

Lunar and Planetary Science Conference, March 18th, 2015

COMMUNITY USER WORKSHOP
ON PLANETARY LIBS (CHEMCAM)
DATA

LIBS Data Processing Level-1



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Cousin, S. Maurice, R. C. Wiens, and the
ChemCam Team

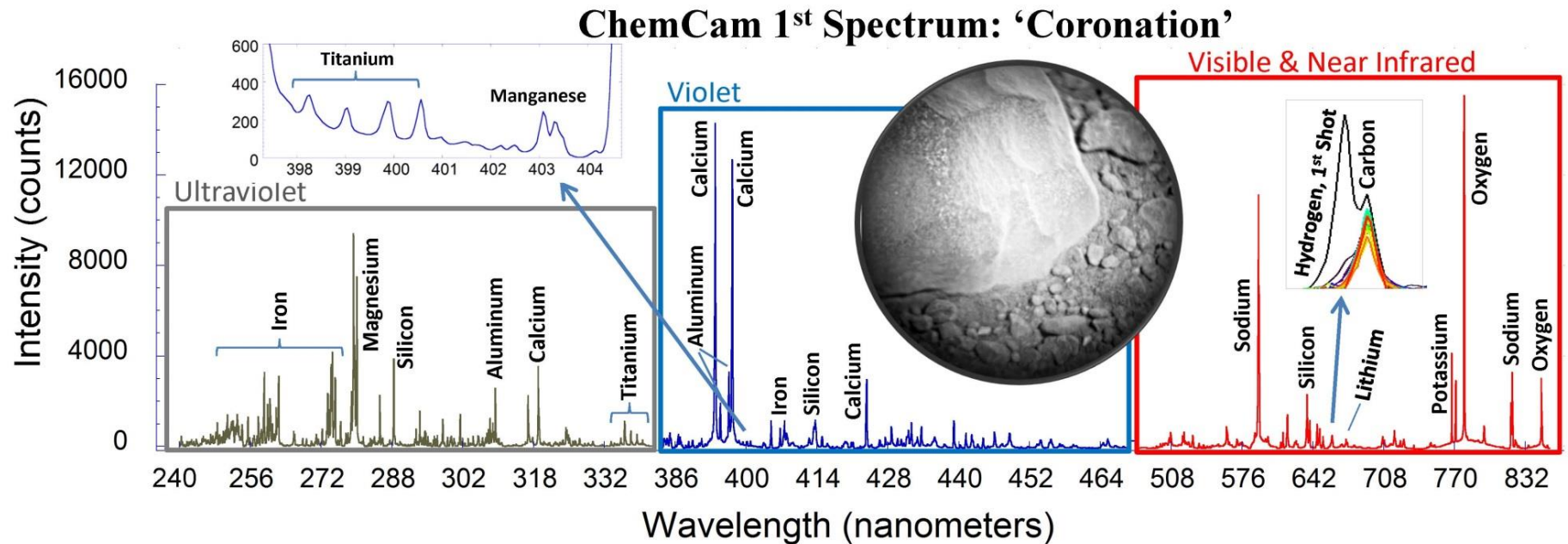
ChemCam Software - Level 1

- Steps in reduction
 - Dark removal
 - Noise removal
 - Wavelength calibration
 - Continuum extraction and subtraction
 - Conversion from counts to photons
 - Element lines identification

