Towards the “Ideal Spectrograph” for Atmospheric Observation Satellites

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New Developments in DOAS-Type Satellite Instruments: See …

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Differential Optical Absorption Spectroscopy
- Principles and Applications, Springer 2008

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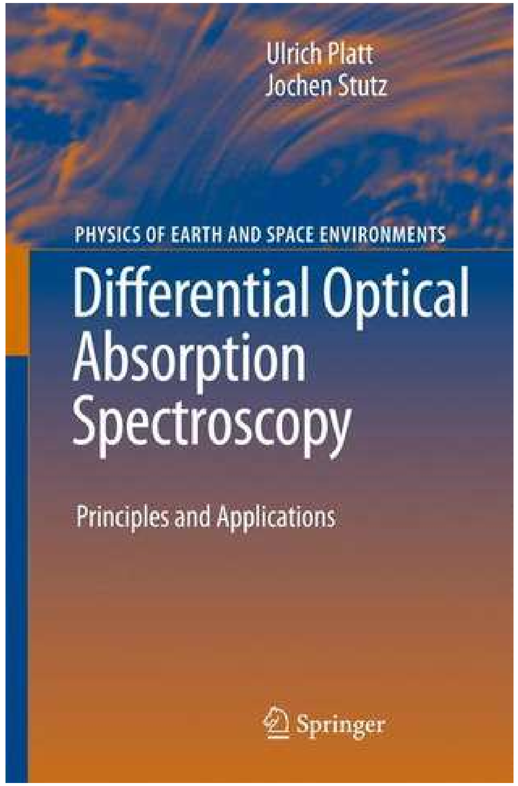
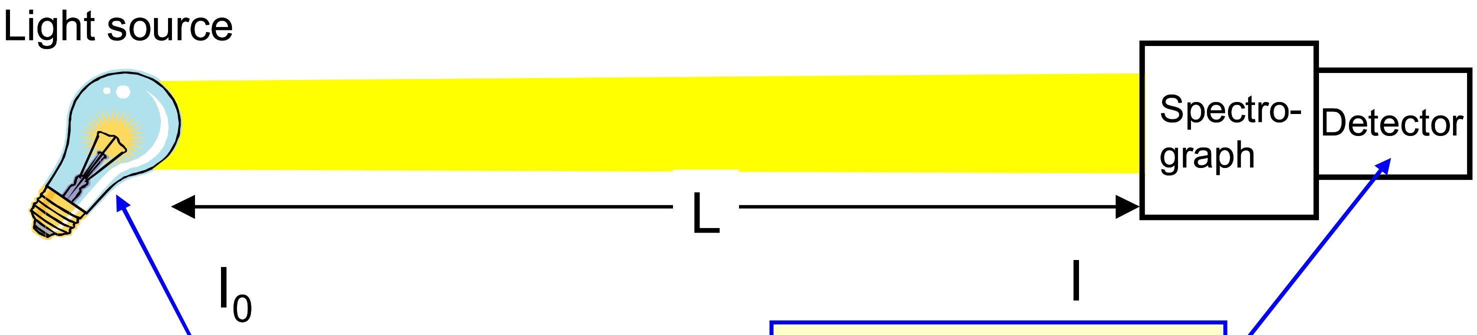
ISBN 978-3-540-21193-8

2nd Edition: **Differential Optical Absorption Spectroscopy** - Principles and Applications.
U. Platt & J.Stutz, Springer,
ISBN: 978-3-662-68637-9 **October, 2024**



Spectroscopy Applications - The Meaning of ‚Ideal‘:



There is enough light from the sky

Modern detectors are shot-noise limited

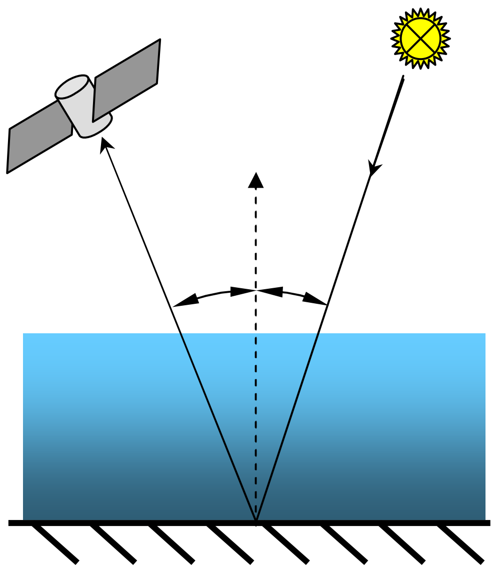
$I = I_0 \cdot e^{-\bar{c}\cdot L\cdot\sigma}$ Lambert-Beer's Law

$\bar{c}$=average trace gas concentration

L =length of light path

σ=absorption cross section

Actual arrangement:



For details see:
Platt U., Wagner T., Kuhn J., and Leisner T. (2021), The “Ideal” Spectrograph for Atmospheric Observations, Atmos. Meas. Tech. 14, 6867–6883, https://doi.org/10.5194/amt-14-6867-2021

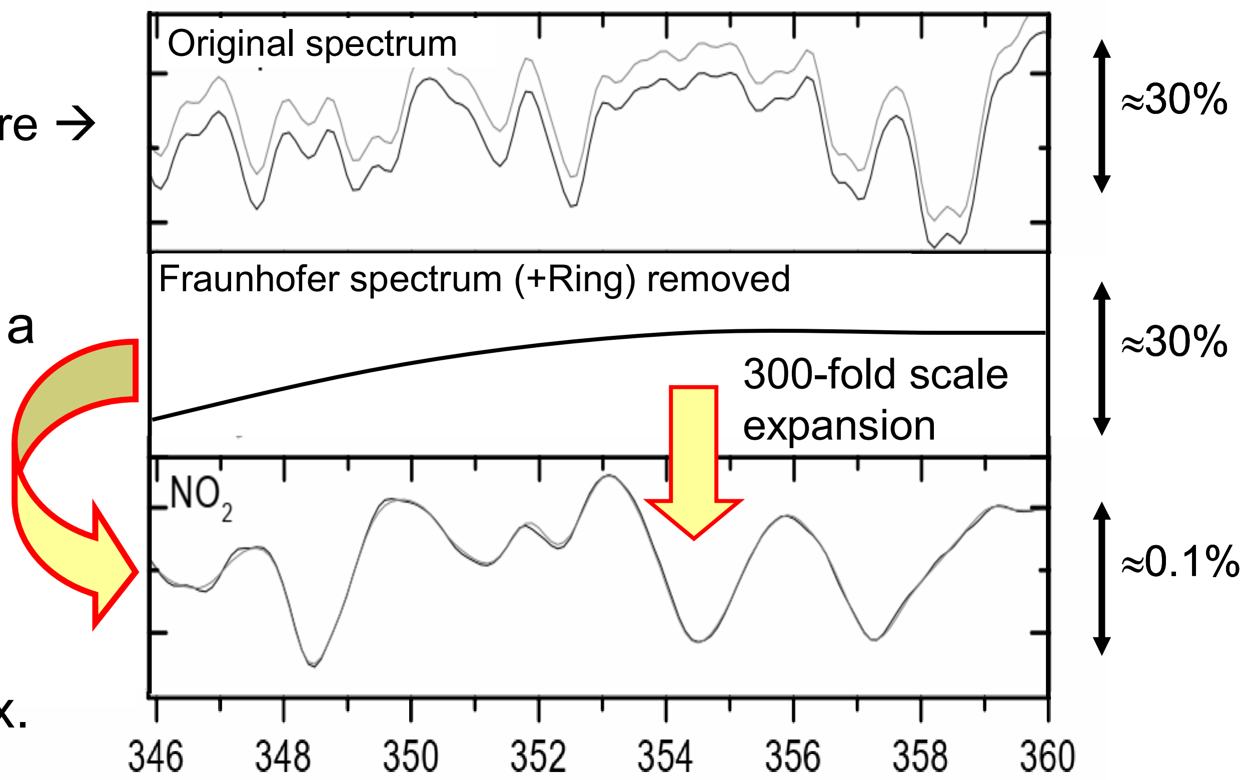
The Differential Absorption Spectroscopy Problem

Fraunhofer Structure →

Extract Information from a (nearly) smooth line

→ Interpret very small ($\approx 10^{-4}$) intensity differences

→ Need $\approx 10^8$ photons/px.



Doktoral Thesis H.Harder 1999

The central problem: **The Shot noise limit!**

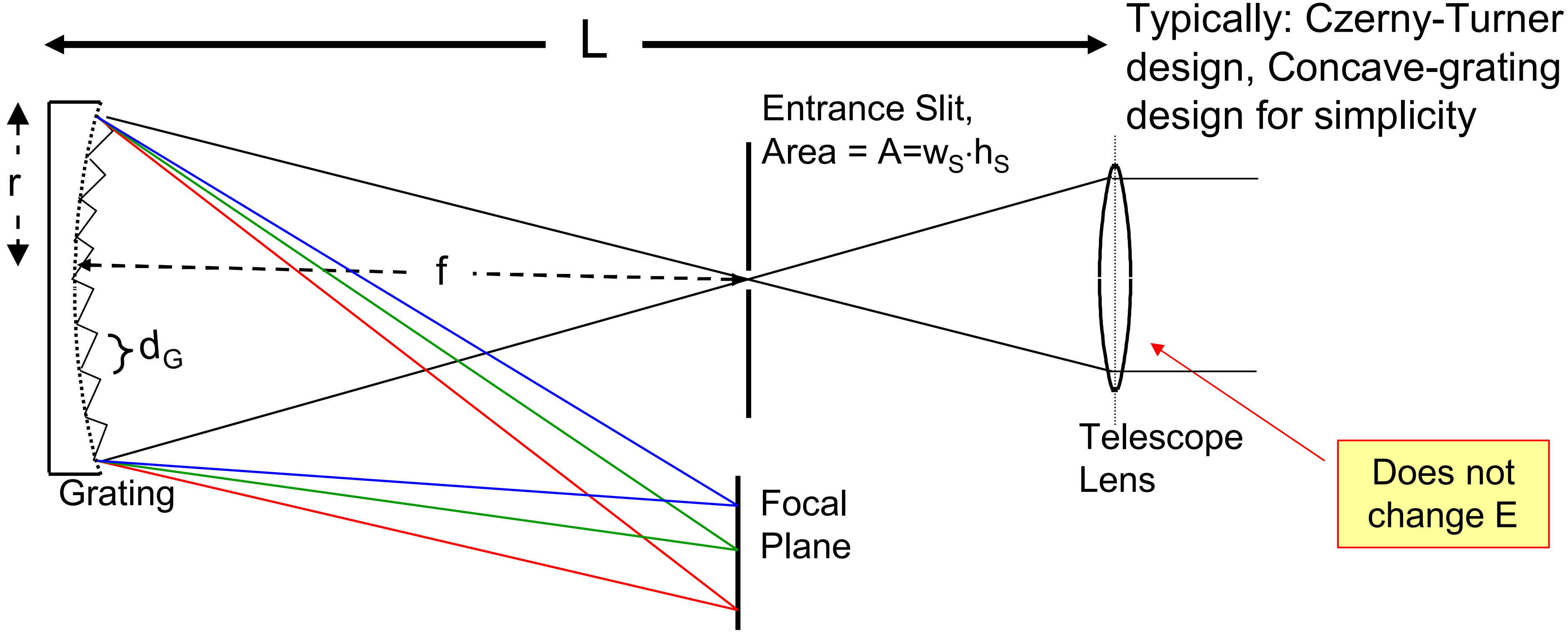
Shot noise: $$N_{SN} = \sqrt{N} \Rightarrow S/N = \frac{N}{\sqrt{N}} = \sqrt{N},\ N = \text{No. of Photons}$$

Solution: → **More light throughput!**

→ **how to get more light**?

Imaging Grating Spectrograph (plus Telescope)

Typically: Czerny-Turner design, Concave-grating design for simplicity



Total size of the spectrograph $L = a \cdot f$, with $a \approx 1.3$

F-Number (F/#):

$$F = \frac{f}{2r}$$

Étendue E:

$E = \Omega \cdot A$ with:

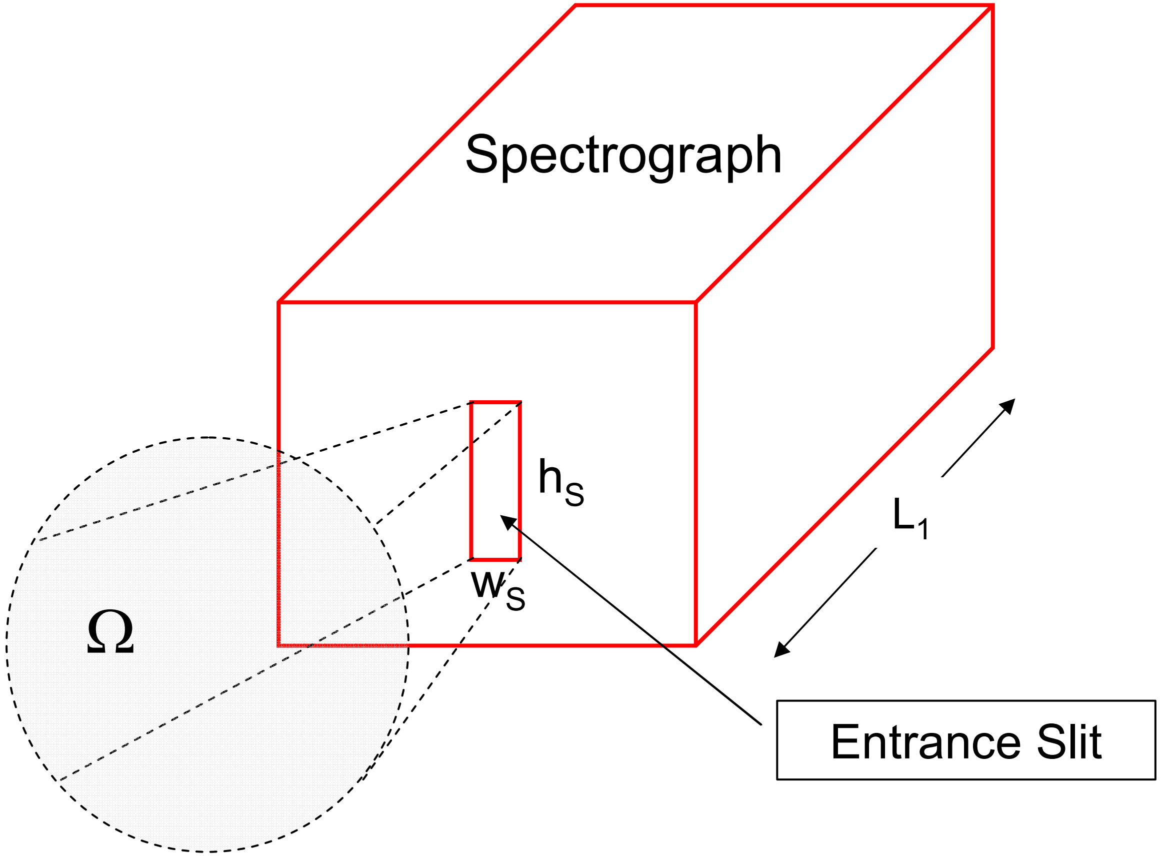
$$\Omega \approx \frac{\pi r^2}{f^2} = \frac{\pi}{4F^2}$$

Resolving power: $\frac{\lambda}{\Delta\lambda} \approx \frac{f}{w_S}$

(assuming 1st order and $d_G \cdot \cos\alpha \approx \lambda$)

λ= wavelength, α= angle of incidence on grating

The Relevant Points



Étendue E:

$E = \Omega \cdot A_S$ with:

$$\Omega \approx \frac{\pi r^2}{f^2} = \frac{\pi}{4F^2}$$

$$A_S = w_S \cdot h_S$$

$$E \approx \frac{\pi}{4F^2} \cdot w_S \cdot h_S$$

How to improve Spectrograph light throughput?

1) Optimize spectrograph
   - Better grating efficiency (typ. 20 – 80%)
   - Higher detector quantum efficiency (typ. 20 – 80%)
   - Higher mirror reflectivity (typ. ≈80%)
   - Fewer optical elements (e.g. Czerny-Turner spectrograph has >3 surfaces)

2) Increase Étendue E
   „Better“ (lower) F-number, F/#

3) Increase slit area (h_S, w_S)

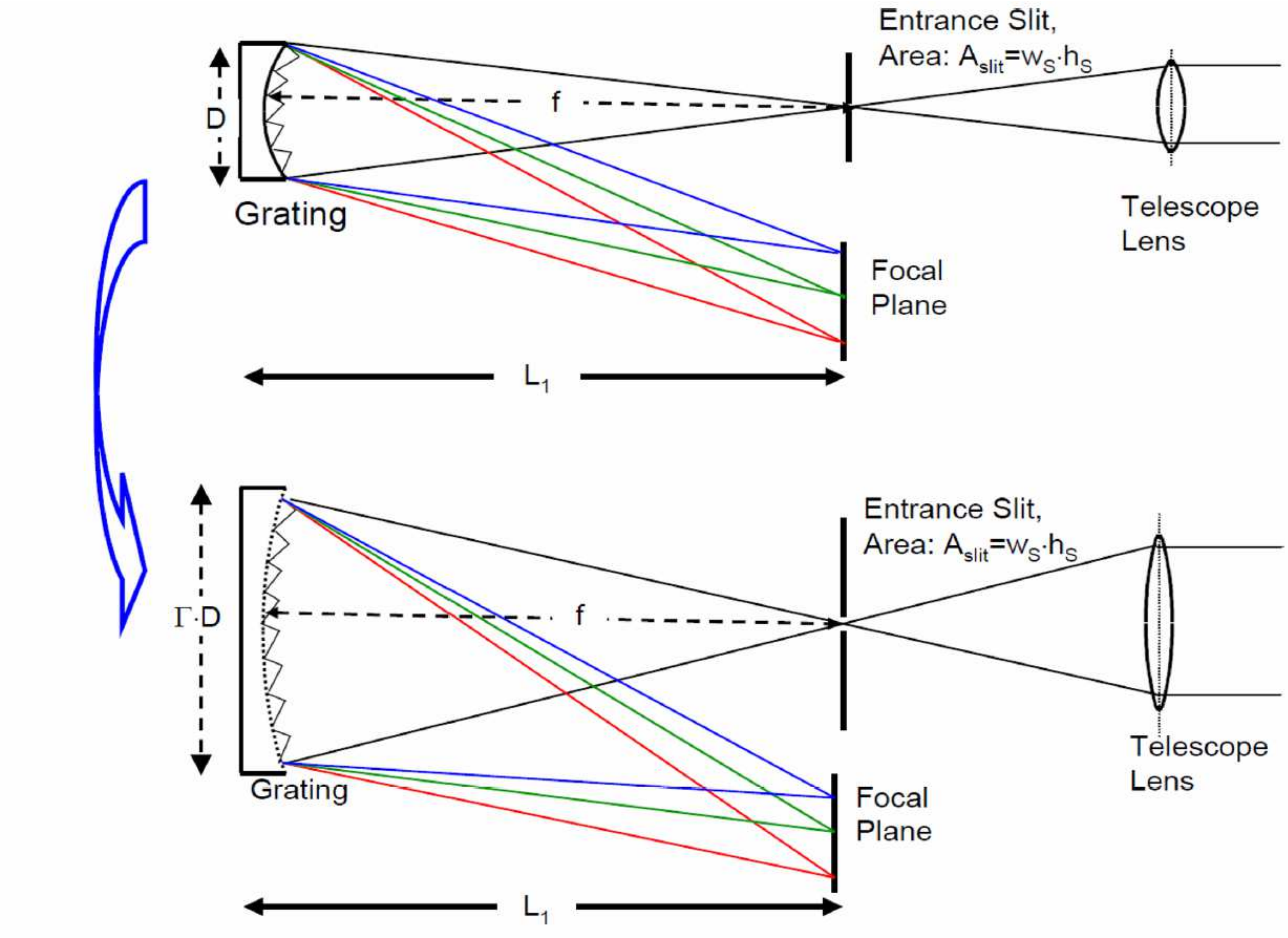
Limited increase in light throughput

4) Increase size of spectrograph, Upscaling
   e.g. larger aperture at same F-Number

5) Other Approaches …

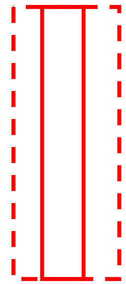
Unlimited increase in light throughput possible

2) Scaling the Spectrograph (Plus Telescope) F-Number



3) Larger Slit-Area?

Étendue E: $E = \Omega \cdot A_S$ with: $A_S = w_S \cdot h_S$



a) Increase w_S?

Problem: w_S determines Spectral Resolution (SR)

Solution: SR preserved if w_S and $g=1/d_G$ vary by same factor!
However: Reduction of d_G limited by wavelength (minimum $d_G \approx \lambda$)

Possible improvement: '**Immersed Grating**'
Wavelength λ_n seen by the grating is: $\lambda_n = \lambda/n$ (=index of refraction)

See e.g. van Amerongen, A.H., Visser, H., Vink, R.J.P., Coppens, T., Hoogeveen, R.W.M.: Development of immersed diffraction grating for the TROPOMI-SWIR Spectrometer, Proc. SPIE, 7826, 78261D-1, doi: 10.1117/12.869018, 2010.

b) Increase h_S?

Problem: larger h_S increases astigmatism → degraded imaging

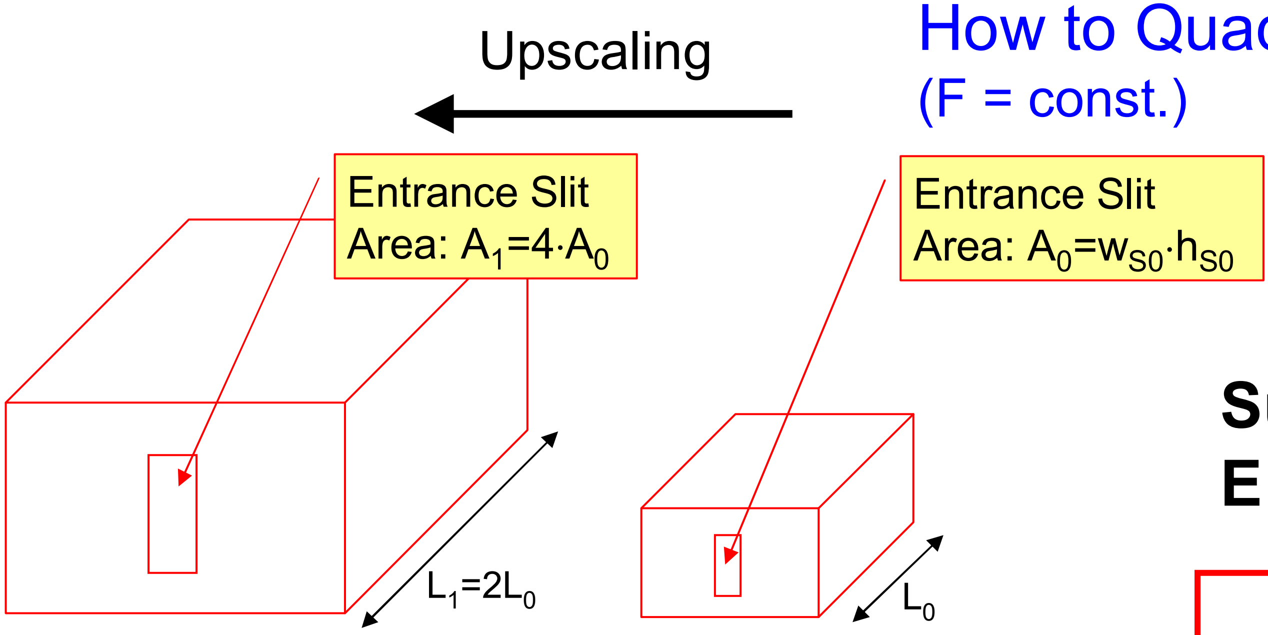
Fastie limit: (Fastie 1952): $h_S \approx w_S \cdot F^2 \underbrace{\approx}_{F=4} 16 \cdot w_S$

Fastie, W.G.: Image Forming Properties of the Ebert Mono-chromator, J. Opt. Soc. Am., 42, 647-651, 1952.

Solutions: large f/#, special optics, Offner design …

4) Upscaling Spectrograph Size (F = const. ⇔ Ω = const.)

