Solving The Rate-Equations

Niall Boohan

Tyndall National Institute of Ireland

January 31, 2020

Overview

Introduction

Introduction

- The aim of this presentation is to introduce a known functioning script to solve the laser-rate equations in Python.
- You may choose to make these calculations in a different programming language but it is still important to start from a well functioning piece of code.
- By the end of this presentation I will have covered what each section of my code does, this will be relatable to other programming languages.

The laser-rate equation overview.

- The laser-rate equation describes how photon (S) & carrier concentration (N) in a laser cavity change with time for a given input current.
- The most basic form has two coupled ODE's, one for S and one for N.
- Each factor in the S or N equation has an associated change in N/s or S/s units associated with it.
- A time base for the calculations is set e.g 1ps. So for every 1ps, the code calculates the change in N or S and adds or subtracts this to the initial or continuing S or N values.

Simple example

$$\frac{dN}{dt} = \frac{I}{eV_a} - v_g g_a \bar{S} - R(N)$$

$$\frac{d\bar{S}}{dt} = v_g g_c \bar{S} + R_{\text{sp}}$$

Figure: [Buus, Amann, and Blumenthal, 2010]

- This is a simple example to make equations' operation more clearer.
- *These are not the equations used in the coded example.*
- N is carrier concentration, I is current, e is unitary charge, g is gain, $\bar{S}$ is photon concentration, R is spontaneous emission rate, ν_g is group velocity.
- Time steps are chosen specifically in code and should be $\sim$ 100 times smaller that the smallest timer interaction.

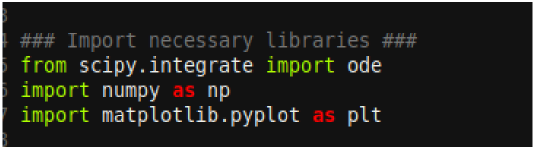
Coding overview

Implementing a pre-packaged solver:

- The example given is in Python, if you do not have a strong preference for a programming language it is best to use Python or MATLAB for simple models to begin with.
- For solving laser-rate equations it is best to start with a template that you know works and is robust and expand it. There are plenty of examples for MATLAB online.
- Link to the codes I have made in Python: https://github.com/boohann/Laser-Rate-Equations-Python/
- Model parameters are passed to the solver which will be written in a low level language (Fortran/C++), so code will solve relatively quickly.
- Implementation is quite similar between Pyhton and MATLAB.

Code — section by section

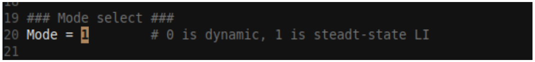
Call libraries



```
### Import necessary libraries ###
from scipy.integrate import ode
import numpy as np
import matplotlib.pyplot as plt
```

- Libraries are repositories of prewritten functions, used heavily in Python.
- Libraries is one way Python can differ from other programming languages, you may not have to call these in languages like MATLAB.
- Always declared at top of script.

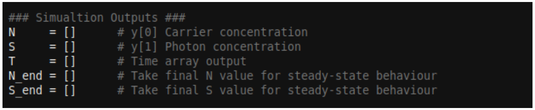
Change code operation



```
### Mode select ###
Mode = 1        # 0 is dynamic, 1 is steadt-state LI
```

- The code has been written to switch between producing an LI for a range of input currents or producing a time dependant trace of photon and carrier concentrations.
- This will be clearer later in the code.

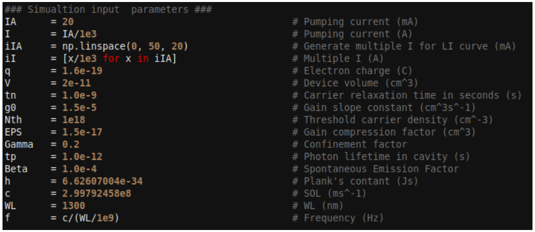
Declaring output storage location



```
### Simualtion Outputs ###
N     = []      # y[0] Carrier concentration
S     = []      # y[1] Photon concentration
T     = []      # Time array output
N_end = []      # Take final N value for steady-state behaviour
S_end = []      # Take final S value for steady-state behaviour
```

- Lists for storing output data from simulation.
- These can be passed to graphing libraries, post-processed or saved and stored.