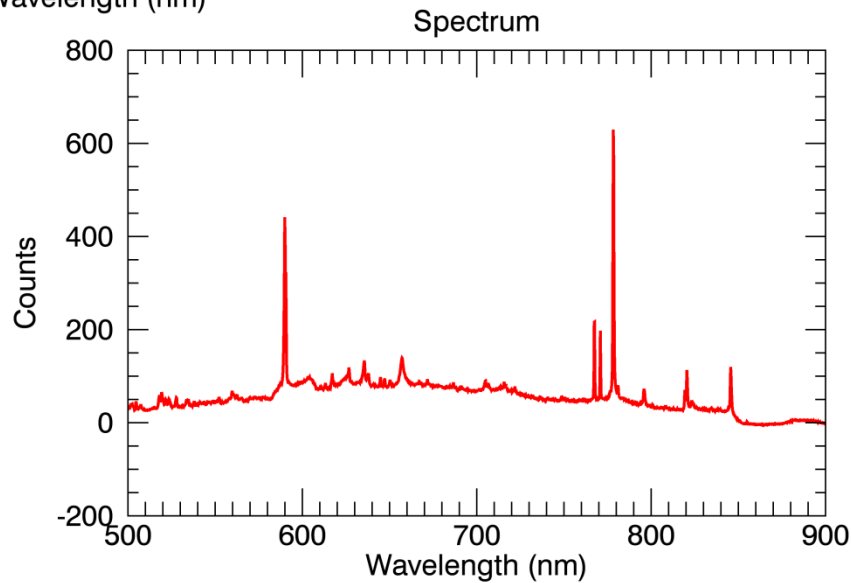
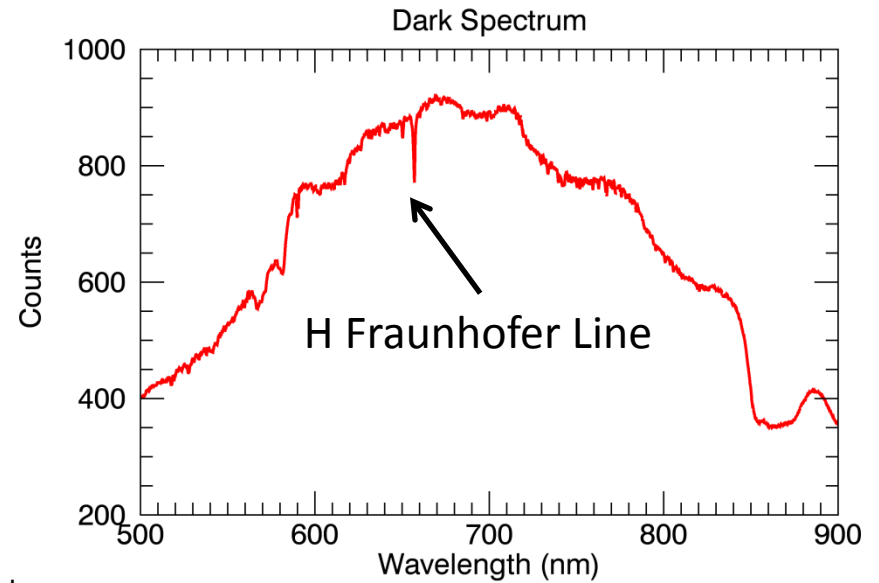
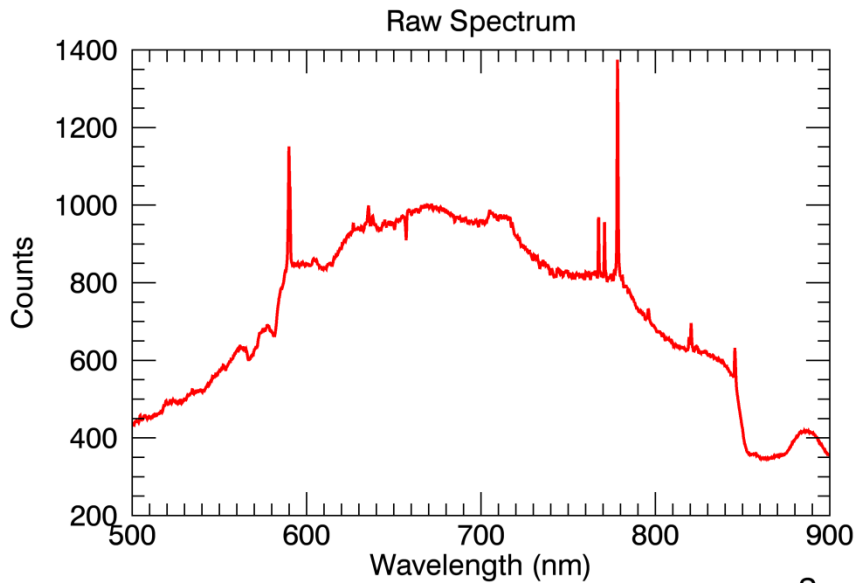
ChemCam Software – Level 2

- Steps in analysis
 - Fit of lines
 - Quantitative estimation
 - Internal standard method
 - Calibration curve, PLS, ...
 - Calibration free
 - Ratios of selected lines
 - Statistical Methods (PCA, ICA, ...)
 - Assign spectrum to a reference library
 - Classification

Coronation (Sol 14)



Coronation (Sol 14)



