Multi-fractal basis for wave-functions approximation in ab-initio calculations

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Abstract: Wavelets and fractals are a powerful new mathematical tool which offers the possibility to treat in a natural way quantities characterized by several length scales. In this article we will show how wavelets can be used to solve partial differential equations which are characterized by widely varying length scales and which are therefore hardly accessible by other numerical methods. The standard way to solve partial differential equations is to express the solution as a linear combination of so-called basis functions. These basis functions can for instance be plane waves, Gaussians or finite elements. Having discretized the differential equation in this way makes it amenable to a numerical solution. Multi-wavelets and multi-fractals are just another basis set which however offers considerable advantages over alternative basis sets.

The electronic spectra of complex atomic systems are non-linear so that even with these simplifications cannot be decrypted using typically used methods.
For example, to describe the effective potential of the uranium atom would need to calculate about 2^{100} Fourier coefficients (and even more in the case of uranium dimer). It is clear that this problem irresistible. At the same time, using the wavelet transform is possible to solve this problem. In particular, potential of uranium dimer a very singular function. It varies by more than 10 orders of magnitude. But now it has become a real recovery task. With the help of wavelet analysis it was possible to calculate it with high reliability and accuracy [1].
The template is used to format your paper and style the using fractal-basis is more effective way for increase quality and speed of calculation than wavelets. For fractal approximation the wave-functions we using Barnsley-Sloan multi-fractal algorithm [2]. Proceed to describe the idea of a compact set (wave-functions) encoding by Barnsley–Sloan method:
Consider a finite set of affine transformations - $S = \{Au \ldots, Ak\}$, that is, transformation A_i - having the form $A_i(x) = xB_i + b_i$, where B_i - square matrices order n; $x_i, b_i \in R_n$, and having the following properties:

1. $A_i(F_0) \subseteq F_0$, *for all* $F \in (F_0)$
2. $||A_i(x)-A_i(y)|| \le \alpha_i||x-y||, \ 0 \le \alpha_i < 1.$

A set S is named an “affine collage”. For a given set F (original wave-functions), we define as combination of sets $S(F) = \{A_1(F), \ldots, A_k(F)\}$, which is called a “collage of F”.
We now define the $f_s(F)$ by the following equation:

$$f_s(F) = \bigcup_{i=1}^{k} A_i(F)$$

This equation is named a “mapping of collage”.
Main property of f_s: for any F_0 have the equality –
$\lim_{m \to \infty} d(f_s^m(F_0), F) = 0$, m - number of iterations.
The affine collage S "encoded" attractor F (wave-functions), and for the restoration of the attractor F on his "code" S with any degree of accuracy, we can take any set F_0 (first approximation) and subject him to the iteration by the “mapping collage” f_s. With a sufficiently large number of iterations will set F_s, which restoring F with arbitrarily high accuracy.
This multi-fractal Barnsley-Sloan algorithm is analog of multiwavelet-coding algorithm, but with some differents: mother functions in fractal algorithm is not defined, this functions find in original set F (in wave-functions). Present work produced in Institute of Dynamic Systems. Thanks a lot to G.I. Zavozina, the director of Informatization Department in Komsomolsk-on-Amur state technical university.

References

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[2] V.A. Bondarenko, “Fractal compression by the Barnsley-Sloan method”, **Letters to JTF**, 12 (1993).