Spectroscopy

Simplest Spectrograph

Light source, eg star or lamp

Slit

Prism

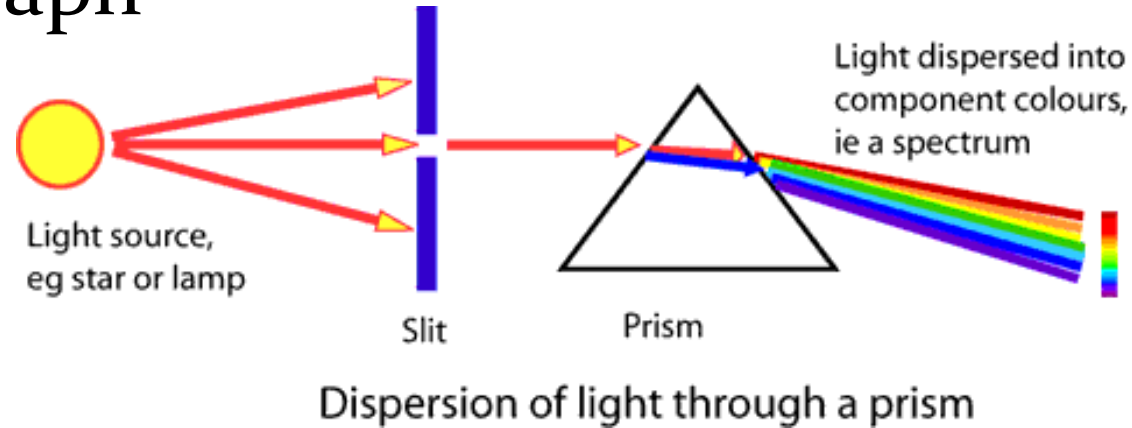Light dispersed into component colours, ie a spectrum

Dispersion of light through a prism

Can do spectroscopy without a slit:
-Objective prism spectroscopy just puts the prism in ahead of the telescope...
      small prism angles, low dispersion
      effective survey space only for the brightest targets
   high background, but high throughput.

Overlapping dispersed images of everything in the field

EUCLID/NISP will employ slitless spectroscopy
between 0.9 and 1.8um using grisms

JWST NIRISS has a slitless spectroscopy mode from 0.8-2.2um
with a resolving power R~ 150 and order sorting filters.
Choice of 1 or 2 orthogonal grisms to help deblend objects
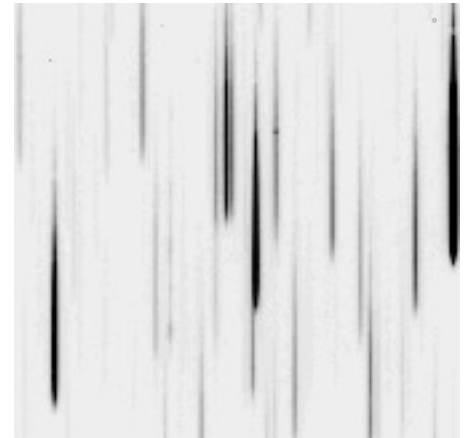
Reflection grating with groove spacing d

$$d\sin\theta + d\sin i = \lambda$$
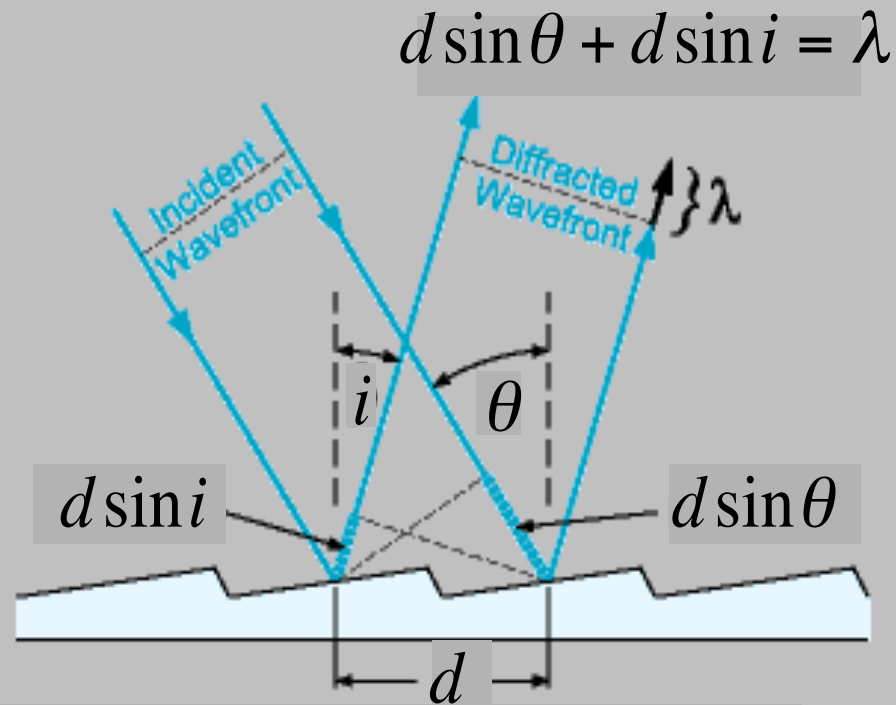
Grating Equation:

$$\sin\theta + \sin i = \frac{m\lambda}{d}$$
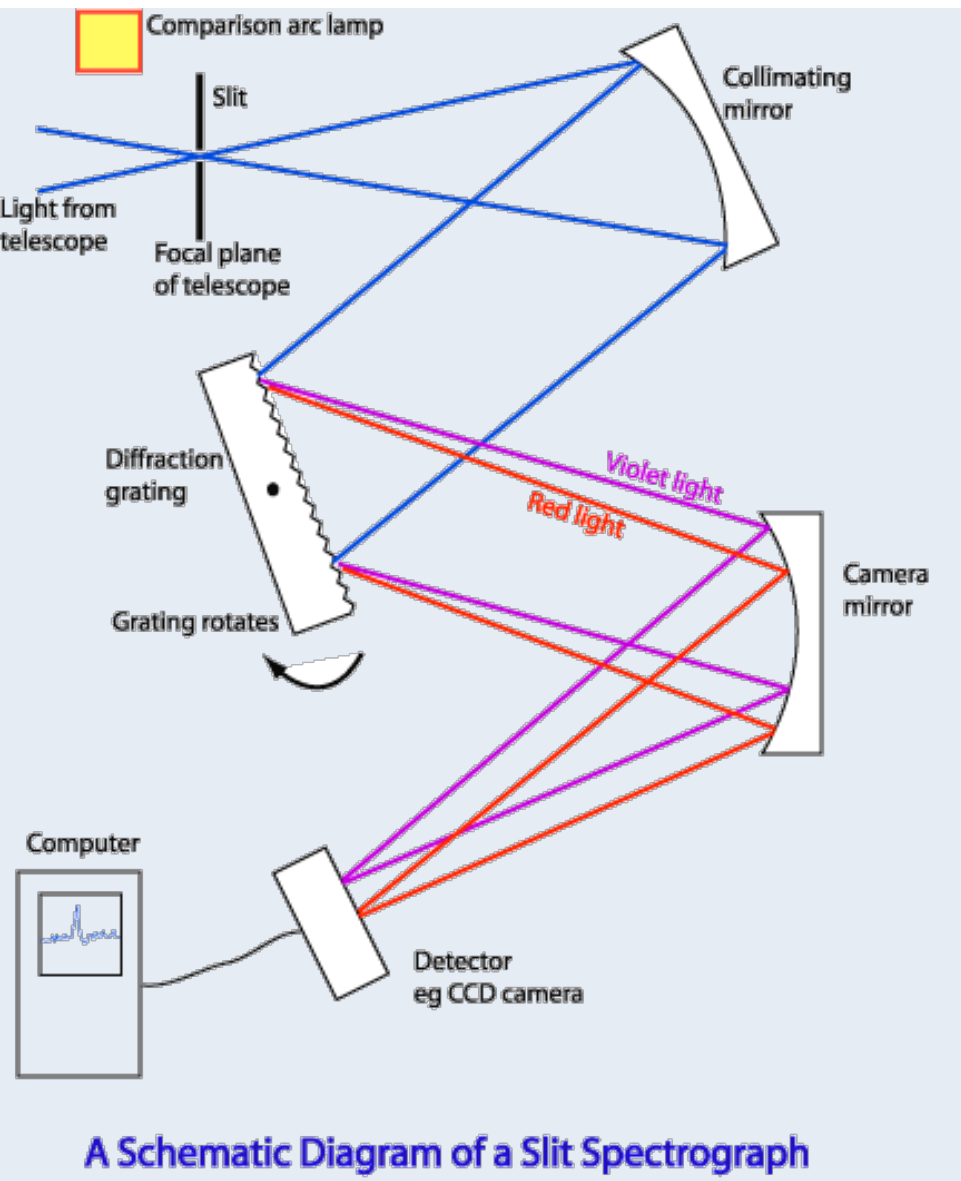
Dispersion: $d\theta/d\lambda = m/d\cos\theta$

In the diffraction limit,
Resolving Power: $R = mN$
Where N is the number of grooves illuminated

For a diffraction-limited grating, resolving power is increased by increasing the number of grooves with a larger grating or higher line density or operating at higher orders

Real Spectrographs

A Schematic Diagram of a Slit Spectrograph

After passing through the entrance slit, the light is collimated by a mirror (or lenses) and directed to a grating. The dispersed light is focussed on the detector by a camera mirror (or lenses) effectively forming a dispersed image of the slit. Then slit width normally defines the resolution.
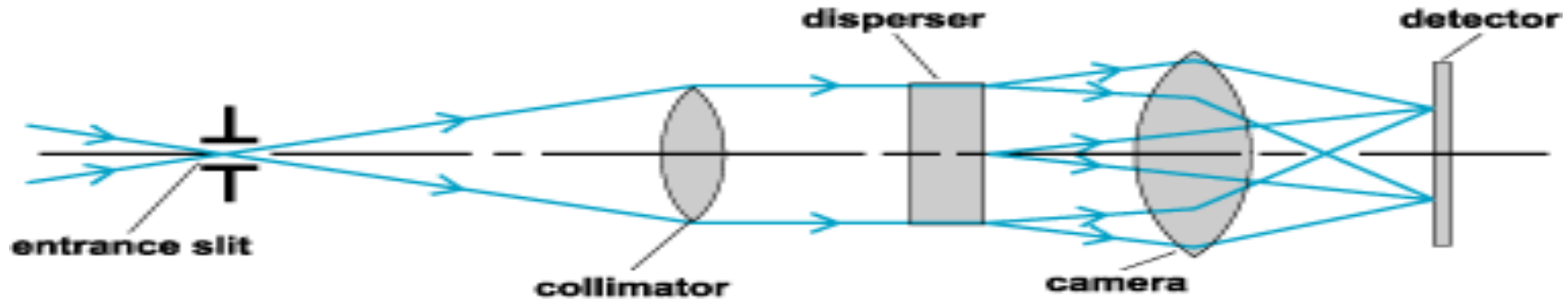
Bandpass filters are used to limit the dispersion order and prevent overlapping orders.

Throughput is lower than simple imaging due to slit losses, more surfaces and grating efficiency.

Field of view limited to the length of the slit.

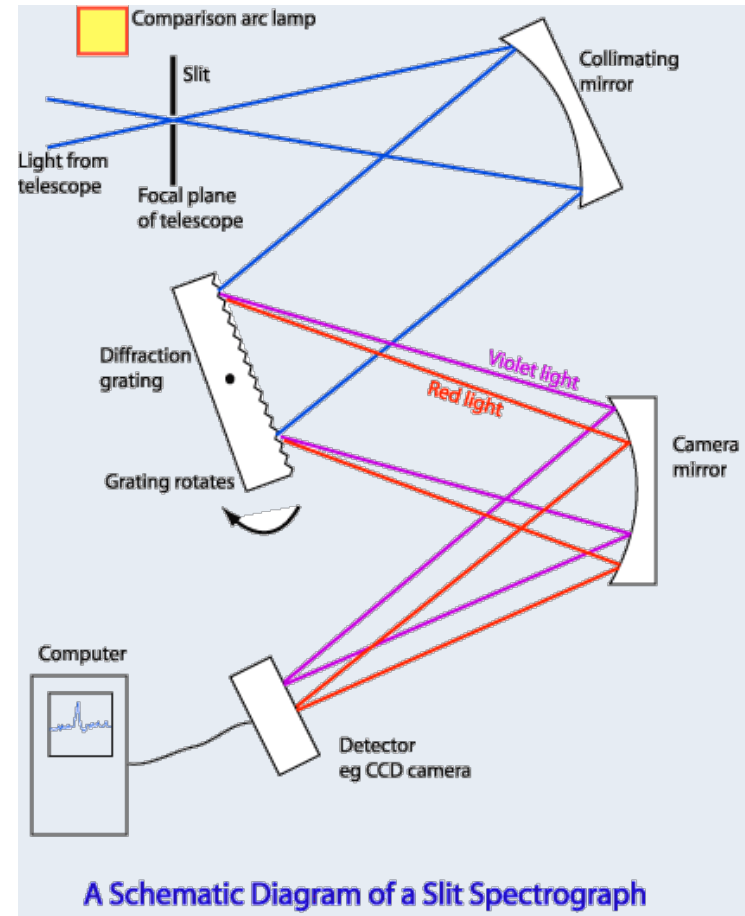Optics can be reflective or transmissive...
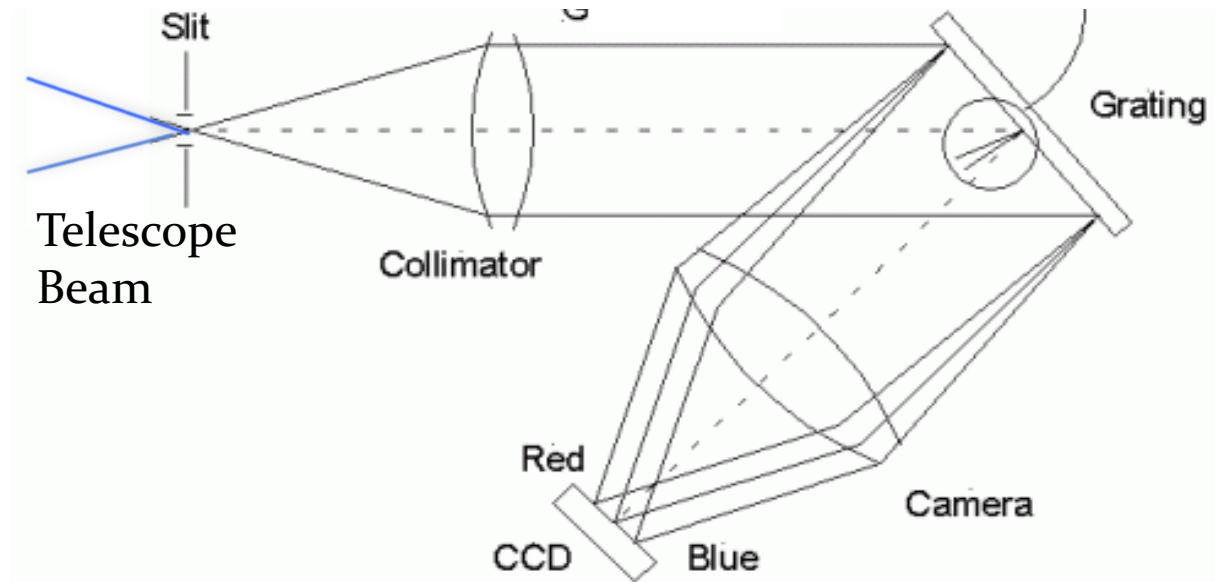
Instrument Layout

- Transmissive optics can be prism, grism, grating (including Volume Phase holographic grating)
- Grism: a grating replicated onto a prism so that the prism compensates for the grating diffraction angle to provide dispersion in the order of interest around the optical axis
- VPH has sinusoidal modulations in the refractive index of dichromated gelatin imprinted into bulk of the material, so provide accurate fringe structures up to ~6000 lines/mm. They have very high efficiency

Grism operation

Grisms can be rotated into the instrument beam   for low resolution spectroscopy in instruments with a collimated space. A slit or slit mask is required in the telescope focal plane.

