Qpack2 / ARTS + Atmlab

Patrick Eriksson

Department of Earth and Space Sciences
Chalmers University of Technology
SE-41296 Gothenburg, Sweden

+

NDACC workshop, Bern, 2013-01-10

What is Qpack2?

- A retrieval environment
  - applies MAP (maximum a posteriori)
    - also known as OEM
  - user interface is Matlab code
- Scope
  - single spectrum observations
  - batch inversion of measurement time series
  - any observation geometry
- Publicly available
  - don't forget to cite Qpack and ARTS (+ modules?)
- Tailored to this community!

Involved software

- ARTS
  - a general forward model for longwave radiation
  - C++
- Atmlab
  - a compilation of Matlab code
  - stand-alone functions + different “systems”
- Qpack2
  - distributed as part of Atmlab
  - mainly an interface to some Atmlab systems
- *PyARTS*
  - *a python interface to ARTS*

Outline

Versions

Qpack vX.Y uses ARTS vX.Y

- Version 1
  - an attempt for a general 1D retrieval environment
  - used for Odin-SMR, and by Bremen, MeteoSwiss and ?
  - no development, not considered below

- Version 2.0
  - compared to v1:
    - \- dedicated treatment of limb sounding, error classification, special plotting functions, conditional simulations
    - \+ batch inversions, definition of a priori climatologies, more sensor characteristics, more species retrieval units, more flexible definition of input and output
  - present “stable” version (only bug fixes)

- Version 2.1
  - development version (new features are added here)

Using Qpack is simple!

- A retrieval

```
>> [Q,O] = my_q_fun;
>> Y = my_y_fun;
>> L2 = qpack2( Q, O, Y );
```

- All variables are structures
  - for batch cases, `Y` and `L2` are arrays

- To simulate spectra matching a priori:

```
>> Y.Y = [];
>> Ysim = qpack2( Q, O, Y );
```

- Example output ⇒

Data types:

- retrieved variables
- retrieval characteristics
  - a priori
  - errors
  - measurement response, AVKs
- convergence, “costs”
- atmospheric data
- auxiliary data

- You can control the content!

```
          year: 2008
         month: 2
           day: 25
     converged: 1
            dx: 1.3642e-06
          cost: 0.9972
        cost_x: 4.0910e-04
        cost_y: 0.9968
             f: [1279x1 double]
             y: [1279x1 double]
            yf: [1279x1 double]
            bl: [1279x1 double]
species1_name: 'O3'
   species1_p: [45x1 double]
   species1_x: [45x1 double]
  species1_xa: [45x1 double]
   species1_e: [45x1 double]
  species1_eo: [45x1 double]
  species1_es: [45x1 double]
  species1_mr: [45x1 double]
   species1_A: [45x45 double]
     fshift_x: 9.1261e+03
    fshift_xa: 0
     fshift_e: 8.9386e+03
    fshift_eo: 8.7913e+03
    fshift_es: 1.6161e+03
    ...
```

measurement data

- Spectrum
- Observation geometry
- Time and place
- Hydrostatic equilibrium ref. point
- Thermal noise

- Example data ⇒

- If `Y.Y = [];`
  the “a priori spectrum” is
  instead calculated

```
       DAY: 25
         F: {}
      HOUR: {}
     HSE_P: 10000
     HSE_Z: 16000
  LATITUDE: 45
 LONGITUDE: 2.7183
    MINUTE: {}
     MONTH: 2
    SECOND: {}
    TNOISE: 0.0500
         Y: [1279x1 double]
      YEAR: 2008
        ZA: 70
Z_PLATFORM: 10500
```

Why a separate structure?