Dark removal

Noise estimation and removal

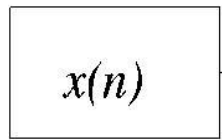
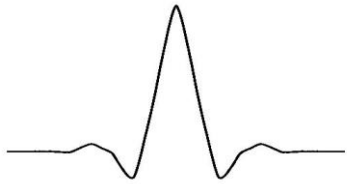
- Undecimated wavelet transform
- Noise estimation at each wavelet scale
- Hard thresholding at σ for each scale
- Sum of thresholded wavelet scales

Continuum estimation

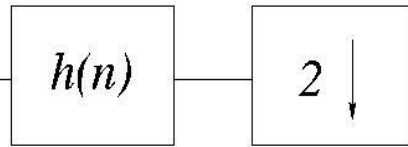
- Undecimated wavelet transform
- All scales above threshold level
- Identification of local minima
- Cubic splines interpolation

Bi-orthogonal wavelet transform

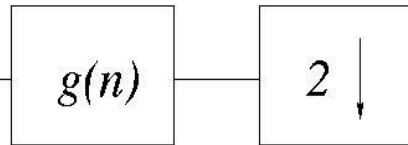
$h(n)$: Scaling function



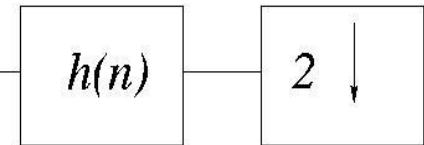
Smooth scale 1



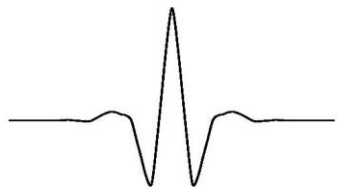
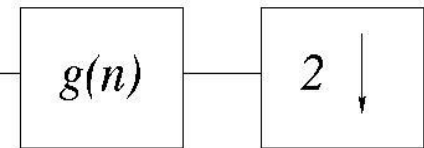
Details scale 1



