

peakmoment

July 30, 2025

1 CH1 MIRI/JWST

1.1 JWST/MIRI Spectral Analysis Script

```
[1]: #CH1
import numpy as np
import matplotlib.pyplot as plt
from spectral_cube import SpectralCube
from astropy import units as u
from scipy.signal import find_peaks
from tqdm import tqdm
import os
from astropy.wcs import WCS
from astropy.wcs.utils import proj_plane_pixel_scales

output_dir = "moment_maps_per_peak"
os.makedirs(output_dir, exist_ok=True)

# Define dictionary: wavelength (Å) -> label
lines = {
    5.5100: 'H$_{2}$ (0-0) S(7)',
    6.1076: 'H$_{2}$ (0-0) S(6)',
    6.9084: 'H$_{2}$ (0-0) S(5)',
}

# --- Step 1: Load JWST cube ---#####
#Change only /path-to-data-directory and file name (i.e. file_dir) here.
# data_dir = '/path-to-data-directory/'
# file_dir = '*****_miri_ch1-****' #your JWST IFU file name, without adding_
# ↪ "_s3d.fits"
data_dir = '/Users/somnathdutta/Desktop/outflow_analysis/JWST/Data/
↪MAST_2024-09-18T0222/JWST/'
file_dir = 'jw01854-c1007_t002_miri_ch1-shortmediumlong' #Change this Only
file_fits = '/' + file_dir + '_s3d.fits'
fitsfile = data_dir + file_dir + file_fits
```

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#fits.info(fitsfile) # 1 SCI 1 ImageHDU 89 (43, 51, 3438)
↳float32
cube = SpectralCube.read(fitsfile, hdu='SCI').with_spectral_unit(u.micron)
#cube = cube.to(u.Jy)
#flux_unit = cube.unit.to_string() # e.g., 'Jy / beam' or 'MJy / sr'

# --- Convert MJy/sr to Jy/pixel ---
# pixel_scale_arcsec = 0.11#96 # Adjust if needed based on the channels
# pixel_area_sr = ((pixel_scale_arcsec * u.arcsec) ** 2).to(u.sr)

# Get pixel area in steradians from SpectralCube's WCS
pixel_area_sr = cube.wcs.proj_plane_pixel_area() # returns an astropy Quantity
↳in steradians

cube = cube.to(u.MJy/u.sr) # Standardize unit
cube = cube * pixel_area_sr # Convert to MJy
cube = cube.to(u.mJy) # Final unit: mJy
cube_next = cube

flux_unit = cube.unit.to_string() # Will now be 'mJy'

wavelengths = cube.spectral_axis.to(u.micron).value # shape: (N_lambda,)
ny, nx = cube.shape[1:]

#--- Step 2: Circular mask ---#####
# -Define central pixel of spectrum extraction and radius-
x0, y0 = 13, 35 # central pixel of spectrum extraction
#radius = 3 # aperture radius in pixels, comment if using arcsec-based
↳radius

# Compute pixel scale and aperture radius in pixels,
#comment this section if you are using pixel-based radius as indicated above
pixel_scales = proj_plane_pixel_scales(cube.wcs.celestial) # degrees/pixel
pixel_scale_arcsec = pixel_scales[0] * 3600 # arcsec/pixel (assuming square
↳pixels)
aperture_radius_arcsec = 0.5 #arcsec
radius_pix_aperture = aperture_radius_arcsec / pixel_scale_arcsec
print(f"Aperture radius: {aperture_radius_arcsec}\" = {radius_pix_aperture:.2f}
↳pixels")
radius = radius_pix_aperture

## Use below section to varify or any error in above section
# aperture_radius_arcsec = 0.2 # aperture radius in arcseconds
# # === Extract spaxel size from WCS ===

