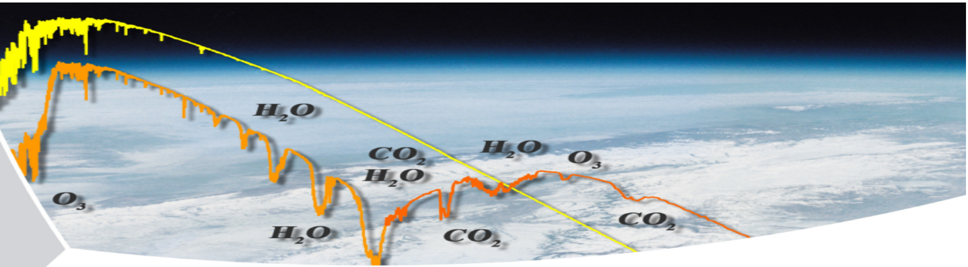


HGF — PEL Atmosphere Workshop II

WP1100 — Radiative Transfer

Past and Future

Franz Schreier, Mayte Vásquez, Thomas Trautmann
Sebastián Gimeno García, Pascal Hedelt

DLR — Remote Sensing Technology Institute

Oberpfaffenhofen, GERMANY

April 2013

Outline

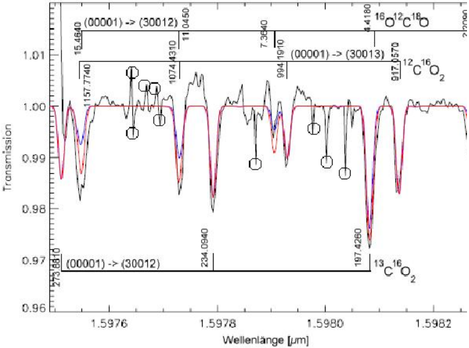
1. Past
2. Future

GARLIC (SQuIRRL) for Venus Transit Spectroscopy

- Transit June 2004
  Vacuum Tower Telescope
  Tenerife
- Emergency call:
  "We have spectra, but no model"

  ... and `SQuIRRL` goes to Berlin!
- *P. Hedelt, DLR–PF,*
  Diploma Thesis, 2006

  Analysis of CO_2 SWIR region:
  isotope abundances,
  field-of-view,
  tangent altitudes, . . .



black: observed; red, blue: modeled
circles: dead pixels

GARLIC — Generic Atmospheric Radiation Lbl Infrared Code

Line shapes:	Voigt, VanVleck$\otimes$Doppler, Lorentz
Line data:	HITRAN, HITEMP, GEISA, JPL, ...
Continua:	H_2O (CKD), CO_2, N_2, O_2, “dry air” (Liebe)
Geometries:	Limb, uplooking, downlooking (refraction optional)
Instruments:	Spectral response: FTS, Heterodyne, Fabry–Perot, ...
	Field-of-view: Box, Gauss, Trapez, ...
Implementation:	FORTRAN 2008, *all data* read from external files
Verification:	AMIL2DA (mid IR, $\rightarrow$), IRTMW01 (μWave, $\rightarrow, \uparrow, \downarrow$), ...
Jacobians:	Automatic differentation
Extensions:	(multiple) scattering infrared radiative transfer: *M. Vasquez:* cloudy planetary atmospheres

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GARLIC — Recent Advances

- SQuIRRL – R.I.P.
- Fortran 90 re-implementation of SQuIRRL
  - dynamic array allocations
  - easier to maintain: structures
- lbl — optimized ∀ IR
  - Humlicek-Weideman Voigt
  - “multi” grid cross sections
  - multi-threading — OpenMP
- CIA collision-induced absorption
- Weighting functions
- Background sources: more flexible

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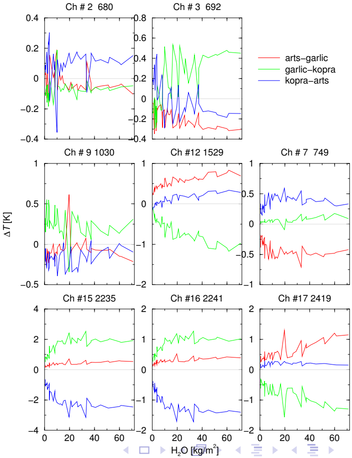
ARTS — GARLIC — KOPRA:
– 42 “Garand” atmospheres,
– 19 HIRS channels



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Outlook:

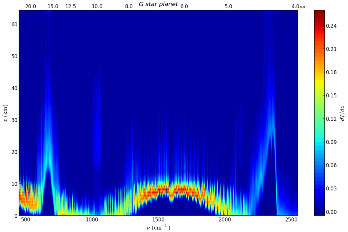
- Continua: MT-CKD
- FPGA
- 2D/3D atmospheres
- Collisional narrowing: Rautian, Galatry, . . .
- Line mixing
- non-LTE

