Doyle-Fuller-Newman (DFN) Full Order Model (FOM) Tutorial

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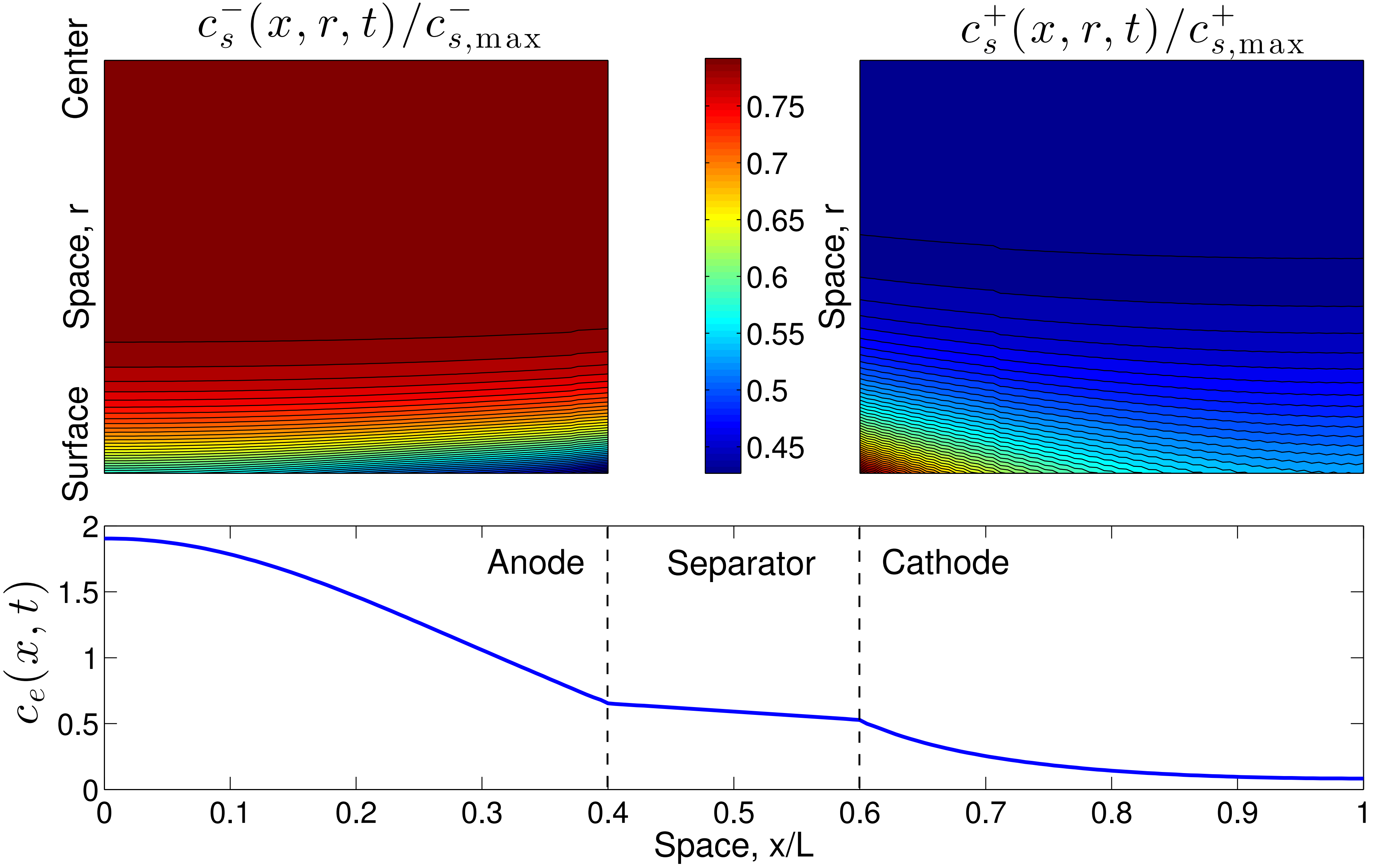
Sample Output



Background

This code is Matlab implementation of electrochemical model equations found in

- Doyle, Marc, Thomas F. Fuller, and John Newman. "Modeling of galvanostatic charge and discharge of the lithium/polymer/insertion cell." Journal of the Electrochemical Society 140.6 (1993): 1526-1533.
- Fuller, Thomas F., Marc Doyle, and John Newman. "Simulation and optimization of the dual lithium ion insertion cell." Journal of the Electrochemical Society 141.1 (1994): 1-10.
- Thomas, Karen E., John Newman, and Robert M. Darling. "Mathematical modeling of lithium batteries." Advances in lithium-ion batteries. Springer US, 2002. 345-392.
- and more…

What it does

- Simulates
  - Terminal voltage [V]
  - Solid & electrolyte concentrations [mol/m^3]
  - Solid & electrolyte potentials [V]
  - Internal temperature [K]
- Generates
  - Various static plots and animations
- Takes as input
  - An applied electric current time-series (time, current)
- Requires
  - A parameter file, which defines electrochemical model parameters
  - OCP functions, electrolyte conductivity & diffusivity fcns
- *Assumes user is proficient with Matlab*

What it does ***NOT*** do

- Provide polished user-interface. This code is for developers, and is under development.
- Simulate
  - Blended cathode materials
  - Different particle sizes
  - non Li-ion chemistries (e.g. NiMH)
  - Battery pack geometries
  - Mechanical stress
  - Aging
- Include the model identification code (PSO)
- Some of these features are under-development
- Keep your expectations reasonable please ☺

Tutorial Outline

1. Parameter file
2. Material function files
3. Input current data
4. Main script to run DFN model
5. Generate plots and animations

