The Paper-and-Code Bundle Concept in Atmospheric Radiation Science

Sergey Korkin (UMBC & NASA GSFC, sergey.v.korkin@nasa.gov), **Andrew M. Sayer** (UMBC & NASA GSFC), **Amir Ibrahim** (NASA GSFC), and **Alexei Lyapustin** (NASA GSFC)

Abstract

The modern workforce is under relentless pressure to constantly acquire new skills and knowledge necessary to get the job done. Atmospheric science is not exempt. A typical practitioner must not only understand atmospheric physics (which alone has many branches) and its underlying mathematics (sophisticated), but also details of numerical techniques, and possess basic software engineering skills (for code development). **Many classic books and papers** in all branches of atmospheric and computer science **are available.** But that is partially the **problem: there are too many.** When switching between branches of atmospheric science (due to collaboration or change of projects), **nobody has time for deep immersion in relevant literature.** Also, successful completion of a project still requires **understanding at the level of code developer** (because using ***"black boxes"*** and ***"spaghetti codes"*** is unprofessional, risky, and counterproductive). Many of these theoretical **papers are not written from the point of view of turning theory into workable, maintainable code.**

In this talk **we discuss two papers** describing numerical simulation of two fundamental physical processes in the atmosphere: multiple scattering of solar light, and absorption by atmospheric trace gases. Following the format of "*Numerical Recipes*" by *Press* et al., **our papers bundle small pieces of necessary theory with corresponding snippets of code**. These are arranged in an order that is natural for code development, which is often opposite of the natural order for laying out the theoretical basis. **The first paper has been published in 2022**, while the second is a work in progress which we intend to finish in 2024. **The goal of both papers is to simplify the transfer of knowledge** from seniors to juniors, and exchange skills between experts from different branches of Earth science. The codes are open source to be a learning resource available to all.

What is the problem?

RT ~~model~~ ~~code~~ solver

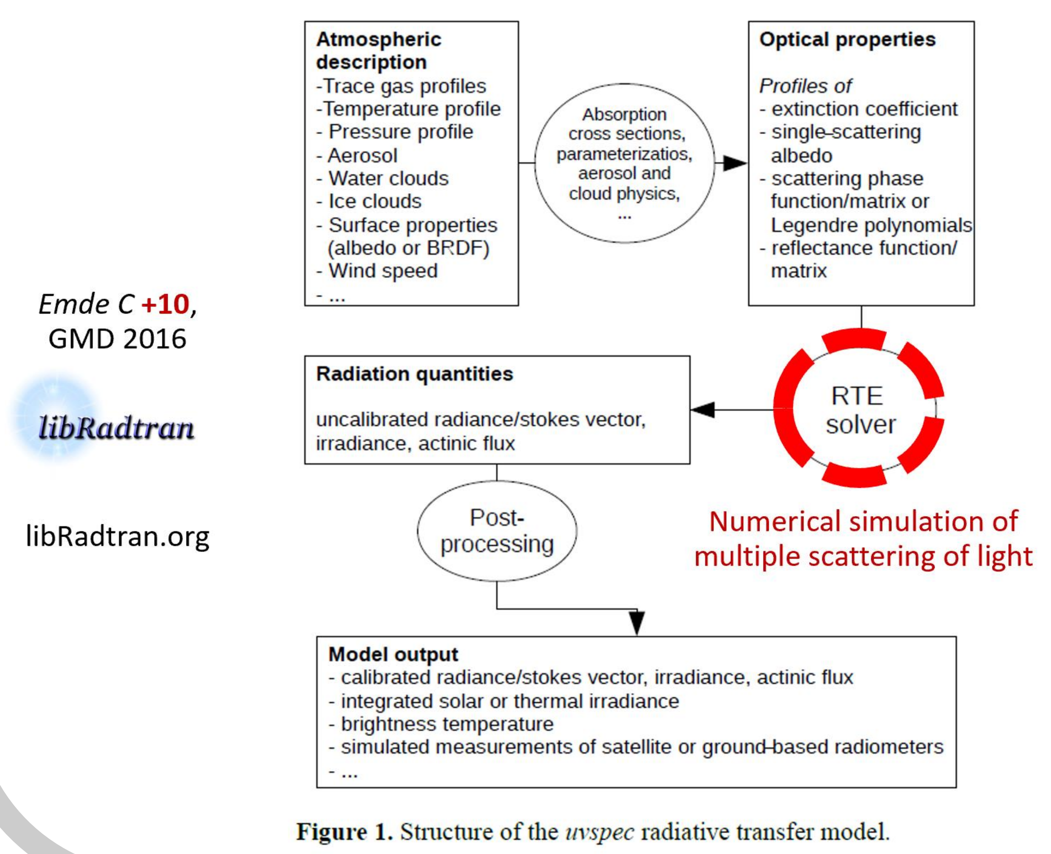
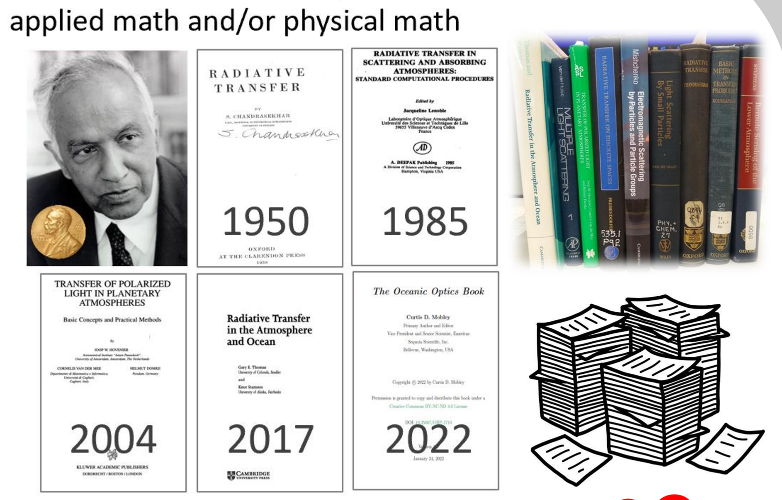


