Software Impacts 11 (2022) 100206

Contents lists available at ScienceDirect

Software Impacts

journal homepage: www.journals.elsevier.com/software-impacts

Original software publication

CRFlowLib — Chemically Reacting Flow Library

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ARTICLE INFO

Keywords:
Chemically reacting flows
Combustion simulation
Thermochemistry reduction
In situ adaptive tabulation

ABSTRACT

The simulation of reactive flows is a very challenging task from the computational point of view, as in addition to taking into account all the complex aspects of fluid dynamics, it requires a detailed description of the chemical kinetics involved in the process. Thus, the use of strategies to reduce simulation time is essential. Among the existing reduction techniques, the In Situ Adaptive Tabulation (ISAT) is one of the most promising since it offers a good compromise between accuracy and cost reduction. This paper presents the CRFlowLib, a computational package to simulate chemically reacting flows using ISAT algorithm

Code metadata

Current code version	2.0
Permanent link to code/repository used for this code version	https://github.com/SoftwareImpacts/SIMPAC-2021-165
Permanent link to Reproducible Capsule	https://codeocean.com/capsule/2804669/tree/v1
Legal Code License	MIT license
Code versioning system used	git
Software code languages, tools, and services used	C and Fortran
Compilation requirements, operating environments & dependencies	Ubuntu, GSL 2.6, SUNDIAL 5.0.0 and Chemkin-II
If available Link to developer documentation/manual	https://github.com/americocunhajr/CRFlowLib
Support email for questions	americo.cunhajr@gmail.com

1. Introduction

Typically, computational models used to predict the behavior of reactive flows (or systems) solve the balance equations of continuum mechanics supplemented by constitutive models (fluid behavior, turbulence, radiation, kinetic mechanisms, equations of state, etc.), initial and boundary conditions, and an adequate geometric representation of the domain of interest. The solution of combustion problems typically require chemical kinetic mechanisms with n_s species, which evolve according to n_r elementary reactions. It is then necessary to integrate $5+n_s$ partial differential equations. Due to strong nonlinearities and coupled transport phenomena at multiple scales, arising from the complex physics underlying these reactive systems, the process of calculating the response of the associated computer model is quite complex and extremely costly [1–3]. In this context, over the past decades, the technical-scientific literature has shown increasing efforts to develop reduced-order computational models for simulating reactive systems with detailed chemical kinetics [4,5].

The methodology known as In Situ Adaptive Tabulation (ISAT) was proposed in 1997 by S. B. Pope [6], and may be considered a milestone on the simulation of reactive flows, as it enables to accelerate calculations involving chemical kinetics by factors that can reach up to the impressive value of three orders of magnitude, with a controllable loss of accuracy. This technique consists of creating, progressively (in situ), a binary search tree that stores (tabulates) information from the reactive flow simulation for posterior use. A search is performed along this tree whenever the integration of model equations is required, and a tabulated solution is retrieved. If the information retrieved from the tree is satisfactory, in a sense defined by a user-prescribed tolerance — the retrieved solution is within a certain precision ellipsoid, which controls the amplification of approximation errors – a linear extrapolation using the values tabulated is used to provide an approximate

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https://doi.org/10.1016/j.simpa.2021.100206
Received 14 November 2021; Received in revised form 3 December 2021; Accepted 13 December 2021

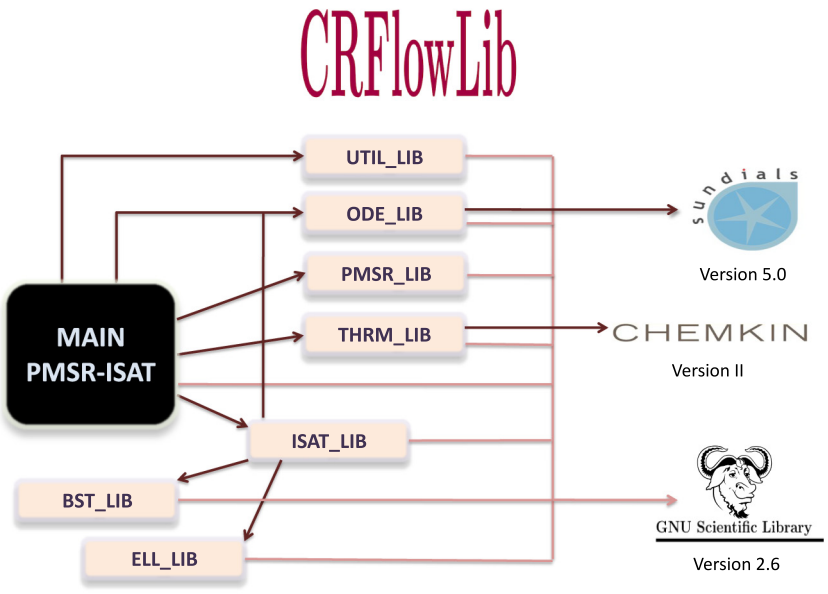

Fig. 1. Schematic representation of PMSR-ISAT main program and CRFlowLib libraries, with an indication of their internal and external dependencies.

solution. This approximate solution has a second-order local error in time, thus ensuring that the global error is first-order. The algorithm also includes an adaptive strategy for updating the binary tree (learning process), with a focus on refining the approximations as the simulation progresses. This adaptive feature allows this algorithm to be seen as a machine learning technique (or an evolutionary algorithm) [4,6,7]. An open ISAT implementation for simulating reactive systems is introduced in this paper, as part of a more general computational package known as *CRFlowLib — Chemically Reacting Flow Library*, that is used to simulate transient homogeneous reactors such as PaSR — Partially Stirred Reactor, and PMSR — Pairwise Mixing Stirred Reactor.