- OEM is a separate module in Atmlab
- In simplest case, only required active choice is

```
O.linear = true;
```

- Available iteration strategies:
  - linear
  - Gauss-Newton
  - Marquardt-Levenberg ($\mathbf{D} = \mathbf{S}_{\mathbf{x}}^{-1}$)

- Atmospheric and spectroscopic data
- Sensor data
- Definition of retrieval quantities
  - retrieval grids
  - a priori uncertainty (corresponding part of $\mathbf{S_x}$)
  - atmospheric a priori "climatology"
  - include in `L2`?
- Atmospheric a priori "climatologies" are interpolated automatically, following date and position in `Y`
- Several input formats allowed, e.g.

```
>> Q.F_GRID = 'f_grid_111ghz.xml';
>> Q.F_GRID = f0 + 1e6*linspace(-100,100,1);
```

Covered instrument characteristics

- Arbitrary altitude and zenith angle
- Antenna pattern
- Mixer and sideband response
- Spectrometer channel response
- Polarisation response

- Frequency switching
- (Beam switching)

- Correlation of thermal noise

Examples on covered physics

- All relevant gases
- Handles several spectroscopic formats
  - HITRAN (old + new), JPL, ARTS specific
- A number of line shapes
- A number of absorption models built-in
  - H_2O, O_2, N_2 and liquid water
  - MPM, PWR, CKD ...
- "On-the-fly" or pre-calculated absorption
- Spherical Earth
- Refraction
- Winds

Available retrieval quantities

- Atmospheric gases
  - supported units: VMR, ND, “rel” and “logrel”
- Atmospheric temperature
  - semi-analytic expression now used
  - hydrostatic eq. is included, but not refraction
- Polynomial baseline fit
- Spectrometer frequencies: shift and stretch

<u>For v2.1 also:</u>

- Sinusoidal baseline fit
- Winds
- Pointing off-set

Possible extensions / applications

- Zeeman
  - being implemented
  - so far no analytic Jacobians with polarised absorption
- Data reduction
  - binning and “transformation matrix” (e.g. Hotelling)
- Any requests?
- Time series inversions?
  - more in presentation by Ole Martin

Documentation

- A small user manual exists
- ARTS and Atmlab systems documented separately
  - mainly built-in documentation
- Email list
- Start with the demo script!

Outline

This is ARTS!

- Flexible
  - important for users
- Modular
  - important for developers
- Documented
  - important for all
- Maintained
  - important for users

How is flexibility and modularity achieved?

- ARTS works somewhat as a scripting language
  - in contrast to keyword based programs
- ARTS operates with variables, methods and agendas
- “Hello world” in ARTS:

```
Arts{
 StringCreate( s )
 StringSet( s, "Hello World" )
 Print( s )
}
```

Scope

Limitations apply, e.g. MC demands 3D

- Full polarisation (1-4 Stokes elements)
- 1D, 2D or 3D atmosphere
- Free geoid + surface topography (no “flat Earth” approx.)
- All observation geometries covered
- Broad coverage of sensor responses
- Many weighting functions provided (very slow if scattering)
- Two modules for handling scattering (DOIT and MC)

Main applications

- Microwave emission observations
  - including scattering and tomographic retrievals
- Applicable in the IR range
- Basic treatment of radio link budgets
- Applicable for other planets
  - two last features being added as part of an ESA study

- Operational inversions:
  - Odin-SMR (standard + off-line tropospheric)
  - UTH from AMSU-B type instruments
  - several ground-based strato/mesospheric radiometers

Outline

Examples on function sets

- Plotting
  - including interface to GMT
- Time formats
- Basic physics
  - including constants
- Forward model related
  - line shapes, conversion to T_b ...
- Properties related to water
- Reading of satellite data
- Collocations of satellite observations
- Mie scattering
- Interface to ARTS-2 (Qarts)
- Retrievals
  - `oem.m`
  - Qpack2

Retrievals using Atmlab

- Qpack2 $\approx$
  - Qarts + `oem.m` + atmdata

- The underlying retrieval system more general
  - 2D limb inversions planned
  - most code in place

Summary

- ARTS and Atmlab general, open source, softwares
- Some features of Qpack2:
  - broad coverage of instrumental characteristics
  - a number of retrieval quantities
  - batch inversions
  - automatic extraction of a priori data

Thank you!