Programing Using High Level Design With Python and FORTRAN: A Study Case in Astrophysics

Eduardo S. Pereira¹, Oswaldo D. Miranda²
Instituto Nacional de Pesquisas Espaciais - Divisão de Astrofísica, Av. dos Astronautas 1758, São José dos Campos, 12227-010 SP, Brazil
Received on September, 2011 / accepted on *****, 2010

Abstract

In this work, we present a short review about the high level design methodology (HLDM), that is based on the use of very high level (VHL) programing language as main, and the use of the intermediate level (IL) language only for the critical processing time. The languages used are Python (VHL) and FORTRAN (IL). Moreover, this methodology, making use of the oriented object programing (OOP), permits to produce a readable, portable and reusable code. Also is presented the concept of computational framework, that naturally appears from the OOP paradigm. As an example, we present the framework called PYGRAWC (Python framework for Gravitational Waves from Cosmological origin). Even more, we show that the use of HLDM with Python and FORTRAN produces a powerful tool for solving astrophysical problems.

Keywords: Computational Physics, Cosmology, Programming Methodology, HLDM.

1. INTRODUCTION

Python [1, 2] is a very-high level dynamic language programing. The Python interpreter is available for different operational systems (OS). This means that is possible to write a code which can run in different OS without requiring any modification. However, in order to have the best performance, the critical computational part of the code should be written in a compiled language like c/c++ or FORTRAN. This way of writing codes is called of

---
¹duducosmo@das.inpe.br
²oswaldo@das.inpe.br
high level design (HLD) \[3, 4\]. Another important fact is that, in general, 80% of the runtime is spent in 20% of the code (Pareto Principle) \[5\]. Thus, the use of a VHL for the principal part of the code permits a more agile processing. Although the HLD goes beyond of a mixing of different languages, an important feature of HLD is related to the use of oriented object programming paradigm, OOP, working together an Unified Modeling Language (UML) class diagram.

2. The High Level Design

The first step to write an efficient code consists in dividing the problem in classes. In this section we present programs that make this task easier, as for example, \textit{dia} \[6\] and \textit{dia2code} \[7\]. The first one permits us to write class diagrams, and with the second program we can generate a frame code. That is, the class in the diagram image which is converted to a class in code structure. Through this section these concepts will become clearer.

2.1 Planning Before Programing

We start this section showing an example of class diagram\[3\]. Through this paper, we will use an example derived from \textit{cosmology}. In particular, the main characteristics of a cosmological model are: the age of the Universe, the scale factor which describes how the radius of the Universe evolves with time, and the density of matter/energy.

The class diagram that represents this cosmological model is showed in the figure\[1\]. The attributes of this class are the cosmological parameters, at the present, for total matter (\texttt{self.omegam} - \(\Omega_m\)), barionic matter (\texttt{self.omegab} - \(\Omega_b\)), dark energy (\texttt{self.omegal} - \(\Omega_{\Lambda}\)) and Hubble parameter (\texttt{self.h} - \(h\) \[4\]).

The file is saved with the name \textit{cosmo.dia}. Now, it is possible to generate a structured code with \textit{dia2code} (see \[7\] for details), using the command \texttt{dia2code cosmo.dia -t Python}. The code generated by this example, and all examples used in this article, can be downloaded from \[8\]. It is possible to generate c++ and java structured code choosing the name of the equivalent language from the \textit{dia2code} command.

\[3\] All documentation about how to install and use the \textit{dia} software can be found in \[6\].

\[4\] The Hubble constant at the present time is written in terms of \(h\) by \(H_0 = 100h\ \text{km s}^{-1}\ \text{Mpc}^{-1}\) (where 1 Mpc = 3.086 \times 10^{24} \text{cm}).
However, this way to structure a code class is only a start point. It is necessary to do a better organization and fill the methods with the equivalent operations.

Figure 1: \textit{cosmo.dia}, an example of class diagram for the basic characteristics of a cosmological model.
2.2 Mixing Python and FORTRAN

There is a very useful tool, called f2py [9], which permits to do a wrapper of a FORTRAN 77 code to Python. That is, it compiles the FORTRAN subroutine in a format which can be used by Python module. The f2py is contained in the package numpy [10]. Below, we present a simple example:

C FILE hiword.f
  subroutine hiword(a,b)
    real*8 a,b
    cf2py intent(in) a
    cf2py intent(out) b
    b = a*a
    write(6,* ) 'b = ',b,', a = ',a
    return
  end

The comment cf2py allows the f2py wrapper can be identified with both the input and output variables in the function hiword. Giving the name hiword.f to the file contained in the above code, we can compile it from the following command:

f2py -c hiword.f -m hiword

In this case, the -c means compile, and -m generate a Python module with name hiword. Below, we present an example how to call the function hiword in a Python code.

[1] >>> import hiword
[2] >>> print hiword.__doc__
[3] >>> This module 'hiword' is auto-generated with f2py (version:2).
[4] >>> Functions:
[5] >>> b = hiword(a)
[6] >>> hiword.hiword(5)
[7] >>> b = 25.000000000000000 , a = 5.0000000000000000
[8] >>> 25.0

The text in front of >> represents what is printed in the display. For more details and examples see [9].
2.2 Optimizing the Code for Multi-Core Machines

Another interesting fact about Python is that it has a lot of modules. One of this is the *multiprocessing* that permits to write a parallel code in an easy way. As an example of using this module in scientific computing, consider the following equation:

\[
f(x) = \int_{a}^{b} g(x, k) dk,
\]

(1)

where \(a \leq k \leq b\).

