



pySME usage – a quick guide

Mingjie Jian

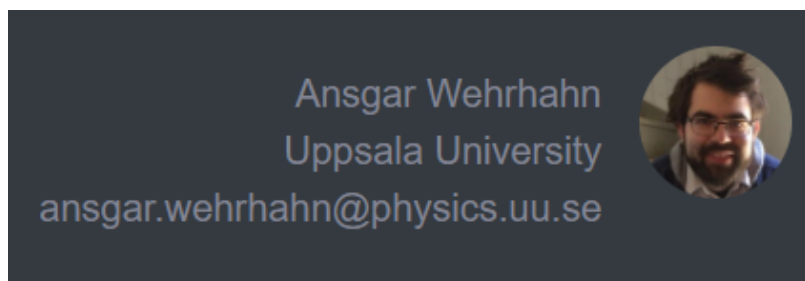
Stockholm University

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PySME

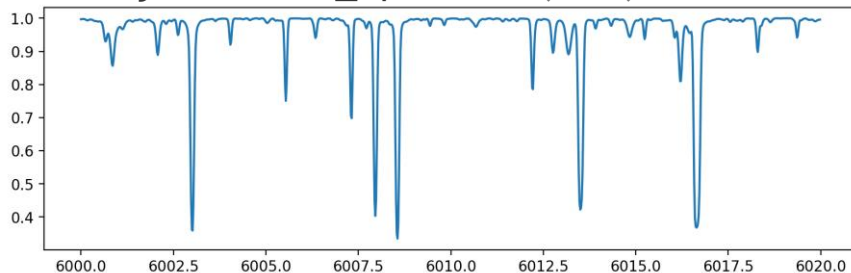
Spectroscopy Made Easier

- Spectroscopy Made Easy: spectral synthesis and parameter determination (C++ and Fortran)
 - [Valenti & Piskunov 1996](#)
- IDL wrapper: IDLSME
- Python wrapper: pysme



Spectral synthesis

- `from pysme.sme import SME_Structure`
- `from pysme.linelist.vald import ValdFile`
- `from pysme.synthesize import synthesize_spectrum`
- `sme = SME_Structure()`
- `sme.teff, sme.logg, sme.monh = 5772, 4.44, 0`
- `sme.linelist = ValdFile('line.list')`
- `sme.wave = np.arange(6000, 6020, 0.02)`
- `sme = synthesize_spectrum(sme)`