2. Software details

CRFlowLib is a hybrid code, with libraries implemented in ANSI C and Fortran 77 languages, fully modularized, with commented routines and functions. To ensure its functionality, it was tested and debugged, following good practices of scientific computing and software engineering [8]. Currently, version 2.0, is composed of several modules and depends on 3 external libraries: (i) GNU Scientific Library version 2.6, which is a set of open-source libraries for scientific computing [9]; (ii) Chemkin-II, a Fortran library for chemical kinetics calculations [10]; and (iii) SUNDIALS: Suite of Nonlinear and Differential/Algebraic Equation Solvers version 5.0.0, which is a set of open-source libraries, with extremely robust routines, for numerical integration of nonlinear differential equations [11], with development and maintenance performed by Lawrence Livermore National Laboratory. A description of the functionality of each of these modules is provided below:

- `ckthrm.f`: library with routines to perform calculations related to chemical kinetics;
- `thrm_lib.c`: library with routines to perform calculations related to chemical kinetics;
- `pasr_lib.c`: library with routines to define a PaSR homogeneous reactor model
- `pmsr_lib.c`: library with routines to define a PMSR homogeneous reactor model
- `bst_lib.c`: library with routines to manipulate binary search trees;
- `ell_lib.c`: library with routines to manipulate ellipsoids;
- `ode_lib.c`: library with routines to integrate the dynamics of a chemical reactor;
- `isat_lib.c`: library with routines to accelerate the calculation of chemical kinetics;
- `util_lib.c`: library with general utility routines;
- `main__conp.c`: program to calculate the equilibrium of a constant pressure reactor;
- `main__pmsr-di.c`: program to simulate a PMSR homogeneous reactor via direct integration;
- `main__pmsr-isat.c`: program to simulate a PMSR homogeneous reactor via ISAT;
- `main__pmsr-isat-di.c`: program to estimate the global error induced by ISAT algorithm.

The modular structure of the CRFlowLib package, the dependency relationship between different libraries and programs, as well as the dependency on external libraries, can be seen in Fig. 1. Note that it is very natural to use CRFlowLib libraries in other simulators, the programmer needs to call the underlying routines in the main module of the other code. Also, as modern compilers allow direct calls to routines written in C to be made in a program developed in C++ or Fortran, the main module does not necessarily need to be written in ANSI C, developments in these other languages are also straightforward.

3. Impact overview

CRFlowLib was developed at Pontifical Catholic University of Rio de Janeiro (PUC-Rio), between 2006 and 2010, during the first author's undergraduate and master courses, [8,12], under the supervision of the second author. It was conceived to be an open library for reactive flow simulation, starting with the implementation of ISAT to simulate transient homogeneous reactors [8,13,14]. Due to its modular structure and open-source nature, extensions are relatively simple to implement, so that the package can be coupled with other existing simulators, as was done in [15], which used this ISAT library to simulate soot formation upon combustion of a methane–air gas mixture.

Although the ISAT is a well-established technique for acceleration of thermochemistry calculations in reactive flows simulation [4,7], perhaps because of the associated mathematical complexity, there are few open implementations of its algorithm available on the internet. For instance, the Wikipedia [16] mentions two Fortran implementations,

the pioneer one by Prof. S. B. Pope and collaborators [17] (which currently has implemented the improved version of ISAT [7]), developed by the Turbulence and Combustion Group at Cornell, an adaptation of Pope's code [18], to make it compatible with the Cantera library [19], and the present ANSI C implementation available at CRFlowLib package [20] (with the classic version of ISAT [6]). To the best of the author's knowledge, CRFlowLib is the only open code that has an ISAT algorithm implemented in the ANSI C language, which is a notable feature due to the computing power and flexibility of this low-level language.

4. Final remarks

CRFlowLib is a computational package that provides an extensive framework to analyze several types of reactive systems. Its modular and customizable architecture makes it attractive to be coupled with existing open simulators (e.g. Open FOAM [21], FEniCS [22], etc.), which opens up a wide horizon of potential applications. In this sense, we believe that this package is an important tool to simulate reactive systems with complex thermochemistry, with the potential to bring advances in the basic and applied research in this field.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

The authors are indebted to the Brazilian agencies National Council for Scientific and Technological Development (CNPq), Coordination for the Improvement of Higher Education Personnel (CAPES), and Research Support Foundation of the State of Rio de Janeiro (FAPERJ) for the financial support given to this research. During this work L. F. Figueira da Silva was on leave from Institut Pprime, Centre National de la Recherche Scientifique (CNRS).

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