J. Comp. Int. Sci. (2015) 6(1):1-2
http://epacis.net/jcis/PDF_JCIS/JCIS-EN0015.pdf
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Pan-american Associacion of Computational Interdisciplinary Sciences

Special Editorial Note

On the meaning of the *Minimum Information Principle* in scientific computing

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Received on April 20, 2015 / Accepted on April 28, 2015

The reading of the three articles[1] published in this issue made me reflect on the importance of Kolmogorov-like complexity[2] in scientific computing, especially those related to the formal tools (and devices) for simulation and analysis of large amounts of data. Although there is a huge (and not so simple) apparatus for hardware, software and midware involved in any computational scientific work, usually, the mathematical computational performance[3] is not explicitly addressed by most researchers; and one of the main reasons for this technical negligence is particularly easy to understand: there is still a huge lack of both practical principles and methodologies of computational complexity that can (and should) be used straight in (and perhaps automatically[4]) by scientists from interdisciplinary areas based on computer science (where computational physics is maybe the most striking example).

Although in practice we deal with the need to practice parsimony as a major scientific conduct, there is still a gap between this epistemological concept and its direct application in the design, detailing, development and application of an analytical mathematical tool that deals with digital scientific information. With the advent of science that depends on the large amount of data (Data Science from Big Data[5]) this deficiency is getting critical. Thus, from a comprehensive search in the vast and diverse scientific literature, it appears that there is no an appropriate *Minimum Information Principle* (MIP) that is well defined and useful to scientific computing. From a practical point of view, we feel the lack of an useful MIP that allows the scientist to qualify (and maybe to quantify), in a straightforward way, the mathematical computational complexity of a 4V-analytical scientific task. So let me try to shed here some small beam of initial light on the problem. Let us briefly discuss some practical examples.

Say we want to observe an effect, process or regime from a spatially three-dimensional simulation (e.g., the fully developed plasma turbulence regime from a MHD simulation). A first question would be: what is the minimum required size grid for observing a given effect of interest (i.e., in a such case, what is the minimum amount of voxels that will compose our minimum physical hypercube?). A second question, considering the example given, could be the following: (ii) given a resolution in time, what is the minimum amount of time

[1]These are three interesting and excellent papers that fit perfectly to the scope of JCIS. The former presents a method for scientific data extrapolation and the other two deal with high performance computing in physics simulation.

[2]the Algorithmic Complexity or *Kolmogorov Complexity* of a string of bits is defined as the length of the shortest program that computes or outputs the string object, where the program is run on some stated universal computer.

[3]Here the main subject is the mathematical structure as the underlying algorithm content.

[4]The *Machine Learning* is one of the few areas of knowledge where we find a practical interpretation of *minimum information*, which we can call *principle*.

[5]The data base and data mining involving the so-called 4 Big "V": volume, variate, velocity and value.

steps which the simulation should achieve? Note that if there is a qualitative criterion from a *principle of minimum information* into this context, it may be possible to be implied in the answer to the first question, also the answer to the second one.

Lets consider also an example related to data analysis. Consider a square gradient field, generated from a given square matrix, containing vectors that can be identified by their respective phases and norms. Let's say one of the analysis operations is to remove the symmetrical pairs and then count the vectors that are left[6]. The task then is: for each vector, the algorithm should seek its symmetrical pair (that is, one in the square gradient lattice that has the same module and phase shifted by π) and then once found implies the pair is removal. How many ways and criteria are in order to find each symmetric pair? Which criterion results in the minimum amount of comparisons? If one uses the amount of remaining vectors to characterize a measurement parameter on the pattern of the gradient field, how each criterion would affect the robustness of such a parameter?

Note that in the above examples (both from scientific computing) we are not necessarily referring to the concept of information related to entropy or probability[7]. Moreover, the quality of information is associated with the concept of effort (work) and quantitatively it is associated with the deterministic number of bits involved in a such computational work. Therefore, in the formulation of a MIP for scientific computing it should prevail a more deterministic approach than statistics. Thus, in this scope, our required MIP must certify that in cases of analytical and\or simulation redundancy, we must seek the solution that minimizes the computational time and this time, in a way, can be interpreted as the deterministic case of a Kolmogorov-like complexity [8]. Actually, the need is to bring the concept of computational complexity to the level of the mathematical operation before it be translate to a classical computational algorithm. Then by simplicity we can call *mathematical algorithm* the core subject of an useful and practical MIP for scientific computing purposes which can be announced as follows:.

Let Ω_{Nj} be one logical-mathematical operation applied to a mathematical input object M_I resulting in a mathematical output object M_O. If there are N_j ways to operate on M_I (for $j > 1$) resulting in equivalents M_O, then one must implement the N_k way which is the one that minimizes the operational amount of information Q of M_I.

If the amount of information Q translates into bits, this principle should ensures that N_k minimizes the deterministic component of Kolmogorov complexity, which in practical terms can be translated as the processing time (τ) spent in the basic operation on M_I which implies M_O:

$$\Omega_{N_j} \mapsto M_I \Rightarrow M_O \mid j = k \quad when \quad N_k \downarrow \tau, \tag{1}$$

where $N_k \downarrow \tau$ means that Ω_{N_k} minimizes τ.

I conclude this note with a challenge to the reader. Apply the principle as it is announced in expression (1) to the example of vector removal described above and found that, based on the more general case, we find at least four equivalent logical mathematical ways to operate on M_I, which are as follows: N_1, when there is no a global lattice symmetry reference, implying *each with all*; N_2 considering all axes of bilateral symmetry (horizontal, vertical and the two diagonals), implying *each with only three*; N_3 considering only two axes of symmetry, implying *each with only two*; and N_4 considering only one axis of symmetry or only the center of the matrix, implying *each with only one*. Therefore, assuming that M_O for $j = 1, ..., 4$ are equivalent, we have as a solution the case $k = 4$.

This special Editorial Note has been reviewed by Professor N.L. Vijaykumar whom I thank for the useful suggestions and corrections.

[6]See the technique named *Gradient Pattern Analysis* and the references given in *https* : *en.wikipedia.orgwikiGradient* − *pattern* − *analysis*.

[7]From statistical mechanics, for example, see the Principle of Minimum Information based on the concept of Entropy: R.A. Evans, IEEE Trans. Reliability, 18(3), 87-90, 1969.

[8]Note that, in the fundamental mathematical algorithm level, there is no need to involve the concept of computational *Speed-up*. We can interpret this new principle of minimum information at different levels, where it is desirable that in the first one, the principle and its application are computer architecture independent.