Figure 1. Structure of the *uvspec* radiative transfer model.

- **Radiative Transfer Theory** - a branch of applied math and/or physical math



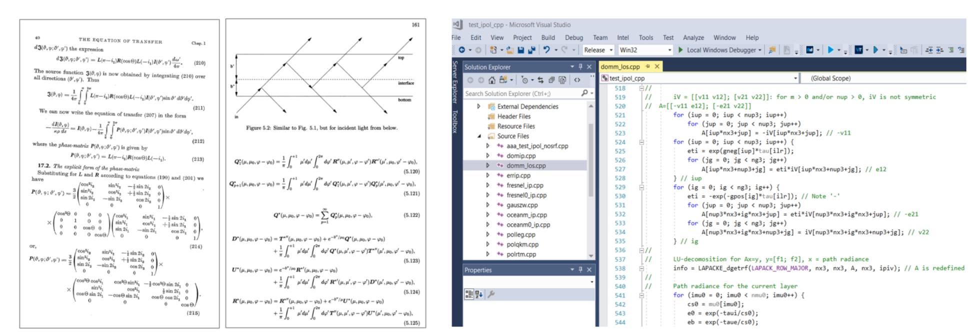
- **Soft- & hardware**

Why is it important ?

- Mission planning (SNR, bands) & data processing

- Mission impose new scientific (e.g., update HITRAN, add new surface) …
- … and software requirements (run faster, create user guide, etc.)