How to Quadruple the Étendue
(F = const.)



Étendue = $4\cdot E_0$

Mass = $8\cdot M_0$

Étendue = E_0

Mass = M_0

Summary:

$E \propto L^2$, $V \propto M \propto L^3$:

$$M \propto V \propto L^3 \propto E^{\frac{3}{2}}$$

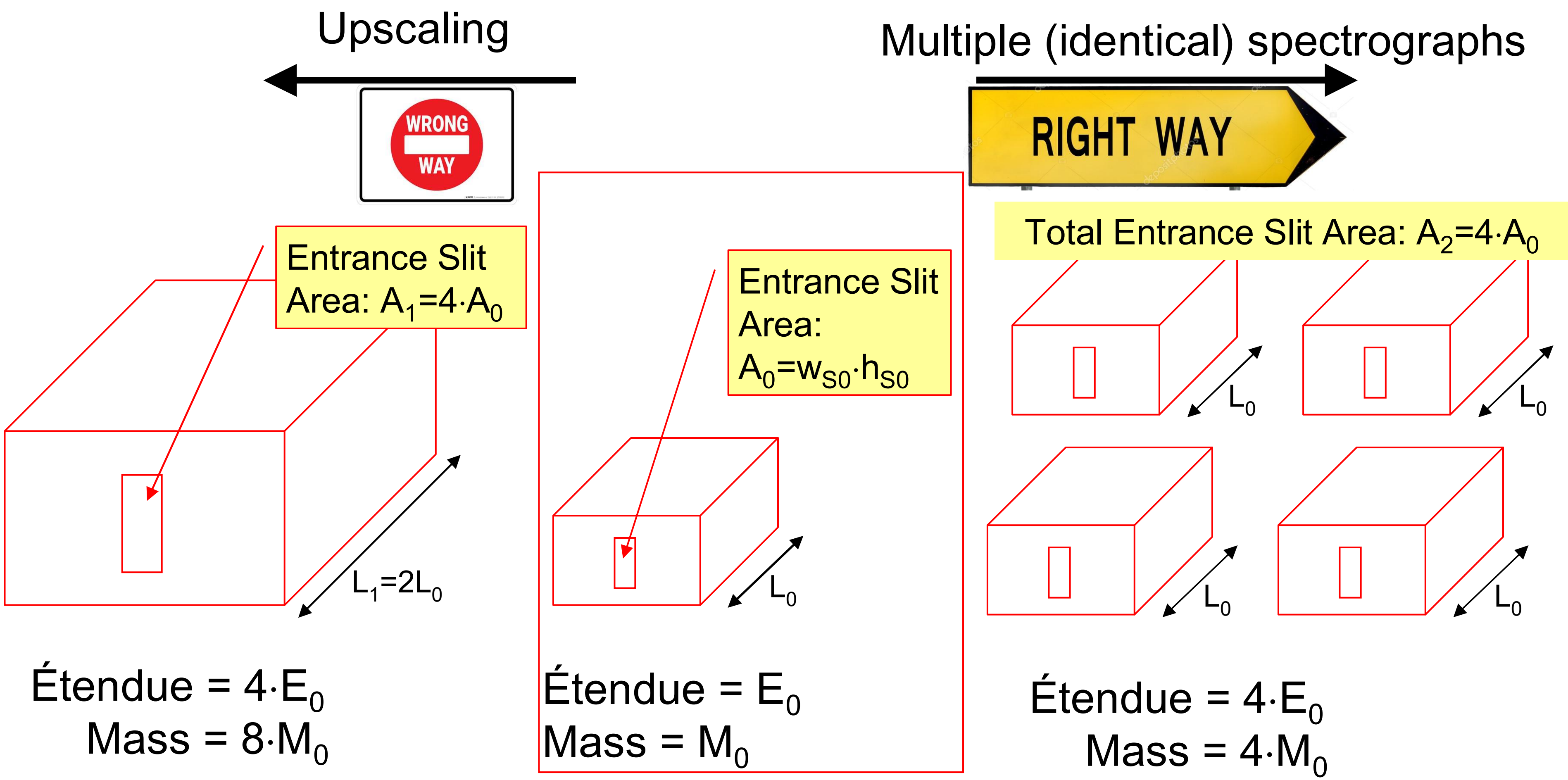
$$\text{or}: \frac{E}{M} \propto \frac{1}{L}$$

Photons/(s · kg)

Since volume and mass of the spectrograph scale with L^3, we have only 50% of photons/s per kg.

5a) Parallel Spectrographs (F = const.)

How to Quadruple the Étendue (F = const.)

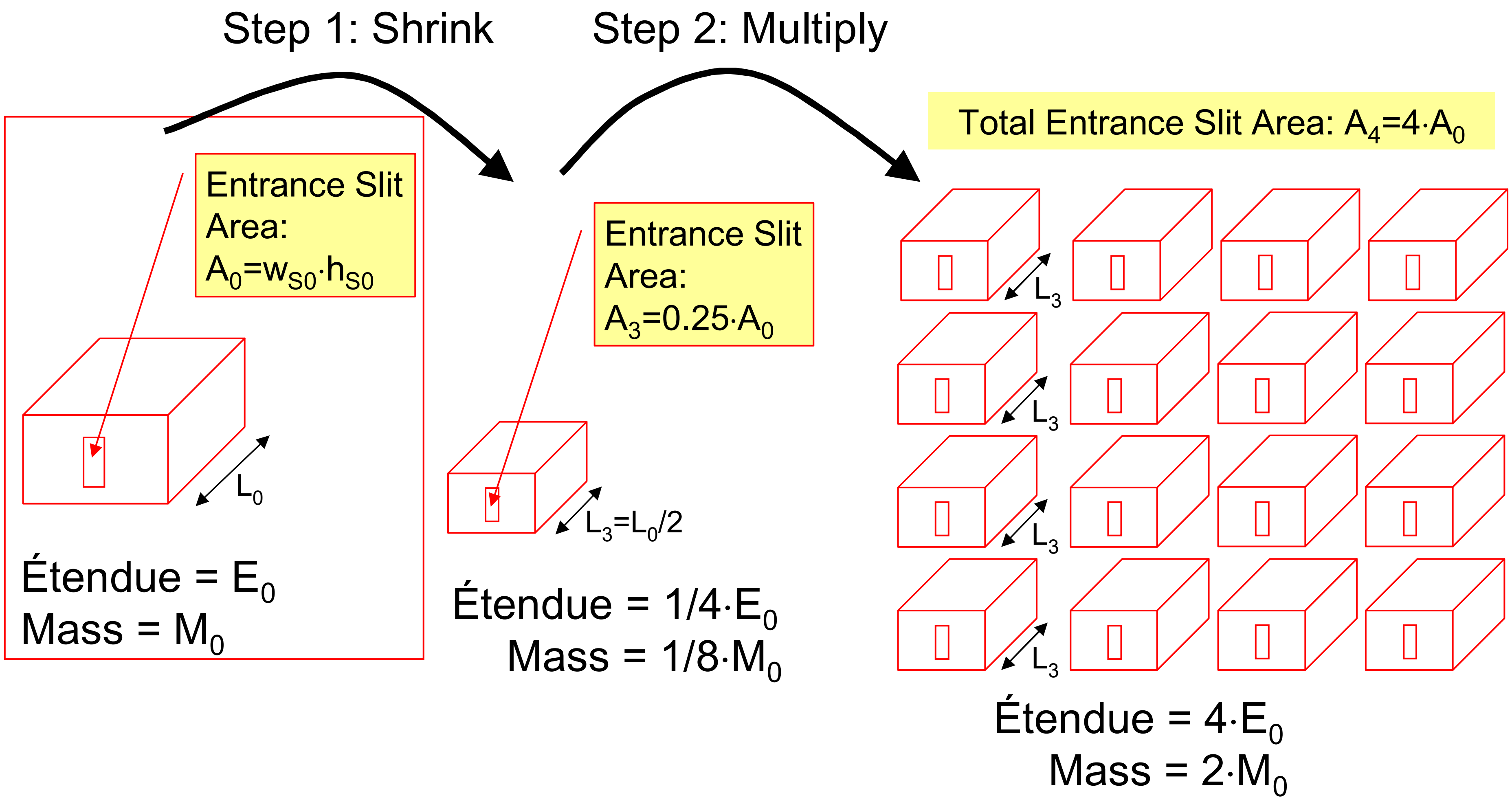


We have 4-times the number of photons/s at 4-times the weight, 100% of photons per kg

And we can still do better …

5b) Parallel Spectrographs (F = const.)

How to Quadruple the Étendue (F = const.)



We have 4-times the number of photons/s at only twice the weight
→ 200% of photons per kg

Scaling Spectrograph Array at Constant Light Throughput

Since $E \propto L^2$ it is a good idea to scale down spectrometer size to $L < L_0$ and to compensate loss in E by increasing the number N of individual spectrometers.

Required number of spectrographs N: $N = \left(\frac{L_0}{L}\right)^2$

Total mass of an array of spectrographs scaled to $L < L_0$:

$$M \cdot N = M_0 \left(\frac{L}{L_0}\right)^3 \cdot \left(\frac{L_0}{L}\right)^2 = M_0 \left(\frac{L}{L_0}\right) \propto L$$

→ Mass (and volume) shrink with scaling, if e.g. a single spectrograph with characteristic dimension L_0 is replaced by an array of N smaller spectrographs, each one scaled down in its linear dimensions to $L_0/(N^{1/2})$.

Example: Replace spectrograph with size=L_0 (Étendue $E=E_0$, mass $M=M_0$) by 100 spectrographs with size $L_1=L_0/10$, each one will have $E_1=E_0/100$ and mass $M_1=M_0/1000$ → **Total mass: $M_1=M_0/10$**

How to Improve Spectrometer Light Throughput - Summary

Scaled Property	**Mass (M) – Étendue (E) Relationship**	**Aspect Ratio Preserved**	**Comment**
1 Optimize Spectrograph	E independent of M	Yes	Only limited improvement possible
2a Mirror size (area), F-number	$M \propto L^2 \propto E \quad \text{or} \quad E \propto M$	No	Very limited scaling, conflict with 3
2b Focal length F-number	$M \propto \frac{1}{E} \quad \text{or} \quad E \propto \frac{1}{M}$	No	Very limited scaling, conflict with 3
3 Slit area	E independent of M	Yes	Very limited scaling, conflict with 2
4 Spectrograph size	$M \propto E^{\frac{3}{2}} \quad \text{or} \quad E \propto M^{\frac{2}{3}}$	Yes	**No limit to scaling**
5 Number of spectrographs, N_{Sp}	$M \propto N_{Sp}$ and $M \propto E$	Yes	**No limit to scaling**

How far can we shrink a Spectrograph?

Limits to the shrinking of spectrographs:

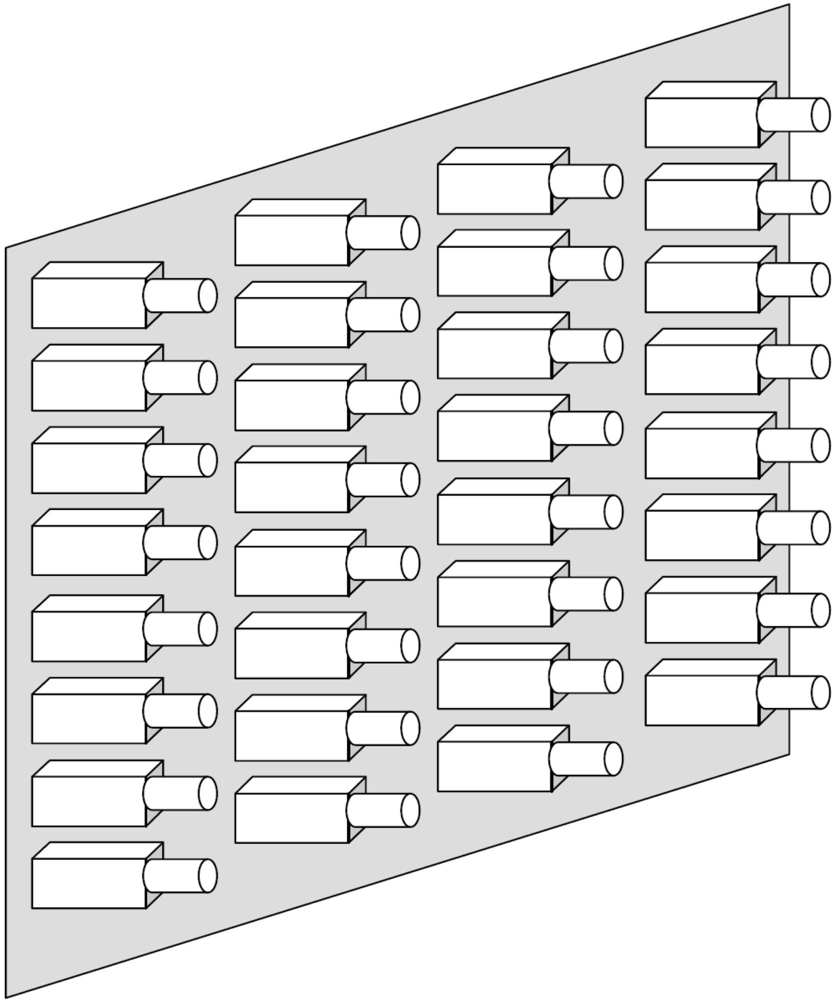
1) Light diffraction at the shrinking entrance slit.
   → Slit widh has to be >$1.22 \cdot F \cdot \lambda$, i.e. typically several μm
2) The grating will loose its resolving power $P_G = \lambda/\Delta\lambda$
   P_G is given by its total number N_G of grooves:

$$P_G = \frac{\lambda}{\Delta\lambda} = N_G = \frac{g}{w_G}$$

   (grating constant g (in grooves/mm) and width w_G (in mm))
   Typical g ≈ 1800 grooves/mm → total number of 36000 grooves and a P_G = 36000. In practice the spectral resolution is about 0.5 nm at 300 nm corresponding to a resolving power $P_{pract} \approx 600$.
3) Very small detector pixels are required
   Typical detector pixel pitch: 12-25 μm, however
   smart phone camera detectors have <1 μm pixel pitch

Summary: Typical satellite spectrographs could be scaled down by $L/L_0 \approx 0.01$
Even miniture spectrographs (like Ocean Insight USB-2000) could be scaled down by $L/L_0 \approx 0.1$

Array of Scaled-Down Parallel Spectrographs



- Mass produced
- Automatic alignment
- Individual electronics
- Spectra of all spectrographs can be co-added
- … or used to improve spatial and temporal resolution

→ For a typical DOAS application mass and volume can be scaled down by a factor 10…100 while maintaining light throughput (E) and spectral resolution

An „Ideal“ Satellite Spectrograph

1) Shrink existing (GOME, OMI, TROPOMI, GEMS, TEMPO…) UV-Vis spectrograph (mass = M_0, etendue E_0) by $L/L_0 = 0.1$
   → need 100 spectrographs with total weight $M/M_0 = 0.1$

2) Replace existing spectrograph by ≈1000 micro spectrographs (of simple design)
   → $M = M_0$ but $E = 10 \cdot E_0$

3) Scanning is achieved by pointing spectrographs + telescope in desired direction

4) Can shrink ground pixel area to 1/10, e.g. from 5.5 x 3.5 km^2 to 2 x 1 km^2 with same S/N-ratio

TROPOMI Imaging

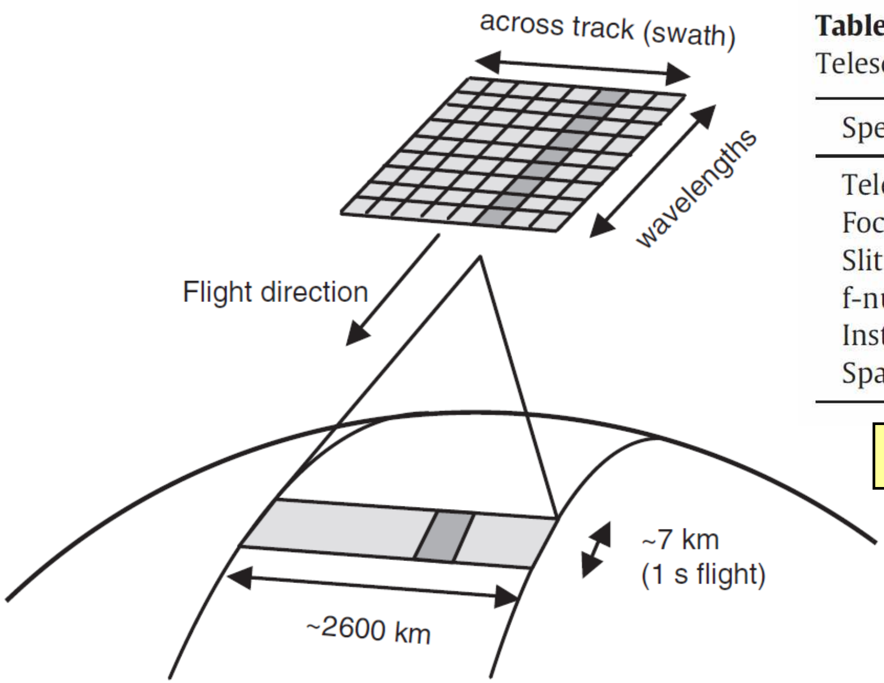


Fig. 1. TROPOMI measurement principle. The dark-gray ground pixel is imaged on the two-dimensional detector as a spectrum. All ground pixels in the 2600 km wide swath are measured simultaneously.

Table 2
Telescope parameters and fields of view.

Spectrometer	UV	UVIS NIR SWIR
Telescope entrance area	25 mm^2	
Focal length (spatial:spectral)	34 mm:68 mm	
Slit size (spatial × spectral)	64×0.56 mm^2	64×0.28 mm^2
f-number (spatial × spectral)	F/9 × F/10	
Instantaneous FOV (spectral)	0.48°	0.24°
Spatial sampling distance (spatial)	0.125°	

Extremely „high“ slit
→ difficult optics, large F

Corresponds to ≈7 km

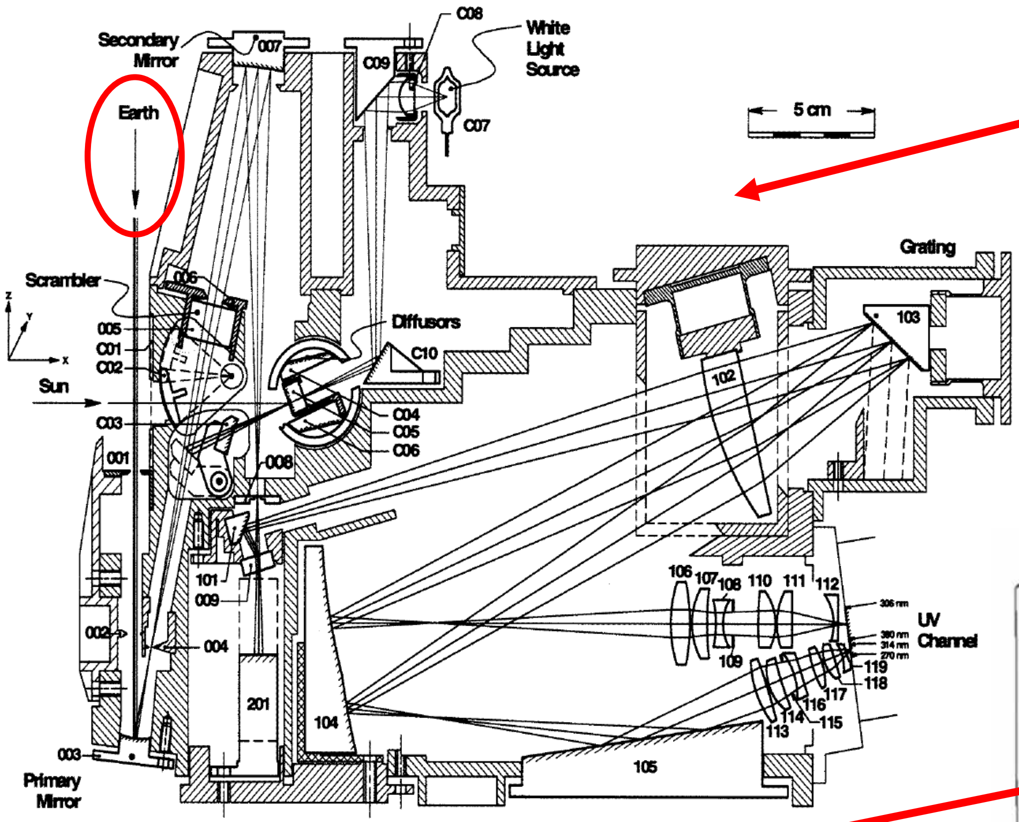
Corresponds to ≈1.7 km

From: Veefkind et al. 2012

Veefkind J.P., Aben I., McMullan K., Förster H., de Vries J., Otter G., Claas J., Eskes H.J., de Haan J.F., Kleipool Q., van Weele M., Hasekamp O., Hoogeveen R., Landgraf J., Snel R., Tol P., Ingmann P., Voors R., Kruizinga B., Vink R., Visser H., and Levelt P.F. (2012), TROPOMI on the ESA Sentinel-5 Precursor: A GMES mission for global observations of the atmospheric composition for climate, air quality and ozone layer applications. Remote Sensing of Environment 120, 70–83.

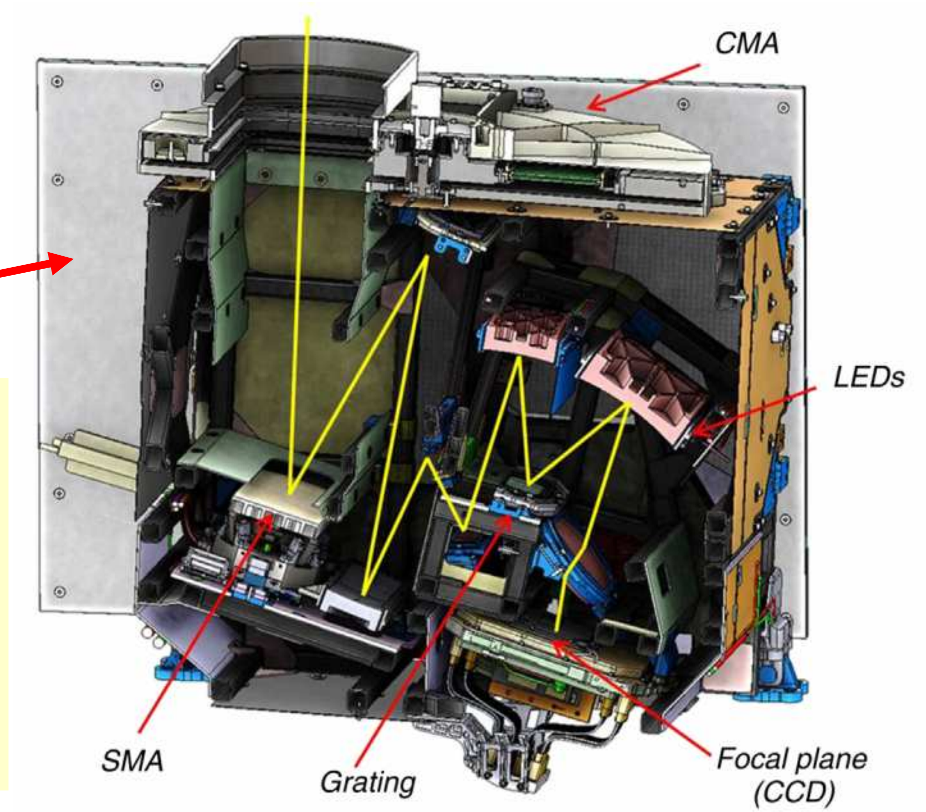
Satellite Spectrometer Optical Design

Incredibly sophisticated!