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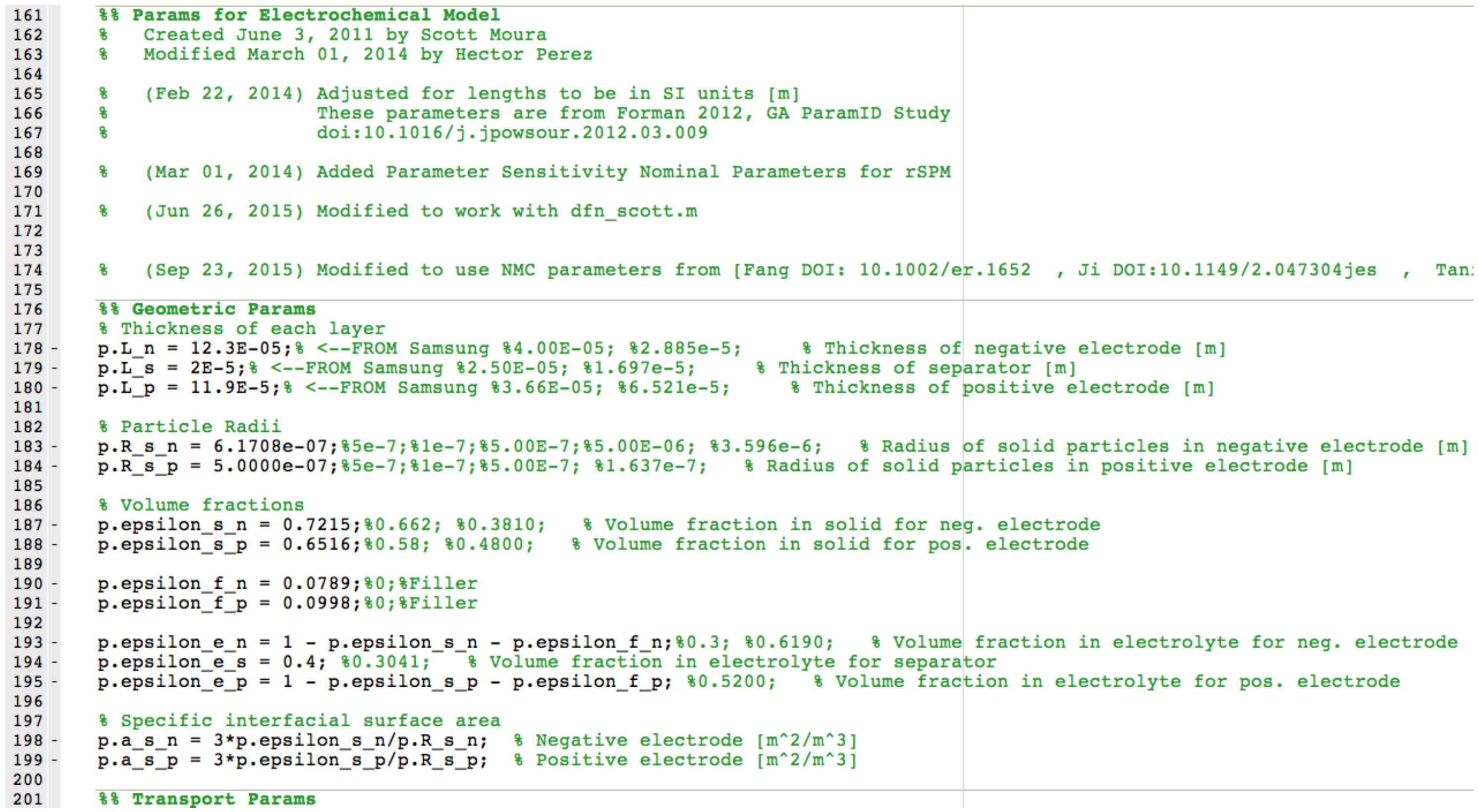
Parameter File

Open `params_NMC_Samsung_new_iteration.m`



```
%% Params for Electrochemical Model
%   Created June 3, 2011 by Scott Moura
%   Modified March 01, 2014 by Hector Perez

%   (Feb 22, 2014) Adjusted for lengths to be in SI units [m]
%                  These parameters are from Forman 2012, GA ParamID Study
%                  doi:10.1016/j.jpowsour.2012.03.009

%   (Mar 01, 2014) Added Parameter Sensitivity Nominal Parameters for rSPM

%   (Jun 26, 2015) Modified to work with dfn_scott.m


%   (Sep 23, 2015) Modified to use NMC parameters from [Fang DOI: 10.1002/er.1652  , Ji DOI:10.1149/2.047304jes   ,  Tan

%% Geometric Params
% Thickness of each layer
p.L_n = 12.3E-05;% <--FROM Samsung %4.00E-05; %2.885e-5;     % Thickness of negative electrode [m]
p.L_s = 2E-5;% <--FROM Samsung %2.50E-05; %1.697e-5;     % Thickness of separator [m]
p.L_p = 11.9E-5;% <--FROM Samsung %3.66E-05; %6.521e-5;     % Thickness of positive electrode [m]

% Particle Radii
p.R_s_n = 6.1708e-07;%5e-7;%1e-7;%5.00E-7;%5.00E-06; %3.596e-6;    % Radius of solid particles in negative electrode [m]
p.R_s_p = 5.0000e-07;%5e-7;%1e-7;%5.00E-7; %1.637e-7;    % Radius of solid particles in positive electrode [m]

% Volume fractions
p.epsilon_s_n = 0.7215;%0.662; %0.3810;    % Volume fraction in solid for neg. electrode
p.epsilon_s_p = 0.6516;%0.58; %0.4800;    % Volume fraction in solid for pos. electrode

p.epsilon_f_n = 0.0789;%0;%Filler
p.epsilon_f_p = 0.0998;%0;%Filler

p.epsilon_e_n = 1 - p.epsilon_s_n - p.epsilon_f_n;%0.3; %0.6190;    % Volume fraction in electrolyte for neg. electrode
p.epsilon_e_s = 0.4; %0.3041;    % Volume fraction in electrolyte for separator
p.epsilon_e_p = 1 - p.epsilon_s_p - p.epsilon_f_p; %0.5200;    % Volume fraction in electrolyte for pos. electrode

% Specific interfacial surface area
p.a_s_n = 3*p.epsilon_s_n/p.R_s_n;  % Negative electrode [m^2/m^3]
p.a_s_p = 3*p.epsilon_s_p/p.R_s_p;  % Positive electrode [m^2/m^3]

%% Transport Params
```

- Embeds scalar parameter values
- Generates a struct object `p`, which is passed throughout the code

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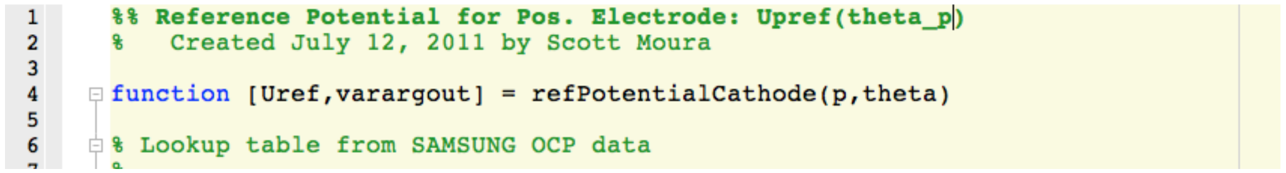
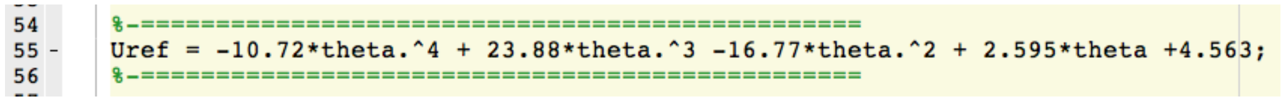
Open Circuit Potential Files

