

## **Software Engineering in Scientific Computation**

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Software in the electronic structures community is by and large a collection of isolated efforts replicated by hundreds of researchers. The resulting code are often inflexible and idiosyncratic, which makes collaborations inefficient, and decreases the productivity of new researchers in the field. There are several factors which contribute to this: the level of programmer training of the researchers, the demands of high performance computing, the limits of the chosen programming language(s), and a lone wolf programming culture are among them. This poster session will describe an effort to engineer a very flexible, easily maintainable, non-commercial, electronic structures code, Socorro. Socorro is currently being written in F90+MPI. Full use is made of the Fortran standard not just for data-hiding, procedural abstraction, and modularization, but also for features such as garbage collection and virtual copying, features we have yet to see discussed in the Fortran language literature. We believe this to be of interest, not just to possible collaborators, but also to any scientist grappling with code organization.