RadLib: a radiative heat transfer model library for CFD

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Abstract

Ca. 100 words

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Nr.	Code metadata description	Metadata
C1	Current code version	TODO 2.1
C2	Permanent link to code/repository used for this code version	*github.com/BYUignite/radlib*
C3	Code Ocean compute capsule	(in review)
C4	Legal Code License	MIT license (MIT)
C5	Code versioning system used	Git
C6	Software code languages, tools, and services used	C++, Python 3
C7	Compilation requirements, operating environments & dependencies	CMake, C++, Python 3, Cython
C8	If available Link to developer documentation/manual	TODO
C9	Support email for questions	davidlignell@byu.edu

Table 1: Code metadata.

1. Motivation and significance

Modeling radiative heat transfer, and particular radiation absorption coefficients, for CFD is complex and challenging. More specifically, combustion simulations are often complicated by the need for accurate radiation modeling, which can be difficult to implement and computationally expensive

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relative to simulation cost. As a result, researchers typically manufacture configurations in which radiation can be safely ignored, which can lead to results inapplicable to practical systems, or use oversimplified models and assumptions, which can produce inaccurate results. Unfortunately, these approaches are neither rigorous nor applicable to real engineering systems.

In some cases, other modes of heat transfer dominate the system, and radiation can be safely neglected, but many practical engineering systems do not allow this. Simple jet flames, for example, demonstrate both possibilities: early in a flame's development, convection typically dominates heat transfer and dictates flame behavior; late-stage flame phenomena like soot behavior and flame sheet breakthrough, however, increasingly depend on the magnitude of radiative heat losses and cannot be simulated accurately without a radiation model.

Like combustion, the core mechanisms of radiation are physically and mathematically complex. Unlike other modes of heat transfer, it is governed by a set of integro-differential equations that depend on both direction and wavelength. Only the simplest systems have analytic solutions, and most practical systems require a numerical solution. Ray tracing (Monte Carlo) solutions are very accurate but extremely computationally expensive, and often require high-performance computing resources to execute. Modeling assumptions are common and can reduce simulation cost at the expense of accuracy, depending on their validity for the system in question.

Currently, there is no convenient or easy-to-use access point for CFD radiation models. As such, we present RadLib, a modular library of radiation models that can be applied alongside various simulation tools. RadLib focuses on calculation of radiation absorption coefficients, often the most difficult and time-consuming portion of radiation calculations, which permits its use with various solvers. The models are fully implemented and validated and all use a common interface, allowing researchers easy and convenient access to radiation modeling tools regardless of the field of application.

2. Model descriptions

RadLib includes three models of varying complexity and accuracy to calculate the radiation absorption coefficients and their weighting factors for each gas considered by the model. Radiation absorption coefficients are typically calculated using correlations relating them local properties such as temperature, total pressure, or species partial pressure, depending on the model. Correlations come from curve fits to high-resolution radiation property databases. At present, RadLib considers up to four gas species (H_2O,

CO, CO_2, and CH_4) and, optionally, soot volume fraction in its calculation of absorption coefficients and weighting factors.

Once the radiative absorption coefficients are calculated, they are then used to solve the radiative transfer equation (RTE), which depends on the simulation configuration and assumptions. Solving the RTE is not the focus of this software, but RadLib's example cases do employ a simple implicit trapezoid method solver to calculate the radiative heat flux and volumetric heat source profiles between two parallel planes. [MORE DESCRIPTION OF SOLVER GOES HERE?]

[OTHER THINGS THAT APPLY TO ALL MODELS GO HERE]

[MAYBE INCLUDE SOME BASIC INFO ON LBL?]

2.1. Planck Mean absorption coefficients

RadLib's simplest model uses Planck Mean absorption coefficients calculated from the correlations given on the TNF Workshop site [1]. The temperature-dependent correlations are based on the RADCAL model in [2]. The TNF radiation model is also documented in [3].

Planck Mean absorption coefficients are commonly used to model radiation, especially in combustion systems, because the model is relatively easy to implement, computationally inexpensive, and reasonably accurate in many cases. The TNF Workshop correlations were developed for use with an optically thin radiation model, which assumes that radiation passes through a medium mostly undisturbed. In cases where the optically thin assumption applies, such as simple hydrogen jet flames, this model and the associated Planck Mean absorption coefficients can produce accurate results [4]. In cases where the optically thin assumption is not reasonable, including many other combustion scenarios, this model does not produce accurate results. For example, it significantly overpredicts radiative losses from the TNF library's CH_4 flames [5, 6, 7].