Open

- `refPotentialAnode.m`
- `refPotentialCathode.m`



```
%% Reference Potential for Pos. Electrode: Upref(theta_p)
%   Created July 12, 2011 by Scott Moura

function [Uref,varargout] = refPotentialCathode(p,theta)

% Lookup table from SAMSUNG OCP data
```



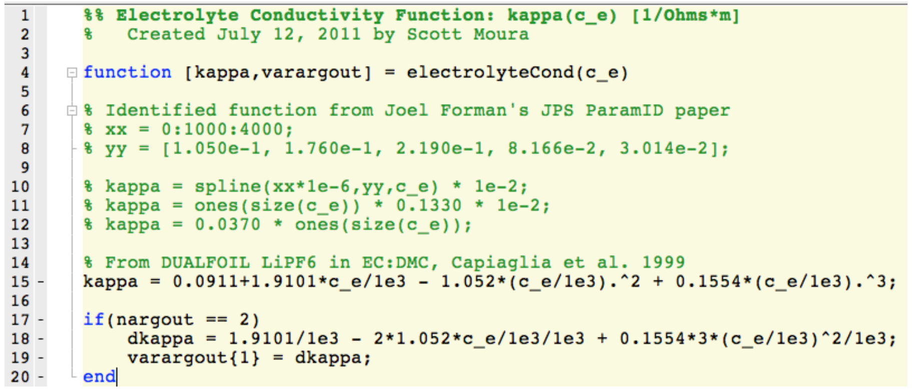
```
%-================================================
Uref = -10.72*theta.^4 + 23.88*theta.^3 -16.77*theta.^2 + 2.595*theta +4.563;
%-================================================
```

- Implements open circuit potentials for each electrode material
- Computes OCP, and it's derivative.

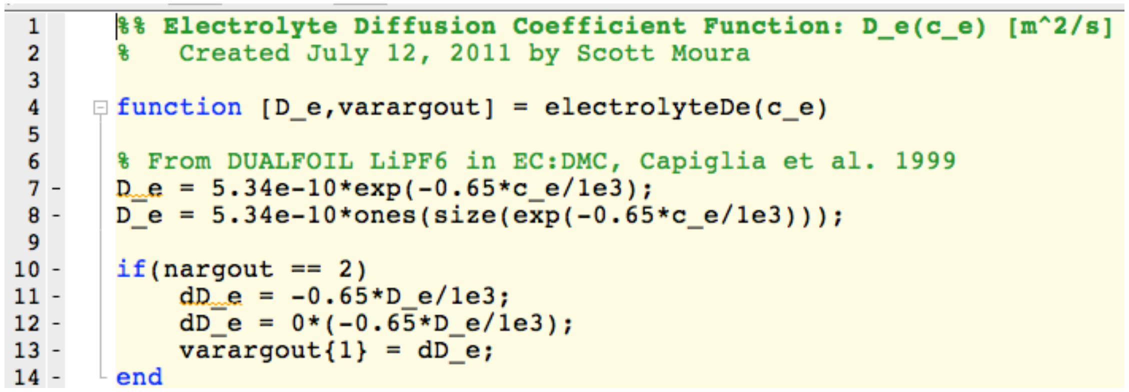
Electrolyte Conductivity & Diffusivity

Open

- `electrolyteCond.m`
- `electrolyteDe.m`



```
%% Electrolyte Conductivity Function: kappa(c_e) [1/Ohms*m]
%   Created July 12, 2011 by Scott Moura

function [kappa,varargout] = electrolyteCond(c_e)

% Identified function from Joel Forman's JPS ParamID paper
% xx = 0:1000:4000;
% yy = [1.050e-1, 1.760e-1, 2.190e-1, 8.166e-2, 3.014e-2];

% kappa = spline(xx*1e-6,yy,c_e) * 1e-2;
% kappa = ones(size(c_e)) * 0.1330 * 1e-2;
% kappa = 0.0370 * ones(size(c_e));

% From DUALFOIL LiPF6 in EC:DMC, Capiaglia et al. 1999
kappa = 0.0911+1.9101*c_e/1e3 - 1.052*(c_e/1e3).^2 + 0.1554*(c_e/1e3).^3;

if(nargout == 2)
    dkappa = 1.9101/1e3 - 2*1.052*c_e/1e3/1e3 + 0.1554*3*(c_e/1e3)^2/1e3;
    varargout{1} = dkappa;
end
```



```
%% Electrolyte Diffusion Coefficient Function: D_e(c_e) [m^2/s]
%   Created July 12, 2011 by Scott Moura

function [D_e,varargout] = electrolyteDe(c_e)

% From DUALFOIL LiPF6 in EC:DMC, Capiglia et al. 1999
D_e = 5.34e-10*exp(-0.65*c_e/1e3);
D_e = 5.34e-10*ones(size(exp(-0.65*c_e/1e3)));

if(nargout == 2)
    dD_e = -0.65*D_e/1e3;
    dD_e = 0*(-0.65*D_e/1e3);
    varargout{1} = dD_e;
end
```

- Electrolyte conductivity & diffusivity are functions of local concentration
- Computes conductivity/diffusivity and it's derivative

