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**Petascale electronic structure code with a new parallel eigen-solver** EMIL BRIGGS, WENCHANG LU, MIROSLAV HODAK, YAN LI, CT KELLEY, JERZY BERNHOLC, NCSU — We describe recent developments within the Real Space Multigrid (RMG) electronic structure code. RMG uses real-space grids, a multigrid pre-conditioner, and subspace diagonalization to solve the Kohn-Sham equations. It is designed for use on massively parallel computers and has shown excellent scalability and performance, reaching 6.5 PFLOPS on 18k Cray compute nodes with 288k CPU cores and 18k GPUs. For large problems, the diagonalization becomes computationally dominant and a novel, highly parallel eigen-solver was developed that makes efficient use of a large number of nodes. Test results for a range of problem sizes are presented, which execute up to 3.5 times faster than standard eigensolvers such as Scalapack. RMG is now an open source code, running on Linux, Windows and MacIntosh systems. It may be downloaded at .

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