Introduction

SFIT Retrieval Workshop

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NCAR, Boulder, CO

November 2019

Outline

- Past SFIT /Retrieval / Error Analysis Workshops
- What we hope to do here
- Structure of SFIT vs Batch processing
- Outline of this workshop

Previous SFIT2 / SFIT4 / Retrieval IRWG Workshops 1/3

SFIT2 Workshop
May 2000 BIRA, Brussels, Belgium, hosted by M. De Maziere

Attendees:
Nicolas Jones, Steve Wood, Curtis Rinsland, Clive Rodgers, Nikita Pougatchev, Frank Hase, Yongjing Zhao, Justus Notholt, Claude Camy-Peyret, Sebastien Payan, Johan Mellqvist, William Bell, Emmanuel Mahieu, Philippe Demoulin, Francine Melen, Rudy Zander, Ralf Sussmann, Wolfgang Wimmer, Merritt Deeter, Leonid Yourganov

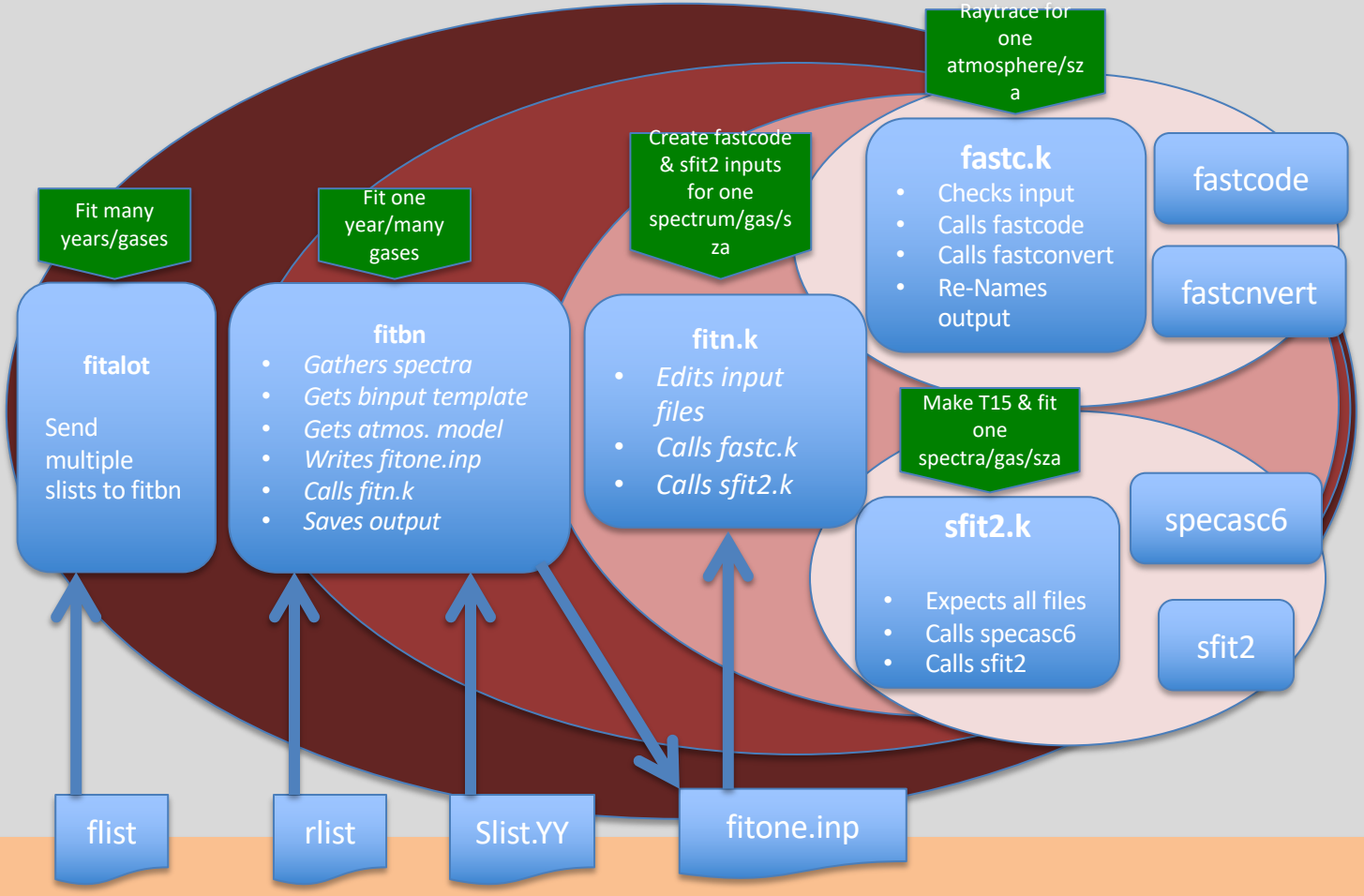
- ✓ "Participants who have some sfit2 experience are requested to bring along one or two transparencies to briefly say something about what they have learned in the context of their local conditions."
- ✓ "The biggest need is for a new document advising on "good practice" points for use with SFIT2."
- ✓ Marked the beginning of wide use of profile retrievals for IRWG type high resolution solar spectra
    - Quick reference on basic formulae.doc
    - Averaging Kernels and errors.doc