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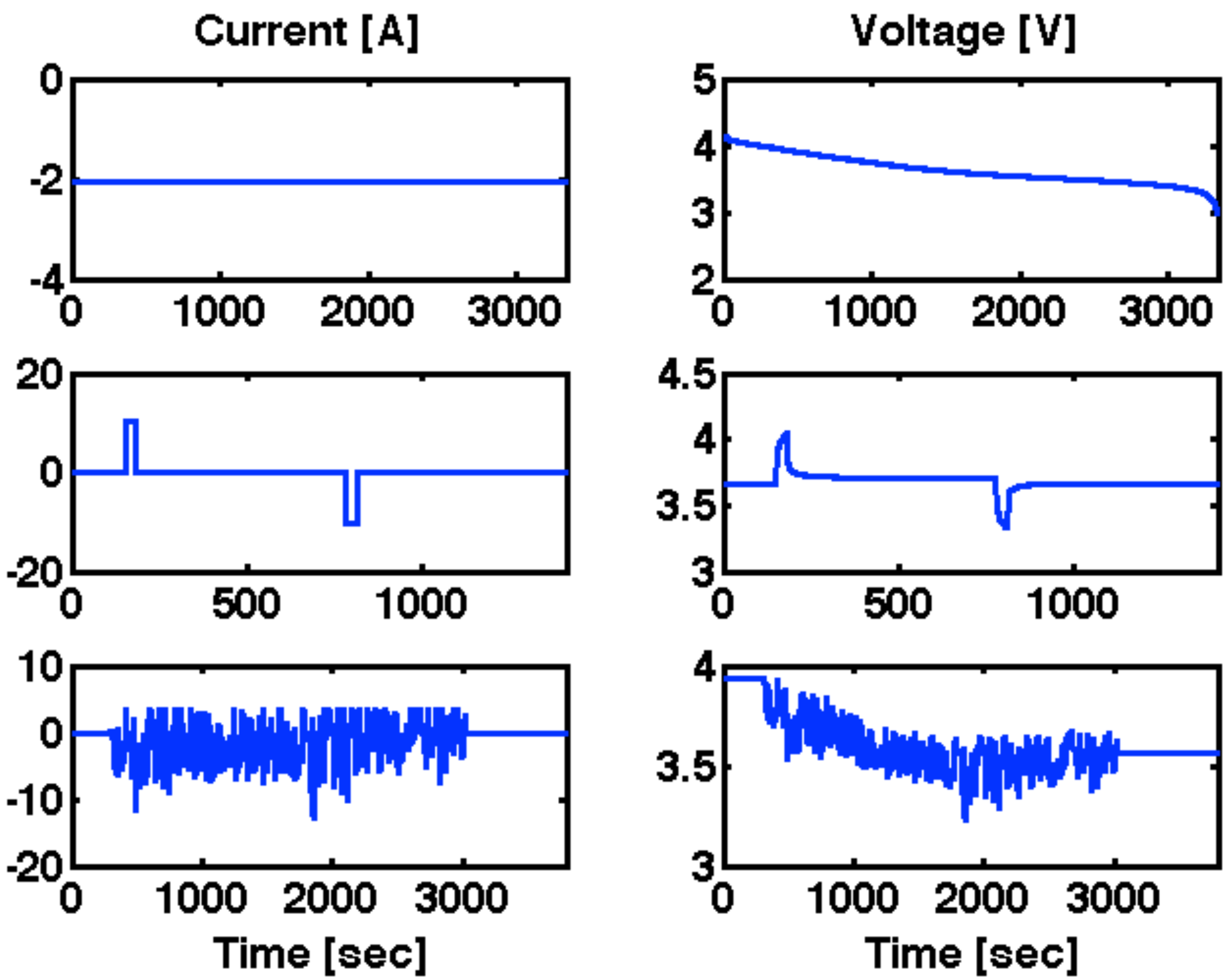
Input current files

- All experimentally collected data is located in: `data/Int_Obs/` directory
- Samples:

1C Discharge
`data/Int_Obs/1C_data_Oct_26_2015_05_sample.mat`

5C Pulses
`data/Int_Obs/dfn_5c.mat`

UDDS drive cycle
`data/Int_Obs/UDDS_data_Oct_26_2015_Sample_05sec.mat`



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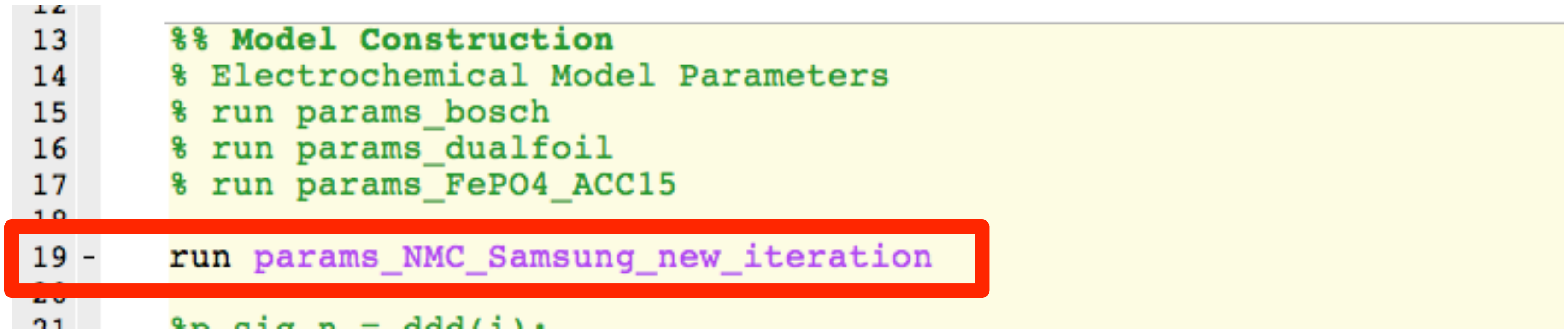
Main Script

- Open dfn_scott_testing_Satadru.m

This is the main script that runs the DFN model

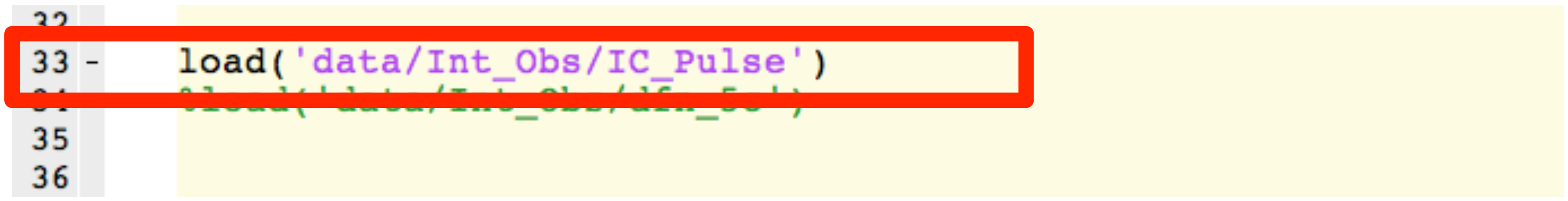
1. To input parameter file, go to line 19. Enter desired parameter file.



```
13      %% Model Construction
14      % Electrochemical Model Parameters
15      % run params_bosch
16      % run params_dualfoil
17      % run params_FePO4_ACC15
18
19 -    run params_NMC_Samsung_new_iteration
20
21      %p_sig_n = ddd(i);
```

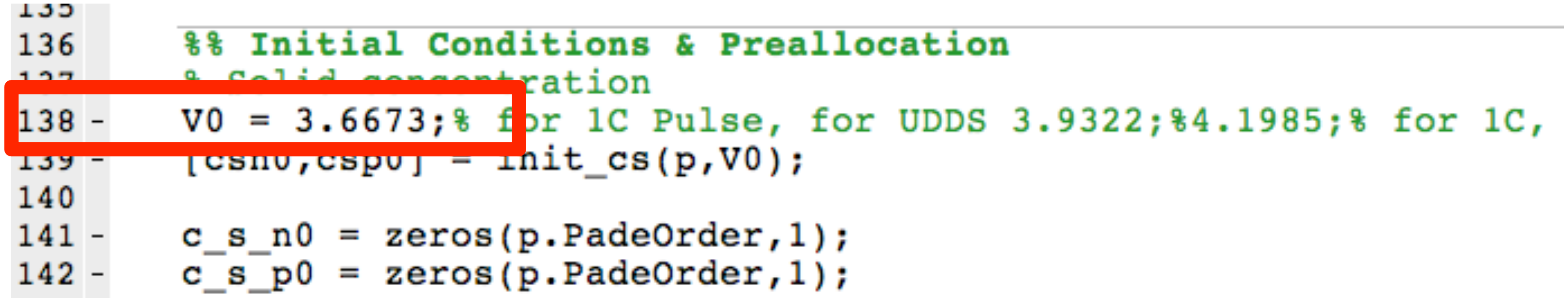
Main Script

2. To load input current, go to line 33. Enter desired input current file.



```
32
33 -    load('data/Int_Obs/IC_Pulse')
34      %load('data/Int_Obs/dfn_50')
35
36
```

