

Towards Unified Error Reporting (TUNER)

This is an application in reply to the ISSI/ISSI-BJ Joint Call for Proposals 2017 for International Teams in Space and Earth Sciences to the ISSI in Berne and refers to Earth Sciences using space data.

Abstract

The project “Towards Unified Error Reporting” (TUNER) aims at providing consistent and intercomparable error estimates for atmospheric temperature and composition measurements from space. Currently multiple retrieval methods are used by the different instrument groups, and along with this various approaches to error estimation are applied. Resulting errors are not always intercomparable. Some kinds of uncertainties are sometimes not reported at all. The different altitude resolutions and the different content of prior information in the data products is a particular problem.

Current scientific activities with satellite Earth observation data have a strong focus on validation and merging of data sets. The construction of long-term satellite data time series is of particular interest in the context of climate change. For all these satellite-data based activities the reliable characterization of the data in terms of uncertainties, altitude resolution, content of *a priori* information and error covariances is essential. While concepts exist to solve these problems in theory, these are only applicable to a subset of the algorithms used by the various groups.

Instead of dreaming of being provided with the perfect rigorous error estimates by all groups, it seems more adequate to face the fact that for some processors the rigorous error estimates cannot be provided and workarounds have to be developed instead. These include: calibration of the error estimates to each other in order to make them inter-comparable; assessment of altitude resolutions where no averaging kernels are provided; estimation of systematic or parameter errors for data sets where they are not routinely provided; and development of recipes to make retrieval errors comparable for instruments with different altitude resolutions.

The success of this project depends on the participation of representatives from each retrieval group in order to have first hand information about algorithms and corresponding metadata and to make sure that the recommendations developed in the frame of this project will be finally accepted by the respective groups.

1 Scientific Rationale, Goals, and Timeliness of the Project

Global data sets on atmospheric temperature and composition as provided by satellites play an increasing role in the context of climate change. Methods to make best use of the data include merging of data from different sources into long-term time series, data assimilation, model validation etc. The quantitative use of satellite data depends on reliable data characterization in terms of metadata such as retrieval error estimates, altitude resolution, and content of prior information. This is of concern for all quantitative applications, like validation, data assimilation, or diagnosis of model results, but particularly of concern to the generation of merged data products. In the latter case, the optimal weight of a parent data set in the merged data depends inversely on the uncertainty.

Thus, inadequate error estimates directly affect the merged climate data product. When merging data with different vertical resolutions reported profile error estimates are not directly comparable. The content of *a priori* information in the retrievals is a particular challenge.

A rigorous method of error estimation is available [1]¹ but it is only applicable to retrievals that use optimal estimation or similar approaches which provide the required diagnostic matrices. However, there are numerous data products to which this methodical framework is inapplicable.

Another unsolved problem is that validation studies often provide evidence that the theoretical error estimates are too optimistic, which hints at missing error sources in the error estimation procedure. These inconsistencies, however, are not usually taken as a basis for refinement of the error budget. Natural variability of the atmospheric state and non-optimal co-location of the compared measurements are often blamed for these inconsistencies without providing further quantitative assessments.

Within the ‘Towards Unified Error Reporting (TUNER)’ project the various error estimation methods for temperature and trace gas retrievals shall be scrutinized and compared. Related satellite missions under consideration are MIPAS, Odin/OSIRIS, OMPS-LP, Odin/SMR, AIRS, SBUV, AURA/MLS, SOFIE, SABER, AURA/TES, GOME, SCIAMACHY, GOME-2, ACE-FTS and GOMOS. Recipes shall be developed which allow to adjust the uncertainty estimated from the various instruments to each other to make them consistent and intercomparable.

