

EDP: a program for projecting electron densities from VASP onto planes

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Summary

The electron density is a fundamental concept in electronic structure calculations, as it provides a detailed description of the distribution of electrons in a material or molecule. In many electronic structure methods, the electron density is used as the basic quantity from which other properties such as the energy, potential, and forces can be derived. The electron density provides insight into chemical bonding and reactivity and understanding the electron density (and its redistribution upon chemical bond breaking or formation) is crucial for predicting and interpreting the properties of materials and molecules. ([Martin, 2004](#))

The electron density is a scalar field, which means that it is a function that assigns a scalar value to each point in space. In the case of the electron density, this scalar value represents the probability density of finding an electron at that point in space. Specialized visualization tools and techniques are often required to effectively visualize scalar fields such as the electron density. These tools may include contour plots, isosurface rendering, and volume rendering, among others. Visualizing the electron density is essential for gaining insights into the electronic properties and behavior of materials and molecules.

EDP is a C++-based command-line utility designed to perform the projection of the electron density scalar field onto a plane. Subsequently, this plane is rendered onto a canvas using a color map and stored as a PNG file.

Statement of need

The visualization of scalar fields using contour plots or heat maps is ubiquitous in science and engineering and plenty of general purpose programs such as Open Data Explorer ([Thompson et al., 2004](#)) and ParaView ([Ahrens et al., 2005](#)) readily accomodate this task. There exist also programs that specifically cater to VASP, such as Vesta ([Momma & Izumi, 2011](#)) and `sisl` ([Papior, 2023](#)). These programs are typically designed for interactive use, `sisl` being a notable exception, and utilize a graphical user interface of some sort. In contrast, EDP is a C++-based command-line tool that carries out the projection of the electron density scalar field as stored in VASP ([Hafner, 2008](#)) CHGCAR or PARCHG file onto a plane. This plane is then rendered onto a canvas using a color map and stored as a PNG file. EDP uses a minimal set of dependencies, i.e. Boost ([Koranne, 2011](#)), Cairo ([Cairo, 2005](#)), TCLAP ([Smoot et al., 2009](#)), and Eigen3 ([Guennebaud et al., 2010](#)), which are all readily available on modern Linux-based operating systems.

EDP was designed to be used by researchers and students working in computational materials modelling using the VASP software. It has already been used in a number of scientific publications ([Filot et al., 2016](#); [Vogt et al., 2019](#); [Zijlstra et al., 2019](#)). EDP is designed with ease of use in mind. The projection planes can be defined with respect to the atomic

coordinates, which are available in the structure block of CHGCAR and PARCHG files. This allows for users to efficiently define projection plane intersecting one or more atoms of interest. This feature is especially relevant to chemists who study the electron density to understand bonding patterns and explain chemical reactivity.

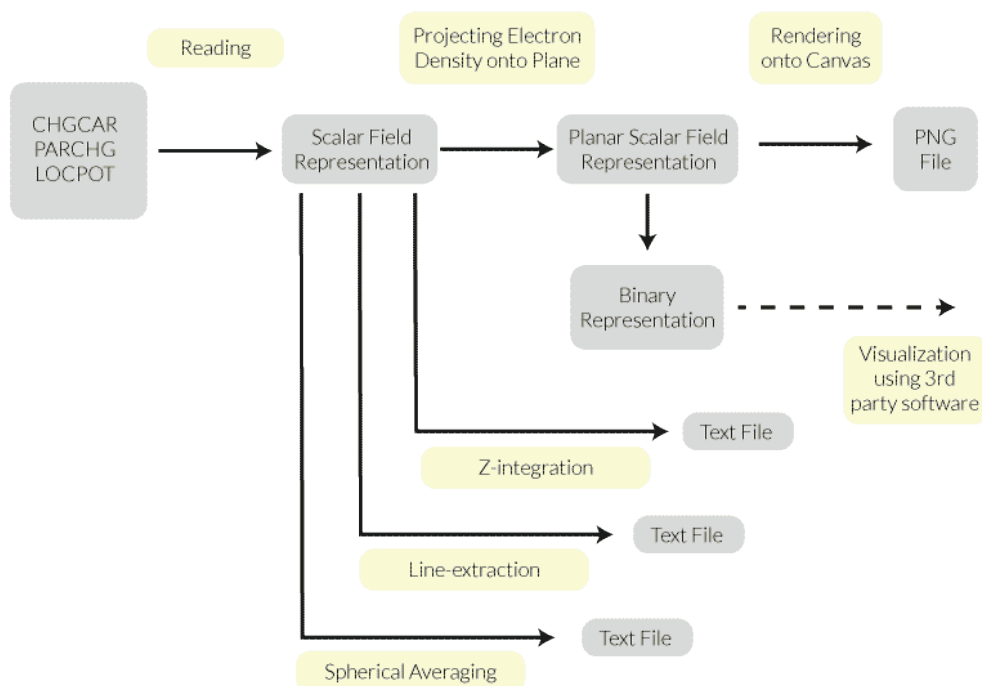


Figure 1: Schematic overview of the pipeline of the EDP program.

In addition to the projection of electron density onto a plane, the EDP tool offers a range of additional features, as illustrated in Figure 1. These features include averaging or sampling operations on the electron density. For example, the tool can integrate the electron density over xy-planes to generate the averaged electron density as a function of the z-coordinate. This feature is particularly useful for researchers studying slab models, which have applications in catalysis and material science.

Additionally, EDP allows for the production of one-dimensional projections. Users can define a line in three-dimensional space on which the electron density is projected, enabling the study of the electron density alongside a chemical bond. Alternatively, EDP can average the electron density over a sphere. In this case, the user specifies a position, and spheres of increasing size are generated up to a set radius. For each sphere, the average electron density is established by sampling grid points that correspond to the integration points of the 23rd order Lebedev quadrature. (Lebedev, 1976) The resulting data is the averaged electron density as a function of the distance to the atom. This feature is useful for studying lateral interactions between adsorbates through the electron-electron repulsion phenomenon (Zijlstra et al., 2019).

While the visualization of the projection plane can be done directly using EDP (which utilizes the Cairo library (Cairo, 2005)), the projection's raw data is also saved as a separate output. This provides users with the flexibility to leverage third-party tools such as matplotlib (Hunter, 2007) or Matlab (The MathWorks Inc., 2022) for visualization purposes, or use the raw data for additional analysis.

An extensive user guide including examples, compilation instructions and documentation of

the command-line arguments is available at <https://edp.imc-tue.nl/>.

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