PRELIMINARY EVALUATION OF ABAQUS, FLUENT, AND CUFLOW PERFORMANCE ON BLUE WATERS

Allocation: Illinois/0.1 Mnh
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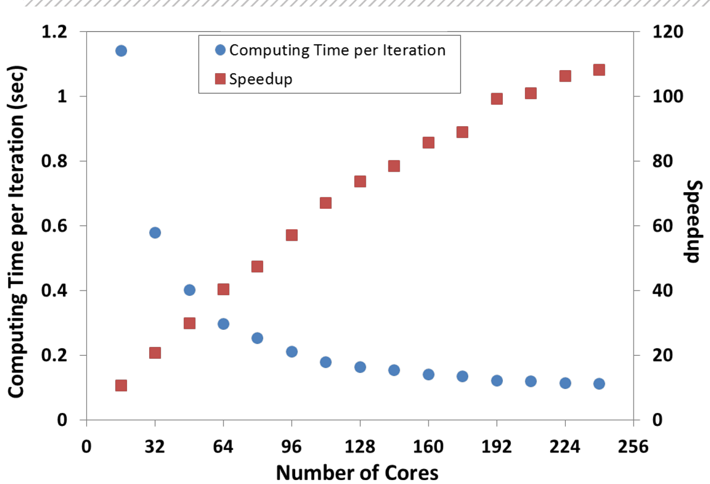
EXECUTIVE SUMMARY:

This project advances the state-of-the-art in computationally intensive models of turbulent flow, mechanical behavior, heat transfer, and solidification in the continuous casting of steel. These models provide practical insight into how to improve this important manufacturing process. The performance of and preliminary results from the commercial codes FLUENT and ABAQUS and an in-house code are presented. FLUENT has been tested with a 3-D, two-phase turbulent flow simulation, and demonstrates a speed-up factor of about 100 with 256 cores. ABAQUS/ Standard has limited speed-up capabilities because of its direct solver and works best with about 64 cores; the vast amount of memory on Blue Waters has improved the simulation time of a thermo-mechanical model of the mold and waterbox by a factor of about 40. A maximum speed-up factor of 25 has been observed on a single Blue Water XK7 node for the in-house GPU code for flow simulations.



INTRODUCTION

Continuous casting is used to produce 95% of steel in the world in the form of semi-finished shapes such as slabs, blooms, billets, beam blanks, and sheets. Even small improvements to this process can have a wide impact. Most defects arise in the mold region of the casting process due to the entrapment of inclusion particles into the solidifying shell and crack formation in the newly solidified steel shell. These defects persist into the final products and cannot be removed. Thus, the best method to improve steel products is to fully understand the mechanisms of defect formation and find operation conditions that avoid these problems.

Owing to the high temperatures and harsh commercial environment, it is difficult to conduct comprehensive measurements in the manufacturing process. Accurate and efficient computational models are needed to optimize various process variables (nozzle geometry, steel and gas flow rates, electromagnetics, taper of the mold walls, etc.). In addition to improving the manufacturing process, development and validation of better computational methodologies is useful in the modeling of many other processes.

METHODS AND RESULTS

For the stress analysis, several runs with a mesh of 375,200 elements, 754,554 nodes, and 2,263,662 degrees of freedom (DOFs) were completed on Blue Waters with implicit ABAQUS, which allows input and use of the phase field. The CPU time for one Newton iteration, consisting of 0.57 Tflop, is presented in Table 1 for different numbers of threads. The optimum number of threads is ~64. Efficiency appears to be limited by the FEM assembly process, coupling between DOFs during solving, or communication across processors. Results from this model match with plant inclinometer measurements on the cold-face exterior [11].

