Spekwin32 – Securing the future by developing a successor
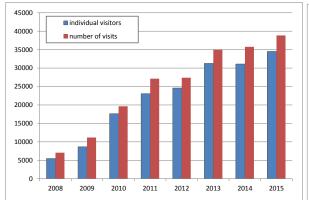
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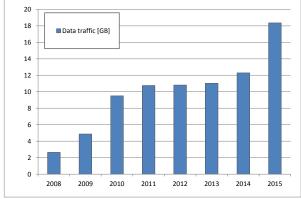
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1   Motivation

When Spekwin32 as optical spectroscopy software was first put to use in early 2000, it was just a little tool for me and about five fellow PhD students from my physical chemistry workgroup at Universität Konstanz. Within the following year it found more users throughout the chemistry department and finally the first (German only) website was created end of 2001. Its first citation in a published outside scientific work (a PhD thesis) was in 2004, which was the same year when I created an English version of the software and also the website. During all the years since, website traffic and download numbers were steadily growing, as well as its user base in academic and industrial settings. The range of functionalities, the performance and the ease-of-use were continuously improved. In the year 2010, the commercial licensing scheme was introduced, which earns enough revenues to pay the expenses since then, but not much more. And stays far away from any relationship with expenditure of time, obviously.

This is today's picture (as of 02/2016):

- An estimated 10,000 – 15,000 satisfied users from all over the world, 95% thereof academics.
- About 5000 individuals downloading the software per year.
- Direct interaction, support, problem solving with about 400 individual users every year
- 110+ scientific publications mentioning the use of Spekwin32
- 70+ companies purchased commercial licenses since 2010
- File size of installation file rising from 1.1MB in 2001 to 1.9 MB in 2016
- 1 person handling everything during his *spare time*

From the beginning, I always kept these four goals in mind while developing Spekwin32:

- Free the data from the spectrometer
- Bring all sorts of spectra together
- Visualize/ analyse multiple spectra at once
- Be useful, or else get out of the user's way

Now, you say: fine, software going strong! Why should there be a need to change anything?

Because it is also growing old and reaches the limitation of its outdated foundations. Read more about this in the next chapter!

2   Modernization

2.1   New development environment, new technology level

2.1.1   Development platform

Spekwin32 is developed in Object Pascal, currently by using Delphi 4.0 from 1998. It is working great and is smoothly running on Win 7, Win 8.1 and even Win10, but still becomes outdated now. The successor will be developed using Embarcadero Delphi XE5, which is up-to-date with current development technologies.

2.1.2   32bit vs. 64bit, Unicode

While the current 32bit Spekwin32 performs well even on 64bit platforms, there are some advances to have a native 64bit application, created with an up-to-date 64bit compiler. For use on older systems, a 32bit version of the successor will also be created. The new development tool allows full Unicode support, which simplifies import of modern data files and interaction with other software.

2.1.3   Modern FileOpen/ FileSave dialogs

The change to the up-to-date Delphi version brings the possibility to use today's standard FileOpen and FileSave dialogs. This is quite a nuisance with the current Spekwin32.

2.1.4   Internationalization/ Localization

The possibility of having versions in different languages will be build right into the core of the software. For the initial version, two languages are planned: English and German. Further languages will be introduced, provided that there is a need for it and native speaking & educated users are found, that are willing to help.

2.1.5   Windows Certificate

Currently, during each installation of Spekwin32, Windows issues an "unknown publisher" warning, with increasing alarmism for the newer Windows versions. In order to produce a digitally signed installation file for going through installation without troubles, it is necessary to register as publisher and purchase a Microsoft authenticode certificate.

2.2   New name & icon

The name "Spekwin32" sounded like some advanced technology in 1999, because the 16bit ancestor was called "Spekwin"; however it is definitely outdated now. Same with the icon: it was a joke on the previous 16bit-Spekwin icon, which comprised a light bulb. The new icon's flash was intended to remind of Spekwin32's greatly enhanced processing speed.

Spekwin (16bit)   Spekwin32 (32bit)   Spectragryph (64bit), not finalized

The current name of *Spekwin32* gives rise to confusion and is not really unique, because there is other software like *SpecWin* from Instrument Systems, *WinSpec32* from Roper, *Spectrawin* from Horiba and so on. The new name *Spectragryph* is unique, hitherto unknown and fuses in its name the spectral graphing purpose with the iconic gryphon shape, which I use since many years here and there and in the social web.

2.3 New look & feel

The new user interface will consist of a basically flat design with clear shapes and reduced colours, thus omitting the shiny, flashy, shadow-casting 3D-rendered icons of the Win XP/ Win7 era. The menu functions and icons will be mainly organized in ribbons, as known from Office 2010. Some functions like zooming around in the plot will be touch-enabled.

2.4 More interactivity

For most functions, there is a dialog window with some options, but the effect of the functions is only seen after executing the function and closing the dialog window. It is much more user-friendly to show some kind of preview or live-view for the function's effect on the spectral data, thus allows direct parameter optimization and in consequence speeds things up and reduces workload. As an example, this was already implemented for the recently developed "Advanced Baselining" function.

2.5 Multiple plot windows

Easy overlay of multiple spectra within a single plot will always stay a key feature. However, there are situations where putting spectra into multiple plots is desirable. Therefore, the new version will have multiple plots, organized in browser-like "tabs". It should be possible to also transfer spectral between the tabs.

