Generalizing numerical calculations

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There are two main approaches to the solution of physical problems: mathematical analysis and numerical computations. Mathematical derivations are usually considered to be on a higher plane. Classic derivations like the Pierce planar gun require sophisticated operations and give broad insights into the design of a variety of charged-particle injectors. In contrast, numerical solutions may have application only to specific systems, and the perception is that the computer does all the thinking. On the other hand, many mathematical derivations lead to complex series expressions that give little insight and must be evaluated numerically for specific cases. Similarly, numerical results can achieve considerable generality with preliminary analysis. This tutorial has two functions:

- Illustrate an application to scaling parameters to a numerical solution.
- Show how Windows batch files may be used to control a large set of calculations.

We will consider the simple example of the transit time Δt of a charged particle in a planar acceleration gap with a uniform electric field. At high voltages, relativistic effects are important. The solution becomes more complex because the particle's mass changes crossing the gap. The **Trak** program provides high accuracy results by dividing the trajectory into hundreds of steps and interpolating the final state crossing the exit boundary. The parameters for the calculation are the gap width d, the applied voltage V_o, the particle rest mass m_o and charge q. Relativistic effects are important when the parameter

$$\alpha = \frac{qV_o}{m_o c^2} \tag{1}$$

is comparable to or greater than unity. In the limit $\alpha \gg 1$, the transit time is

$$\Delta t \approx \frac{d}{c}. \tag{2}$$

In the non-relativistic limit ($\alpha \ll 1$), the distance traversed by a particle in time Δt is $d = a\Delta t^2/2$ where the acceleration is $a = eV_o/dm_o$. The transit time is therefore

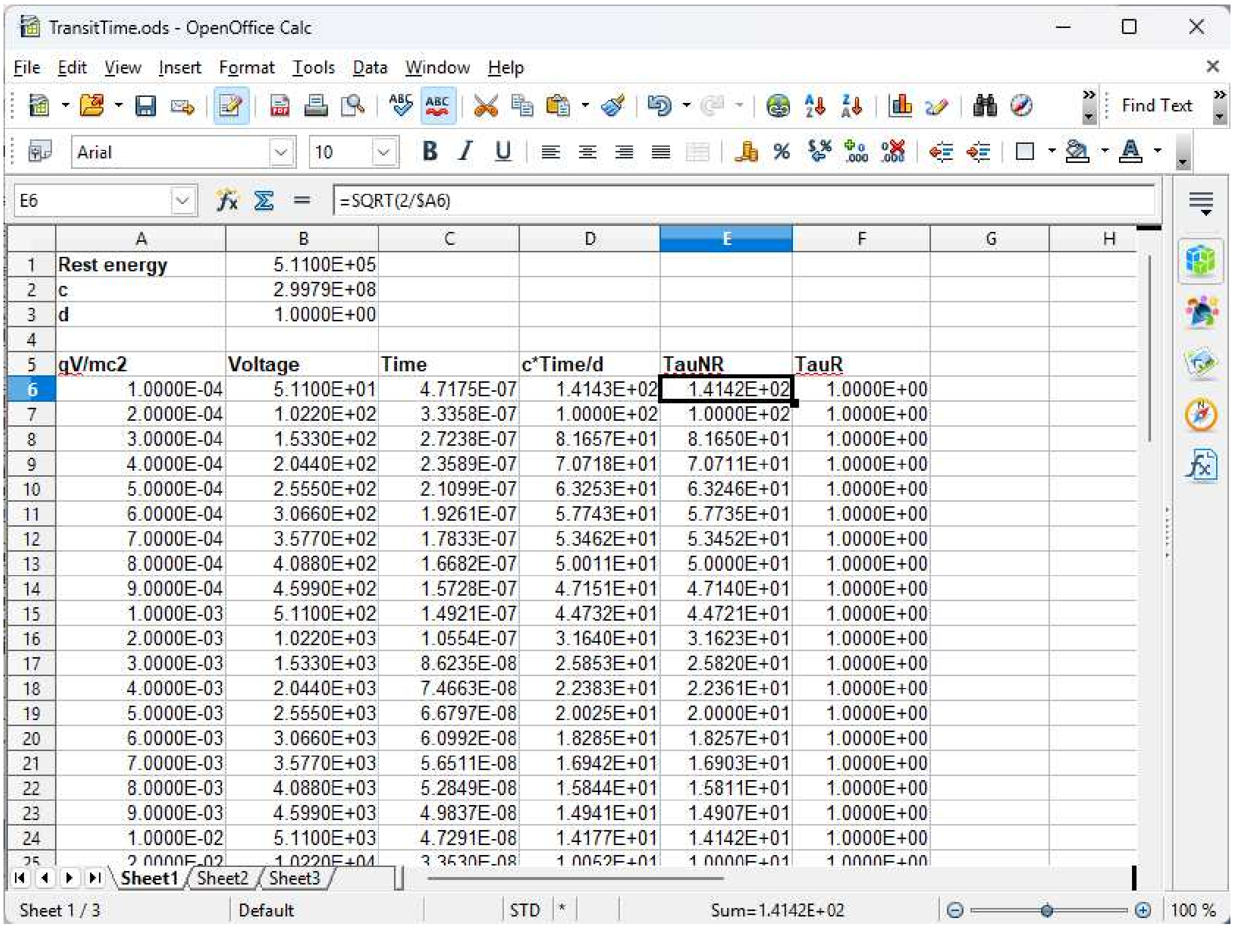
$$\Delta t = d\,\sqrt{\frac{2m_o}{qV_o}} = \frac{d}{c}\,\sqrt{\frac{2m_oc^2}{qV_o}}. \tag{3}$$