OMI, From:

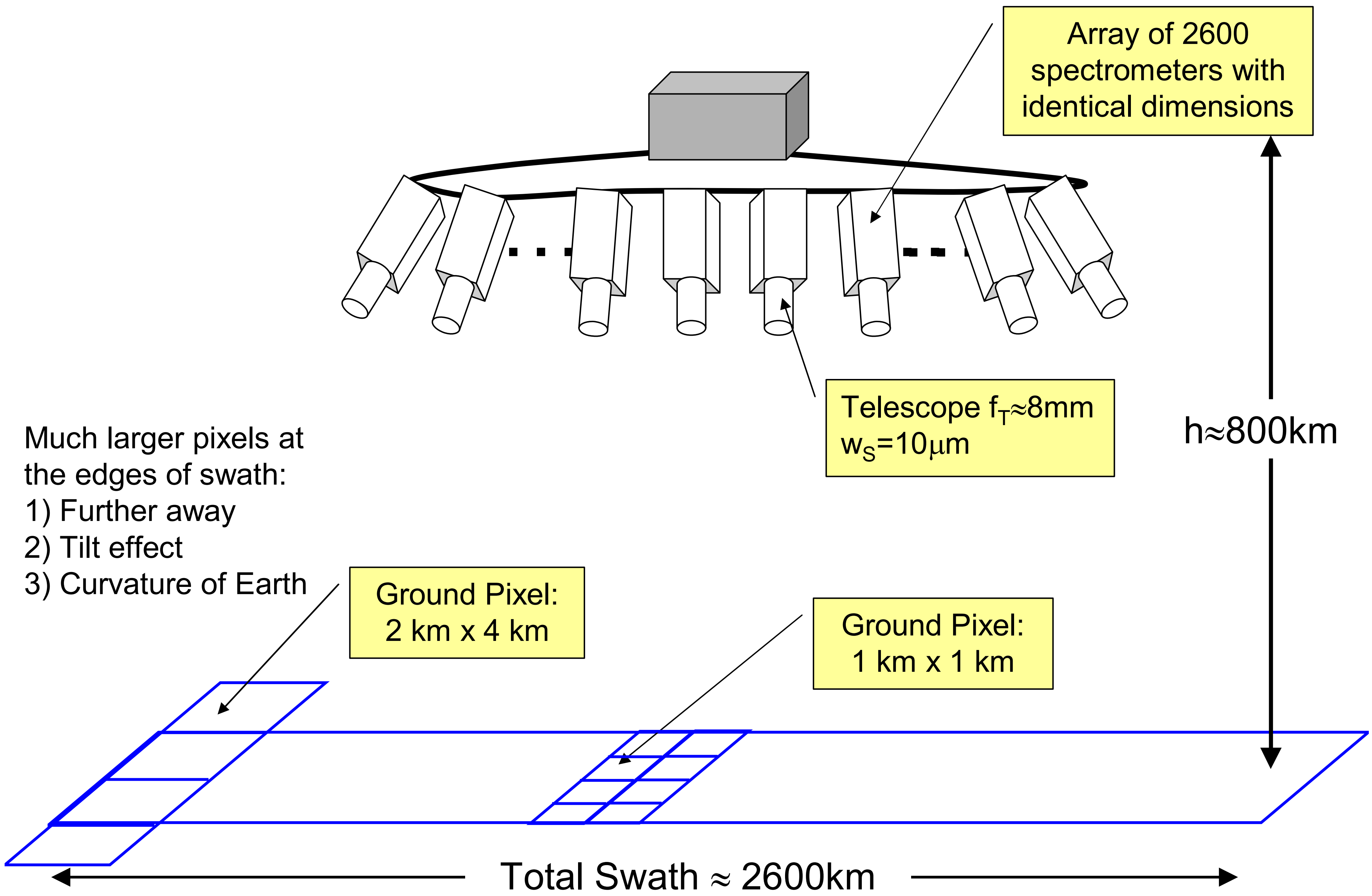
Dobber M.R., Dirksen R.J., Levelt P.F., van den Oord G.H.J., Voors R.H.M., Kleipool Q., Jaross G., Kowalewski M., Hilsenrath E., Leppelmeier G.W.,de Vries J., Dierssen W., and Rozemeijer N.C. (2006), Ozone Monitoring Instrument Calibration, IEEE Trans. Geosci. Remote Sensing 44 (5), 1209.



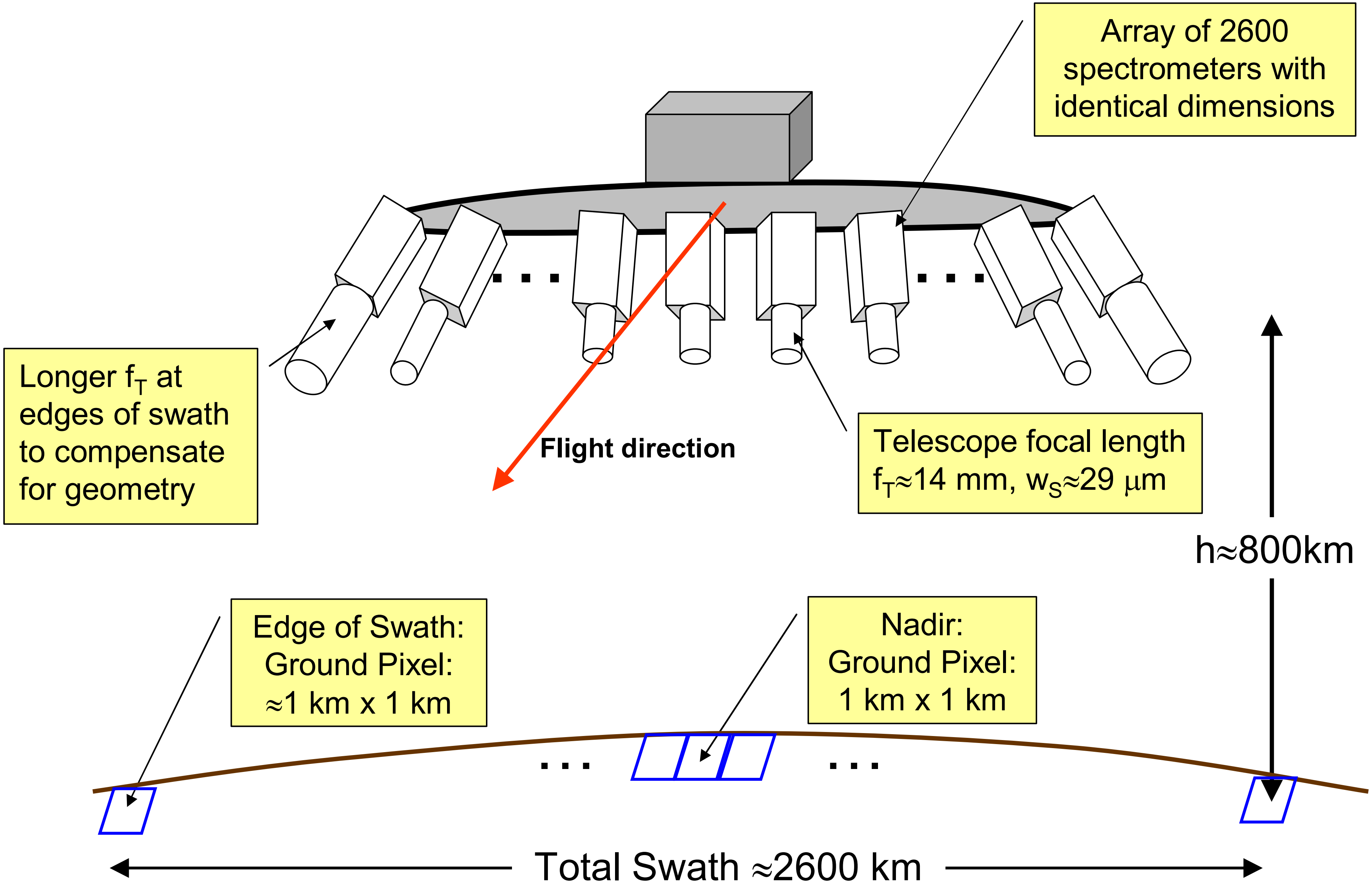
GEMS, From:

Won Jun Choi, Kyung-Jung Moon, Jongmin Yoon, Ara Cho, Sang-kyun Kim, Seounghoon Lee, Dai ho Ko, Jhoon Kim, Myung Hwan Ahn, Deok-Rae Kim, Sang-Min Kim, Ji-Young Kim, Dennis Nicks, Jeong-Su Kim, “Introducing the geostationary environment monitoring spectrometer,” J. Appl. Remote Sens. 12(4), 044005 (2019), doi: 10.1117/1.JRS.12.044005.

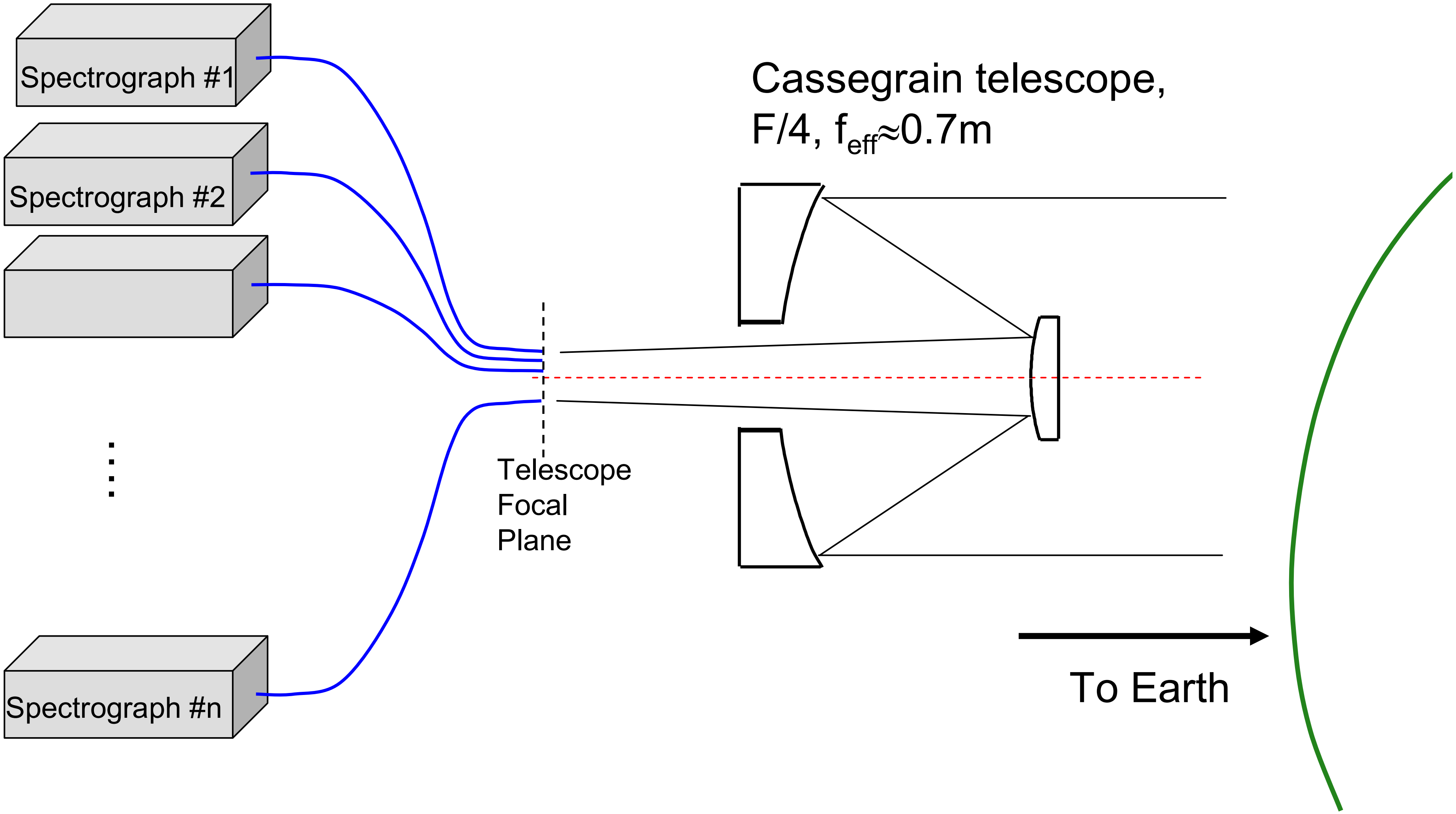
An „Ideal“ LEO Satellite Spectrometer (1)



An „Ideal" LEO Satellite Spectrometer (2)



Geostationary Satellite Instruments (1)



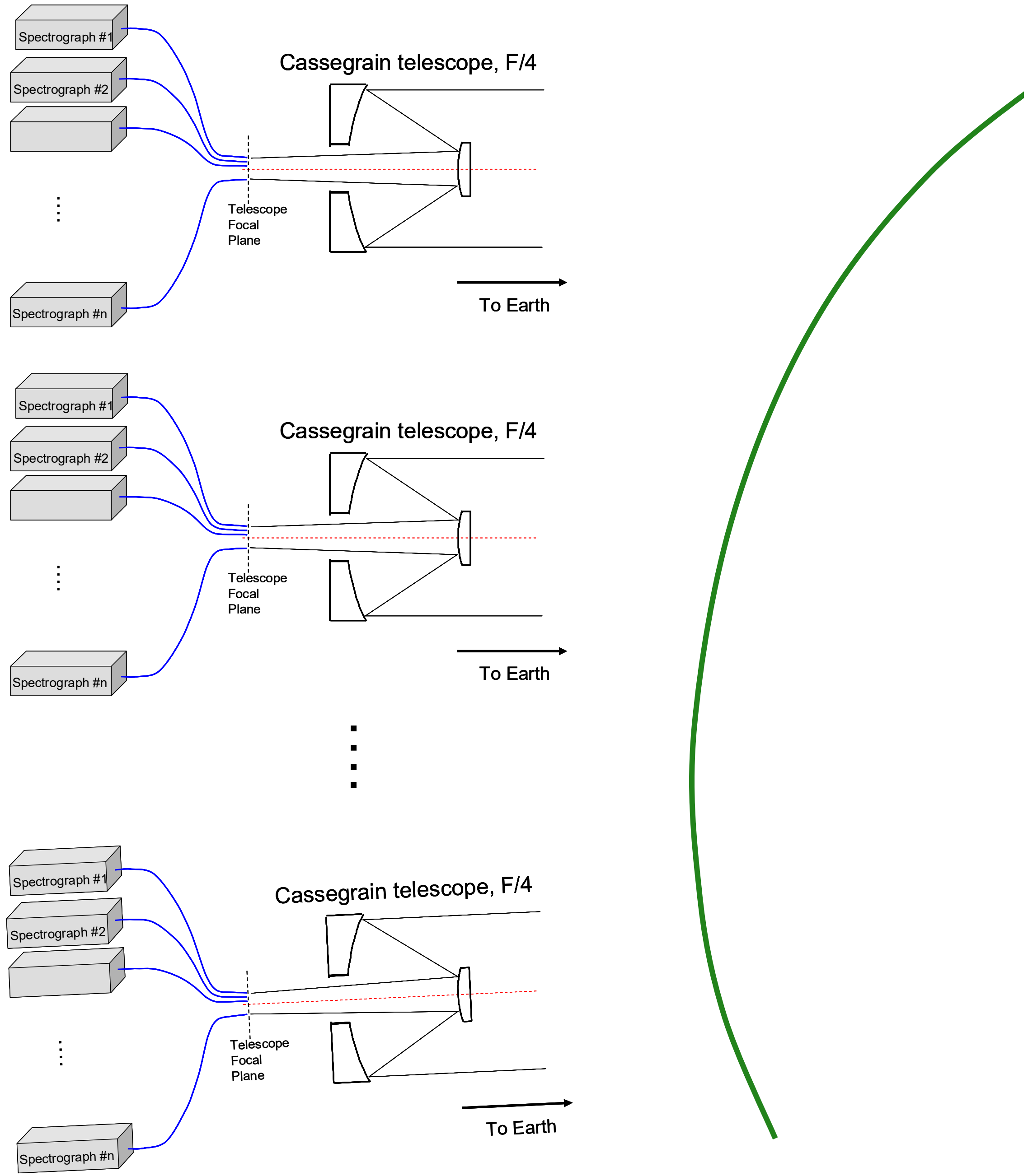
→ The spectrograph system could be build 1-2 orders of magnitude lighter

However the telescope is heavy (due to great height) → Solution …

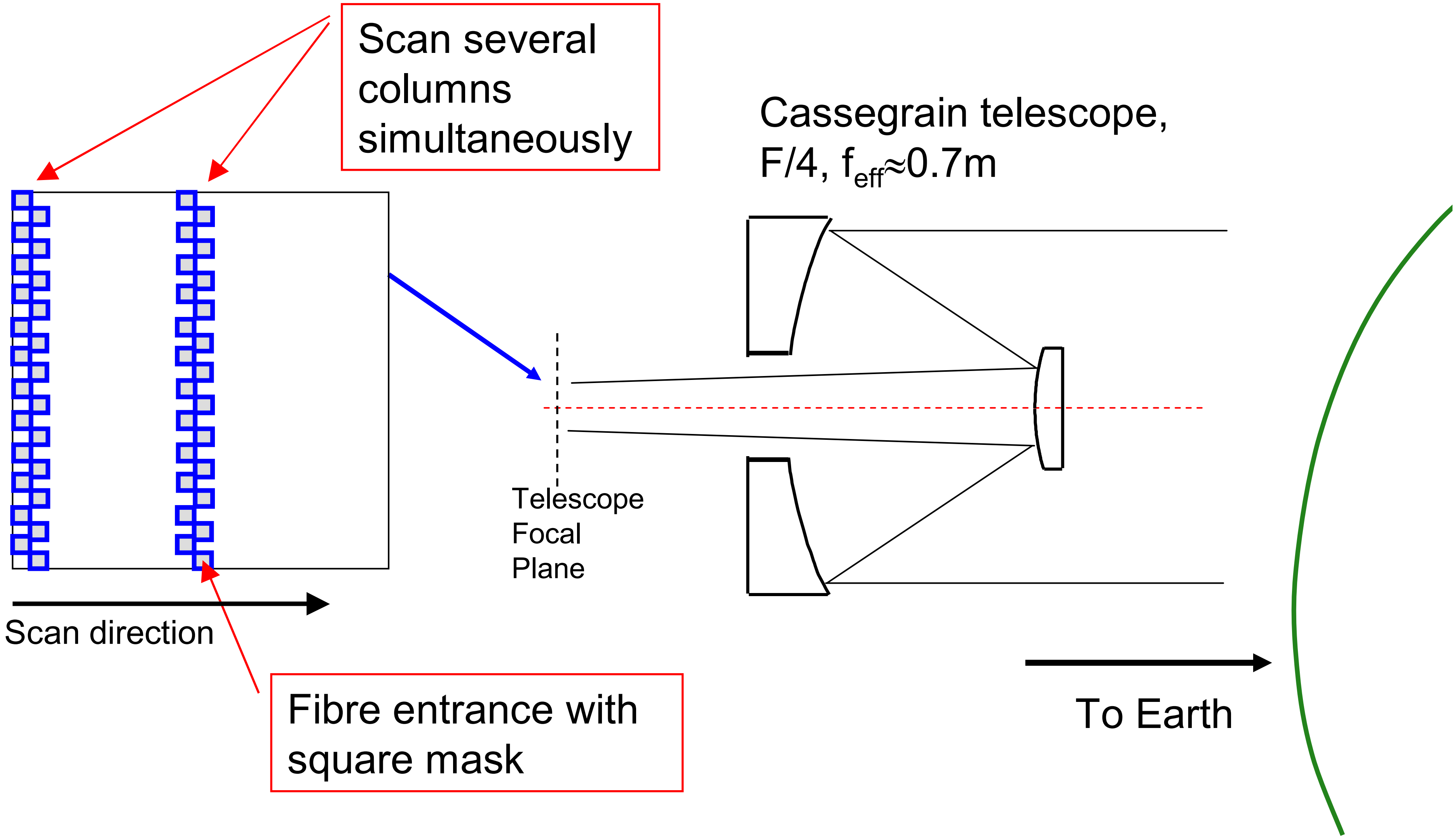
Geostationary Satellite Instruments (2)

Use array of m scaled-down telescopes, each one supplying n/m spectrographs

→ Same scaling rules as for spectrographs apply to telescopes



Geostationary Satellite Instruments (3)



→ Shorter scan period

What About Completely Different Solutions?

1) New Technology: „Detector only“ Spectrograph
2) Old Technology: Fabry-Pérot Spectrograph
3) …

An Ultracompact Spectrograph

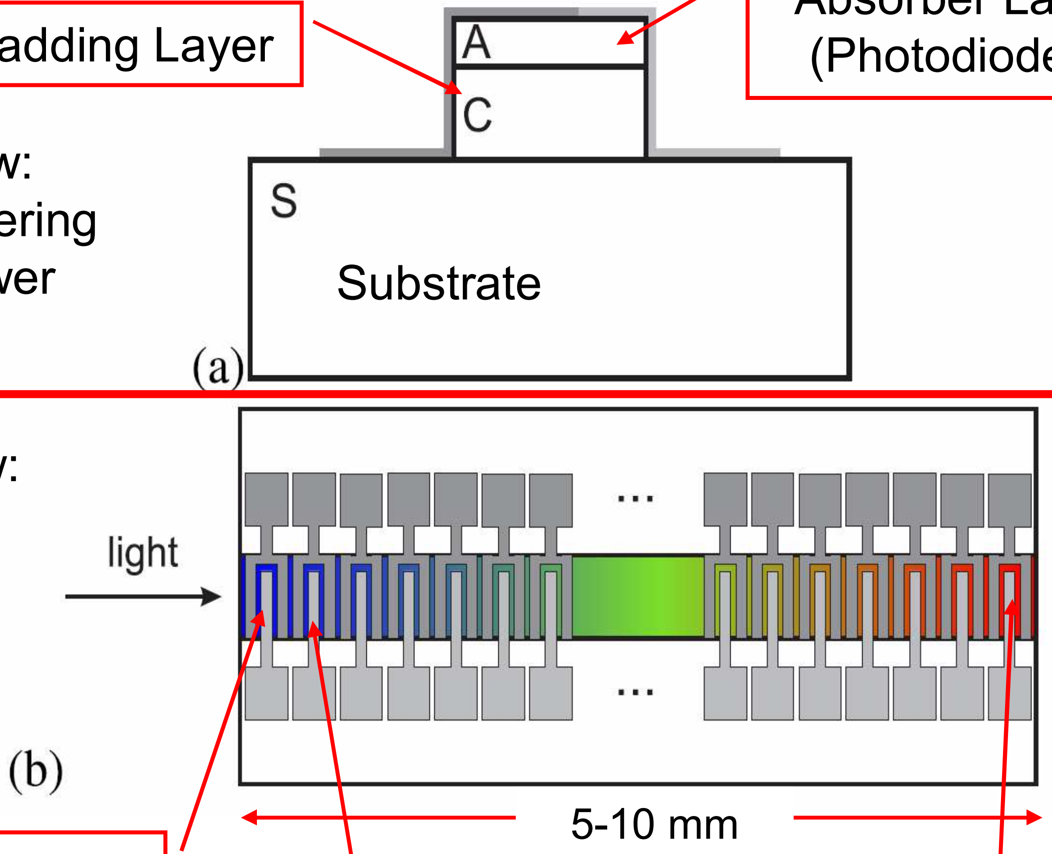
waveguide-based photodetector (WGPD)

- Entirely new type of spectrograph
- Large F/#
- Waveguide (can couple to fiber)
- No dispersive elements
- All photons used (in principle)
- Works in the near UV (or visible)
- Sub-nm (10 meV) spectral resolution expected

Cladding Layer

Absorber Layer (Photodiodes)

Side View:
Light entering from viewer direction



Top View:

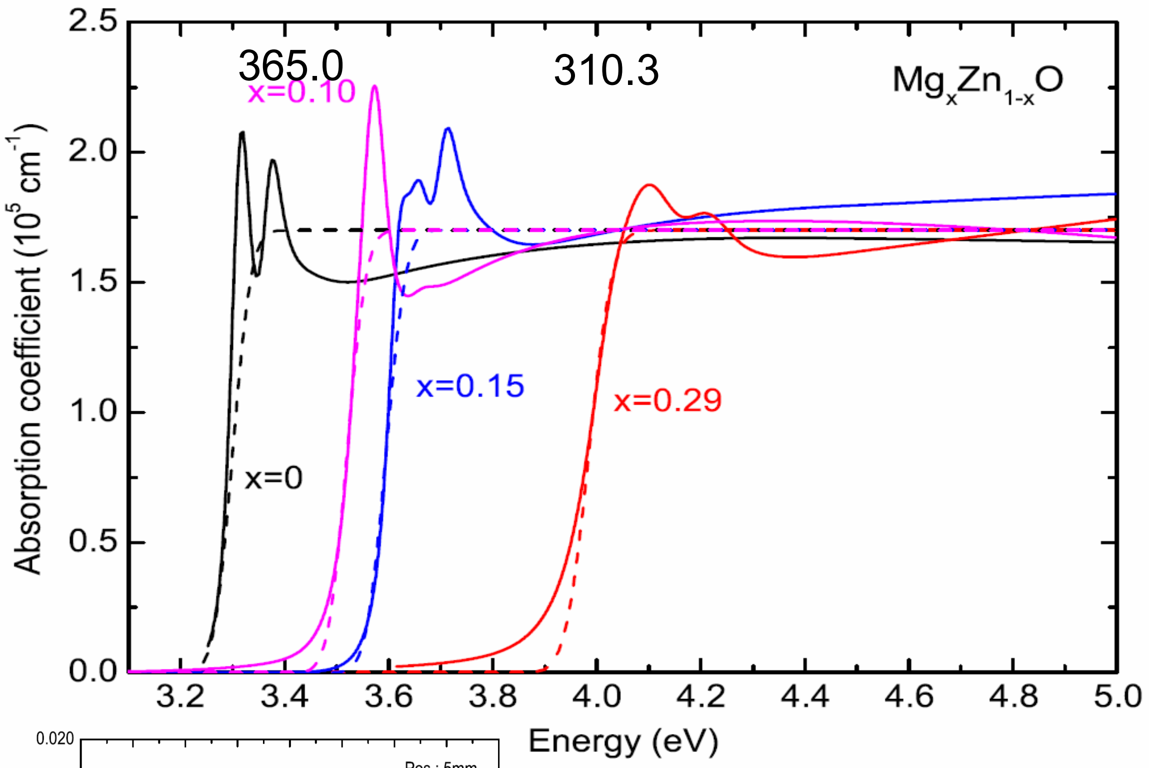
Large Bandgap, absorbs shortest wavelength, transparent to longer wavel.