- Grism grating equation: $m\lambda = d(n \sin\alpha + \sin \beta)$
- From the geometry : $\alpha = -\beta = \theta = A$
- And so $m\lambda = d(n-1) \sin\theta$
- Thus   the prism apex angle : $\sin A = m\lambda / d(n-1)$
- And different orders can be employed with different A

Seeing-limited instruments

- The slit width defines how much light is admitted.
- The entrance slit is imaged onto the detector and the slit width usually defines the resolution delivered by the instrument.
- A wide slit
  - admits more light (and more background light).
  - It may also mean that the target underfills the slit so that the spectral resolution is is given by the profile of the object instead of the width of the slit and so may vary from object to object.

Comparison arc lamp

Slit

Collimating mirror

Light from telescope

Focal plane of telescope

Diffraction grating

Violet light

Red light

Camera mirror

Grating rotates

Computer

Detector eg CCD camera

A Schematic Diagram of a Slit Spectrograph

Spectral Resolution

- Want to sample the resolution, $\Delta\lambda$, with at least 2 pixels for proper sampling.
- Telescope focal plane scale is $206265/f.D_{tel}$ arcsec/mm
- Spectrograph acts as an optical relay with magnification $= f_{cam}/(f_{coll} \cos\theta)$
  - Where the $\cos\theta$ term is the anamorphic magnification that arises from the diffraction angle
- Large slit widths on large telescopes need very fast optics
- VLT Nasmyth is f/17 => 0.5 arcsec slit has width 330μm in the focal plane.
- VIMOS images a 0.5" slit on to 2.5 CCD 15μm pixels with an f/1.8 camera.

Grating Choice

- Match grating dispersion to the camera pixel scale and f-ratio to provide the required resolution
- Grisms can provide low resolving powers <3000
  - e.g. VIMOS Grisms have 200 < R < 2500 with a 1 arcsec slit
- Grating maximum resolving power : Nm.
- High resolution spectrographs usually use Echelles - gratings used at high order (m~ 60), but relatively low groove density (10s of lines/mm rather than thousands)
  - High order means steep angles, and large dimensions
  - E.g. R4 grating with $i = 75^\circ$ and R up to 200,000
  - Generally used with cross-dispersing elements (prisms or gratings) to separate the diffraction orders and permit wide wavelength coverage at high resolution.
  - Located in stable locations, Nasmyth, Coude or fibre-fed in a controlled environment for high-stability, high precision observations (e.g. RV measurements for exoplanets)

- Echellogram – output from a cross-dispersed echelle
- X-dispersion normal to the echelle dispersion separates orders.
- Typically have curved orders and order separation that increases with decreasing wavelength
- Need large format detectors to sample the full range at high resolution
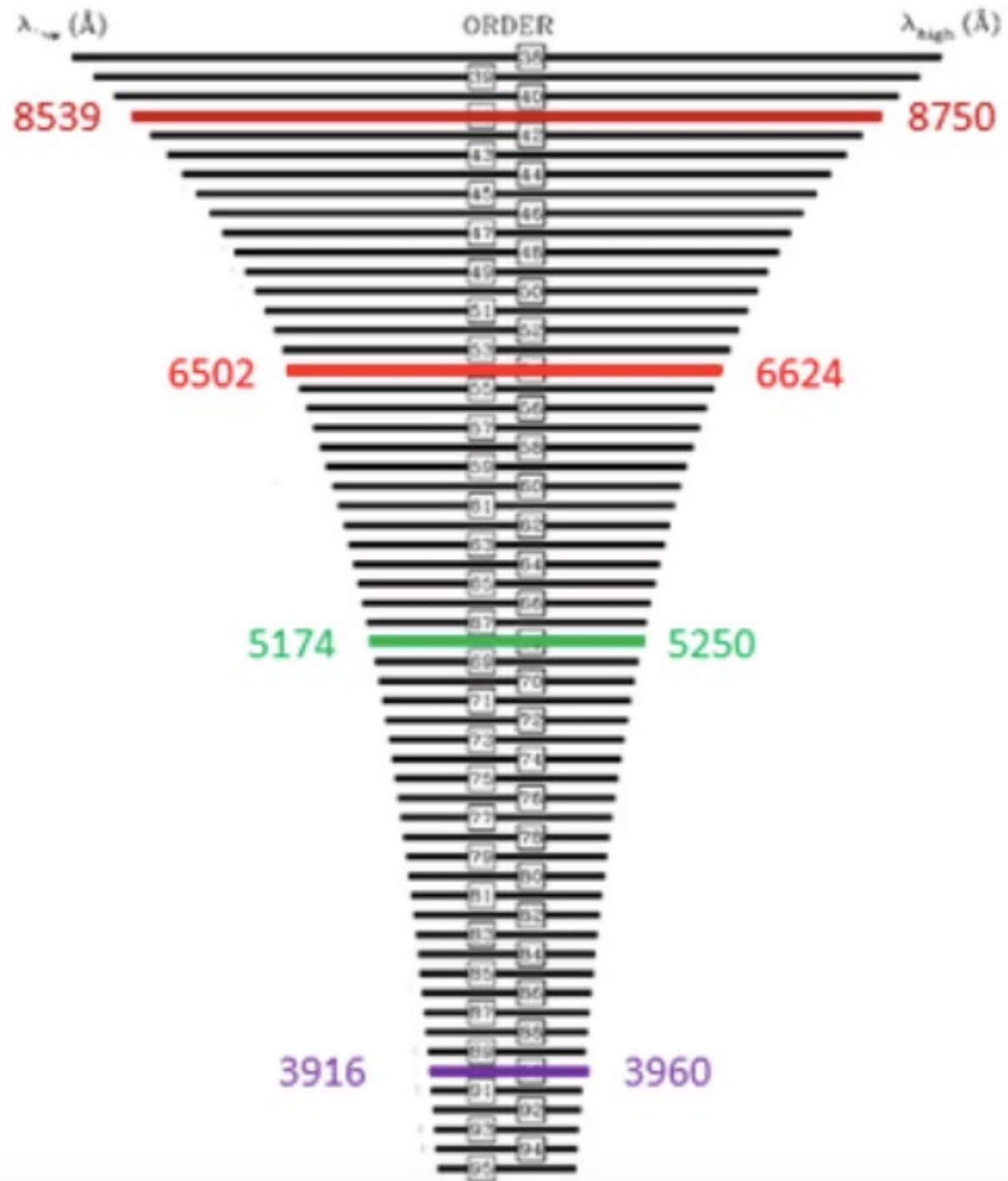
VLT ESPRESSO Optical Layout
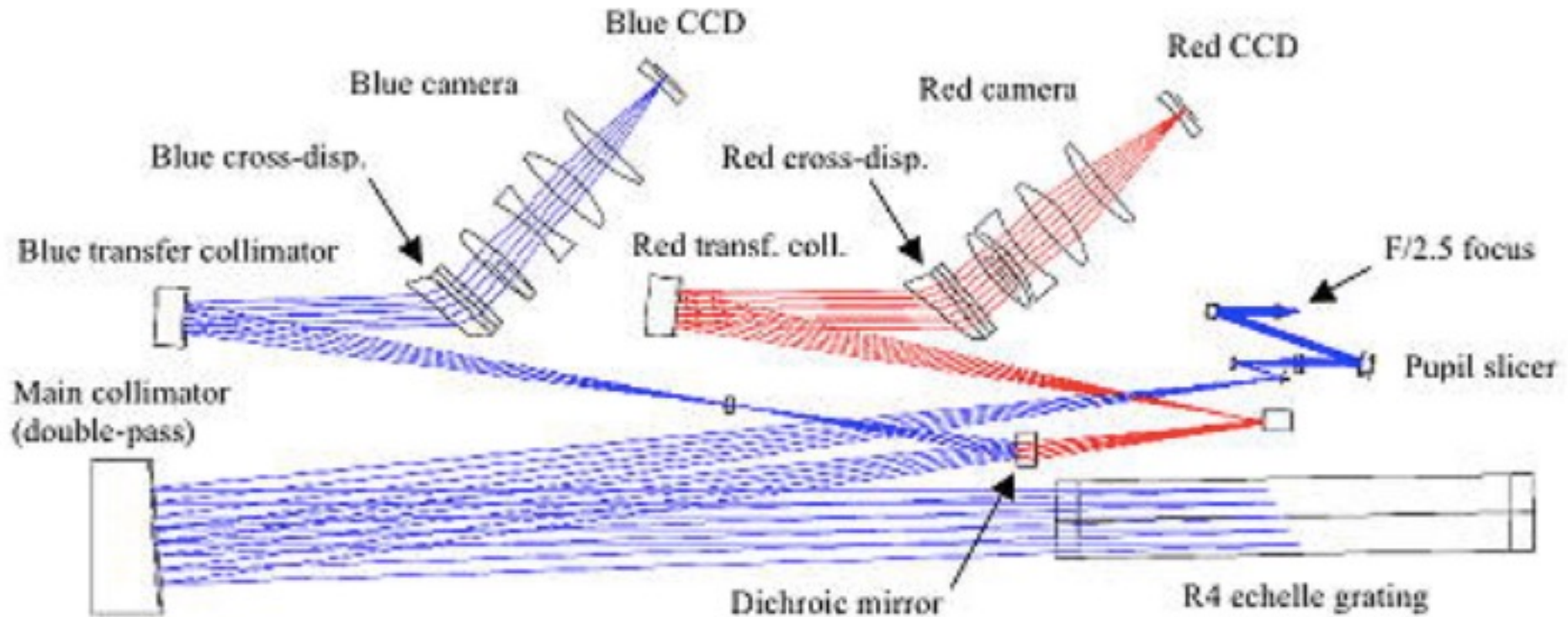
- Two arm spectrograph optimised for blue and red spectral regions
- Located at the incoherent combined focus of the 4 VLT telescopes
- Temperature-controlled environment – goal is for precision of 10cm/s
- Echelle gratings mosaiced together to provide a large format

Maximising Efficiency

A grating (unless cross-dispersed) only covers one order in wavelength without overlap – a bandpass filter may be used to prevent overlap.

So the whole CCD range (0.3 – 1.0um) cannot be covered in a single setting.

Splitting the light into two arms with a dichroic mirror, typically 0.3-0.55um and 0.55-1.0 um, allows complete spectral coverage.

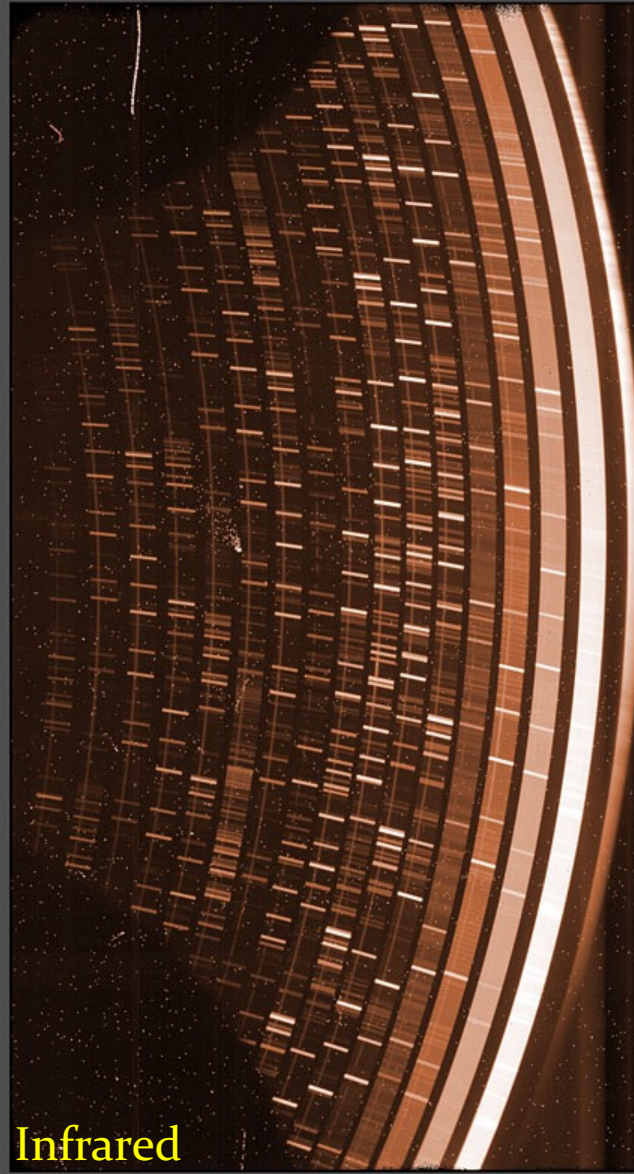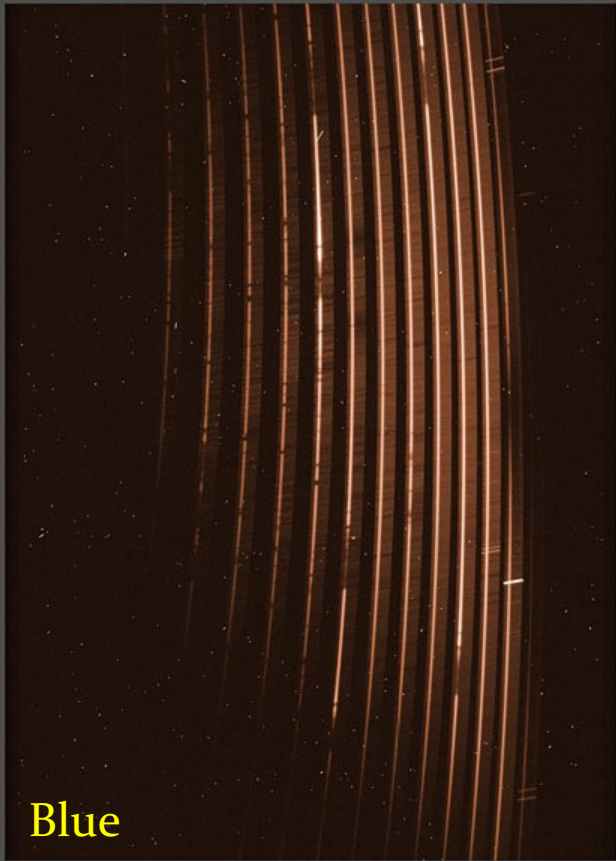It also permits optimised coatings and CCD detector properties for the Blue and Red spectrograph arms.