3. To set initial voltage, go to line 138.

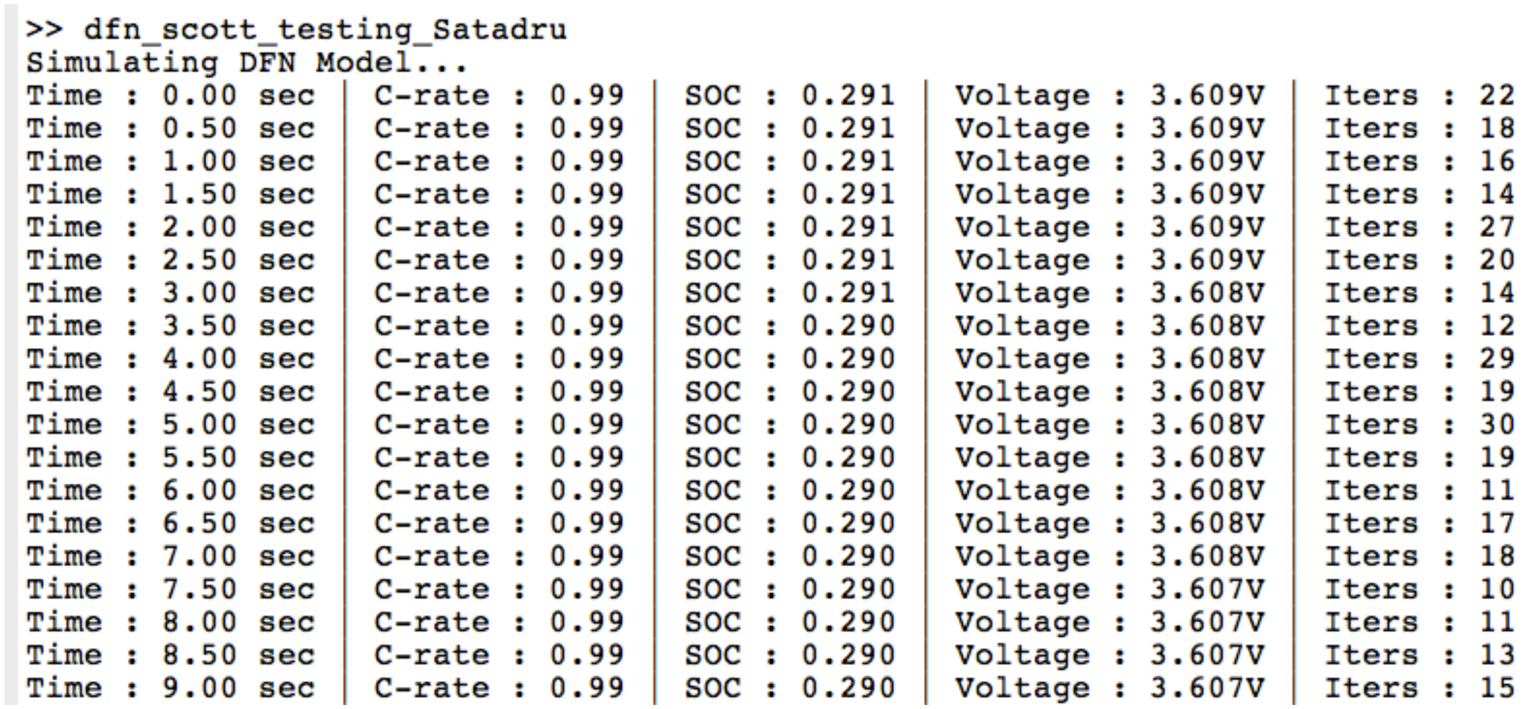


```
135
136     %% Initial Conditions & Preallocation
137     % Solid concentration
138 -   V0 = 3.6673;% for 1C Pulse, for UDDS 3.9322;%4.1985;% for 1C,
139 -   [csn0,csp0] = init_cs(p,V0);
140
141 -   c_s_n0 = zeros(p.PadeOrder,1);
142 -   c_s_p0 = zeros(p.PadeOrder,1);
```

