
Nd = 1e23 * (x > xm);

% avoid zero doping
D = Nd - Na;

% initial guess for n, p, V, phin, phip
V_p = -1;
V_n = 0;

Fp = V_p * (x <= xm);
Fn = Fp;

p = abs (D) / 2 .* (1 + sqrt (1 + 4 * (ni./abs(D)) .^2)) .* (x <= xm) + ...
    ni^2 ./ (abs (D) / 2 .* (1 + sqrt (1 + 4 * (ni ./ abs (D)) .^2))) .* (x > xm);

n = abs (D) / 2 .* (1 + sqrt (1 + 4 * (ni ./ abs (D)) .^2)) .* (x > xm) + ...
    ni ^ 2 ./ (abs (D) / 2 .* (1 + sqrt (1 + 4 * (ni ./ abs (D)) .^2))) .* (x <= xm);

V = Fn + Vth * log (n / ni);

% scaling factors
xbar = L;          % [m]
nbar = norm(D, 'inf'); % [m-3]
Vbar = Vth;        % [V]
mubar = max (u0n, u0p); % [m2 V-1 s-1]
tbar = xbar^2 / (mubar * Vbar); % [s]
Rbar = nbar / tbar; % [m-3 s-1]
Ebar = Vbar / xbar; % [V m-1]
Jbar = q * mubar * nbar * Ebar; % [A m-2]
CAubar = Rbar / nbar^3; % [m6 s-1]
abar = 1/xbar;      % [m-1]

% scaling procedure
l2 = e0 * Vbar / (q * nbar * xbar^2);
theta = ni / nbar;

xin = x / xbar;

```

```

Din = D / nbar;
Nain = Na / nbar;
Ndin = Nd / nbar;
pin = p / nbar;
nin = n / nbar;
Vin = V / Vbar;
Fnin = Vin - log (nin);
Fpin = Vin + log (pin);

tnin = tn / tbar;
tpin = tp / tbar;

u0nin = u0n / mubar;
uminnin = uminn / mubar;
vsatnin = vsatn / (mubar * Ebar);

u0pin = u0p / mubar;
uminpin = uminp / mubar;
vsatpin = vsatp / (mubar * Ebar);

Nrefnin = Nrefn / nbar;
Nrefpin = Nrefp / nbar;

Cnin      = Cn / CAubar;
Cpin      = Cp / CAubar;

anin      = an / abar;
apin      = ap / abar;
Ecritnin  = Ecritn / Ebar;
Ecritpin  = Ecritp / Ebar;

% tolerances for convergence checks
toll = 1e-3;
maxit = 1000;
ptoll = 1e-12;
pmaxit = 1000;

% solve the problem using the full DD model
[nout, pout, Vout, Fnout, Fpout, Jnout, Jpout, it, res] = ...
    secs1d_dd_gummel_map (xin, Din, Nain, Ndin, pin, nin, Vin, Fnin, Fpin, ...
        12, er, u0nin, uminnin, vsatnin, betan, Nrefnin, ...
        u0pin, uminpin, vsatpin, betap, Nrefpin, theta, ...
        tnin, tpin, Cnin, Cpin, anin, apin, ...
        Ecritnin, Ecritpin, toll, maxit, ptoll, pmaxit);

% Descaling procedure
n = nout*nbar;
p = pout*nbar;
V = Vout*Vbar;

```

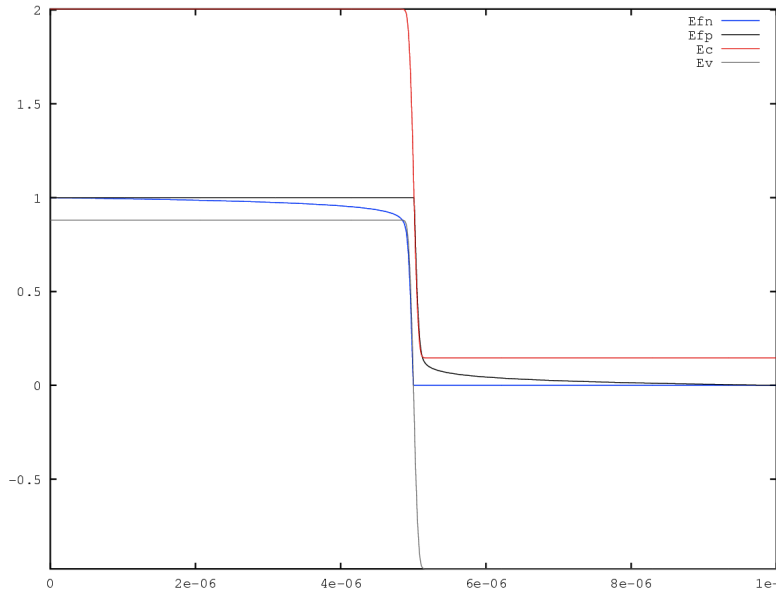



Figure 1: Figure produced by demo number 1 for function secs1d_dd_gummel_map