Smaller Bandgap

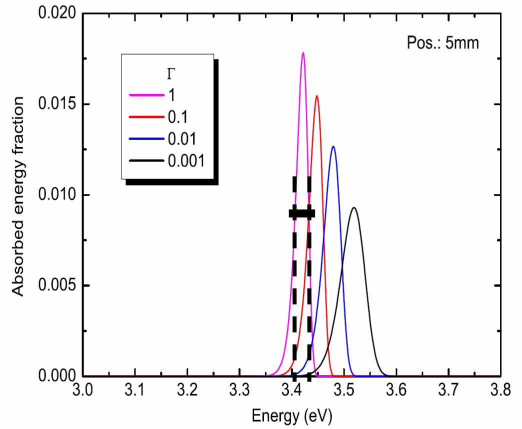
Smallest Bandgap

Grundmann M. (2019), Monolithic Waveguide-Based Linear Photodetector Array for Use as Ultracompact Spectrometer, IEEE Transactions on Electron Devices 66 (1).

Semiconductor Band-Edges & Spectral Resolution



$$1eV \;\square\; 1241\,nm$$

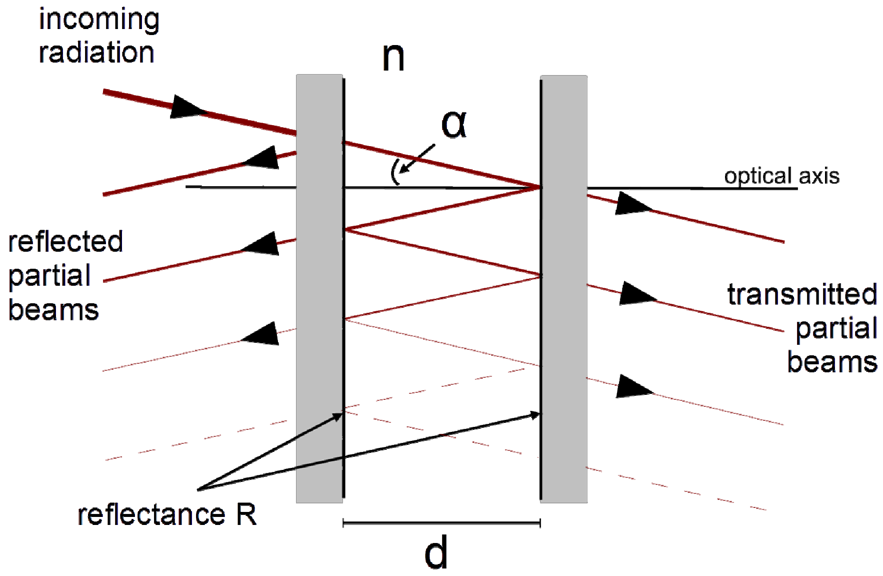


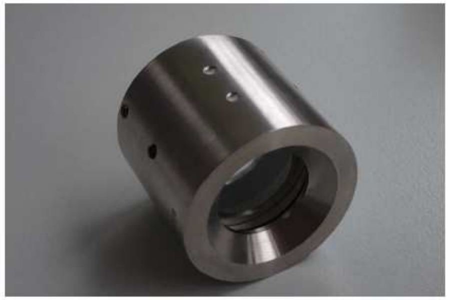
$$\frac{\Delta E}{E} \approx \frac{\Delta\lambda}{\lambda} \approx \frac{0.03}{3.1} \approx 0.01 \Leftrightarrow \Delta\lambda \approx 3.6\,nm$$

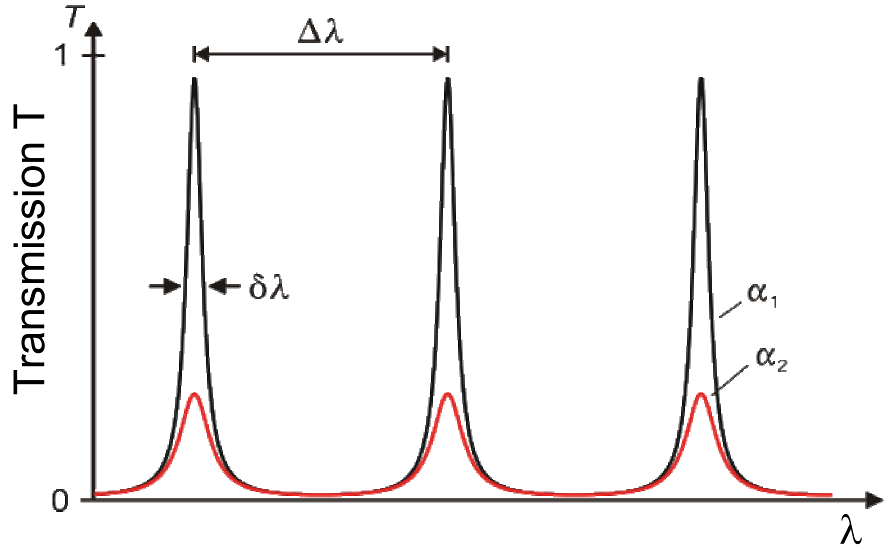
From: Grundmann 2019

2) Fabry-Pérot Spectrograph

Pérot, A. and Fabry, C.:
Astrophys. J. 9, 87-115, 1899.







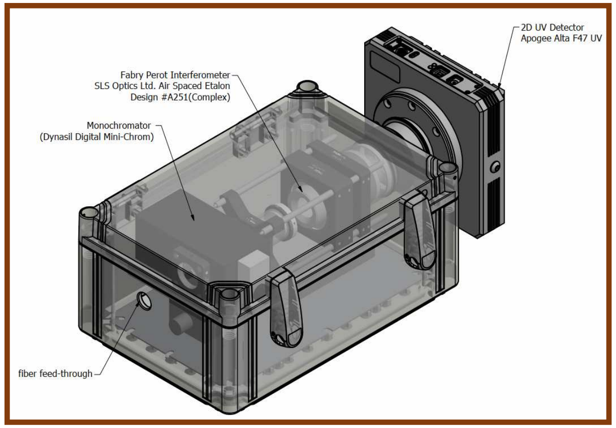
Kuhn J., Bobrowski N., Wagner T., and Platt U. (2021), Mobile and high spectral resolution Faby-Perot interferometer spectrograph for atmospheric remote sensing, Atmos. Meas. Tech. 14, 7873–7892, doi: https://doi.org/10.5194/amt-14-7873-2021

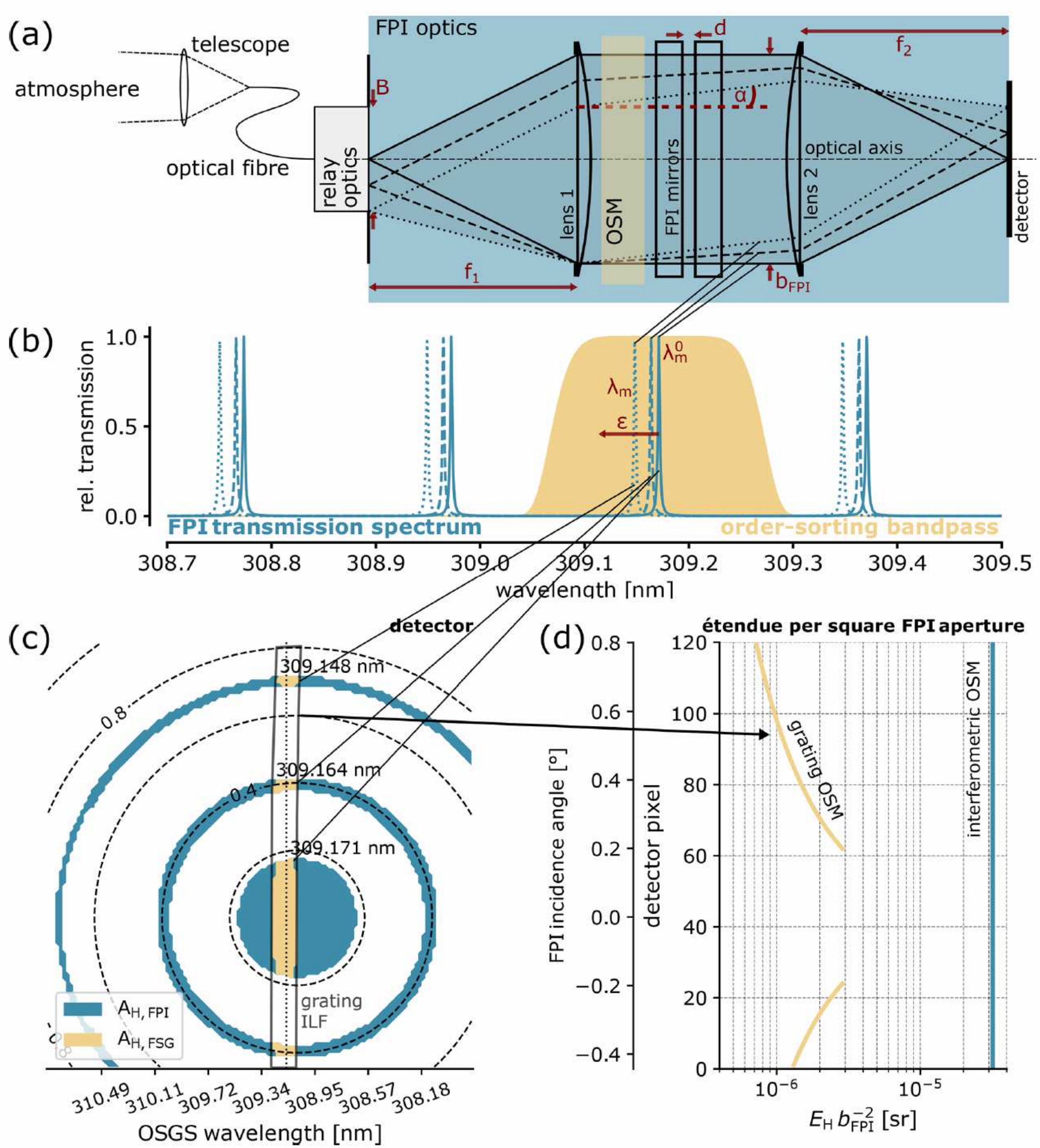
Free spectral range: $\Delta\lambda \approx \dfrac{\lambda^2}{2 \cdot nd\cos(\alpha)}$

Finesse: $F = \dfrac{\Delta\lambda}{\delta\lambda} \approx \dfrac{\pi\sqrt{R}}{1-R}$

… high finesse → high resolution

Our high Res. Fabry Pérot Interferometer Spectrograph





Kuhn J., Bobrowski N., Wagner T., and Platt U. (2021), Mobile and high spectral resolution Faby-Perot interferometer spectrograph for atmospheric remote sensing, Atmos. Meas. Tech. 14, 7873–7892, doi: https://doi.org/10.5194/amt-14-7873-2021

Which Type of Spectrometer is the Best?

Formulas have been established which express the flux given by a spectrometer as a function of the effective resolving power and of the dimension of the dispersive system (area of the base of the prism, or area of the grating, or area of the plates of the etalon). It is thus possible to compare the luminosities of the three types of instruments with, in each case, equal resolving power and equal dimension. This comparison reveals a great superiority of the grating over the prism for all regions of wavelengths, and a great superiority of the etalon over the grating.

Jacquinot (1954)

In other words:

$$\mathrm{P}\left(\mathrm{Etalon}\right) >> \mathrm{P}(\mathrm{Grating}) >> \mathrm{P}(\mathrm{Prism})$$

Jacquinot, P. (1954), The Luminosity of Spectrometers with Prisms, Gratings, or Fabry-Perot Etalons, J. Opt. Soc. Am., 44, 761–765, https://doi.org/10.1364/josa.44.000761.

Summary

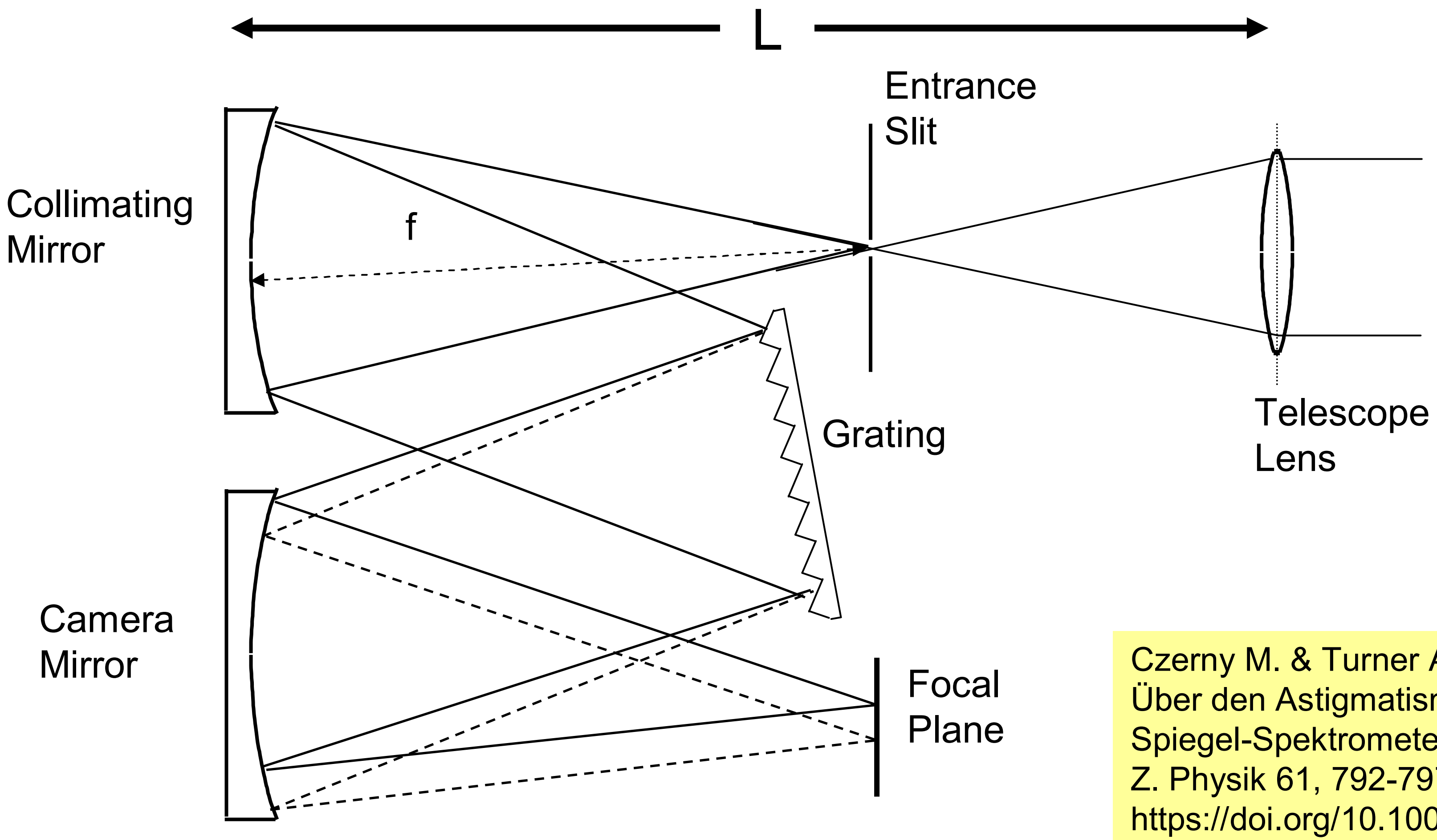
- Arrays of massively parallel spectrographs can solve the problem of achieving high light throughput with compact and lightweight instruments
- Existing designs could be made more compact by applying this approach
- Problem of mass-producing micro-spectrometers has to be solved
- LEO: Much simpler telescope design, since only a small telescope field of view is required.
- Adaptive field of view for the edges of the swath (need ≈2600 km swath for a daily coverage by a LEO instrument) in order to reduce the variation in ground pixel size across the swath.
- GEO: Multiple spectrometers + Multiple telescopes could
  - considerably reduce instrument mass
  - allow smaller ground pixels
  - allow faster scan

  } Or combination thereof

For details see:
Platt U., Wagner T., Kuhn J., and Leisner T. (2021), The "Ideal" Spectrograph for Atmospheric Observations, Atmos. Meas. Tech. 14, 6867–6883, https://doi.org/10.5194/amt-14-6867-2021

Thank You!

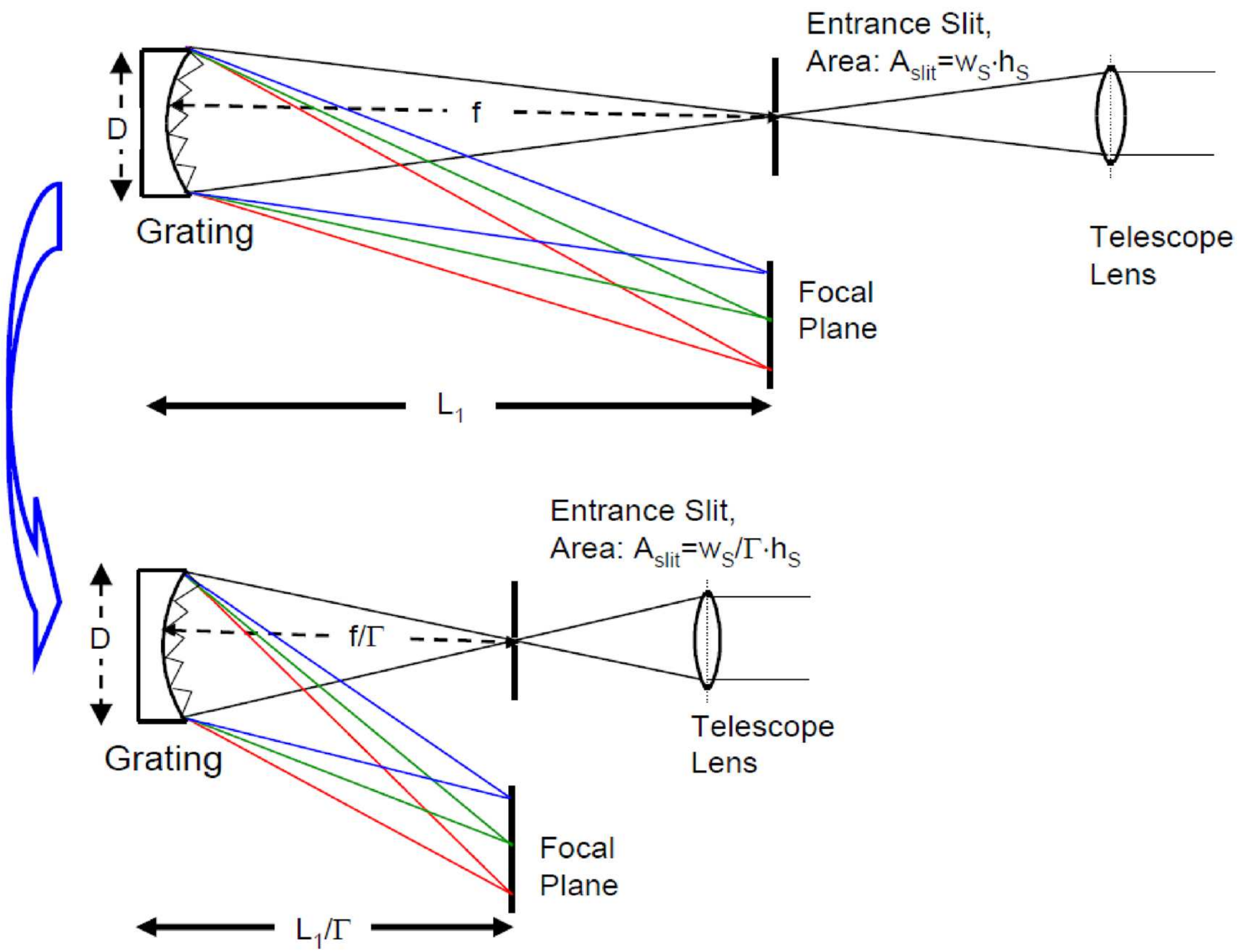
Typical design of a Czerny Turner Spectrograph plus Telescope



Czerny M. & Turner A.F. (1930), Über den Astigmatismus bei Spiegel-Spektrometern, Z. Physik 61, 792-797, https://doi.org/10.1007/BF01340206.

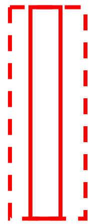
The size of the spectrograph L is largely dominated by the focal length f with $L = a \cdot f$, $a \approx 1.3$

2b) Scaling the Spectrograph (Plus Telescope) F-Number



3a) Larger Slit-Area by Increasing Slit Width w_S?

Étendue E:



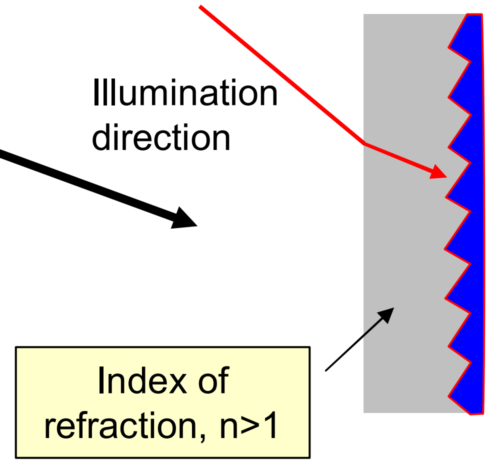
$E = \Omega \cdot A_S$ with: $A_S = w_S \cdot h_S$

Increase w_S?

Problem: w_S determines Spectral Resolution (SR)

Solution: SR preserved if w_S and $g=1/d_G$ vary by same factor!
However: Reduction of d_G limited by wavelength (minimum $d_G \approx \lambda$)

Possible improvement: '**Immersed Grating**'



Wavelength λ_n seen by the grating is: $\lambda_n = \lambda/n$

→ d_G can be reduced (and g be increased) by factor n

Diamond: $n \approx 2.4$?

→ Limited gain!

See e.g. van Amerongen, A.H., Visser, H., Vink, R.J.P., Coppens, T., Hoogeveen, R.W.M.: Development of immersed diffraction grating for the TROPOMI-SWIR Spectrometer, Proc. SPIE, 7826, 78261D-1, doi: 10.1117/12.869018, 2010.

