SPIKE Relase Notes

0.99.3 - March 2019

- Development of Interactive tools, to be used within Jupyter - *should be extended in further releases* -
  - a tool for displaying multiresolution 2D FT-ICR-MS data-sets
  - simple interface in Jupyter for 1D NMR
  - (that part is not tested in python 2)
- `scale="auto"` in 2D display, choose a level `autoscalethresh` (default is 3) times above the noise floor.
- added `gaussenh` apodisation plugin for one-command gaussian enhancement.
- improved display of FTMS spectra
- improved `findnoiselevel` and `findnoiselevel_2D`
- modified `absmax` in NPKData - now a property
- added phase parameters to NMRAxis: `.P0` and `.P1`
- removed the old Visu2D program - use the jupyter notebook rather !

0.99.2 - January 2019

- added number of local peaks in bucketing
- improved Bruker importer and added support for NEO/TopSpin 4.0 files
- improved the `.set_unit()` method
- improved importing DOSY processed with TopSpin
- corrected a bug for min value in bucketing
- changed pylint/QC defaults -> new values (and corrected a bad bug)
- cleaned the code a little

0.99.1 - November 2018

- added the sane algorithm
- added the pg-sane algorithm
- added the `NPKData.set_unit(unit)` method for pipelining
- added the `NPKData.load_sampling(axis)` method for pipelining
- improved spinit support
- corrected a few bugs
- `NPKData.save_csv()` now works in python 3
- `NPKData.copy()` is now more robust

0.99 - April 2018 - temp release branch

We have been developping a lot this last year, and published quite a few results. The program is now quite stable in most of its features. Additions and improvements were added to the repository in the `devel` branch, however we neglected

updating the more official `default` branch. This release is an effort to bring everything into normal mode, and hopefully, preparing a 1.0 version !

New in 0.99:

- SPIKE is now fully compatible with python 2 AND python 3
- added the SANE noise denoising algorithm and plugin.
  - an improvement to urQRd
  - more faithfull to small signal intensity
  - slightly different optimum parameters (optimal rank slightly smaller, less iterations needed)
- added the handling of NUS 2D FTICR acquisition
- added the PALMA DOSY processing algo and plugin (NMR).
- added a Linear Prediction plugin
- added the first trial for a m/z calibration plugin (MS)
- added import from SpinIt (NMR)
- added a primitive set of interactive tools to be used in Jupyter notebooks (`INTER.py`)
- added the possibility to pass a complete dictionary to matplotlib in the .display() method
- added the .center() method for NPKData
- added a plugin implementing a subset of Topspin commands: xf1, xf2, xfb. (NMR)
- added an line fitter, still very exploratory, only 1D Lorentzian for the moment
- added more controls on plots (new_fig and mpldic arguments of `.display()`)
- added a Spinit importer (preliminary) (NMR)
- added a compress mode in Solarix importer (MS)
- added new automatic tests
- improved and extended the Bucketing plugin, with extended features
- improved the baseline correction code
- improved import/export to Topspin/Bruker NMR files
- improved automatic phaser `.apmin()` (NMR)
- improved the plugin mechanism - with added documentation
- corrected the extract() method which was broken

- corrected a bug when importing Topspin/Bruker NMR datasets, where $NC was not used. (NMR)
- corrected a bug and improved 3 parameters FT-ICR calibration (MS)
- corrected the extract function for NPKData
- corrected a bug with contour plots and matplotlib version > 1.5.0
- modified (improved?) plugin loading code, with additional plugin documentation
- modified the way None values are stored into hdf5 files
- modified `.extract()` code to work in current axis unit
- modified `.mean()` to return complex value is axis is complex
- improved python 3 compatibility. It is not finished yet, but most of the program is python 2/python 3 independent, some parts are still missing,
- known bugs
- `NPKData.extract()` method not fully tested
- `NPKData.save_csv()` is buggy in python 3

0.9 - 8 sept 2016

never reached the normal distribution - doc partly redundant with 0.8.3

- added a baseline correction plugins, already quite developed, with 3 different methods
- added an automatic phasing plugin, `.apmin()` still exploratory (NMR)
- added a wavelet filtering plugin (requires the PyWavelet library)
- added a 3D zoom plugin (requires the Mayavi library)
- added export to Topspin/Bruker files, and added import of processed Topspin files (NMR)
- added the upgrade of files from previous version
- added the `d.axis?.cpxsize` : the size of an axis expressed in spectroscopic points (real of complex) different from `d.axis?.size` which is the size of an axis expressed in data points so
- `d.axis?.cpxsize == d.axis?.size` is axis is real
- `d.axis?.cpxsize == d.axis?.size/2` is axis is complex
- improved the Peak-Picker (mostly the output capabilities)
- improved processing.py for nicer spectra, and possibly faster processing (MS)
- improved visu2D.py, for a greater stability and improved selection syntax
- corrected a bug in `.conv_n_p()` (NMR)
- and many small bugs as well