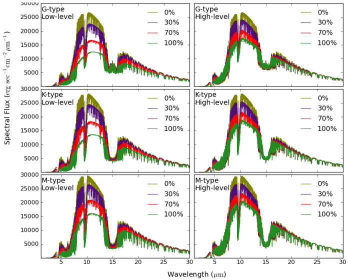
PhD Thesis

Radiative transfer in cloudy planet atmospheres

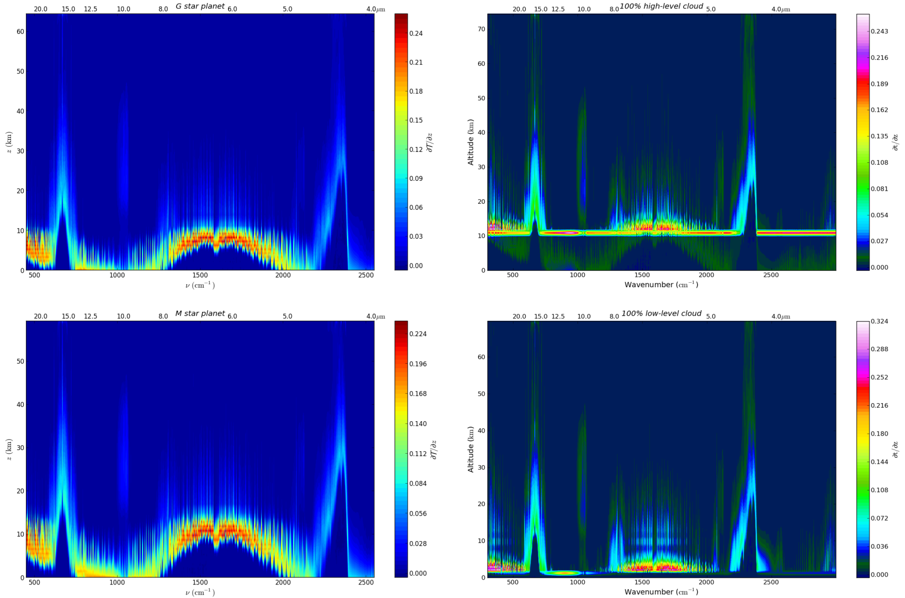
SORTRA = GARLIC + DISORT

- SCIA–Venus observations & modeling:
  Adv. Space Research 2013
- Infrared radiative transfer in atmospheres of Earth-like planets around F, G, K, and M stars
  Input: "Kitzmann atmospheres"
  1. Clear-sky thermal emission spectra and weighting functions
     Astronomy & Astrophysics 2013
  2. Thermal emission spectra influenced by clouds
     A&A, hopefully accepted soon!?!

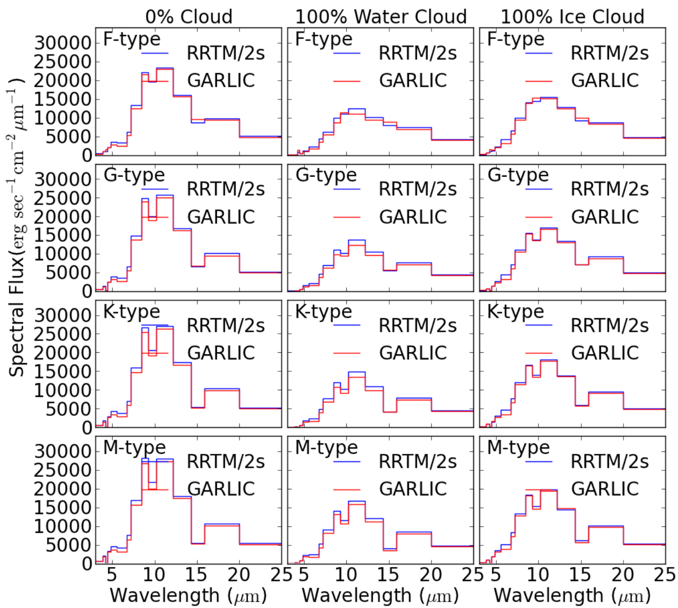




FGKM Star Planets: Weighting Functions



FGKM Star Planets: Lbl vs. Correlated-k



Where are we?