Previous SFIT2 / SFIT4 / Retrieval IRWG Workshops 2/3

IRWG – NORS Retrieval & Error Analysis Workshop
January 2013 NCAR, Boulder, CO hosted by J Hannigan

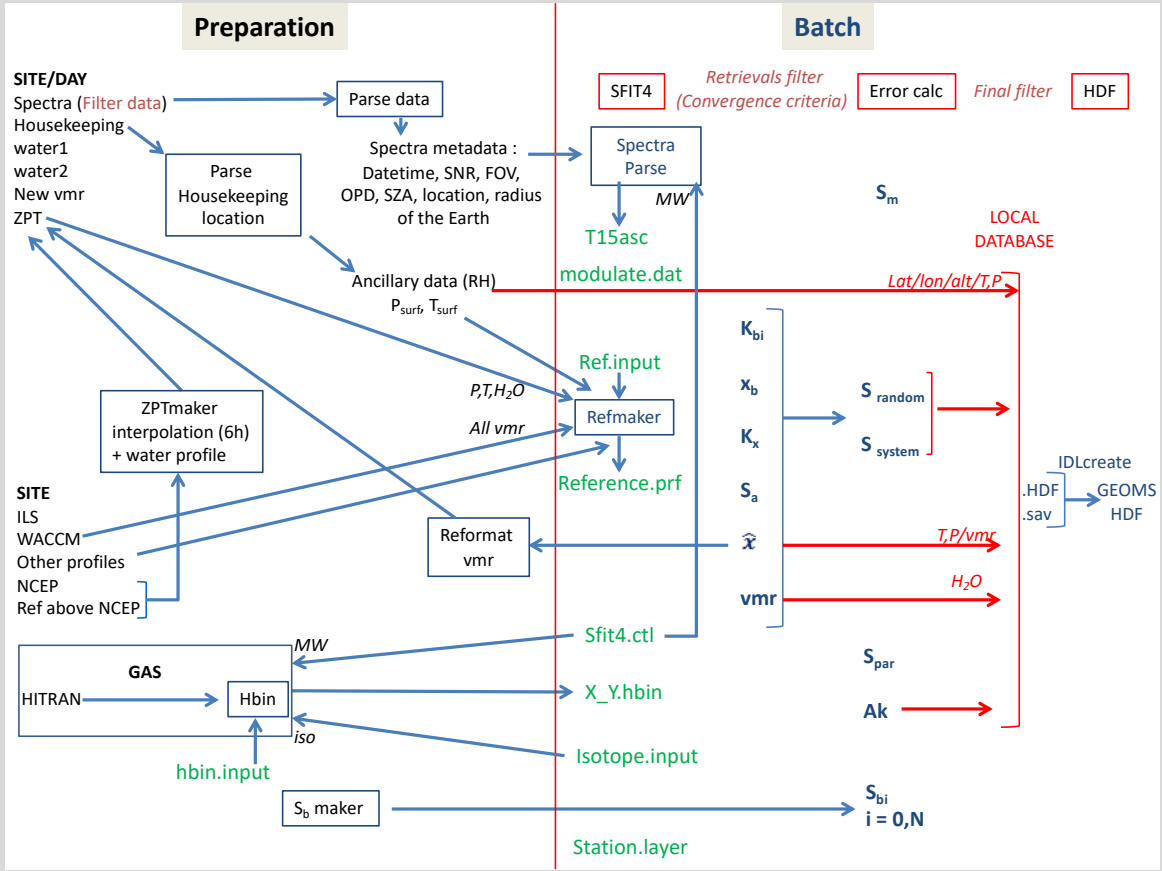
- Shortly after the adoption of the standard retrieval parameters for all 10 NDACC species
- Move to SFIT4
- Beginning of OE error estimation
  - How would we do this efficiently?
- Definition of batch processing
  - Collected batch processing techniques from many goups to optimize a set of procedures that would be acceptable / useful to all groups

Nested Scripts for Calling Spectra Process & Fitting Codes



Previous SFIT2 / SFIT4 / Retrieval IRWG Workshops 2/3

Interconnect diagram for requirements of the SFIT4 batching processing.