0.8.3 - April 2016

- ALL spectro.
  - added a new `cpxsize` property, associated to axes and dataset, which counts complex and real entries
  - added: display and peak display now accept a color and markersize arguments
  - improved plugins, plugins with a filename starting with _ do not load
  - improved: automatic baseline correction algorithms have been improved (`Algo/BC.py`)
  - `finnoiselevel()` set of functions has been rewritten (`util/signal_tools.py`)
  - standard test now includes testing for `multiprocessing` - *DOES NOT WORK ON ALL DISTRIBUTION* if it is your case, set `use_multiprocessing = False` in test.mscf
- NMR
  - added: BrukerNMR now imports TopSpin processed dataset (1r, 2rr)
  - improved: and corrected Laplace axes - for a new DOSY module to come...
  - corrected: conv_n_p() was wrong and has been corrected
  - corrected: `gm_apod()` was wrong and has been corrected_
  - corrected: an error in GifaFile access under Windows
- MS
- processing.py (2D FTMS) now includes parallel processing in F2 (helping in certain cases)
- and gives sharper lineshape thanks to kaiser() apodisation
- files from the previous program version (0.7.x) can now be upgraded and read. just do `python -m spike.File.HDF5File update your_file.msh5`
- improved `.report()` for FTMS datasets

0.8.2 - 2 Feb 2016

- corrected a bug in processing when running under MPI parallel
- added warning in set_col() and set_row() if type do not match.
- starting to work on the documentation

0.8.1 - 24 Jan 2016

- corrected a bug for Orbitrap related to offsetfreq.

0.8.0 - 23 Jan 2016

- first clean version using the new HDF5 file set-up **WARNING**
  - HDF5 files created with this version cannot be read with previous versions

  - HDF5 files created with previous versions cannot be read with this version - this should be fixed later - File now contains acquisition parameters files in the attached hdf5 sub-group
- datasets now carry store and retrieve the parmeters imported from manufacturers file in d.params
- improved FTMS calibration using 1, 2, and 3 parameters calibration : calibA calibB calibC, retrieve by Import from experimental file
- improved FTMS Hz unit, added the d.axis.offsetfreq parameter
- corrected fine details of F1 demodulation and added the parameter freq_f1demodu
- unittests extended, in particular in visu2D
- Starting with this version
  - a stable version will be maintained, downloadable as a zip file in the download page https://bitbucket.org/delsuc/spike/downloads
  - Two developpement branches will be used, the `default` for the stable version - improved for bugs, and the `devel` branche, used for developping the new features.

0.7.1 - 5 Jan 2016

- greatly improved internal compression of msh5 files and speed of processing.py
- many small corrections and bug fixes.

0.7.0 - November 2015

- a plugin mechanism has been created which allows to add very simply new features to the program
  - most new features are implemented through this mechanism
- the organisation of the spectral axes has been complete modified, with the introduction of a Unit class
  - each axis holds its own series of possible units (called .units)
  - and the current unit used for display and selection
  - many commands now have a zoom= ketword that works in the current unit
  - additionnaly, there are itoc and ctoi unit converters
- Thanks to this, NMR data-sets are now correctly handled, DOSY are still in progress and should come soon
  - addtionnaly a plugin for Bruker NMR processing is now implemented
- A complete 1D and 2D peak-picker is now implemented, with many controls and features
- New baseline correction algo have been implemented
- the sane algorithm, which is an evolution from urQrd has been separated from urQRd, so both algo can now be used independently
- Tests have been reorganized and improved

- Importers have been extended - parameters are now brought back to the user
- many others

0.6.4 - march 2015

- added Bruker NMR import
- clean-up of the module, still going on
- Tests improved

0.6.3 - march 2015

- first installeable release

0.6.0 - dec 2014

- Fork to SPIKE
- Large improvements of the display program, renamed visu2D
- Corrected a bug in the hypercomplex modulus, resulting in splitting in 2D-FT-ICR
- many improvements everywhere

0.5.1 - 26 mar 2014

- processing2.py renamed to processing.py with added features
  - urQRd
- source code reorganized by folders

0.5.0 - 24 mar 2014

- starting new devl effort
- published ! version of urQRd

0.4.1 - 27 Sep 2012

- final (?) version of urQRd
- added data arithmetic
- many other optimisation

0.4.0 - 20 apr 2012 -

new version processing2.py (temporary name) this one

- processing is performed in steps, F2 from infile to interfile (intermediate file) and F1 from interfile to outfile

- steps are optionnal, F2 or F1 can be performed alone - allowing denoising on the interfile
- processing is faster and mpi enabled - speed-up are better for very large files
- has a better way of computing the smaller spectra - done by downsampling - faster and nicer
- vignette is now 1024x1024 - can be changed using SIZEMIN in config file

0.3.11 - 29 mar 2012

Small tools have been added to modify configuration files and to mix processing.py and ipython visualisation

0.3.10 - 22 jan 2012

processing is now (hopefully) bug free and RAPID !

0.3.9 - 18 jan 2012

fticrvisu.py, processing working, getting all parameters correctly from FTICR-Data and Apex

0.3.8 - 13 jan 2012

fticrvisu.py, processing working, corrected after Marie came

0.3.7 - 12 dec 2011

correction of Gifa file bug, bug in Apex for narrow band data-sets, changes in msh5 file format

0.3.6

3 Oct 2011 - added HDF5 file format (.msh5), multiresolution files, configuration files (.mscf), fticrvisu

0.3.5

5 Sept 2011 - added cadzow in MPI / savitsky-golay / HDF5 still in progress

0.3.4

26 July 2011 - added autotests / savehdf5 first version

0.3.3

12 July 2011 - first reliable/taged FTICR version