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# wcs = WCS(cube.header)
# cdelt1 = np.abs(wcs.wcs.cdelt[1]) * 3600 # RA spaxel size in arcsec
# cdelt2 = np.abs(wcs.wcs.cdelt[2]) * 3600 # Dec spaxel size in arcsec
# mean_spaxel_size = (cdelt1 + cdelt2) / 2.0
# radius = aperture_radius_arcsec / mean_spaxel_size #in pixel
# print(f"Using aperture radius: {aperture_radius_arcsec} → {radius_pix:.2f}␣
→pixels")

yy, xx = np.mgrid[0:ny, 0:nx]
mask = (xx - x0)**2 + (yy - y0)**2 <= radius**2
#####

# #####

# --- Step 3: Extract summed spectrum within aperture ---
data = cube.unmasked_data[:, mask] # shape: (N_lambda, N_pixels)
spectrum = np.nansum(cube._data[:, mask], axis=1) # _data is a Quantity array

# --- Step 4: Define continuum-fitting regions (line-free) ---
continuum_windows = [(4.8, 5.2), (7.5, 8.0)] # micron; adjust based on your␣
→data

# Create boolean mask to select continuum regions
cont_mask = np.zeros_like(wavelengths, dtype=bool)
for wmin, wmax in continuum_windows:
    cont_mask |= (wavelengths >= wmin) & (wavelengths <= wmax)

# Extract continuum points
wave_cont = wavelengths[cont_mask]
flux_cont = spectrum[cont_mask]

# --- Step 5: Polynomial fit to continuum ---
degree = 1 # linear fit; use 2 for quadratic if needed
coeffs = np.polyfit(wave_cont, flux_cont, deg=degree)
continuum_fit = np.polyval(coeffs, wavelengths)

# --- Step 6: Estimate noise and detect peaks ---
residuals = spectrum - continuum_fit
noise = np.nanstd(residuals[cont_mask]) # sigma from continuum regions
sigma_given = 5
threshold = continuum_fit + sigma_given * noise

peaks, properties = find_peaks(spectrum, height=threshold)

# --- Step 7: Plot ---

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plt.figure(figsize=(10, 5))
plt.plot(wavelengths, spectrum, label='Observed Spectrum')
plt.plot(wavelengths, continuum_fit, 'k--', label=f'Polyfit Continuum
↳(deg={degree})')
#plt.axhline(continuum_fit.mean() + 5 * noise, color='red', linestyle='--',
↳label='10 Threshold')
plt.plot(wavelengths, continuum_fit + sigma_given * noise, 'r--',
↳label=f'{sigma_given} Threshold')
plt.plot(wavelengths[peaks], spectrum[peaks], 'ro', label='Detected Peaks')

#####
# Annotate using the dictionary
for wave, label in lines.items():
    #plt.axvline(wave, color='red', linestyle='--', alpha=0.5)
    plt.text(wave - 0.06, max(spectrum)*0.65, label, rotation=90,
↳verticalalignment='bottom', color='red')

