SECS1D

CARLO DE FALCO AND RICCARDO SACCO

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 (>= 3.0.0), bim (>= 0.0.0),
Autoload:	No

Contents

Part 1. Mathematical models

1. Full model

1.1. Conservation laws.

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

2. Constitutive relations

2.1. Currents.

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

2.2. Mobilities.

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

2.3. Production terms.

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

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

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

3. Simplified model used for Newton's method

3.1. **Conservation laws.**

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

4. Constitutive relations

4.1. **Currents.**

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

4.2. **Production terms.**

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

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

5. Scaling factors/adimensional parameters

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

$$\widehat{u} := \frac{u}{\overline{u}}$$

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

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

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

We also introduce the following adimensional numbers

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

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

Part 2. 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
            u0n, uminn, vsatn, Nrefn electron mobility model coefficients
            u0p, 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 unction 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);         % [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;         % [m^6 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, ...
                            l2, 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;
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
```

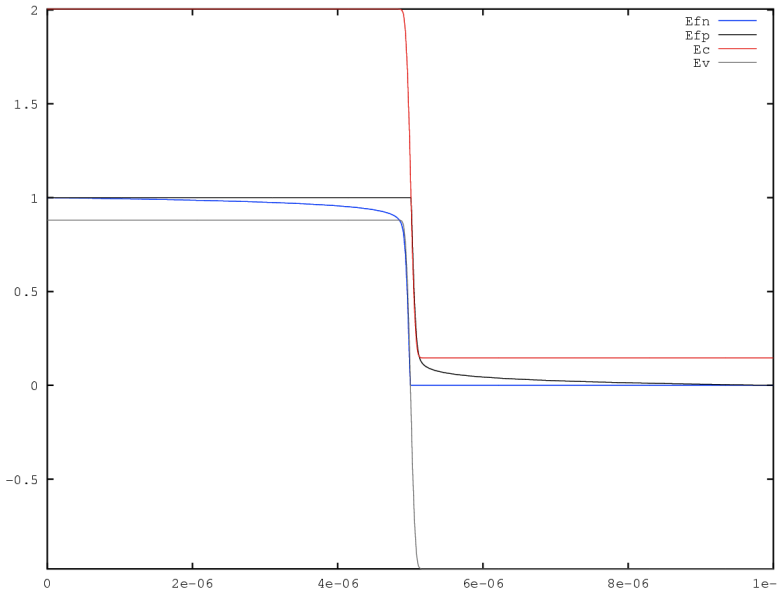

FIGURE 1. Figure produced by demo number 1 for function secs1d_dd_gummel_map

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 iterarion convergence test
      maxit           maximum number of Gummel 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
```

6.4. **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;              % [m^6 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;

% 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
```

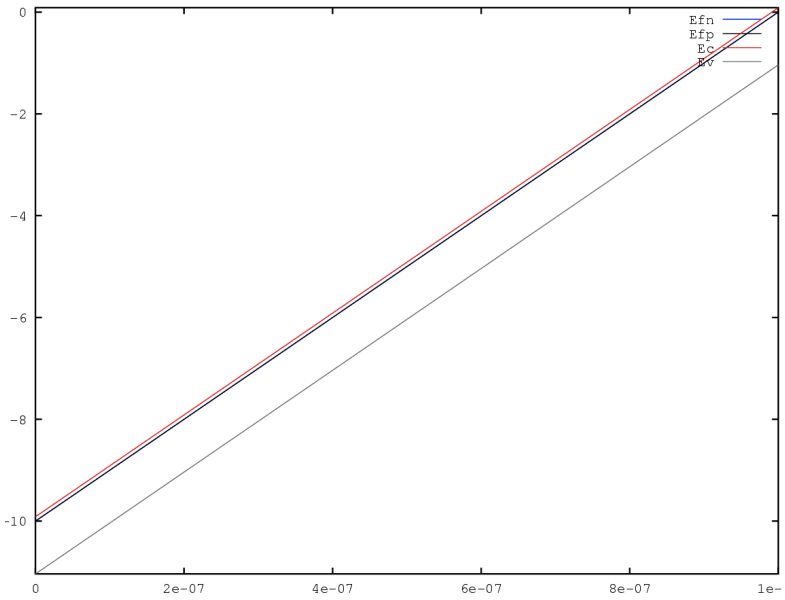

FIGURE 2. Figure produced by demo number 1 for function secs1d_dd_newton

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;
NelSiO2 = 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
    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)
```

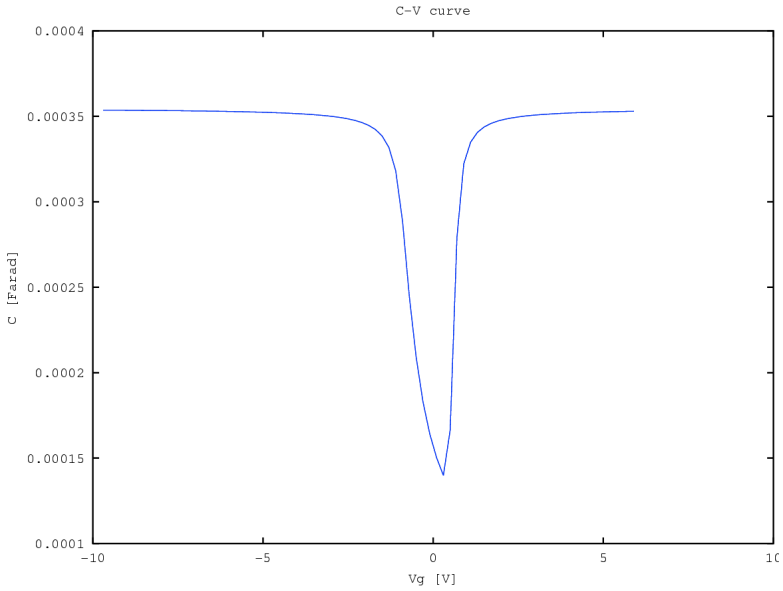

FIGURE 3. Figure produced by demo number 1 for function secs1d_nlpoisson_newton

```
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
```

Appendix A. Licence

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Version 2, June 1991

Preamble

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