The following specific actions are foreseen:

1. A systematic assessment of the error estimation schemes used by the different groups will be made and their adequacy will be evaluated. In particular, approximated methods of error estimation will be tested against the full matrix-based scheme. What is adequate for one mission can be inadequate for another.
2. Standards for estimating parameter errors and systematic errors will be developed. These issues require additional clarification, as became evident from the analysis of replies to a related questionnaire distributed among the instrument scientists during preparation of this proposal. A further important issue is to identify the most adequate way to compare errors for instruments with different vertical resolutions and to communicate the *a priori* content of the data to the user.
3. In this project we will use high resolution in-situ measurements and model simulations (already available) to gain information about magnitude and patterns of natural variability in order to accurately attribute and isolate a fraction of the residual differences due to the natural variability.
4. Unexplained differences (i.e. explained neither by error bars nor by natural variability) between measurements will be investigated. If the same quantity is measured by three or more instruments, correction factors for the precision estimates of each instrument can be obtained by solving a system of linear equations. These correction factors minimize the unexplained differences between the measurements.
5. For some satellite data sets the quantities necessary to evaluate the full error budget are not available (particularly parameter errors and averaging kernels). Alternative ways of error estimation will be tested

¹However, parts of this method have been challenged by [2].

(perturbation studies; emulation of the respective data processors by other processors which have the full matrix formalism available). For data products without averaging kernels, altitude resolutions will be estimated and approximate averaging kernels will be constructed.

6. Standards on the unified and unambiguous reporting of the estimated retrieval errors will be developed.
7. A tutorial document will be created to help data users to correctly account for the uncertainties in the data. The focus will be on the correct combination of different error components, grid interpolation issues, and the application of averaging kernels.

This methodical work shall be applicable to all trace gases and most other state variables (temperature, aerosols, etc) measured by the instruments involved but since almost all instruments measure ozone, it seems adequate to select this particular gas as a paradigm case for methodical development.

TUNER has been selected as an emerging SPARC activity. TUNER-ISSI will be embedded in the overarching TUNER-SPARC activity. It may now be the last chance to carry out these activities, because for most of the missions of the “Golden Age of Earth Observation” the retrieval experts are still available but it is not at all clear how long they will still have the opportunity to work on their missions. Any delay may imply loss of expert knowledge.

2 List of the Expected Output

1. Recommendations addressed to instrument scientists including recipes for error estimation which lead to intercomparable, consistent error estimates;
2. Recommendations addressed to data users including recipes on how to transform the error estimates and averaging kernels when the profile data are interpolated from the native altitude grid to a user-defined grid; recipes on how to deal with error estimates of data of different altitude resolution; recipes on how to use error covariances when available.
3. Approximate averaging kernels for data products where the averaging kernels are not routinely produced.
4. The error estimation approaches developed in the framework of this project will be implemented by some groups and their applicability will be tested. Complete error budgets will be provided for selected data sets.
5. Journal papers based on the results of this project shall be published in a special issue of the journal “Atmospheric Measurement Techniques”. One executive editor of this journal has already encouraged submission of a proposal for this special issue.

The metadata (uncertainty estimates including error correlations and averaging kernels) and related documentations will be essential for scientists who intend to validate satellite data, to construct a merged data product, to assimilate the data, to analyze time series, or to validate models.

3 Added Value by ISSI

Due to the nature of this project (which is harmonization and unification of error estimation methods), its success will critically depend on communication between the involved scientists. The ISSI facilities and communicational/computational resources are ideal to bring the experts together for productive meetings. It is important to have dedicated meetings for the TUNER project to guarantee concentrated work. The obligations, strict schedule, etc required by the ISSI rules will guarantee that progress will be made.

4 Schedule

4.1 Preliminary and Overarching Activities

In preparation to this project, a questionnaire has been distributed among the satellite groups with a list of questions regarding to error estimation and reported metrics. Based on the collected responses, some aspects

of error reporting were found most challenging by the instrument community, including the treatment of parameter errors, altitude resolution and error covariance. Thus TUNER will specifically focus on resolving these issues. A TUNER-SPARC meeting has been scheduled for June 2017. It will be open to the entire team and will cover a wider range of topics than those listed above. During this meeting, a detailed work plan will be decided and the work-packages will be distributed to the participating experts.

4.2 Activities directly linked to TUNER-ISSI

While the general TUNER project includes also data users, modelers, etc., the TUNER ISSI International team meetings will be mainly limited to the instrument and retrieval scientists and the agendas will be focused on the instrument related topics. Within ISSI the focus will be on coordination of the activities and harmonization of the concepts. For technical work, it is assumed that at least some of the participating groups will allocate external funding.