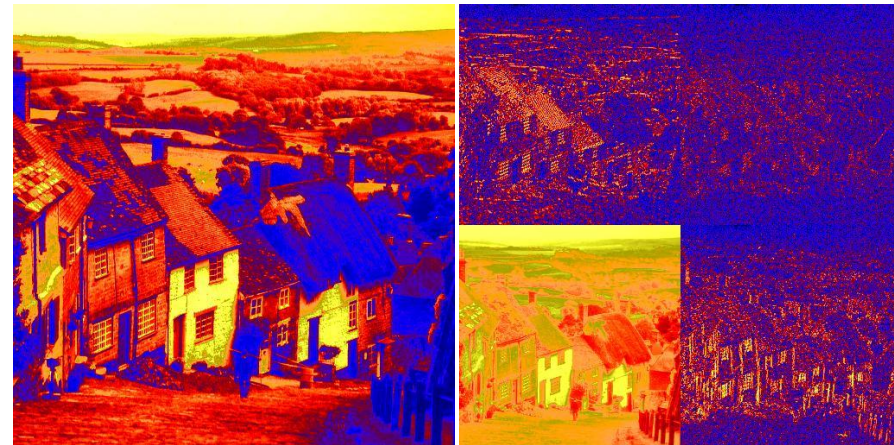
Smooth scale 2



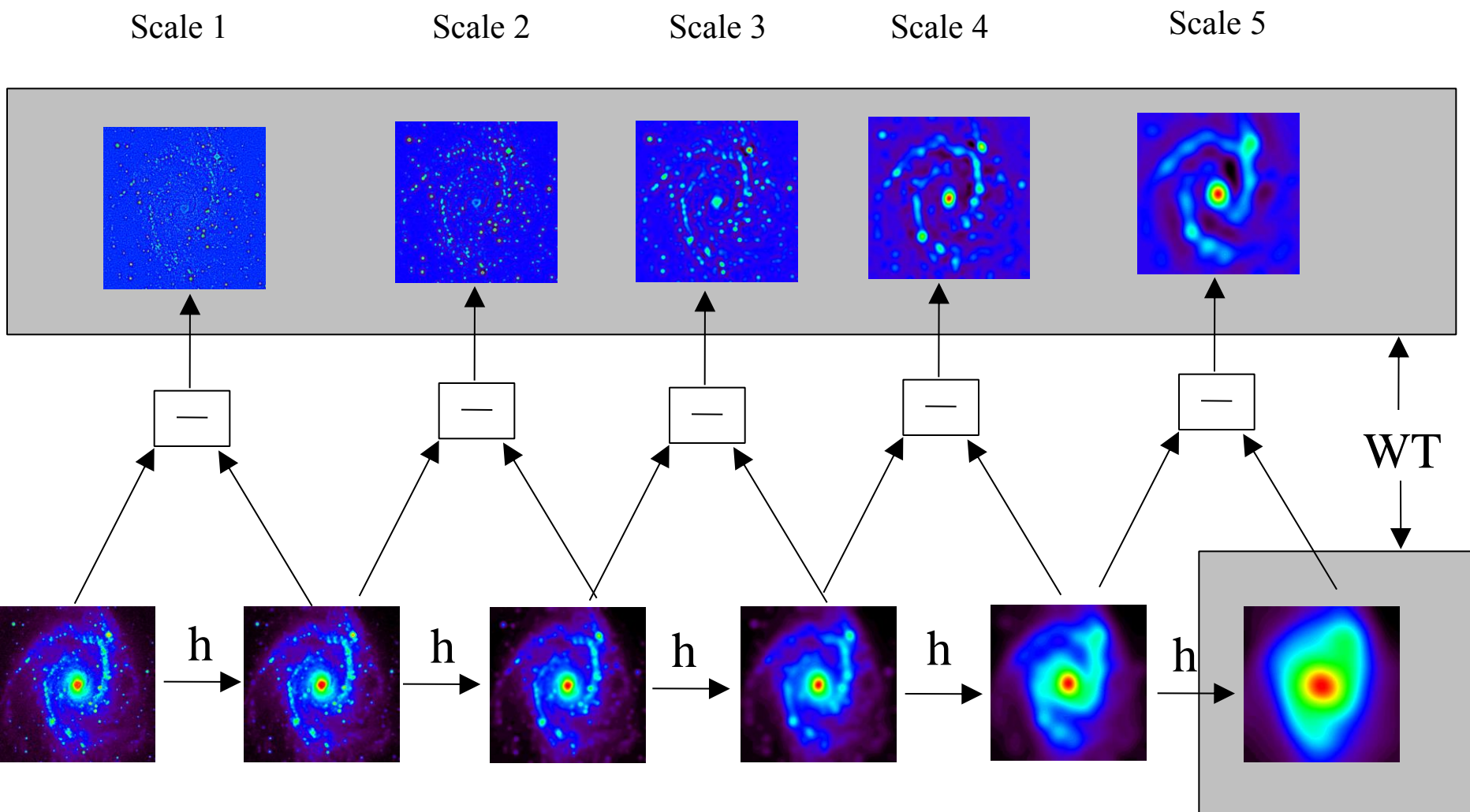
Details scale 2

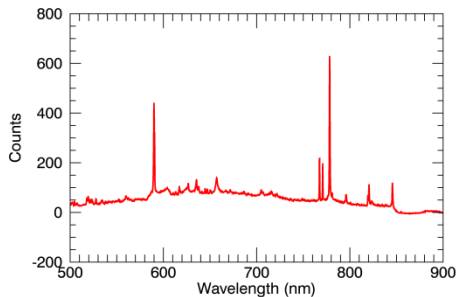


$g(n)$: Wavelet function



Undecimated isotropic wavelet transform





$$I(x, y) = c_j(x, y) + \sum_{j=1}^J w(j, x, y)$$

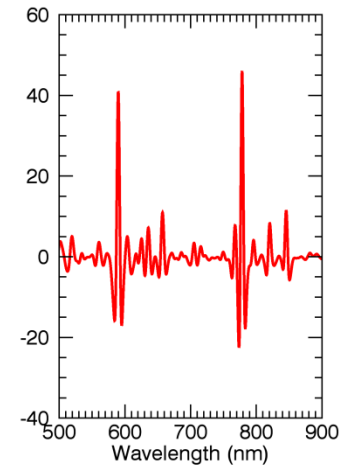
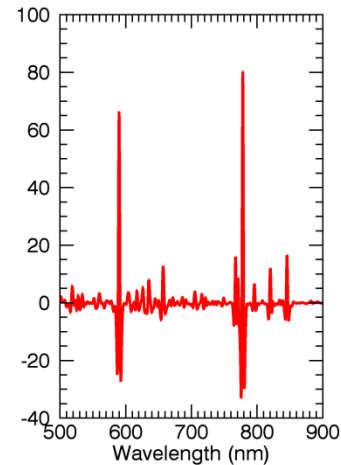
