Infrared remote sensing of atmospheres of Earth-like planets

Feasibility of Atmospheric Retrievals

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   - Jacobians for G- and M-Star planets
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What is this presentation about

Overview on what I've been working over the last seven weeks and which methods have been used to obtain information on following questions:

- what kind of *spectral signatures* can we expect from *potentially habitable terrestrial planets*, particular form *their atmospheres*
- what influence do changes in different atmospheric constituents (e.g. CO2, H2O, temperature) have on radiation transfer (RT) (*J-functions (jacobians)*)
- are the columns (atm. parameter e.g. CO2, H2O, temperature) of the *J-matrices statically related* to each other, and if in what manner
- what are the *singular values* $\sum$ of the J-functions and how do the *condition numbers* χ behave when omitting a column
- how does the *ILS* affect the values of $\sum_{[i]}$ and $\chi_{[i]}$

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Lbl-RT-calculations in the IR-region

To *simulate high resolution spectra* of earthlike exoplanet atmospheres, a fundamental knowledge of RT in atmospheres is required;
all known *interactions* between radiation and atmospheric constituents as well as effects caused by *pressure-* and *temperature-broadening* have to be taken under account;
so the main *input-parameters* which have to be defined for each calculation in each level* are

- Pressure*
- Temperature*
- Molecule-density*
- Molecule absorption-cross-sections[1]

[1] e.g. HITRAN 2004, GEISA 2003 - databases for lineparameters of 39 molec.

Lbl-RT-calculations in the IR-region

This is the *basic equation* on calculating the RT in the IR-region of the spectrum

$$I_\nu(s) = I_0 * e^{-\mu_\nu(s_0,s)} + \int_{s0}^{s} ds' B(\nu, T(s')) e^{-\mu_\nu(s',s)} k(\nu; s') n(s') \qquad (1)$$

where μ is defined as the absorption cross section

$$\mu_{i,s}(\nu) = \int_{s0}^{s} ds' k_i(\nu) n_i(s) \qquad (2)$$

Defining the Garlic input files

Output of eq.: 1 is among others dependent of the input atmospheric conditions and profiles;

so initially I used I established a *well defined vertical profile* of the following atmospheric constituents for the input-files

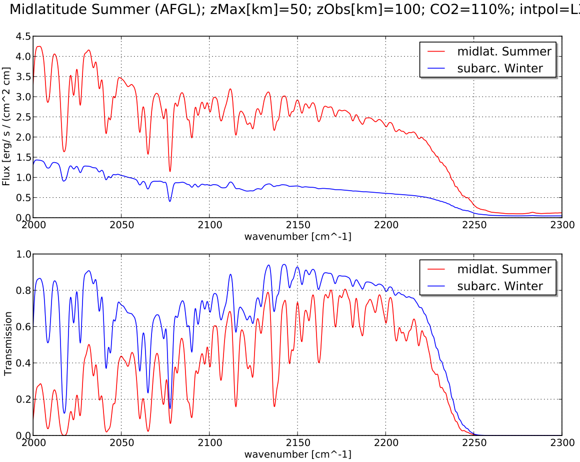
---

readout from standard atmospheric file

- CO2
- H2O
- O3
- Pressure
- temperature

Outputs of Garlic RT-calculations for [AFGL]

Magnitude of influence on radiation by different states of the *earth atmosphere* with standard atmospheric input [AFGL - atmospheric reference model] at wavenumbers from 2000 - 2300 [cm^{-1}];



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- calculated standard-atmospheres of exoplanets orbiting different stars;
- my calculations are based on the *G-Star* and *M-Star* due to their controversal lapse rates above $10^2[mb]$
- the points connected by the straight lines define the *coarse (NZ=3) vertical temperature profile* as given to the input-file

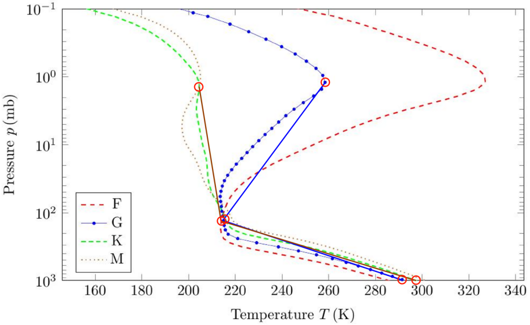


Abbildung: Temperature profiles of exoplanet atmospheres [3]

