

Handout: Handy Computer Tools

T. Satogata: June 2011 USPAS Accelerator Physics

June 13, 2011

This is a description of a few computational tools that I've found to be very useful as a working physicist. This handout is more to note that these tools exist, and to indicate how they might be used in class. It is not meant to replace full documentation for any of these tools, nor is it meant to imply that any of these tools are any better or worse than what you might already be using!

1 Mathematica

Mathematica is the industry standard among symbolic manipulation codes, and it also does arbitrary-precision calculations. If you are fortunate enough to have a license (usually through a lab or student/educational discount), you probably already know how to use it. Matrices are entered with curly brackets, e.g. $\{\{1, L\}, \{0, 1\}\}$, and matrix multiplication and vector dot products are performed using a period, e.g. "a.b". Functions are capitalized and use square brackets to surround arguments, and `Simplify[]` is used to aggressively simplify algebraic expressions. One common stumbling block for a beginner is that the trace function is `Tr[]`; `Trace[]` is used to trace variables, not to calculate matrix traces.

```
In[12]:= qdh = {{1, 0}, {1 / (2 * f), 1}}
In[13]:= qfh = {{1, 0}, {-1 / (2 * f), 1}}
In[14]:= d = {{1, L / 2}, {0, 1}}
In[21]:= Simplify[qfh.d.qdh.qdh.d.qfh]
Out[21]= {{1 -  $\frac{L^2}{8 f^2}$ ,  $L + \frac{L^2}{4 f}$ }, { $\frac{L (-4 f + L)}{16 f^3}$ ,  $1 - \frac{L^2}{8 f^2}$ }}
In[31]:= Tr[Simplify[qfh.d.qdh.qdh.d.qfh]]
Out[31]=  $2 - \frac{L^2}{4 f^2}$ 
```

Figure 1: A simple Mathematica FODO cell calculation.

2 Wolfram Alpha

The **Wolfram Alpha** "Computational Knowledge Engine" includes an interface to some simple but powerful and convenient Mathematica tools, including numerical and symbolic analysis:

<http://www.wolframalpha.com>

Its big drawback is that you cannot define variables, but it has two big advantages: it's free, and it's in a browser so it's portable. It's extremely useful for one-off calculations, particularly when you can edit your entry in a text editor and then cut and paste it into the Alpha query window. See Fig. (2) for a simple FODO cell matrix calculation in Alpha.



Figure 2: A simple FODO cell calculation, and a calculation of required magnetic field to bend a $q = e$, $p = 3 \text{ GeV}/c$ particle through a bending radius of $\rho = 10 \text{ m}$ in Wolfram Alpha.

Both **Google** and Alpha also serve as excellent symbolic calculators and unit converters. For example, type

$$3 \text{ GeV}/c / (1.602e - 19 \text{ Coulombs} * 10\text{m}) \text{ in Tesla} \tag{1}$$

to calculate that it takes a 1 T magnet to bend a $q = e$, $p = 3 \text{ GeV}/c$ particle with a bending radius of $\rho = 10 \text{ m}$. Also see Fig. (2). These nice online unit-friendly calculators will often get confused about certain symbols. For example, they get confused between e as the base of natural logarithms vs the charge of the electron. In the above example I just used a number I know, but Alpha also will recognize it if you type q_e .

Alpha also gives some comparisons to magnetic induction and polarization. Such a magnet would be comfortably under saturation if made out of good iron, but would be horribly saturated and probably infeasible if made out of nickel.

3 yacas

Recall that one of Wolfram Alpha's drawbacks is that it only evaluates single statements; it's not really a full free interpreter. Fortunately there are a few free symbolic algebra interpreters out there of varying complexity. Perhaps the most lightweight is **yacas**, yet another computer algebra system, available with source code from

<http://yacas.sourceforge.net>

yacas is no longer being maintained, but it is still useful. You can download the source code and compile it fairly easily for a simple command-line interpreter. There is also a console view (beneath the "My Yacas" tab on the above website) that can be used from a web browser connected to the internet. The syntax is close to Mathematica, but $:=$ is used for variable assignment, functions delineate arguments with parentheses, and $*$ is used for matrix multiplication.

Yacas also does not simplify algebraic expressions by default, so you will find yourself using `Simplify()` in almost every evaluation. Yacas also has a hard time automatically reducing polynomial fractions, as seen in Fig. (3). Nonetheless, it is useful for simple symbolic and

algebraic calculations, and it can also perform numerical evaluation. However, yacas does not integrate with common plotting programs such as **gnuplot**.