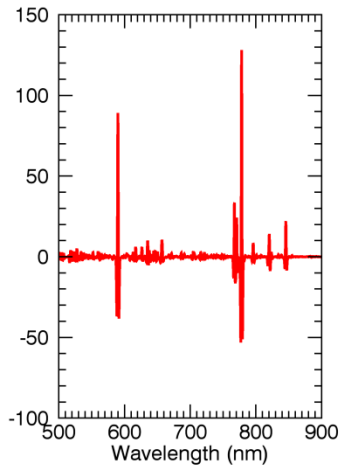
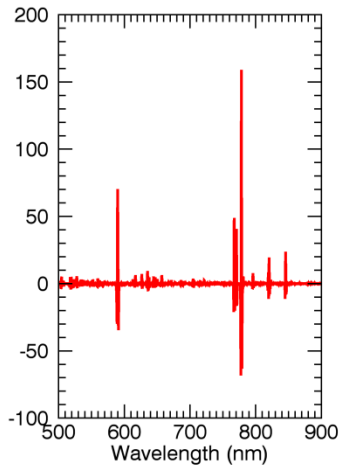
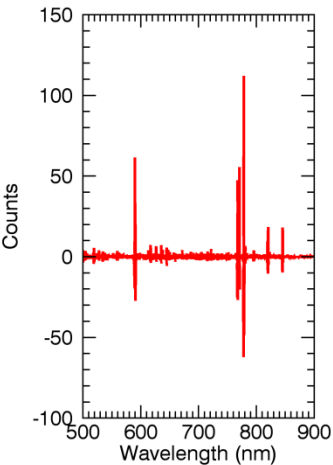
Scale 1

Scale 2

Scale 3

Scale 4

Scale 5



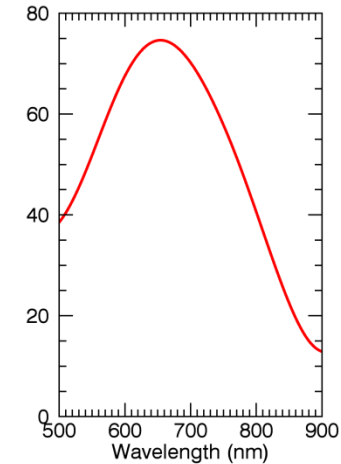
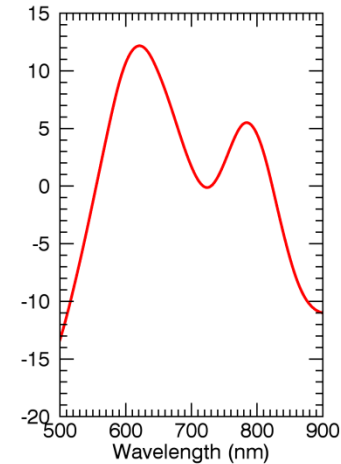
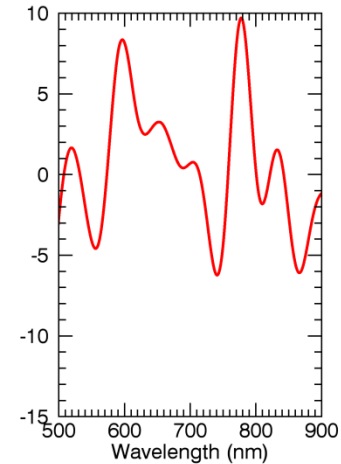
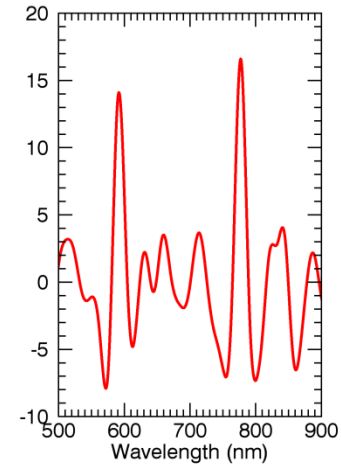
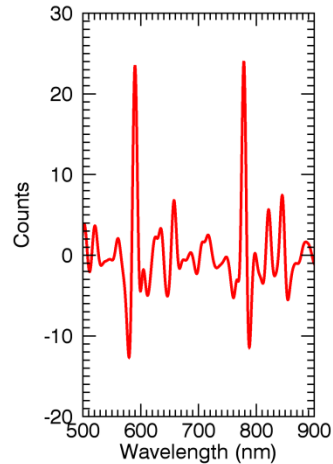
Scale 6