If we define the dimensionless transit time $\tau = c\Delta t/d$, then τ approaches unity when $\alpha \gg 1$ and is given by

$$\tau = \sqrt{\frac{2}{\alpha}}, \tag{4}$$

when $\alpha \ll 1$. The scaling relationships suggest a solution strategy. First, calculate transit times for a specific particle (q and m_p) and a specific gap width d over a range of voltage V_o. Then, make tables and graphs of results in terms of the parameters α and τ. These results can then be applied to any particle type, voltage or gap spacing.

The **Trak** calculation in planar symmetry is performed for an electron in a solution box of length in x of $d = 1.0$ m with an arbitrary width in y of 0.2 m. The x boundaries have fixed voltages and



TransitTime.ods - OpenOffice Calc

E6 =SQRT(2/$A6)

	A	B	C	D	E	F	G	H
1	Rest energy	5.1100E+05						
2	c	2.9979E+08						
3	d	1.0000E+00						
4								
5	qV/mc2	Voltage	Time	c*Time/d	TauNR	TauR		
6	1.0000E-04	5.1100E+01	4.7175E-07	1.4143E+02	1.4142E+02	1.0000E+00		
7	2.0000E-04	1.0220E+02	3.3358E-07	1.0000E+02	1.0000E+02	1.0000E+00		
8	3.0000E-04	1.5330E+02	2.7238E-07	8.1657E+01	8.1650E+01	1.0000E+00		
9	4.0000E-04	2.0440E+02	2.3589E-07	7.0718E+01	7.0711E+01	1.0000E+00		
10	5.0000E-04	2.5550E+02	2.1099E-07	6.3253E+01	6.3246E+01	1.0000E+00		
11	6.0000E-04	3.0660E+02	1.9261E-07	5.7743E+01	5.7735E+01	1.0000E+00		
12	7.0000E-04	3.5770E+02	1.7833E-07	5.3462E+01	5.3452E+01	1.0000E+00		
13	8.0000E-04	4.0880E+02	1.6682E-07	5.0011E+01	5.0000E+01	1.0000E+00		
14	9.0000E-04	4.5990E+02	1.5728E-07	4.7151E+01	4.7140E+01	1.0000E+00		
15	1.0000E-03	5.1100E+02	1.4921E-07	4.4732E+01	4.4721E+01	1.0000E+00		
16	2.0000E-03	1.0220E+03	1.0554E-07	3.1640E+01	3.1623E+01	1.0000E+00		
17	3.0000E-03	1.5330E+03	8.6235E-08	2.5853E+01	2.5820E+01	1.0000E+00		
18	4.0000E-03	2.0440E+03	7.4663E-08	2.2383E+01	2.2361E+01	1.0000E+00		
19	5.0000E-03	2.5550E+03	6.6797E-08	2.0025E+01	2.0000E+01	1.0000E+00		
20	6.0000E-03	3.0660E+03	6.0992E-08	1.8285E+01	1.8257E+01	1.0000E+00		
21	7.0000E-03	3.5770E+03	5.6511E-08	1.6942E+01	1.6903E+01	1.0000E+00		
22	8.0000E-03	4.0880E+03	5.2849E-08	1.5844E+01	1.5811E+01	1.0000E+00		
23	9.0000E-03	4.5990E+03	4.9837E-08	1.4941E+01	1.4907E+01	1.0000E+00		
24	1.0000E-02	5.1100E+03	4.7291E-08	1.4177E+01	1.4142E+01	1.0000E+00		
25	2.0000E-02	1.0220E+04	3.3530E-08	1.0052E+01	1.0000E+01	1.0000E+00		

Sheet 1 / 3 Default STD * Sum=1.4142E+02 100 %

Figure 1: Spreadsheet to record input and output quantities for the numerical calculation and to generate scaled quantities.