Because RadLib does not specify case geometry or medium, there is no optically thin assumption inherent in its use of the Planck Mean absorption coefficients. However, the correlations were developed with the intention of use with an optically thin assumption, and, as a result, depend only on local temperature values. RadLib users must take care to consider these limitations before using this model.

2.2. Weighted sum of gray gases (WSGG)

The basic assumption of weighted sum of gray gases (WSGG) models in general is that the non-gray behavior of gas mixtures, in this case H_2O and CO_2, can be modeled by a weighted sum of several gray gases and one transparent gas (which represents the spectral windows between absorption bands). RadLib uses the WSGG model presented by Bordbar et al. [8, 9], which uses correlations based on the HITEMP 2010 database [10]. RadLib, in accordance with the Bordbar et al. WSGG method cited above, uses a mixture of four gray gases and one transparent gas. Absorption coefficients are calculated by

$$K_i = \sum_{k=0}^{4} d_{i,k} M_r^k, \tag{1}$$

where K_i is the absorption coefficient for species i, $d_{i,k}$ is a species-specific correlated model coefficient, and M_r is the molar ratio $Y_{\mathrm{H_2O}}/Y_{\mathrm{CO_2}}$. The weight factors are calculated by

$$a_i = \sum_{j=0}^{4} b_{i,j} T_r^j, \tag{2}$$

where a_i is the weighting factor for species i and T_r is a normalized temperature equal to T/T_{ref} with $T_{ref} = 1200$K. The value of $b_{i,j}$ is calculated by

$$b_{i,j} = \sum_{k=0}^{4} C_{i,j} M_r^k, \tag{3}$$

where $C_{i,j}$ is another correlated model coefficient and M_r is the molar ratio $Y_{\mathrm{H_2O}}/Y_{\mathrm{CO_2}}$ as above. The model coefficients $d_{i,k}$ and $C_{i,j}$ can be found in the literature [8, 9]. RadLib uses the updated model coefficients from [9], which extends the model presented in [8] to include all possible values of the H_2O-CO_2 molar ratio.

2.3. Rank Correlated SLW (RCSLW)

The Spectral Line Weighted-sum-of-gray gases (SLW) model represents a family of global approaches to radiative heat transfer in high-temperature gases that also includes Absorption Distribution Function (ADF) and Full Spectrum k-distribution (FSK) models, all of which are based on the same fundamental principle in modeling the gas absorption spectrum [11]. In order to extend their spectral models from uniform conditions (isothermal, homogeneous gases) to nonuniform conditions (non-isothermal, non-homogeneous gases), these models take a reference approach in which local gas states are corrected relative to a reference state. Reference approaches, however, generally lack consistent reference states and can yield significant errors in cases with large spatial temperature gradients [12]. The Rank Correlated SLW (RCSLW) model is a unique extension of the generalized SLW model that does not require a specified gas reference state and preserves the emission term of the spectrally integrated RTE. Recent comparison of advanced SLW modeling approaches revealed that "the Rank Correlated SLW model is the most robust of all models, and demonstrates that it can achieve accurate solutions with as few as 3–5 gray gases" [13]. A brief overview of the general SLW and RCSLW models will be given here; detailed discussion can be found in the literature [14, 15, 16, 17, 18, 11, 12, 19].

The radiative transfer equation (RTE) for an absorbing, emitting, and non-scattering medium along a given path length s in a direction $\hat{\Omega}$ is given by

$$\frac{dI_\eta}{ds} = -\kappa_\eta I_\eta + \kappa_\eta I_{b\eta}, \tag{4}$$

where I_η is the radiative spectral intensity, $I_{b\eta}$ is the Planck spectral distribution of blackbody intensity, and κ_η is the spectral absorption coefficient of the medium. Integrating with respect to wavenumber and subdividing the absorption cross-section into gray gases gives the SLW form of the RTE:

$$\frac{dI_j}{ds} = -\kappa_j I_j + a_j \kappa_j I_b, \qquad j = 0, 1, ..., n. \tag{5}$$