M0: Kickoff teleconference; the purpose of the teleconference is to define the first steps and to schedule the TUNER-ISSI-related activities. We assume that this kickoff-teleconference will take place after the TUNER-SPARC meeting (after June 2017).

M1-M4: Based on existing validation papers, an assessment of the adequacy of the error estimation schemes will be made.

M5: First ISSI International Team meeting: Reporting of Results of the error assessment; identification of workaround strategies for missing metadata, identification of the best strategy for each instrument.

M6-M14: Formulation and development of recommendations for error estimation and reporting; generation of workaround tools.

M15: Second ISSI International Team meeting: Revision of the workarounds; Discussion and revision of error estimation recommendations; planning of publications.

M16-M24: Generation of unified error reports for data sets of involved satellite missions. Publication of results.

Mx-My reads from month x to month y after kickoff.

5 Team

5.1 General Rationale

It is not possible to include a representative of each satellite instrument considered. However, care has been taken to include at least one representative of each type of instrument / retrieval scheme in order to have adequate expertise onboard. These experts are supposed to collect information also from instrument teams not directly included in the TUNER project.

In this phase of the project the scope will be restricted to passive space-borne sensors. Extension towards other missions (LIDAR, radio occultation, in situ, other platforms) is left for possible follow-up activities.

The SPARC-TUNER activity includes also scientists not directly involved in a particular space mission (modelers etc). SPARC-ISSI will draw upon their expertise and they are intended to be admitted to the TUNER-ISSI meetings as self-supported experts.

5.2 List of Team Members

1. Thomas von Clarmann (KIT/IMK; MIPAS; team leader);
2. Adam Bourassa (Univ. Saskatchewan; Odin/OSIRIS);
3. Doug Degenstein (Univ. Saskatchewan; OMPS-LP and Odin/OSIRIS);
4. Patrick Eriksson (Chalmers; Odin-SMR);
5. Fredrick Irion (NASA-JPL, AIRS);
6. Natalya A. Kramarova (NASA-GSFC, SBUV and OMPS-LP);
7. Nathaniel Livesey (NASA-JPL; AURA-MLS);
8. Tom Marshall (SOFIE, SABER);
9. Vivienne Payne (NASA-JPL; AURA-TES);
10. Alexei Rozanov (Univ. Bremen; GOME, SCIAMACHY, GOME-2);
11. Patrick Sheese (Backup: Kaley Walker) (Univ. Toronto; ACE-FTS);
12. Viktoria Sofieva (Finnish Meteorological Institute, GOMOS);

Some further self-supported experts will complement the team.

6 Facilities required

- Meeting room with projector;
- Access to the Internet;
- (ideally but not mandatory) online access to relevant journals which are not open access, particularly J. Geophys. Res., including back issues.

7 Financial Support Required

Per diem and accommodation for 12 team members for 2 one-week meetings at ISSI, Berne; in addition 2 return railway tickets Karlsruhe-Berne (2nd class, Halbtaxabo and Bahncard50 available) for the team leader. Young scientist support according to the ISSI rules.

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A CVs of the Team Members

PD Dr. Thomas von Clarmann

Contact: thomas.clarmann@kit.edu

phone: +49-721-60825946

fax: +49-721-60824742

Affiliation: Karlsruhe Institute of Technology, Institute of Meteorology and Climate Research (KIT/IMK);

Role in the project: Team leader; Expert for MIPAS;

Current Position: Head of the IMK satellite remote sensing group (since 1995);

Former Positions: Postdoc, then staff scientist at Forschungszentrum Karlsruhe (1990-1995);

Education: Habilitation in meteorology (2003, Karlsruhe, Germany);

Dr. rer. nat (equivalent to PhD) (1989, Karlsruhe, Germany);

Diploma in meteorology (1986, Munich, Germany);

Services in National and/or International Committees: Member of MIPAS-QWG, ALTIUS-MAG;

Honors: “La Recherche 2014 – Environment” by the French journal La Recherche, for the ACP paper on combined IASI and GOME-II ozone retrievals.

