

Engineering PFLOTRAN for Scalable Performance on Cray XT and IBM BlueGene Architectures

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We describe PFLOTRAN -- a code for simulation of coupled hydro-thermal-chemical processes in variably saturated, non-isothermal, porous media -- and the approaches we have employed to obtain scalable performance on some of the largest scale supercomputers in the world. We present detailed analyses of I/O and solver performance on Jaguar, the Cray XT5 at Oak Ridge National Laboratory, and Intrepid, the IBM BlueGene/P at Argonne National Laboratory, that have guided our choice of algorithms.