But at the cost of greater complexity and cost

X-shooter on the VLT covers the visible and near-IR from 0.3 to 2.4um with 3 arms, Blue, Red, IR, each optimised for throughput
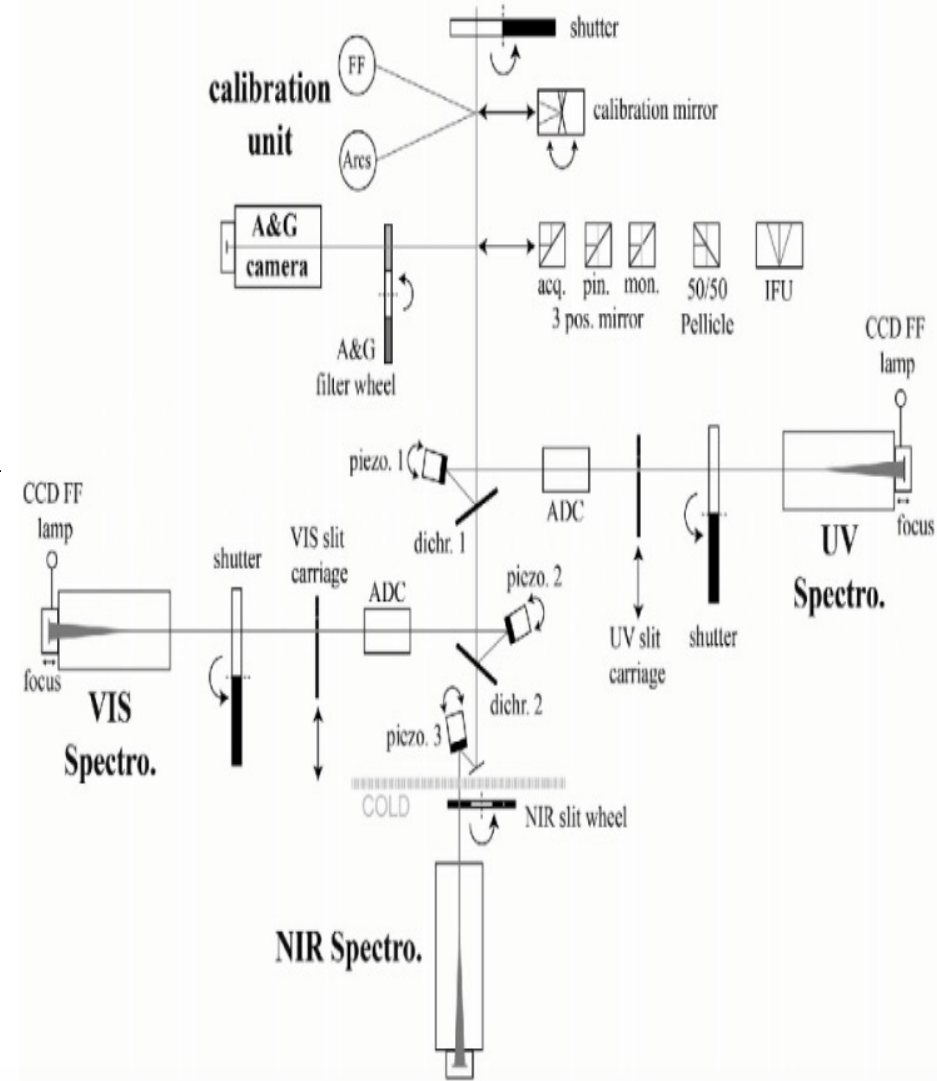
X-Shooter schematic

see Vernet et al. 2011, A&A, 536A, 105

Raw X-shooter spectrum of a Quasar. The wavelength increases from bottom to top of each spectrum, and from left to right. The spectrum of the quasar is the thin bright lines visible in each of the orders. The short bright nearly horizontal lines are atmospheric airglow lines while the thermal emission increases sharply above 2um in the right hand spectrum

Calibration requirements:
Wavelength: Arc lamps

- Need reference lines with well known wavelengths spread through the free spectral range

- Traditionally done with calibration lamps
  - HeAr, ThAr, U-Ne, etc., etc.
  - Pro: well known technology, relatively cheap
  - Con: irregularly located lines, line blends, warm-up time/stability, limited lifetime
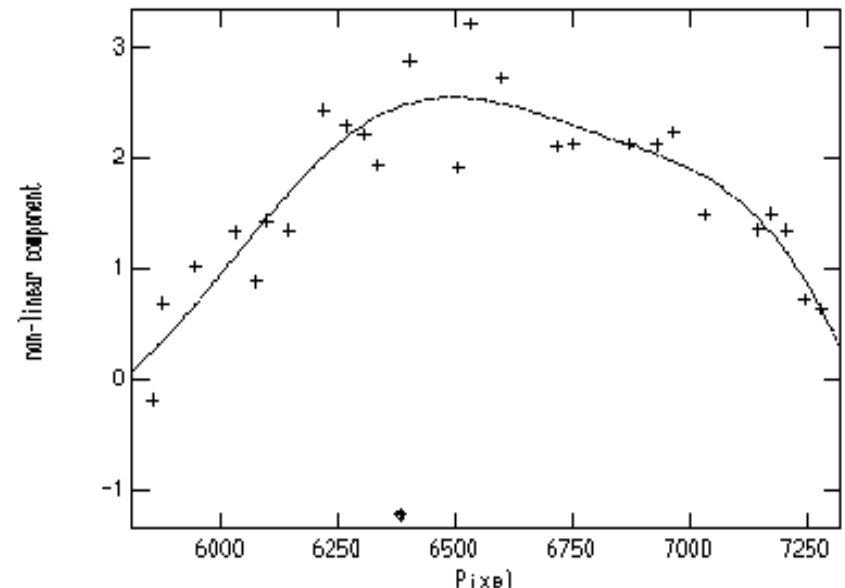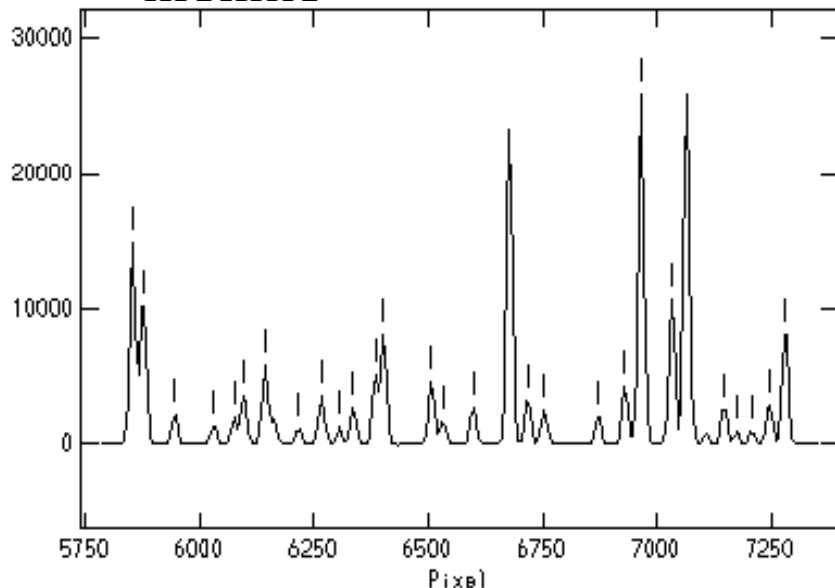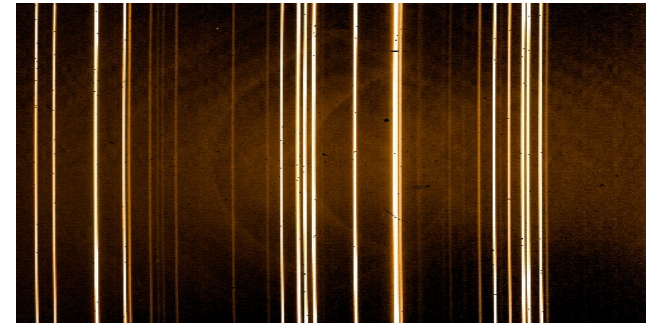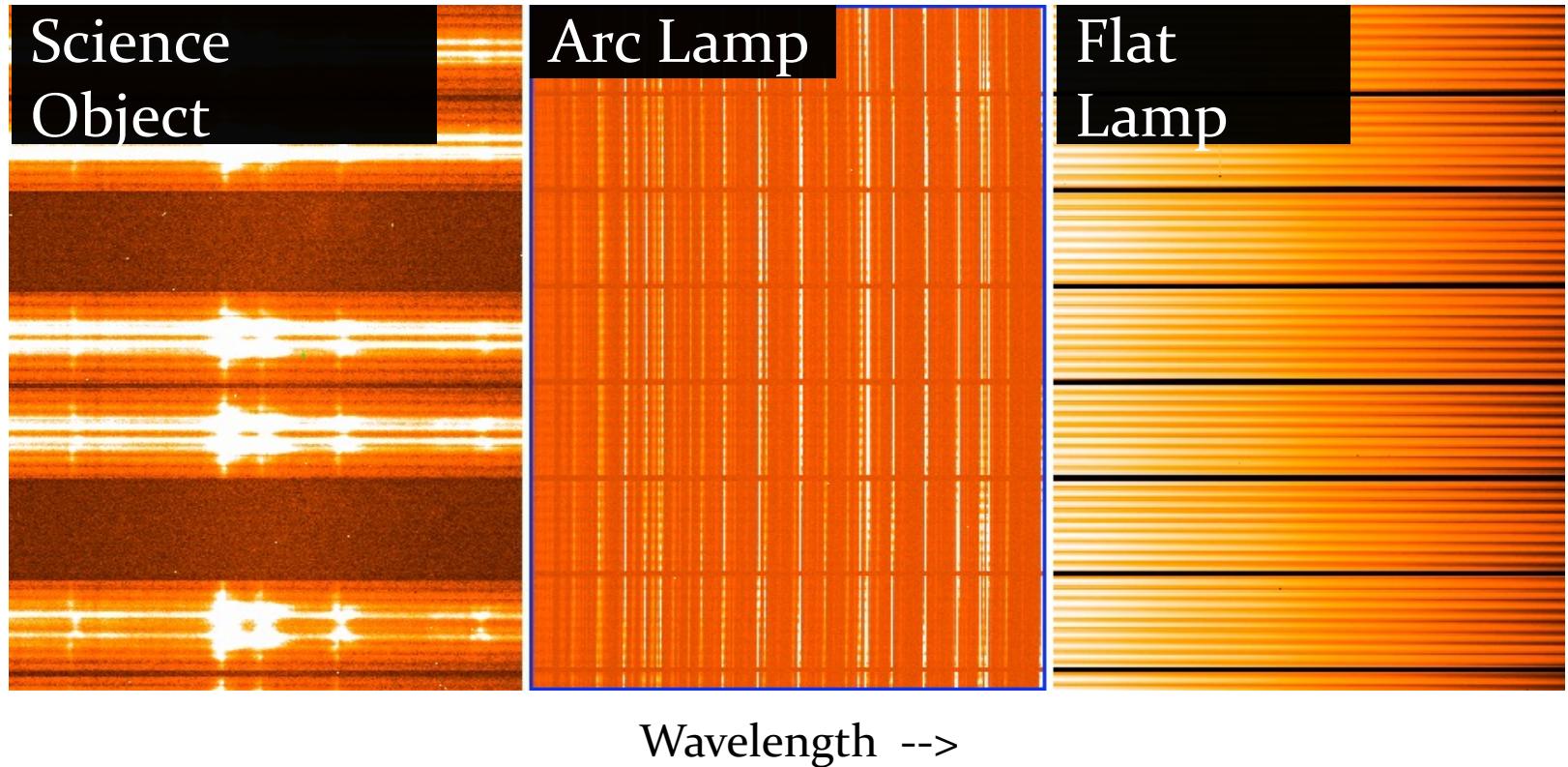
Spectral Calibration