3b) Larger Slit-Area by Increasing Slit Height h_s?

Étendue E:

$E = \Omega \cdot A_S$ with: $A_S = w_S \cdot h_S$

Increase h_S? → Problem: larger h_S increases astigmatism

Quantification by Fastie (1952): empirical relationship between astigmatism as defined as the difference Δf between the sagittal focal length f_s and the meridional focal length f_m (see also Kuhn et al. 2021):

$$\Delta f \approx 0.1 \cdot \frac{f}{F^2}$$

Width of astigmatic spread: $\Delta L = \Delta f / F$. Causing additional width of the image Δw (in dispersion direction): $\Delta w = \Delta L \cdot h_S / f$. With the grating clear aperture 2r we obtain:

$$\Delta w \approx \Delta L \cdot \frac{h_S}{2r} = \frac{\Delta f}{F} \cdot \frac{h_S}{2r} = 0.1 \cdot \frac{f}{F^3} \frac{h_S}{2r} = 0.1 \cdot \frac{h_S}{F^2}$$

Allowing an additional width $\Delta w = w_S/10$ (and corresponding slight degradation in spectral resolution) we obtain:

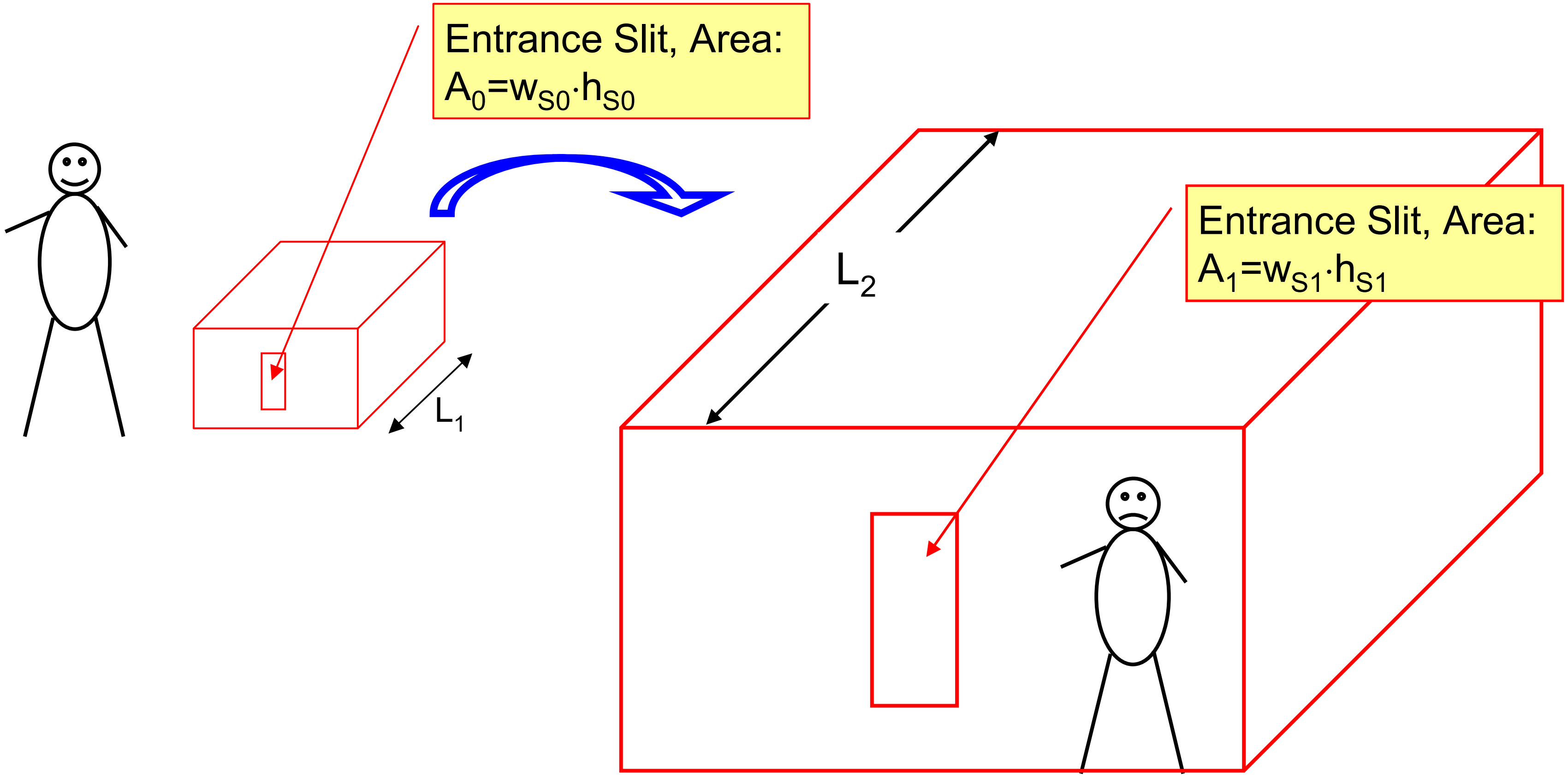
$$\frac{w_S}{10} \approx 0.1 \cdot \frac{h_S}{F^2} \quad \text{or} \quad h_S \approx w_S \cdot F^2$$

Fastie, W.G.: Image Forming Properties of the Ebert Monochromator, J. Opt. Soc. Am., 42, 647-651, 1952.

→ **Slit height h_S is limited**, e.g. a typical F = 4 spectrograph with w_S = 50µm would allow $h_S \approx F^2 \cdot w_S = 16 \cdot w_S \approx 0.8$ mm (for 10% resolution degradation)

Solution 4 to the Light-Throughput Problem

Scale up size, keeping F-number - and thus Ω - constant:



Problem:

$$M \propto V \propto L^3 \propto E^{\frac{3}{2}} \Leftrightarrow M \propto E^{\frac{3}{2}}$$

Example: Scaling up to $L_1=10\cdot L_0$

Gives 100-fold light throughput but requires 1000-times higher mass

4) Upscaling Spectrograph Size (F = const.)

Assume a spectrograph entrance slit with width w and height h, area $A_S = h_S \cdot w_S$ and aperture solid angle Ω.
→ Étendue E of the instrument given by:

$$E = \Omega \cdot A_S$$

Ω = const. when spectrograph is scaled

Change of light throughput (i.e. E) when spectrograph size is changed:

$$E = \Omega \cdot A_S \left(\frac{L}{L_0}\right)^2 = E_0 \left(\frac{L}{L_0}\right)^2 \propto L^2 \Leftrightarrow L \propto E^{\frac{1}{2}}$$

However, volume and mass of the spectrograph scale with L^3, i.e.:

$$M \propto V = M_0 \left(\frac{L}{L_0}\right)^3 \propto L^3$$

Summary: $E \propto L^2$, $V \propto M \propto L^3$:

Photons/(s · kg)

$$M \propto V \propto L^3 \propto E^{\frac{3}{2}} \text{ or } \frac{E}{M} \propto \frac{1}{L}$$

Micro Spectrometer & Scaling

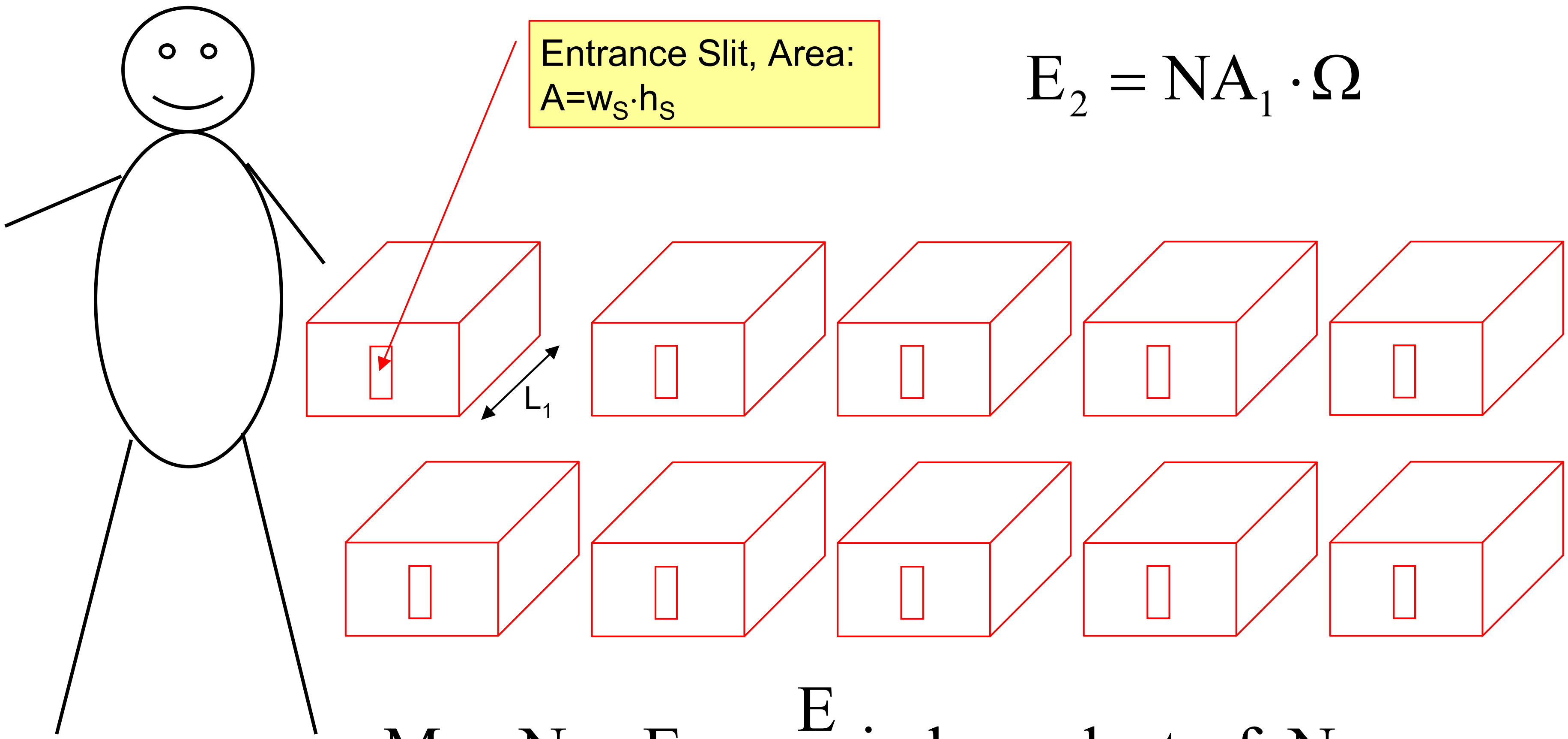
Avrutsky I., Chaganti K., Salakhutdinov I., and Auner G. (2006), Concept of a miniature optical spectrometer using integrated optical and micro-optical components, Appl. Opt. 45 (30), 7811-7817.

Danz N., Höfer B., Förster E., Flügel-Paul T., Harzendorf T., Dannberg P., Leitel R., Kleinle S. and Brunner R. (2019), Miniature integrated micro-spectrometer array for snap shot multispectral sensing, Optics Express 27 (4), https://doi.org/10.1364/OE.27.005719.

Park Y. and Choi S.H.(2013), Miniaturization of optical spectroscopes into Fresnel microspectrometers, J. of Nanophotonics 7, DOI: 10.1117/1.JNP.7.077599

Solution 5 to the Light-Throughput Problem

Array of N identical Spectrometers (with same F-numbers, F_1):



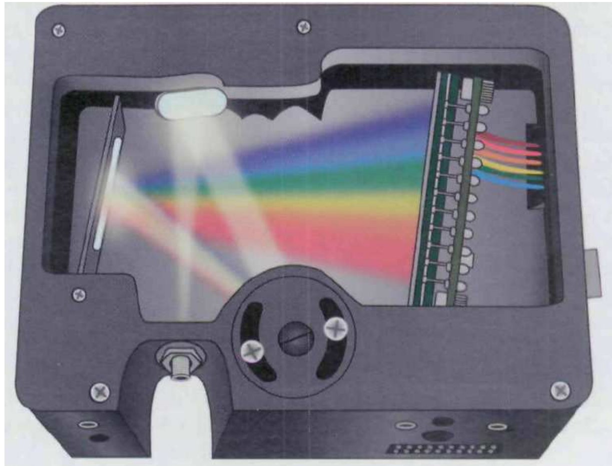
$$E_2 = NA_1 \cdot \Omega$$

$$M \propto N \propto E \text{ or } \frac{E}{M} \text{ independent of } N$$

Example: 10-fold light throughput requires 10-times higher mass

However, it is even better …

Example: Shrink a Miniature Spectrograph?



Example:
Ocean Insight USB2000 instrument with f=70 mm, slit with w_S = 0.05 mm by h_S = 0.5 mm.
Aperture is F/4 corresponding to
$\Omega \approx 0.25^2/4 \cdot \pi \approx 0.0491$ sr.

→ Etendue ≈0.00123 mm^2sr.

The grating typically has 1800 grooves/mm resulting in a total number of 36000 grooves and a theoretical resolving power $P_{G,theo}$ = 36000 >> $P_{G,\ prakt} \approx 600$.

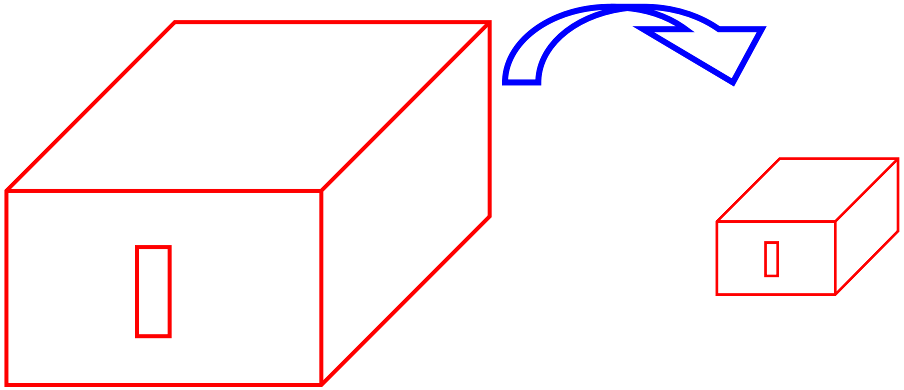
Detector pixels: ≈12 µm (ILX511)
→ use commercial camera detectors with ≈ 1 µm pixels (see e.g. Wilkes et al. 2018)

Summary: Even such rather small spectrographs probably could be scaled down by $L_1/L_0 \approx 0.1$

Summary: Shrink & Multiply

Step 1: shrink spectrograph

$$M \propto L^3 \propto E^{\frac{3}{2}} \text{ or } \frac{E}{M} \propto \frac{1}{L}$$



$$L_1 = 0.1 \cdot L_0$$

$$E_1 = 10^{-2} E_0,\ M_1 \rightarrow 10^{-3} M_0,$$

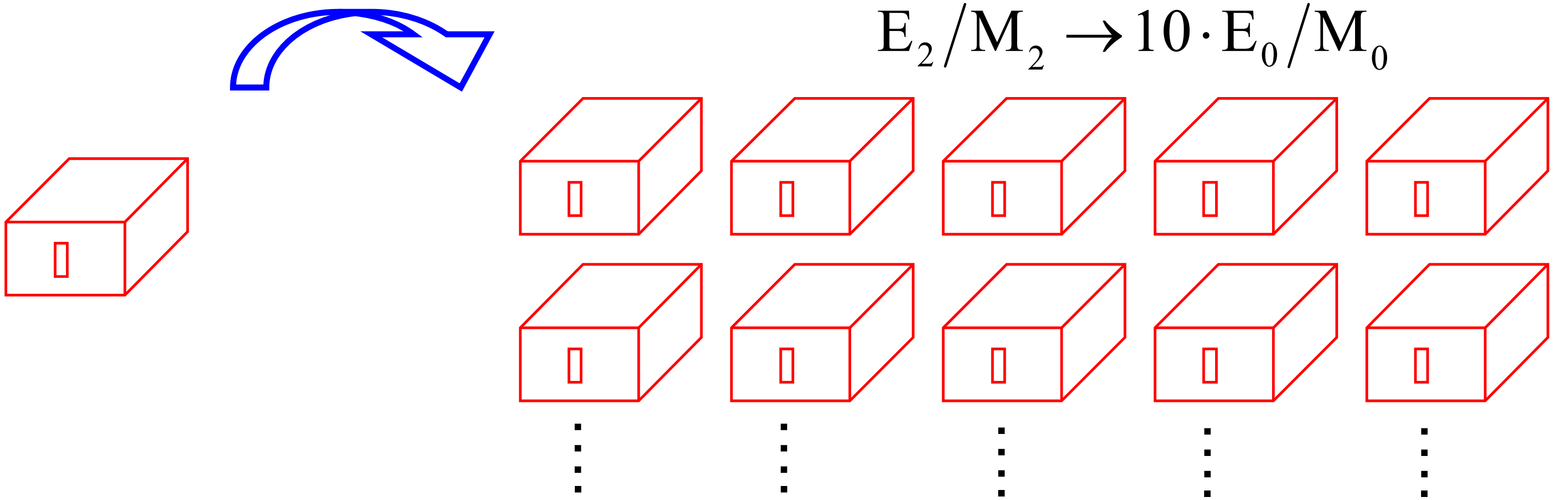
$$E_1 / M_1 = 10 \cdot E_0 / M_0$$

Step 2: multiply spectrograph

$$N = 100 \Rightarrow \text{final}\, E_2 :$$

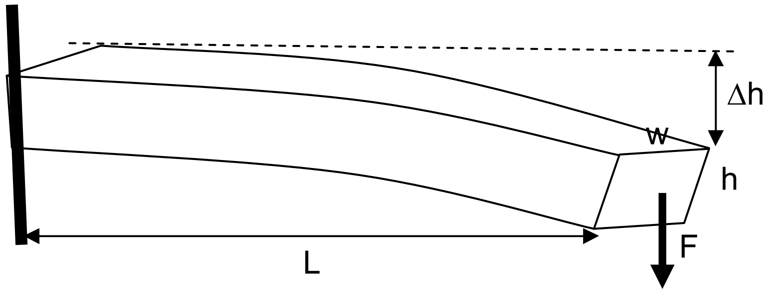
$$E_2 = 100 \cdot 10^{-2} E_0,\ M_2 = 100 \cdot 10^{-3} M_0,$$

$$E_2 / M_2 \rightarrow 10 \cdot E_0 / M_0$$



Is it true that the spectrometer mass scales with L^3?

For simplicity, we assume the spectrometer to behave like a bar with length L, width w, and height h on which an external force acts.

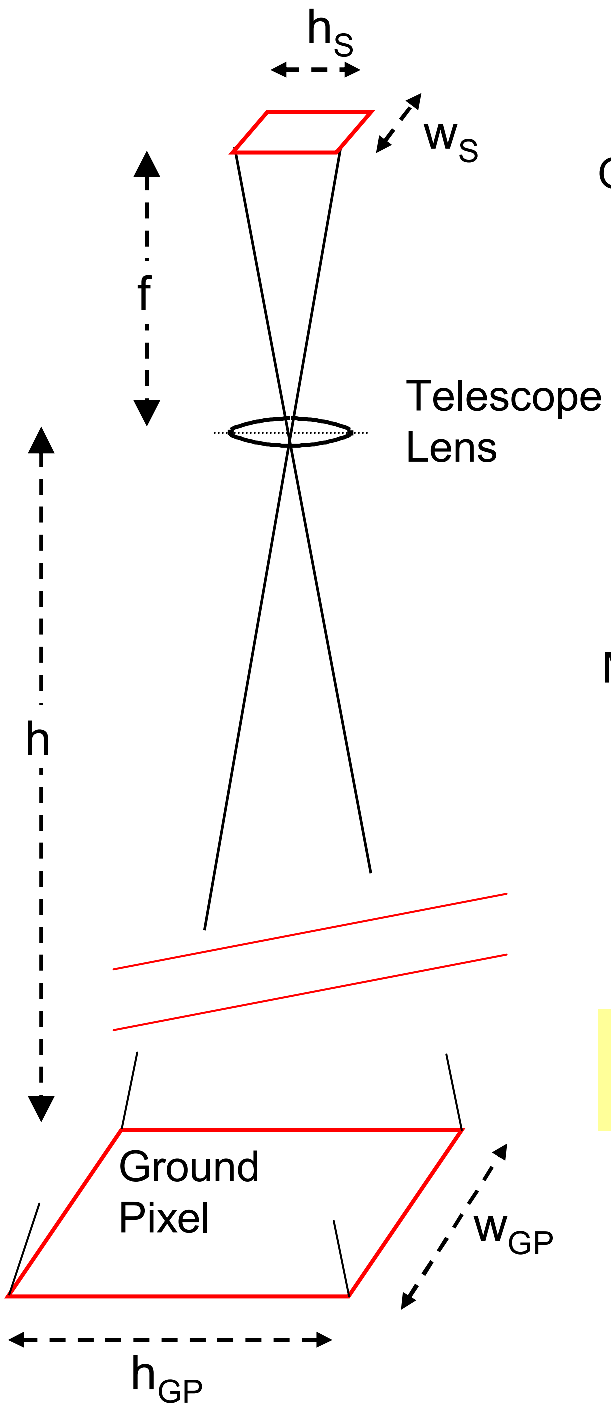


→ Apply the famous case of bending a bar, (see most physics textbooks, e.g. Meschede 2015). When scaling the initial length L_0 of the bar to some other length L by a factor L/L_0 and likewise w_0 to $w=w_0 \cdot L/L_0$ and h_0 to $h=h_0 \cdot L/L_0$ we can calculate the scaling of Δh since:

$$\Delta h \propto L^3, \ \Delta h \propto h^{-2}, \ \Delta h \propto w^{-1}$$

And:

$$\Delta h \propto \frac{L^3}{L^2 \cdot L} = \text{const.}$$



Satellite Imaging

OMI/TROPOMI – type instrument for 1 km ground pixel size:

$$f = h \cdot \frac{w_S}{w_{GP}} = \frac{h}{w_{GP}} \cdot w_S \approx \frac{8 \cdot 10^5}{10^3} \cdot 0.1\text{mm} \approx 80\text{mm}$$

For F=4 a telescope diameter of D=20 mm would be required. Actually TROPOMI has F=9 …10

Miniature spectrometer instrument for 1 km ground pixel size:

$$f = \frac{h}{w_{GP}} \cdot w_S \approx \frac{8 \cdot 10^5}{10^3} \cdot 0.01\text{mm} \approx 8\text{mm}$$

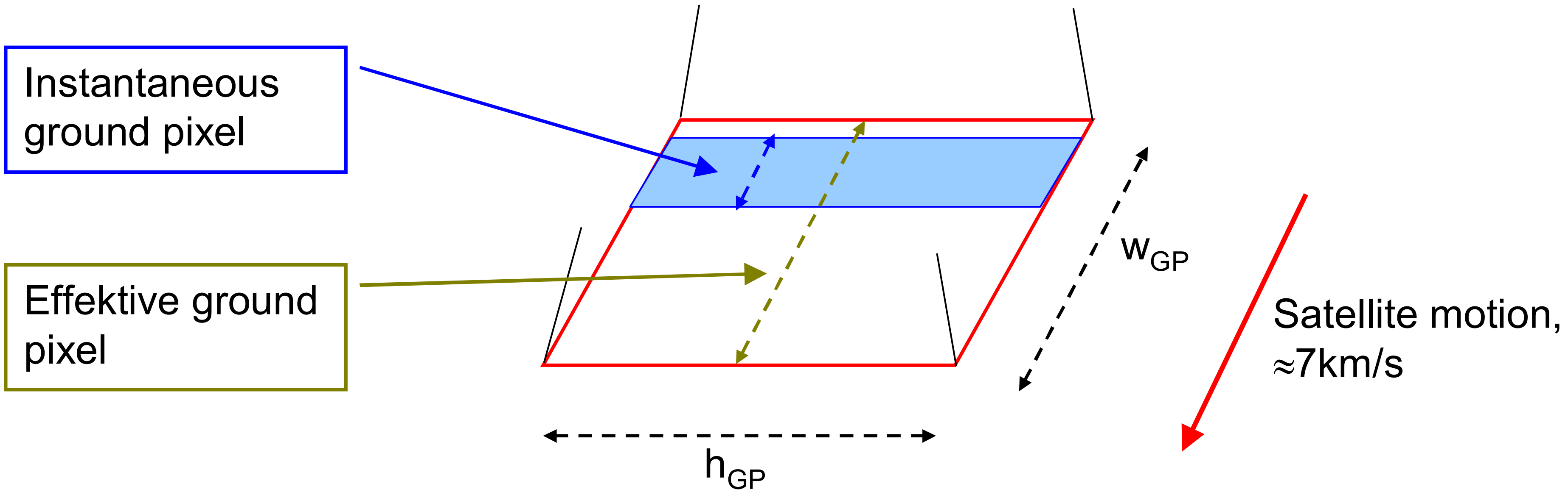
For F=4 a telescope dia. of D=2 mm would be required.