Scale 7

Scale 8

Scale 9

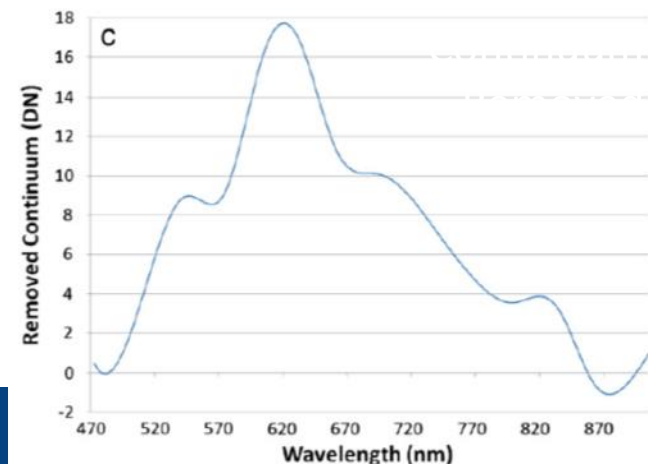
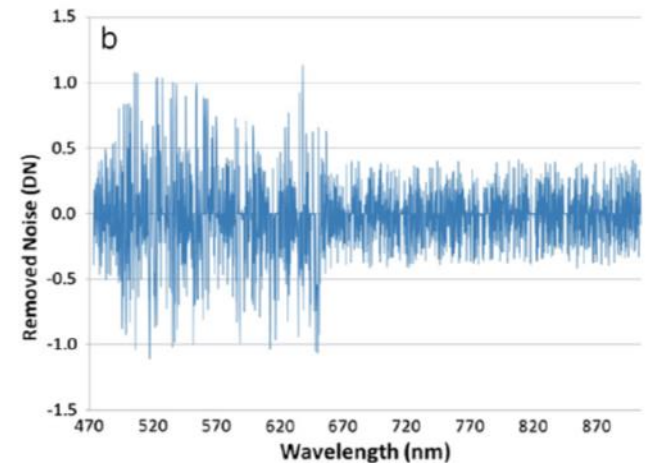
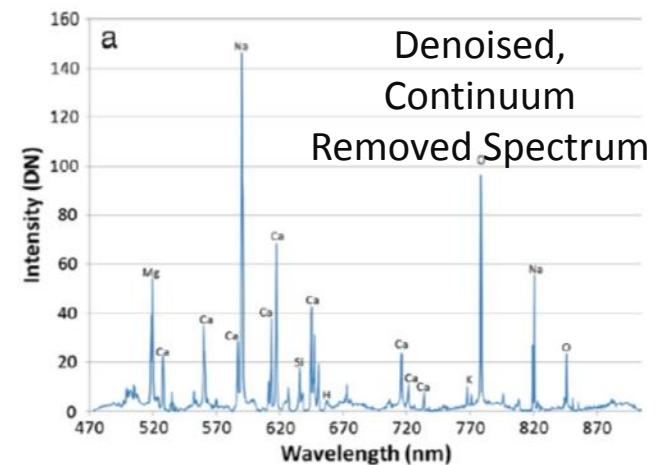
Scale 10



Dark Subtraction, Noise Removal, Continuum Removal

- “Dark” spectrum (no-laser) is subtracted from the LIBS spectrum.
- Noise removed using wavelet transform
- Continuum signal caused by Bremsstrahlung and ion-electron recombination needs to be removed:
 - Continuum defined by wavelet decomposition and fitting a spline to local minima in wavelet space.
- Background signal is distance-dependent, so removal partially corrects for distance.