Some studies with lbl infrared simulations:

- P. Hedelt: Venus transit observations 2004 A+A 2011
- P. von Paris et al.: Warming the early Earth – CO2 reconsidered PSS 2008
- H. Rauer et al.: Potential biosignatures in super-Earth atmospheres I. Spectral appearance of super-Earths around M dwarfs A+A 2011
- P. von Paris et al.: Spectroscopic characterization of the atmospheres of potentially habitable planets: GL 581 d as a model case study A+A 2011
- L. Grenfell et al.: Sensitivity of biomarkers to changes in chemical emissions in the Earth's Proterozoic atmosphere Icarus 2011
- P. Hedelt et al.: Spectral features of Earth-like planets and their detectability at different orbital distances around F, G, K stars A+A 2013
- P. von Paris et al.: Characterization of potentially habitable planets: Retrieval of atmospheric and planetary properties from emission spectra A+A 2013

Outline

1. Past
2. Future

What's next???

HGF Alliance "Planetary Evolution and Life" 2008–2013

- "Near-term" — "simple" extension of Mayte's work:
  - NIR transmission/reflection of cloud covered exoplanets
  - Multiple cloud layers
  - CO_2 ice clouds
  - Gliese 581 d: impact of clouds?
  - Fluxes: plane-parallel approximation vs. full spherical
  - Clouds: 'simple" vs. multiple scattering

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  - NIR transmission/reflection of cloud covered exoplanets
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  - Gliese 581 d: impact of clouds?
  - Fluxes: plane-parallel approximation vs. full spherical
  - Clouds: 'simple" vs. multiple scattering
- "Long-term" — remote sensing
  - Temperature sounding and weighting functions: (impact of (unknown) CO_2 concentration and surface pressure)
  - Retrieval feasibility studies (cf. PvP A&A 2013)
  - Analysis of real observations (e.g., hot Jupiters and Neptunes)
  - ......
- ...and our neighbors?
  - Venus transit 2012 ?
  - Venus, Mars Express?

Retrieval Methodology

Schwarzschild equation (negl. background, clouds, instrument, ...)

$$I(\nu) = \int_0^\infty \mathrm{d}z \; B(\nu, T(z)) \underbrace{\frac{\partial}{\partial z} \exp\left(- \int_0^z \mathrm{d}z' \sum_m k_m(\nu; p(z'), T(z')) \; n_m(z') \right)}_{\partial \mathcal{T}(\nu;z)/\partial z}$$

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Discretization:

- finite number m of observations: measurement vector $\boldsymbol{y}$
- quadrature points *or* expansion coefficients *or* ...: state vector $\boldsymbol{x}$

Nonlinear least squares problem

$$\min_{\boldsymbol{x}} \left\| \boldsymbol{I}_{\mathrm{obs}} - \boldsymbol{I}_{\mathrm{mod}}(\boldsymbol{x}) \right\|^2$$

Regularization

- Discretization of radiative transfer integral equation $\Longrightarrow$
  Least squares problem $\min_{\mathbf{x}} \|\mathbf{F}(\mathbf{x}) - \mathbf{y}\|^2$
- Ill posed problem
  - Data cannot provide sufficient information
  - Extremely strong sensitivity of solution to perturbations of data

  $\longrightarrow$ Need additional information about the solution
- Generalization of the minimization problem
  - Optimal estimation (Rodgers 1976):
    Statistically combine *a priori* and retrieved profile

$$\min_{\mathbf{x}} \left((\mathbf{F}(\mathbf{x}) - \mathbf{y})^T \mathbf{S}_y^{-1} (\mathbf{F}(\mathbf{x}) - \mathbf{y}) + (\mathbf{x} - \mathbf{x}_a)^T \mathbf{S}_a^{-1} (\mathbf{x} - \mathbf{x}_a) \right)$$

  - Tikhonov regularization (1963):
    Introduce *'smoothness'* conditions on profile

$$\min_{\mathbf{x}} \left(\|\mathbf{F}(\mathbf{x}) - \mathbf{y}\|^2 + \lambda^2 \|\mathbf{L}\mathbf{x}\|^2 \right)$$

  - Fit of parameterized function (e.g. column density fit)
    $\Longrightarrow$ reduced number of unknowns

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    ?¿? a priori for exo-planets ?¿?
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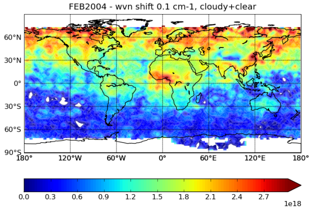
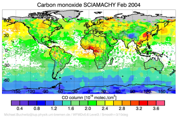
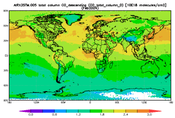
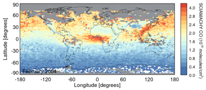
GARLIC and Atmospheric Inverse Problems

- BIRRA Beer InfraRed Retrieval Algorithm
  column density nonlinear least squares for nadir nir (SCIAMACHY)