- Simultaneous measurement of calibration spectrum gives highest precision. Depending on the application, different techniques can be used:
  - Atmospheric features –sky lines
  - Arc lamps, typically Ar, Th etc
  - Fabry-Perot etalons, constant wavenumber interval and brightness
  - gas cells – imprint an absorption spectrum e.g. I_2 on the spectrum
  - Laser frequency combs – new technology for very high stability
- For highest accuracy, need the calibration light to travel through the same optical path as the science target
- LFC may provide stability at cm/s velocities
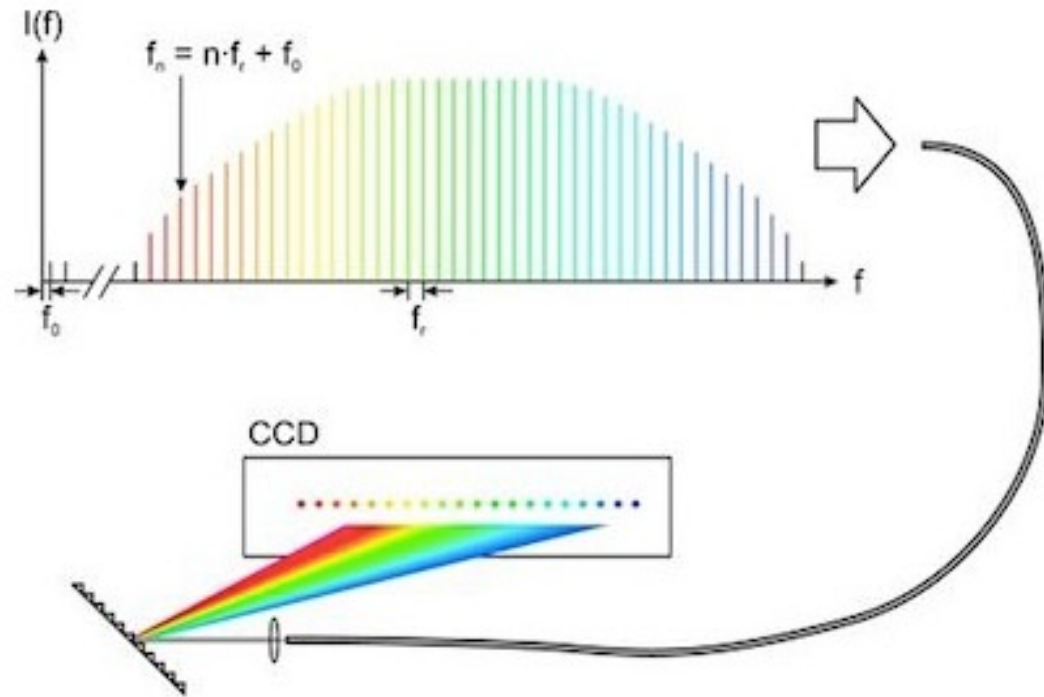
The frequency difference (f_r) between two neighboring lines in a frequency comb is always exactly the same. It is kept stable by comparing it with an atomic clock. The comb light is guided to the spectrograph in an optical fiber. The light is separated into its its frequency components by the spectrograph and imaged on the CCD detector. The comblike spectrum appears as a row of dots, of which each dot corresponds exactly to one line of the frequency comb. This "laser ruler" can now be used to calibrate the spectrograph. (Image: T. Wilken)

Calibration: fit spatial and wavelength distortions and rebin the data

Wavelength -->

- Apply wavelength calibration (position dependent) and rebin data to linear scale
- Pipelines may use models for sky spectrum and fits to raw data (better control of noise terms)
- Also need dark and bias removal, flat field correction, cosmic ray clean-up etc. And correct for distortions, curved orders etc.

Correction for sky emission

- Blank sky is not black, even in space, but from the ground the atmosphere is the main contributor, especially in the IR
- Need to "sky" subtract to give the clean object spectrum – subtract detector rows above and below the target
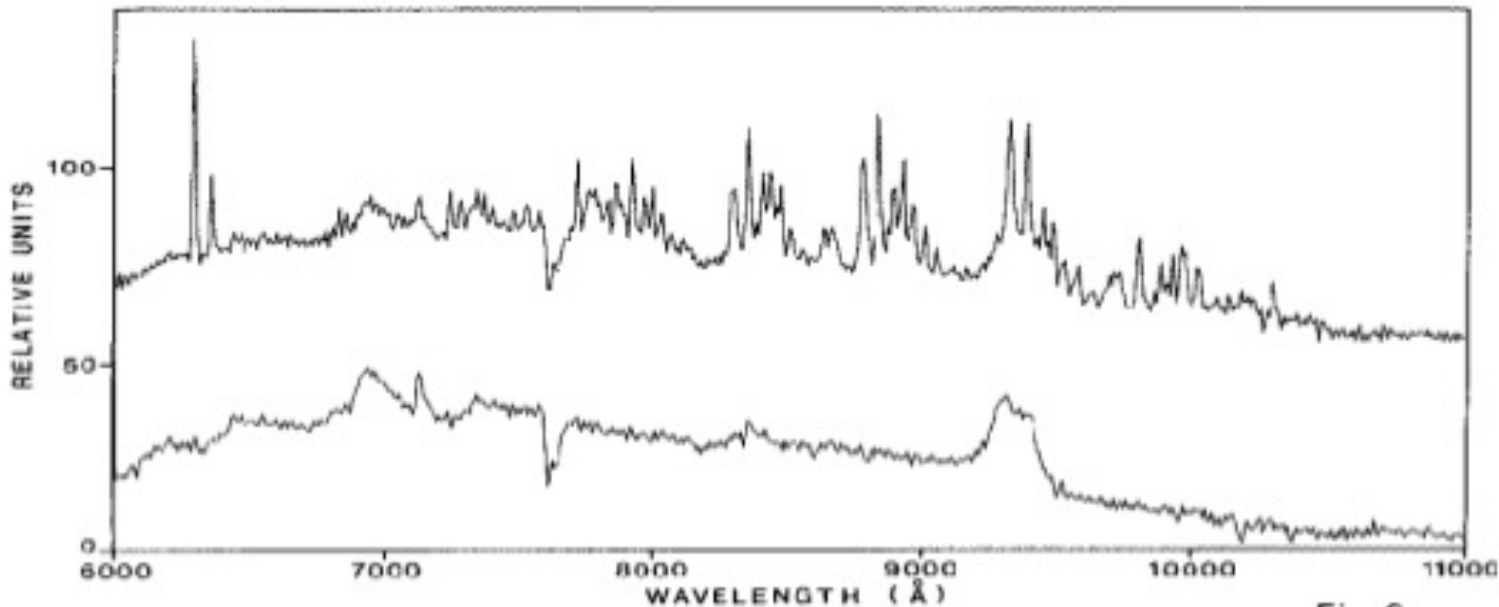
- Observation of V=16.5 mag (bright) QSO: most of the structure in the raw spectrum is due to the Earth's atmosphere

Sky subtraction: spatial/temporal

spectral direction ➔

spatial (long slit) ⬇
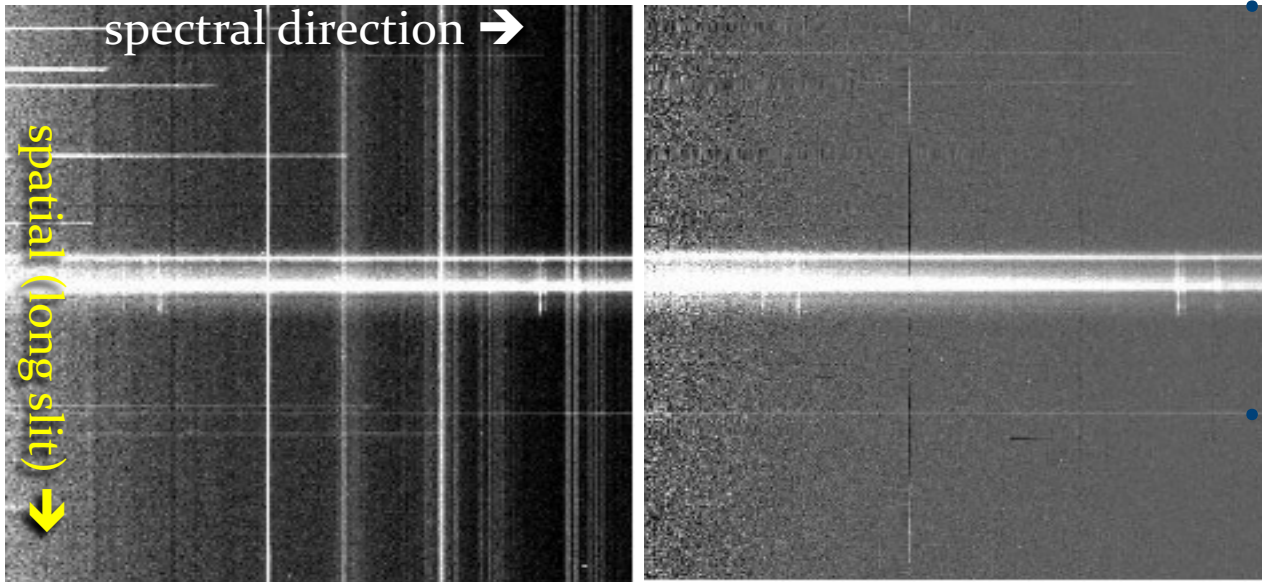
- Left: long-slit spectrum before sky subtraction (object central)

Sky emission lines run vertically. Smooth fit is subtracted

- Right: after sky subtraction. Some residuals due to pixelation, wavelength error, and slit variations remain

- Use sky measurement from nearby patch of sky
- However, optical path not entirely identical
- Use separate sky exposures by moving telescope
  - but sky changes on short time
- Use both by switching back-and-forth (nod-and-shuffle on detector)

Flux Calibration

- Absolute flux calibration
  - Usually done with spectro-photometric standard stars
  - Hot stars with only smooth spectral features, White Dwarfs and F stars in the near-IR
  - Absolute calibration of best cases now ~1% RMS using space (Hubble)
  - Only a handful available, need large offsets and atmosphere corrections
  - Most applications are happy to achieve 5% accuracy
  - Gaia mission may help setting a better all sky (relative) calibration system

- Continuum normalization – Equivalent width measurements
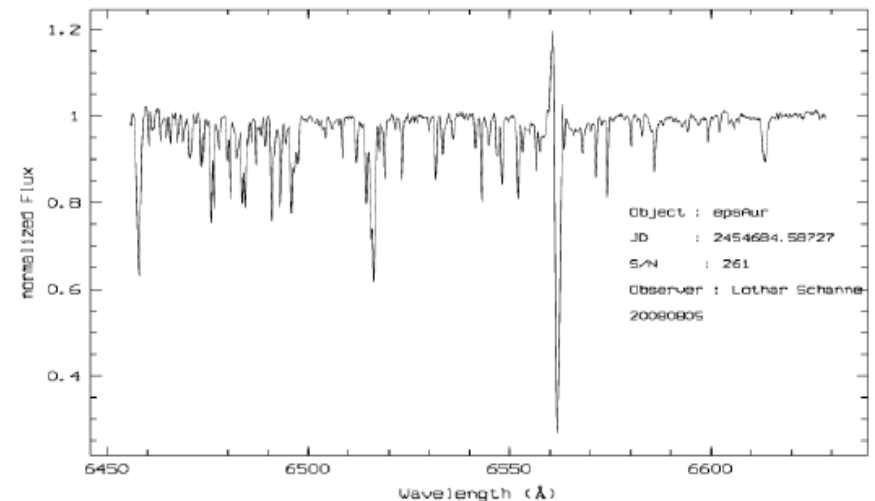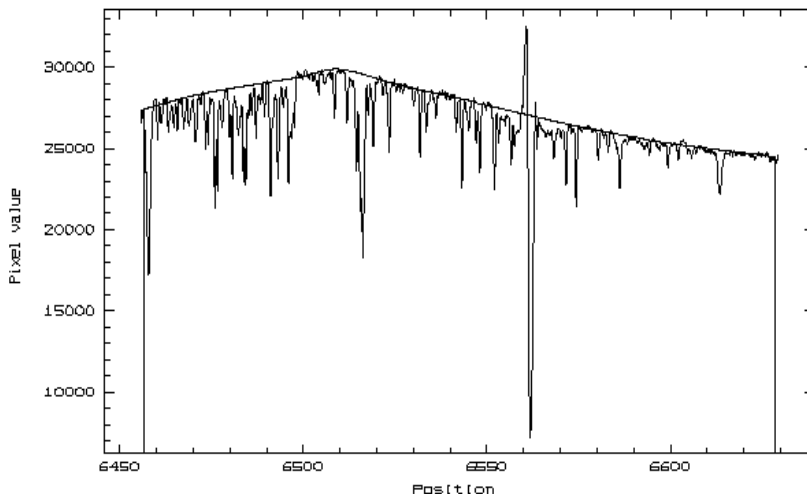
Resolving out the sky emission lines

E. Oliva et al.: The sky emission in the near infrared
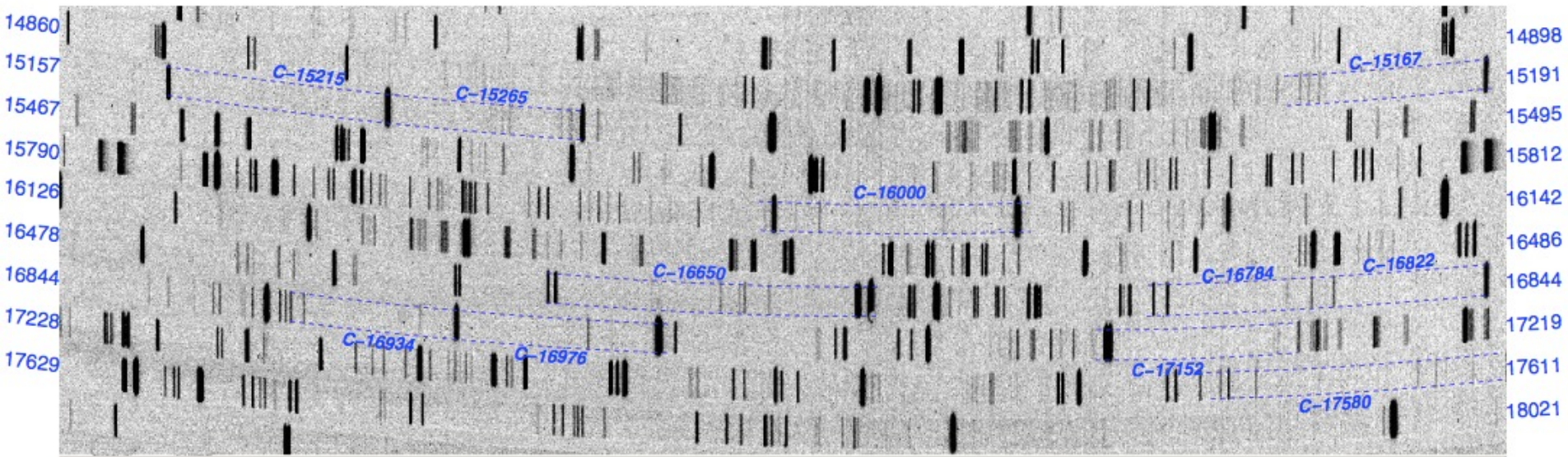
- At R >3000, the bright OH airglow lines at near-IR wavelengths start to become resolved. Careful selection allows sensitive spectroscopy or narrow-band imaging in the spectral fragments between the lines.

