

# Urbana-OORI: a new paradigm for the electronic-structure code development

Yong-Hoon Kim and Richard M. Martin

*Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801*

## Abstract

We report recent progress in our electronic-structure code construction project, Urbana-OORI (object-oriented real-space initiative). It has two main features: (1) The components are highly reusable by the *object-oriented* design. (2) For the physical and computational transparency, they are mainly *real-space* based. The object-oriented design decouples the lower-numerical level, grid-based objects, and the higher-abstract level, physical objects appear in the electronic-structure calculations such as orbitals and the density. The object-oriented feature further makes each component of the two levels be easily combined with new objects introduced in the other level. The higher level currently performs regular self-consistent Kohn-Sham calculations, and the lower-level is grid-based objects that should be easily combined with different types of higher-level calculations such as tight-binding or order- $N$  method or even non-electronic-structure computations. We show the powerfulness of the new formalism by using it to implement<sup>1</sup> the self-consistent-loop multigrid method we have recently proposed<sup>2</sup>.

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<sup>1</sup>**Y.-H. Kim**, I.-H. Lee, and R. M. Martin, Comput. Phys. Comm., in press. (physics/9911031)

<sup>2</sup>I.-H. Lee, **Y.-H. Kim**, and R.M. Martin, Phys. Rev. B **61**, (2000).