the boundaries in y assume a Neumann condition to define a planar electric field. The reference electrostatic calculation in **EStat** has an applied voltage equal to the electron rest energy in eV, $V_o = 510998.95$ V. The **Trak** input file `TransitTime.TIN` has the following content:

```
FIELDS
  EFILE: TransitTime.EOU %1
  DUNIT:   1.0000E+00
END
PARTICLES TRACK
  PLIST
*   Mass    Charge   KEng     x       y     z    ux   uy   uz
    0.0      -1.0     0.0   1.0E-6  0.00 0.00 0.00 0.00 0.00
  END
END
DIAGNOSTICS
  PARTLIST
END
ENDFILE
```

The symbol %1 represents a multiplication factor for the input electric field, in this case the value of α. The procedure is to determine a large set of transit time values by calling **Trak** from a Windows batch file multiple times with α as a pass parameter. The output data is used to construct tables and graphs of τ as a function of α. We'll first consider generating and displaying the data and then discuss batch file techniques.

Figure 1 show one possible approach to data manipulation by using a spreadsheet. Physical parameters for the specific calculation are shown at top-left: the electron rest energy in eV, the speed of light and the gap width. Column A lists the set of 46 values of α spanning five orders of magnitude (0.0001 to 10.0). Column B displays α times the rest energy, equal to applied voltages for electron acceleration. Column C lists the values of electron transit in seconds determined by **Trak** for each electric field multiplication factor. Column D lists the normalized transit time τ. The remaining columns show values of τ in the non-relativistic (Eq. 4) and ultra-relativistic limits.

The data in Columns D, E and F can used to create spreadsheet plots or copied and pasted into a scientific plotting program to create graphs like Fig. 2. The figure shows the calculated normalized transit time along with the non-relativistic (orange) and relativistic (blue) predictions. The lower end of the voltage range was omitted because the agreement between the code and prediction was almost exact.

To conclude, we'll discuss some Windows batch file techniques to carry out solution sets in **Trak** and to arrange data in a useful form. A convenient method to create and to run basic batch files is with the *Task* commands in **FPController**. Clicking *Create task* opens the dialog of Fig. 3. Entering the values shown and clicking *OK* produces the file `TransitTime.BAT` with the content

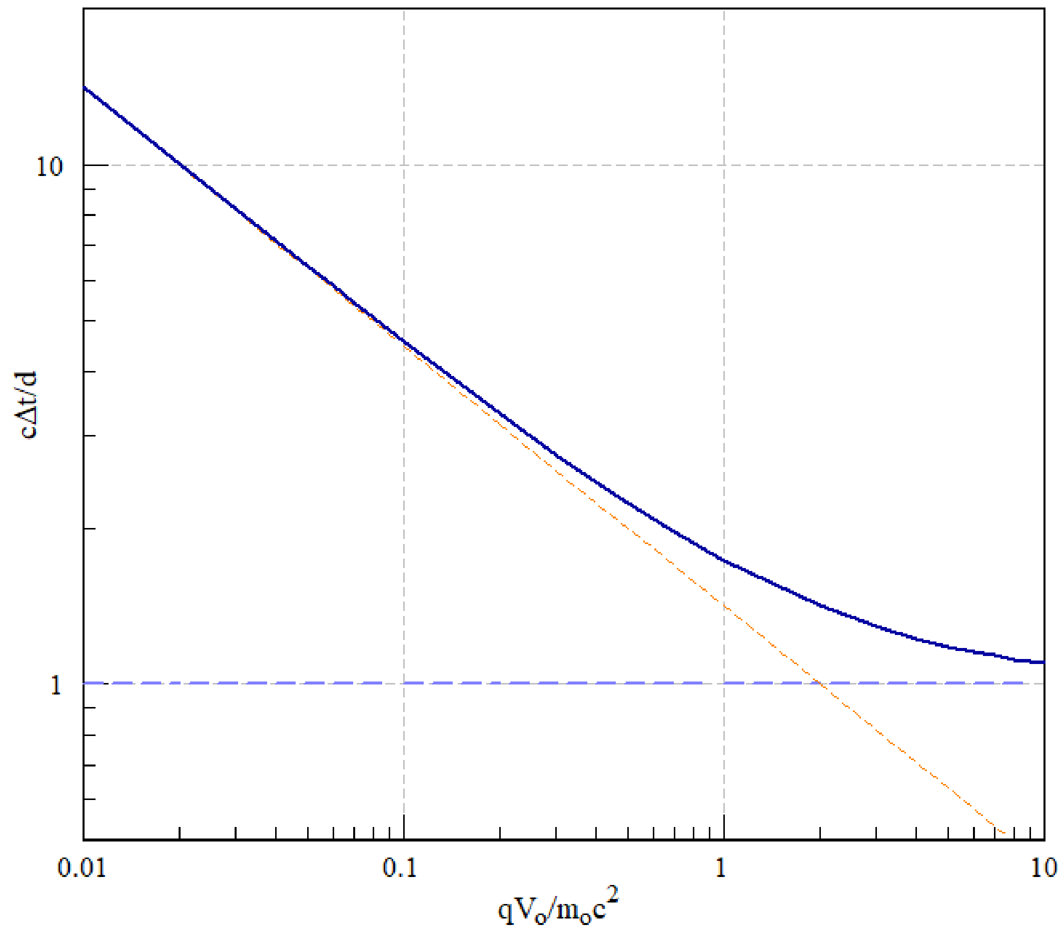


Figure 2: Plot of normalized transit time τ as a function of the normalized applied voltage α. Ornage line: non-relativistic limit. Blue line: relativistic limit.

