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Electronic structure code based on existing parallel AMR infrastructure[1] JEAN-LUC FATTEBERT, RICH HORNUNG, ANDY WISSINK, FRANCOIS GYGI, CASC, Lawrence Livermore National Laboratory — Following the first developments in real-space methods for electronic structure calculations, various efforts have been carried out in the past ten years to improve efficiency using local adaptive mesh refinement (AMR), in particular for finite physical systems. So far, the complexity of AMR codes has limited these efforts to serial calculations of relatively small problems. One way of overcoming this barrier is to build a code based on an existing parallel AMR infrastructure. We will report our progress in developing a parallel Finite Element electronic structure code based on the C++ SAMRAI (Structured Adaptive Mesh Refinement Application Infrastructure) library developed at Lawrence Livermore National Laboratory (www.llnl.gov/casc/SAMRAI).

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