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Open release of the DCA++ project[1] URS HAEHNER, ETH Zurich, RAFFAELE SOLCA, Swiss National Supercomputing Center, PETER STAAR, IBM Research - Zurich, GONZALO ALVAREZ, THOMAS MAIER, MICHAEL SUMMERS, ORNL, THOMAS SCHULTHESS, ETH Zurich, Swiss National Supercomputing Center — We present the first open release of the DCA++ project, a highly scalable and efficient research code to solve quantum many-body problems with cutting edge quantum cluster algorithms. The implemented dynamical cluster approximation (DCA) and its DCA$^+$ extension with a continuous self-energy capture nonlocal correlations in strongly correlated electron systems thereby allowing insight into high-T_c superconductivity. With the increasing heterogeneity of modern machines, DCA++ provides portable performance on conventional and emerging new architectures, such as hybrid CPU-GPU and Xeon Phi, sustaining multiple petaflops on ORNL's Titan and CSCS' Piz Daint. Moreover, we will describe how best practices in software engineering can be applied to make software development sustainable and scalable in a research group. Software testing and documentation not only prevent productivity collapse, but more importantly, they are necessary for correctness, credibility and reproducibility of scientific results.

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Urs Haehner
ETH Zurich

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