#####

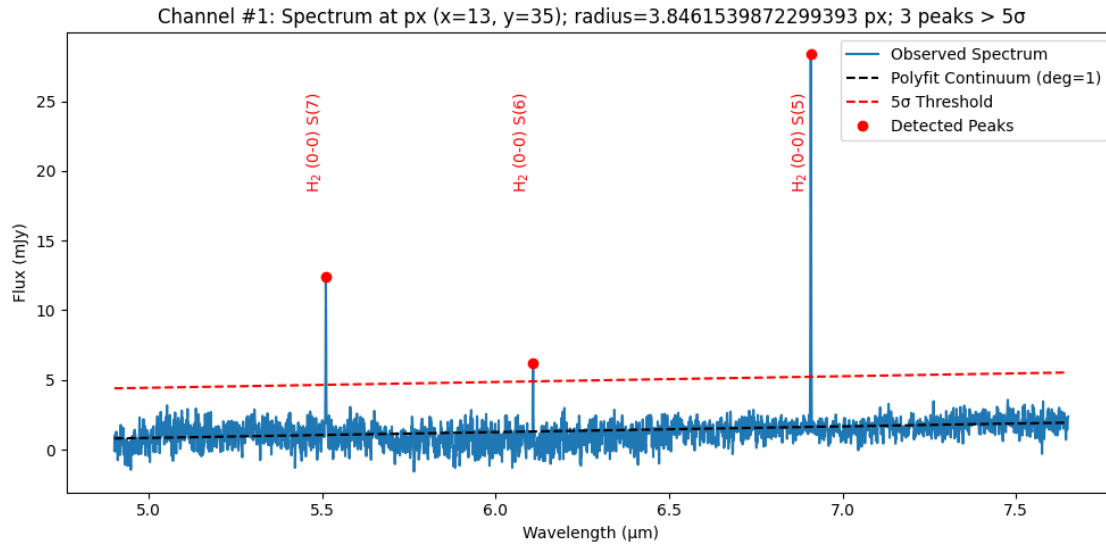
plt.xlabel('Wavelength (m)')
#plt.ylabel('Flux')
plt.ylabel(f'Flux ({flux_unit})')
plt.title(f'Channel #1: Spectrum at px (x={x0}, y={y0}); radius={radius} px;
↳{len(peaks)} peaks > {sigma_given} ')
#plt.title(f'Channel #1: Spectrum at px (x={x0}, y={y0});
↳radius={aperture_radius_arcsec} arcsec; {len(peaks)} peaks > {sigma_given} ')
plt.legend()
plt.tight_layout()
plt.savefig(f"{output_dir}/full_spectra_{file_dir}.png", dpi=200)
plt.show()

# --- Optional: Print peak info ---
print("Detected Peak Wavelengths (m):")
print(np.round(wavelengths[peaks], 4))
detected_peaks_wavelengths = wavelengths[peaks]

# --- Print peak results ---
#print(f"\n estimated from continuum: {sigma:.4g}")
print(f"Detected peaks (wavelength ([m]), flux ({flux_unit})):")
for wl, flux in zip(wavelengths[peaks], spectrum[peaks]):
    print(f"{wl:.4f} m\t{flux:.4g}")
#CH1

```

Aperture radius: 0.5" = 3.85 pixels



Detected Peak Wavelengths (m):

[5.51 6.1076 6.9084]

Detected peaks (wavelength ([m]), flux (mJy)):

5.5100 m 12.4

6.1076 m 6.181

6.9084 m 28.41

1.2 JWST MIRI Channel Moment Map Generator (per Emission Line)

```
[2]: #CH1
import numpy as np
import matplotlib.pyplot as plt
from astropy.io import fits
from astropy import units as u
from spectral_cube import SpectralCube
from astropy.visualization import simple_norm
from tqdm import tqdm
from matplotlib.patches import Circle

# --- Load the JWST cube ---
#Comment this section, since this cell#2 will take input from the output of
#above cell#1
# fitsfile = '.....'
# cube = SpectralCube.read(fitsfile, hdu='SCI').with_spectral_unit(u.micron)

# detected_peaks_wavelengths = [...] # your detected peak wavelengths in
# microns
# x0, y0 = ... # aperture center pixel coordinates
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# radius = ... # aperture radius in pixels
# output_dir = 'output_directory_path'
# flux_unit = cube.unit # or specify flux unit string

delta1 = 0.1 # micron; continuum window half-width, adjust if needed
gap1 = 0.014 # micron; gap between line and continuum windows, adjust if
↳needed.

for i, peak in enumerate(detected_peaks_wavelengths):
    wavelengths = cube.spectral_axis.to(u.micron).value
    ny, nx = cube.shape[1:]

    # Circular mask for aperture
    yy, xx = np.mgrid[0:ny, 0:nx]
    mask = (xx - x0)**2 + (yy - y0)**2 <= radius**2

    # Extract summed spectrum within aperture
    spectrum = np.nansum(cube._data[:, mask], axis=1)

    # Define continuum windows
    cont_windows = [
        (peak - delta1 - gap1, peak - gap1),
        (peak + gap1, peak + delta1 + gap1)
    ]