Envisat Medal by ESA, 2003;

Award (Jahresprämie für wissenschaftliche Leistungen) by Forschungszentrum Karlsruhe for work on MIPAS-B, 1993

Relevant publications:

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Prof. Dr. Douglas A. Degenstein

Contact: doug.degenstein@usask.ca

phone: +1 (306) 966-6447

fax: +1 (306) 966-6400

Affiliation: University of Saskatchewan;

Role in the project: Team co-leader; expert representing Odin-OSIRIS and OMPS-LP;

Current Position: Professor of Physics and Engineering Physics at the University of Saskatchewan (1999-present);

Education: PhD in Atmospheric Remote Sensing (1999, University of Saskatchewan, Canada);

B.Sc. in Engineering Physics (1993, University of Saskatchewan, Canada);

B.Sc. in Computer Science (1988, University of Saskatchewan, Canada);

Services in National and/or International Committees: Past member of the Space and Atmospheric Environments Advisory Committee (SAEAC); OSIRIS PI;

Relevant publications:

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Dr. Nathaniel J. Livesey

Contact: Nathaniel.J.Livesey@jpl.nasa.gov

phone: +1 818 354 4214

fax: +1 818 393 5065

Affiliation: NASA Jet Propulsion Laboratory and California Institute of Technology;

Role in the project: Team co-leader; expert for the Microwave Limb Sounder (MLS) instruments on Aura and UARS;

Current Position: Principal Investigator for Aura MLS.

Education: D. Phil in Atmospheric Physics (1995), University of Oxford, United Kingdom.

B.A. degree in physics (1991), University of Oxford, United Kingdom

Services in National and/or International Committees: MLS science team, Aura science team

Honors: 2006 NASA Exceptional Achievement Medal “In recognition of exceptional accomplishment for the design and implementation of the retrieval algorithms for the Aura Microwave Limb Sounder to extract critical atmospheric information.”

1999 NASA Exceptional Achievement Medal “For development of data processing algorithms that allowed reduction in Upper Atmosphere Research Satellite Microwave Limb Sounder operational power consumption, and enabled the delivery of the MLS version 5 data, the most ambitious version of UARS MLS data products.”

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Prof. Dr. Adam E. Bourassa

Contact: adam.bourassa@usask.ca

phone: +1-306-966-1418

fax: +1-306-966-6400

Affiliation: University of Saskatchewan;

Role in the project: Expert for OSIRIS;

Current Position: Associate Professor, University of Saskatchewan, Canada (2008-present);

Former Positions: Research Scientist, Science Systems and Applications, Inc., NASA-Langley, Hampton, Virginia (2007-2008);

Education: Ph.D. Physics and Engineering Physics (2007, Saskatchewan, Canada);

Services in National and/or International Committees: OSIRIS Deputy-PI, CATS Science Team;

Relevant publications:

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Prof. Dr. Patrick Eriksson

Contact: patrick.eriksson@chalmers.se

phone: +46-31-7721832

fax: +46-31-7721884

Affiliation: Chalmers University, Gothenburg;

Role in the project: Expert for Odin-SMR;

Current Position: Professor, Chalmers University of Technology;

Former Positions: Other research positions at Chalmers University of Technology, post doc at Bremen University;

Education: PhD in Environmental Sciences and MSc in Engineering Physics, both at Chalmers University of Technology, Sweden;

Services in National and/or International Committees: Member of Odin-SMR science team and Metop SG MWI/ICI science advisory group.

Relevant publications:

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Dr. Fredrick W. Irion

Contact: bill.irion@jpl.nasa.gov

phone: +1 818-393-4337

fax: +1 818.354.3223

Affiliation: NASA Jet Propulsion Laboratory;

Role in the project: Expert for AIRS;

Current Position: Research Scientist with NASA JPL (since 2004);

Former Positions: Scientist with NASA JPL (1999-2004);

Caltech Post-Doctoral Scholar (1996-1999);

Staff Researcher, California Institute of Technology (1996);

Graduate Research Assistant, California Institute of Technology (1989-1995);

Education: B.A.Sc, Chemical Engineering, University of Ottawa (1988);

M.S., Chemical Engineering, California Institute of Technology (1992);

Ph.D., Chemical Engineering with minor in Planetary Science, California Institute of Technology (1996);

Relevant publications:

F. W. Irion, M. Brown, G. C. Toon and M. R. Gunson, Increase in atmospheric CHF₂Cl over southern California from 1985 to 1990, *Geophys. Res. Lett.*, 21, 1723-1726, 1994.