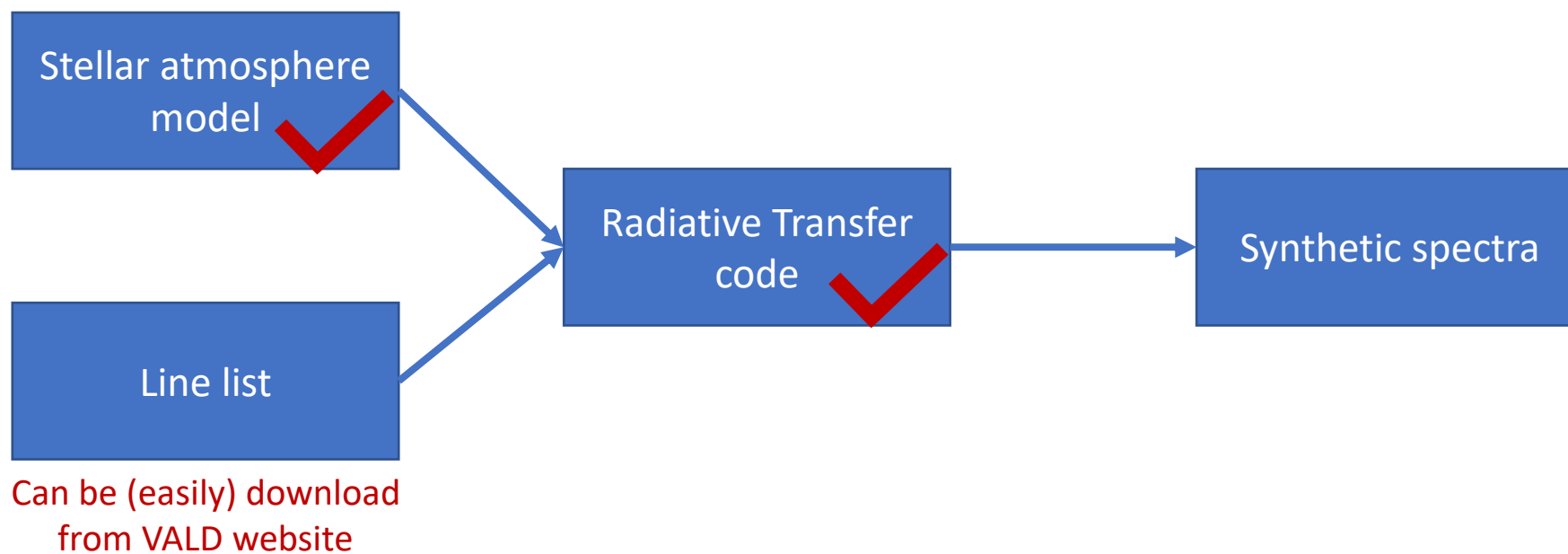
Parameter fitting

- `from pysme.sme import SME_Structure`
- `from pysme.solve import solve`
- `sme = SME_Structure()`
- `sme.teff, sme.logg, sme.monh = 5772, 4.44, 0`
- `sme.linelist = ValdFile('line.list')`
- `sme.wave = wave_observe`
- `sme.spec = flux_observe`
- `sme_fit = solve(sme_fit, ['teff', 'logg', 'monh', 'vmic', 'vsini'])`
- `sme_fit = solve(sme_fit, ['abund Mg', 'abund Al'])`

```
INFO - teff      6852.00437 +- 73.763
INFO - logg      4.32846 +- 0.10283
INFO - monh     -0.01311 +- 0.030663
INFO - vmic      2.16246 +- 0.11556
INFO - vsini     3.39724 +- 0.84919
INFO - v_rad     [0.] +- [[0. 0.]]
```

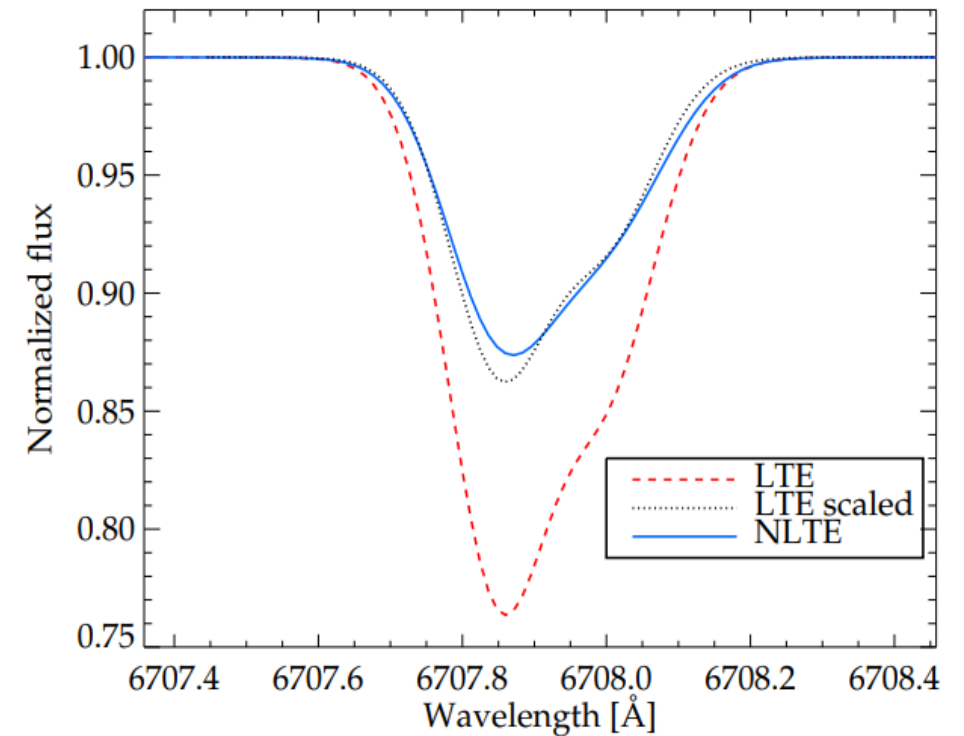
easy to use

- MOOG, Turbospectrum, ...
 - pymoog



accurate

- Local thermal equilibrium
 - Can use Saha-Boltzman distribution
 - Simplify the calculation
 - Not correct for some spectral lines
- Non-LTE / NLTE
 - Use pre-computed departure coefficient grids
 - Correct population