- Oliva et al (2015) identify a few promising regions and suggest that the underlying H-band continuum level is ~300 photons/m²/arcsec²/um/sec

Effects of the Earth's Atmosphere

- Atmospheric absorption
  - Varies with time and zenith angle
  - Calibrated by measuring standard stars at different zenith distances or by modeling
- Atmospheric dispersion
- For long-slit: rotate slit along parallactic angle (perpendicular to the ground)
- Atmospheric differential refraction
  - Image scale shear over a large field of view
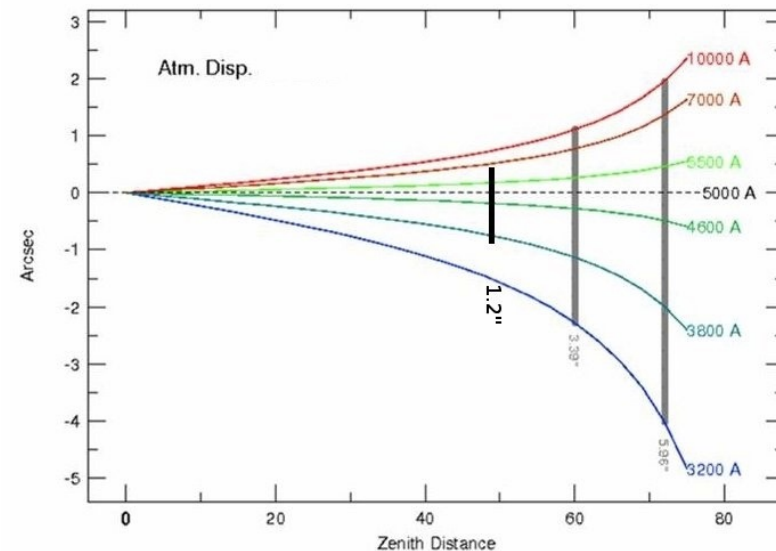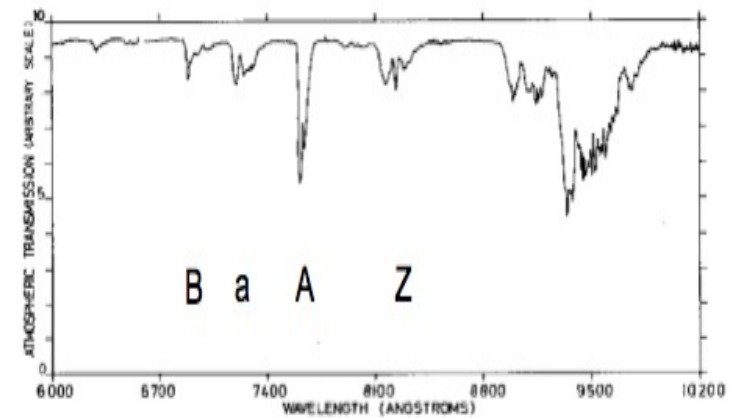
Atmospheric Transmission

Accurate flux measurements depend on good correction for atmospheric transmission.

Need to be aware of line wavelengths in air or vacuum and to use the correct form for doppler shift (optical or radio definitions)

Transmission, especially at the edge of the IR windows, can vary rapidly with wavelength.

The radial velocity at the time of observation can make a big difference, moving the line position from a region of good to poor transmission.

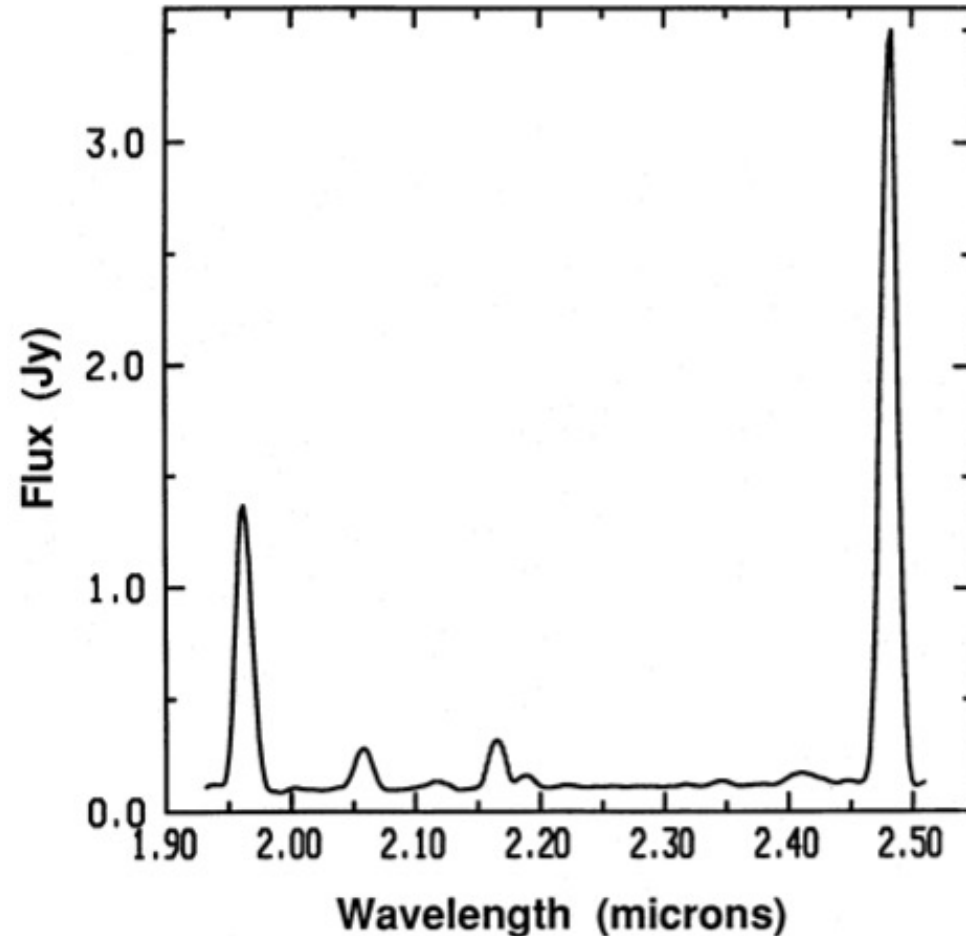e.g. the [Si VI] and [Si VII] forbidden lines at the edge of the K-band

FIG. 1.—An extended K band spectrum of NGC 6302 taken with the FIGS spectrometer on the AAT using a 5".9 square aperture with a 60" north-south chop. The strong lines at 1.96 μm and 2.48 μm are due to [Si VI] and [Si VII], respectively. Also visible are lines due to He I at 2.058 μm, a blend of He I and H_2 $S(1)$ at 2.12 μm, H I Brγ at 2.166 μm, He II at 2.189 μm, and the H_2 Q-branch at 2.41 μm.

(Ashley & Hyland 1988)

K- Band Transmission, Mauna Kea

K Band Transmission - Mauna Kea

[Si VI] coronal line at 1.962μm

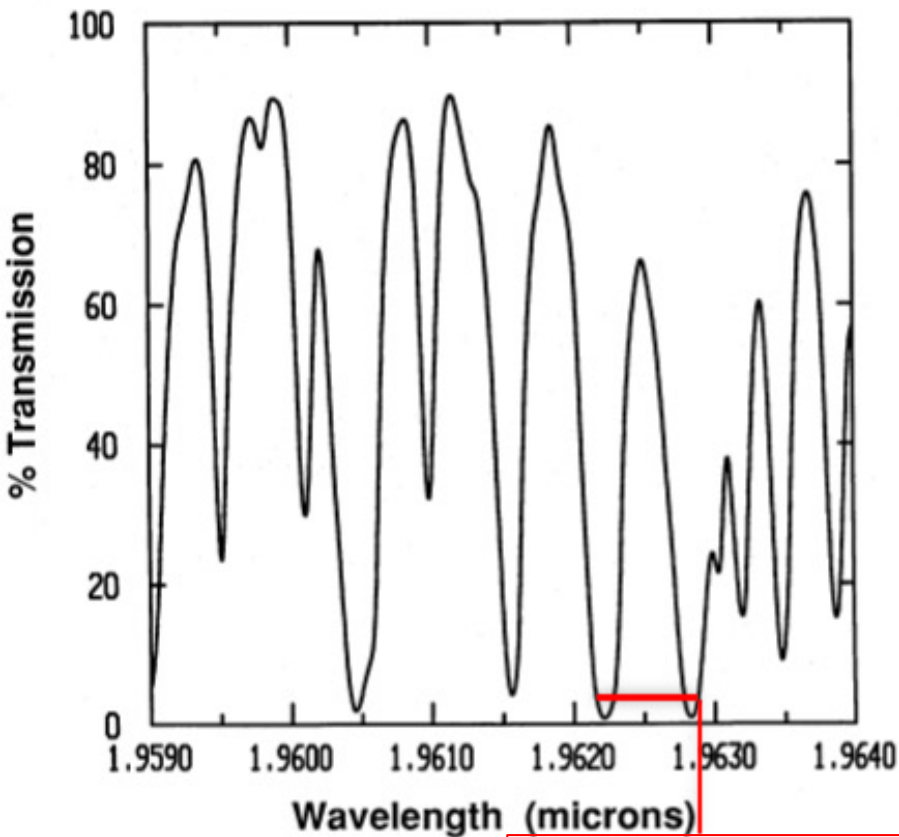[Si VII] coronal line at 2.485 μm
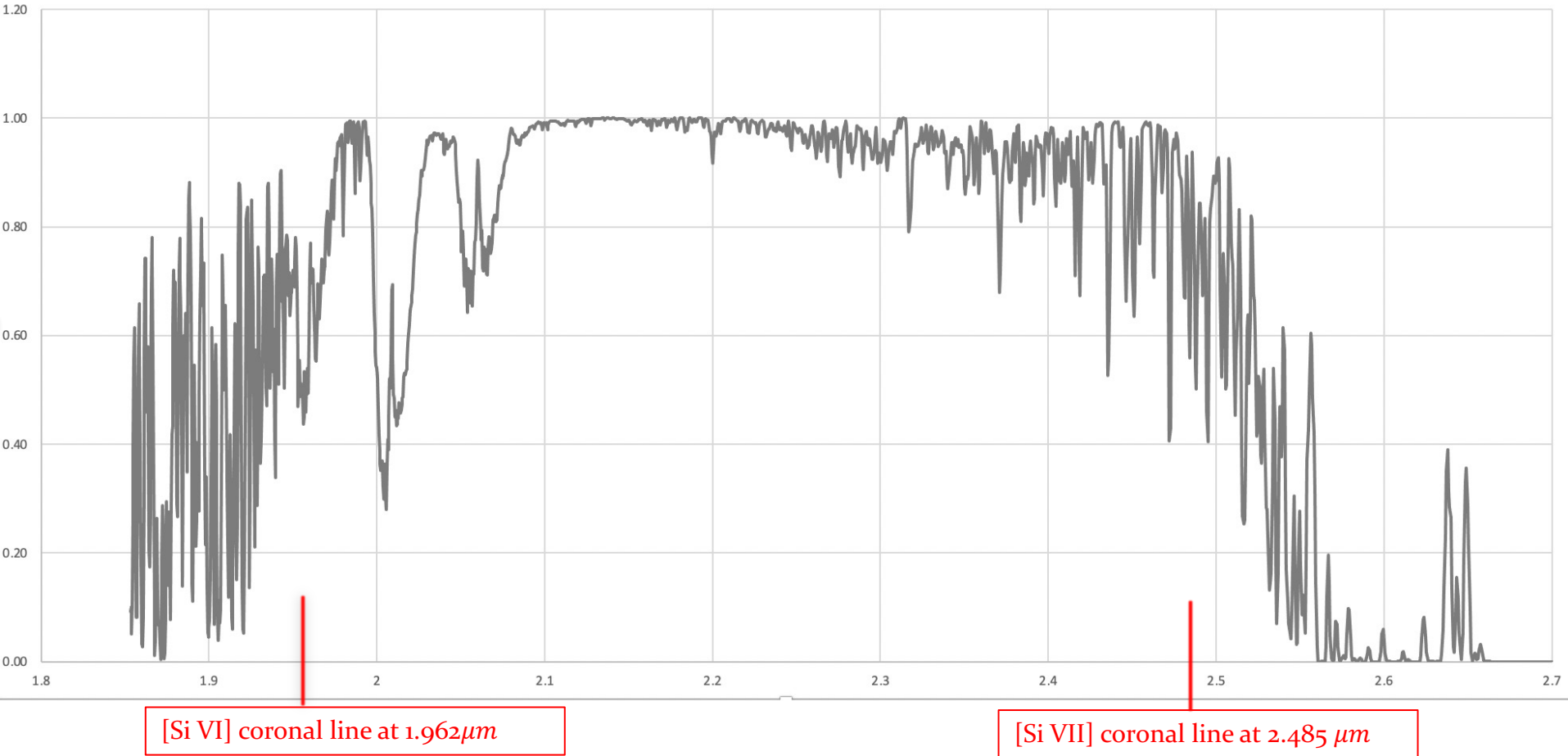
FIG. 4   [Si VI] coronal line at 1.96287 μm

FIG. 5

FIG. 4.—The approximate transmission of the Earth's atmosphere near the observed rest wavelength of the [Si VI] line. The nominal line center is at 1.9613 μm. Depending on the position of the Earth in its orbit, the line emitted by NGC 6302 could be shifted from the nominal center by amounts varying from -0.0006 μm to -0.0001 μm. The line wavelength itself could be in error by up to ± 0.0020 μm.
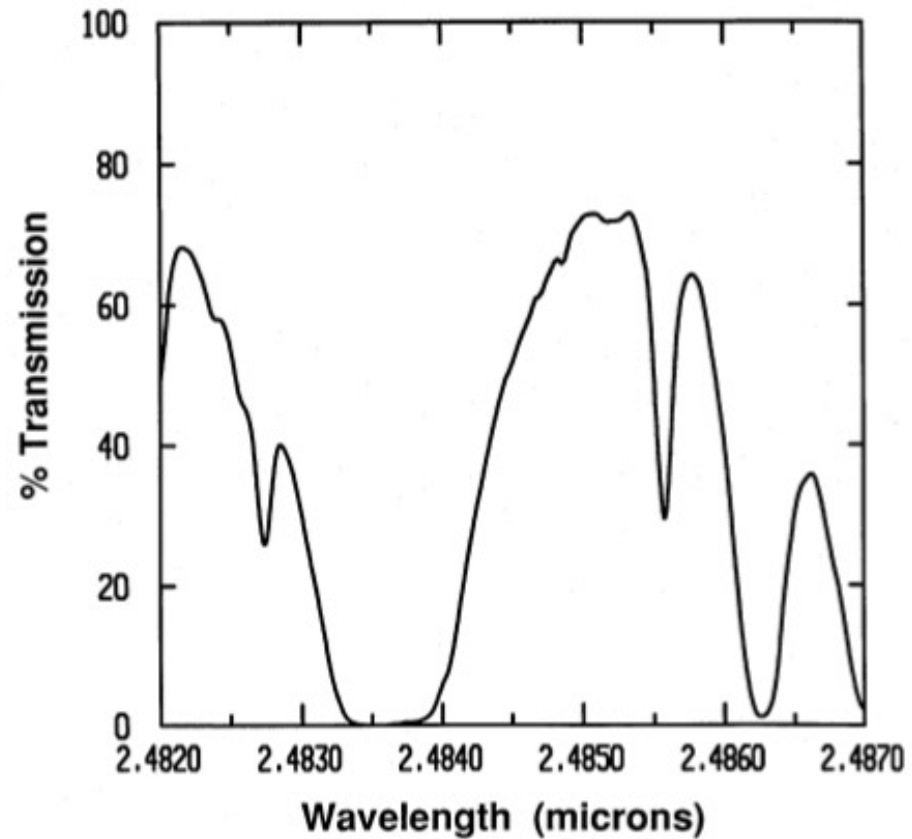
FIG. 5.—Approximate transmission of the Earth's atmosphere near the observed rest wavelength of the [Si VII] line. The nominal line center is at 2.4852 μm.