```

Fn  = V - Vth*log(n/ni);
Fp  = V + Vth*log(p/ni);
dV  = diff(V);
dx  = diff(x);
E   = -dV./dx;

% band structure
Efn = -Fn;
Efp = -Fp;
Ec  = Vth*log(Nc./n)+Efn;
Ev  = -Vth*log(Nv./p)+Efp;

plot (x, Efn, x, Efp, x, Ec, x, Ev)
legend ('Efn', 'Efp', 'Ec', 'Ev')
axis tight

```

6.3 secs1d_dd_newton

```
[n, p, V, Fn, Fp, Jn, Jp, it, res] = secs1d_dd_newton (x, D, Vin, nin,  
                                                    pin, l2, er, un,  
                                                    up, theta, tn, tp,  
                                                    Cn, Cp, toll, maxit)
```

Solve the scaled stationary bipolar DD equation system using Newton's method

```
input:
  x          spatial grid
  D          doping profile
  pin        initial guess for hole concentration
  nin        initial guess for electron concentration
  Vin        initial guess for electrostatic potential
  l2         scaled Debye length squared
  er         relative electric permittivity
  un         electron mobility model coefficients
  up         electron mobility model coefficients
  theta      intrinsic carrier density
  tn, tp, Cn, Cp  generation recombination model parameters
  toll       tolerance for Gummel iteration convergence test
  maxit      maximum number of Gummel iterations

output:
  n          electron concentration
  p          hole concentration
  V          electrostatic potential
  Fn         electron Fermi potential
  Fp         hole Fermi potential
  Jn         electron current density
  Jp         hole current density
  it         number of Gummel iterations performed
  res        total potential increment at each step
```

6.4 Demo 1 for function secs1d_dd_newton

```
% physical constants and parameters
secs1d_physical_constants;
secs1d_silicon_material_properties;

% geometry
L = 1e-6; % [m]
x = linspace (0, L, 10)';
sinodes = [1:length(x)];
```

```

% dielectric constant (silicon)
er = esir * ones (numel (x) - 1, 1);

% doping profile [m-3]
Na = 1e20 * ones(size(x));
Nd = 1e24 * ones(size(x));
D = Nd-Na;

% externally applied voltages
V_p = 10;
V_n = 0;

% initial guess for phin, phip, n, p, V
Fp = V_p * (x <= L/2);
Fn = Fp;

p = abs(D)/2.*(1+sqrt(1+4*(ni./abs(D)).^2)).*(D<0)+...
    ni^2./(abs(D)/2.*(1+sqrt(1+4*(ni./abs(D)).^2))).*(D>0);

n = abs(D)/2.*(1+sqrt(1+4*(ni./abs(D)).^2)).*(D>0)+...
    ni^2./(abs(D)/2.*(1+sqrt(1+4*(ni./abs(D)).^2))).*(D<0);

V = Fn + Vth*log(n/ni);

% scaling factors
xbar = L; % [m]
nbar = norm(D, 'inf'); % [m-3]
Vbar = Vth; % [V]
mubar = max(u0n, u0p); % [m-2 V-1 s-1]
tbar = xbar^2/(mubar*Vbar); % [s]
Rbar = nbar/tbar; % [m-3 s-1]
Ebar = Vbar/xbar; % [V m-1]
Jbar = q*mubar*nbar*Ebar; % [A m-2]
CAubar = Rbar/nbar^3; % [m6 s-1]
abar = xbar^(-1); % [m-1]

% scaling procedure
l2 = e0*Vbar/(q*nbar*xbar^2);
theta = ni/nbar;

xin = x/xbar;
Din = D/nbar;
Nain = Na/nbar;
Ndin = Nd/nbar;
pin = p/nbar;
nin = n/nbar;
Vin = V/Vbar;
Fnin = Vin - log(nin);

```

```

Fpin = Vin + log(pin);

tnin = tn/tbar;
tpin = tp/tbar;

% mobility model accounting scattering from ionized impurities
u0nin = u0n/mubar;
uminnin = uminn/mubar;
vsatnin = vsatn/(mubar*Ebar);

u0pin = u0p/mubar;
uminpin = uminp/mubar;
vsatpin = vsatp/(mubar*Ebar);

Nrefnin = Nrefn/nbar;
Nrefpin = Nrefp/nbar;

Cnin      = Cn/CAubar;
Cpin      = Cp/CAubar;

anin      = an/abar;
apin      = ap/abar;
Ecritnin  = Ecritn/Ebar;
Ecritpin  = Ecritp/Ebar;

% tolerances for convergence checks
ptoll = 1e-12;
pmaxit = 1000;