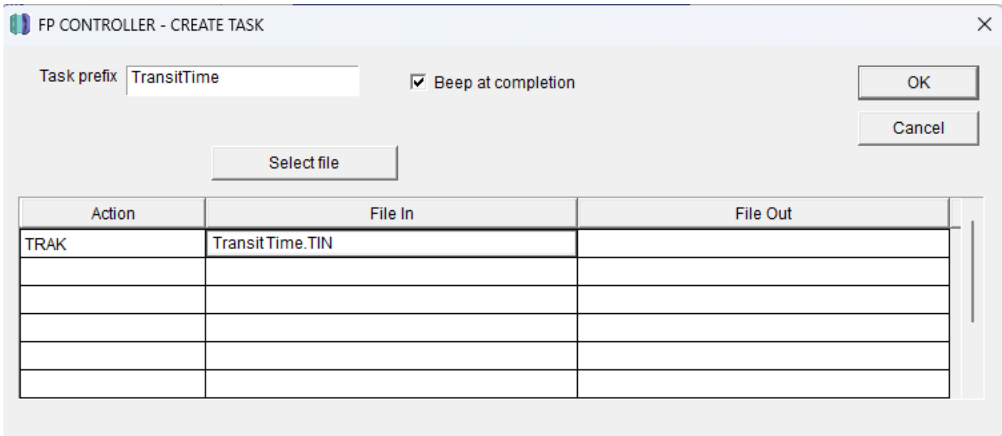


Figure 3: The Create task dialog of FPControl with settings to define the initial setup of TransitTime.BAT.

```
REM FP Controller batch file, Field Precision
START /B /WAIT C:\fieldp/tricomp/trak.exe TransitTime
START /B /WAIT C:\fieldp\NOTIFY.EXE
IF EXIST TransitTime.ACTIVE ERASE TransitTime.ACTIVE
```

To perform a set of forty-six calculations and to record the results of interest in a convenient form, we need to make two modifications[1]. First, replicate the *Start* command line to run **Trak** forty-six times and add the multiplication factors from Column *A* of the spreadsheet as pass parameters:

```
START /B /WAIT C:\fieldp/tricomp/trak.exe TransitTime 1.0E-4
START /B /WAIT C:\fieldp/tricomp/trak.exe TransitTime 2.0E-4
START /B /WAIT C:\fieldp/tricomp/trak.exe TransitTime 3.0E-4
...
```

There are two problems running the batch file in this form.

- The transit time is listed in the *Momentum table* of the listing file `TransitTime.TLS` in response to the *PartList* command. Each run erases the output files of the previous one, so that only the final file remains.
- The listing file documents extensive information about the run. The appropriate text line in the *Momentum Table* is one of over one hundred lines in the file. If each listing file is renamed and saved, it would take considerable work to pick the single numbers of interest.

Both issues can be resolved with a standard Windows batch command. The batch file is modified to this form.

[1]The best way to edit batch files is with a text editor such as **ConText** with advanced features like column selection and macros.

```
IF EXIST Abstract.txt ERASE Abstract.txt
START /B /WAIT C:\fieldp/tricomp/trak.exe TransitTime 1.0E-4
findstr /l /c:"0.0000E+00  0.0000E+00  0.0000E+00" TransitTime.TLS >> Abstract.txt
START /B /WAIT C:\fieldp/tricomp/trak.exe TransitTime 2.0E-4
findstr /l /c:"0.0000E+00  0.0000E+00  0.0000E+00" TransitTime.TLS >> Abstract.txt
...
```

The *findstr* command identifies lines of text in the file `TransitTime.TLS` that contains a specific string pattern. In this case, the pattern is the start of the line in the *Momentum Table* given by

```
/c:"0.0000E+00  0.0000E+00  0.0000E+00"
```

The /l parameter specifies that the string should be interpreted literally rather than as a regular expression. The text

```
 >> Abstract.txt
```

specifies that the text line should be redirected and added to the file `Abstract.txt`. After the run, the file contains forty-six data lines with transit times in the last column. This column can be grabbed with a text editor and added to the spreadsheet as Column *C*. Input files for the calculations are available at: `https://www.fieldp.com/example_library/TransitTime.html`