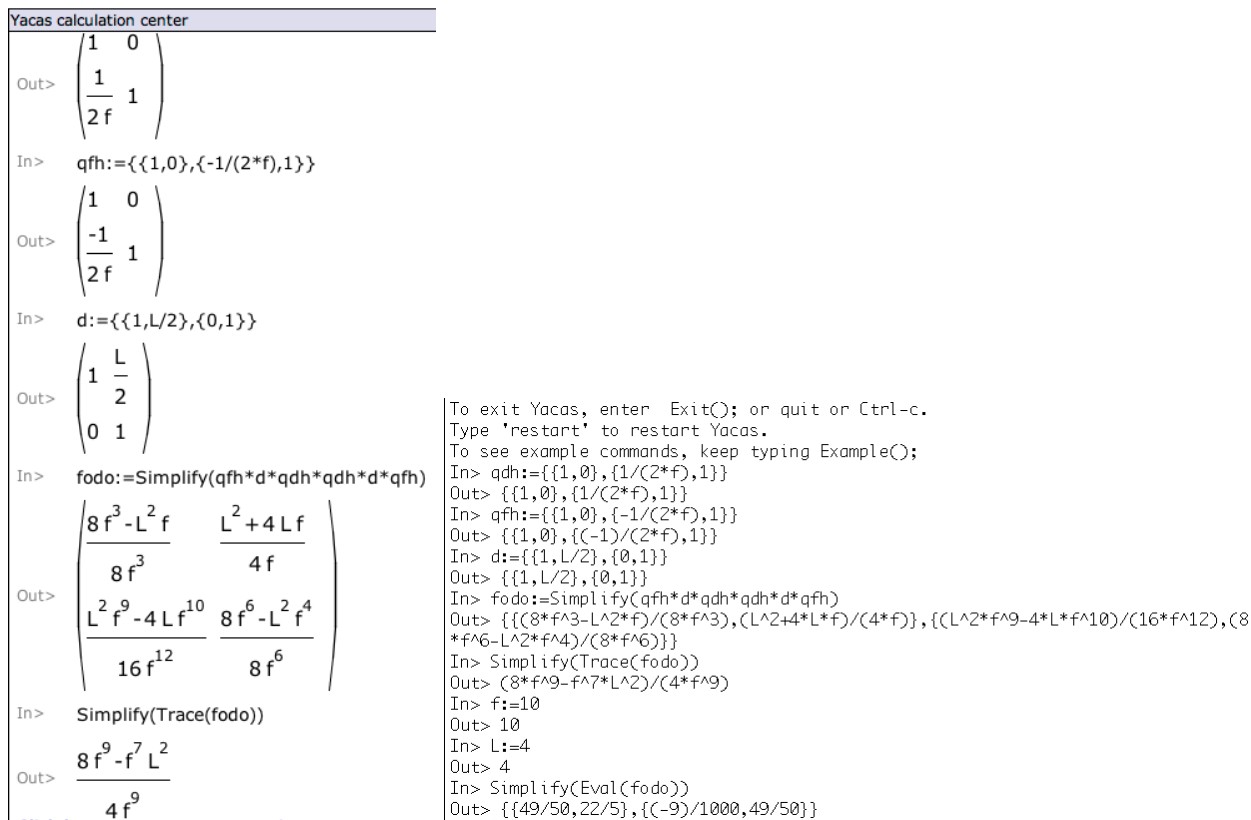


Figure 3: A simple FODO cell calculation in the web interface (left) and terminal interface (right) to yacas. The terminal interface example also shows numerical evaluation.

4 maxima

maxima is much more heavyweight (the user's guide is nearly 1000 pages long), but is also very well-supported and free. It is derived from Macsyma, a symbolic algebra system developed by MIT and DOE from the late 1960's to 2000. It is available with source code from

<http://maxima.sourceforge.net>

maxima's symbolic interpreter is implemented in LISP, no surprise since it originated at MIT. The syntax is thus a bit more arcane to those who are familiar with the Mathematica expression style; it will be more familiar to those who program elisp in emacs. For example, assignments are made with `:`, not with an equals sign as in Mathematica or `:=` as in yacas. Matrices are declared with the `matrix()` function. Instead of `Simplify()`, you should generally use `factor(expand())` around most algebraic expressions to simplify them as much as possible. All statements must end with a semicolon; you can get very confused if you forget it as the interpreter will look like it's hung waiting for your input. An example interpreter session is shown in Fig. (4).