In many cases \(g(x, k)\) can not be written in a separated form. In this case, the integral equation must be evaluated for each \(x\) in a given range \([x_0, x_f]\). However, we can divide the range \([x_0, x_f]\) by the number of central processor units (CPU) of a cluster compute (or multi-core machine), and so we can calculate \(f(x)\) in parallel mode. In the figure 2, it is showed the class diagram of *ppvector*, that is a class we developed to do this type of operation in parallel model, for multi-core machine, based on the module *multiprocessing*. The source code can be downloaded from [11].

![ppvector](image)

Figure 2: *ppvector*, a Python module for construction of parallel scientific code in a multi-core machine.

The code below shows the use of *ppvector*:

```python
import multiprocessing as mpg
from ppvector import ppvector
from scipy.integrate import romberg

np=10000; zmax=20.0; deltaz=zmax/np

g= mpg.Array(’d’,[0 for i in range(np)]) # The d indicate double precision
```

---

[11]: URL1
```python
z = mpg.Array('d', [zmax-i*deltaz for i in range(np)])

# Define a function that will be calculate the integral in parallel
# k is the starter point of the sub-range
# E is the length of the range
# n is the number of CPU's of machine
def f(x):
    def f2(k):
        return (x+k)**(-2.0)
    return romberg(f2, 5.0, 20.0)

def fun(k, E, n):
    k2 = k + E
    for i in range(k, k2 + 1):
        zloc = z[k]
        g[k] = f(zloc)

C1 = ppvector(np, fun)  # Star the ppvector class
C1.runProcess()  # Executing the parallel calculus.
```

The function `Array`, of `multiprocessing` module, allocates a matrix in a global memory which can be accessed by all CPU's. In line 25 is passed on the length of the vector and the function that divides the job in sub-ranges. In line 26, the parallel code is called and executed.

### 3. Python Framework for Cosmological Gravitational Waves - PYGRAWC

A framework is a set of classes, interfaces and patterns to solve a group of problems. It is like a little application with statical and dynamical structures to solve a set of restrict problems. So, a framework is more than a simple library (we refer the reader to [12, 13, 14]).

In figure 3 is presented the class diagram of the core of PyGrWC. It is a framework that we are developing to study gravitational waves from cosmological origin. Here, it is only showed the class name and the relation among their several components.

The class `cosmo` describes the background cosmology. The class `PressSchechter` is based on a Press-Schechter-like formalism [15] and it
describes both the evolution of dark matter halos and the infall of barionic matter in these halos. The class csfr describes the evolution of the cosmic star formation rate. The class smbh describes the evolution of supermassive black holes in the centers of galaxies. The classes bhestelar and bhmassivo calculate the stochastic background of gravitational waves generated by: the collapse of stars to form black holes [15] and the growth of supermassive black holes (in progress). All details about the astrophysical model and the results obtained from this framework can be seen in [15, 16, 17].
4. Final Considerations

In this work is presented a High Level Design methodology (HLD), that consists in the mixing of a very-high level interpreted language (VHL) with an intermediated compiled language (IL). Using tools of software engineering, like UML, and also framework concept, we can write efficient scientific codes without spending a lot of time in the development phase. Here, it was used Python (VHL) and Fortran (IL) and it was showed that this combination can be easily done giving excellent results, as can be seen by the presentation of Python framework for Gravitational Waves from Cosmological origin (PyGraWC).

Acknowledgments: E.S. Pereira would like to thank the Brazilian Agency CAPES for support. O.D. Miranda would like to thank the Brazilian Agency CNPq for partial support (grant 300713/2009-6)

References

[1] http://www.Python.org/ <accessed in 09 September 2011>
[2] GUPTA, R, 2002. Making Use of Python. Wiley Publishing.
[3] HINSEN, K, LANGTANGEN, HP, SKAVHAUG, O, ØDEGÅRD, Å, 2006. Using BSP and Python to simplify parallel programming. Future Generation Computer Systems. 22: 123-157.
[4] HINSEN, K, 2007. Parallel scripting with Python. Computing in science & engineering. Nov./Dec. 82-89.
[5] BEHNEL, S, BRADSHAW, R, CITRO, C, DALCIN, L, SELJEBOTN, D, SMITH, K., Cython: The Best of Both Worlds. CISE, 13, 2, 31-39.
[6] http://projects.gnome.org/dia/ <accessed in 09 September 2011>
[7] http://dia2code.sourceforge.net/ <accessed in 09 September 2011>
[8] https://duducosmos@github.com/duducosmos/pereira_miranda_jcis2012.git <accessed in 10 September 2011>
[9] PETERSON,P, 2009. F2PY: a tool for connecting Fortran and Python programs IJCSE, 4, 4, 296-305.

[10] http://www.scipy.org/ <accessed in 09 September 2011>

[11] https://duducosmos@github.com/duducosmos/ppvector.git <accessed in 09 September 2011>

[12] FAYAD, M. E. 2000. Introduction to the computing surveys electronic symposium on object-oriented application frameworks. ACM Comput. Surv., 32,1,1-9.

[13] Fayad, M. E., SCHIMIDT, D. C. 1997. Object-oriented application frameworks. Commun.ACM, 40, 10, 32-38.

[14] GOVONI, D. 1999. Java Application Frameworks. John Wiley & Sons.

[15] PEREIRA, ES, MIRANDA, OD, 2011. Supermassive Black Holes: Connecting the Growth to the Cosmic Star Formation Rate. accept in Mon. Not. R. Astron. Soc. Letter.

[16] PEREIRA, ES, MIRANDA, OD, 2010. Stochastic background of gravitational waves generated by pre-galactic black holes. Mon. Not. R. Astron. Soc. 401: 1924-1932.

[17] PEREIRA, ES, MIRANDA, OD, 2010. Massive Black Hole Binary Systems in Hierarchical Scenario of Structure Formation. International Journal of Modern Physics D. 19: 1271-1274