Here, n is the number of gray gases in the model and I_j is the intensity of gray gas j. κ_j is the gray gas absorption coefficient, which can be calculated as $\kappa_j = N\sqrt{C_{j-1}C_j}$, where C_{j-1} and C_j are supplemental absorption cross-sections used to discretize the absorption spectrum [15]. The gray gas weights corresponding to each absorption coefficient are given by $a_j = F(C_j) - F(C_{j-1})$, where $F(C_j)$ is the absorption line blackbody distribution function (ALBDF) for species j, calculated from the detailed absorption spectrum of that species. The absorption cross-sections are chosen with respect to a thermodynamic reference state, which makes generalized SLW methods reference approaches. Once Equation 5 is solved for each gray gas species, to total radiative intensity I can be calculated by summing the gray gas intensities:

$$I = \int_{\eta=0}^{\infty} I_\eta d\eta = \sum_{j=1}^{n} I_j. \tag{6}$$

The Rank-Correlated SLW (RCSLW) model avoids specifying a reference state by relating thermodynamic states to one another instead. If two arbitrary absorption cross-sections define identical wavenumber intervals, the two cross-sections (neither of which is designated a reference cross-section) can be said to be rank-correlated. The inverse ALBDF, defined such that $C[F(C, \phi_g, T_b), \phi_g, T_b] = C$ and $F[C(F, \phi_g, T_b), \phi_g, T_b] = F$ for a given gas thermodynamic state ϕ_g and blackbody temperature T_b, is proven to have this property and can also be called the rank-correlated reordered absorption cross-sections [12]. As a result, the inverse ALBDF can be used to construct cross-section intervals for the RCSLW model that do not rely on a defined reference state or spectrum. RadLib's RCSLW model uses Method 1.2.2 as defined and recommended in [12]

3. Software Description

RadLib is an object-oriented C++ class library that includes both C++ and Python interfaces. The RadLib package contains five subdirectories (upon initial download): `source` contains the RadLib source code; `build` contains installation files; `examples` contains instructive example cases, including a simple interface and solver for a parallel planes geometry; `data` contains ALBDF data tables required for the RCSLW model; and `docs` contains files used to generate code documentation with Doxygen (optional).

The `source` and `examples` directories are further divided into `C++` and `Python` subdirectories to differentiate between interfaces. There are three interface options for using this code: C++, Python, and Cython-wrapped Python. C++ interfaces are located within the `examples/c++` folder, while Python interfaces are located within the `examples/python` folder. When running examples with Python, the Cython-wrapped version is the default; to run the regular Python version without the Cython wrapper, edit the comments near the top of the example files (i.e `ex_S1.py`). The C++ interface produces the fastest-running code, followed by the Cython-wrapped Python interface and then the regular Python interface. [INSERT RUNTIME COMPARISONS HERE]

RadLib installation is automated with CMake. First, navigate to the `radlib/build` directory. If the user requires an installation location other than the default `radlib/installed` directory, edit the `user_config` file before running CMake. To compile the package, run the command `cmake -C user_config ../source`. Upon successful completion, run `make` and then `make install` to complete the process. The generated C++ library file is located at `radlib/installled/lib/libradlib.a`.

Figure 1 illustrates the basic structure use of the RadLib package within a generic example using the provided interfaces. The RadLib library generates absorption coefficients and their weighting factors for use within the appropriate RTE, but does not specify any particular geometry, making it a versatile tool for any simulation that requires radiative heat transfer, regardless of configuration. The interfaces, solver, and examples included with the library serve to illustrate its use and validate the implementation and results.