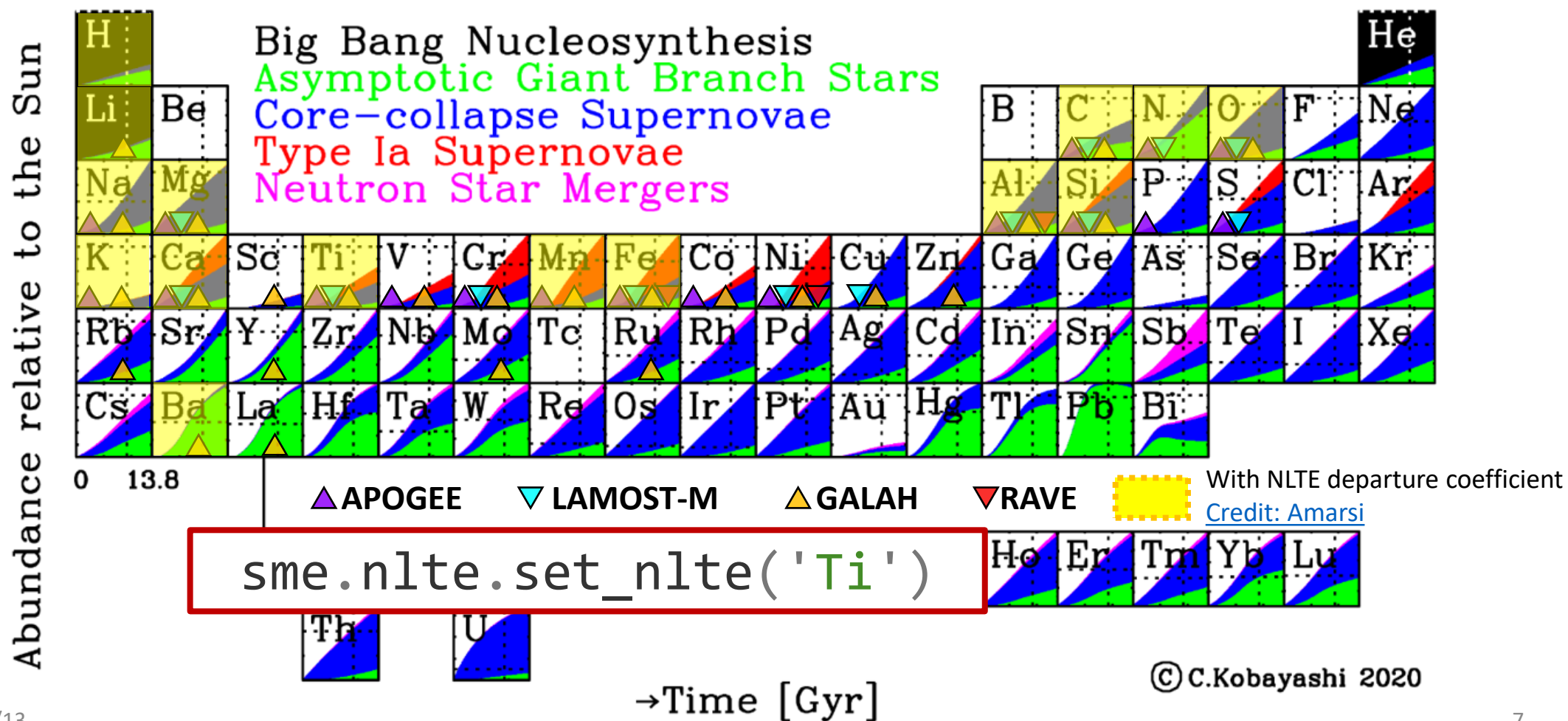
Lind+2013



PySME

Spectroscopy Made Easier

accurate

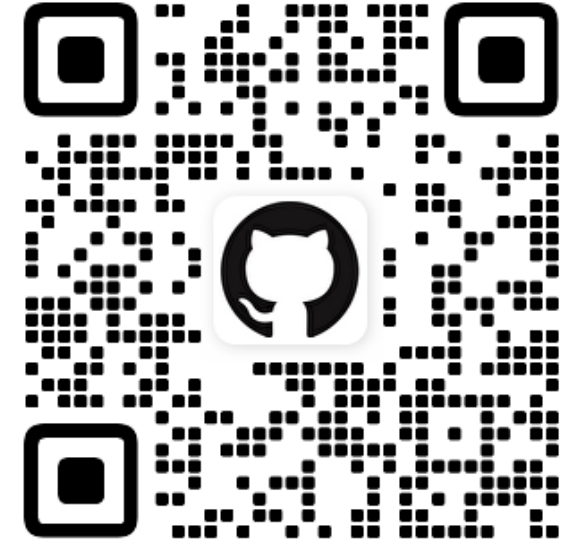


pySME how-tos

How to use pySME? Questions and answers

How to install pysme?

- For now: Mingjie's github
 - git clone <https://github.com/MingjieJian/SME>
 - cd SME
 - pip install .
- Long-term: `pip install pysme-astro`
- How large of the disk volume is needed?
 - 5-50G (in ~/.sme)



github.com/MingjieJian/SME

How to generate a synthetic spectra?

- `from pysme.sme import SME_Structure`
- `from pysme.linelist.vald import ValdFile`
- `from pysme.synthesize import synthesize_spectrum`
- `sme = SME_Structure()`
- `sme.teff, sme.logg, sme.monh = 5772, 4.44, 0`
- `sme.linelist = ValdFile('line.list')`
- `# Either`
- `sme.wran = [[6700, 6800]]`
- `# Or`
- `sme.wave= np.array(6700, 6800, 0.02)`
- `sme = synthesize_spectrum(sme)`
- `wave, flux = sme.wave[0], sme.synth[0]`
- Make the wavelength range of wave/wran consistent with that of the line list.
- Avoid using large number of lines in synthesis – it would take ages. Consider doing it chunk by chunk.

How to set the elemental abundances?

