AIMPAC2: A next-generation QTAIM code

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The Quantum Theory of Atoms in Molecules (QTAIM) originated by Professor R.F.W. Bader and colleagues over 30 years ago, has seen growing acceptance and use in the chemistry, physics, and materials science communities, and has spawned multiple independent software implementations. This project addresses the need for a flexible common core of QTAIM and QCT (Quantum Chemical Topology) functionality, to encapsulate the best available algorithms and discourage unnecessary duplication of effort. The new collaboratively developed AIMPAC2 code (evolving directly from the Bader group's original AIMPAC code), will also allow a vastly extended range of analyses to be performed across a wide range of fields in the physical sciences, yielding deeper insights into behavior and properties of molecules and materials. This talk will outline the current state, development roadmap and future of AIMPAC2, before its general release to the scientific community, including theoretical developments such as our new Ehrenfest Force partitioning [1-4].

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