    # Continuum mask for fitting
    cont_mask = np.zeros_like(wavelengths, dtype=bool)
    for wmin, wmax in cont_windows:
        cont_mask |= (wavelengths >= wmin) & (wavelengths <= wmax)
    wave_cont = wavelengths[cont_mask]
    flux_cont = spectrum[cont_mask]

    if len(wave_cont) < 2:
        print(f"Not enough continuum points around peak {peak:.6f} m for fit.
↳Skipping...")
        continue

    # Fit continuum to full spectrum for residual calculation
    coeffs = np.polyfit(wave_cont, flux_cont, deg=1)
    continuum_fit = np.polyval(coeffs, wavelengths)

    # Residual spectrum
    residual_spectrum = spectrum - continuum_fit

    # Estimate noise sigma from continuum residuals
    residual_continuum = residual_spectrum[cont_mask]
    noise_sigma = np.nanstd(residual_continuum)

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# Define spectral slab including peak and continuum windows
lambda_min = (peak - delta1 - gap1) * u.micron
lambda_max = (peak + delta1 + gap1) * u.micron
cube2 = cube.spectral_slab(lambda_min, lambda_max)
wavelengths2 = cube2.spectral_axis.to(u.micron).value

# Sum spectrum in aperture from cube2
spectrum2 = np.nansum(cube2._data[:, mask], axis=1)

# Residual spectrum in cube2 range
continuum_fit2 = np.polyval(coeffs, wavelengths2)
residual_spectrum2 = spectrum2 - continuum_fit2

# Select channels with residual > 3 sigma
significant_channels = np.where(residual_spectrum2 > 3 * noise_sigma)[0]

#####
# Integrated flux from actual spectrum (not continuum-subtracted), in
→aperture, for channels > 3 sigma
delta_lambda = np.mean(np.diff(wavelengths2)) # micron per channel
num_sig_channels = len(significant_channels)

if num_sig_channels > 0:
    integrated_flux = 0.0
    for ch in significant_channels:
        # sum flux in aperture at this channel
        flux_ch = np.nansum(cube2._data[ch, mask])
        integrated_flux += flux_ch * delta_lambda # flux * wavelength
→channel width (m)

    print(f"Integrated flux (actual spectrum) at peak {peak:.4f} m over
→{num_sig_channels} channels >3 : {integrated_flux:.3e} [{flux_unit}·m]")
else:
    print(f"No >3 channels at peak {peak:.4f} m for integrated flux
→calculation.")
#####

#####
# Integrate the residual spectrum in m units for channels above 3
delta_lambda = np.mean(np.diff(wavelengths2)) # average spectral
→resolution in m
flux_contsub = np.sum(residual_spectrum2[significant_channels]) *
→delta_lambda
print(f"Continuum-subtracted integrated flux at {peak:.4f} m:
→{flux_contsub:.3e} [{flux_unit}·m]")

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# Get peak residual flux at the channel closest to the line center (peak)
peak_idx = np.argmin(np.abs(wavelengths2 - peak))
peak_flux_subtracted = residual_spectrum2[peak_idx]
print(f"Peak flux (continuum-subtracted) at {peak:.4f} m:␣
↪{peak_flux_subtracted:.3e} [{flux_unit}]")
#####

# Print channels and channel widths above 3 sigma
channels_wavelengths = wavelengths2[significant_channels]
if len(significant_channels) > 1:
    channel_widths = np.diff(wavelengths2) # differences between channels
    selected_channel_widths = channel_widths[significant_channels[:-1]]
else:
    selected_channel_widths = np.array([])

print(f"Peak {i+1} at {peak:.4f} m: {len(significant_channels)} channels >␣
↪3 ")
print("Channels (m):", channels_wavelengths)
if len(selected_channel_widths) > 0:
    print("Channel widths (m):", selected_channel_widths)
else:
    print("Channel widths (m): N/A (only one significant channel)")

if len(significant_channels) == 0:
    print(f"No channels above 3 for peak {peak:.4f} m, skipping moment␣
↪maps.")
    continue