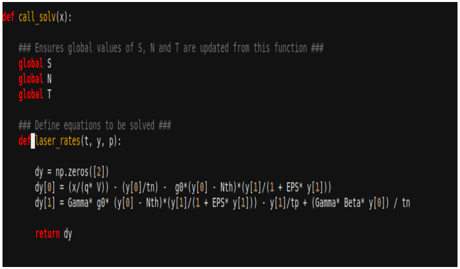
Declaring input parameters



```
### Simualtion input  parameters ###
IA      = 20                                        # Pumping current (mA)
I       = IA/1e3                                    # Pumping current (A)
iIA     = np.linspace(0, 50, 20)                    # Generate multiple I for LI curve (mA)
iI      = [x/1e3 for x in iIA]                      # Multiple I (A)
q       = 1.6e-19                                   # Electron charge (C)
V       = 2e-11                                     # Device volume (cm^3)
tn      = 1.0e-9                                    # Carrier relaxation time in seconds (s)
g0      = 1.5e-5                                    # Gain slope constant (cm^3s^-1)
Nth     = 1e18                                      # Threshold carrier density (cm^-3)
EPS     = 1.5e-17                                   # Gain compression factor (cm^3)
Gamma   = 0.2                                       # Confinement factor
tp      = 1.0e-12                                   # Photon lifetime in cavity (s)
Beta    = 1.0e-4                                    # Spontaneous Emission Factor
h       = 6.62607004e-34                            # Plank's contant (Js)
c       = 2.99792458e8                              # SOL (ms^-1)
WL      = 1300                                      # WL (nm)
f       = c/(WL/1e9)                                # Frequency (Hz)
```

- Different input parameters are best declared at the top to make changing these values easier.
- Note: different values for current for steady-state or dynamic operation.

Inputting equations into solver



```
def call_solv(x):

    ### Ensures global values of S, N and T are updated from this function ###
    global S
    global N
    global T

    ### Define equations to be solved ###
    def laser_rates(t, y, p):

        dy = np.zeros([2])
        dy[0] = (x/(q* V)) - (y[0]/tn) -  g0*(y[0] - Nth)*(y[1]/(1 + EPS* y[1]))
        dy[1] = Gamma* g0* (y[0] - Nth)*(y[1]/(1 + EPS* y[1])) - y[1]/tp + (Gamma* Beta* y[0]) / tn

        return dy
```

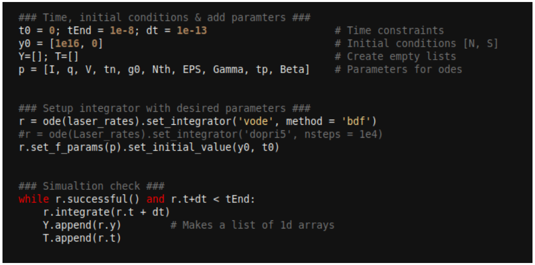
$$\frac{dN(t)}{dt} = \frac{I(t)}{qV} - \frac{N(t)}{\tau_n} - g_0(N(t) - N_t)\frac{1}{(1+\varepsilon S(t))}S(t) \qquad (1)$$

$$\frac{dS(t)}{dt} = \Gamma g_0(N(t) - N_t)\frac{1}{(1+\varepsilon S(t))}S(t) - \frac{S(t)}{\tau_p} + \frac{\Gamma \beta N(t)}{\tau_n} \qquad (2)$$

[Cartledge and Srinivasan, 1997]

- The first function (def) allows the entire solver to be called repeatedly for varying input current to calculate an LI curve.
- The second function (def) defines the equations we will input into our solver.
- "global" ensures T, N and S values are updated.