Wiens et al., 2013



Conversion from counts to photons

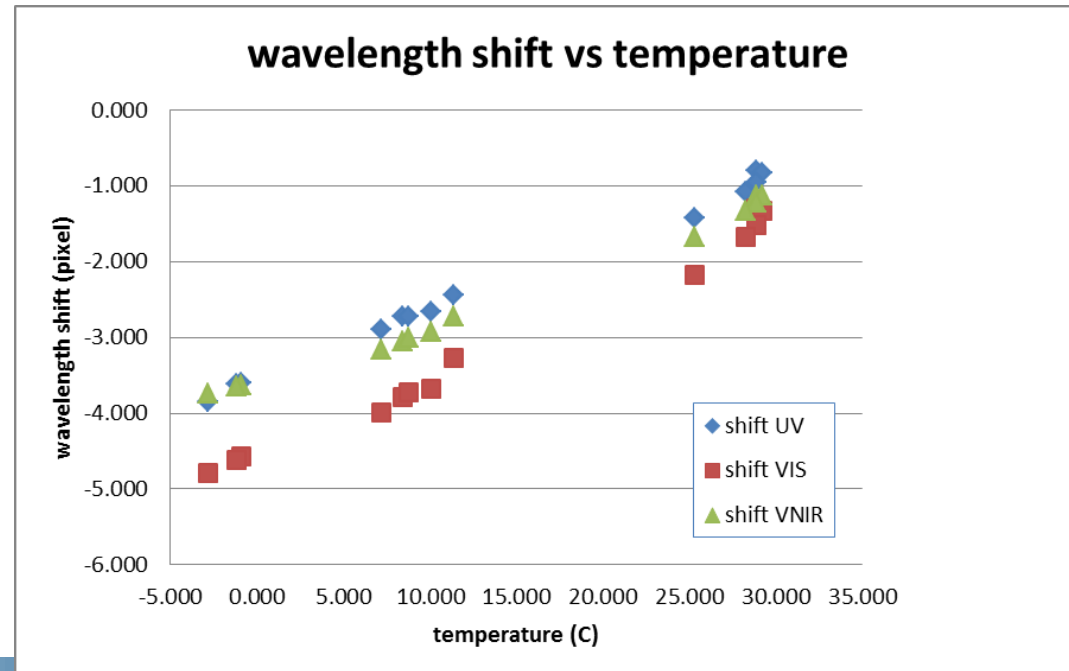
$$DN = L \times A \times \Omega \times \Delta\lambda \times \Delta t \times \sigma + \text{Off}$$

- DN is the digital number (intensity in counts)
- L is the photon spectral radiance in photons/second/cm²/sr/μm wavelength
- A is the source area imaged, in cm²
- Ω is the solid viewing angle in sr
- Δλ is the detector wavelength bin width in μm
- Δt is the integration time in seconds
- σ is the amplified conversion gain in DN/photon
- Off is the offset provided in the analog-to-digital conversion electronics
- L and Ω are inversely dependent upon the distance from the ChemCam telescope to the target while A is increasingly dependent on distance

Wavelength Calibration

- Ti spectrum used as reference because emission lines are present in UV, VIS, and VNIR spectral ranges.
 - Establishes baseline channel-wavelength calibration
- Ti calibration target on Mars provides flight data for wavelength calibration
- Channel wavelength shifts as a linear function of spectrometer temperature
 - Varies from -2C to 30C, depending upon time of day on Mars and season

- For each pixel, find relationship between wavelength and temperature
- Apply shift and interpolate to get calibrated spectrum.



Line identification

- Spectrum to database
 - Localisation of individual peaks
 - Search in library
- Database to spectrum
 - Correlation of region of spectrum (multiple lines) with elemental synthetic spectrum
 - Identification of multiple set of lines

NIST Data Base

http://physics.nist.gov/PhysRefData/ASD/lines_form.html

The screenshot shows a Firefox browser window displaying the NIST Atomic Spectra Database Lines Form. The browser's address bar shows the URL `physics.nist.gov/PhysRefData/ASD/lines_form.html`. The page features a navigation menu with categories like 'DATA' (ASD, LINES, LEVELS) and 'INFORMATION' (List of SPECTRA, GROUND STATES & IONIZATION ENERGIES, Bibliography, Help). The main heading is 'NIST Atomic Spectra Database Lines Form', with a note that it is best viewed with the latest versions of web browsers and JavaScript enabled.

The form includes several input sections:

- Spectrum:** A text input field with a dropdown menu and a hint: "e.g., Fe I or Na;Mg; Al or mg i-iii".
- Wavelength/Wavenumber:** Fields for 'Lower Wavelength' and 'Upper Wavelength', each with a corresponding 'or Upper Wavenumber (in cm⁻¹)' and 'or Lower Wavenumber (in cm⁻¹)' field.
- Units:** A dropdown menu currently set to 'nm'.
- Buttons:** 'Reset input' and 'Retrieve Data'.
- Dynamic Plots:** A section with options for 'Line Identification Plot' and 'Saha-LTE Spectrum', and input fields for 'Electron Temperature T_e (eV)', 'Electron Density N_e (cm⁻³)', and 'Ion Temperature T_i (eV)'. A checkbox for 'Doppler-broadened spectrum' is also present.
- Grotrian Diagram:** A section with 'Java subwindow size' options (640 x 640, 800 x 640, 1024 x 768, 1280 x 1024), checkboxes for 'Group by configurations | Term multiplicity' and 'Show only radiatively linked levels', and a 'Make Grotrian Diagram' button (noting it requires Java2).
- Output Options:** A dropdown menu for 'Format output' set to 'HTML (formatted)'. The 'Additional Criteria' section shows 'Lines' set to 'All'.

