Turbulent stellar convection simulations on the new Canadian computer Niagara

Falk Herwig (fherwig@uvic.ca), Robert Andrassy (University of Victoria) and Paul Woodward (University of Minnesota)
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At the end of March and beginning of April our research team had early test user access to the new Compute Canada computer Niagara operated by SciNet at the University of Toronto. Niagara has 1500 40-core Intel Skylake nodes in a dragonfly architecture machine.

What is the science?

For our early access opportunity on Niagara we chose a problem that we had not worked on before, the core convection during the hydrogen-core burning phase in a massive star with a mass 25 times that of the Sun. The nature of the transition region at the boundary between the convective core and the stable envelope is still poorly known. Recently, NASA's Kepler space mission has revealed intriguing observational constraints on the internal mixing processes through very high-precision monitoring of minuscule fluctuations of the light from individual stars. This asteroseismology data is being used to probe the internal properties of stars, just as seismology is used on Earth to probe underground for geological properties. Our simulations aim to (1) improve our general understanding of convection in stars, to (2) provide first-principles based insight into the physics of mixing at the core convection boundary, and (3) to start providing detailed 3D simulation-based understanding of the light oscillations that the Kepler mission and future missions like TESS are measuring of a very large number of stars.

What have we learned so far?

We have performed a simulation of turbulent core-convection in a massive star that provides unprecedented detail of the convective flow in its natural three-dimensional full sphere geometry. The simulation will also provide a detailed picture of the physics of mixing at the convective boundary and the oscillations in the stable envelope above the core. The convective motions in the core are propelled by heating associated with the nuclear hydrogen burning reactions. Fluid elements in the center of the star rise due to the buoyancy they gain from nuclear heating. Initially fluid elements rise and descend in all directions. However, quickly a large scale flow pattern in the form of a global dipole mode develops that is best observed in a rendering of the radial velocity (Figure 1). The large scale flow consist of two giant cells in which the fluid flow proceeds through the center of the entire sphere. Once the flow approaches the convective boundary it has to turn around as stability of the stratification beyond the boundary prohibits any substantial convective fluid motion to proceed beyond the boundary. The flow is redirected by

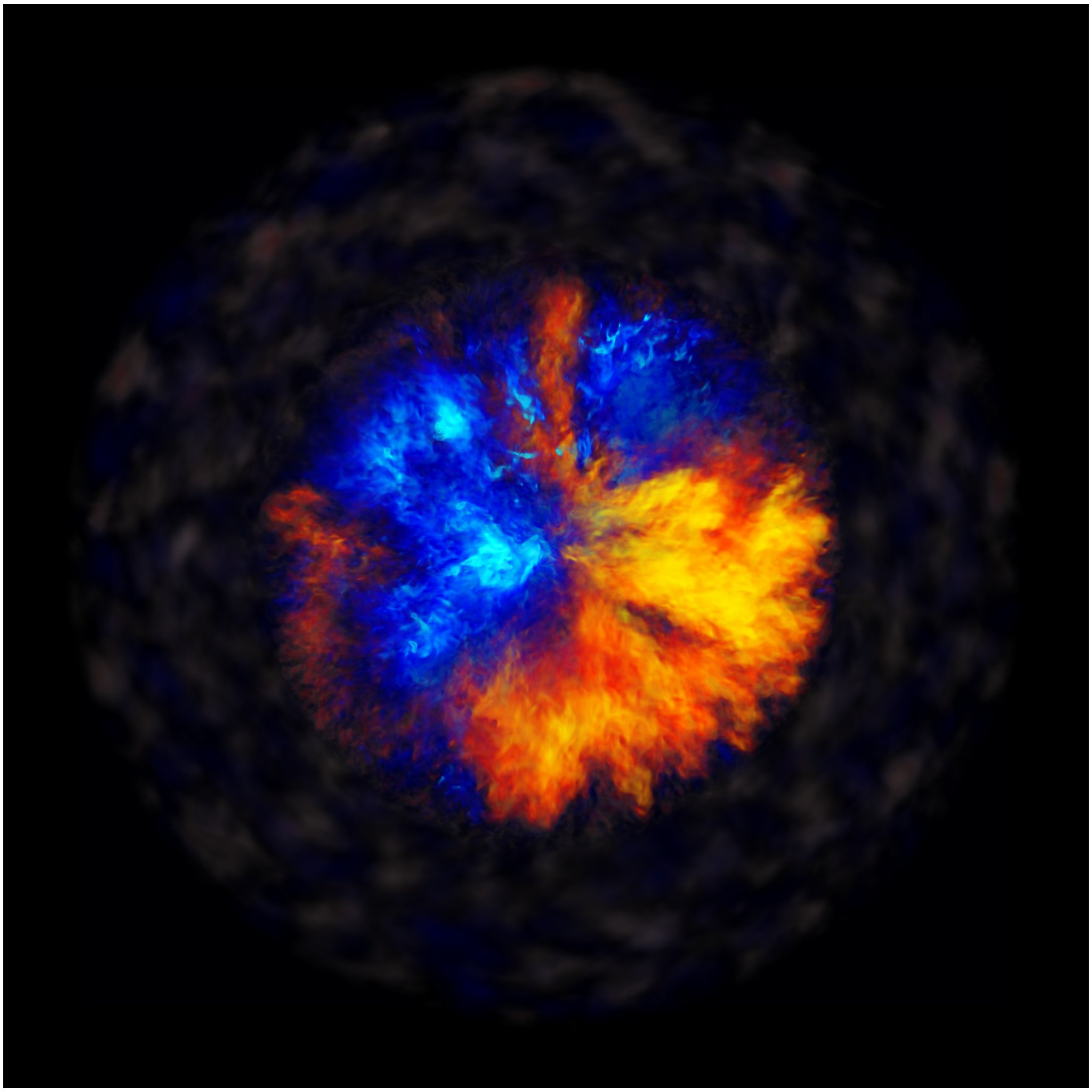

Figure 1: Radial velocity at 37.7 days of star time (dump 320). Orange-red is outward flow, blue-turquoise is inward-directed flow. The giant dipole mode is directed from the top-left to the bottom right.