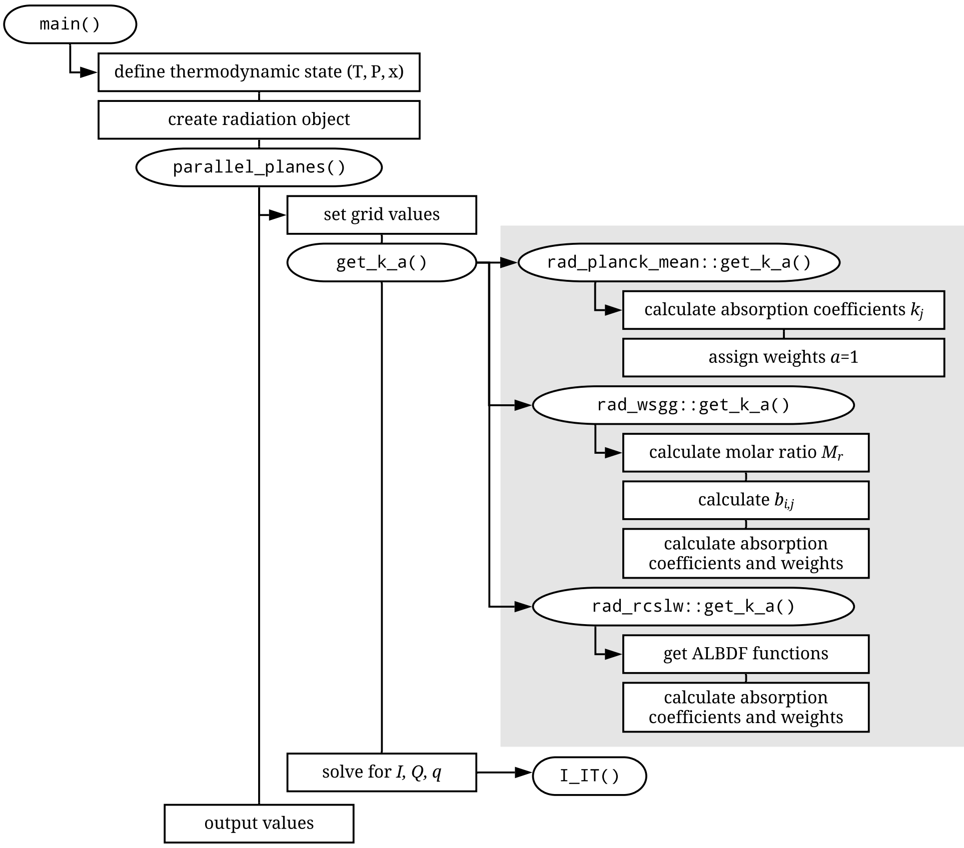

Figure 1: Example workflow diagram. Highlighted areas are part of the RadLib library; other areas represent example infrastructure for using the package.

Example	T(K)	y_{H2O} y_{CO2} (mole frac.)	L (m)	T_{walls} (K)
S1	$T(x<0.5)=2000$; $T(x>0.5)=300$	$y_{CO2}=0.1$, $y_{H2O}=0.2$	0.5-2.5	cold, cold
S2	T=1000	$y_{CO2}(x<0.5)=0.4$, $y_{CO2}(x>0.5)=0.1$ $y_{H2O}=0.0$	0.5-2.5	cold, cold
S3	$T(x)=4000x(L-x)/L^2+800$	$y_{H2O}(x)=0.8x(L-x)/L^2+0.12$ $y_{CO2}=0$	1	800, 800
S4	middle third triangular to 2500	$y_{H2O}=0.1$, $y_{CO2}=0$	0.3	500, 500
S5	$T(x)=1000+500\cos(\pi x/L)$	$y_{H2O}=0.1$, $y_{CO2}=0$	2	1500, 500
B3	$T(x)=400+1400\sin(\pi x/L)^2$	$y_{H2O}(x)=0.0001+0.9999\sin(\pi x/L)^2$ $y_{CO2}=1-y_{H2O}$	1	400, 400

Table 2: Summary of example cases presented. S1-S5 are from [12]; B3 is from [9]. All cases use $P=1$ atm and black walls.

4. Illustrative Examples

Several examples are presented to illustrate the behavior of the models. The examples show heat flux q or volumetric heat source Q in one one-dimensional configurations with varying gas compositions and temperatures. We compare the PM, WSGG, and RCSLW models for each example. The examples correspond to those presented by Solvojov et al. (S) [12] and Bordbar et al. (B) [9], and the number of each example corresponds to the example number in the respective reference. A ray-tracing code is used to solve the radiative transport equation between two parallel plates. Table 2 summarizes the cases. Example S1 is a hot slab next to a cold slab where the cold slab's thickness varies; Example S2 is isothermal with a thick slab of high CO_2 next to a thin slab of low CO_2 with variable thickness; Example S3 uses parabolic temperature and H_2O mole fraction profiles; Example S4 has a triangular temperature profile between equally-spaced isothermal regions; Example S5 uses a half-sinusoid temperature profile that decreases from 1500 to 500 K; and Example B3 has symmetric temperature and H_2O mole fraction profiles with central peaks of 1800 K and 1, respectively (with $y_{CO2}=1-y_{H2O}$). Each case is presented alongside the line-by-line (LBL) data presented in the references.