NIST Data Base

http://physics.nist.gov/PhysRefData/ASD/lines_form.html

Ca I	395.002	15	3.34e+06	C
Ca I	395.817	17	9.8e+06	C
Ca II	396.959	220	1.4e+08	C
Ca I	397.369	8		
Ca I	397.483	18	1.75e+07	C
Ca II	409.826	50	9.9e+06	D
Ca I	409.969	15	1.3e+07	D
Ca I	409.973	15	1.5e+06	D
Ca II	411.098	60	1.2e+07	D
Ca II	411.144	30	1.9e+06	D
Ca II	420.736	40	4.3e+06	D
Ca II	422.126	50	8.5e+06	D
Ca I	422.792	50	2.18e+08	B+

C-Quest

C-QuEST - ChemCam - Quick Element Search Tool v2.5.0 (16 Aug 2012)

File Help

Databases

NIST
 Martian (Agnes Cousin)

Wavelength (nm)

UV (240-341) VIS (381-469) VNIR (471-905)

Min 0 Max 1,000

Periodic Table

SELECT ALL CLEAR ALL Major Trace Organic (CHNOPS) Other

Information

20: Calcium

Ca shows several important lines.
Here are the most ones, observed for each spectral range :
- UV : 315.978 nm and 318.025 nm
- VIS : 393.477 nm, 396.959 nm and 422.792 nm are the most important among others
- VNIR : lot of Ca lines. The most easy ones to detect are the triplet at 610.441, 612.39 and 616.3 nm with an increasing intensity, and a second triplet at 644.085, 645.159 and 646.436-646.557 nm with a decreasing intensity.
All these lines are well defined with no interferences.
The most important Ca lines in all the spectrum are those at 393.477 nm and 396.959 nm, but they can suffer some auto-absorption effects.

26: Iron

Db	Elt	Ionization_deg	Wavelength	Intensity (rel)
Martian	Fe	I	382.891	123.040
Martian	Mg	I	383.339	348.572
Martian	Fe	I	383.531	119.010
Martian	Mg	I	383.938	550.271
Martian	Fe	I	384.214	124.963
Martian	Fe	I	384.435	170.888
Martian	Fe	I	384.789	180.731
Martian	Fe	I	385.105	25.079
Martian	Mg	II	385.148	27.250
Martian	Fe	I	385.191	25.079
Martian	Si	II	385.711	97.816
Martian	Fe	I	385.747	97.816
Martian	Fe	I	386.100	99.896
Martian	Fe	I	386.662	29.485
Martian	Fe	I	387.360	28.300
Martian	Fe	I	387.912	42.953
Martian	Fe	I	387.967	87.629
Martian	Fe	I	388.738	87.009
Martian	Fe	I	388.815	38.716
Martian	Fe	I	388.961	29.944
Martian	Mg	I	389.668	25.116
Martian	Fe	I	389.676	11.379
Martian	Fe	I	390.081	16.824
Martian	Al	II	390.178	126.093
Martian	Fe	I	390.405	40.857
Martian	Si	I	390.663	92.265
Martian	Fe	I	390.759	7.718
Martian	Fe	I	392.137	17.891
Martian	Fe	I	392.402	21.324
Martian	Fe	I	392.903	27.216
Martian	Fe	I	393.141	28.136
Martian	Ca	II	393.477	2,055.650
Martian	Al	I	394.512	1,719.220
Martian	Fe	I	394.989	16.226
Martian	Fe	I	395.228	7.751
Martian	Fe	I	395.757	28.646
Martian	Fe	I	395.780	28.646
Martian	Al	I	396.264	2,529.360
Martian	Fe	I	396.774	22.027
Martian	Ca	II	396.959	3,839.890
Martian	Fe	I	397.038	139.231
Martian	Fe	I	397.887	13.207

Nb lines : 166

Print Spectra

Agnès presentation

To be continued with level 2
Thank you