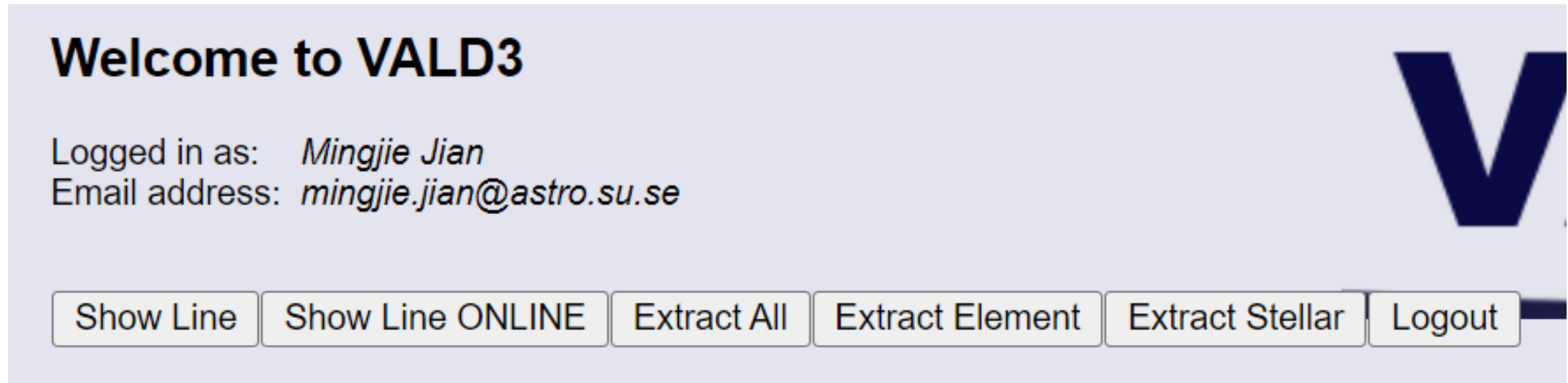
- `sme_fit.abund['P'] += [P/Fe] - sme_fit.monh`
- `sme_fit.abund['Be'] = A(Be) - sme_fit.monh`
- Always check if `sme_fit.abund` looks reasonable after you modify it!

How to apply broadening?

- Microturbulence
 - `sme.vmic`
- Macroturbulence
 - `sme.vmac`
- Stellar rotation
 - `sme.vsini`
- Instrumental broadening
 - `sme.ipstype = gauss/sinc/table`
 - `sme.ipres = 50000`

How to get my line list?

- pysme is compatible with the VALD line list database:
 - <http://vald.astro.uu.se/~vald/php/vald.php>
- Register an account then log in.



How to get my line list?

Show Line ONLINE

Show Line - ONLINE EXTRACTION - EXPERIMENTAL

Approximate wavelength
 Å (air)

Wavelength window
 Å (air)

Element [+ ionization]

Linelist configuration

☒ Default
☐ Custom

Isotopic scaling of oscillator strength

☒ On
☐ Off

*(Takes precedence over the default value set in the **unit selection** dialog)*

How to get my line list?

Extract All

Starting wavelength :	<input type="text"/>	Å (air)
Ending wavelength :	<input type="text"/>	Å (air)
Extraction format :	<input type="radio"/> Short format <input checked="" type="radio"/> Long format <input type="radio"/> Email <input checked="" type="radio"/> FTP	
Retrieve data via		
Hyperfine structure	<input checked="" type="checkbox"/> Include HFS splitting	
Require lines to have a known value of :	<input type="checkbox"/> Radiative damping constant <input type="checkbox"/> Stark damping constant <input type="checkbox"/> Van der Waals damping constant <input type="checkbox"/> Landé factor <input type="checkbox"/> Term designation	
Linelist configuration	<input type="radio"/> Default <input checked="" type="radio"/> Custom	
Unit selection	Energy unit: eV - Medium: air - Wavelength unit: angstrom - VdW syntax: default	
Optional comment for request	<input type="text"/>	
<input type="button" value="Submit request"/>		<input type="button" value="Reset form"/>

- FTP: Maximum 100000 lines per query.
- Avoid too many lines
 - Remove unnecessary molecular lines (e.g, TiO for FGK type stars)
 - Query the database chunk by chunk.

How to fit paras?

- `from pysme.sme import SME_Structure`
 - `from pysme.solve import solve`
 - `sme = SME_Structure()`
 - `sme.teff, sme.logg, sme.monh = 5772, 4.44, 0`
 - `sme.linelist = ValdFile('line.list')`
 - `sme.wave = wave_observe`
 - `sme.spec = flux_observe`
 - `sme.uncs = uncs_observe`
 - `sme_fit = solve(sme_fit, ['teff', 'logg', 'monh', 'vmic', 'vsini'])`
 - `sme_fit = solve(sme_fit, ['abund Mg', 'abund Al'])`
- ← Always think of what parameters to fit and which wavelength ranges to use!
- ↓

Line list

The VALD short\long format output

Line list loading and manipulation

- `sme.linelist = ValdFile('line.list')`

	species	wlcent	gflog	excit	j_lo	e_upp	j_up	lande_lower	\
655774	Pr 2	4800.0060	-3.868	0.2162	5.0	2.7985	5.0	0.86	
655776	Pr 2	4800.0072	-3.090	0.2162	5.0	2.7985	5.0	0.86	
655785	La 1	4800.0170	-0.640	1.2350	3.5	3.8173	2.5	0.89	
655786	Fe 2	4800.0171	-1.231	12.8714	3.5	15.4536	3.5	1.24	
655790	CH 1	4800.0210	-2.532	1.0838	20.5	3.6660	20.5	99.00	
...	