# Build continuum-subtracted cube for full cube2 spectral range
n_lambda, ny, nx = cube2.shape
contsub_cube = np.full((n_lambda, ny, nx), np.nan)
continuum_map = np.full((ny, nx), np.nan)

# Pixel-wise continuum fitting for cube2 wavelengths
valid_idx = np.where(cont_mask)[0]
for y in tqdm(range(ny), desc=f"Peak {i+1}/
↪{len(detected_peaks_wavelengths)}"):
    for x in range(nx):
        spec = cube2[:, y, x].value
        if np.all(np.isnan(spec)):
            continue
        # Use continuum indices relative to cube2 spectral axis
        cont_mask_cube2 = np.zeros_like(wavelengths2, dtype=bool)
        for wmin, wmax in cont_windows:
            cont_mask_cube2 |= (wavelengths2 >= wmin) & (wavelengths2 <=␣
↪wmax)
        spec_cont = spec[cont_mask_cube2]

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        valid = ~np.isnan(spec_cont)
        if np.sum(valid) < 2:
            continue
        coeffs_pix = np.polyfit(wavelengths2[cont_mask_cube2][valid],
        spec_cont[valid], deg=1)
        fitted_full = np.polyval(coeffs_pix, wavelengths2)
        consub_cube[:, y, x] = spec - fitted_full
        continuum_map[y, x] = np.polyval(coeffs_pix, peak)

    cube_sub = SpectralCube(data=consub_cube * cube.unit, wcs=cube2.wcs).
    with_spectral_unit(u.micron)

    # Compute moment maps from only channels above 3 sigma
    consub_mask = np.zeros(n_lambda, dtype=bool)
    consub_mask[significant_channels] = True
    if np.sum(consub_mask) < 1:
        print(f"No channels above 3 sigma for peak {peak:.4f} m after
        selection. Skipping moment maps.")
        continue

    moment0_orig = cube2.spectral_slab(wavelengths2[significant_channels[0]]*u.
    micron,
                                     wavelengths2[significant_channels[-1]]*u.
    micron).moment(order=0)
    moment0_sub = cube_sub.
    spectral_slab(wavelengths2[significant_channels[0]]*u.micron,
                 wavelengths2[significant_channels[-1]]*u.micron).moment(order=0)

    # Plotting
    fig, axs = plt.subplots(1, 4, figsize=(20, 5), gridspec_kw={'wspace': 0.5})
    fig.suptitle(f"JWST/MIRI Channel#1: Peak #{i+1} at {peak:.4f} μm",
    fontsize=16, y=0.92)

    # Panel 1: Zoomed spectrum with continuum fit and windows
    axs[0].plot(wavelengths, spectrum, color='black', label='Spectrum')
    axs[0].plot(wavelengths, continuum_fit, 'r--', label='Continuum fit')
    for wmin, wmax in cont_windows:
        axs[0].axvspan(wmin, wmax, color='skyblue', alpha=0.3)
    axs[0].set_xlim(cont_windows[0][0], cont_windows[1][1])
    axs[0].set_xlabel('Wavelength (m)')
    axs[0].set_ylabel(f'Flux [{flux_unit}]')
    axs[0].set_title(f'Zoomed Spectrum around Peak @ {peak:.4f} m')
    axs[0].legend()

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    axs[0].grid(True)
    axs[0].set_aspect(aspect=1.0 / axs[0].get_data_ratio())