Casassus, Roche & Barlow (2000) give 1.96287 um for [Si VI], and discuss the effects of radial velocity and different observation frames.

Need to plan observations to account for these effects

Multiplexing... Multi-object spectroscopy

- Single long slit can only usually accommodate 1 or 2 objects in a single observation
- Want to maximise the amount of information collected in a single observation (preferably for the smallest cost!)
- Reformatting prior to the spectrograph slit via:

  - Multislits
  - Optical Fibres
  - Other optical components to give integral field spectroscopy, image slicers etc

Image slicer changes the format from the input bundle (right) to the linear fibre array forming the spectrograph entrance slit below
(e.g. Cyclops: Horton et al 2012)

Improves light gathering, and allows narrower slit for higher resolution.
Can be done with mirrors or fibres.
Can include wavelength calibration and sky fibres in the bundle.
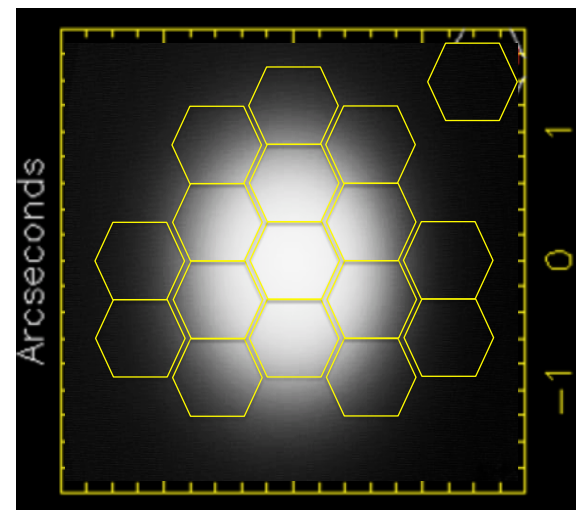
Lenslets allow close-packing of on-sky elements (spaxels) without compromising the outer cladding/buffer layers of the fibres…

…and allows pupil-injection of light from the telescope, giving increased stability for observations at high spectral resolution…
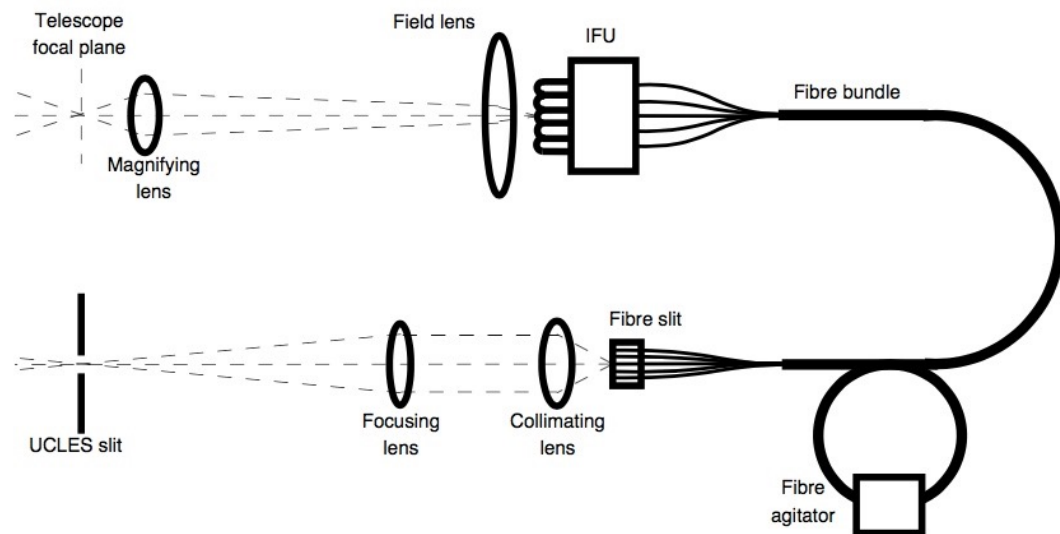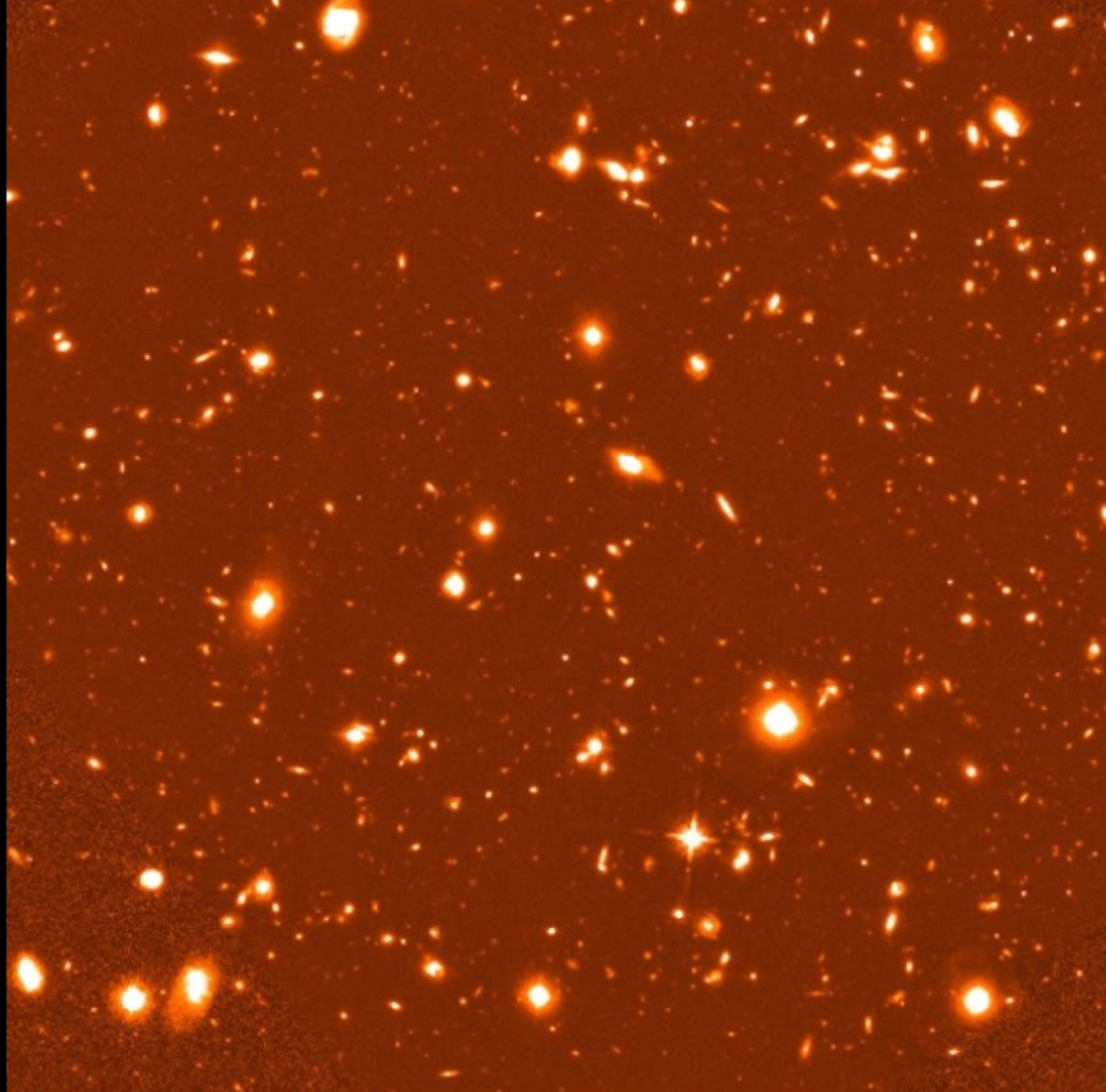
Multi-Slit approach

- 2-dimensional collimator (full-field pupil re-imaging system... Often used in IR imagers anyway!)
- Slit masks need to be cut offline (laser cutting)
  - Need accurate positions and map to coordinates
- Or addressable micro-shutters as on JWST/NIRSPEC
- Slit profiles
- Thermal stability issues
- Grating configuration (grisms)
  - Generally restricted to low resolution (prism angles)
- IR instruments: cryogenic slit masks
  - Cycle time issues
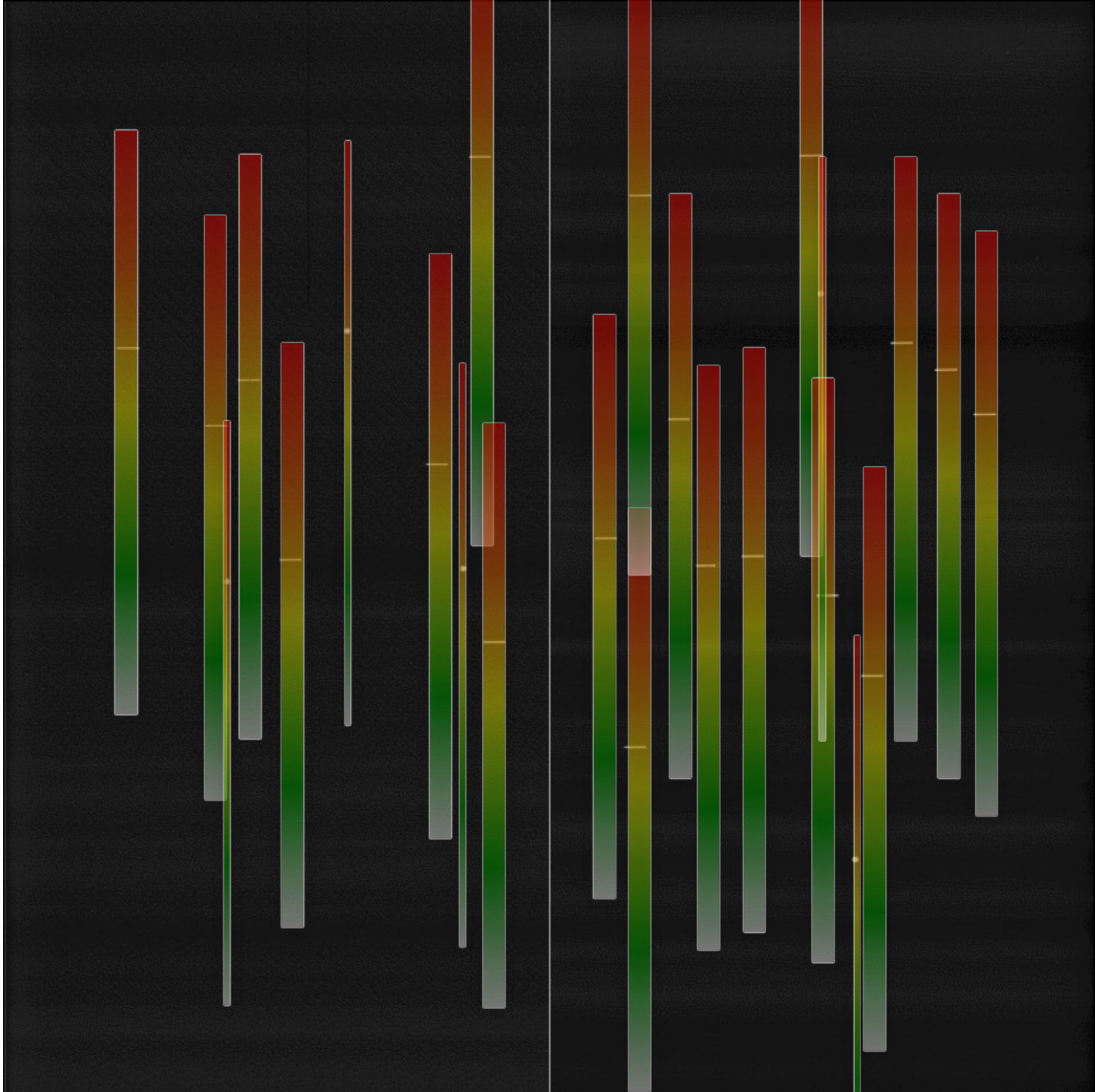 - On-instrument storage volume

Sky image

From which
science targets
and alignment
stars are
identified

Corresponding
slit-mask
image

Holes used for
alignment stars
-these will
produce
BRIGHT
spectra in the
final data

Multi-Slit approach - summary

Pros:

- Efficiency
- Sky sampling
    - Subtraction efficiency?
- Mask generator offline
- Imaging capability
    - No astrometric issues
- Interesting new technologies - microshutters
- Spatial information retained along slits (e.g. rotation curves)

Cons:

- Limited Resolution(?)
- 2D collimator (transmissive)
- Spectrograph at telescope focal station
    - Size/mass/moment/flexure
    - Scaling
- Bandpass filters
- Spectral cross-talk
- Alignment stars
- Offline mask generation
    - No real-time decisions
- Doesn't scale well...