- The line list object is very similar with `pandas.DataFrame`.
 - `linelist[linelist['species'] == 'Fe 1']`
 - `linelist[linelist['species'] != 'TiO 1']`
 - `linelist[linelist['wlcent'] > 5500]`


Line list – VALD download

- Only use “long” format if using NLTE
 - Since short format will lose the term configuration required by NLTE calculation.
- When using “extract stellar”
 - Set the detection threshold to ~ 0.001 (0 means all lines included, 1 means no lines included).

Line list – ValdFile object 1

- acknowledgement
 - Acknowledgement string for using VALD
- add
 - Add a new line to the existing linelist
- append
 - Append a linelist to this one
- atomic
 - list(float) of size (nlines, 8): Data array passed to C library
- citation_info
 - Self explained
- columns (? property)
- cull
 - Remove lines from the linelist that are weaker than the cutoff
- cull_percentage
 - Remove a percentage of the lines in the linelist, removing the weakest lines first
- extra
 - list(float) of size (nlines, 3): additional line level information for NLTE calculation
- from_dict

But it doesn't work for VALD line list – maybe need external line depth?



Line list – ValdFile object 2

- fom_IDL_SME
 - extract LineList from IDL SME structure keywords
- guess_format (?)
- identify_valdtype
 - Determines whether the file was created with extract_all, extract_stellar, or extract_element and whether it is in long or short format
- index (?)
- load
 - Read line data file from the VALD extract service
- loads (?)
- lulande
 - list(float) of size (nlines, 2): Lower and Upper Lande factors
- medium (?)
- mro
 - Return a type's method resolution order.
- parse_abund
 - Parse VALD abundance lines from a VALD line data file
- parse_columns (?)
- parse_header
 - Parse header line from a VALD line data file
 - and sets the internal parameters

Line list – ValdFile object 3

- `parse_line_error`
 - Transform Line Error flags into relative error values
- `parse_linedata`
 - Parse line data from a VALD line data file
- `parse_nlines (?)`
- `parse_references (?)`
- `parse_valdatmo`
 - Parse VALD model atmosphere line from a VALD line data file
- `sort`
 - Sort the linelist
- `species`
 - `list(str)` of size (nlines,): Species name of each line
- `string_columns`
 - Self explained
- `to_dict`
 - Self explained
- `trim`
 - Remove lines from the linelist outside the specified wavelength range

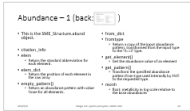
VALD linelist format – 1

species:	A string identifier including the element and ionization state or the molecule
atom number:	Identifies the species by the atomic number (i.e. the number of protons) ignored in the radiative transfer calculations and therefore does not need to be set
ionization:	The ionization state of the species, where 1 is neutral (?)
wlcent:	The central wavelength of the line in Angstrom
excit:	The excitation energy in ?
gflog:	The log of the product of the statistical weight of the lower level and the oscillator strength for the transition.
gamrad:	The radiation broadening parameter
gamqst:	A broadening parameter
gamvw:	van der Waals broadening parameter
lande:	The lande factor
depth:	An arbitrary depth estimation of the line
reference:	A citation where this data came from

VALD linelist format – 2

lande_lower:	The lower Lande factor
lande_upper:	The upper Lande factor
j_lo:	The spin of the lower level
j_up:	The spin of the upper level
e_upp:	The energy of the upper level
term_lower:	The electron configuration of the lower level
term_upper:	The electron configuration of the upper level
error:	An uncertainty estimate for this linedata

The SME structure - 1



- abund ->
 - elemental abundances
- accft
 - leastsquares_ftol
- accgt
 - leastsquares_gtol
- accrt
 - float: minimum accuracy for synthethized spectrum at wavelength grid points in sme.wint
- accwi
 - float: minimum accuracy for linear spectrum interpolation vs. wavelength.
- accxt
 - leastsquares_xtol



- atmo ->
 - model atmosphere data
- atomic
 - Atomic linelist data, usually passed to the C library
- citation
 - A method, self explained
- citation_info
 - A string, self explained
- cont
 - continuum intensities
- create_citation
 - A method, self explained
- cscale
 - Continumm polynomial coefficients for each wavelength segment

The SME structure – 2

- `cscale_bounds`
 - bounds for the continuum parameters
- `cscale_degree`
 - Polynomial degree of the continuum as determined by `cscale_flag`
- `cscale_flag`
 - Flag that describes how to correct for the continuum
- `cscale_ftol`
 - tolerance for the continuum least squares fit
- `cscale_gtol`
 - tolerance for the continuum least squares fit
- `cscale_jac`
 - str: jacobian approximation used in the continuum fit
- `cscale_loss`
 - str: loss function for the continuum fit
- `cscale_method`
 - str: least squares method used in the continuum fit