Garlic input-file with coarse temperature profile

for the analysis of the exoplanet-atmospheres I established a *well defined vertical profile* of the following atmospheric constituents, but a *coarse* vertical *temperature-profile*:

---

readout from standard atmospheric file

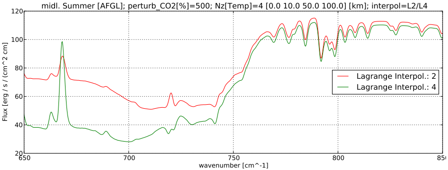
- CO2
- H2O
- O3
- Pressure

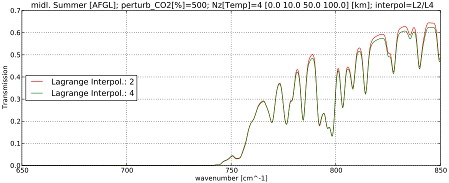
readout from coarse defined atmospheric file

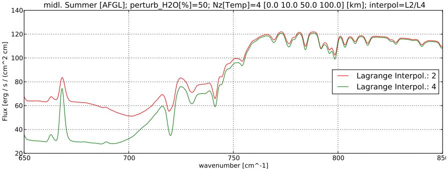
- Temperature $_{[Surface]}$
- Temperature $_{[Tropopause]}$
- Temperature $_{[Stratopause]}$

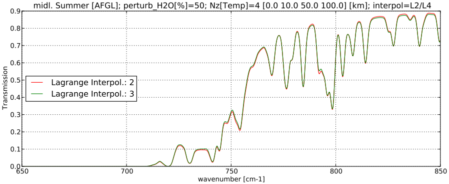
Outputs of Garlic for coarse temperature-profile

Differences in flux and transmission caused by the selected *interpolation method* for a *coarse vertical temperature profile*









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Determining the Jacobians

Definition

Partial derivative of all columns of the flux-matrix $\mathbf{y} = (\mathbf{n} \times \mathbf{x}_i)$, whereat $\mathbf{x}_i$ is the atm. parameter i and $\mathbf{n}$ the number of wavelength values on which the flux/transmission was determined:

$$J_j(x_i) = \frac{\partial y_j}{\partial x_i} \tag{3}$$

this was the analytical formula, so I used the numerical expression to calculate the Jacobian J_i for each derivative i

$$J_i(x) = \frac{y(x + \delta x_i) - y(x)}{\delta x_i} \tag{4}$$

at which δx_i is the **perturbation**.

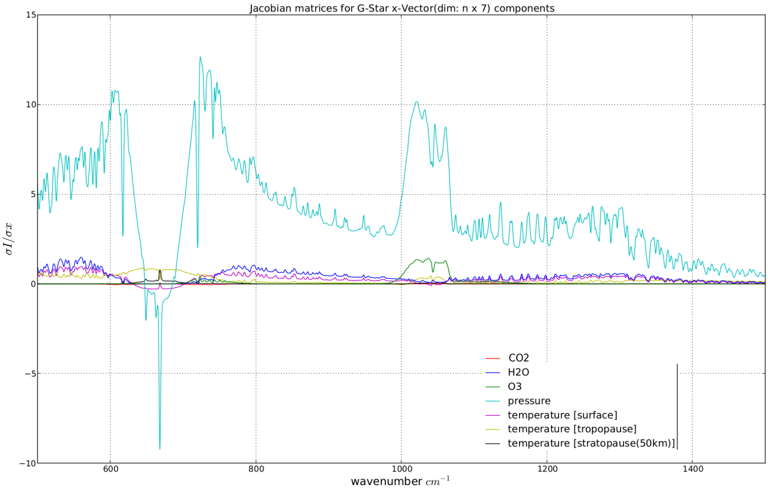
Chosen parameters for the Jacobians

The plot on the next slide will show the jacobians for a G- and M-Star and the following parameters of **x**:

