Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2024-0027

Vol. **36**, No. 1, pp. 274-318
July 2024

COMPUTATIONAL SOFTWARE

AFEPack: A General-Purpose C++ Library for Numerical Solutions of Partial Differential Equations

Zhenning Cai[1], Yun Chen[2], Yana Di[3,4], Guanghui Hu[5,*], Ruo Li[6,7,*], Wenbin Liu[8], Heyu Wang[9], Fanyi Yang[10], Chengbao Yao[11] and Hongfei Zhan[12]

[1] *Department of Mathematics, National University of Singapore, Singapore.*
[2] *Shenyang National Laboratory for Material Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, Liaoning Province, China.*
[3] *Research Center for Mathematics, Beijing Normal University, Zhuhai, China.*
[4] *Guangdong Key Laboratory of IRADS, BNU-HKBU United International College, Zhuhai, China.*
[5] *State Key Laboratory of Internet of Things for Smart City and Department of Mathematics, University of Macau, Macao SAR, China.*
[6] *CAPT, LMAM and School of Mathematical Sciences, Peking University, Beijing, China.*
[7] *Chongqing Research Institute of Big Data, Peking University, Chongqing, China.*
[8] *Division of Business and Management, BNU-HKBU United International College, Zhuhai, China.*
[9] *School of Mathematical Sciences, Zhejiang University, Hangzhou, Zhejiang Province, China.*
[10] *School of Mathematics, Sichuan University, Chengdu, China.*
[11] *Northwest Institute of Nuclear Technology, Xian, Shaanxi Province, China.*
[12] *School of Mathematical Sciences, Peking University, Beijing, China.*

Received 3 February 2024; Accepted (in revised version) 6 May 2024

Abstract. AFEPack is a general-purpose C++ library for numerical solutions of partial differential equations. With over two decades development, AFEPack has been successfully applied for scientific and engineering computational problems in a variety of areas such as computational fluid dynamics, electronic structure calculations, computational micromagnetics. In this paper, design philosophy of the library, algorithms and data structures used in the discretization of governing equations, numerical linear algebra for the discretized system, as well as the pre-processing and post-processing of the simulations, will be described systematically for the AFEPack. The realization of two main features of the library, i.e., adaptive mesh methods and parallel computing,

*Corresponding author. *Email addresses:* garyhu@um.edu.mo (G. Hu), rli@math.pku.edu.cn (R. Li)

will be introduced in detail. The potential of the library for large scale scientific/engineering problems would be demonstrated by several examples. The future works on developing the library will also be discussed.

AMS subject classifications: 65M08, 65M60, 65N08, 65N30, 65-04

Key words: AFEPack, C++ library, partial differential equations, scientific/engineering computing, software.

Program summary

Program title: AFEPack
Software licence: GPL 2.0
CiCP scientific software URL:
Developer's repository link: `http://dsec.pku.edu.cn/~rli/software.php`
Programming language(s): C, C++
Nature of problem: Numerical methods for partial differential equations have been playing a more and more important role in both scientific exploration and engineering applications, and the development of related numerical software is urged to catch up with the rapid development of hardware, as well as numerical algorithms.
Solution method: A C++ library entitled *AFEPack* is developed for the purpose. The package was designed originally based on finite element methods, and has been extended to finite volume methods, discontinuous Galerkin methods, spectral elements, etc. Features of the package include adaptive mesh techniques, and parallel computing. Based on AFEPack, several specific-purpose packages have been developed in computational fluid dynamics, electronic structure calculations, etc.

1 Introduction

Besides the theory and experiments, computational science has been becoming an indispensable methodology for science exploration. As an essential component of computational science, numerical solutions of partial differential equations (PDEs) have been playing an increasingly important role, not only in science exploration, but also in engineering applications, entertainments, etc.

Towards the scientific and engineering numerical simulations, there have been many mature software, covering a variety of research and application areas. For example, in computational fluid dynamics, Ansys Fluent [48], COMSOL [50], Autodesk CFD [49], etc., are popular commercial software, while OpenFOAM [35], SU2 [10], GeoClaw [4], etc., are popular open-source ones. In electronic structure calculations, there are commercial software such as Gaussian [51], Q-Chem [52], and Jaguar [53], and open-source software such as VASP [11], Quantum ESPRESSO [8], and ABINIT [1].