The SME structure – 3

- `cscale_type`
 - str: Flag that determines the algorithm to determine the continuum
- `cscale_xscale`
 - array of 'jac', Scale of each continuum parameter
- `cscale_xtol`
 - float: tolerance for the continuum least squares fit
- `fitparameters`
 - list: parameters to fit
- `fitresults`
 - Fitresults: fit results data
- `from_dict`
- `gam6`
 - float: van der Waals scaling factor
- `h2broad`
 - bool: Whether to use H2 broadening or not
- `id`
 - str: DateTime when this structure was created


The SME structure – 4

- `import_mask`
 - Import the mask of another sme structure and apply it to this one
- `ip_x`
 - array: Instrumental broadening table in x direction
- `ip_y`
 - array: Instrumental broadening table in y direction
- `ipres`
 - float, array: Instrumental resolution for instrumental broadening
- `iptype`
 - str: instrumental broadening type
- `leastsqares_ftol`
 - float: minimum accuracy of the best fit cost
- `leastsqares_gtol`
 - float: minimum accuracy of the gradient of the least squares fit
- `leastsqares_jac`
 - str: leastsqares jacobian calculation, see `scipy least_squares` for details, default: '2-point'
- `leastsqares_loss`
 - str: leastsqares loss to use, see `scipy least_squares` for details, default: 'linear'

The SME structure – 5

- `least_squares_method`
 - str: least_squares method to use, see `scipy least_squares` for details, default: 'dogbox'.
- `least_squares_xscale`
 - str, arraylike: leastsquare x-scale to use, see `scipy least_squares` for details, default: 1
- `least_squares_xtol`
 - float: minimum accuracy of the parameters in the fitting procedure
- `linelist`
 - LineList: spectral line information
- `load`
 - Load SME data from disk
- `log`
 - float: surface gravity in $\log_{10}(\text{cgs})$
- `mask`
 - `liffe_vector` of shape (nseg, ...): mask defining good and bad points for the fit
- `mask_bad`, `mask_cont`, `mask_good`, `mask_line`, `mask_vrad`

The SME structure – 6

- meta
 - dict: Arbitrary extra information
- monh
 - float: metallicity in log scale relative to the base abundances
- mu
 - $\mu = \cos(\theta)$ values to calculate radiative transfer at μ values
- nlte -> 
 - NLTE: nlte calculation data
- nmu
 - Number of μ array
- normalize_by_continuum
 - bool: Whether to normalize the synthetic spectrum by the synthetic continuum spectrum or not
- nseg
 - int: Number of wavelength segments

The SME structure – 7

- `save`
 - Save the whole SME structure to disk.
- `spec`
 - observed spectrum
- `species`
 - Names of the species of each spectral line
- `specific_intensities_only`
 - bool: Whether to keep the specific intensities or integrate them together
- `synth`
 - synthetic spectrum
- `system_info`
 - information about the host system running the calculation for debugging
- `teff`
 - float: effective temperature in Kelvin
- `telluric`
 - telluric spectrum that is multiplied with `synth` during the fit

The SME structure – 8

- `to_dict`
- `uncs`
 - uncertainties of the observed spectrum
- `version`
 - str: PySME version used to create this structure
- `vmac`
 - float: macro turbulence in km/s
- `vmic`
 - float: micro turbulence in km/s
- `vrad`
 - radial velocity of each segment in km/s
- `vrad_bounds`
 - float: radial velocity limits in km/s
- `vrad_flag`
 - flag that determines how the radial velocity is determined
- `vrad_ftol`
 - tolerance for the radial velocity least squares fit
- `vrad_gtol`

The SME structure – 9

- `vrad_jac`
 - str: jacobian approximation used in the radial velocity fit
- `vrad_limit`
- `vrad_loss`
 - str: loss function for the radial velocity fit
- `vrad_method`
 - str: least squares method used in the radial velocity fit
- `vrad_xscale`
 - array or 'jac': scale of the vrad parameter
- `vrad_xtol`
 - float: tolerance for the radial velocity least squares fit
- `vsini`
 - projected rotational velocity in km/s
- `wave`
 - wavelength
- `wran`
 - beginning and end wavelength points of each segment

Abundance – 1 (back:)

- This is the `SME_Structure.abund` object.
- `citation_info`
- `elem`
 - Return the standard abbreviation for each element.
- `elem_dict`
 - Return the position of each element in the raw array
- `empty_pattern()`
 - Return an abundance pattern with value `None` for all elements.
- `from_dict`
- `fromtype`
 - Return a copy of the input abundance pattern, transformed from the input type to the 'H=12' type.
- `get_element()`
 - Get the abundance value of an element
- `get_pattern()`
 - Transform the specified abundance pattern from type used internally by SME to the requested type.
- `monh`
 - float: metallicity in log scale relative to the base abundances