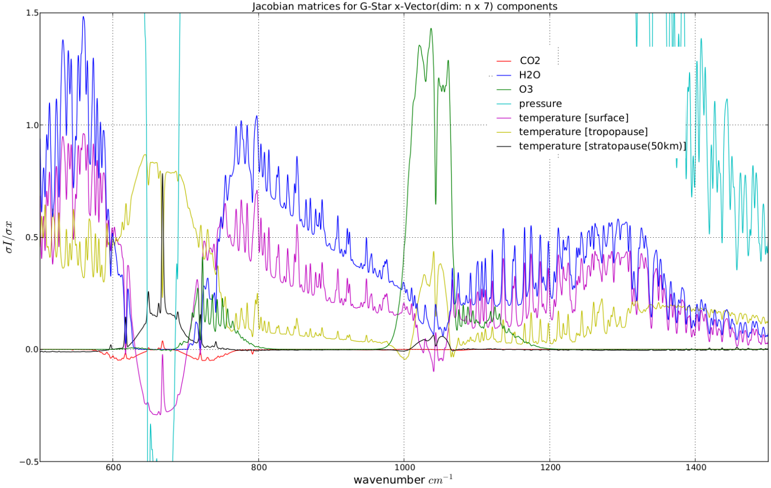
variable δx_i	addition	multiplication	remark
δCO2	$+10$	-	add 10 units to the initial values across the whole vertical CO2 profile (standard-profile) - i.e. creating an offset
δ H2O	-	1.1	multiply the initial profile values by a factor of 1.1 across the whole vertical H2O profile (standard-profile)
δ O3	-	1.1	same as for H2O (standard-profile)
δT[surface]	$+10$	-	add 10 units [K] to the initial value on the surface-level on the coarse profile
δT[tropopause]	$+10$	-	add 10 units [K] to the initial value at the tropopause level (ca. $10^2[hPa/mb]$ respectively 15 [km]) on the coarse profile
δT[stratopause]	$+10$	-	add 10 units [K] to the initial value at the tropopause level (ca. $10^1[hPa/mb]$ respectively 50 [km]) on the coarse profile
δpressure [p]	-	2.0	double the initial profile values across the whole vertical profile (standard-profile)

$$J(x) = \left(\frac{\sigma I(x)}{\sigma CO_2}; \quad \frac{\sigma I(x)}{\sigma H_2O}; \quad \frac{\sigma I(x)}{\sigma O_3}; \quad \frac{\sigma I(x)}{\sigma T_{[surf]}}; \quad \frac{\sigma I(x)}{\sigma T_{[tropop]}}; \quad \frac{\sigma I(x)}{\sigma T_{[stratop]}}; \quad \frac{\sigma I(x)}{\sigma p} \right)$$