Multi-Fibre Approach

- Position one end of optical fibres in the telescope focal plane to intercept light from stars or galaxies and then arrange the other end as a pseudo-slit, feeding a spectrograph.
- Sky fibres are mixed with object fibres and the fibre outputs are separated to reduce cross-talk
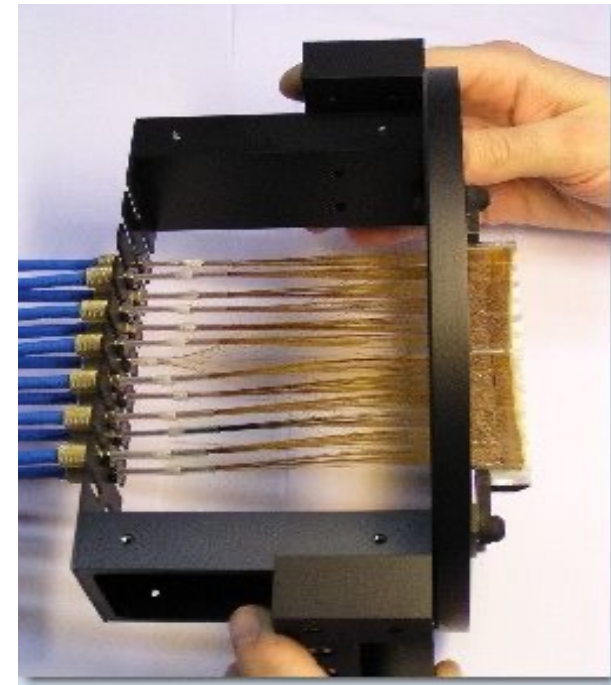
FLAMES & 6DF

Robot positioner places fibres on a curved plate
Fibre positions to observe objects in the Field are configured in software
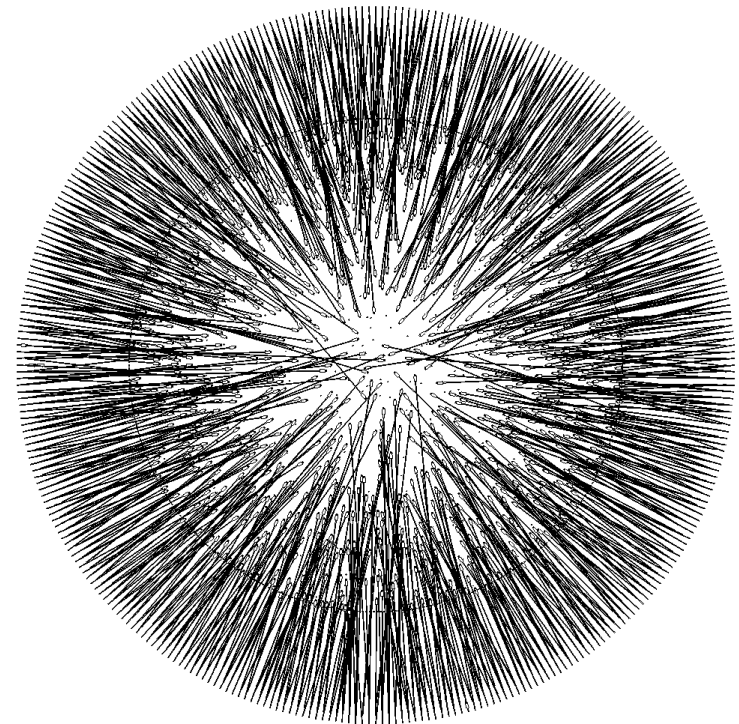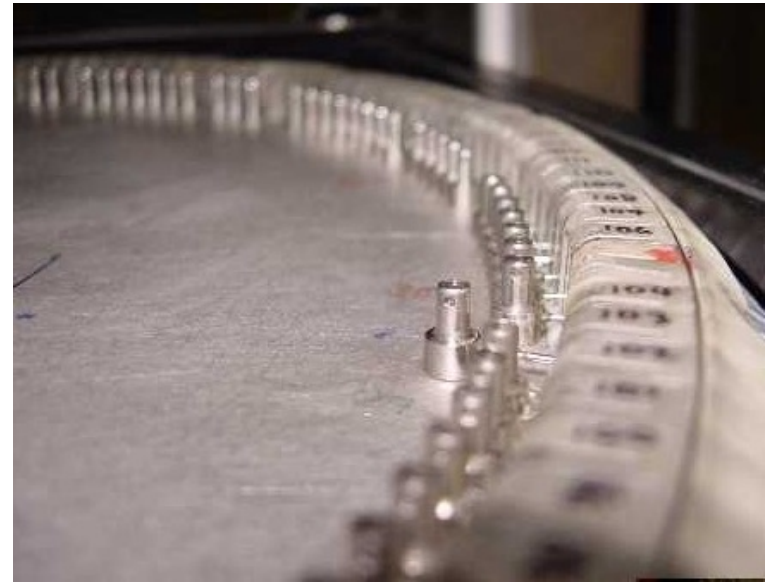
The plate may be curved in order to maximise throughput – aligned with the beam at all field positions

Cooled spectrographs for IR observations

Careful matching of fibre output f-ratio to spectrograph input.

Fast beams to minimise focal ratio degradation

+ WEAVE...

Multi-Fibre approach - summary

Pros:
- Efficiency
- Can access large field without increasing optics size
- 1-D collimator
- Spectrograph where you like... (Large, Stable, as many as you can afford)
- Range of bandpass/resolutions easier
- Lots of options for addressing the focal plane
- All spectra can have the same sampling/resolution/coverage
- Can change plans in the middle of the night (relatively) easily...

Cons:
- FRD and absorption loss
- No imaging capability
  - Need imaging data
- Cost of positioner(s) & Fibres
- Sky subtraction can need some care

Integral field spectroscopy

Reformat the focal plane a different way:

Fully sample the variation of spectral properties within a single object at seeing-limited or corrected spatial resolution

3-D spectroscopy – spectral + 2 spatial

Moving on... other ways to re-format the focal plane

Integral Field Spectroscopy

Divides the field in two dimensions

Telescope focus	Spectrograph input	Spectrograph output

Lenslet array — Pupil imagery

Spectra must not overlap → less information density in datacube

Fibre array — Fibres — slit

Datacube

y
λ
x

Image slicer — Micro-mirrors — slit
1 2 3 4

Only the image slicer retains spatial information within each slice/sample → high information density in datacube

Both designs maximise the spectrum length and allows more efficient utilisation of detector surface.

Only the Fibre array slicer gives full flexibility to decouple the input and output geometries, allowing maximal choice of wavelength coverage and spectral resolution

Centre for Ådvanced Instrumentation

Principle of the Image Slicer

(used in MPE 3D, SINFONI)

2nd mirror stack

input from telescope

Light loss at
mirror boundary

slicer
stack

located in telescope
focal plane

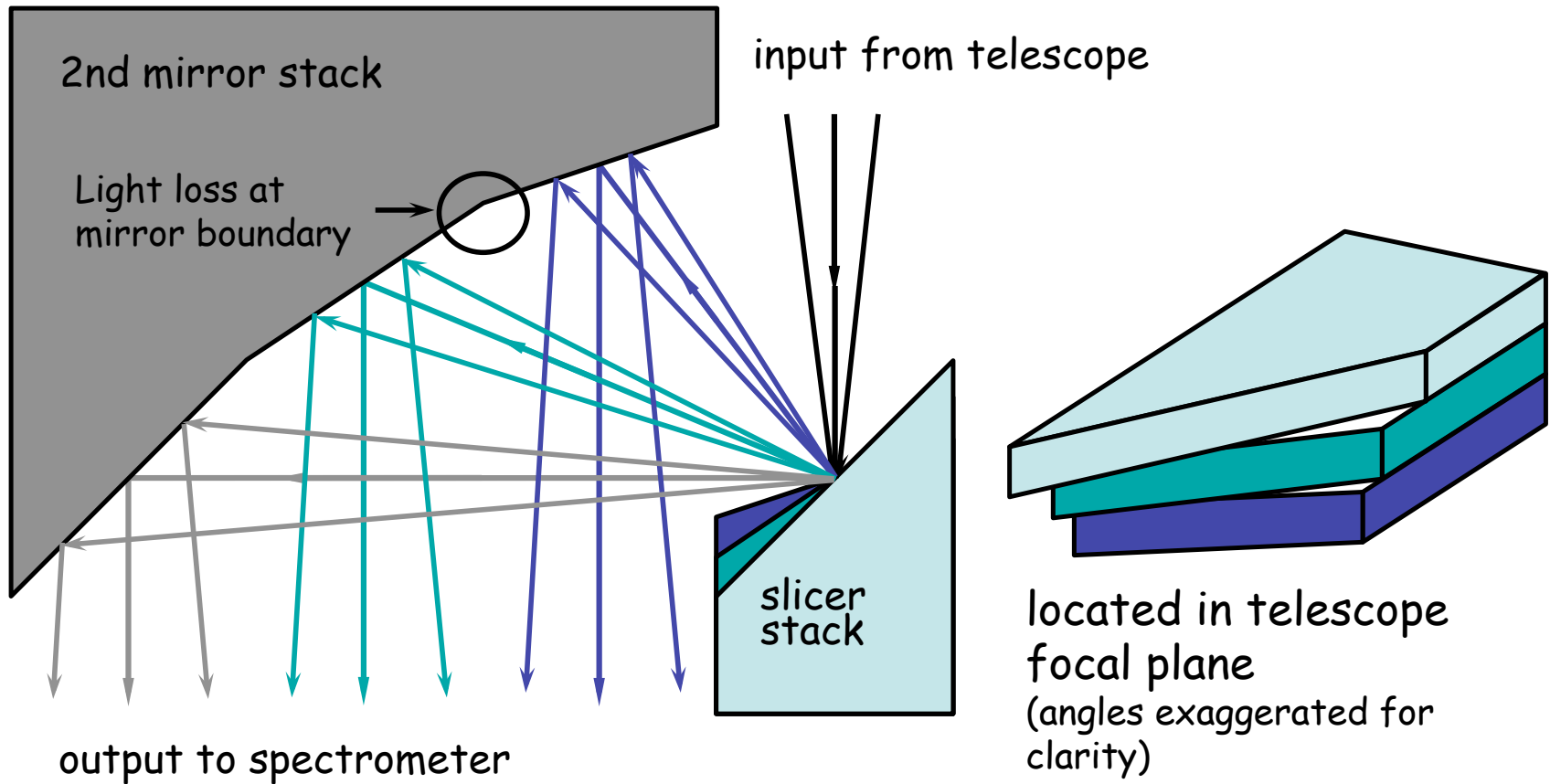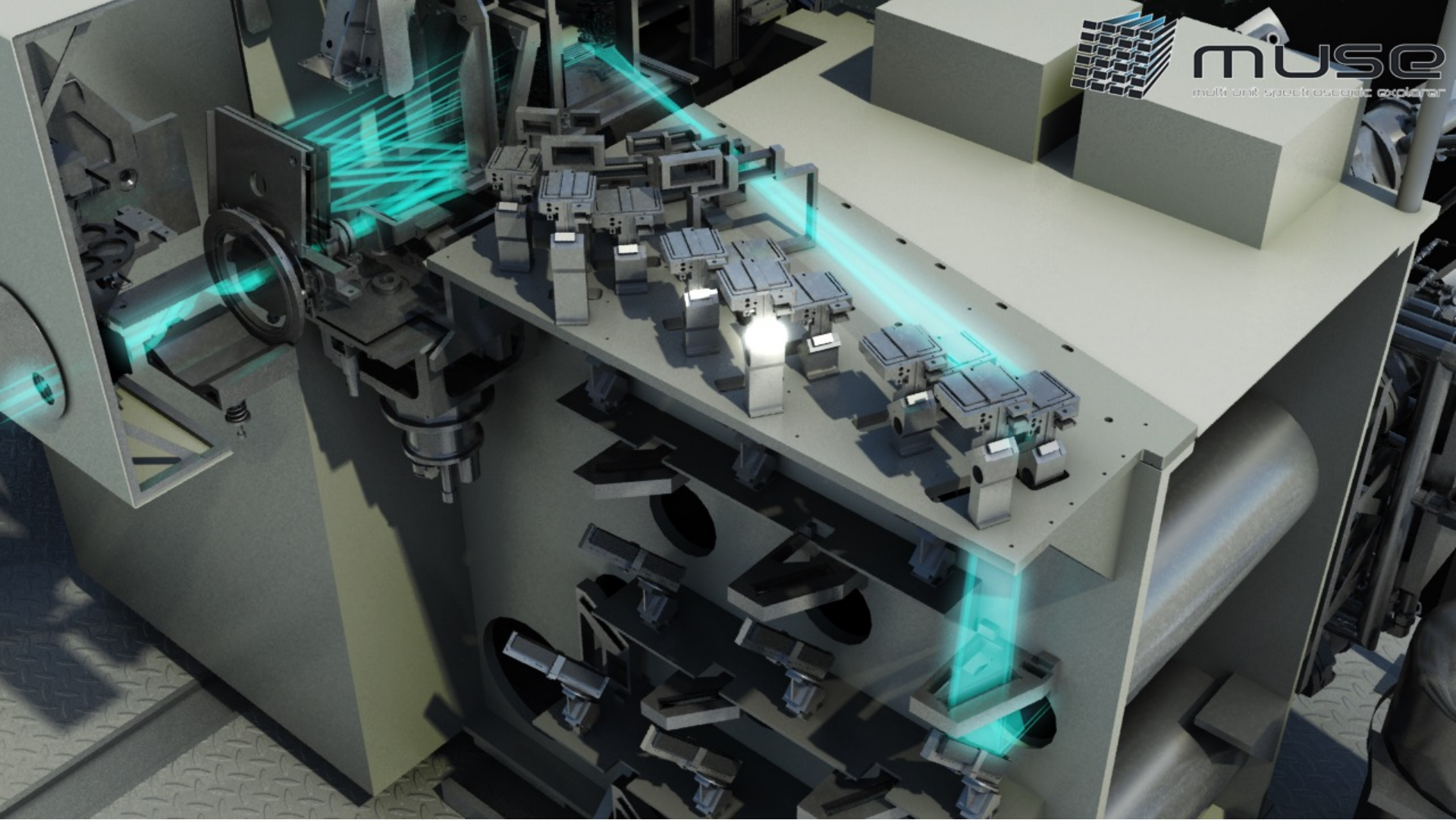(angles exaggerated for
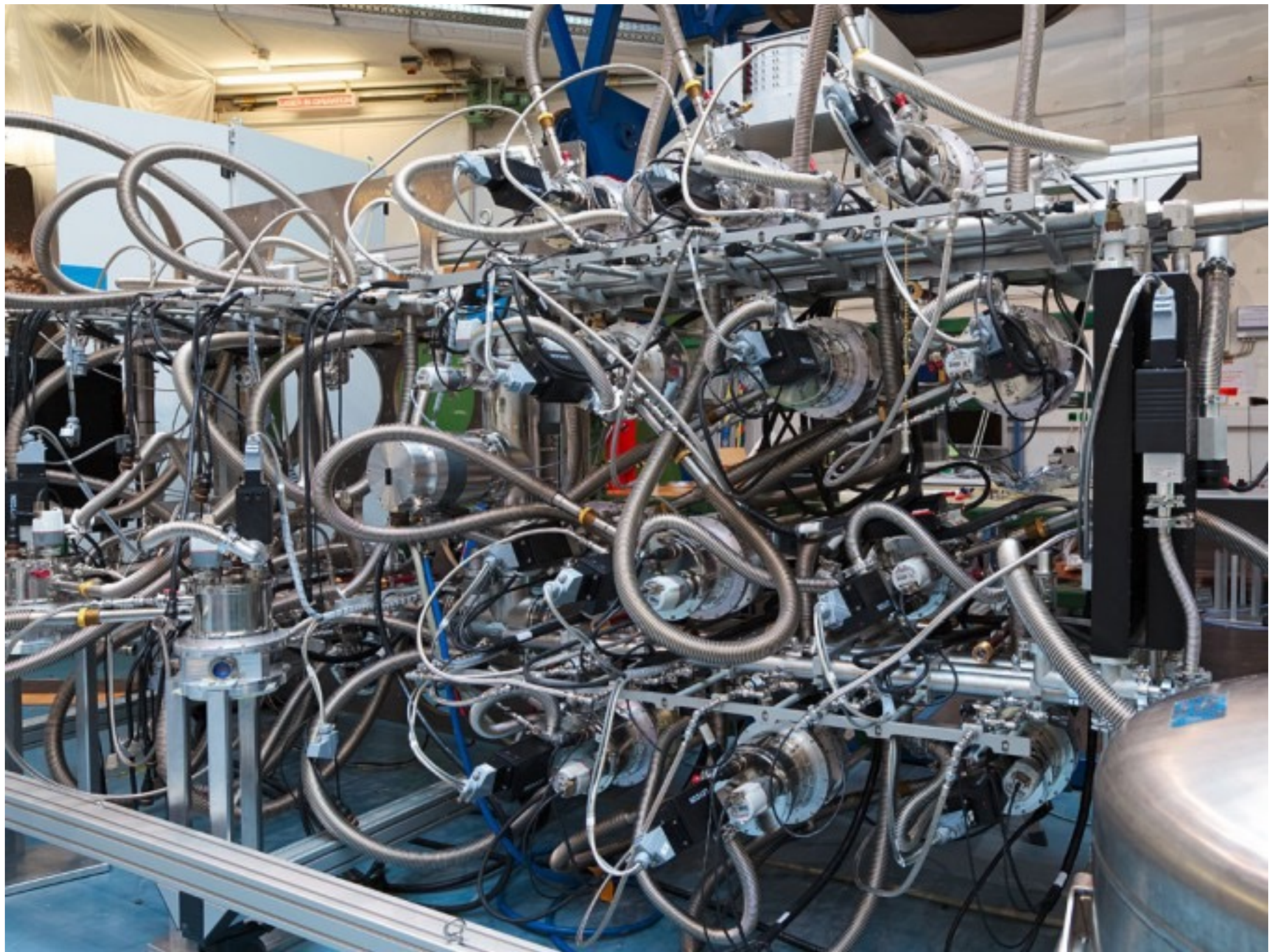clarity)

