The True Bottleneck of Modern Scientific Computing in Astronomy

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Abstract. We discuss what hampers the rate of scientific progress in our exponentially growing world. The rapid increase in technologies leaves the growth of research result metrics far behind. The reason for this lies in the education of astronomers lacking basic computer science aspects crucially important in the data intensive science era.

1. Motivation

Present-day astronomical instruments and large surveys produce the data flow increasing exponentially in time. The CPU power required to analyse these data is also growing with the same pace following the Moore’s law; the same applies to the data storage volume per price unit. However, in astronomy we do not see the exponential avalanche of scientific results produced with this computational power. This suggests the presence of a bottleneck somewhere in the loop: \textit{if we consider the system containing three modules “A”, “B”, and “C” so that “A” is connected to “C” via “B”, then optimizing features in module “A” or “C” will not produce a change in the performance of the system until the performance problems in module “B” are addressed.}

Where is the true bottleneck of the scientific computing? Astronomers as many other scientists, prefer to develop their computational codes and software systems (including database solutions) themselves often having no coding skills, insufficient background in algorithms and computational science.

2. Code Writing: Astronomers vs Software Engineers

2.1. Scientific Software by Scientists

Most computer programs developed by astronomers without computer science background, regardless of their purposes (numerical modelling or simulations, data reduction or visualisation, etc.) often have some specific common features. \textbf{(a)} They are usually written in \textit{Fortran-95, -90, -77} (or even prehistoric \textit{Fortran-4} and -66). Sometimes high-level languages (e.g. \textit{IDL, MATLAB}) are used. Primitive building
scripts are used instead of Makefiles or more advanced building solutions (e.g. ant, or maven for Java). Code is non-portable.

(b) They often contain the goto statement every 10–20 lines; names of variables do not follow any conventions, i.e. _a1, a2, aa1_; the code is unreadable: no or bad indentations, very long function bodies and/or source files. There is a lot of hard-coding of file and device names, file system paths.

(c) They are undocumented and full of “intuitive” algorithmic solutions, such as “re-invented” sorting and search algorithms, which sometimes end up quite far from what computer science students learn at school.

(d) The “multi-layered” code structure is another typical feature. When the author is returning to the same program after several months or years, he/she often finds that the existing procedure/function calls do not satisfy his/her needs, however is not willing to modify them to keep the backward compatibility. Then, a wrapper routine is created which is calling some underlying procedures/functions in a slightly different way. As a result, after several such periods of development, one can find multiple (undocumented) interfaces to the same functional blocks.

(e) **However**, at the end the program does what it is supposed to, because the author knows exactly what it should do. Even though it may sometimes crash during run-time or have very poor performance.

### 2.2. Scientific Software by IT Engineers

The software developed by IT engineers in research is notably different. Here the quality of the final product strongly depends on the job of a project manager.

(a) Usually it is done using a “real” programming language: C/C++/Java, primarily because it is virtually impossible to find an IT professional developing in Fortran.

(b) All necessary solutions for computational algorithms are conventional because the developer at least heard about the “Art of the computer programming” (Knuth 1978).

(c) The code is usually well organized and structured; correct indentations and variable naming conventions are used; sometimes the author follow one of the coding styles (e.g. GNU). Therefore, the code becomes readable and comprehensible.

(d) The quality and completeness of the documentation strongly depends on the project manager’s competence. It can be from none to nearly perfect.

(e) **However**, the author often does not understand the physical principles behind the algorithm or particular features of the instrumentation making the data looking as they are, therefore some bad surprises are possible. For example, some arithmetic bugs leading to the results which are wrong by many orders of magnitude from what is expected cannot be spotted by a software engineer because for him/her it is “just a number”. This may dramatically slow down the development.

### 2.3. Databases by Scientists

The worst class of software solutions is probably DBs developed by researchers.

(a) Often they contain custom implementation in Fortran or IDL of re-invented indexing solutions and primitive requests to the data. Indices and data tables are stored in a proprietary undocumented binary format.

(b) If an existing database management system (DBMS) is used, then the DB usually contains one or several flat tables without mutual links, i.e. no data model.
(c) DB constraints are not used for consistency checks, in some rare cases they are implemented externally in a DB management interface (also often written in Fortran).
(d) User interfaces, both application programming interface (API) and web front-end are undocumented, have very low usability and terrible design.