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Dr. Natalya A. Kramarova

Contact: natalya.a.kramarova@nasa.gov

phone: +1-301-614-5115

fax: +1-301-614-5903

Affiliation: NASA Goddard Space Center;

Role in the project: Expert for SBUV and OMPS;

Current Position: Lead Research Scientist, Science Systems and Applications Inc., NASA Goddard Space Center, Greenbelt, MD, USA;

Education: Ph.D. Degree in Physics and Mathematics (2007), Moscow State University, Moscow, Russia;
MS degree in physics (2000), Moscow State University, Moscow, Russia;

Advisory boards, panels, etc.: OMPS LP Science Team;

Relevant publications:

Kramarova, N. A., Bhartia, P. K., Frith, S. M., McPeters, R. D., and Stolarski, R. S.: Interpreting SBUV smoothing errors: an example using the quasi-biennial oscillation, *Atmos. Meas. Tech.*, 6, 2089-2099, doi:10.5194/amt-6-2089-2013, 2013.

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Mr. Benjamin T. Marshall

Contact: b.t.marshall@gats-inc.com
phone: +1-757-952-1045
fax: +1-757-873-5924

Affiliation: GATS

Role in the project: Expert for SABER and SOFIE;

Current Position: Chief Technology Officer, GATS, Newport News, Virginia (1986-present);

Former Positions: Data Analyst, SASC, Inc. (later to become Hughs-STX and now part of Raytheon), NASA-Langley, Hampton, Virginia (1982-1986);

Education: M.S. Geophysics (1981), Georgia Institute of Technology;

Services in National and/or International Committees: SABER and SOFIE Science Teams;

Honors: NASA Group Achievement Awards for SABER and LIMS data analysis, 2003;

Relevant publications:

Marshall, B. T., Deaver, L. E., Thompson, R. E., Gordley, L. L., McHugh, M. J., Hervig, M. E., and Russell, J. M. III, Retrieval of temperature and pressure using broadband solar occultation: SOFIE approach and results, *Atmos. Meas. Tech.*, 4, 893-907, 2011.

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Dr. Vivienne H. Payne

Contact: Vivienne.H.Payne@jpl.nasa.gov

phone: +1 818 354 0353

fax: +1 818 393 5065

Affiliation: NASA Jet Propulsion Laboratory;

Role in the project: Expert for the Aura Tropospheric Emission Spectrometer;

Current Position: Group Supervisor, Tropospheric Composition, JPL.

Education: D. Phil in Atmospheric Physics (2006), University of Oxford, United Kingdom;

M.Phys degree in Physics (2001), University of Edinburgh, United Kingdom;

Services in National and/or International Committees: TES science team, Aura science team, Suomi-NPP science team;

Honors: NASA Group Achievement Awards for contributions to the success of the Global Precipitation Measurement Mission (2015) and the Aura Tropospheric Emission Spectrometer (2014);

Relevant publications:

Oetjen, H., V. H. Payne, J. L. Neu, S. S. Kulawik, D. P. Edwards, A. Eldering, H. M. Worden and J. Worden, A joint data record of tropospheric ozone profiles from Aura-TES and MetOp-IASI, *Atmos. Chem. Phys.*, 16, 10229-10239, doi:10.5194/acp-16-10229-2016 (2016)

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Dr. Alexei Rozanov

Contact: alex@iup.physik.uni-bremen.de
phone: +49-421-21862084
fax: +49-421-21862070

Affiliation: University of Bremen;

Role in the project: Expert for SCIAMACHY, GOME, GOME-2, OMPS;