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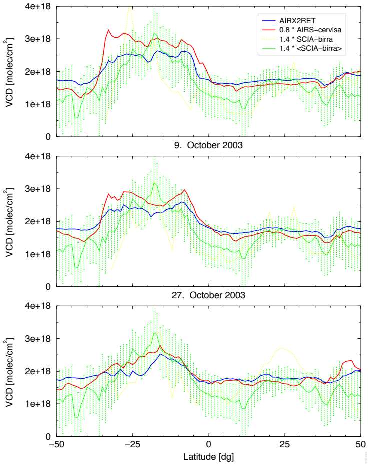

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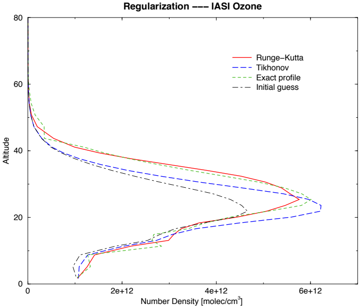

A. Doicu, M. Hess, M. Szopa

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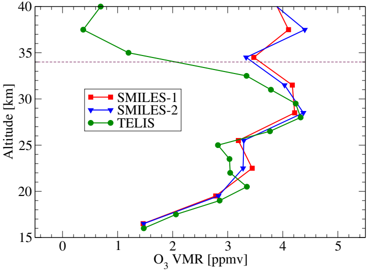
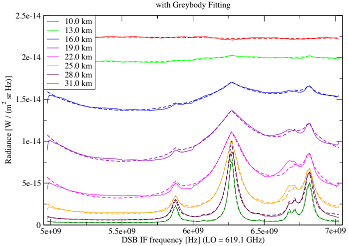
- PILS Profile Inversion for Limb Sounding
  TELIS — TeraHertz Limb Sounder





Jian Xu

Exoplanets Retrievals — Additional Challenges

Earth

- Climatologies etc. for initial guess and/or a priori

Exoplanets

- no climatologies!
  unknown constituents?
  atmos model $\longrightarrow$ init guess?

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- Climatologies etc. for initial guess and/or a priori
- Local view (1D atmosphere sufficient)
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- Observations repeatable
- "Easy" verification & validation
- Everything known (almost)

Exoplanets

- no climatologies! unknown constituents? atmos model $\longrightarrow$ init guess?
- Global view: disk-averaged spectrum
- "Sub-optimal" spec range, low resolution, high noise
- A single observation?
- Validation ???
- Everything unknown

Exoplanets Retrievals — Workpackages

- Set-up state vector
  - Select parameters to retrieve
  - Appropriate discretization
- Analyze conditioning, correlations, ...
  Information content (weighting fct., PCA, SVD, ...)
- Constraints
  - Smoothness, positivity, ...
  - "Physical" constraints
- Implementation
  - Derivative code
  - Inverse problem solver
- Earth-shine, Mars, Venus, Titan, ... for verification & validation
- Analyse exoplanet spectra
  (and observation, reduction, calibration ...)

Temperature profiles of exoplanet atmospheres

- 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

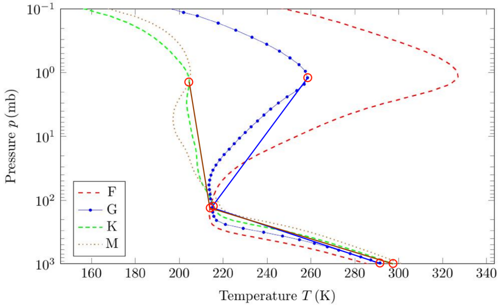

Abbildung: Temperature profiles of exoplanet atmospheres [3]

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

Summary

Looking back — forward modeling

- SQuIRRL $\longrightarrow$ GARLIC
  faster, more flexible, ...
- SQuIRRL in Berlin:
  exoplanets (and young Earth) spectral signatures
- SORTRA:
  - lbl with multiple scattering
  - Validation: Venus SCIA
  - FGKM planets: clear + cloudy

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Looking forward — inversion

- Feasibility:
  information content analysis
  $\rightarrow$ "optimized" state vector
- Constraints:
  atmos. modeling ?
- Solver: Least squares ?
- ... and cloud studies ...

Where are we now . . . and where to go ?

Now: First Steps

- Berlin:
  Nonlinear least squares (LM)
- OP:
  Long expertise @ Earth
  μWave – IR – UV
  First studies: correlation

Soon: Science and Tools

A Versatile Retrieval System

- constrained least squares etc.
- forward model (incl. deriv):
  - molecules – lbl
  - clouds – scattering
- transmission & emission
  SWIR & TIR

Collaborations

- WP1200 — 1D atmosphere modelling
- WP1300 — 3D atmosphere modelling
  (and retrieval @ MPS)