Abundance – 2

- `pattern`
 - Abundance pattern in the initial format
- `set_pattern_by_name()`
 - Set the abundance pattern to one of the predefined options
- `set_pattern_by_value()`
 - Set the abundance pattern using an dict of pattern value
- `solar`
 - Return solar abundances of asplund 2009
- `to_dict`
 - Convert abundance pattern to dict.
- `totype`
 - Return a copy of the input abundance pattern, transformed from the 'H=12' type to the output type.
- `type`
 - Self explained.
- `update_pattern`
 - Update the abundance pattern for several elements at once
 - Be careful on the format

Atmosphere – 1

- This is the `SME_Structure.atmo` object.
- `abund`
 - elemental abundances. May be different from `SME_structure.abund`
- `citation`
- `citation_info`
- `create_citation`
- `depth`
 - str: flag that determines whether to use `RHOX` or `TAU` for calculations
- `dtype (?)`
- `from_dict`
- `geom`
 - str: the geometry of the atmosphere model
- `height`
 - array: height of the spherical model
- `interp`
 - str: flag that determines whether to use `RHOX` or `TAU` for interpolation

Atmosphere – 2

- logg
- lonh
 - L/H value
- method
 - str: whether the data source is a grid or a fixed atmosphere
- monh
- names
 - The names of the attributes
- ndep
 - N of depth
- opflag
 - opacity flags
- radius
 - float: radius of the spherical model
- rho
 - array: density profile
- rhox
 - array: mass column density

Atmosphere – 3

- source
 - str: datafile name of this data, or atmosphere grid/file
- tau
 - array: continuum optical depth
- teff
- temp
 - array: temperature profile in Kelvin
- to_dict
- vturb
 - float: turbulence velocity in km/s
- wlstd
 - float: wavelength standard deviation
- xna
 - array: number density of atoms in $1/\text{cm}^{**3}$
- xne
 - array: number density of electrons in $1/\text{cm}^{**3}$

NLTE – 1

- This is the `SME_Structure.nlte` object.
- `abund_format`
 - str: which abundance format to use for comparison
- `citation`
- `citation_info`
- `create_citation`
- `elements`
 - list: elements for which nlte calculations will be performed
- `first (?)`
- `flags`
 - array: contains a flag for each line, whether it was calculated in NLTE (True) or not (False)
- `from_dict`

NLTE – 2

- `get_grid`
 - Read and interpolate the NLTE grid for the current element and parameters
- `grid_data`
- `grids`
 - dict: nlte grid datafiles for each element
- `min_energy_diff`
 - float: difference between energy levels that are still matched. If None will default to the smallest non zero difference between energy levels in the grid.
- `remove_nlte`
 - Remove an element from the NLTE calculations
- `selection`
 - str: which selection algorithm to use to match linelist and departure coefficients
- `solar`
 - str: defines which default to use as the solar metallicities
 - Not used now?

NLTE – 3

- `sub_grid_size`
 - array of shape (4,): defines size of nlte grid cache. Each entry is for one parameter `abund`, `teff`, `logg`, `monh`
- `to_dict`
- `update_coefficients`
 - pass departure coefficients to C library

Line by line description for solve

- 730: the fun is `_residuals`, used for calculating the residual between observed and synthesized spectra;
- 731: `jac` is the Jacobian matrix of the fun, i.e., residuals. Here `jac` is a callable, so `pysme` have its own way to calculate the Jacobian matrix, and `least_square` function will directly use it. Note that it is the same as "2-point".
- `x0` is the initial parameter values.

```
728         with print_to_log():
729             res = least_squares(
730                 self._residuals,
731                 jac=self._jacobian,
732                 x0=p0,
733                 bounds=bounds,
734                 loss=sme.leastsquares_loss,
735                 f_scale=self.f_scale,
736                 method=sme.leastsquares_method,
737                 x_scale=sme.leastsquares_xscale,
738                 # These control the tolerance, for early termination
739                 # since each iteration is quite expensive
740                 xtol=sme.accxt,
741                 ftol=sme.acfft,
742                 gtol=sme.accgt,
743                 verbose=2,
744                 args=(sme, spec, uncs, mask),
745                 kwargs={
746                     "bounds": bounds,
747                     "segments": segments,
748                     "step_sizes": step_sizes,
749                     "method": sme.leastsquares_jac,
750                 },
751             )
752             # The jacobian is altered by the loss function
753             # This lets us keep the original for our uncertainty estimate
754             res.jac = self._latest_jacobian
755
```

Line by line description for solve

- bounds is the bounds on the paras. pysme will give bounds on Teff, logg and monh depend on the grids, on velocities from 0 to c, no abunds if available (?).
- loss is the loss function for estimating how similar the spectra are. pysme use linear loss function.
- f_scale is the scaled factor for the spectra, but no effect with loss=linear (?). pysme has a setting of f_scale (a number).

```
728         with print_to_log():
729             res = least_squares(
730                 self._residuals,
731                 jac=self._jacobian,
732                 x0=p0,
733                 bounds=bounds,
734                 loss=sme.leastsquares_loss,
735                 f_scale=self.f_scale,
736                 method=sme.leastsquares_method,
737                 x_scale=sme.leastsquares_xscale,
738                 # These control the tolerance, for early termination
739                 # since each iteration is quite expensive
740                 xtol=sme.accxt,
741                 ftol=sme.accft,
742                 gtol=sme.accgt,
743                 verbose=2,
744                 args=(sme, spec, uncs, mask),
745                 kwargs={
746                     "bounds": bounds,
747                     "segments": segments,
748                     "step_sizes": step_sizes,
749                     "method": sme.leastsquares_jac,
750                 },
751             )
752             # The jacobian is altered by the loss function
753             # This lets us keep the original for our uncertainty estimate
754             res.jac = self._latest_jacobian
755
```