The examples are provided with the RadLib code and implemented in both C++ and Python. A Juptyer notebook is provided with the Python examples that runs the examples, displays the plots, and saves the plots to PDF files. Python and Cython versions of the one-dimensional solver `parallel_planes.py` are provided for convenience.

These cases are intended to illustrate the use of the RadLib library and are not exhaustive. Details about these examples and their motivations can be found in their respective references. While ommitted here for brevity, the implemented WSGG and RCSLW models give essentially identical results to those presented in [12, 9] such that these examples also serve as a validation of the implementation of the models.

Figure 2 shows comparative results for the different radiation models for these cases. In general, the PM model performs poorly compared to the WSSGG and RCSLW models. A notable exception is Example S4. In Example S2, the PM $q(L)/\sigma T^4$ is off scale at an essentially constant at a value of unity. The PM absorption coefficient is 27.4 atm^{-1}m^{-1}, giving optical thicknesses of 0.09 and 0.36 m in the thick and thin layers, respectively, which are relatively small compared to the isothermal domain size greater than 0.5 m. Example S5 omits the PM model to more clearly show the behavior of the WSGG and RCSLW models. For that example, the PM values follow the shape of the other curves but Q varies from around -80 at $x = 0$ to a peak of 200 at x=1.5 m, and dropping to 100 kW/m^3 at $x = 2$ m. In all examples, four gray ($n = 4$) and one clear gas are computed for the RCSLW models to give a consistent comparison to the WSGG model. Example S5 shows the sensitivity of the RCSLW model to the number of gases used. When n is increased to eight the RCSLW model improves to show nearly perfect agreement with the LBL data in Example S2. In all Examples, the RCSLW model is initialized using the mean temperature and composition on the domain. In Example S5, the RCSLW model converges to the LBL solution when the model is initialized using the maximum temperature instead of the average temperature.

5. Impact

Radiative heat transfer models are historically difficult to implement in CFD codes due to their complexity and high computational costs. Neglecting radiation or using simple models like the optically thin assumption is adequate for some cases with simple geometry or limited chemical reactions, but most simulations of interest to engineers and researchers require more advanced radiation modeling to yield accurate results. In such cases, radiation models that are incorrectly implemented or inappropriate for the simulation parameters can become additional sources of error that may be extremely difficult to separate from existing sources or error. Currently, researchers that require detailed radiation modeling must code and validate it themselves at the expense of valuable research time and funding.

RadLib makes researchers' work easier by consolidating various approaches into a modular library of interchangeable, prevalidated radiation models. Additionally, RadLib's modular framework is designed to easily accommodate new models as well, allowing researchers to compare new or existing models with very little overhead. Sometimes, it is not clear which radiation model may be the best fit for a particular simulation. When simulations are especially complex or computationally expensive, researchers may have