% solve the problem using the Newton fully coupled iterative algorithm
[nout, pout, Vout, Fnout, Fpout, Jnout, Jpout, it, res] = secs1d_dd_newton (xin, Din,
                                                                    Vin, nin, pin, l2, er,
                                                                    u0nin, u0pin, theta, tnin,
                                                                    tpin, Cnin, Cpin, ptoll, pmaxit);

% Descaling procedure
n      = nout*nbar;
p      = pout*nbar;
V      = Vout*Vbar;
Fn      = V - Vth*log(n/ni);
Fp      = V + Vth*log(p/ni);
dV      = diff(V);
dx      = diff(x);
E      = -dV./dx;

% compute current densities
[Bp, Bm] = bimu_bernoulli (dV/Vth);
Jn      = q*u0n*Vth .* (n(2:end) .* Bp - n(1:end-1) .* Bm) ./ dx;
Jp      = -q*u0p*Vth .* (p(2:end) .* Bm - p(1:end-1) .* Bp) ./ dx;
Jtot    = Jn+Jp;

```

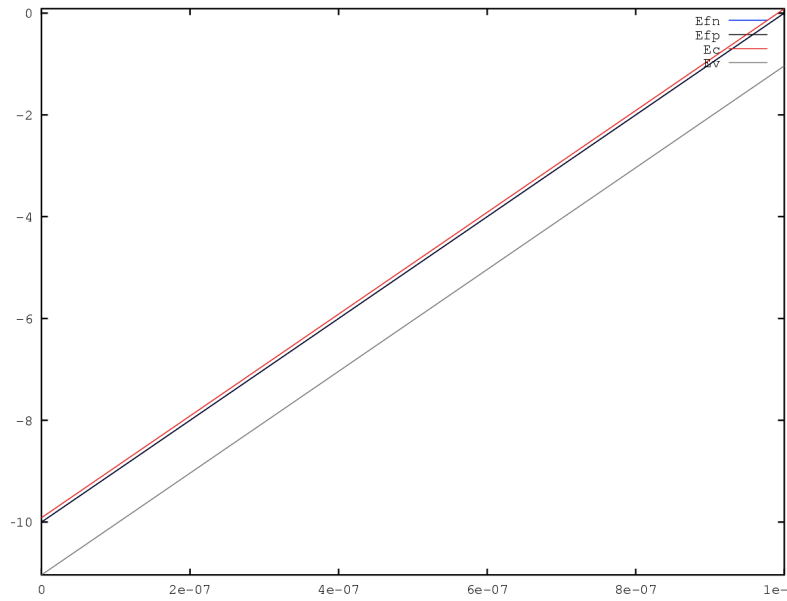


Figure 2: Figure produced by demo number 1 for function secs1d_dd_newton

```
% band structure
Efn = -Fn;
Efp = -Fp;
Ec  = Vth*log(Nc./n)+Efn;
Ev  = -Vth*log(Nv./p)+Efp;

plot (x, Efn, x, Efp, x, Ec, x, Ev)
legend ('Efn', 'Efp', 'Ec', 'Ev')
axis tight
```

7 Non-linear Poisson solver

7.1 secs1d_nlpoisson_newton

```
[V, n, p, res, niter] = secs1d_nlpoisson_newton (x, sinodes, Vin, nin, pin,  
                                                Fnin, Fpin, D, l2, er, toll, maxit)
```

```
input:
    x        spatial grid
    sinodes   index of the nodes of the grid which are in the semiconductor subdomain
              (remaining nodes are assumed to be in the oxide subdomain)
    Vin       initial guess for the electrostatic potential
    nin       initial guess for electron concentration
    pin       initial guess for hole concentration
    Fnin      initial guess for electron Fermi potential
    Fpin      initial guess for hole Fermi potential
    D         doping profile
    l2        scaled Debye length squared
    er        relative electric permittivity
    toll      tolerance for convergence test
    maxit     maximum number of Newton iterations

output:
    V         electrostatic potential
    n         electron concentration
    p         hole concentration
    res       residual norm at each step
    niter     number of Newton iterations
```

7.2 Demo 1 for function secs1d_nlpoisson_newton

```
secs1d_physical_constants
secs1d_silicon_material_properties

tbulk= 1.5e-6;
tox = 90e-9;
L = tbulk + tox;
cox = esio2/tox;

Nx = 50;
Nel = Nx - 1;

x = linspace (0, L, Nx)';
sinodes = find (x <= tbulk);
xsi = x(sinodes);
```

```

Nsi = length (sinodes);
Nox = Nx - Nsi;

NelSi = Nsi - 1;
NelSi02 = Nox - 1;

