SPIKE Relase Notes

0.99.21 - Feb 2021

- plugin which implements .diagonal() for computing the diagonal of 2D FTICR spectra
- small correction in urQRd - thanks to Will Kew
- correction when reading Apex MS dataset for pulse frequency limits - thanks to Maria van Agthoven
- correction ThermoFisher/Orbitrap import code - thanks to Will Kew
- small corrections when opening files

0.99.20 - Nov 2020

- corrected a bad bug which corrupted F1 calibration when loading a 2D-FTICRMS experiment this bug was introduced in the 0.99.14 release but was not detected at that time

0.99.19 - May 2020

- corrected a bug in BrukerNMR importer...

0.99.17 - April 2020

- corrected a bug in BrukerMS importer...

0.99.16 - April 2020

- FTICR a new Apex0 bruker importer - to access old datasets, with the "NMR" setup (acqus pdata ...)
- FTICR a global BrukerMS importer - Import1D - Import2D
- a few corrected bugs

0.99.15 - March 2020

This release introduces a major modification in the organisation of the `NPKData` object - which is the central object on which everything is organized.

Previously `NPKData.NPKData` was the standard class, which created NMR object, and other classes (such as `FTICR.FTICRData` or `Orbitrap.OrbiData`) inherited from this class and had to overloaded a few things. `NPKData` held also all `Axis` definition, both generic and for NMR.

Now,

- `NPKData._NPKData` is a generic object - agnostic about the spectroscopy
- `NPKData` holds also the definitions of generic Axes (`Axis` but also `TimeAxis` and `LaplaceAxis`)
- `NMR.NMRData` is the new class for NMR data-sets, `NMR` also contains the definitions for all NMR related Axes.

- `FTICR.FTICRData` and `Orbitrap.OrbiData` now inherit from the `_NPKData` class (through `FTMS`).

In consequence, to create an NMR dataset from scratch, now do:

```
NMR.NMRData(...)
```

where you were using `NPKData.NPKData` previously

and do

```
NPKData._NPKData(...)
```

to create an empty dataset not associated to any spectroscopy

This should have been done long ago - but I'm so lazy...

Other modifications - This set-up allows to better adapt compound experiments (LC-NMR LC-MS ...) - jupytext extension was added to jupyter Notebooks - means that a python copy is maintained - only this copy is version controlled - still improvements in notebooks - - NMR: improvement in the SpinIt importer - FTICR: added a Bo attribute - added the NbMaxPeaks flag in Peak display - added the self.kind attribute in the Axis class - easier to use than self.NMR ! - small bugs corrections - adding a complex value to a complex datasets was wrong in complex mode. - tests in python 2.7 are abandoned - but very few python 3 features are really used... - REMARK, it was always mentionned that version 1.0 would be rolled out when interactive functions in notebooks would be really usefull. It will be the next big release probably !

0.99.14 - October 2019 - not released on pypi -

- NMR: lots of improvements in Proc1DNMR notebooks
- improvements in NoteBook for mouse interactivity (click and scroll)
  - requires the additional ipympl module

0.99.13 - October 2019 - not released on pypi -

- MS: added the EasyDisplayFTICR2D for non programers !
- improvements in NoteBook interactivity
- added smoothing in spline baselinecorrection

0.99.12 - September 2019

The 0.99.11 had a bug in the display of 1D NMR experiment - the 0.99.12 corrects it.

0.99.11 - September 2019

- NMR: added a Notebook for processing of DOSY
- many improvement in the interactive Notebooks, and in the interactive library (still work to do though)

- added autpoints computation for spline baseline correction
- corrected axis placement in spectral display (you should not have inverted axis anymore)
- corrected a bug when computing projections

0.99.10 - August 2019

- changed calibration in FTICR-MS - now should better correspond to Bruker, both for linear and quadratic
  - be carefull, the definitions are slightly modified, this should be taken into account when reading files, however you should verify the calibration stored into previous files
- added Proc2DNMR Notebook - preliminary!
- continued to improve other Notebooks
- added skewness and kurtosis in bucket lists (optional)
- improved Test suite (should mostly work under Windows now)
- corrected peak-picker so that width is FWMH after centroid
- added an option in Peaks.pk2pandas to output or not the uncertainties

0.99.9 - June 2019

- improved many aspect of the interactive Notebooks
- improved Proc1DNMR Notebook
  - added peak-picker
  - added integration
  - added bucketing
- Integrate: plugin for 1D NMR data integration
- added peak lists export to pandas
- added limit to the number of peak to be displayed on screen (default 1000)

0.99.8 - April 2019

- corrects a BIG BUG which hampers the import of 1D NMR data-sets,

0.99.7 - April 2019

Please do not use, see above - first version of Interactive Notebooks: - ProcessFTICR-MS - DisplayFTICR2D - Process1DNMR - The new BrukerMS importer tries Solarix importer and falls back to Apex importer if it fails - improved Interactive tools - improved FTICR importers to accept `my_expt.d/fid` as well as `my_expt.d` - improved peak-picker behavior - improved error messages in FTICR importers - cured a bug in Apex.Importxx for a special xml format

0.99.6 - April 2019

- extended and improved tests - finalized installation through PYPI

- support for distribution via pip - you can now do `pip instal spike_py` and spike installed globally on your system.
- still struggling with correct calibration routines for FTICR ! - proceed carefully ! -
- phase() speeded-up by a factor 20 !
- added a autothresh scaling to peakpicking (catching peaks "autothresh" times above the noise level - default is 3)
- slight improvement of peak list reporting (additional key words: format="report" and format="full")
- a bug in extract of complex 1D data-sets was corrected
- added the figure keyword to peaklist display

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)
- added the setup.py prgm, SPIKE is now a regular installable program - still working on it ! -
- `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