→ **From a standpoint of imaging** there is no problem to build a system with smaller ground pixels

However, measurement time is a problem!

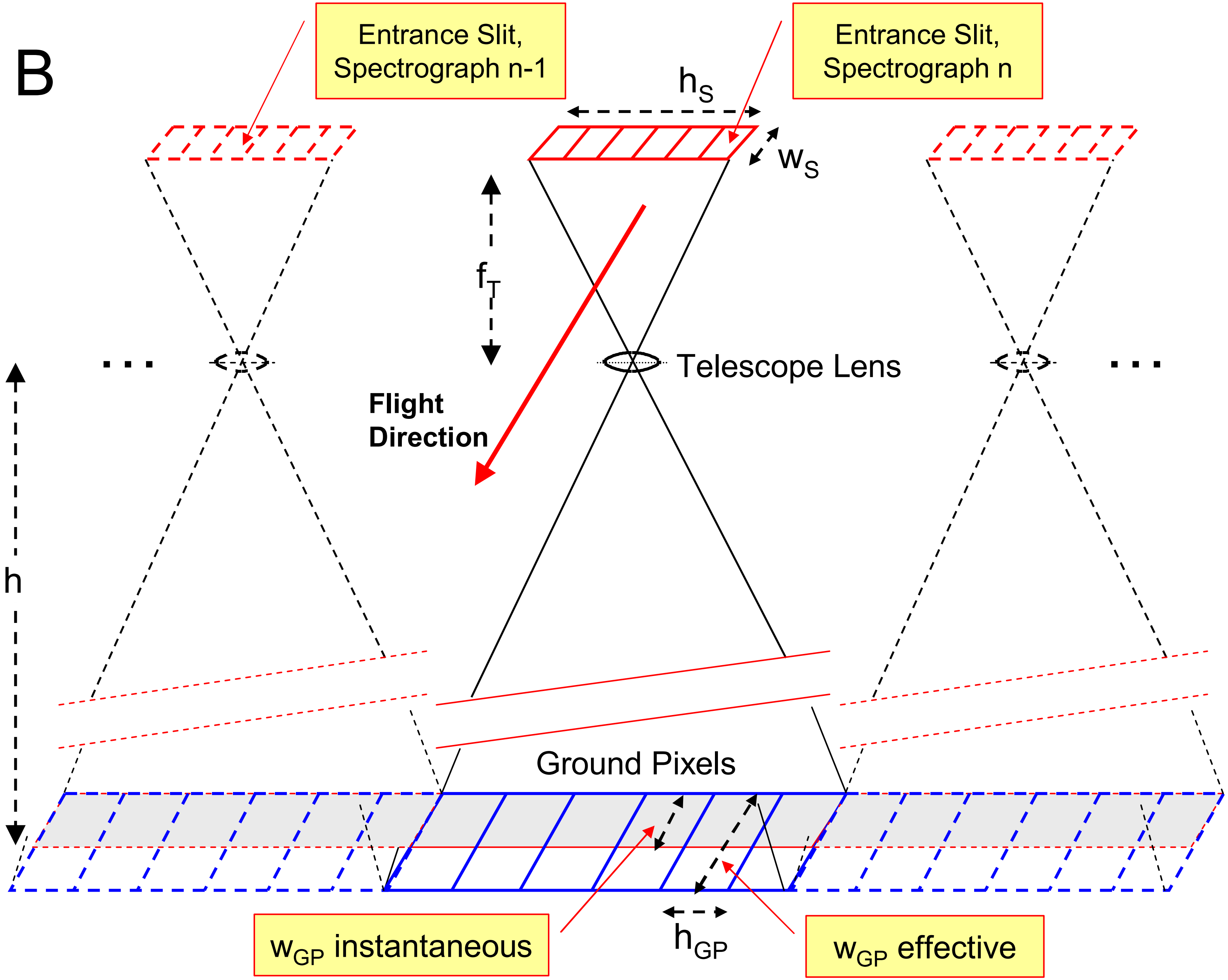
For w_{GP}=1km max. 1/7s would be permissible

Instantaneous Ground Pixel vs. Effective Ground Pixel



Along-track extension of the Instantaneous ground pixel should be small (?) compared to that of the effective ground pixel.

An „Ideal" Satellite Spectrometer (2)



„Ideal“ Satellite Spectrometers

See: Platt etal. (2021), AMT 14, 6867–6883, https://doi.org/10.5194/amt-14-6867-2021

[1]see Veefkind et al. 2012 and Dobber et al. 2006

[2]not applicable in this context due to intermediate imaging

[3]calculated from telescope F-number and entrance area as given by Dobber et al. 2006

[4]For 60% of the pixels (centre 1600 km of swath) the necessary extension of f_T is < 2.

Property \ Instrument	TROPOMI-Type[1]	Scaled 1	Scaled 2
Nominal ground pixel dimensions at nadir, km^2	7 x 3.5	7 x 4.3	1 x 1
Instantaneous ground pixel dimensions at nadir, (area), km^2	1.7 x 3.5 (11.9)	1.6 x 4.3 (6.9)	0.5 x 1 (0.5)
Ground pixel dimensions at edge of swath km^2	7 x 12.7	7 x 4.3	1 x 1
Spectrograph focal length, mm	≈ 200	20	20
Spectrograph F-Number	≈ 9.5	4	4
Entrance slit w x h, mm x mm	NA[2]	0.029 x 0.46	0.029 x 0.46
Number of spectrographs + telescopes per instrument	1	200	2600
Ground pixels per spectrograph	576	6	8
No. of spectrographs observing the same ground pixel	1	2	8
Total number of ground pixels	576	600	2600
Total étendue, (mm^2sr)	E_0 (≈0.103)	≈1.27 E_0(0.131)	≈16.5·E_0 (≈1.7)
Étendue per pixel, mm^2sr	0.000179[3]	0.00011	0.0006548
Telescope focal length f_T at nadir, (f_T at edge of scan), mm	NA[2]	14.3 (52[4])	46.1 mm (167.7[4])
Telescope diameter, (dia. at the edge of scan), mm	NA[2]	3.6 (13)	11.52 (42)
Exposure time τ_{exp}, s	1	1	0.14
Signal per pixel (signal/noise, SNR) relative to TROPOMI	1 (1)	1.3 (1.1)	0.51 (0.72)
Approximate total volume, litres	100	ca. 1.4	50-100
Approximate total mass	M_0 (≈100 kg)	M_0/100	M_0

From the TROPOMI Spectrograph to the "Ideal Spectrograph"

TROPOMI: f≈200mm, F≈10, N_{SP}=1, E_{rel}=1, M_{rel}=1

Ideal Spectrograph 1: f=20mm, F=10, N_{SP}=2600, E_{rel}=26

→ Volume scaling factor $\Gamma_V \approx 1000$

→ M_{rel}=2.6

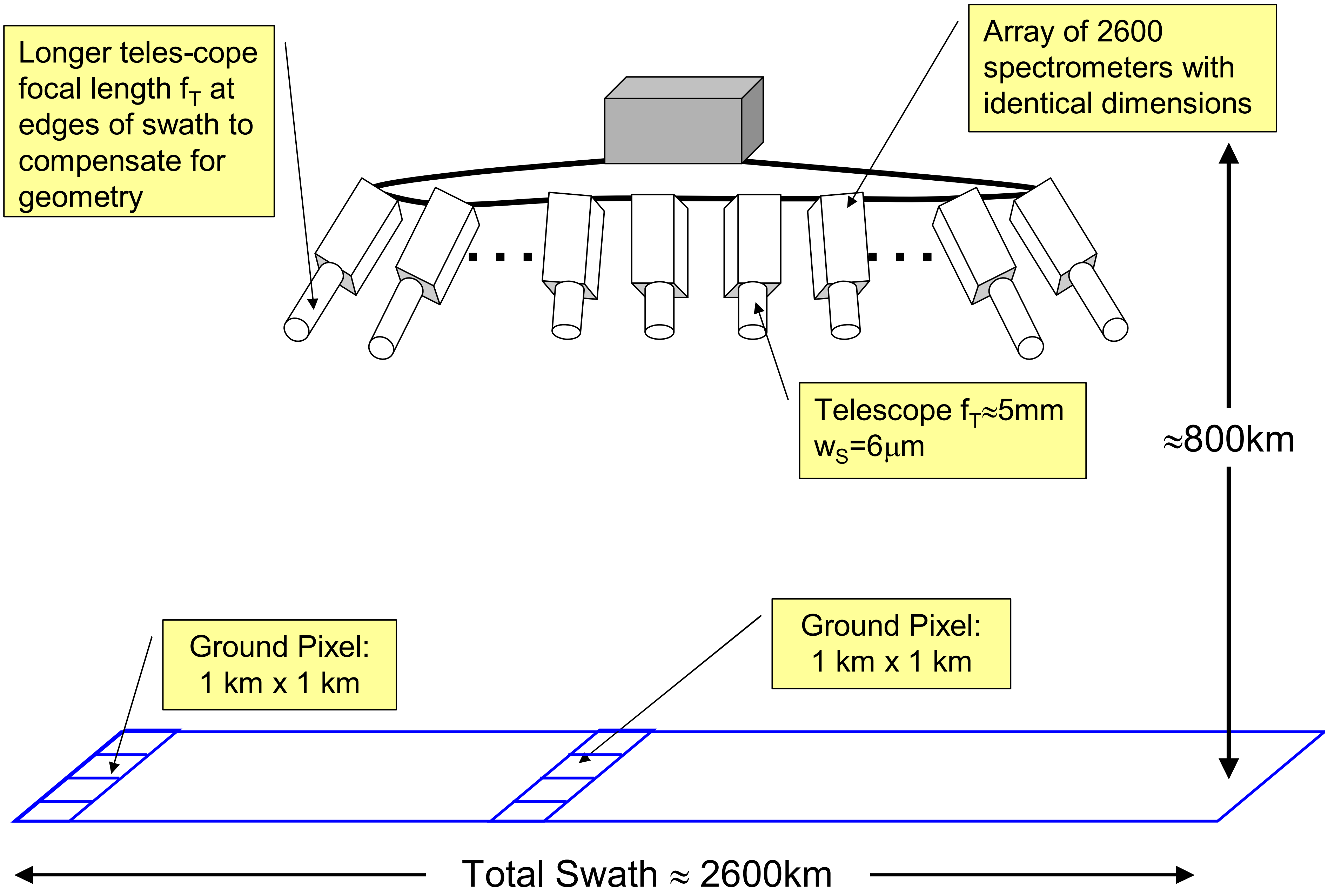
More than enough to compensate for shorter exposure time

→ At only 2.6-times more mass the resolution could be improved from 3.5x7km^2 to 1x1km^2 with somewhat better SNR

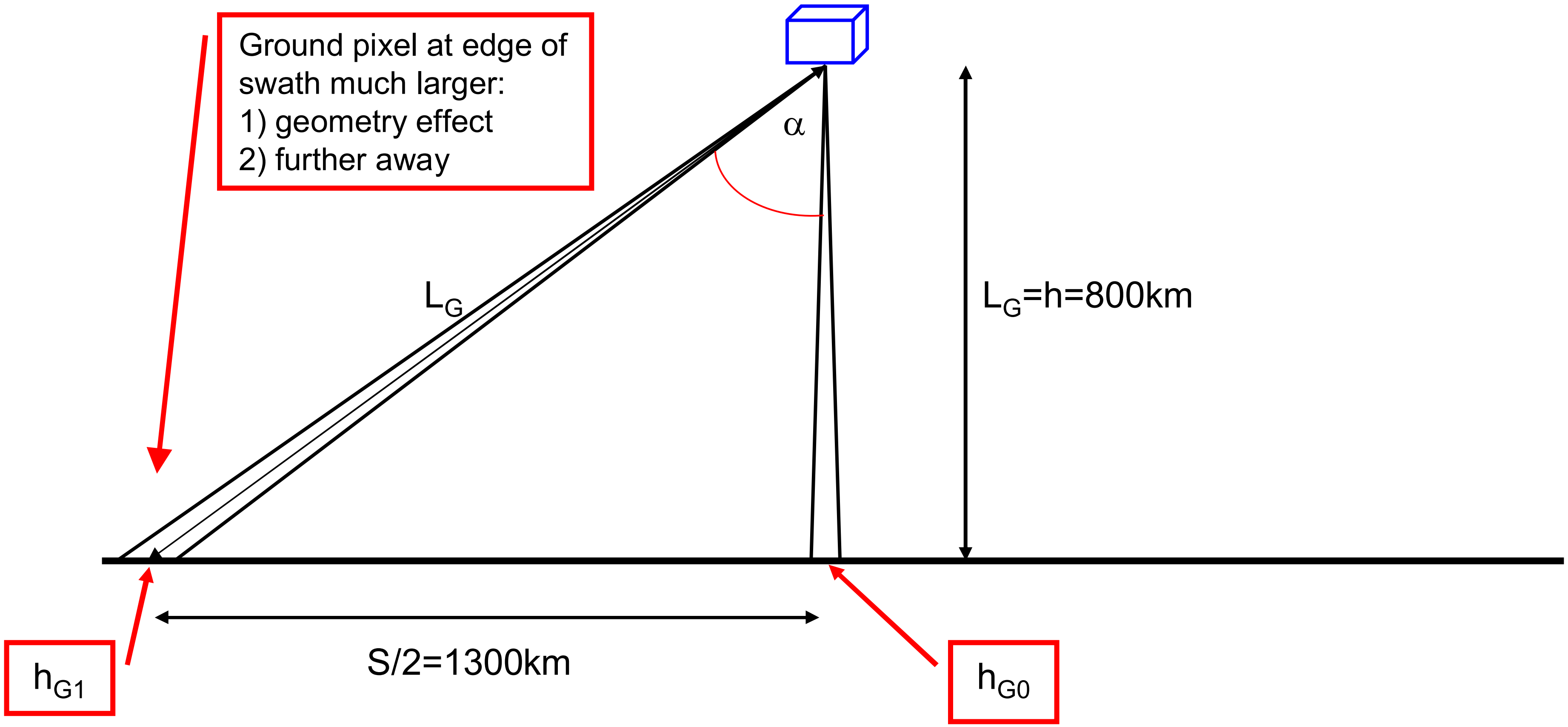
Further advantages:

- Simpler optics design,
- Option to enhance to F=4
- Nearly uniform ground pixel size

An „Ideal“ Satellite Spectrograph



Ground Pixel Size

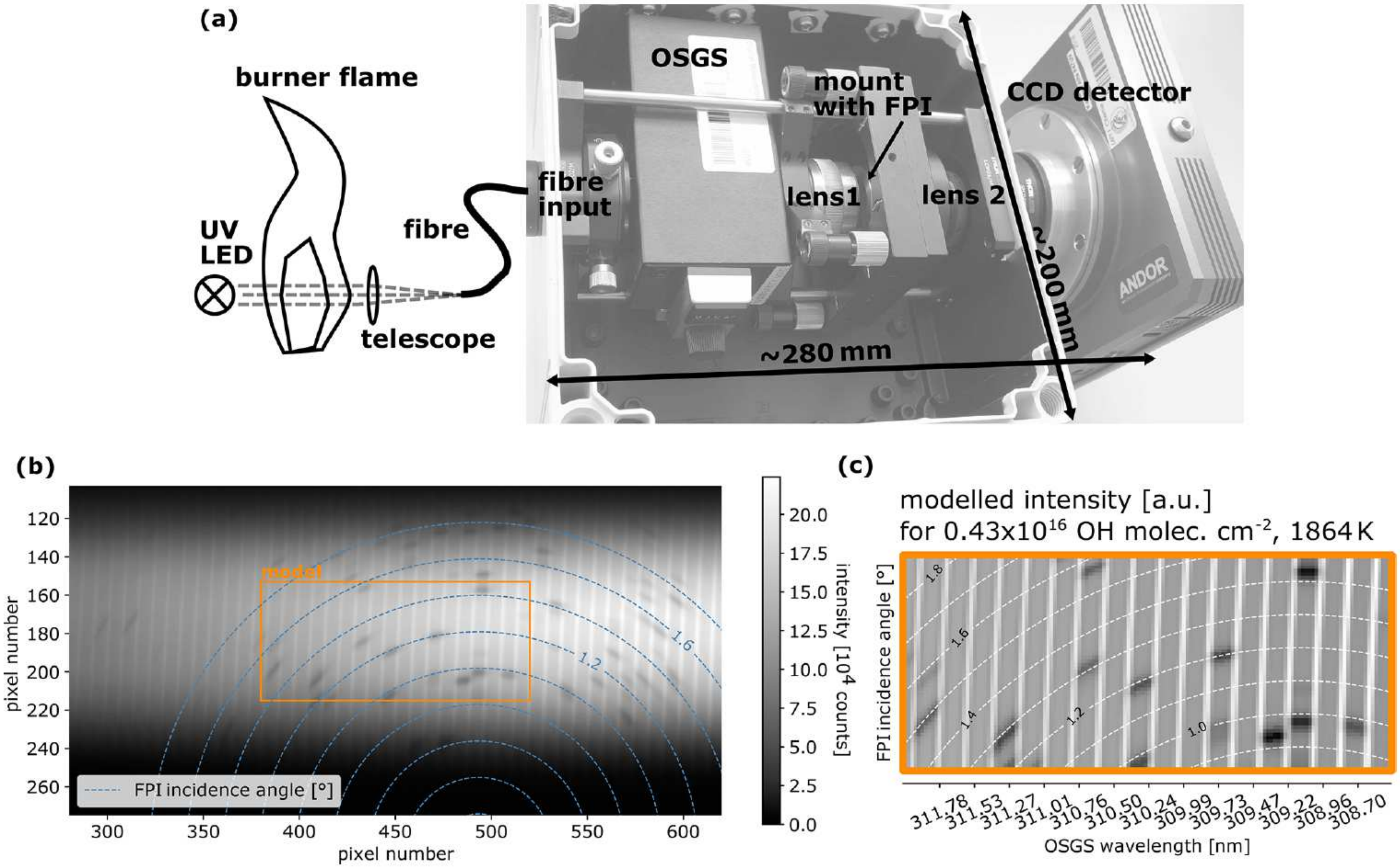


$$L_G = \sqrt{\frac{S^2}{4} + h^2} \approx 1526 \text{ km} \approx 1.91 \cdot h$$

$$h_{G1} = \frac{1.91 \cdot h_{G0}}{\cos\alpha} \approx 3.28 \cdot h_{G0}$$

$$\alpha = \arctan\left(\frac{S}{2h}\right) \approx 54.4^\circ$$

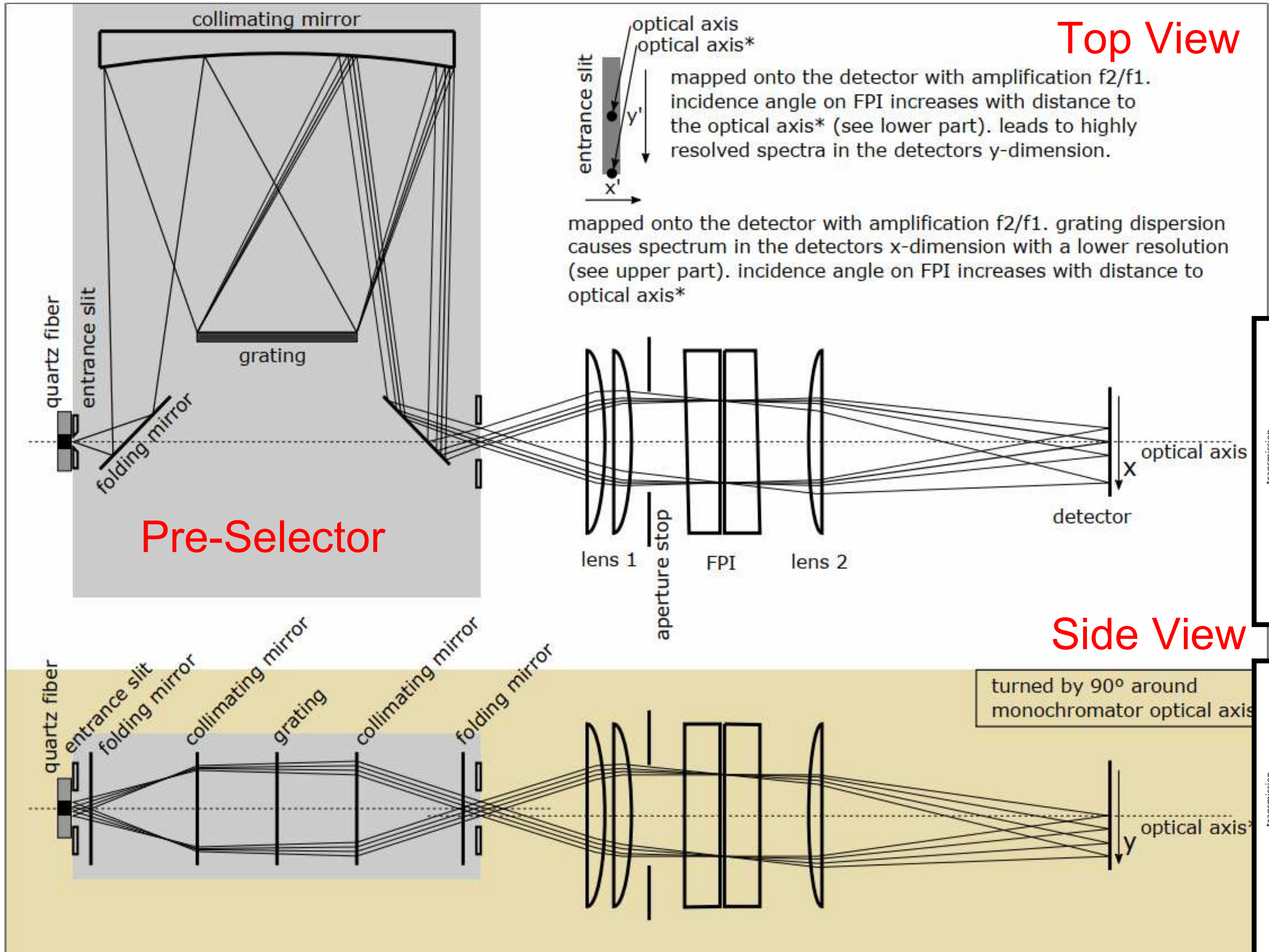
Fabry Pérot Interferometer Spectrograph - Prototype

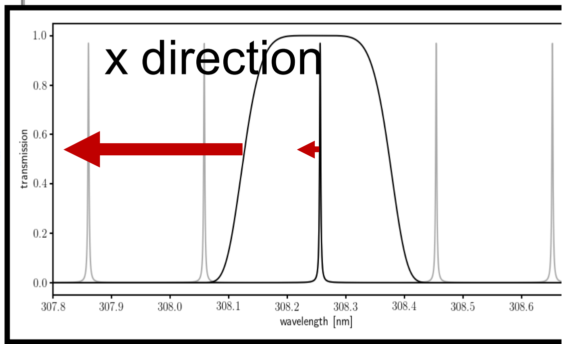


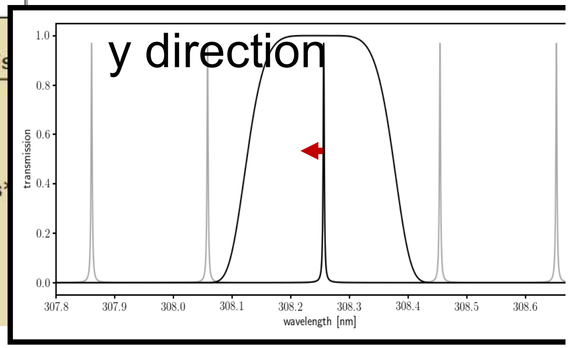
From: Kuhn J., Bobrowski N., Wagner T., and Platt U. (2021), Mobile and high spectral resolution Faby-Perot interferometer spectrograph for atmospheric remote sensing, AMT 14, 7873–7892.