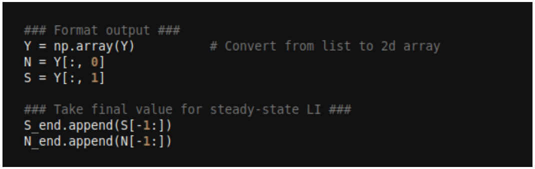
Running the solver



```
### Time, initial conditions & add paramters ###
t0 = 0; tEnd = 1e-8; dt = 1e-13                       # Time constraints
y0 = [1e16, 0]                                        # Initial conditions [N, S]
Y=[]; T=[]                                            # Create empty lists
p = [I, q, V, tn, g0, Nth, EPS, Gamma, tp, Beta]      # Parameters for odes


### Setup integrator with desired parameters ###
r = ode(laser_rates).set_integrator('vode', method = 'bdf')
#r = ode(Laser_rates).set_integrator('dopri5', nsteps = 1e4)
r.set_f_params(p).set_initial_value(y0, t0)


### Simualtion check ###
while r.successful() and r.t+dt < tEnd:
    r.integrate(r.t + dt)
    Y.append(r.y)         # Makes a list of 1d arrays
    T.append(r.t)
```

- First block of code defines time extents, initial conditions and organises our parameters into the solver.
- The second block of code calls the integrator (vode) and method (bdf) with initial conditions and parameters. It is best not to change solver and method unless absolutely necessary.
- The third block of code runs the solver while it is within the time extents and not diverging.

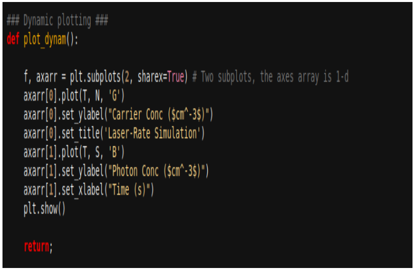
Saving outputs



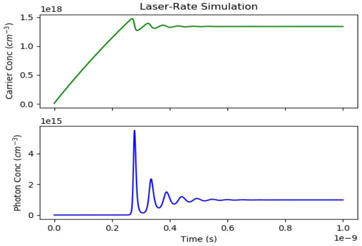
```
### Format output ###
Y = np.array(Y)          # Convert from list to 2d array
N = Y[:, 0]
S = Y[:, 1]

### Take final value for steady-state LI ###
S_end.append(S[-1:])
N_end.append(N[-1:])
```

- This section of code outputs the data into the structures we defined at the beginning of the script.
- A save to data file routine could be added here if required.

Dynamic output

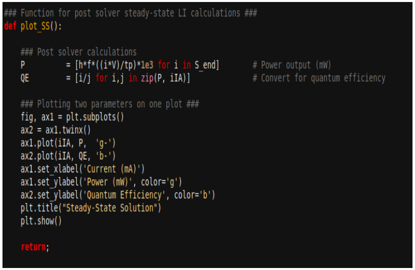


```
### Dynamic plotting ###
def plot_dynam():

    f, axarr = plt.subplots(2, sharex=True) # Two subplots, the axes array is 1-d
    axarr[0].plot(T, N, 'G')
    axarr[0].set_ylabel("Carrier Conc ($cm^-3$)")
    axarr[0].set_title('Laser-Rate Simulation')
    axarr[1].plot(T, S, 'B')
    axarr[1].set_ylabel("Photon Conc ($cm^-3$)")
    axarr[1].set_xlabel("Time (s)")
    plt.show()

    return;
```

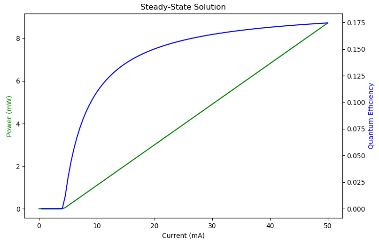


- This routine plots the dynamic photon and carrier concentrations (Vs time).
- The solver is run for one input current.
- Generally this routine should be run up to $1e^{-9}s$, so the dynamic behaviour can been seen clearly.