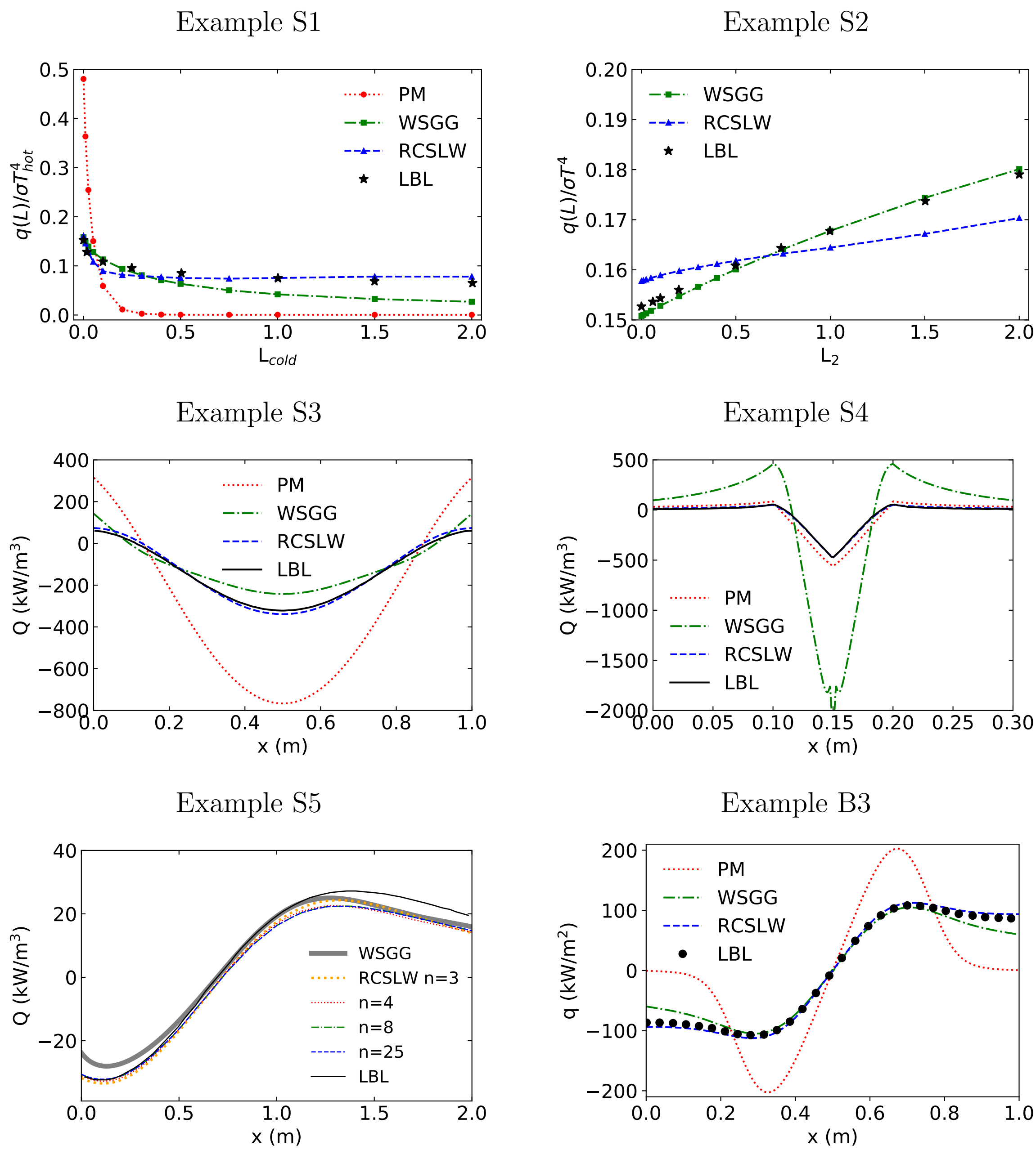

Figure 2: Results for examples summarized in Table 2.

to extrapolate from theory and literature to choose an appropriate radiation model rather than testing for their specific case. RadLib is designed to ease both of these obstacles by facilitating comparison between radiation models through a common interface and providing a practical means of testing various models without the restriction of prespecified geometry or case parameters. With RadLib, researchers can put more of their time and effort into useful results rather than code or model development.

Currently, RadLib is only used within the authors' research group, where it is applied to combustion CFD simulations using the One-Dimensional Turbulence (ODT) model [20], but its design and structure as a C++ library allows it to be incorporated easily into existing codes. It can be applied to research questions in various other fields involving radiative heat transfer as well, including energy engineering or atmospheric and climate sciences. Radiation is a universal phenomenon, and RadLib can assist researchers in many areas with systems and processes that involve heat transfer.

6. Conclusions

Set out the conclusion of this original software publication.

7. Conflict of Interest

There are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

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Current executable software version

Nr.	**(Executable) software metadata description**	**Metadata**
S1	Current software version	1.0
S2	Permanent link to executables of this version	https://github.com/BYUignite/radlib
S3	Legal Software License	MIT license (MIT)
S4	Computing platforms/Operating Systems	Linux, OS X, Microsoft Windows
S5	Installation requirements & dependencies	CMake, C++, Python 3, Cython
S6	If available, link to user manual - if formally published include a reference to the publication in the reference list	https://github.com/BYUignite/radlib
S7	Support email for questions	davidlignell@byu.edu

Table 3: Software metadata.