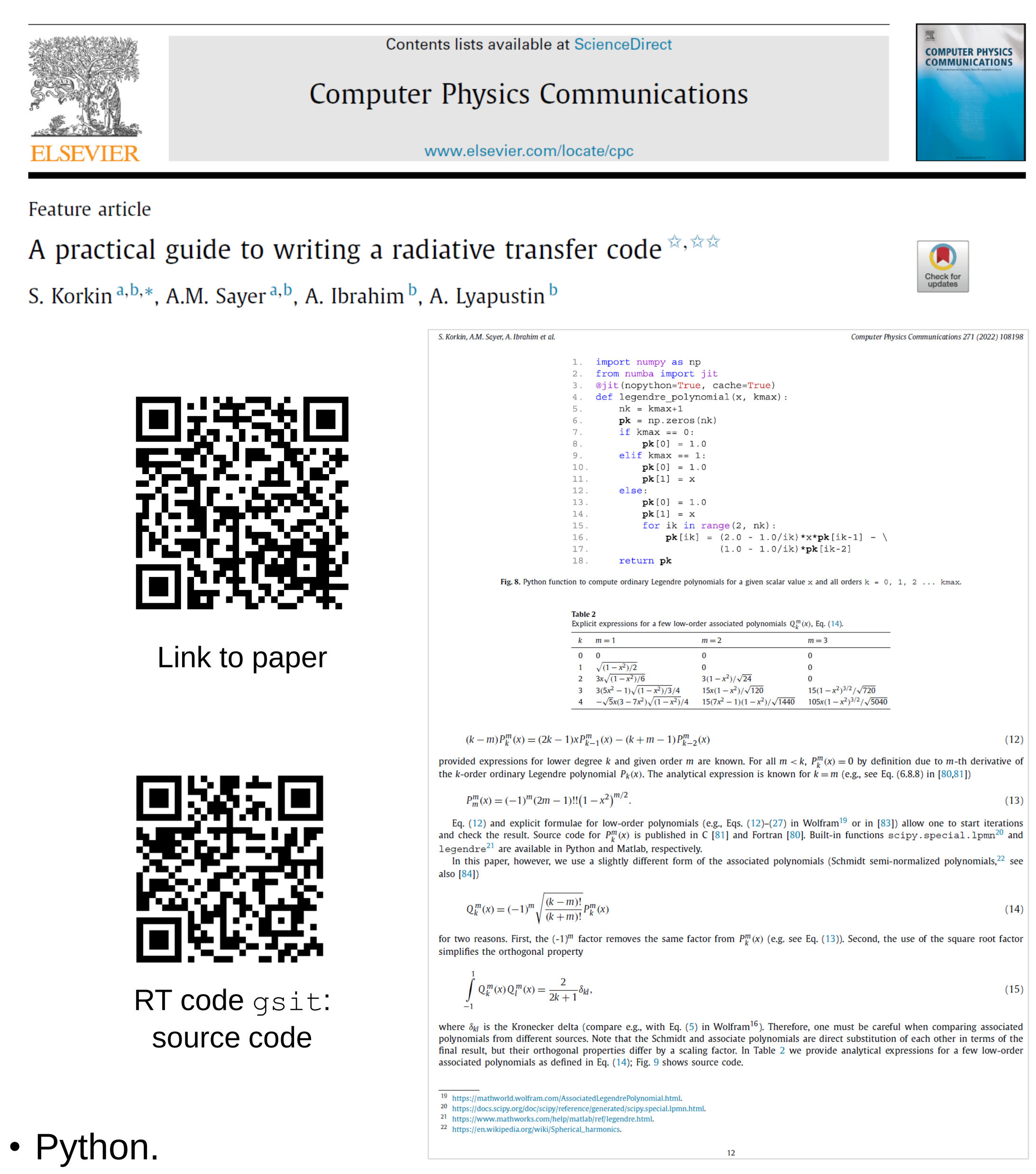
You need to get the RT work done "quickly"…



… but not at the expense of quality (understanding)

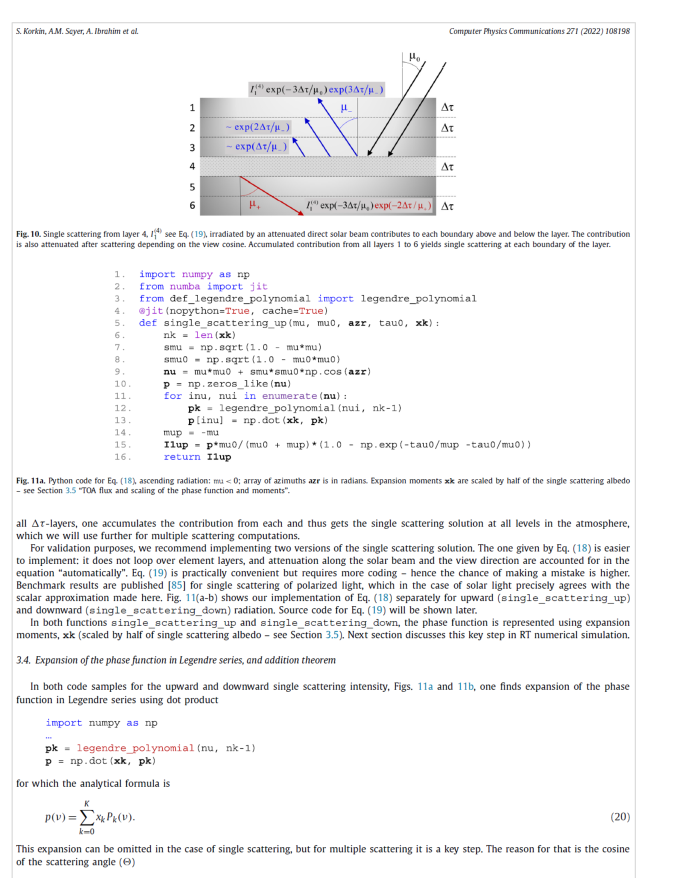
What do we propose? To bundle paper & code!