LI output

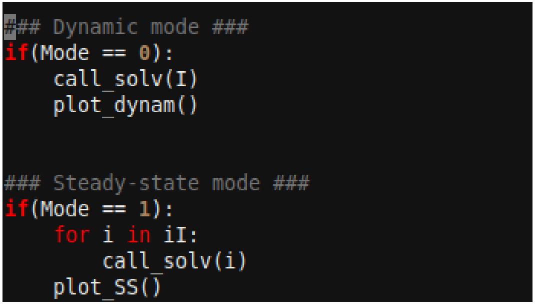


```
### Function for post solver steady-state LI calculations ###
def plot_SS():

    ### Post solver calculations
    P          = [h*f*((i*V)/tp)*1e3 for i in S_end]        # Power output (mW)
    QE         = [i/j for i,j in zip(P, iIA)]               # Convert for quantum efficiency

    ### Plotting two parameters on one plot ###
    fig, ax1 = plt.subplots()
    ax2 = ax1.twinx()
    ax1.plot(iIA, P,  'g-')
    ax2.plot(iIA, QE, 'b-')
    ax1.set_xlabel('Current (mA)')
    ax1.set_ylabel('Power (mW)', color='g')
    ax2.set_ylabel('Quantum Efficiency', color='b')
    plt.title("Steady-State Solution")
    plt.show()

    return;
```



- This routine plots the steady-state output power Vs input current.
- The solver is run for a range of input current $(0 \rightarrow 50mA)$.
- Generally this routine should be run up to $1e^{-8}s$, so the laser is in a stable operating point when power value is extracted.
- Post-processing of data is taking place to convert photon concentration to output power.

"Main" section

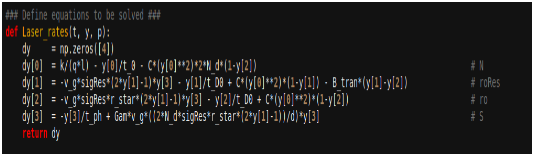


```
### Dynamic mode ###
if(Mode == 0):
    call_solv(I)
    plot_dynam()


### Steady-state mode ###
if(Mode == 1):
    for i in iI:
        call_solv(i)
    plot_SS()
```

- This portion of the code is implementing the two different operational modes of the code.
- It can be noted for the LI operation the solver is called repeatedly for an increasing input current.

Code extension

Extending the code



```python
### Define equations to be solved ###
def Laser_rates(t, y, p):
    dy     = np.zeros([4])
    dy[0]  = k/(q*l) - y[0]/t_0 - C*(y[0]**2)*2*N_d*(1-y[2])                                    # N
    dy[1]  = -v_g*sigRes*(2*y[1]-1)*y[3] - y[1]/t_D0 + C*(y[0]**2)*(1-y[1]) - B_tran*(y[1]-y[2])     # roRes
    dy[2]  = -v_g*sigRes*r_star*(2*y[1]-1)*y[3] - y[2]/t_D0 + C*(y[0]**2)*(1-y[2])                 # ro
    dy[3]  = -y[3]/t_ph + Gam*v_g*((2*N_d*sigRes*r_star*(2*y[1]-1))/d)*y[3]                        # S
    return dy
```

- The main aim of this presentation was to introduce a simple functioning solver for the laser-rate equations.
- A basic functioning template can then be extended in any number of ways to model various laser parameters.
- It can then be included with various other further models such as travelling-wave models or scattering matrix method models to capture higher levels of laser behaviour.

Bibliography

Bibliography

Buus, Jens, Markus-Christian Amann, and Daniel J. Blumenthal (2010). *Fundamental Laser Diode Characteristics*. Pp. 7–41. ISBN: 0471208167. DOI: 10.1109/9780470546758.ch2.

Cartledge, J. C. and R. C. Srinivasan (1997). “Extraction of DFB laser rate equation parameters for system simulation purposes”. In: *Journal of Lightwave Technology* 15.5, pp. 852–860. ISSN: 1558-2213. DOI: 10.1109/50.580827.

The End