output to spectrometer

image slicer preserves the pupil of input beam

Then if you scale all this up to 90,000 spaxels you fill the entire Nasmyth platform on the VLT...
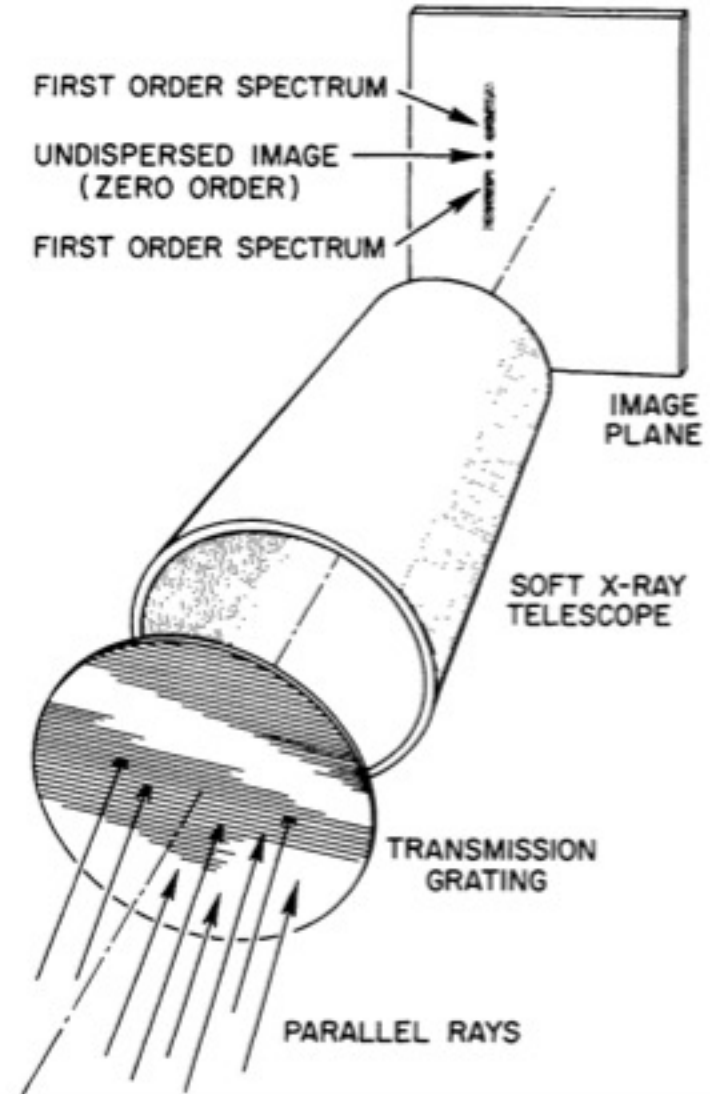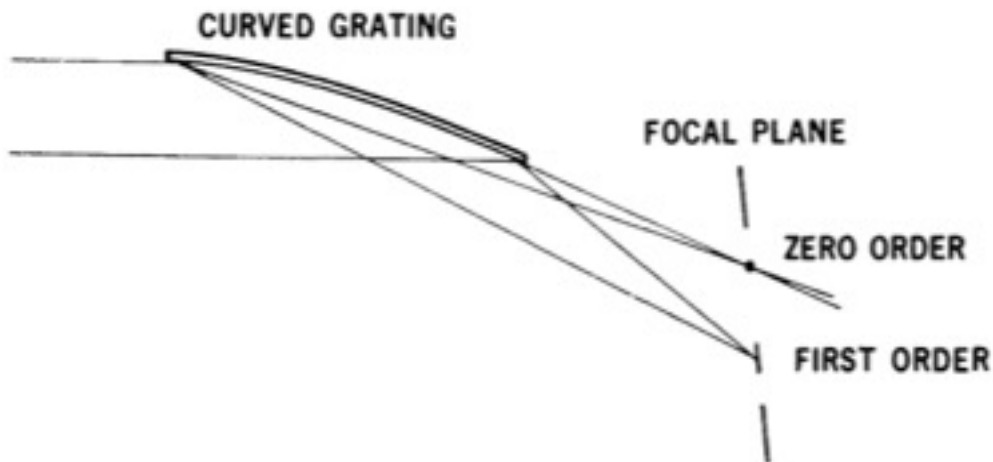

Fixed, stable spectrographs, image is rotated optically (throughput)

X-Ray Space Telescopes : Spectroscopy

- Grating Spectrometers - Groove spacings ~200nm from grids of gold wires
- Slitless spectroscopy so different objects are at different positions

- Or grazing incidence gratings used with a grazing incidence nested telescope

FIRST ORDER SPECTRUM

UNDISPERSED IMAGE (ZERO ORDER)

FIRST ORDER SPECTRUM

IMAGE PLANE

SOFT X-RAY TELESCOPE

TRANSMISSION GRATING

PARALLEL RAYS

CURVED GRATING

FOCAL PLANE

ZERO ORDER

FIRST ORDER

Chandra

Advanced Charged Coupled Imaging Spectrometer (ACIS):

Ten CCD chips in 2 arrays provide imaging and spectroscopy; imaging resolution is 0.5 arcsec over the energy range 0.2 - 10 keV;
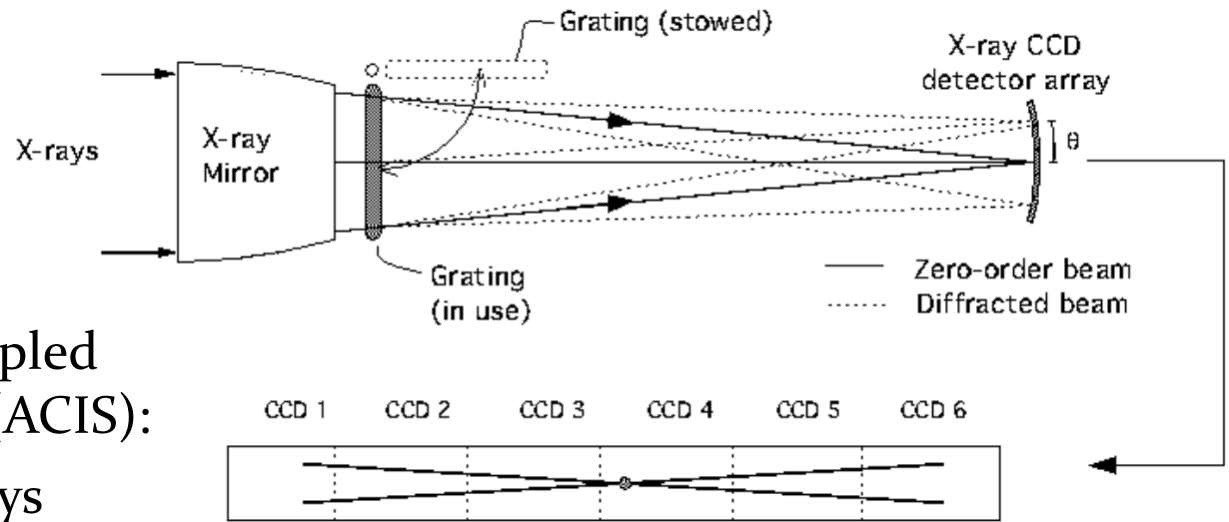
Gratings inserted into focused X-ray beam;

High Energy Transmission Grating (HETG) provides spectral resolution of 60-1000 over energy range 0.4 - 10 keV

Low Energy Transmission Grating (LETG)provides spectral resolution of 40-2000 over the energy range 0.09 - 3 keV

X-ray Spectroscopy

Micro-calorimeter detectors, cooled to ~60 mK give good spectral resolution (temperature increase on photon absorption is proportional to photon energy)

Hitomi had energy resolution of ~6eV at soft X-ray bands (0.3-12 keV) and obtained just one spectrum before being lost.

The replacement XRISM mission is planned for launch in 2023
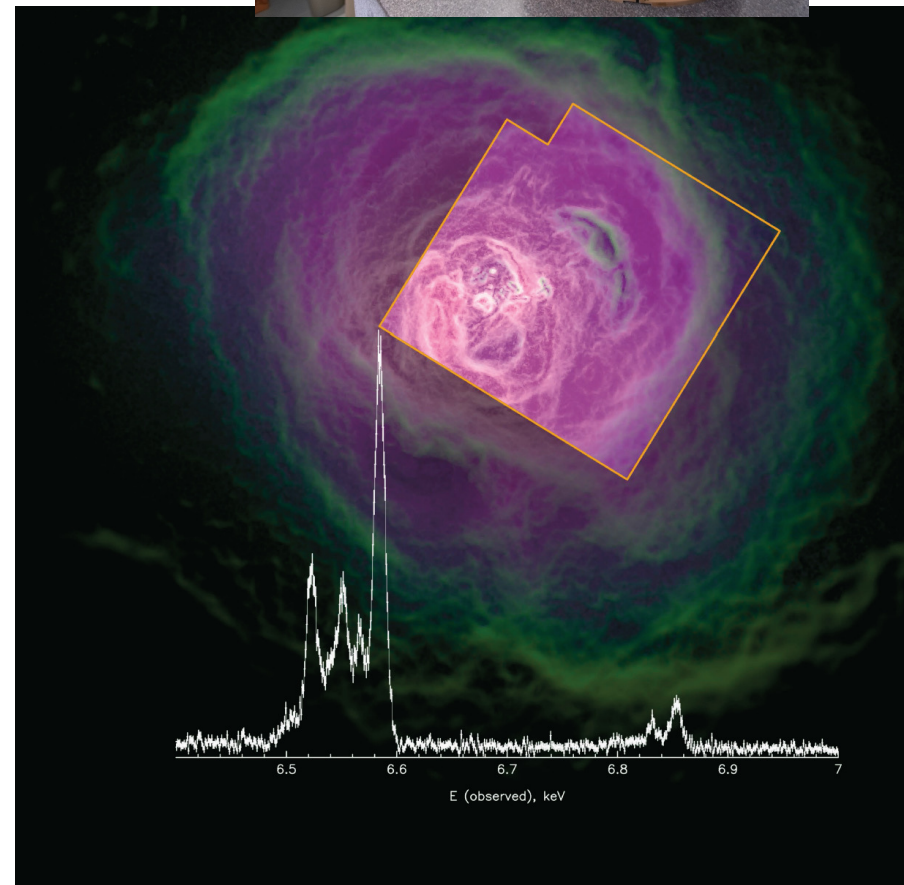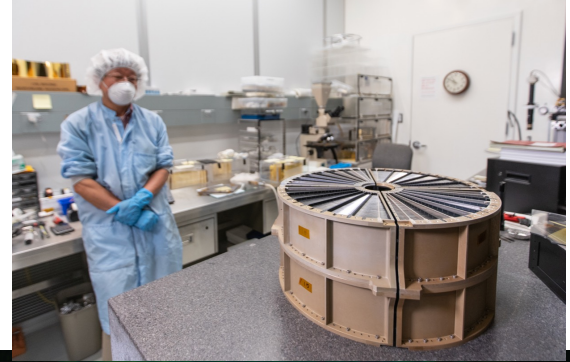
The Perseus cluster shows emission from FeXXIV (left) and FeXXV (right) with a velocity dispersion of 160 km/s

Microwave and Radio Frequencies

- Heterodyne systems – coherent detection
- Spectral images with interferometers
- Very high resolving power - $>10^8$ routinely available
  - Ideal for Galactic kinematics and Galactic structure
  - Isotopic measurements
- Spectral range usually determined by correlator bandwidth – several GHz

Spectral Extraction

- Spectra tend to have significant variations in S/N with wavelength
- Optimal extraction is an art
- Compromise between S/N, spectral fidelity and photometric accuracy – see K Horne 1986 PASP
- Calibrations depend upon science usage
  - Wavelength/velocity precision down to 1 m/sec or less
  - Atmospheric absorption correction – may not be necessary for redshift determination, equivalent widths