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## Abstract & Motivation

Rigorous protocols for instrument absolute calibration and data processing, developed and maintained by a dedicated international team for over three decades, have established AERONET as the global standard for aerosol research. **Software has been, and will continue to be, a crucial contributor to the project's success.**

### How about [ scientific ] software ?

Select appropriate topic of the abstract

- AERONET networks, operation, calibration, and instrumentations
- Ground Networks (SKYNET, Pandora, MPLNET, SPARTAN, ASCENT, AirNow, others) synergic deployment, science, and applications
- Atmospheric aerosols properties retrievals and applications using AERONET and other similar measurements.
- Satellite Validation and Calibration with AERONET data
- Model evaluation and assimilation using AERONET data
- AERONET data in applications (i.e., Air Quality, Climate, renewable energy, etc.)
- Nighttime aerosol monitoring using AERONET and its applications
- Maritime Aerosol Network (MAN) data and applications
- AERONET-OC Network, data, and application
- Innovative Applications of AERONET Data
- Advances in Instrumentation and Technology
- Collaborative Research and Partnerships
- others

Overlooked?  
Forgotten?  
Ignored?  
Underappreciated?

"Scientists spend an increasing amount of time building and using software. However, most scientists are never taught how to do this efficiently. As a result, many are unaware of tools and practices that would allow them to write more reliable and maintainable code with less effort."

Write program for people, not computers. ...  
Wilson + 12 (Canada, UK, US), "Best Practices for Scientific Computing", PLOS Biology (2014)

Maybe "it works" well and needs no further development ?

"The more frequently a program is changed, the more difficult it is to maintain its correctness. Scientific programs are frequently changed throughout their lifetimes, not just when they're young. For most scientific programs, the rate of change doesn't decrease significantly even after many years. Like sharks, scientific programs that aren't moving are dead."

Dubois, "Maintaining correctness in scientific programs", Computing in Science & Engineering (2005)

AERONET relies on various software including data processing (primarily implemented in C-language), and research (forward and inverse modelling - mostly in Fortran). This disparity between C and Fortran, and the lack of support for modern software development tools (Python, Intel MKL high-performance mathematical library, Doxygen) disrupts seamless data flow and hampers research progress.

Furthermore, scientific software serves both as a research tool and an object of study. As science evolves, the software undergoes modifications, often incorporating "temporary" patches that persist indefinitely within the codebase without proper documentation. Decades of extensive development without systematic cleanup inevitably turn software into "black boxes" with "spaghetti code".

"...several authors have argued that the "gap" or "chasm" between software engineering and scientific programming is a serious risk to the production of reliable scientific results, as demonstrated in a number of case studies."

Storer, "Bridging the Chasm: A Survey of Software Engineering Practice in Scientific Programming", ACM Computing Surveys (2017)

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"...we also demonstrate how moving to programming languages with high momentum, like modern C++, can help improve the sustainability, interoperability, and performance of research software."

Anzt et al., "Then and Now: Improving Software Portability, Productivity, and 100 x Performance", Computing in Science & Engineering (2024)

## Radiative Transfer (RT): Multiple Scattering of Sunlight



**2015**

NASA Earth Science Division  
Dr. Sergey Korkin  
GISTAR  
Goddard Space Flight Center  
National Aeronautics and Space Administration  
Greenbelt, MD 20771

**SELECTED**

Dear Dr. Korkin:  
We have assigned the evaluation of your proposal number Year Request to Code for V3 AERONET Reprocessing (18182119) to the following members of the Science Mission Directorate's Earth Science Division as members of NASA Earth Science's National Science Team (NST):  
Researcher: Alexander Straych (2024052014), Program Element A 30, Research Training Theory for Earth Science, NASA received a total of 12 proposals in response to the RTA and selected 22. A peer review panel evaluated all received proposals as well as the status of the current science objectives and improvements to Earth Science goals and objectives, as well as an analysis of cost.

**2017**

Journal of Quantitative Spectroscopy and Radiative Transfer  
Volume 180, October 2017, Pages 291-300

Vector radiative transfer code SORD: Performance analysis and quick start guide  
Sergey Korkin<sup>a,\*</sup>, Alexei Lyapustin<sup>b</sup>, Alexander Straych<sup>c</sup>, Brent Holben<sup>d</sup>, Alexander Babushnikov<sup>e</sup>

**vRT solver SORD:**

- Successive orders (replaced the original SOS vRT)
- Fortran 90/95
- Emphasis on the code "quality" for easy support:
  - Readability, comments
  - Structure
  - 50+ Tests (automatic mode)
  - Other people will read it!
- Interface between the solver and inversion code
- Publicly available: [https://github.com/korkins/SORD\\_QSRT\\_2017](https://github.com/korkins/SORD_QSRT_2017)