Jacobians for G-Star-Planet atmosphere

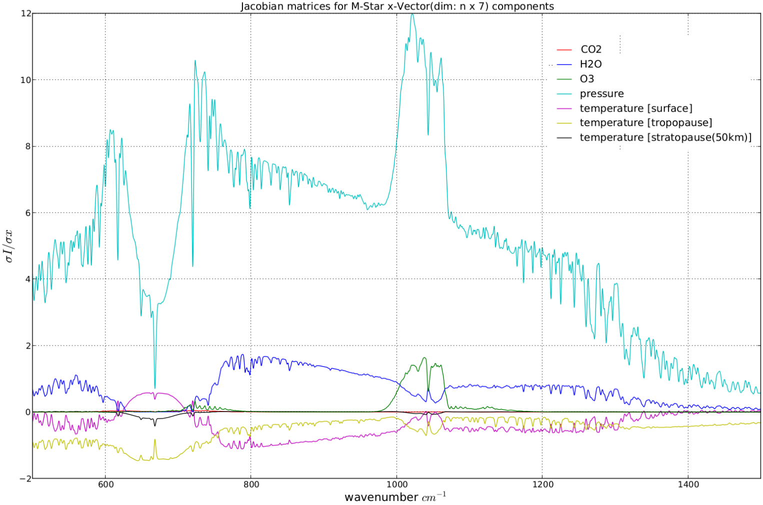


Jacobians for G-Star-Planet atmosphere

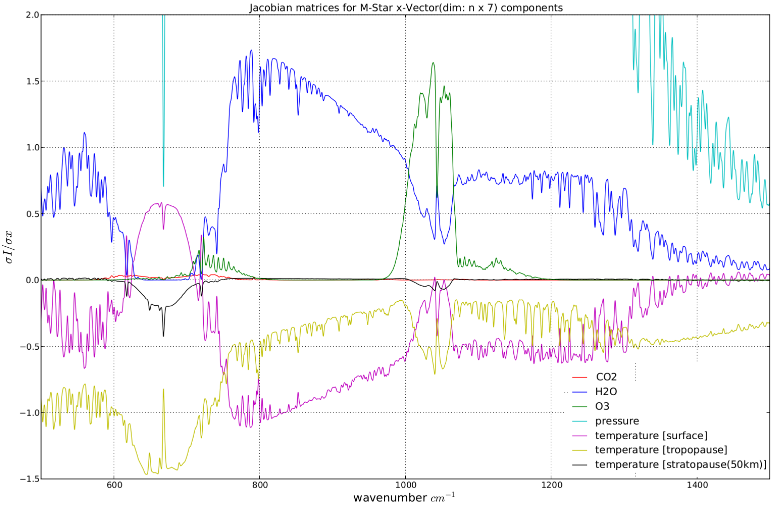


correl

Jacobians for M-Star-Planet atmosphere



Jacobians for M-Star-Planet atmosphere



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Covariance- and Correlationmatrices

The covarianz and correlation coefficient were used to describes the statistical properties of the calculated jacobianmatrices

Definition

The covarianz is defined as followed:

$$Cov_{[i,k]} = [J(x_i)^T J(x_k)]^{-1}$$

Covariance describes:

- how much two random variables change together (positive or negative)
- the signum indicates the linear realtionship between two variables

Definition

The correlation coefficient is defined as followed:

$$Corr_{[i,k]} = \frac{Cov_{[i,k]}}{\sqrt{Cov_{[i,i]} Cov_{[k,k]}}}$$

Correlation coefficient describes:

- positive or negative **linear** relationship between the two variables
- is defined between $-1 \leq Corr_{[i,k]} \leq 1$
- values of zero indicate no linear (but perhaps square) relationships

Correlationmatrix for G- and M-Star-Planet atmosphere

Correlationmatrix for atm. parameters of **G-Star-Planet**							
Relate	CO2	$T_{surface}$	$T_{tropopause}$	$T_{stratopause}$	H2O	O3	p
CO2	1.0000e+00	-1.54e-01	-4.32e-01	2.88e-02	1.04e-01	1.64e-02	-6.34e-01
$T_{surface}$	-	1.0000e+00	-1.46e-01	-5.06e-01	9.16e-01	-2.27e-01	5.58e-01
$T_{tropopause}$	-	-	1.0000e+00	5.39e-01	-1.33e-01	-1.43e-02	1.20e-01
$T_{stratopause}$	-	-	-	1.0000e+00	-3.96e-01	8.93e-02	-3.00e-01
H2O	-	-	-	-	1.0000e+00	-2.39e-01	4.06e-01
O3	-	-	-	-	-	1.0000e+00	4.41e-01
pressure	-	-	-	-	-	-	1.0000e+00

The table shows the correlation coefficient K for each combination of columns of the jacobian;

Correlationmatrix for atm. parameters of **M-Star-Planets**							
Relate	CO2	$T_{surface}$	$T_{tropopause}$	$T_{stratopause}$	H2O	O3	p
CO2	1.0000e+00	3.71e-01	-7.17e-01	-4.34e-01	-3.49e-01	-6.23e-02	3.14e-01
$T_{surface}$	-	1.0000e+00	-6.09e-01	-6.85e-01	-9.50e-01	8.01e-02	-4.58e-01
$T_{tropopause}$	-	-	1.0000e+00	6.55e-01	4.55e-01	5.48e-02	-5.10e-02
$T_{stratopause}$	-	-	-	1.0000e+00	5.03e-01	-1.43e-01	4.71e-02
H2O	-	-	-	-	1.0000e+00	-8.9930e-02	4.92e-01
O3	-	-	-	-	-	1.0000e+00	5.73e-01
pressure	-	-	-	-	-	-	1.0000e+00

green cells indicate $\|K\| \geq 0.5$;

G-planet ; M-planet

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Singular Values Decomposition