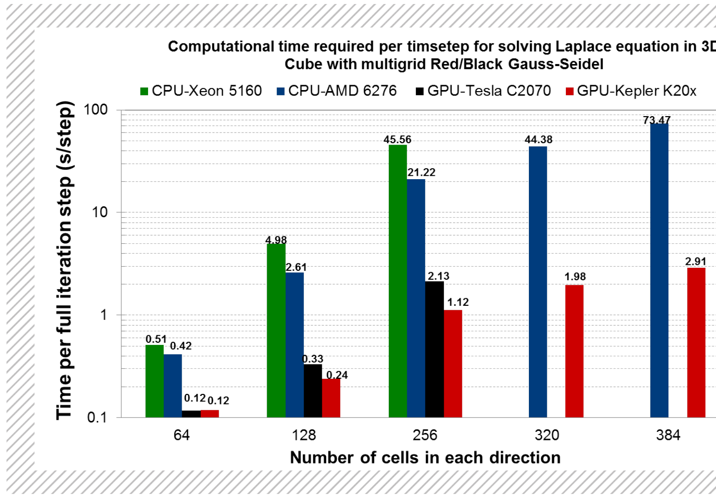
To evaluate performance of the commercial package, FLUENT, for fluid flow modeling on Blue Waters, argon-steel two-phase turbulent flows in a continuous casting mold was modeled on several computers. The test consisted of 0.66 million hexahedral mapped computational cells and ~8.4 million DOFs. One hundred iterations of FLUENT ran about 108 times faster on 240 nodes on Blue Waters than on a single-core Dell Precision T7600 workstation. Further simulations on Blue Waters with a different number of computer nodes showed almost linear speed-up with more nodes (Fig. 2). Results from this model show that dithering (oscillation) of the slide gate to lessen clogging also causes mold flow oscillations, which may become unstable at certain frequencies (Fig. 3) [12].

For the in-house GPU code, CUFLOW, the pressure Poisson equation (PPE) solver was tested on a single Blue Waters XK7 node by solving a heat conduction problem in a 3-D cube. The solver uses V-cycle multi-grid technique and a red/black successive over-relaxation (SOR) method. Both CPU and GPU versions were developed and tested. Increasing grid size from 0.26 million to 0.56 billion cells increased speedup to a maximum of 25 (Fig. 4). The model is being applied to predict the entrapment locations of inclusion particles in the solidified strand for conditions where measurements were obtained at an operating commercial caster [13].

WHY BLUE WATERS

All of the models used in this work are very computationally demanding. For the stress analysis part, multi-scale thermal-mechanical simulations of mechanical behavior the solidifying steel shell are being conducted using ABAQUS/Explicit. By aiming to capture physical phenomena involving detailed behavior on the small scale of the microstructure, this model requires advanced computational resources like Blue Waters.

For the fluid flow simulation, the Navier-Stokes equations are solved using the finite volume method for large eddy simulations (LES) incorporating the multi-phase flow via Eulerian-Lagrangian coupling [7-8]. Our previous LES simulations with about 1.5 million cells requires about 4 months to simulate only 30 seconds of model time on high-end workstations [9-10]. Proper mesh resolution requires over 10 million cells, and resolving the main periodic frequencies identified in plant experiments require over 60 seconds of model time. Thus, we explore the feasibility of using FLUENT on Blue Waters, with the help of ANSYS, Inc.



# THREADS	DAYS REQUIRED
32	6.80
64	5.25
128	5.50
256	5.50

FIGURE 1 (LEFT): FLUENT computational cost on Blue Waters (per iteration) with speed-up relative to a lab workstation.

FIGURE 2 (RIGHT): PPE solver performance on Blue Waters CPU and GPU.

TABLE 1: ABQUS runs on BW. CPU time required for 1 second simulation for different numbers of threads

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Hibbeler, L. C., B. G. Thomas, R. C. Schimmel, and H. H. Visser, Simulation and Online Measurement of Narrow Face Mold Distortion in Thin-Slab Casting. *Proc. 8th European Continuous Casting Conf.* , Graz, Austria, June 23-26, 2014.

Liu, R., and B. G. Thomas, Model of Transient Multiphase Turbulent Flow with Surface Level Fluctuations and Application to Slide-Gate Dithering in Steel Continuous Casting. (in preparation)

Jun, K., and B. G. Thomas, Prediction and Measurement of Turbulent Flow and Particle Entrapment in Continuous Slab Casting with Electromagnetic-Braking Flow-Control Mold. (in preparation).

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