    # Panel 2: Original Moment-0 Map
    norm0 = simple_norm(moment0_orig.value, 'linear', percent=85)
    im0 = axs[1].imshow(moment0_orig.value, origin='lower', cmap='inferno',
↳ norm=norm0)
    axs[1].set_title('Original Moment-0 Map')
    axs[1].set_xlabel('X Pixel')
    axs[1].set_ylabel('Y Pixel')
    cbar0 = plt.colorbar(im0, ax=axs[1], fraction=0.046)
    cbar0.set_label(f'Flux [{moment0_orig.unit}]')
    # Add a circle
    circle = Circle((x0, y0), radius, edgecolor='cyan', facecolor='none',
                    lw=1.5, transform=axs[1].transData, zorder=99)
    axs[1].add_patch(circle)
    #####

    # Panel 3: Fitted Continuum Map
    norm1 = simple_norm(continuum_map, 'linear', percent=85)
    im1 = axs[2].imshow(continuum_map, origin='lower', cmap='plasma',
↳ norm=norm1)
    axs[2].set_title(f'Fitted Continuum Map @{peak:.4f} μm')
    axs[2].set_xlabel('X Pixel')
    axs[2].set_ylabel('Y Pixel')
    cbar1 = plt.colorbar(im1, ax=axs[2], fraction=0.046)
    cbar1.set_label(f'Flux [{cube2.unit}]')

    # Panel 4: Continuum-Subtracted Moment-0 Map
    norm2 = simple_norm(moment0_sub.value, 'linear', percent=85)
    im2 = axs[3].imshow(moment0_sub.value, origin='lower', cmap='inferno',
↳ norm=norm2)
    axs[3].set_title('Continuum-Subtracted Moment-0 Map')
    axs[3].set_xlabel('X Pixel')
    axs[3].set_ylabel('Y Pixel')
    cbar2 = plt.colorbar(im2, ax=axs[3], fraction=0.046)
    cbar2.set_label(f'Flux [{moment0_sub.unit}]')

    plt.savefig(f"{output_dir}/moment_maps_peak_{i+1}_{peak:.4f}.png", dpi=200,
↳ bbox_inches='tight')
    plt.show()
    plt.close()

    # Save FITS files
    header = cube_sub.wcs.celestial.to_header()
    fits.writeto(f"{output_dir}/moment0_original_{peak:.4f}.fits", moment0_orig.
↳ value, header, overwrite=True)

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```
fits.writeto(f"{output_dir}/continuum_map_{peak:.4f}.fits", continuum_map,
↳header, overwrite=True)
fits.writeto(f"{output_dir}/moment0_subtracted_{peak:.4f}.fits",
↳moment0_sub.value, header, overwrite=True)

