Office of Science
U.S. DEPARTMENT OF ENERGY

Fundamental Algorithms for Advanced Applications in Science and Technology

SciDAC
Scientific Discovery through Advanced Computing

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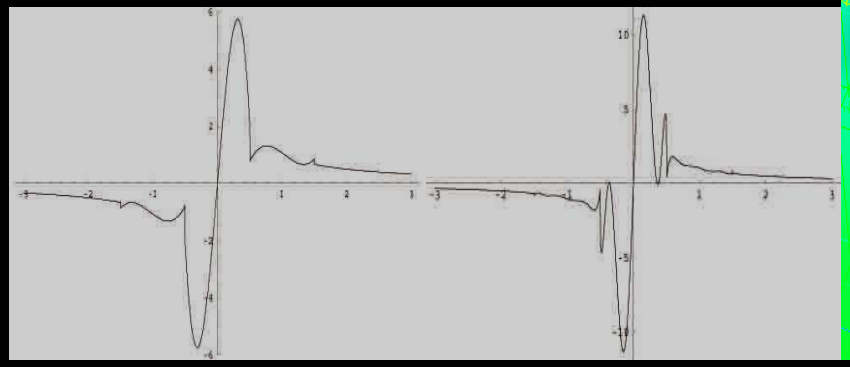
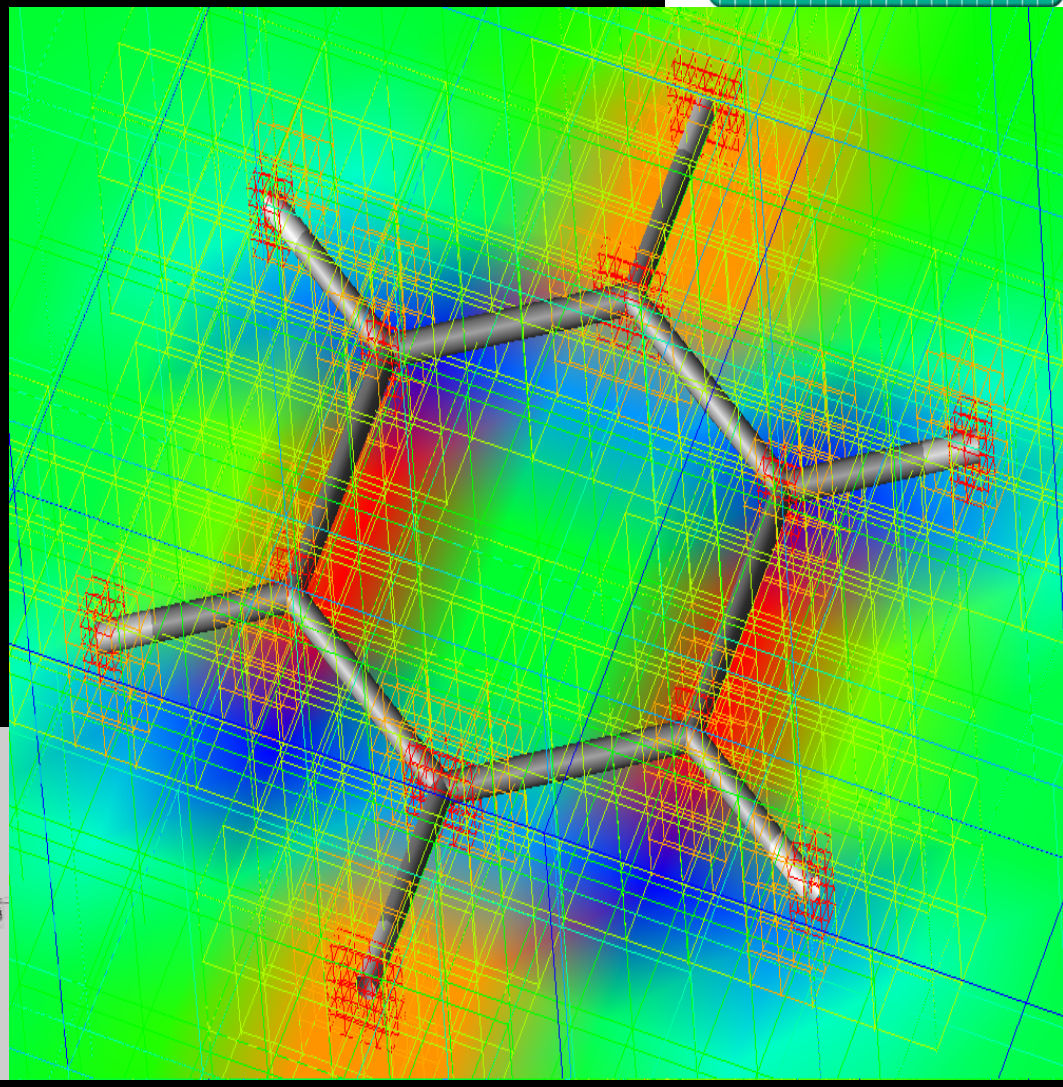
We are developing fast, O(N), multiwavelet and low separation rank based methods for solving problems in computational chemistry. Some of the desirable mathematical features are:

- Higher accuracy, reliability and ease of use.
- Fully adaptive in order and space.
- Spectral precision.
- Multiresolution analysis using multiwavelets.
- Sparse representation of operators and functions.
- Numerical regularization of singular operators.



Multiwavelet regularization of the Hilbert transform using 3 and 7 multiwavelets.



Adaptive grids are automatically generated for molecular orbital simulations. An orbital of benzene and a slice through that orbital are shown.