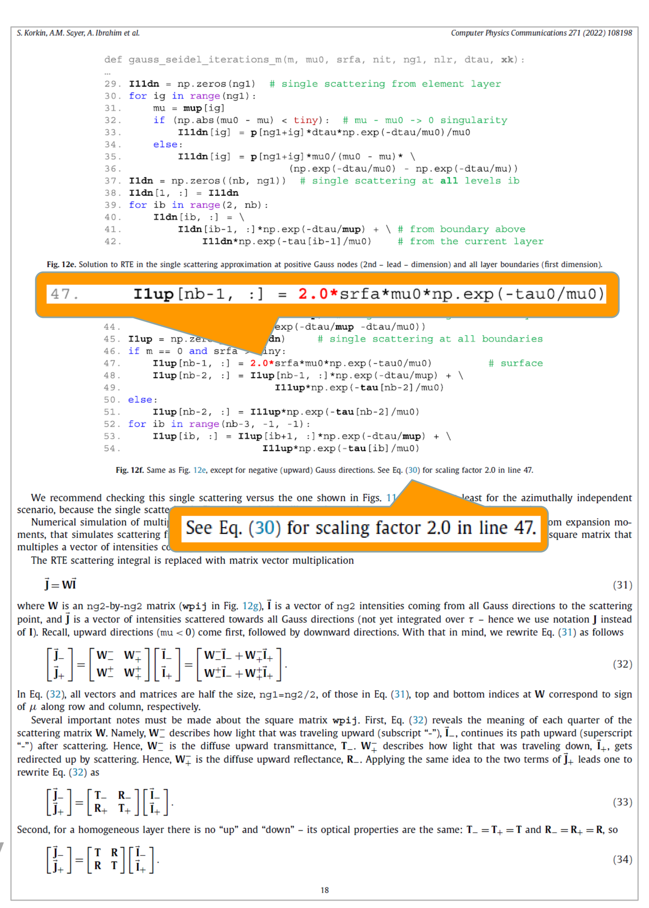
1. Multiple Scattering of Sunlight



General "strategy":

- Collocate equations (only necessary) with code snippets (short).
- Arrange these in an order natural for code development (e.g., starting from low-level function without dependencies).
- Find the right balance: practically valuable but not overcomplicated. Skip "necessary" but complicated physical effects for later paper(s).
- Provide reproducible tests (including unit tests for low-level functions).
- Try predict where the reader may have problems (likely, where you had!). Aim for ~1 month of work (full time). FYI: a typical NASA ROSES proposal is up to 3 yrs – coding for multiple scattering & spectroscopy & single scattering by particles (all together) should be done within 10% of the time.





- Python.
- Multiple scattering of monochromatic Solar light.
- Method of Gauss-Seidel iterations: relatively easy to code -- like successive orders: 2 methods for the price of one.
- User-defined solar-view geometry at TOA & BOA.
- Isotropic (Lambertian) surface.
- Single scattering correction.

- No polarization
- No BRDF (but we explain equations)
- No vertical profile (but we give algorithm)
- No truncation
- No Mie / spheroids
- No absorption spectroscopy

2. Line-by-Line Atmospheric Absorption Spectroscopy (in preparation)

- We have used LBL solver from Interpolation and Profile Correction (IPC) Method by *A. Lyapustin*, J. Atm Sci, 2003 -- QR-code:
- HPOSS22: "The paper-and-code bundle as a new paradigm supporting the TOPS initiative in Earth Science" (status = "selectable") -- thank you for considering our proposal