Main Script

4. You are ready! Run the m-file.

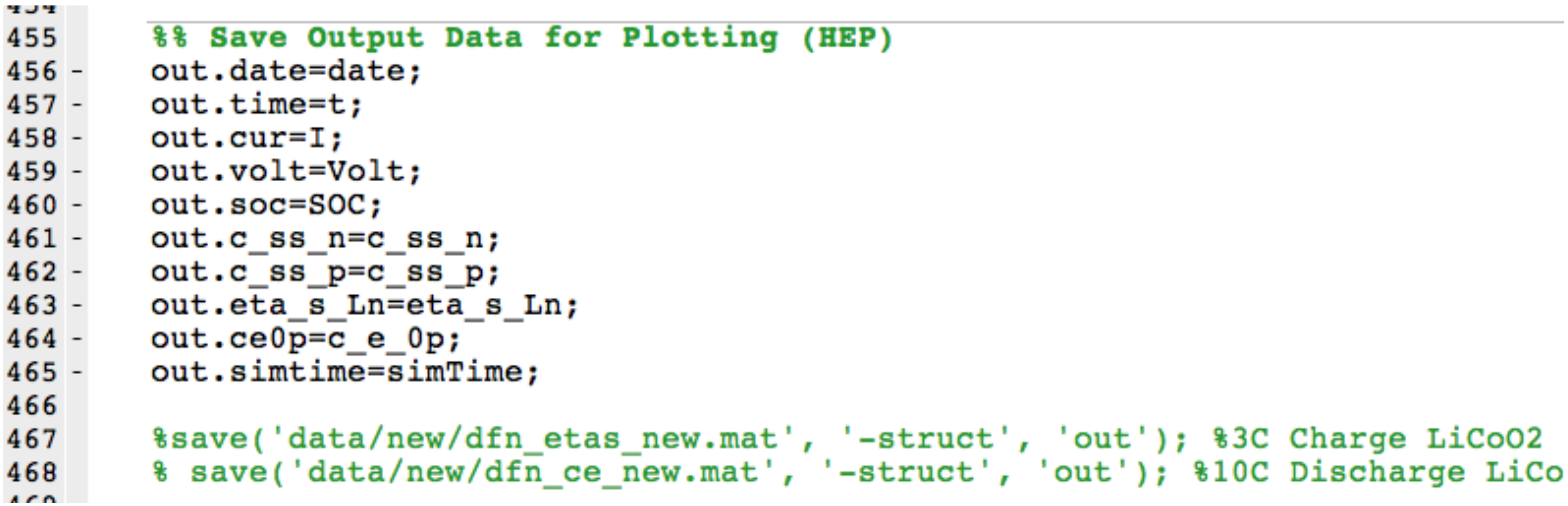
The command window output will look like…



```
>> dfn_scott_testing_Satadru
Simulating DFN Model...
Time : 0.00 sec | C-rate : 0.99 | SOC : 0.291 | Voltage : 3.609V | Iters : 22
Time : 0.50 sec | C-rate : 0.99 | SOC : 0.291 | Voltage : 3.609V | Iters : 18
Time : 1.00 sec | C-rate : 0.99 | SOC : 0.291 | Voltage : 3.609V | Iters : 16
Time : 1.50 sec | C-rate : 0.99 | SOC : 0.291 | Voltage : 3.609V | Iters : 14
Time : 2.00 sec | C-rate : 0.99 | SOC : 0.291 | Voltage : 3.609V | Iters : 27
Time : 2.50 sec | C-rate : 0.99 | SOC : 0.291 | Voltage : 3.609V | Iters : 20
Time : 3.00 sec | C-rate : 0.99 | SOC : 0.291 | Voltage : 3.608V | Iters : 14
Time : 3.50 sec | C-rate : 0.99 | SOC : 0.290 | Voltage : 3.608V | Iters : 12
Time : 4.00 sec | C-rate : 0.99 | SOC : 0.290 | Voltage : 3.608V | Iters : 29
Time : 4.50 sec | C-rate : 0.99 | SOC : 0.290 | Voltage : 3.608V | Iters : 19
Time : 5.00 sec | C-rate : 0.99 | SOC : 0.290 | Voltage : 3.608V | Iters : 30
Time : 5.50 sec | C-rate : 0.99 | SOC : 0.290 | Voltage : 3.608V | Iters : 19
Time : 6.00 sec | C-rate : 0.99 | SOC : 0.290 | Voltage : 3.608V | Iters : 11
Time : 6.50 sec | C-rate : 0.99 | SOC : 0.290 | Voltage : 3.608V | Iters : 17
Time : 7.00 sec | C-rate : 0.99 | SOC : 0.290 | Voltage : 3.608V | Iters : 18
Time : 7.50 sec | C-rate : 0.99 | SOC : 0.290 | Voltage : 3.607V | Iters : 10
Time : 8.00 sec | C-rate : 0.99 | SOC : 0.290 | Voltage : 3.607V | Iters : 11
Time : 8.50 sec | C-rate : 0.99 | SOC : 0.290 | Voltage : 3.607V | Iters : 13
Time : 9.00 sec | C-rate : 0.99 | SOC : 0.290 | Voltage : 3.607V | Iters : 15
```

Main Script

5. After running, the simulation outputs of interest are saved to struct object `out`. Go to line 467, uncomment, and save to a user-specified filename.



```
455     %% Save Output Data for Plotting (HEP)
456 -   out.date=date;
457 -   out.time=t;
458 -   out.cur=I;
459 -   out.volt=Volt;
460 -   out.soc=SOC;
461 -   out.c_ss_n=c_ss_n;
462 -   out.c_ss_p=c_ss_p;
463 -   out.eta_s_Ln=eta_s_Ln;
464 -   out.ce0p=c_e_0p;
465 -   out.simtime=simTime;
466
467     %save('data/new/dfn_etas_new.mat', '-struct', 'out'); %3C Charge LiCoO2
468     % save('data/new/dfn_ce_new.mat', '-struct', 'out'); %10C Discharge LiCo
```

Main Script – Ex: HEV Validation

To reproduce the model vs. experiment validation on the Samsung HEV cycle…

1. Use `params_NMC_Samsung_new_iteration.m`
2. Load `data/Int_Obs/Samsung_HEV_data.mat` cycle
3. Initialive model voltage to equal initial voltage from experimental data on line 138.
4. Run `dfn_scott_testing_Satadru.m`
5. The model will require 30min or so. After it's finished, then the last code (line 507) will compute the RMS error between experiments and model

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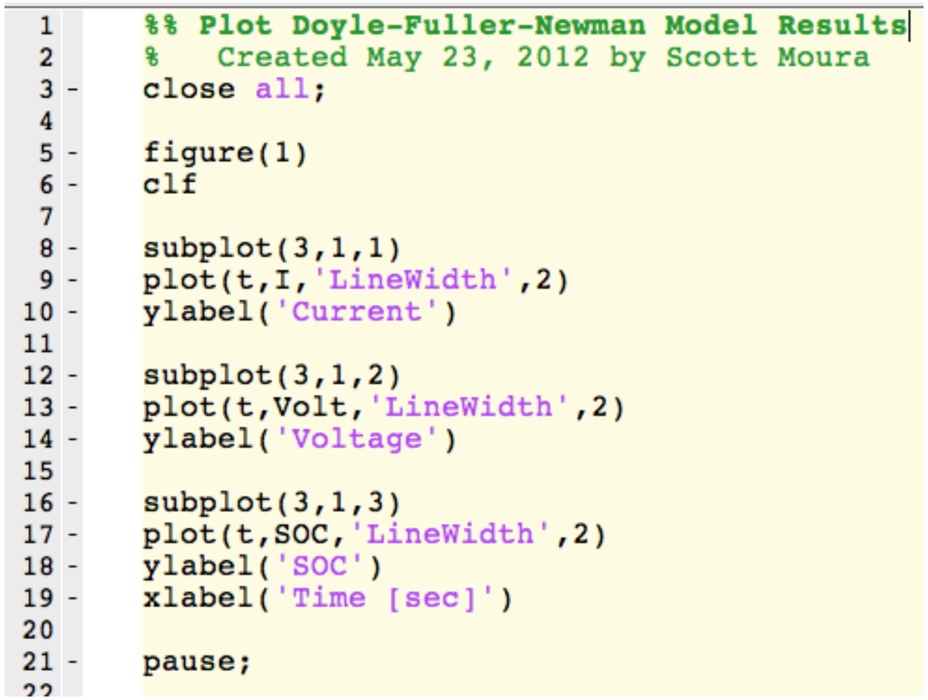
Generate Plots and Animations