Current Position: Head of the IUP Bremen SCIAMACHY limb group ;

Education: Dr. rer. nat (equivalent to PhD) (2001, University of Bremen, Germany);
Diploma in physics (1994, University of St. Petersburg, Russia, 1994);

Services in National and/or International Committees: SCIAMACHY-QWG;

Relevant publications:

Gebhardt, C., Rozanov, A., Hommel, R., Weber, M., Bovensmann, H., Burrows, J. P., Degenstein, D., Froidevaux, L., and Thompson, A. M.: Stratospheric ozone trends and variability as seen by SCIAMACHY from 2002 to 2012, *Atmos. Chem. Phys.*, 14, 831-846, doi:10.5194/acp-14-831-2014, 2014.

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Dr. Patrick E. Sheese

Contact: psheese@atmosph.physics.utoronto.ca
phone: +1-416-978-7796

Affiliation: University of Toronto;

Role in the project: Expert for ACE-FTS;

Current Position: Research Associate, University of Toronto, Canada (2013-present);

Former Positions: Postdoctoral Fellow, University of Toronto, Canada (2010-2013);
Postdoctoral Fellow, University of Saskatchewan, Canada (2009-2010);

Education: Ph.D. in Earth and Space Science (York University, Toronto, Canada);
B.Sc. in Physics and Astronomy (York University, Toronto, Canada);

Relevant publications:

Sheese, P. E., K. A. Walker, C. D. Boone, P. F. Bernath, L. Froidevaux, B. Funke, P. Raspollini, and T. von Clarmann, ACE-FTS ozone, water vapour, nitrous oxide, nitric acid, and carbon monoxide profile intercomparisons with MIPAS and MLS, *J. Quant. Spectrosc. Radiat. Transf.*, 186, 62-80, 2017.

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Dr. Viktoria Sofieva

Contact: viktorija.sofieva@fmi.fi

phone: +358-29-5394698

fax: +358-29-5393146

Affiliation: Finnish Meteorological Institute;

Role in the project: Expert for GOMOS;

Current position: Senior research scientist (since 2000), Earth Observation Department, Finnish Meteorological Institute;

Education: Doctor of Science in Technology (Helsinki University of Technology, 2005);

Master of Science (Moscow Institute of Physics and Technology, 1990);

Services in National and/or International Committees: GOMOS-QWG, ALTIUS Science Team;

Relevant publications:

Sofieva, V. F., Kalakoski, N., Pivrinta, S.-M., Tamminen, J., Laine, M., and Froidevaux, L.: On sampling uncertainty of satellite ozone profile measurements, *Atmos. Meas. Tech.*, 7, 1891-1900, doi:10.5194/amt-7-1891-2014, 2014, <http://www.atmos-meas-tech.net/7/1891/2014/>

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Prof. Dr. Kaley A. Walker

Contact: kaley.walker@utoronto.ca

phone: +1-416-978-8218

fax: +1-416-978-8905

Affiliation: University of Toronto;

Role in the project: Back up expert for ACE-FTS;

Current Position: Associate Professor, Department of Physics, University of Toronto, Toronto, CANADA (2011-present);

Former Positions: Assistant Professor, Department of Physics, University of Toronto, Toronto, CANADA (2006-2011);

Research Assistant Professor, Department of Chemistry, University of Waterloo, Waterloo, CANADA (2001-2006);

Education: Ph.D. in Physical Chemistry (1998, University of British Columbia, Vancouver, CANADA);

B.Sc. in Honours Applied Chemistry (1992, University of Waterloo, Waterloo, CANADA);

Services in National and/or International Committees: Deputy Mission Scientist for ACE; SCISAT/ACE science team;

Relevant publications:

Sheese, P. E., K. A. Walker, C. D. Boone, P. F. Bernath, L. Froidevaux, B. Funke, P. Raspollini, and T. von Clarmann, ACE-FTS ozone, water vapour, nitrous oxide, nitric acid, and carbon monoxide profile intercomparisons with MIPAS and MLS, *J. Quant. Spectrosc. Radiat. Transf.*, 186, 62-80, 2017.

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