**2020**

AERONET Version 3 aerosol retrieval algorithm, associated uncertainties and comparisons to Version 2  
Alexander Straych<sup>a</sup>, Brent Holben<sup>b</sup>, Thomas F. Eck<sup>c</sup>, David M. Giles<sup>d</sup>, Poo Sathiaraj<sup>e</sup>, Sergey Korkin<sup>f</sup>, Alexei Lyapustin<sup>g</sup>, Alexander Babushnikov<sup>h</sup>, Mikhail Spiridonov<sup>i</sup>, and Brent Holben<sup>j</sup>

**SORD supported AERONET V3 reprocessing**

"We want it faster" (never ending requirement) & we need:

- to run it on a supercomputer
- to add fluxes, mix land & ocean
- TOA reflectance (was not provided on output by default)
- output "in the middle" of atmosphere (MLO observatory), etc.
- Multiple SZAs for MLO calibration (averaging)
- Add Cirrus to Aerosol & Rayleigh mix

**2024**

Implementation of the truncation/correction method on the AERONET polarized radiative transfer solver  
M. Momoi<sup>a</sup>, A. Siniuk<sup>b</sup>, T. Lapyonok<sup>c</sup>, E. Lind<sup>d</sup>, O. Dubovik<sup>e</sup>, S. Korkin<sup>f</sup>

**Faster SORD:**

- Did you see a poster by M. Momoi (GRASP) on Tuesday?
- Extension of Nakajima & Tanaka's technique (1988); with polarization Ota et al (2010) – both utilize DOM
- Phase matrix truncation + correction of higher orders of scattering (3 orders)
- No help from the original developer, who believes that:
  - The ONLY VALID MEASUREMENT OF CODE QUALITY: WTF/minute

**ROSES RST Proposal:**

"Fast Polarized RT Code for V3 AERONET Reprocessing"  
PI: S. Korkin, Collaborators: A. Lyapustin, A. Siniuk, and B. Holben

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Mid-2018: end of the proposal = end of support for RT code. If HQ supports AERONET shouldn't the code get something?

### Proposed To-do List for AERONET's RT Code (Solver):

Job Type	Task	Purpose
Software	Translate into C	Seamless integration with data processing part
Software	Documentation	Future support & development cost minimization
Software	GitHub / GitLab	Same + debugging + NASA's Open-Source Science
Software	Professional code review	Bring expertise from a skilled software engineer
Model	Spherical-shell	Low SZA & VZA; hybrid scan
Model	Linearization	Jacobians for inversion
Model	Output at given height	Elevated stations (e.g., MLO)
Science	Skip polarization in higher scattering orders	Further acceleration
Computing	Interface for parallel runs	Faster calculation of the Jacobians and/or data processing
Computing	Support of GPU	Yet more faster runs

- Document code(s) as "paper-and-code bundle"
  - Collocate necessary equations with short code snippets
  - Arrange these in an order natural for code development starting from low-level function without dependencies
  - Provide reproducible final and unit tests
  - Try predict where next developer may have problems
- Open-source code vs. open knowledge & experience: <https://github.com/korkins/gsit>

Computer Physics Communications  
Feature article  
A practical guide to writing a radiative transfer code

S. Korkin<sup>a,b,\*</sup>, A.M. Sayer<sup>a,b</sup>, A. Ibrahim<sup>b</sup>, A. Lyapustin<sup>b</sup>

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## LBL Atmospheric Absorption

(1) Original LBL code is part of another package:

HITRANonline  
Journal of Quantitative Spectroscopy and Radiative Transfer  
A practical guide to coding line-by-line trace gas absorption in Earth's atmosphere

(2) Paper under review: "A Practical Guide to Coding Line-by-line Trace Gas Absorption in Earth's Atmosphere"

2a: one Voigt line  
2b: Gas cell (no line mix)  
2c: MODTRAN profiles

(3) Open-source code for LBL absorption in gas cell (GCELL.cpp) and atmosphere (ASPECT.cpp):

Practical example for OCI: scaling of OT(WW) = WW x OT(1.43 cm) / 1.43 vs. true calculation

[https://github.com/korkins/aspect\\_gcell](https://github.com/korkins/aspect_gcell)

## Light Scattering by Spheroids

**Acknowledgments:**

- SK received FORTRAN sources from T. Lapyonok & O. Dubovik in September 2012 (AL received it way before)
- MAIAC has used the sources since then: SK – as is, AL – dropped polarization and converted the sources into C
- From O. Dubovik (private communication 2023/10/23 over email): "...we do have new version and plan to have radically new one ..."
- Anyone interested should refer to the GRASP website for a newer version of the (so called) spheroidal or DLS package

**Reasons for refactoring:**

- SK is learning things
- Numerical optimization (for our tasks)
  - Integrate over the size parameter  $x = r/\lambda$ , not  $r$
  - Use the fixed kernels grid – drop all splines
  - Improved interpolation of "polarized" elements
  - Remove ASCII format & hard-coded parameters
  - Fixed kernels generator – must be a separate code
- Clean up the code, convert to C (phase matrix)

**One Slide Documentation: In → Out**

Test Case 1  
Test Case 2

<https://github.com/korkins/spheroids> (code creating Fixed Kernels is yet to be refactored)