Our high Res. Fabry Pérot Interferometer Spectrograph

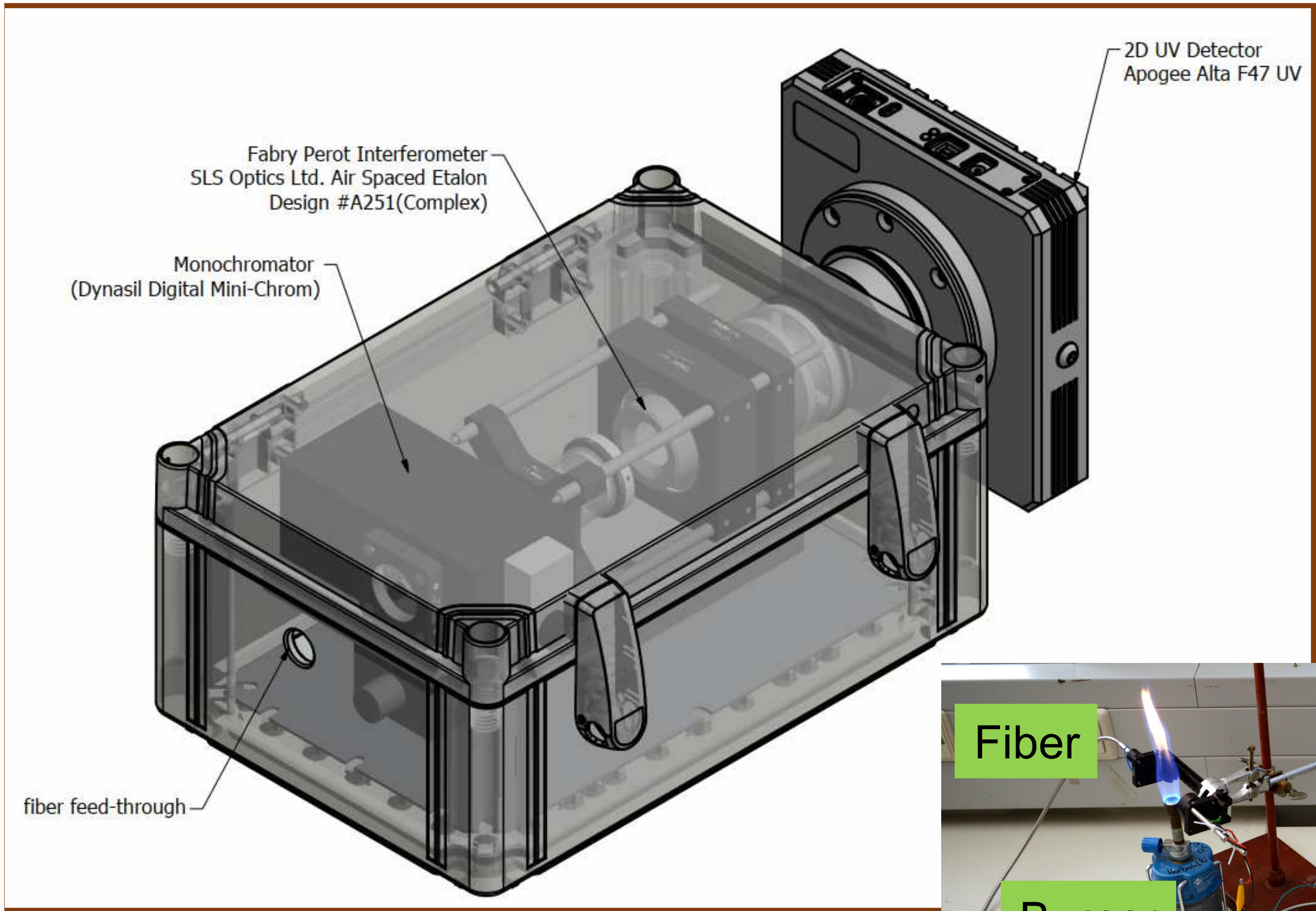
Combination of grating spectrometer (~0.3 nm resolution) and high finesse FPI (~2 pm resolution) to an ‚Echelle‘-type spectrograph



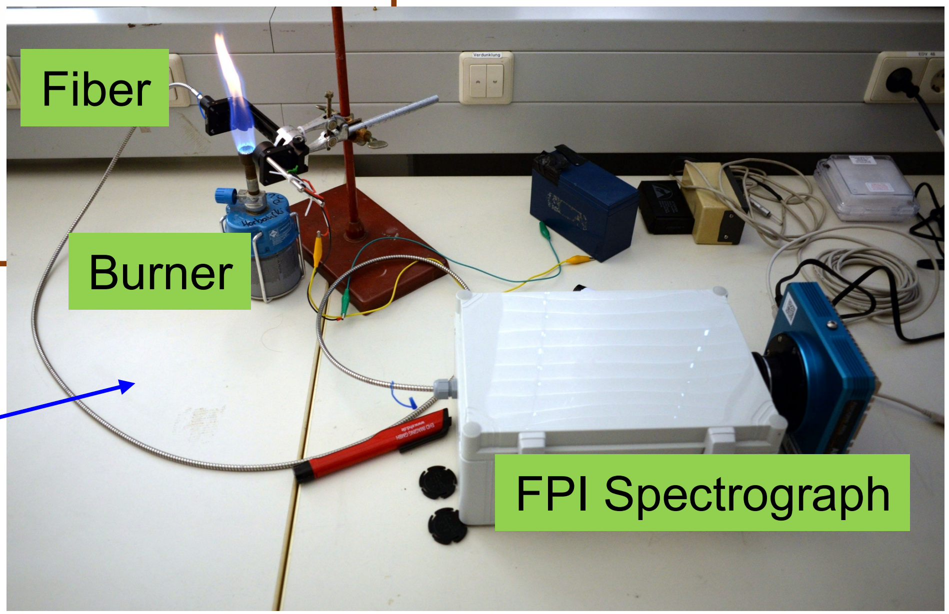




Fabry Pérot Interferometer Spectrograph - Prototype

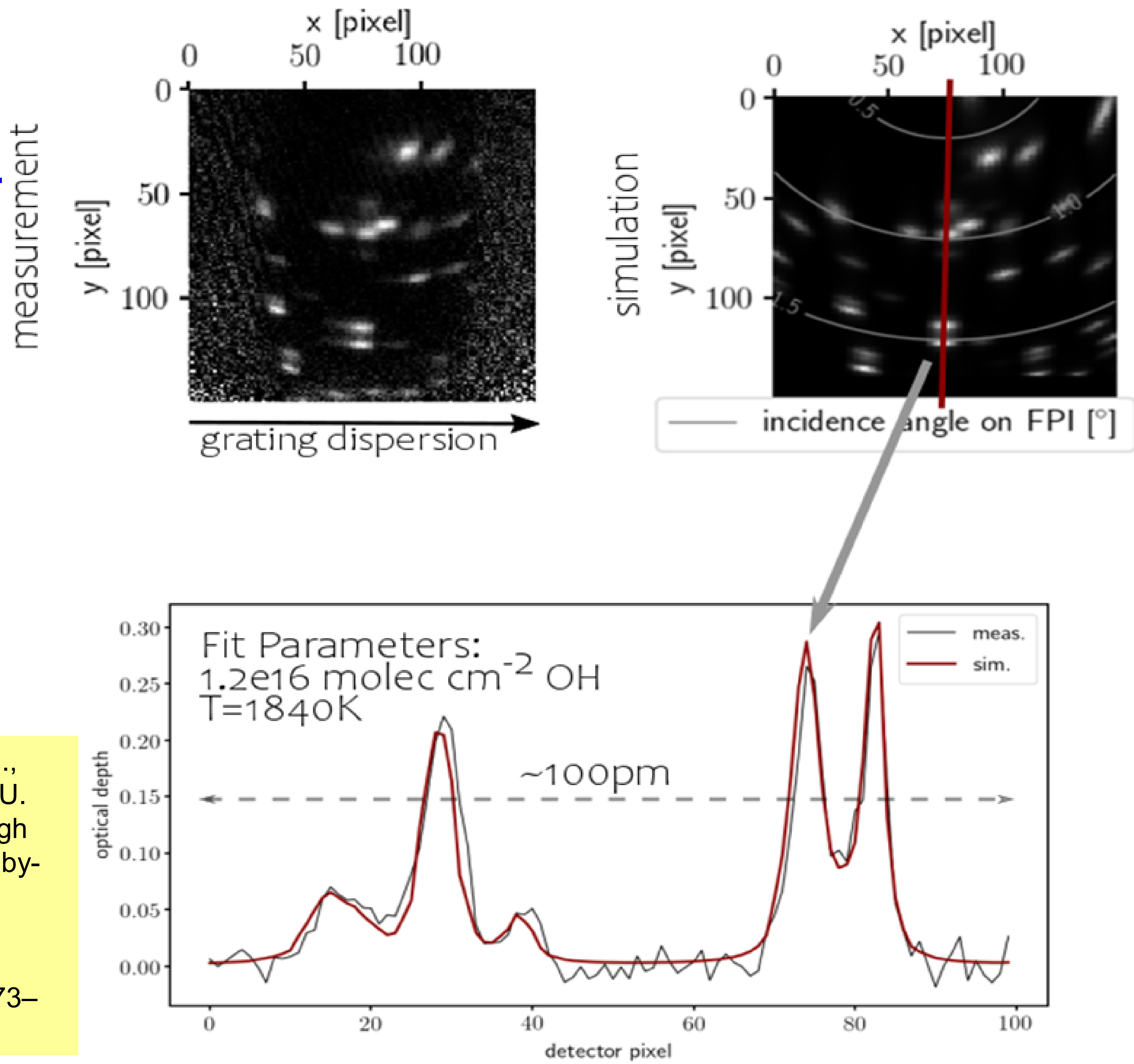


- Shoebox size
- Can be connected to a telescope
- 2pm spectral resolution



Laboratory setup to record OH-spectrum in a flame

FPI Validation with Flame-OH



Kuhn J., Bobrowski N., Wagner T., and Platt U. (2021), Mobile and high spectral resolution Faby-Perot interferometer spectrograph for atmospheric remote sensing, AMT 14, 7873–7892.

Low Res. Fabry Pérot Interferometer Spectrograph

Free Spectral Range:

$$\Delta\lambda \approx \frac{\lambda^2}{2n \cdot d\cos(\alpha)} \Leftrightarrow d \approx \frac{\lambda^2}{2n \cdot \Delta\lambda\cos(\alpha)}$$

$\text{Example}: \Delta\lambda = 50\text{nm},\ \lambda = 300\text{nm}$

$d \approx 0.9\mu\text{m}$

Finesse:

$$F = \frac{\Delta\lambda}{\delta\lambda} \approx \frac{\pi\sqrt{R}}{1-R} \Leftrightarrow d \approx \frac{\lambda^2}{2n \cdot \Delta\lambda\cos(\alpha)}$$

$\text{Example}: \delta\lambda = 0.5\text{nm},$

$\Rightarrow F = 100 \Rightarrow R = 0.97$

FPI Aperture angle about 20° → Ω comparable to F=4

→ $\Omega_{\text{Spectrograph}} \approx \Omega_{\text{Fabry-Pérot}} \approx 0.04\text{Sr}\cdot\text{mm}^2$

However:

$A_{\text{Spectrograph}} \approx 0.04\text{mm}^2$ $\quad$ $A_{\text{Fabry-Pérot}} \approx 60\text{mm}^2$

$E_{\text{Fabry-Pérot}} \approx 10^4 \cdot E_{\text{Spectrograph}}$

Possibilities 2a and 2b are really the same …

The change of the spectrometer with initial étendue E_0, initial focal length f_0 and optics diameter D_0 to Γ_1 f_0 with constant optics diameter D_0, can be thought of as a two step process:

1) Scale the entire spectrometer with preserved aspect ratio (according to case 1 in Table 1) by a linear factor Γ_1 (for example Γ_1=1/2)
→ E will be reduced to $(\Gamma_1)^2$ (i.e. to ¼ E_0) while the mass will change from M_0 to $M_0 \cdot (\Gamma_1)^3$ (i.e. to $M_0/8$). Note that the slit dimensions are also scaled by Γ_1.

2) Then increase D by factor $1/\Gamma_1$ (according to case 2a in Table 1)
→ in this step E and mass will increase by factor $1/(\Gamma_1)^2$

In total E would be unchanged, mass will be scaled to $M_0 \cdot \Gamma_1$ (i.e. to $4 \cdot M_0/8 = M_0/2$).

Since we assumed that in case 2b (see Table 1) the slit width is scaled, but not the slit height we have to change the slit height from $\Gamma_1 \cdot h_0$ to ist original value h_0.

→ The final E will be E_0/Γ_1, (i.e. $E = 2E_0$) thus $E \propto 1/M$ as given in equation 9

The “Ideal Spectrograph” for Atmospheric Observations

Ulrich Platt[1,2], Thomas Wagner[2], Jonas Kuhn[1,2], and Thomas Leisner[3]
[1]Heidelberg University, Institute of Environmental Physics, [2]Max Planck Institute for Chemistry, Mainz,
[3]Karlsruhe Institute for Technology (KIT), Karlsruhe

Central problem of spectroscopy (DOAS-type) systems: Shot noise limit!

$S/N \propto \sqrt{S}$ → How to collect more light (higher S)?

Bigger Spectrometer is a poor solution, since Size (and Mass) $\propto S^{3/2}$

The ideal spectrograph system:

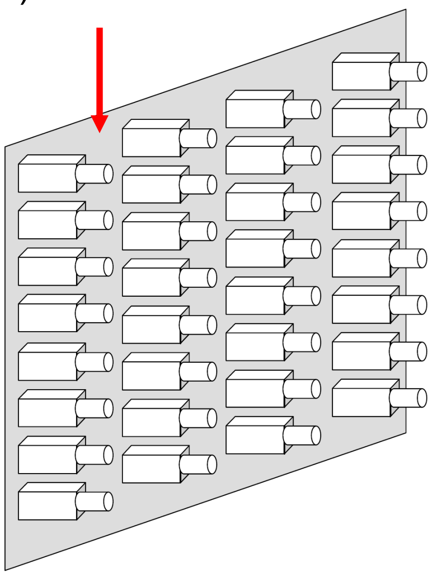
Step 1: Shrink spectrograph as much as possible: gain, since Size $\propto S^{3/2}$
(e.g. 1/10 reduces Size (and mass) to 1/1000, light throughput to 1/100)
→ 10-times more signal per mass

Step 2: Use an array of many spectrographs in parallel: Size $\propto S$

See Platt et al. 2021, AMTD, https://doi.org/10.5194/amt-2020-521

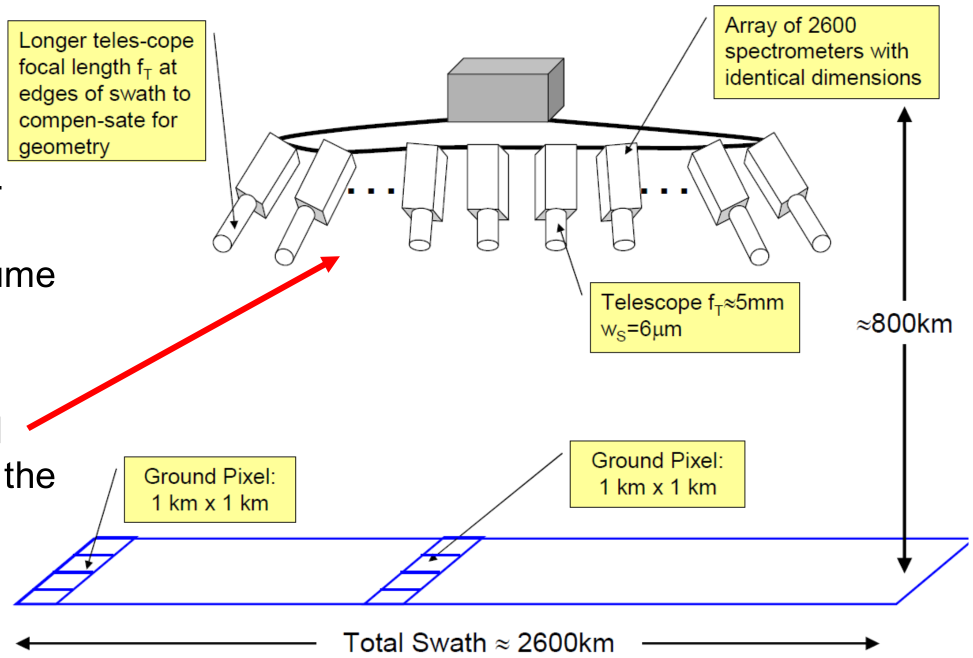
Array of miniature spectrographs:

1) Shrink MAX-DOAS to 1/100 of volume



2) Shrink TROPOMI-Type instrument to 1/100 of mass & volume maintaining light throughput

3) Build 1km² ground pixel instrument with the same mass as TROPOMI



The “Ideal Spectrograph” for Atmospheric Observations

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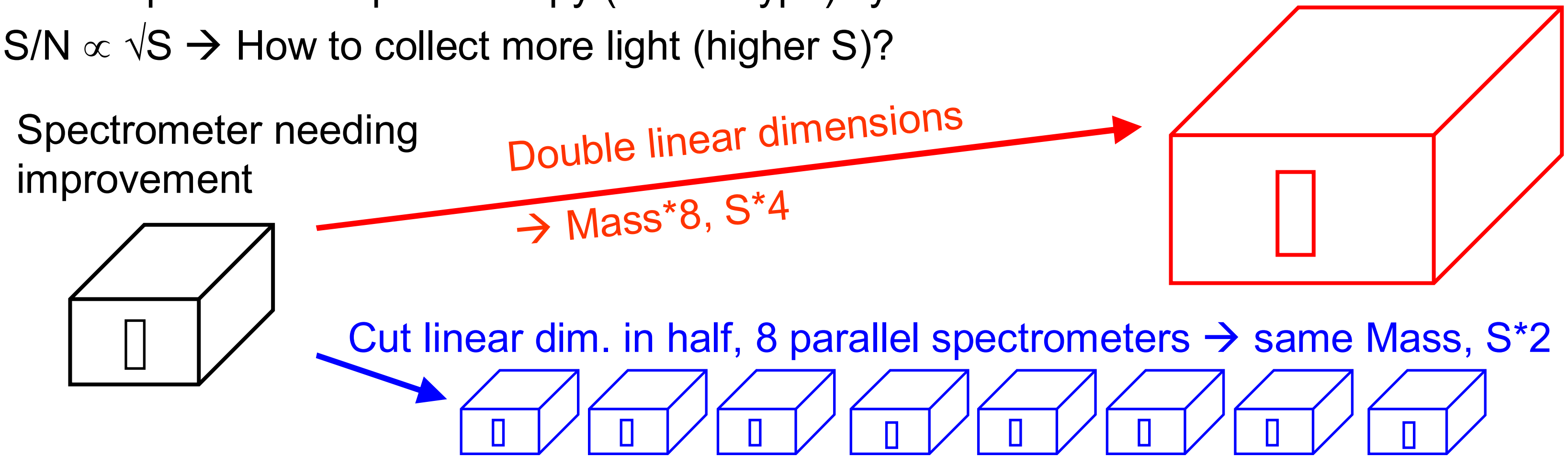

Array of miniature spectrographs:

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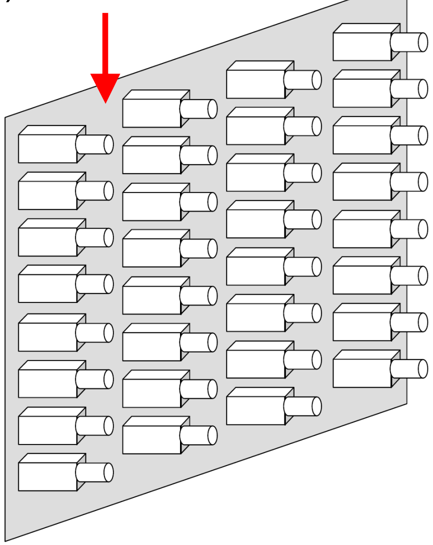

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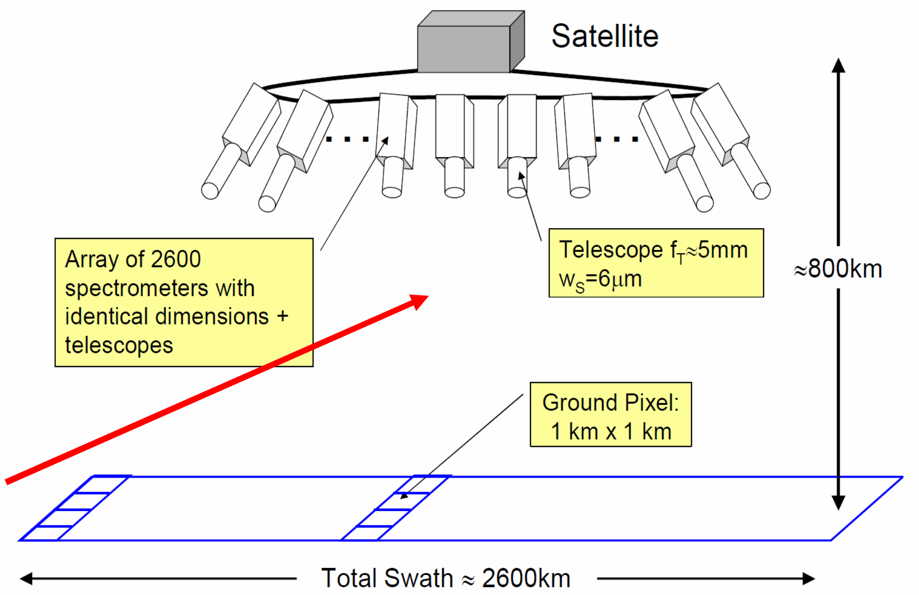
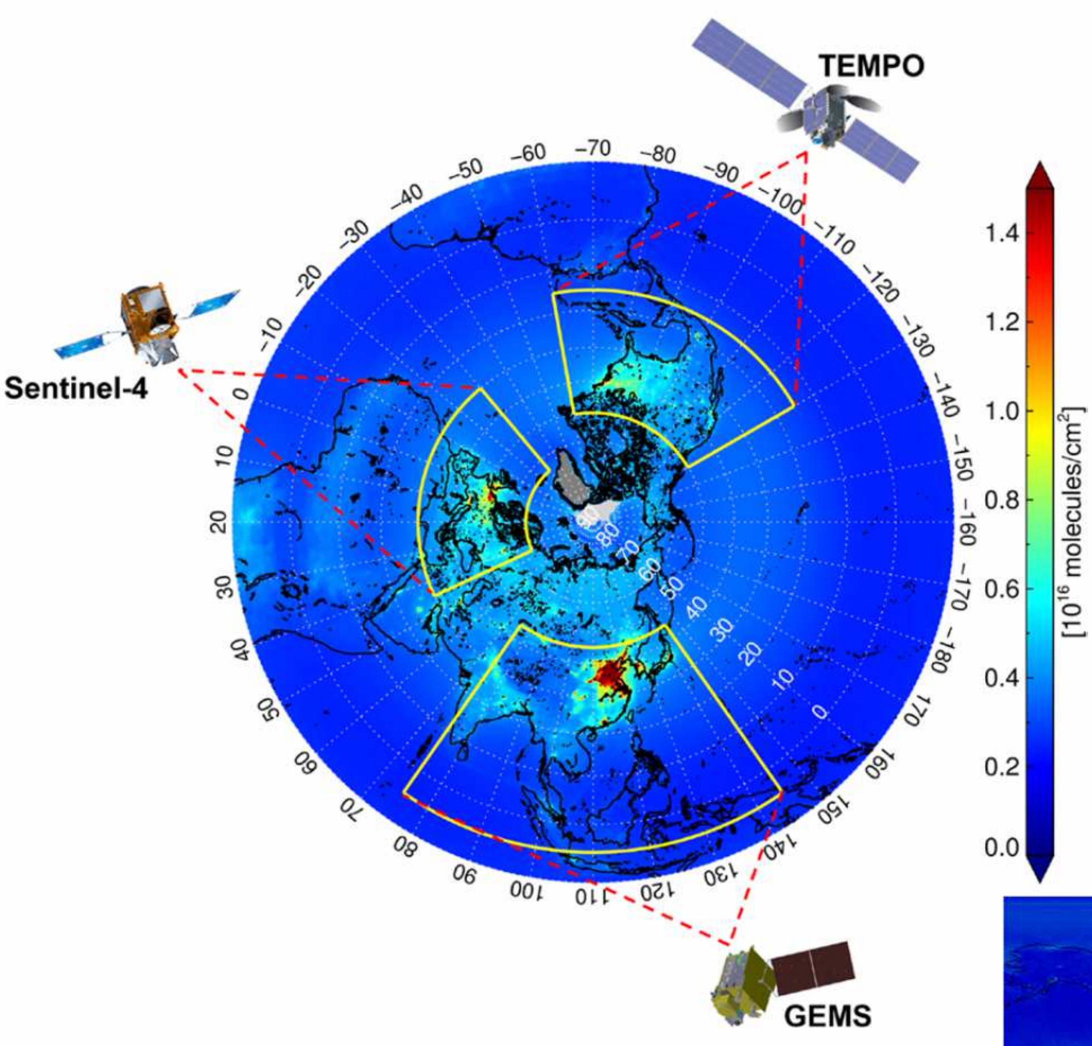
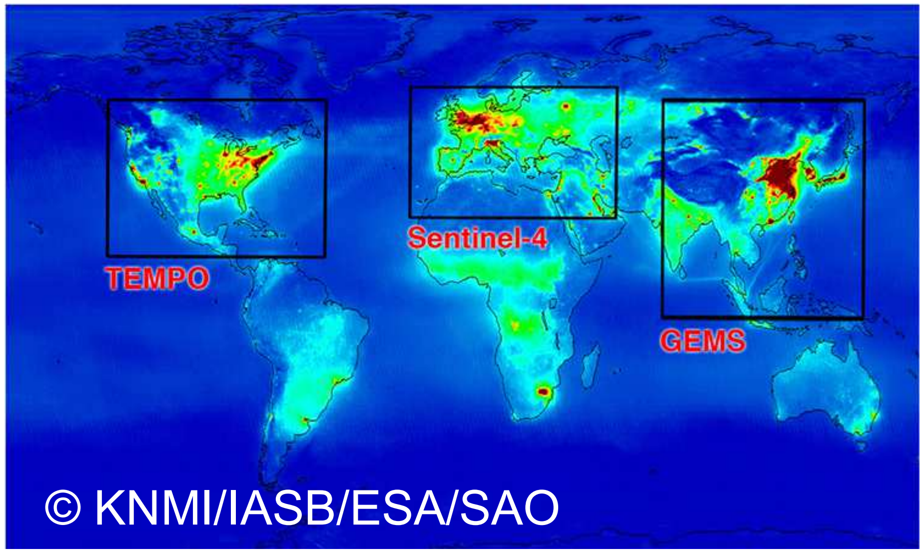