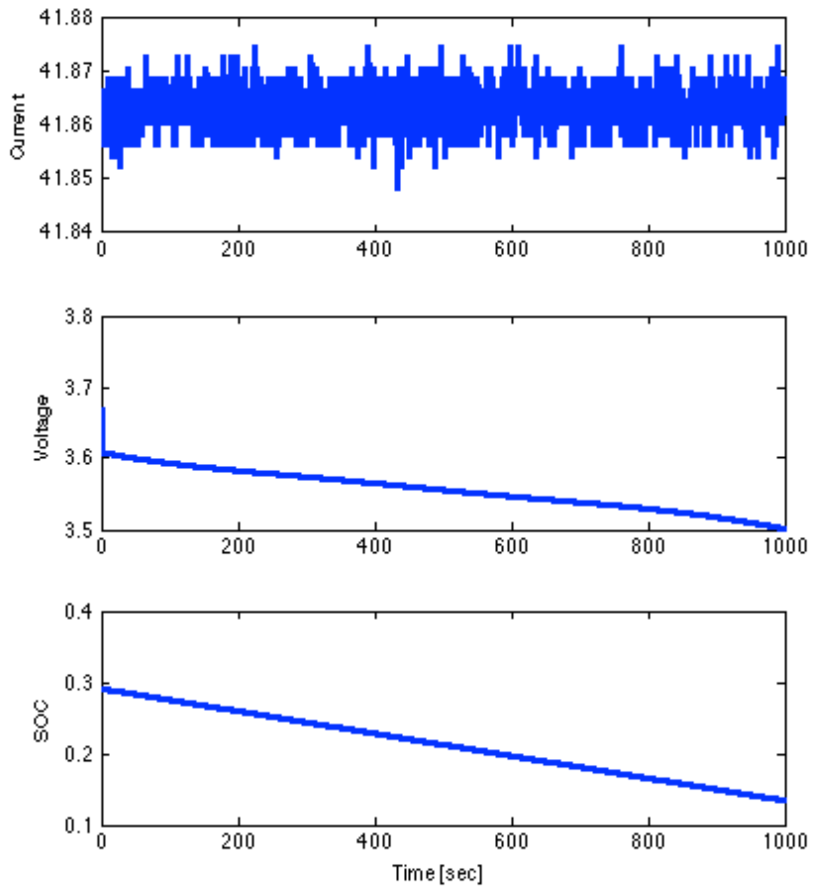
Open `plot_dfn.m`

1. Plot basic outputs: current, SOC, and voltage



```
%% Plot Doyle-Fuller-Newman Model Results
%   Created May 23, 2012 by Scott Moura
close all;

figure(1)
clf

subplot(3,1,1)
plot(t,I,'LineWidth',2)
ylabel('Current')

subplot(3,1,2)
plot(t,Volt,'LineWidth',2)
ylabel('Voltage')

subplot(3,1,3)
plot(t,SOC,'LineWidth',2)
ylabel('SOC')
xlabel('Time [sec]')

pause;
```

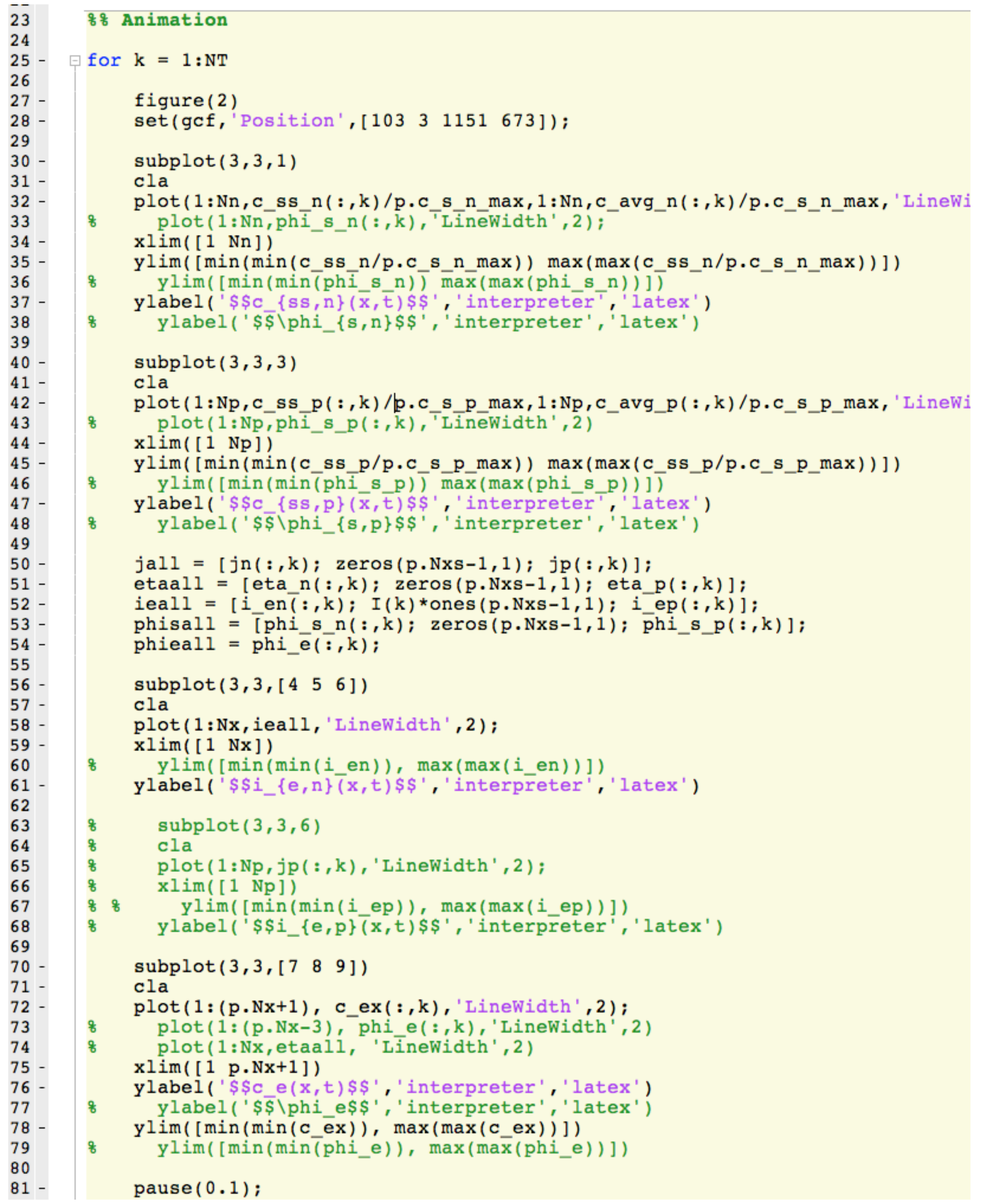
Example: 1C discharge for 1000 sec



Generate Plots and Animations

Open `plot_dfn.m`

2. Animate electrochemical states, e.g. solid & electrolyte concentrations and ionic current. Please feel free to uncomment/comment parts of code to view different echem states.



