WP1100 — Radiative Transfer
Past and Future

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DLR — Remote Sensing Technology Institute
Oberpfaffenhofen, GERMANY

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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!

Analysis of CO\textsubscript{2} SWIR region: isotope abundances, field-of-view, tangent altitudes, ...
Line shapes: Voigt, VanVleck\times 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)
Field-of-view: Box, Gauss, Trapez, . . .
Implementation: FORTRAN 2008, all data read from external files
Verification: AMIL2DA (mid IR, \rightarrow), IRTMW01 (\mu Wave, \rightarrow, \uparrow, \downarrow), . . .
Jacobians: Automatic differentiation
Extensions: (multiple) scattering infrared radiative transfer: M. Vasquez: cloudy planetary atmospheres
GARLIC — Generic Atmospheric Radiation Lbl Infrared Code

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Line data: HITRAN, HITEMP, GEISA, JPL, \ldots
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Geometries: Limb, uplooking, downlooking (refraction optional)
Instruments: Spectral response: FTS, Heterodyne, Fabry–Perot, \ldots
Field-of-view: Box, Gauss, Trapez, \ldots
Implementation: FORTRAN 2008, \textit{all data read from external files}
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Extensions: (multiple) scattering infrared radiative transfer:
M. Vasquez: cloudy planetary atmospheres
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

![Graphs showing temperature changes](image)
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Outlook:
- Continua: MT-CKD
- FPGA
- 2D/3D atmospheres
- Collisional narrowing: Rautian, Galatry, …
- Line mixing
- non-LTE
Where are we?

Oberpfaffenhofen

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

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Some studies with.lbl infrared simulations:

- P. Hedelt: Venus transit observations 2004
- P. von Paris et al.: Warming the early Earth – CO2 reconsidered
- P. von Paris et al.: Spectroscopic characterization of the atmospheres of potentially habitable planets: GL 581 d as a model case study
- L. Grenfell et al.: Sensitivity of biomarkers to changes in chemical emissions in the Earth’s Proterozoic atmosphere
- P. Hedelt et al.: Spectral features of Earth-like planets and their detectability at different orbital distances around F, G, K stars
- P. von Paris et al.: Characterization of potentially habitable planets: Retrieval of atmospheric and planetary properties from emission spectra
Outline

1. Past
2. Future
“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
What’s next???

HGF Alliance “Planetary Evolution and Life” 2008–2013

“Near-term” — “simple” extension of Mayte’s work:
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“Long-term” — remote sensing
- Temperature sounding and weighting functions:
  (impact of (unknown) \( \text{CO}_2 \) 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?
Schwarzschild equation (negl. background, clouds, instrument, ...)
Retrieval Methodology

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

\[ l(\nu) = \int_0^{\infty} \text{d}z \ B(\nu, T(z)) \ \frac{\partial}{\partial z} \exp \left( - \int_0^z \text{d}z' \sum_m k_m(\nu; p(z'), T(z')) n_m(z') \right) \]

\[ \partial T(\nu;z)/\partial z \]

Discretization:

- finite number \( m \) of observations: measurement vector \( y \)
- quadrature points or expansion coefficients or . . . : state vector \( x \)

Nonlinear least squares problem

\[ \min_x \| l_{\text{obs}} - l_{\text{mod}}(x) \|^2 \]
Regularization

- Discretization of radiative transfer integral equation

\[ \text{Least squares problem} \quad \min_x \| F(x) - y \|^2 \]

- Ill posed problem
  - Data cannot provide sufficient information
  - Extremely strong sensitivity of solution to perturbations of data
  \[ \text{Need additional information about the solution} \]

- Generalization of the minimization problem
  - Optimal estimation (Rodgers 1976):
    Statistically combine \textit{a priori} and retrieved profile

\[ \min_x \left( (F(x) - y)^T S_y^{-1} (F(x) - y) + (x - x_a)^T S_a^{-1} (x - x_a) \right) \]

- Tikhonov regularization (1963):
  Introduce \textit{smoothness} conditions on profile

\[ \min_x \left( \| F(x) - y \|^2 + \lambda^2 \| Lx \|^2 \right) \]

- Fit of parameterized function (e.g. column density fit)
  \[ \text{reduced number of unknowns} \]
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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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- **CERVISA**
Column EstimatoR Vertical Ir Sounding Atmosphere
column density nonlinear least squares for nadir tir (AIRS, IASI, ...)

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![Graphs showing VCD variations over time]

- **AIRX2RET**
- **0.8 * AIRS - cervisa**
- **1.4 * SCIA - birra**
- **1.4 * <SCIA - birra>**

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- **VINO** Versatile Inversion for Nadir Observations
  GARLIC + DRACULA for nadir sounding profiles (IASI, GOSAT)

A. Doicu, M. Hess, M. Szopa
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- **PILS** Profile Inversion for Limb Sounding
  TELIS — TeraHertz Limb Sounder

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**Jian Xu**

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### Exoplanets Retrievals — Additional Challenges

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<thead>
<tr>
<th>Earth</th>
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</tr>
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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 ...)

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

<p>| Correlationmatrix for atm. parameters of G-Star-Planet |
|----------------------------------|--|--|--|--|--|--|--|</p>
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<tr>
<th>Relate</th>
<th>CO2</th>
<th>$T_{\text{surface}}$</th>
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<tr>
<td>CO2</td>
<td>1.0000e+00</td>
<td>-1.54e-01</td>
<td>-4.32e-01</td>
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<td>$T_{\text{surface}}$</td>
<td>-</td>
<td>1.0000e+00</td>
<td>-1.46e-01</td>
<td>-5.06e-01</td>
<td>9.16e-01</td>
<td>-2.27e-01</td>
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<td>-</td>
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<td>5.39e-01</td>
<td>-1.33e-01</td>
<td>-1.43e-01</td>
<td>1.20e-01</td>
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<td>$T_{\text{stratopause}}$</td>
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<td>-</td>
<td>1.0000e+00</td>
<td>-3.96e-01</td>
<td>8.93e-02</td>
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<td>pressure</td>
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<td>-</td>
<td>-</td>
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<td>-</td>
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*green cells indicate $|K| \geq 0.5$;*

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Summary

Looking back — forward modeling

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

Looking forward — inversion

Feasibility:
- information content analysis
- "optimized" state vector
Constraints:
- atmos. modeling?
- Solver: Least squares?
  \ldots and cloud studies \ldots
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Where are we now . . . and where to go?

Now: First Steps
- Berlin:
  Nonlinear least squares (LM)
- OP:
  Long expertise @ Earth
  \( \mu \)Wave – 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)