Definition

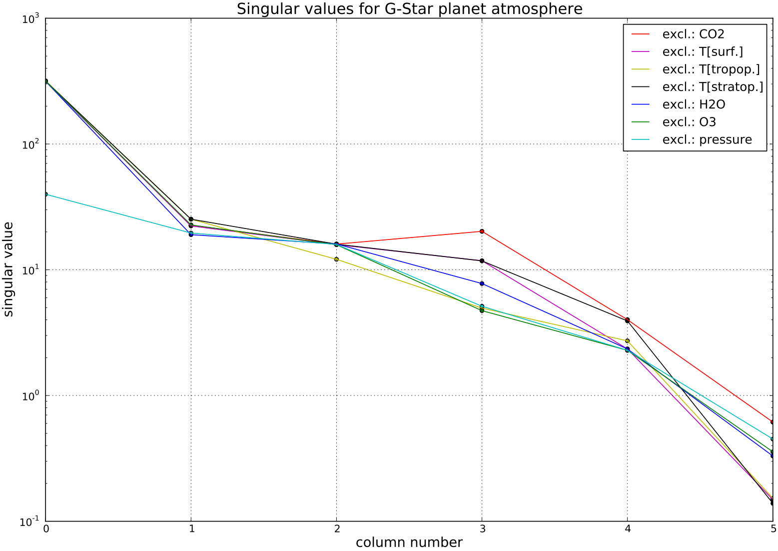
The **SVD** of an (mxn) matrix J is a factorization of the form

$$J = U\Sigma V^*$$

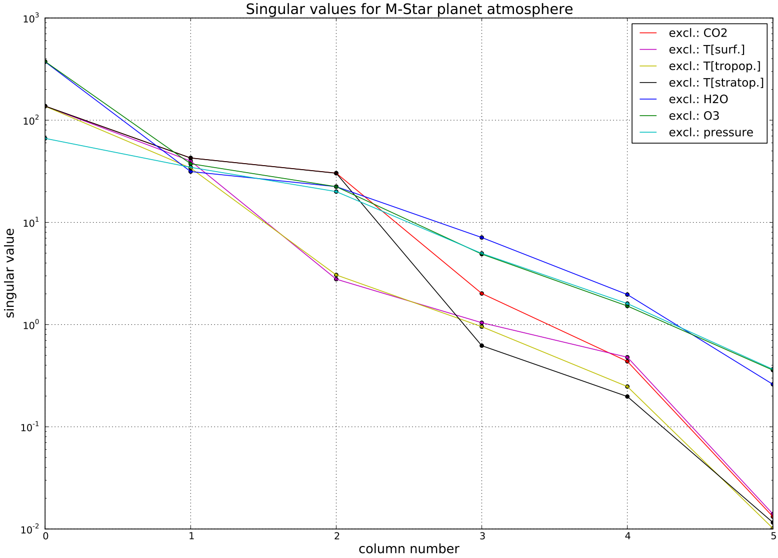
The diagonal entries $\Sigma_{[i,i]}$ of Σ are known as the **singular values** of J

$$\Sigma = \left(\begin{array}{ccc|ccc} \sigma_1 & & & & \vdots & \\ & \ddots & & \cdots & 0 & \cdots \\ & & \sigma_n & & \vdots & \\ \hline & \vdots & & & \vdots & \\ \cdots & 0 & \cdots & \cdots & 0 & \cdots \\ & \vdots & & & \vdots & \end{array}\right)$$

Singular Values $\sum_i$ of Jacobian subsets for G-Star-Planet



Singular Values $\sum_i$ of the Jacobian subsets for M-Star-Planet



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Condition number-χ

Definition

The **condition number** χ measures the worst case of how much the function **b** can change in proportion to small changes in the argument **x**

$$\mathbf{J}(\mathbf{x} + \delta\mathbf{x}) = \delta_{max}\mathbf{b} \quad |\delta\mathbf{x} \to 0$$

and is defined as

$$\chi = \frac{\sigma_1}{\sigma_n}$$

where σ was the singular value of **J**

- a problem/(matrix) with low/high condition number is said to be well/ill-conditioned
- the identity matrix i.e. has a χ of one

