C1 Lithium-Cluster Dynamics under Electron Bombardment – MATLAB

Numerical approach

Simulator: MATLAB (short for MATrix LABoratory) is an environment for technical computing based on matrix and vector operations. One can use it either interactively (by typing the commands directly on the screen) or by programming (creating a m-file of commands). The computations of the following problem were done with MATLAB version 5.3. SIMULINK, an extension to MATLAB offers a graphical modelling environment enabling the user to operate on complex systems on a high abstraction level.

Model: The approach followed in this solution is based on a straightforward SIMULINK model. The graphical model description is given in figure 1.

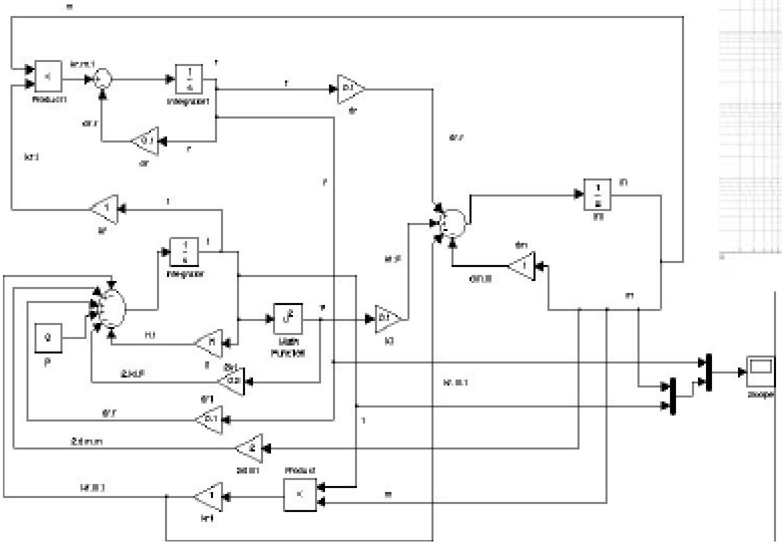

Figure 1: SIMULINK Model

Task a: Simulation of the System: After the model was built with the SIMULINK editor, a MATLAB-file was used to start the simulation. Computation times were determined with the `tic/toc` command. Figure 2 lists the different computing times.

Algorithm	Computing time
Dormand-Prince	1.27 s
mod. Rosenbrock	0,22 s
NDF	0,17 s

Figure 2: Computing times

As the system is stiff, the NDF- and the modified Rosenbrock algorithm are much more efficient, while a classical RK - algorithm (although using a sophisticated stepsize control as in Dormand-Prince algorithm) works inefficient and becomes unstable.

Task b: Parameter Variation: The parameter l_f was changed by use of the following commands (results in fig. 3):

```
for n = 1:5; lf = 10^(2+(n-1)/2);
set_param('comp1/lf', 'Gain', 'lf')
[t, x, y] = sim('comp1');
switch(n)
case 1;  m1(:,1) = x(:,1); t1 = t;
…………
case 5;  m5(:,1) = x(:,1); t5 = t;
end; end
loglog(t1,m1(:,1),t2,m2(:,1),…)
```

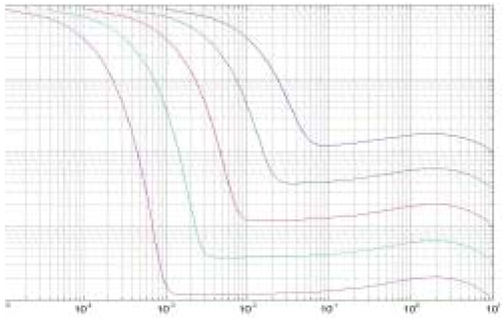

Figure 3: f(l_f, t) vs. t in logarithmic scale for 5 different values of l_f

Task c: Calculation of steady states: The command `trim` computes the equilibrium points of a system, in our case f(r,m,f). `trim` returns a vector [r_s, m_s, f_s] with f(r_s, m_s, f_s) = 0 (results in fig. 4):

```
set_param('comp1/p', 'Value', '10000');
[x] = trim('comp1')
```

The results are given in the following table.

p	rs	ms	fs
0	-0.5*10-12	~0	~0
10000	1000	10	10

Figure 4: Results for steady states

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