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An Open Source Embedding Code for the Condensed Phase ALESSANDRO GENOVA, Rutgers University - Newark, DAVIDE CERESOLI, CNR, ISTM, ALISA KRISHTAL, Rutgers University - Newark, OLIVIERO ANDREUSSI, EPFL, ROBERT DISTASIO, Cornell University, MICHELE PAVANELLO, Rutgers University - Newark — Work from our group [1,2] as well as others [3,4] has shown that for many systems such as molecular aggregates, liquids, and complex layered materials, subsystem Density-Functional Theory (DFT) is capable of immensely reducing the computational cost while providing a better and more intuitive insight into the underlying physics. We developed a massively parallel implementation of Subsystem DFT for the condensed phase [1] into the open-source Quantum ESPRESSO software package. In this talk, we will discuss how we: (1) implemented such a flexible parallel framework aiming at the optimal load balancing; (2) simplified the solution of the electronic structure problem by allowing a fragment specific sampling of the first Brillouin Zone [2]; (3) achieve enormous speedups by solving the electronic structure of each fragment in a unit cell smaller than the supersystem simulation cell, effectively introducing a fragment specific basis set, with no deterioration of the fully periodic simulation. As of March 14, 2016, the code has been released and is available to the public. [1] A. Genova et al., JCP 2014, 141, 174101 [2] A. Genova et al., JPCM 2015, Accepted [3] S. Luber, JCP 2014, 141, 234110 [4] C. Jacob, et al., WIREs 2014, 4, 325

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