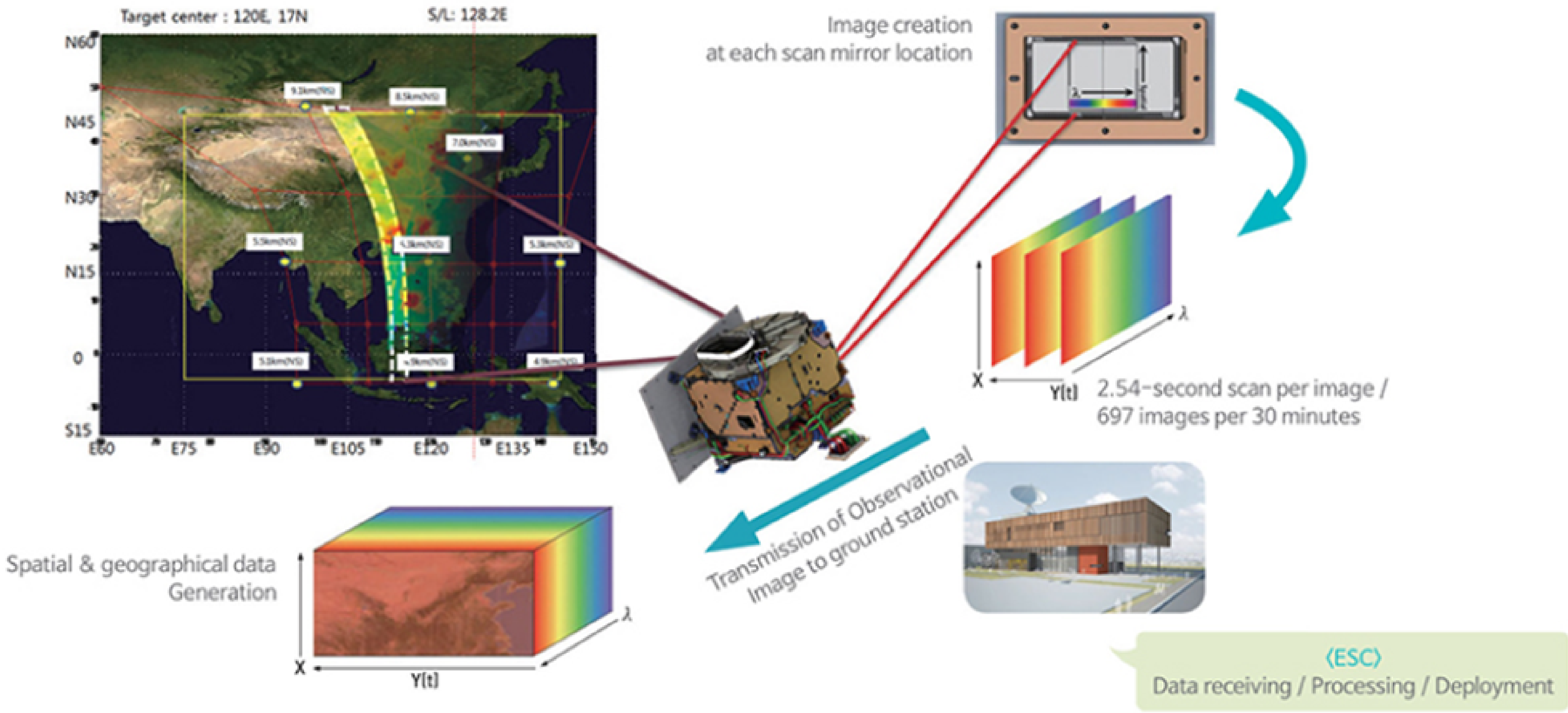
The Geostationary Air Quality Constellation (GEMS, TEMPO, Sentinel-4)



From: Kim et al. (2020) New Era of Air Quality Monitoring from Space, BAMS, https://doi.org/10.1175/BAMS-D-18-0013.1



The Geostationary Environment Monitoring Spectrometer (GEMS)

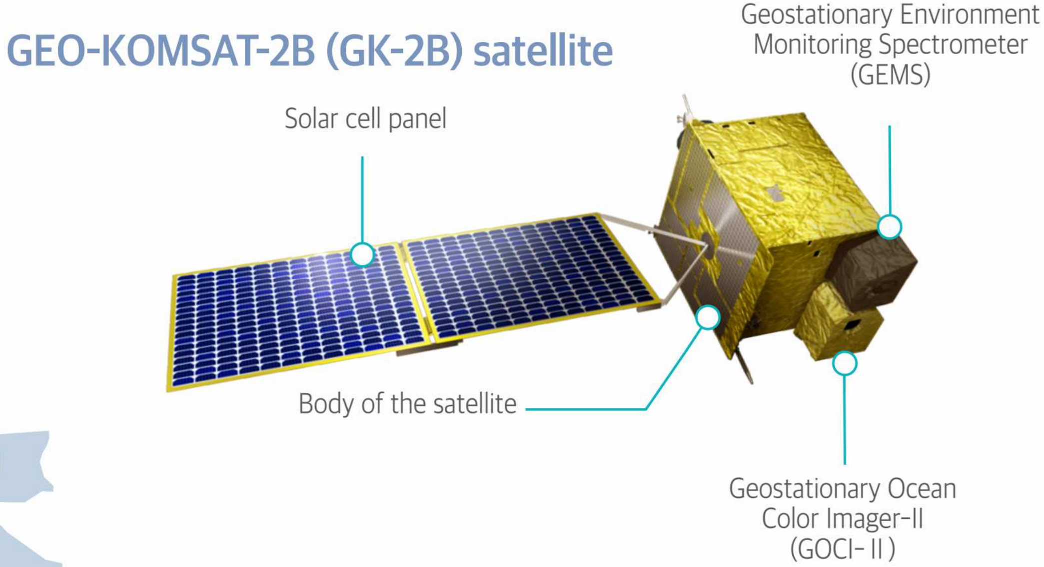


GEMS was launched in February 2020 onboard the GEO-COMPSAT-2B satellite

The UV-Visible hyper spectrometer measures atmospheric composition and climate forcers including sulfur dioxide (SO_2), nitrogen dioxide (NO_2), ozone (O_3) formaldehyde (HCHO), and aerosols

The Geostationary Environment Monitoring Spectrometer (GEMS)

Parameter	Value
Spacecraft	GEO-KOMPSAT-2B
Orbit	Geostationary
Lifetime	> 10 years
Spectral range	300–500 nm
Spectral resolution	0.6 nm
Spectral sampling	0.2 nm
Temporal resolution	1 h
Spatial resolution	$7 \times 8\,km^2$ (gases) at Seoul $3.5 \times 8\,km^2$ (aerosol) at Seoul
Field of regard	$> 5000 \times 5000\,km^2$ (N/S × E/W) N/S range: 5° S–45° N E/W range: 75–145° E
Requirement of polarization factor	< 2 % (310–500 nm) (No inflection point within 20 nm range)



From GEMS Brochure:

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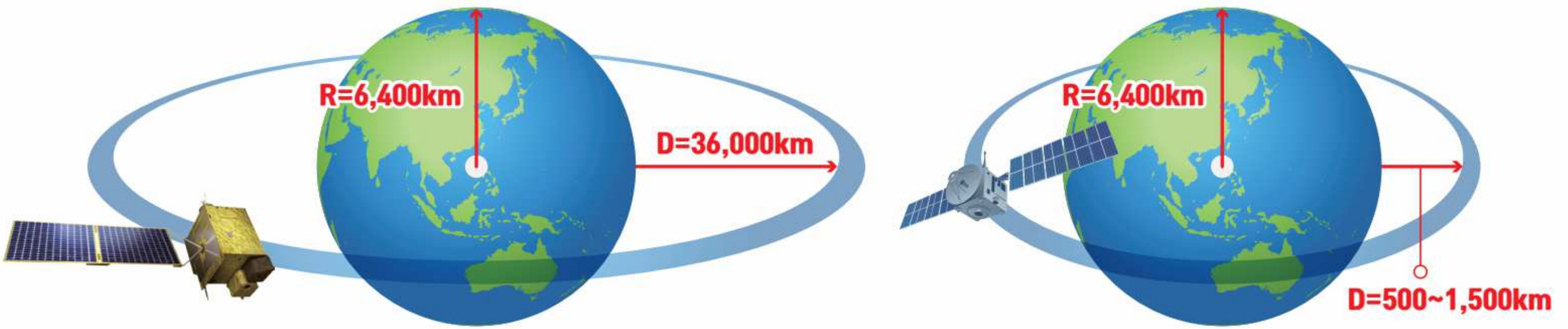
Geostationary (GEO) vs. Low Earth Orbit (LEO)



GK-2B (GEO satellite)	LEO satellite
· Monitoring Asia on average 8 times a day	· Monitoring the Korean Peninsula every 1 to 3 days
· Monitoring air pollutants and climate change causing pollutants	· Monitoring environment in over 10 countries (the U.S and Europe, etc.)

A GEO satellite is placed at an altitude of approximately 36,000km above earth and revolves in the same length of time as the earth requires to rotate, so it appears nearly stationary in the sky as seen by a ground-based observer. GEO satellites consistently monitor targeted areas in daylight.

A LEO satellite is much closer to the earth than GEO-typed one. It takes only 90 to 100 minutes to revolve the earth, which makes LEO-typed satellites suitable to be used for exploring the earth, mobile communication, and meteorological observation.

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Monitoring mode	Half East (HE)	Half Korea (HK)	Full Central (FC)	Full West (FW)
FOR				
Monitoring range	Korean Peninsula, Japan, etc.	Korean Peninsula, Japan, East China, etc.	Korean Peninsula, Japan, China, Southeast Asia, etc.	Korean Peninsula, China, Southeast Asia, some parts of India, etc.
Monitoring hours (UTC)	23~1	0~2	1~3	3~8

Monitoring No.	1	2	3	4	5	6	7	8	9	10	Daily observation times
UTC	23:00	0:00	1:00	2:00	3:00	4:00	5:00	6:00	7:00	8:00	
KST	8:00	9:00	10:00	11:00	12:00	13:00	14:00	15:00	16:00	17:00	
Jan			HE	HK	FC	FW	FW	FW			6
Feb			HE	HK	FC	FW	FW	FW	FW		7
Mar		HE	HK	FC	FC	FW	FW	FW	FW		8
Apr	HE	HK	FC	FC	FC	FW	FW	FW	FW	FW	10
May	HE	HK	FC	FC	FW	FW	FW	FW	FW	FW	10
Jun	HE	HK	FC	FC	FW	FW	FW	FW	FW	FW	10
Jul	HE	HK	FC	FC	FW	FW	FW	FW	FW	FW	10
Aug	HE	HK	FC	FC	FW	FW	FW	FW	FW	FW	10
Sep	HE	HK	FC	FC	FW	FW	FW	FW	FW	FW	10
Oct		HE	HK	FC	FC	FW	FW	FW	FW		8
Nov			HE	HK	FC	FW	FW	FW			6
Dec			HE	HK	FC	FW	FW	FW			5

= No observation

Ex.) In case of 23:00 UTC, the actual monitoring time is UTC 22:45~23:15.

*UTC (Coordinated Universal Time): The standard (KST-9) of the scientific time used in the international community

*KST (Korea Standard Time): 9 hours (UTC+9) ahead of the UTC

From GEMS Brochure: Publication Registration No. 11-1480523-004814-14, NIER-GP2022-059

From: Kim et al. (2020) New Era of Air Quality Monitoring from Space, BAMS, https://doi.org/10.1175/BAMS-D-18-0013.1

GEMS Optomechanical subsystem

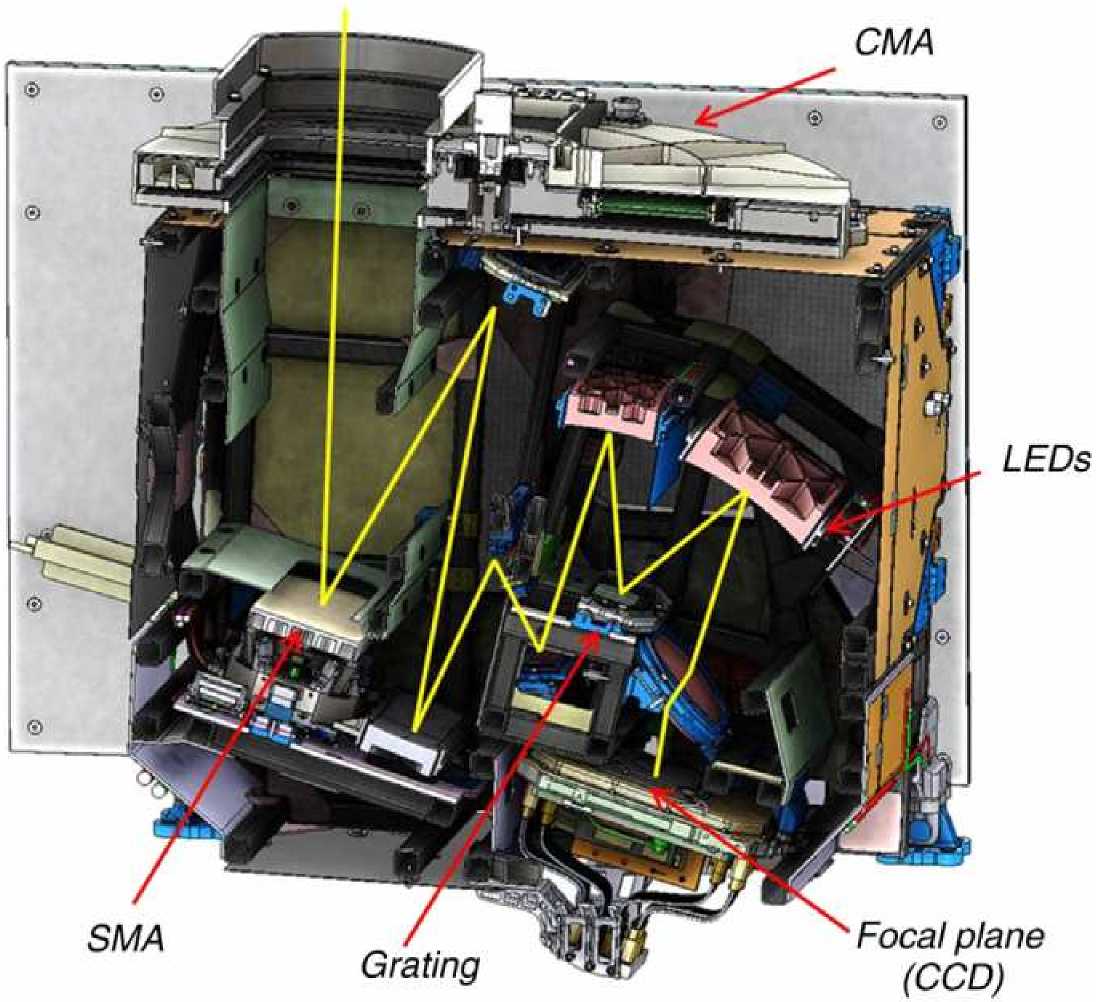
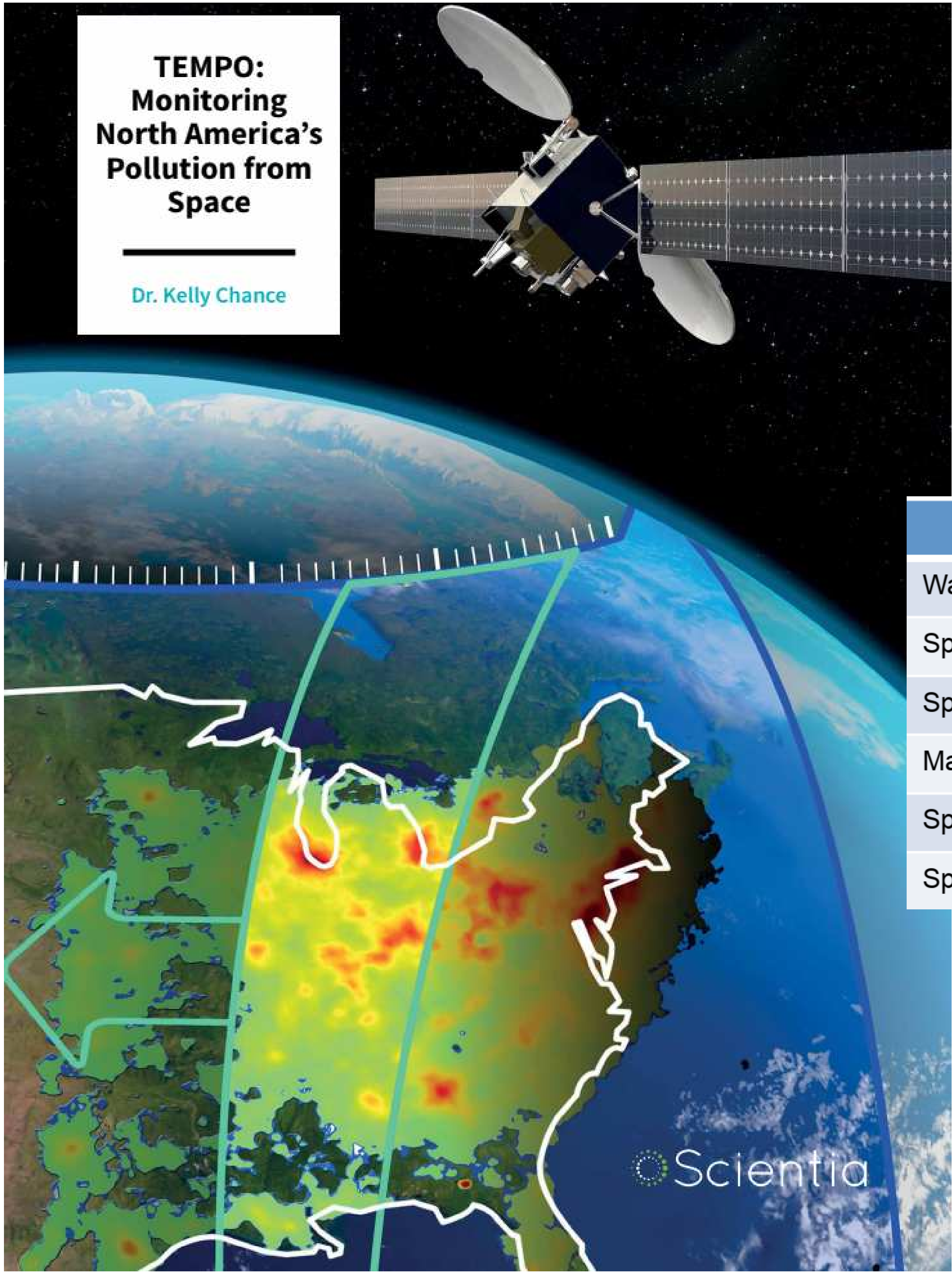


Fig. 4 Optomechanical subsystem of the GEMS.

From: Won Jun Choi, Kyung-Jung Moon, Jongmin Yoon, Ara Cho, Sang-kyun Kim, Seounghoon Lee, Dai ho Ko, Jhoon Kim, Myung Hwan Ahn, Deok-Rae Kim, Sang-Min Kim, Ji-Young Kim, Dennis Nicks, Jeong-Su Kim, “Introducing the geostationary environment monitoring spectrometer,” J. Appl. Remote Sens. 12(4), 044005 (2019), doi: 10.1117/1.JRS.12.044005.



Tropospheric Emissions: Monitoring of Pollution (TEMPO)

TEMPO instrument characteristics	
Wavelength range	290-490 + 540-740 nm
Spectral resolution	0.6 nm FWHM
Spectral sampling	0.2 nm
Maximum S/N	2700 @ 330-340 nm, EOL
Spatial resolution	2.1×4.5 km^2 @ 36.5N, 100W
Spectra per hour	2000 N/S × 1250 E/W

Sentinel-4

Instrumental Payload: SENTINEL-4 Instrument

The MTG-S payload consists of the IRS instrument and of the SENTINEL-4 instrument.

Airbus Defense and Space is the European Space Agency's (ESA) prime contractor for the development and construction of SENTINEL-4, a highly accurate instrument designed to monitor key atmosphere constituent. Airbus Defense and Space lead a team of around 40 subcontractors for the development and construction of SENTINEL-4.

The main characteristics of SENTINEL-4 instrument can be summarised as follows:

Instrument type: passive imaging spectrometer

Number of spectrometric bands: three Ultraviolet (305-400 nm), Visible (400-500 nm) and Near Infrared(750-775 nm) VIS and NIR bands implemented in two spectrometers UVVIS & NIR)

Number of spectrometric channels: 2 (UV-VIS channel; NIR channel)

Configuration: Push broom scanning (scan in the E/W direction).

Field Of View (FOV) E-W: 30°W-46.5°E @ 40°N, N-S: 30°N-65°N

Spatial resolution: 8x8 km2

Spectral resolution: 0.5 nm for the UV-VIS channel; 0.12 nm for the NIR channel

Radiometric accuracy (absolute): 3% (2% goal) of the measured sun irradiance, earth radiance and spectral reflecta

Overall mass: 200 Kg.

Dimensions : 1.1 x 1.4 x 1.6 m3

Design lifetime: 8.5 years

Power Demand: 180 W

Data volume, generated during observation: about 2.0 Terabits per day.

Revisit time: about 60 min.