Chapter 14

PELLPACK:
A PROBLEM SOLVING ENVIRONMENT
FOR PDE BASED APPLICATIONS
ON MULTICOMPUTER PLATFORMS

Elias N. Houstis, John R. Rice, Sanjiva Weerawarana, Ann Christie Catlin, P. Papachiou, KoYang Wang and Margaret Gaitatzes

Abstract
This paper presents the software architecture and implementation of the problem solving environment (PSE) PELLPACK for modeling physical objects described by partial differential equations (PDEs). The scope of this PSE is broad as PELLPACK incorporates many PDE solving systems and some of these, in turn, include several specific PDE solving methods. Its coverage for 1-D, 2-D and 3-D elliptic or parabolic problems is quite broad, and it handles some hyperbolic problems. Since a PSE should provide complete support for the problem solving process, PELLPACK also contains a large amount of code to support graphical user interfaces, analytic tools, user help, domain or mesh partitioning, machine and data selection, visualization, and various other pre- and post-processing tasks. Finally, the PELLPACK PSE integrates several PDE libraries and PDE systems available in the public domain. The system employs several parallel reuse methodologies based on the decomposition of discrete geometric data to map sparse PDE computations to parallel machines. An instance of the system is available as the Web server WebPELLPACK for public use at the http://pellpack.cs.purdue.edu.

1. INTRODUCTION

The concept of a mathematical software library was introduced in the early 70s to support the reuse of high quality software. Although the software library provides some form of abstraction and a facility of reusing software parts, it still requires a level of computing expertise beyond the skills and background of the scientists who usually design manufactured products. This recognition led to a new concept of software reuse referred to as Problem Solving Environments (PSEs). The current PSEs consist of small sets of modules, usually taken from existing libraries, and packaged to handle a predefined class of mathematical
models. In these PSEs the specification of the mathematical model, the problem solving process, and the required pre-processing or post-processing are done with a high level user interface. This interface usually consists of a very high level language and graphical interface that allows the user to specify the problem and visualize the solution in some “natural” form. PSEs and their associated tools have greatly increased the abstraction of computational prototyping for many applications. In this paper we describe the architecture and functionality of a PSE called PELLPACK for solving certain classes of partial differential equations (PDEs) on sequential and multicomputer platforms. PELLPACK provides an interactive graphical user interface for specifying the PDE model, its solution method and post-processing, supported by the Maxima (Energy Science Center, 1995) symbolic system and libraries of sequential and parallel solver codes. Parallel libraries are implemented using MPI, PVM and some machine native communication libraries. A number of well known “foreign” PDE systems have been integrated into PELLPACK. The PDE solvers available in PELLPACK are listed in Table 14.1, along with their Parallel libraries are implemented using MPI, PVM and some machine native communication libraries. domain of applicability. PELLPACK can simulate structural mechanics, semi-conductors, heat transfer, flow, electromagnetic, microelectronics, and many other scientific and engineering phenomena. An expanded version of this paper can be found at http://webppellpack.cs.purdue.edu/doc.

2. SOFTWARE ARCHITECTURE

In this section, we present the architecture of PELLPACK in terms of (1) the level of programming supported, (2) the software subsystems involved, and (3) the software layers used to implement PELLPACK.

2.1 THE PROGRAMMING VIEW

In order to realize the PELLPACK computational environment, we have adopted three levels of programming with standardized data structures and interfaces among the various PDE objects involved in the problem specification and solution processes. At the highest level, the graphical user interface provides application users with knowledge-based, object-oriented editors to define problem components, specify the solution methods and perform various post-processing analyses. The problem and solution specifications are expressed in terms of a high level PDE language, which is used to represent the PDE objects produced by the graphical editors. At the second level, the PELLPACK language processor compiles this high level problem and solution specification into a procedural driver program. In the third level, the driver program