Previous SFIT2 / SFIT4 / Retrieval IRWG Workshops 3/3

SFIT4 – Error Analysis Workshop
June 2013 NEIS, Tsukuba Japan, Hosted by Hideake Nakajima

Goals for the meeting:

a. a core group who are very familiar with a standard processing method, issues and tools,

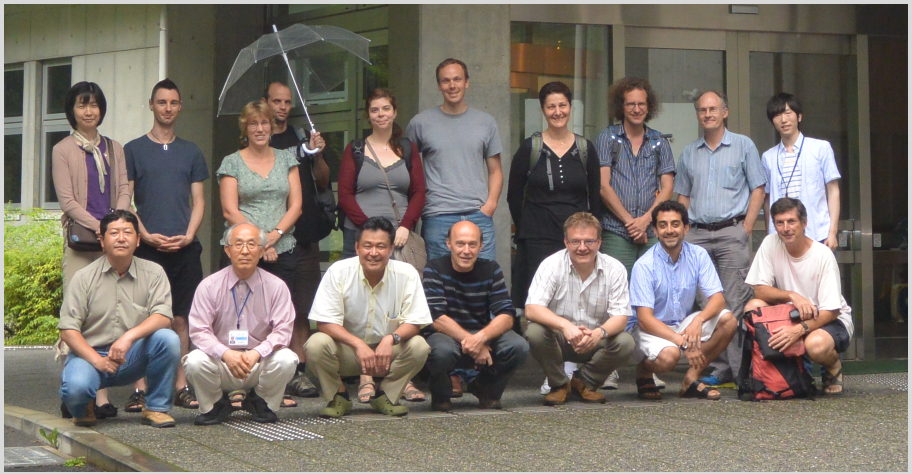
b. a deeper understanding of error issues and limitations

c. further implementation of a general set of tools and documentation required to produce reasonable error estimates and create the IRWG HDF data that would be available to all IRWG/NORS members at the IRWG web site.

d. agreement on and a path toward 'completing' these tools

e. plans to implement these methods back at their home institute for testing, verification and operational use.

- Introduction of the SFIT Processing Environment
- Refinement of Kb calculations
- Bug fixes in SFIT4



What we hope to do here

- Less development, more teaching & learning on all sides
- Answer your questions
- Dig inside how sfit works how to make it work for you
- Test latest version (wiki) V1.0pr & latest linelist including ATM2010910
- A more savvy user community especially as we move towards external processing
- Consolidate and complete documentation
    - We envision 3 documents
        1. SFIT4 Theory, Input, Outputs (many pieces already exist…)
        2. SFIT4 Processing Environment (this generally exists: "Optical Techniques FTS Profile Retrieval Processing")
        3. SFIT4 User Manual, Tips, Examples (some pieces exist…)

Outline of this workshop

Mornings

- Presentations of components of SFIT4 and the processing Environment
- SFIT4 theory, Spectroscopy, forward model, Band, Retrieval parameters
- Including discussions of these

Afternoons

- More open discussions
- Your questions and issues discussed
- Discussions of examples or of earlier presentations or ?

Structure of SFIT4 vs Batch processing 1/

Much more detail to follow, and we all have thousands of spectra to process **but** to start at the beginning: SFIT4 fits one spectrum at a time. So when we talk about SFIT4 or talk about an issue with fitting a spectrum we are talking about just running SFIT4. A user should know what SFIT4 needs to run and what SFIT4 outputs for diagnostics. And this is very different than what the processing environment requires:

- ✓ This leads ease of diagnosing any issue
- ✓ Leads to more direct communication when asking about an issue: ie. What constitutes a *"testcase"*
- ✓ *The structure of SFIT4 and the Processing Environment was specifically designed to be modular & concentric.*

Structure of SFIT4 vs Batch processing 2/

1. **Flexibility** – Exploratory analysis tool

i. S_a (S_a^{-1}) definition / direct input
ii. Background parameters (slope, curvature, zero)
iii. Shifts, by species, by fit
iv. Channeling
v. SNR by region
vi. Multiple regions / SZA
vii. Fit gas by region
viii. Phase, ME
ix. Isotope separation
x. Solar background /shift
xi. Levenberg-Marquardt non-linear iteration scheme
xii. Emission spectra
xiii. Log(vmr) retrieval
xiv. Line mixing (co2, ch4 soon…)
xv. SDV speed dependent Voigt lineshape
xvi. Spectra output by layer / gas
xvii. O2 CIA line data included