Line by line description for solve

- method is the algorithm to perform minimization. pysme default is dogbox.
- x_scale is the scale factor for the wavelength. pysme default is 1.

```
728         with print_to_log():
729             res = least_squares(
730                 self._residuals,
731                 jac=self._jacobian,
732                 x0=p0,
733                 bounds=bounds,
734                 loss=sme.leastsquares_loss,
735                 f_scale=self.f_scale,
736                 method=sme.leastsquares_method,
737                 x_scale=sme.leastsquares_xscale,
738                 # These control the tolerance, for early termination
739                 # since each iteration is quite expensive
740                 xtol=sme.accxt,
741                 ftol=sme.accft,
742                 gtol=sme.accgt,
743                 verbose=2,
744                 args=(sme, spec, uncs, mask),
745                 kwargs={
746                     "bounds": bounds,
747                     "segments": segments,
748                     "step_sizes": step_sizes,
749                     "method": sme.leastsquares_jac,
750                 },
751             )
752             # The jacobian is altered by the loss function
753             # This lets us keep the original for our uncertainty estimate
754             res.jac = self._latest_jacobian
755
```

Line by line description for solve

- xtol is the tolerance for termination by the change of the independent variables (fitting parameters).
- ftol is the tolerance for termination by the change of the dependent variables (flux).
- gtol is the tolerance for termination by the norm of the gradient.
- The iteration will stop if any these three tol are smaller than the threshold (?).

```
728 with print_to_log():
729     res = least_squares(
730         self._residuals,
731         jac=self._jacobian,
732         x0=p0,
733         bounds=bounds,
734         loss=sme.leastsquares_loss,
735         f_scale=self.f_scale,
736         method=sme.leastsquares_method,
737         x_scale=sme.leastsquares_xscale,
738         # These control the tolerance, for early termination
739         # since each iteration is quite expensive
740         xtol=sme.accxt,
741         ftol=sme.accft,
742         gtol=sme.accgt,
743         verbose=2,
744         args=(sme, spec, uncs, mask),
745         kwargs={
746             "bounds": bounds,
747             "segments": segments,
748             "step_sizes": step_sizes,
749             "method": sme.leastsquares_jac,
750         },
751     )
752     # The jacobian is altered by the loss function
753     # This lets us keep the original for our uncertainty estimate
754     res.jac = self._latest_jacobian
755
```

Line by line description for solve

- verbose is the level of algorithm's verbosity, default will display the fitting details.

```
728         with print_to_log():
729             res = least_squares(
730                 self._residuals,
731                 jac=self._jacobian,
732                 x0=p0,
733                 bounds=bounds,
734                 loss=sme.leastsquares_loss,
735                 f_scale=self.f_scale,
736                 method=sme.leastsquares_method,
737                 x_scale=sme.leastsquares_xscale,
738                 # These control the tolerance, for early termination
739                 # since each iteration is quite expensive
740                 xtol=sme.accxt,
741                 ftol=sme.accft,
742                 gtol=sme.accgt,
743                 verbose=2,
744                 args=(sme, spec, uncs, mask),
745                 kwargs={
746                     "bounds": bounds,
747                     "segments": segments,
748                     "step_sizes": step_sizes,
749                     "method": sme.leastsquares_jac,
750                 },
751             )
752             # The jacobian is altered by the loss function
753             # This lets us keep the original for our uncertainty estimate
754             res.jac = self._latest_jacobian
755
```

Output description for solve

- Iteration: iteration number
- nfev: number of the function called
- Cost: the value of target function (`_residuals`)
- Cost reduction: The reduction amount of the target function compared with the last iteration.
 - ftol termination
- Step norm: The change in the norm of independent parameters (fitting parameters)
 - xtol termination
- Optimality: The norm of the gradient.
 - gtol termination

```
INFO - Don't forget to cite your sources. Use sme.citation()
WARNING - SME Structure has no uncertainties, using all ones instead
INFO - Fitting Spectrum with Parameters: abund C
INFO -      Iteration      Total nfev      Cost      Cost reduction      Step norm      Optimality
INFO -          0          1      1.3989e-02
INFO -          1          2      1.3973e-02      1.61e-05      3.75e-02      5.00e-05
INFO - `gtol` termination condition is satisfied.
INFO - Function evaluations 2, initial cost 1.3989e-02, final cost 1.3973e-02, first-order optimality 5.00e-05.
INFO - Abund c      8.42753 +- 0.12672
INFO - v_rad      [0.] +- [[0. 0.]]
```