maxima also has the advantage of integrating well with **gnuplot**, so it can be used to plot fairly complex functions (see pp. 117 and onward of the manual). There are also many nice GUI programs available, such as **wxmaxima**; these give a much nicer display than maxima from the command line.

```

(%i1) d: matrix([[1,L/2],[0,1]);
      [  L ]
      [ 1  - ]
      [  2  ]
      [  0  1 ]
(%o1)
(%i2) qdh: matrix([[1,0],[1/(2*f),1]);
      [ 1  0 ]
      [  1  ]
      [ --- 1 ]
      [ 2 f  ]
(%o2)
(%i3) qfh: matrix([[1,0],[-1/(2*f),1]);
      [ 1  0 ]
      [  1  ]
      [ - --- 1 ]
      [ 2 f  ]
(%o3)
(%i4) fodo: factor(expand(qfh.d.qdh.qdh.d.qfh));
      [ 2 2 ]
      [ L - 8 f L (L + 4 f) ]
      [ - ---- - ---- ]
      [ 8 f 4 f ]
      [ 2 2 ]
      [ L (L - 4 f) L - 8 f ]
      [ ---- - ---- ]
      [ 3 2 ]
      [ 16 f 8 f ]
(%o4)
(%i5) load(funcs)
;
(%o5) /opt/local/share/maxima/5.24.0/share/simplification/funcs.mac
(%i6) tracematrix(fodo);
      2 2
      L - 8 f
      - ----
      2
      4 f
(%o6)
.....

```

Figure 4: A simple FODO cell calculation in the terminal interface for maxima.

5 Matlab

You may also be familiar with **Matlab**, a numerical analysis program that is widely used particularly for signal processing and excellent numerical matrix analysis tools. It excels at analysis of large sparse matrices. Matlab does not perform any symbolic algebra. Matlab can be even more costly than Mathematica, but it is particularly useful for design and modeling of time-varying systems with a powerful graphical environment called **Simulink**.

The **AT accelerator toolbox**, developed at SLAC and available at

<http://ssrl.slac.stanford.edu/at>

is particularly popular for accelerator modeling and high-level controls at many light sources around the world. It is implemented fully within Matlab, and requires Matlab licenses to run.

6 Octave

Since Matlab can be expensive (several thousands of dollars for a single license), there is a free program called **Octave** that replicates much of the numerical and matrix analysis with a very similar syntax. Octave is part of the GNU project but is not directly developed or supported by the FSF (Free Software Foundation). Octave is installed on the Linux systems in our computer labs, and many of the programs in this class's computer labs use octave as an underlying fast matrix calculator. Octave does not have built-in graphics like Matlab does,

so Matlab user interface code (including AT) is not trivially portable to Octave. However, Octave can produce many plots that Matlab can by invoking gnuplot as a plotting tool.

Matlab and Octave have a syntax much closer to C. Assignment is done with = and matrix multiplication is done with *. Matrices are surrounded with square brackets, with commas separating elements and semicolons separating rows. A semicolon at the end of a statement also suppresses output. A simple numerical FODO cell example, including calculation of eigenvalues and phase advance/cell, is shown in Fig. (5).

```

octave-3.0.3:1> f=11.1312;           # focal length [m]
octave-3.0.3:2> l=29.79;          # fodo cell length [m]
octave-3.0.3:3> qdh=[1,0;1/(2*f),1]; # Half defocusing quad matrix
octave-3.0.3:4> qfh=[1,0;-1/(2*f),1]; # Half focusing quad matrix
octave-3.0.3:5> d=[1,l/2;0,1];    # Drift matrix
octave-3.0.3:6> fodo=qfh*d*qdh*qdh*d*qfh # fodo cell, printed
fodo =

    0.104703    49.721456
   -0.019892     0.104703

octave-3.0.3:7> [V,lambda]=eig(fodo) # Find and print eigenvalues, eigenvectors
V =

    0.99980 + 0.00000i    0.99980 - 0.00000i
   -0.00000 + 0.02000i   -0.00000 - 0.02000i

lambda =

    0.10470 + 0.99450i    0.00000 + 0.00000i
    0.00000 + 0.00000i    0.10470 - 0.99450i

octave-3.0.3:8> # Calculate phase advance/cell mu for this FODO cell next
octave-3.0.3:8> mu=acos(real(lambda(1,1)))*360/(2*pi)
mu = 83.990

```

Figure 5: A simple numerical FODO cell calculation in Octave.