Two foci of sfit4 Development

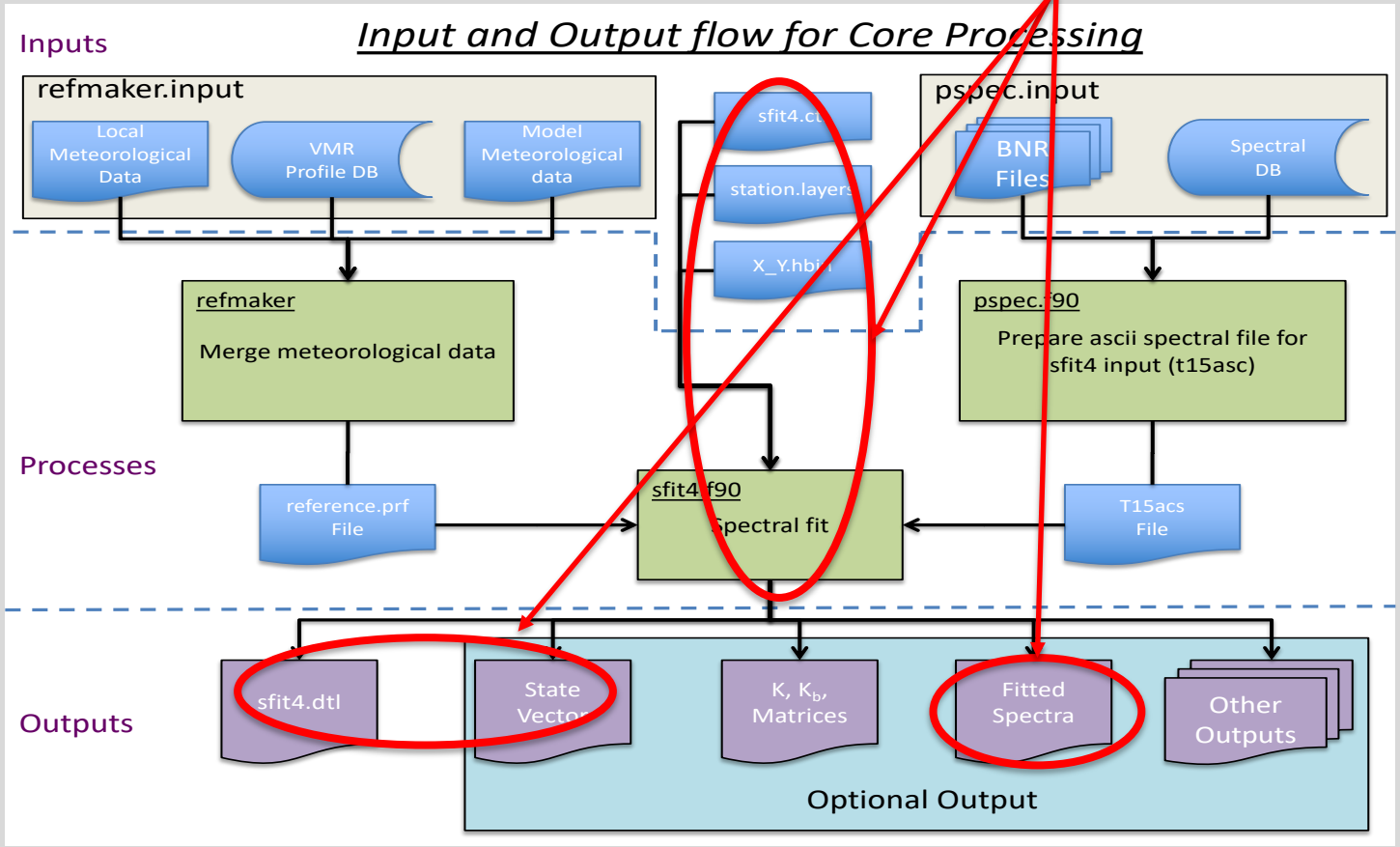
2. Process & I/O **Speed** –

NDACC operational processing

i. Standard layering
ii. Binary HITRAN input
iii. Binary output for HDF ?

