Requirements:

xsltproc
python 2.5 or higher
python modules:

- lxml
- numpy
- matplotlib (optional)

How to get elements tool as git repository:

Open terminal and type:

>>> git clone git@github.com:exciting/elements.git

Now the scripts should be located at ./elements .
For the moment, one has to checkout the experimental branch:

>>> cd elements
>>> git checkout experimental

From now on this directory will be referred to as *ELEMENTSPATH*.

Setup:

The setup consists of a nested python dictionary. See http://exciting-code.org/elements-tool for more information on the general concepts.
In the case that automatic convergence should be performed, two further keys have to be defined:

- autoconvergence:{...} which inherits the main definitions for the convergence
- autoconv:True with the value *True* for autoconvergence switched on, and False else.

Starting calculations:

Execute elements.py with your setup as argument:

>>> ELEMENTSPATH/elements.py setup.py

Now, calculations for the initial parameters are performed. Once finished, the fitting procedure is started, and determined if convergence is reached. While convergence is not reached, the calculation steps are repeated iteratively.

Output:

eos_data.xml	Output for equation of states and parameters for Birch-Murnaghan fit.
auto_conv.xml	Parameters and errors for every convergence step.