σ is the singular value - ref.: SVD

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Condition numbers χ_i

Condition Numbers χ for J(x)

exclude column	-	σCO2	$\sigma T_{surface}$	$\sigma T_{tropopause}$	$\sigma T_{stratopause}$	$\sigma H2O$	$\sigma O3$	σp
G-Star-Planet	2.305e+03	1.394e+02	2.123e+03	2.076e+03	2.280e+03	9.550e+02	8.868e+02	8.840e+01
M-Star-Planet	5.204e+03	6.145e+02	4.887e+03	4.931e+03	4.790e+03	1.432e+03	1.047e+03	1.817e+02

- the χ's for both types of planets are quite different, though there are common variations per parameter
- pressure and CO_2 have the largest effect on the χ of the jacobian
- the relatively large difference in the values of the columns (G-/M-star) could be caused due to different resolutions between the G- and M-Star-Planets input atmospheric data file

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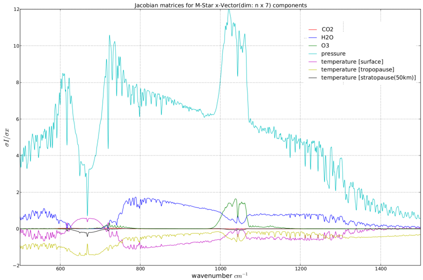
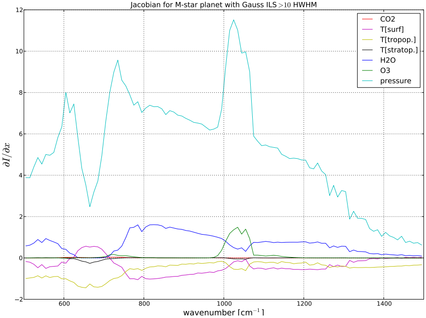
Comparing values at a different ILS (resolution)

- Finally comparing the *jacobians* and χ for an $ILS^2 > 10^1$ *HWHM*
- This has been achieved by *combining 40 consecutive flux values* of the M-Star-planets output within the wavenumber-intervall I from 500-1500 $[cm^{-1}]$ and *recalculate* the flux and further the jacobians and χ_i for all parameters and subsets as an *arithmetic mean* within the new dimension (lenght) of I

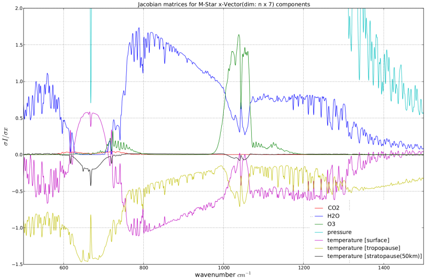
[2] instrument line shape

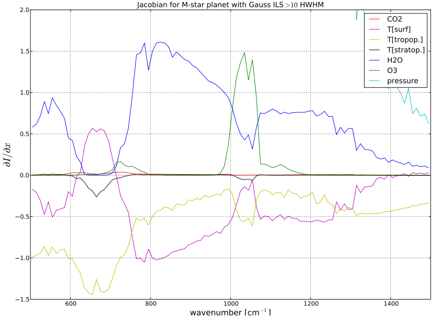
M-Star values at a different ILS





M-Star values at a different ILS





χ of Jacobian and subsets

Condition Numbers χ for J(x) for M-Star-planet

excl. column	-	σCO2	$\sigma T_{surface}$	$\sigma T_{tropopause}$	$\sigma T_{stratopause}$	$\sigma H2O$	$\sigma O3$	σp
$ILS = 1.0[Gauß]$	5.204e+03	6.15e+02	4.887e+03	4.931e+03	4.790e+03	1.432e+03	1.047e+03	1.82e+02
$ILS > 10^1[Gauß]$	2.162e+03	3.06e+02	2.123e+03	2.153e+03	2.082e+03	1.550e+03	1.134e+03	2.01e+02

Conclusion

- the interpolation method has a significant effect on the outputs, particular when using a coarse vertical grid
- jacobians of G- and M-star planets show some common variations though there are some significant differences
- the singular values tend to be lower with the M-star planets calculations
- condition numbers of the M-star planet are higher
- the jacobian of pressure and CO_2 show significant effect on the condition number (by ommitting these values matrix becomes much better conditioned)
- the ILS improves the condition number of the overall jacobian (see the definition of χ), but shows diverse trends omitting a parameter

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Mirart / squirrl / garlic.
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