July 12, 2012

Review comments for the manuscript titled
"Use of general purpose graphical processing units with MODFLOW-2005"

The paper presents the use of a graphical processing unit (GPU) to solve groundwater simulations more efficiently than the currently available MODFLOW-2005 that uses the central processing unit (CPU). The authors explain the application of GPU and use an unstructured preconditioned conjugate gradient (UPCG) solver to demonstrate speedups due to the use of GPU.

The paper presents an innovative approach to solving MODFLOW problems by using GPUs.

Following are some general comments:

1. Specify whether this work is first of its kind in applying GPUs in the field of groundwater modeling or specifically in the application of MODFLOW. Otherwise, cite other works that apply GPUs to solve groundwater simulations. The following two search results were found as a result of a quick Google search.
   http://dl.acm.org/citation.cfm?id=1774588&dl=ACM&coll=DL&CFID=95297384&CFTOKEN=85482675
   http://www.gpucomputing.net/?q=node/14182
2. Define the term speedup in the paper. Speedup is used in many different ways: solver speedup, speedup of parallelized loops, or speedup of total simulation time. Since simulation efficiency is at the core of this paper, it will be useful to mention what the calculated speedups are based on.
3. Are there any drawbacks to using GPUs and how these compare to using CPUs: limitations on the size of the problem; a general cost comparison (twice/thrice) etc.
4. Page 9 mentions that two different machines were used (2.4 GHz and 3 GHz) for comparing the CPU and GPU simulations. Were comparisons made between the two machines by running exactly same simulation runs on the two CPUs (without multithreading and by using 2 cores) to benchmark whether there are inherent differences in the performance of the two machines? Besides the processor speed other factors like bus speed, motherboard, hard drives, etc. could be impacting the results.
5. Did the authors study if a relationship existed between the total number of inner iterations and the speedups in the test simulations? If such a comparison was made, it may be interesting to share that with the readers. That would be an indication to the users as to which problems may reap the benefits of GPU more than others.
6. Was the total number of inner and outer iterations compared between the CPU and GPU simulations? The number should come out to be very similar in all simulations since the only thing GPU is doing is to parallelize the same computations that CPU is doing. This comparison would provide more confidence in the results that no other processes/algorithms besides GPU and its parallelization are responsible for the speedups.
7. There are more robust and faster solvers available besides PCG2 (XMD of MODFLOW-NWT; PCG5 of MODFLOW-SURFACT). It would be interesting to see how the GPU speedup (of 8 when compared to PCG2), compares with faster algorithms used in other solvers like XMD and PCG5.
8. The LMG2 (SAMG) solver is a parallel solver that claims speedups of up to 100 times when compared to the PCG solver (http://www.scai.fraunhofer.de/fileadmin/download/samg/paper/modflow11.pdf; http://www.scai.fraunhofer.de/fileadmin/download/samg/paper/Modflow_Paper.pdf). The

authors may wish to comment about the combination of the GPU technology and the SAMG solver.

9. How does PCG and UPCG sequential simulation compare?
10. Mention that the groundwater simulation results are the same irrespective of the solver/processor used.

Following are some specific comments on the manuscript.

1. Line 35: replace SOR with SSOR.
2. Line 40: also refer to other more efficient solvers, including the XMD, LMG2, and PCG5 solvers.
3. Line 44: it is important to note that speedup in this paper is based on "solver computing time" as defined in the paper. Upon testing, I had found that the loops parallelized took 25-30% of the total simulation time for the problem I was testing. Effectively, 5 times speedup (20%) of 25-30% comes out to 5-6% saving in the total simulation time.
4. Line 92: "a" appears twice.
5. Lines 161 and 163: is there a citation for CUBLAS and BLAS? If these are acronyms, what do they stand for?
6. Line 162: Saad, 2003 is misspelled.
7. Line 173: what is GEMV? Is this an acronym?
8. Lines 193 and 196: Xeon is misspelled.
9. Lines 251-252: is this treatment of RCLOSE applied to PCG solver as well? If not, then the comparison between PCG and UPCG is unfair since the two solvers would converge to different RCLOSE values.
10. Line 317: if MIC is more efficient, was parallelization of the MIC preconditioner attempted? Please make a statement as to why not.
11. Table 3: several values in this table are less than 1, indicating that UPCG is slower than PCG. What is the possible reason of this slowdown?