Structure of SFIT4 vs Batch processing 2/

These (mainly) constitute a fit



Structure of SFIT4 vs Batch processing 3/ map of Input & Output files

```
! --- SET DEFAULT FILENAMES

    TFILE(08) = 'pbpfile'

! --- ISOTOPE SEPARATION FILE
    TFILE(09) = 'isotope.input'

    TFILE(15) = 't15asc'

    TFILE(16) = sfit4.dtl'

! --- STATEVEC
    TFILE(18) = 'statevec'

! --- SET MIXOUTPUT FILENAME AS STATE VECTOR FILENAME + .MXF
    TFILE(17) = TRIM(TFILE(18))//'.mxf'

! --- SAVED SYNTHETIC SPECTRUM
    TFILE(19) = 'synspec.out'

! --- SUMMARY
    TFILE(20) = 'summary'

! --- EMPIRICAL MODULATION FUNCTION
    TFILE(23) = 'ils.dat'

! --- EMPIRICAL PHASE FUNCTION
    TFILE(24) = 'ils.dat'
```

```
! --- DEFAULT COMPLETE SA OUTPUT FILENAME
    TFILE(63) = 'Sa.complete'

! --- DEFAULT K,SE,SA MATRICES OUTPUT FILENAME
    TFILE(66) = 'K.out'

! --- SE OUTPUT
    TFILE(67) = 'Se.out'

! --- DEFAULT K TRANSPOSED FILENAME
    TFILE(68) =  'KT.out'

! ---  LEVENBERG-MARQUARDT DETAILS
    TFILE(70) = 'detail.opt'

! --- LAYERING SCHEME - OUTPUT FROM WACCM PROFILES
    TFILE(71) = 'station.layers'

! --- REFERENCE VMR PROFILES
    TFILE(72) = 'reference.prf'

! --- RAYTRACE DETAILED OUTPUT AKA TAPE6
    TFILE(73) = 'raytrace.out'

    TFILE(74) = 'raytrace.pt'
    TFILE(75) = 'raytrace.ms'
    TFILE(76) = 'raytrace.mix'
    TFILE(77) = 'raytrace.sa'
    TFILE(78) = 'raytrace.pnch'
```

```
! --- CHANNEL OUTPUT
    TFILE(30) = 'chnspec.data1'

    TFILE(40) = 'chnspec.data2'

! --- SET SHORT FILENAME AS SUMMARY FILENAME + .ST
    TFILE(31) = TRIM(TFILE(20))//'.st'

! --- DEFAULT FIRST RETRIEVAL GAS SA OUTPUT FILENAME
! --- OUTPUT DEPENDS ON NAME SA .NORM, .VMR, .PCOL
    TFILE(61) = 'Sa.norm'

! --- DEFAULT SAINV INPUT FILENAME
    TFILE(62) = 'Sainv.input'

! --- RESERVED FOR GASOUT NAME CHANGES - SEE FRWDMDL.F90
    !TFILE(80)
    TFILE(80) = "gas.<gas>.<band>.<scan>.<itr>"

    TFILE(81) = 'AK.out'
    TFILE(82) = 'SM.out'
    TFILE(83) = 'SS.out'
    TFILE(84) = 'A-S.out'
    TFILE(85) = 'AEIGEN.out'

    TFILE(88) = 'PRFS.out'
    TFILE(89) = 'Parm.out'

    TFILE(91) = 'Spec.out'
```

Structure of SFIT4 vs Batch processing 4/4 Testcase

required inputs

sfit4.ctl
Retrieval specific params:
- *Region*
- *Species*
- *State vector*

t15asc4
- *Spectrum specific params:*
- *Date/Time*
- *Solar zenith angle*
- *N spectra*

stations.layers
- *Layering for each site*
- *From WACCM*

reference.prf
- *Z-p-T for reference profiles*
- *Reference (apriori) chemical profiles*

Binary (HITRAN) Line list file

sfit4
Raytracing
Forward Transmission / Emission Model
retrieval

required output

sit4.dtl (detail file)
- *Step-by-step of retrieval process*
- *Verification of inputs*
- *Summary of raytracing*
- *Statevector on every iteration*

spc.all.01.01.final (Spectra output file)
- *This file and others for individual specie plotting*

pbpfile (Spectra output file)
- *Input, output difference spectra*

The Rest of the Workshop

Your feedback is important so we can

i. Improve documentation and

ii. Future workshops

iii. Improve SFIT4 functionality and usability

The workshop is informal and all presentations are open for discussion

Visit: https://wiki.ucar.edu/display/sfit4/

Enjoy the workshop!

end