3 Expansion of functionality

3.1 More file formats

There are always unknown file formats left, some of the more important that should be included:

- Bruker OPUS *.0, *.dpt
- Thermo Nicolet OMNIC *.spa
- ASDI TerraSpec *.asd
- HITACHI *.usd
- Shimadzu *.irs (and *.spc, some kinds)
- Varian Cary Eclipse *.spc
- HP 8453 *.sd

3.2 Individual functions
- Kramers-Krohnig transformation
- Kubelka-Munk transformation
- determination of DNA/protein content
- calculation of labelling efficiency for fluorescent labelled DNA/proteins
- Peak finding based on polynomial fit
- Individual peak labels, editing peak labels, saving peak labels with spectra
- Staggered view, with a vertical offset between spectra
- Support and analyse time series kinetic data

3.3 Chemometrics data preprocessing

For many users, Spekwin32 is useful for executing intermediate steps in preprocessing spectral data for chemometric or statistic purposes. That is, to convert the original (often binary) data, then do parallel processing steps like spike removal, baseline correction, smoothing, normalization, and

finally batch export the spectral into a format recognized by the big chemometrics software packages. To make this application even more attractive, some additional functions will be helpful, especially for NIR applications:

- Detrending
- Standard Normal Variates (SNV)
- Multiplicative Scatter Correction (MSC)
- Generalize Least Squares (GLS)

3.4 Automation, Batch execution of sequence of steps

The above-mentioned use for data pre-processing will benefit much from the possibility of creating a predefined sequence of linked processing steps. This will be done with an easy-to-use interface for defining the step sequence, for adjusting each step's parameters and for saving the final sequence for later use. Once created, this named step sequence can be applied any time to an arbitrary number of spectra at once.

3.5 Spectral File Converter

Introduced for Spekwin32 version 1.72, batch export of loaded spectra is already possible. The successor will have a fully blown converter function, which will be able to convert spectral data files from a folder (with all subfolder optionally) by recursive iterative file search into all available export formats including multi-files and graphics files. A "watchdog function" is possible, doing automated conversion whenever new spectral content is produced in a certain folder.

3.6 Reporting

For use in a production environment, after conversion and pre-processing, two more steps are often needed for spectrum-based quality decisions and documentation:

- Evaluation and assessment of spectrum properties against predefined acceptance criteria. This includes some basic calculations and functions like peak finding or averaging spectral regions.
- Creation of reports for documentation of this status assessment. Actual report layout will be based on configurable report templates, together with the previously defined spectrum evaluation and assessment steps.

3.7 Spectral matching, library search

For spectrum-based identification of unknowns, a spectral similarity search against a database of known samples could be done. This database could be a simple collection of files within folders or else a commercial database format. The matching algorithm has to depend on measurement technology, as Raman spectra have to be compared differently than FTIR or NIR spectra. Spectral matching for UV/VIS absorbance or fluorescence data seems to be less important, since data is mostly too unspecific for successful identification.

3.8 Converting spectrum images

From hobbyists creating DIY spectrometers, amateur astronomers doing star spectroscopy, to gemmologists photographing the output of their hand spectroscope, many are in need of conversion functionality for turning spectrum images into spectral data. Useful functions for this purpose are:

- auto-location or user-assisted location of the spectrum part inside an image (pixel graphics)

- creating an intensity cross-section for the spectrum image, with averaging in perpendicular direction of the spectrum axis
- automated/ user-assisted correction for curved slit images
- calibration of the wavelength scale with user-defined spectral lines
- correction of the detector sensitivity (already there)
- calculation of transmittance/ absorbance from sample + reference spectrum (already there)

3.9   Spectrometer hardware control

For a tool so capable in spectral data handling, controlling spectrometer hardware is a logical next step. To make this a success, adequate information on spectrometer hardware/ firmware communication protocols are mandatory. Some spectrometer manufacturers (like Ocean Optics) provide this for 3rd party developers, so Ocean Optics spectrometers might be a good start for this.

3.10 Other platforms

The new development environment Delphi XE allows developing code for multiple platforms. Currently it is possible to compile for Windows 32/ 64bit, for Mac OS X, iOS and Android. Thus, the software could in principle run on all Windows machines, Mac computers, iPads & iPhones and all Android smartphones and tablets. Which is a quite comprehensive range of devices. Of course, user interface then has to take care for lack of keyboard, touch and gesture functionality and strongly varying screen sizes…

3.11 Summary of new functionalities

From the first 292 responses to the Spekwin32 user feedback initiative , a good overview on the ranking for the above chapters could be found.

As expected, the spectral converter function is desired most, followed by the spectral library search. Report generation and conversion of spectral images are also much desired. Chemometrics data preprocessing and hardware control are seen as the less important areas of development.

Areas of development	Very Important	Important	Neutral	Somewhat Important	Not at all Important	N/A	Sum	Significance
data preprocessing for chemometrics application	55	55	74	25	38	44	291	805
automated execution of processing step sequence	37	80	84	29	30	31	291	845
spectral file converter	164	77	26	9	9	7	292	1233
result assessment + report generation	72	87	68	24	25	16	292	985
spectral matching, library search	131	81	37	18	15	10	292	1141
convert spectrum images, calibration of DIY spectros	77	91	57	19	20	27	291	978
spectrometer hardware control (like Ocean Optics)	43	65	67	23	56	36	290	778
run on other platforms (Mac OS X, iOS, Android)	59	52	79	23	55	23	291	841

4   Funding it

Since three years, I consider doing this, since three years I postponed it. The evenings and week-ends are just too short and too scattered, and my family is too important to me to sacrifice all available time for this. It will take an estimated three months of full-time work to get this ready. Therefore, from April 04, I will do a Kickstarter campaign in order to crowd-fund the development of the brand new modernized successor to Spekwin32.