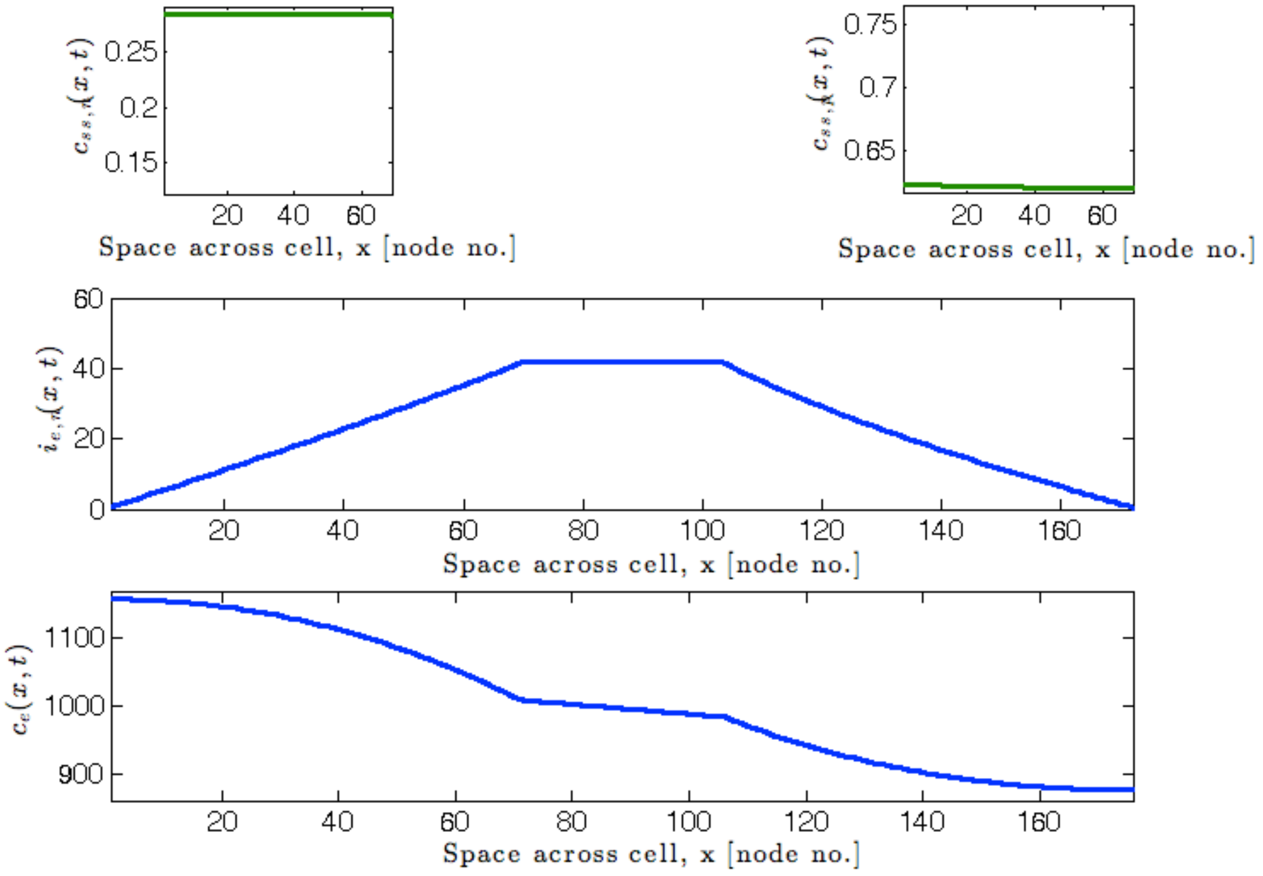
```
%% Animation

for k = 1:NT

    figure(2)
    set(gcf,'Position',[103 3 1151 673]);

    subplot(3,3,1)
    cla
    plot(1:Nn,c_ss_n(:,k)/p.c_s_n_max,1:Nn,c_avg_n(:,k)/p.c_s_n_max,'LineWi
%     plot(1:Nn,phi_s_n(:,k),'LineWidth',2);
    xlim([1 Nn])
    ylim([min(min(c_ss_n/p.c_s_n_max)) max(max(c_ss_n/p.c_s_n_max))])
%     ylim([min(min(phi_s_n)) max(max(phi_s_n))])
    ylabel('$$c_{ss,n}(x,t)$$','interpreter','latex')
%     ylabel('$$\phi_{s,n}$$','interpreter','latex')

    subplot(3,3,3)
    cla
    plot(1:Np,c_ss_p(:,k)/p.c_s_p_max,1:Np,c_avg_p(:,k)/p.c_s_p_max,'LineWi
%     plot(1:Np,phi_s_p(:,k),'LineWidth',2)
    xlim([1 Np])
    ylim([min(min(c_ss_p/p.c_s_p_max)) max(max(c_ss_p/p.c_s_p_max))])
%     ylim([min(min(phi_s_p)) max(max(phi_s_p))])
    ylabel('$$c_{ss,p}(x,t)$$','interpreter','latex')
%     ylabel('$$\phi_{s,p}$$','interpreter','latex')

    jall = [jn(:,k); zeros(p.Nxs-1,1); jp(:,k)];
    etaall = [eta_n(:,k); zeros(p.Nxs-1,1); eta_p(:,k)];
    ieall = [i_en(:,k); I(k)*ones(p.Nxs-1,1); i_ep(:,k)];
    phisall = [phi_s_n(:,k); zeros(p.Nxs-1,1); phi_s_p(:,k)];
    phieall = phi_e(:,k);

    subplot(3,3,[4 5 6])
    cla
    plot(1:Nx,ieall,'LineWidth',2);
    xlim([1 Nx])
%     ylim([min(min(i_en)), max(max(i_en))])
    ylabel('$$i_{e,n}(x,t)$$','interpreter','latex')

%     subplot(3,3,6)
%     cla
%     plot(1:Np,jp(:,k),'LineWidth',2);
%     xlim([1 Np])
% %     ylim([min(min(i_ep)), max(max(i_ep))])
%     ylabel('$$i_{e,p}(x,t)$$','interpreter','latex')

    subplot(3,3,[7 8 9])
    cla
    plot(1:(p.Nx+1), c_ex(:,k),'LineWidth',2);
%     plot(1:(p.Nx-3), phi_e(:,k),'LineWidth',2)
%     plot(1:Nx,etaall, 'LineWidth',2)
    xlim([1 p.Nx+1])
    ylabel('$$c_e(x,t)$$','interpreter','latex')
%     ylabel('$$\phi_e$$','interpreter','latex')
    ylim([min(min(c_ex)), max(max(c_ex))])
%     ylim([min(min(phi_e)), max(max(phi_e))])

    pause(0.1);
```

Generate Plots and Animations

Open `plot_dfn.m`

2. Animate electrochemical states, e.g. solid & electrolyte concentrations and ionic current.

Example: Snapshot of 1C discharge animation



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Closing remarks: This code is under development. Future versions will have enhanced speed, accuracy, usability, etc. Enjoy!