print(" Done: CH1 Moment maps generated for all detected peaks.")
```

Integrated flux (actual spectrum) at peak 5.5100 m over 4 channels >3 :
2.408e-02 [mJy·m]

Continuum-subtracted integrated flux at 5.5100 m: 2.063e-02 [mJy·m]

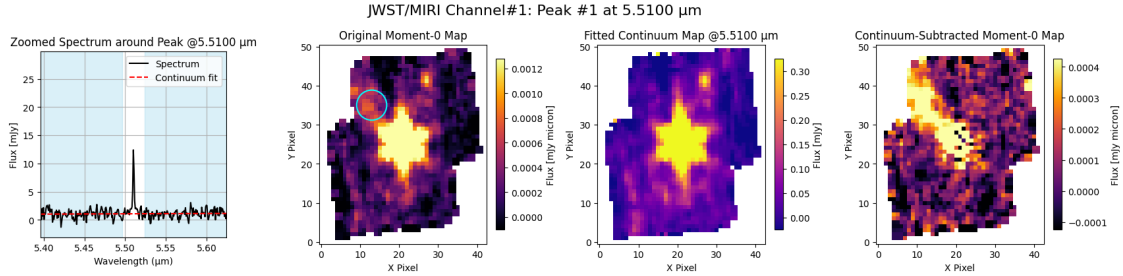
Peak flux (continuum-subtracted) at 5.5100 m: 1.132e+01 [mJy]

Peak 1 at 5.5100 m: 4 channels > 3

Channels (m): [5.50920008 5.51000008 5.51080008 5.51160008]

Channel widths (m): [0.0008 0.0008 0.0008]

Peak 1/3: 100% | 51/51 [00:07<00:00,
7.12it/s]



Integrated flux (actual spectrum) at peak 6.1076 m over 2 channels >3 :
8.425e-03 [mJy·m]

Continuum-subtracted integrated flux at 6.1076 m: 7.204e-03 [mJy·m]

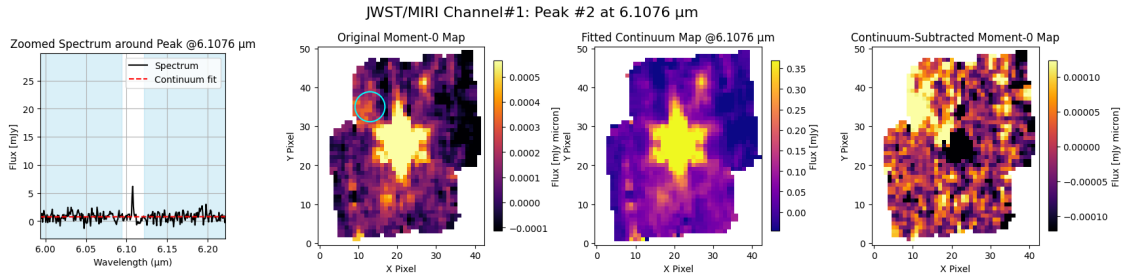
Peak flux (continuum-subtracted) at 6.1076 m: 5.418e+00 [mJy]

Peak 2 at 6.1076 m: 2 channels > 3

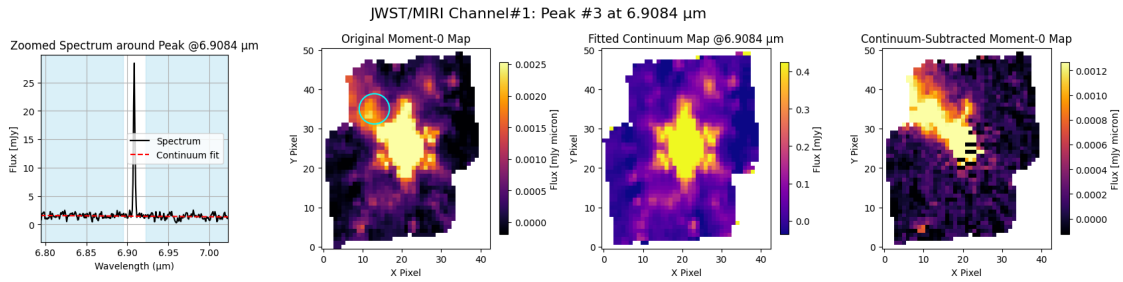
Channels (m): [6.10680006 6.10760006]

Channel widths (m): [0.0008]

Peak 2/3: 100% | 51/51 [00:06<00:00,
7.87it/s]



Integrated flux (actual spectrum) at peak 6.9084 μ m over 6 channels >3 :
6.688e-02 [mJy \cdot m]
Continuum-subtracted integrated flux at 6.9084 μ m: 5.992e-02 [mJy \cdot m]
Peak flux (continuum-subtracted) at 6.9084 μ m: 2.696e+01 [mJy]
Peak 3 at 6.9084 μ m: 6 channels > 3
Channels (μ m): [6.90680004 6.90760004 6.90840004 6.90920004 6.91000004
6.91080004]
Channel widths (μ m): [0.0008 0.0008 0.0008 0.0008 0.0008]
Peak 3/3: 100%| | 51/51 [00:07<00:00,
6.60it/s]



Done: CH1 Moment maps generated for all detected peaks.