3. Bad and Good Examples

For obvious reasons we will not cite the corresponding references for bad examples. The list of good examples is neither exhaustive nor complete.

3.1. Bad Example #1: an Unnamed Galaxy Catalogue
The project is very interesting scientifically and recognised in the community. But...
(a) There is no access interface on the web.
(b) The data are distributed as a set of dozens of FITS tables with a total volume >10Gb and IDL access routines to perform queries on these tables. One has to download nearly everything in order to study just a handful of objects.
(c) Therefore, huge memory requirements if one uses the whole catalogue at once.
(d) Therefore, very slow and inefficient data access and selection.

3.2. Bad Example #2: an Unnamed Database Using PostgreSQL
(a) DB administration and ingestion interface (implemented in Fortran) has a function with over 250 arguments
(b) Inside the DB restore script, to delete a record from a table, instead of
   `DELETE FROM table1 WHERE field1=value1`
   the authors do:
   `pg_dump -t table1 mydb | grep -v value1 | pg_restore -c mydb`
(c) One of the stored procedures which is triggered on `INSERT`, connects externally to the same DB and making some selections using this new connection. Obviously, it cannot see the changes introduced before the trigger had been fired because the transaction has not been committed.

3.3. Good Examples #1: Technologically Advanced Projects
1. HLA - the Hubble Legacy Archive (http://hla.stsci.edu/). Innovative solutions implemented inside HLA include: (a) Virtual Observatory standard interfaces (Simple Image Access Protocol) as a hidden middleware; (b) XSLT transformation of VOTables into AJAX-enabled HTML pages; (c) advanced visualisation tools.
2. SDSS CasJobs (http://cas.sdss.org/CasJobs, Szalay et al. 2002). Efficient and easy-to-use access to a large DB featuring user management, user table upload, I/O of tabular data in different formats, comprehensive SQL query builder.
3. GalexView (http://galex.stsci.edu/GalexView/) – a Flash-based interactive web-access to the GALEX satellite images.
4. Millennium Simulation (http://www.mpa-garching.mpg.de/millennium/ by G. Lemson) – access to the DB containing the results of large cosmological simulations with a comprehensive data model and full SQL access.
5. GalMer (http://galmer.obspm.fr/ Chilingarian et al. 2010) - a DB to access numerical simulations of merging and interacting galaxies. The projects implements a set of Virtual Observatory (VO) standards, features efficient interactive preview visualisation of the datasets on the server side, complex on-the-fly data analysis algorithms.
The JavaScript-powered web-interface working in most modern browsers is integrated with VO tools in order to visualise complex datasets (Chilingarian & Zolotukhin 2008; Zolotukhin & Chilingarian 2008).

3.4. Good Examples #2: Computations, Data Analysis and Visualisation

1. GADGET-2 by V. Springel (2005), a cosmological simulation code that is well documented and easily extensible: there are numerous third-party add-ons implementing different physical phenomena, e.g. radiative transfer, metallicity evolution in galaxies.

2. SExtractor (Bertin & Arnouts 1996): a software to perform object extraction and photometry from CCD images has very intuitive configuration, although outdated documentation. It is relatively clearly coded.

3. TOPCAT/STILTS (Taylor 2005, 2006) – the best available platform independent table manipulation software integrated with VO services and resources.

4. CDS Aladin (Bonnarel et al. 2000) – a VO data browser for images and catalogues.

5. SAOImage DS9 (Joye & Mandel 2003) – probably the most frequently used desktop FITS visualisation software in astronomy implementing some VO data access methods.

4. The Main Message and a Possible Solution

It turns out that all “good examples” were developed either by professional astronomers with very strong IT/CS background or by IT/CS professionals working closely with astronomers for years and understanding astronomy. One cannot simply hire an industrial software engineer to develop astronomical software and/or an archive and/or a database.

A possible solution is to change the teaching paradigm for students in astronomy. Basic courses in algorithms, programming, software development and maintenance have to be made mandatory in the education of modern astronomers and physicists; advanced courses should be recommended to some of them. The Fortran language is now obsolete and we have to accept this. Instead of teaching research students to Fortran programming, one should teach how to interface legacy Fortran code in C/C++.

As soon as this bottleneck is resolved, the avalanche of discoveries will loom.

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