Na = 1e22;
D = - Na * ones (size (xsi));
p = Na * ones (size (xsi));
n = (ni^2) ./ p;
Fn = Fp = zeros (size (xsi));
Vg = -10;
Nv = 80;
for ii = 1:Nv
    Vg = Vg + 0.2;
    vvect(ii) = Vg;

    V = - Phims + Vg * ones (size (x));
    V(sinodes) = Fn + Vth * log (n/ni);

% Scaling
xs = L;
ns = norm (D, inf);
Din = D / ns;
Vs = Vth;
xin = x / xs;
nin = n / ns;
pin = p / ns;
Vin = V / Vs;
Fnin = (Fn - Vs * log (ni / ns)) / Vs;
Fpin = (Fp + Vs * log (ni / ns)) / Vs;

er = esio2r * ones(Nel, 1);
l2(1:NelSi) = esi;
l2 = (Vs*e0)/(q*ns*xs^2);

% Solution of Nonlinear Poisson equation

% Algorithm parameters
toll = 1e-10;
maxit = 1000;

[V, nout, pout, res, niter] = secs1d_nlpoisson_newton (xin, sinodes,
    Vin, nin, pin,
    Fnin, Fpin, Din, l2,
    er, toll, maxit);

% Descaling

```

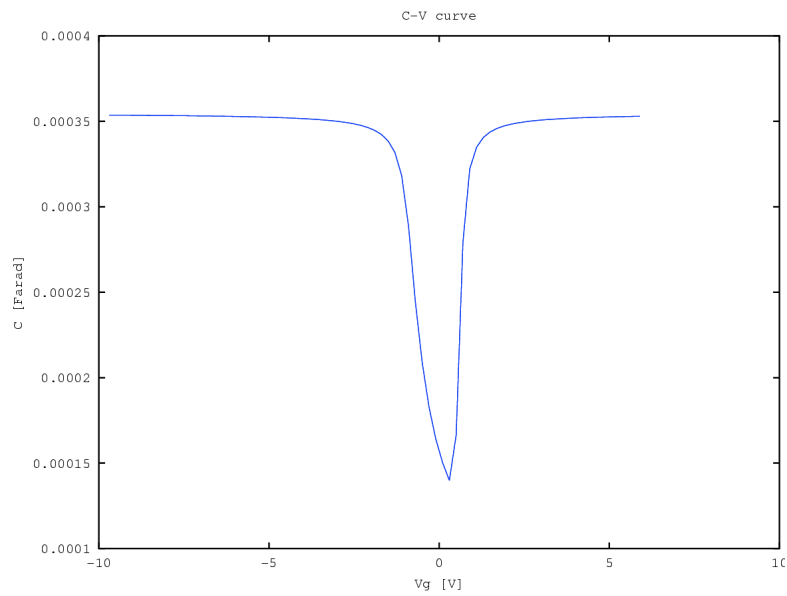


Figure 3: Figure produced by demo number 1 for function secs1d_nlpoisson_newton

```

n      = nout*ns;
p      = pout*ns;
V      = V*Vs;

    qtot(ii) = q * trapz (xsi, p + D - n);
end

vvectm = (vvect(2:end)+vvect(1:end-1))/2;
C = - diff (qtot) ./ diff (vvect);
plot(vvectm, C)
xlabel('Vg [V]')
ylabel('C [Farad]')
title('C-V curve')

```


8 Physical constants and material properties

8.1 secs1d_physical_constants.m

some useful physical constants

Kb = Boltzman constant
q = quantum of charge
e0 = permittivity of free space
hplanck = Plank constant
hbar = Plank constant by 2 pi
mn0 = free electron mass
T0 = temperature
Vth = thermal voltage

8.2 secs1d_silicon_material_properties.m

material properties for silicon and silicon dioxide

esir	= relative electric permittivity of silicon
esio2r	= relative electric permittivity of silicon dioxide
esi	= electric permittivity of silicon
esio2	= electric permittivity of silicon dioxide
mn	= effective mass of electrons in silicon
mh	= effective mass of holes in silicon
u0n	= low field electron mobility
u0p	= low field hole mobility
uminn	= parameter for doping-dependent electron mobility
betan	= idem
Nrefn	= idem
uminp	= parameter for doping-dependent hole mobility
betap	= idem
Nrefp	= idem
vsatn	= electron saturation velocity
vsatp	= hole saturation velocity
tp	= electron lifetime
tn	= hole lifetime
Cn	= electron Auger coefficient
Cp	= hole Auger coefficient
an	= impact ionization rate for electrons
ap	= impact ionization rate for holes
Ecritn	= critical field for impact ionization of electrons
Ecritp	= critical field for impact ionization of holes
Nc	= effective density of states in the conduction band
Nv	= effective density of states in the valence band
Egap	= bandgap in silicon
EgapSio2	= bandgap in silicon dioxide
ni	= intrinsic carrier density
Phims	= metal to semiconductor potential barrier

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