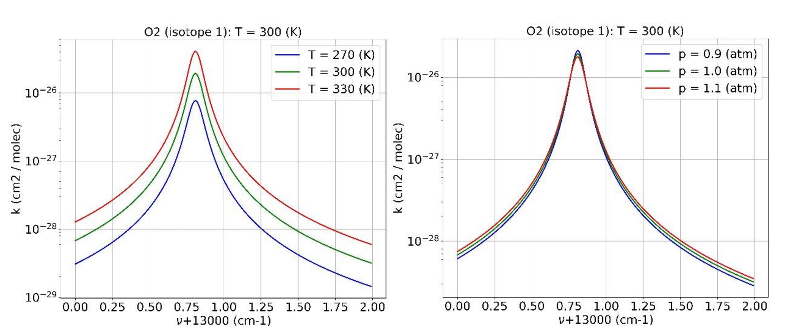
(A) We explain input & output in two modes: gas cell & atmospheric absorption (both use HITRAN)

```
molec_id  nu_usr_min  nu_usr_max  dnu    lcm  T_kelv  p_atm  fmt
6         4081.901    4505.699    0.002  8.0  296.0   1.0    k
```

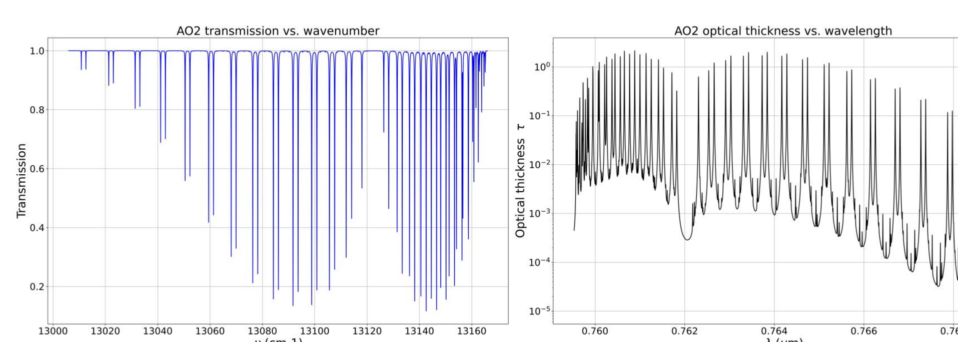
```
molec_id iatm column_amount nu_usr_min nu_usr_max dnu nzkm zkm[] fmt
7        6    -1.0          13050.0    13160.0    0.01 3   0.0 2.5 5.0  txt
```

```
7113000.816219 2.708E-27 1.740E-02.04580.047 1814.01040.67-.007400     b     1     X     1           R 13Q 14     d54644449 5 5 3 1 1     29.0    29.0
```

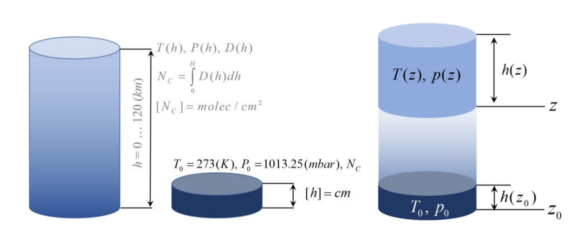
(B) We simulate 1 spectral line (*T* & *p* may vary)



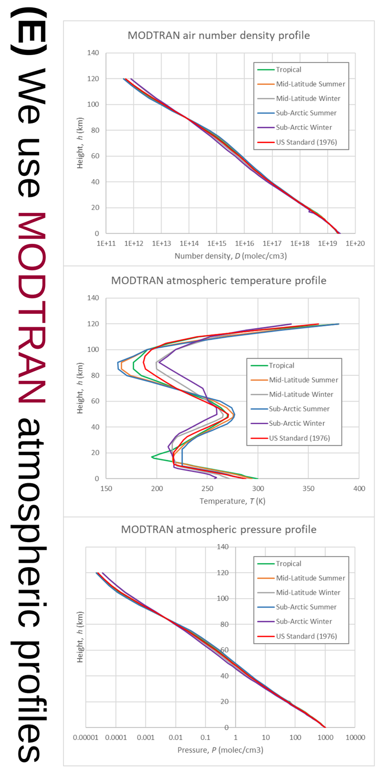
(C) Then we combine many lines to simulate absorption in a gas cell



(D) Atmosphere is a "stack" of gas cells



(E) We use MODTRAN atmospheric profiles



(F) We provide source code bundled with theory and reproducible results for all these steps