the boundary into a horizontal flow which is clearly revealed in the visualization of the horizontal velocity component (Figure 2). The material then flows along the convective boundary in a sweeping motion and approaches the antipode from all sides. Here, the flows are converging and again are confined by the stable layers above the convection zone. The flows must separate from the boundary and turn inward again. In the vorticity rendering (Figure 3) the boundary layer instabilities that are associated with the shear flow of the tangential motions along the boundary and the subsequent boundary layer separation can be identified especially clearly in the bottom-left and top-right quadrants.

The internal gravity waves in the stable layer are particularly well observed in the rendering of the horizontal velocity (Figure 2). These waves have implications for asteroseismology observations of massive stars. Contrary to these well-ordered

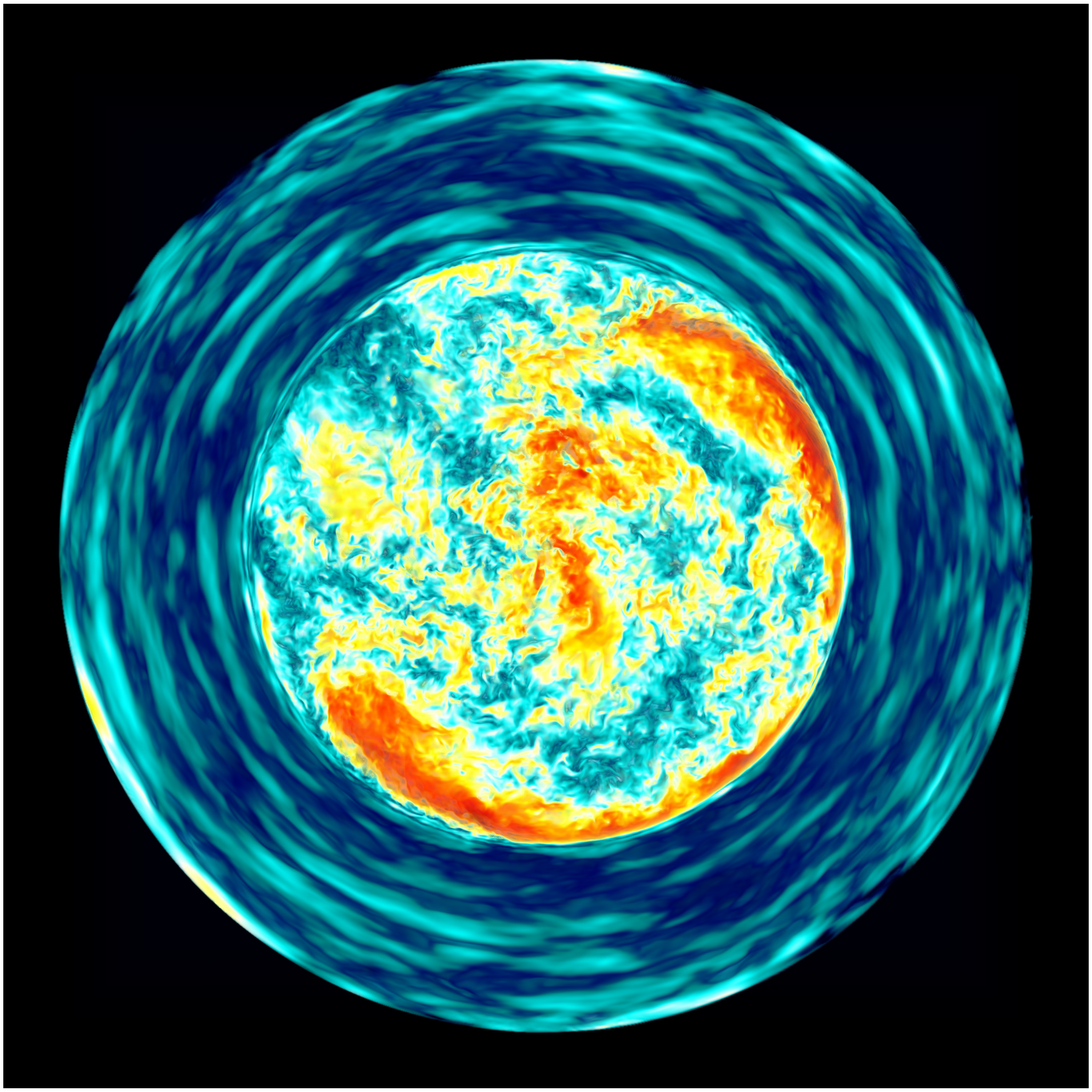

Figure 2 Magnitude of the tangential velocity 37.7 days of star time (dump 320). The outer stable region is characterized by oscillations associated with internal gravity waves. The inner region is dominated by a global dipole mode oriented from top-left to bottom-right in the diagonal direction. This global flow is also reflected in the distribution of the or radial velocity shown in Figure 1.

waves the motions in the convective core are highly turbulent. This is revealed by the fine detail of the vorticity at smaller scales. This high resolving power of the small scales will be needed for a detailed analysis of the mixing processes at the very narrow convective boundary transition layer.

An intriguing early result arose already at the first level of data analysis. Although the stable envelope and the convective core appear to be separated by a rather stiff boundary we observe that material from the stable layer is mixed into the core. Such mixing would provide fresh nuclear fuel for the star and extend its lifetime, with potentially significant observable consequences. The material above is tracked

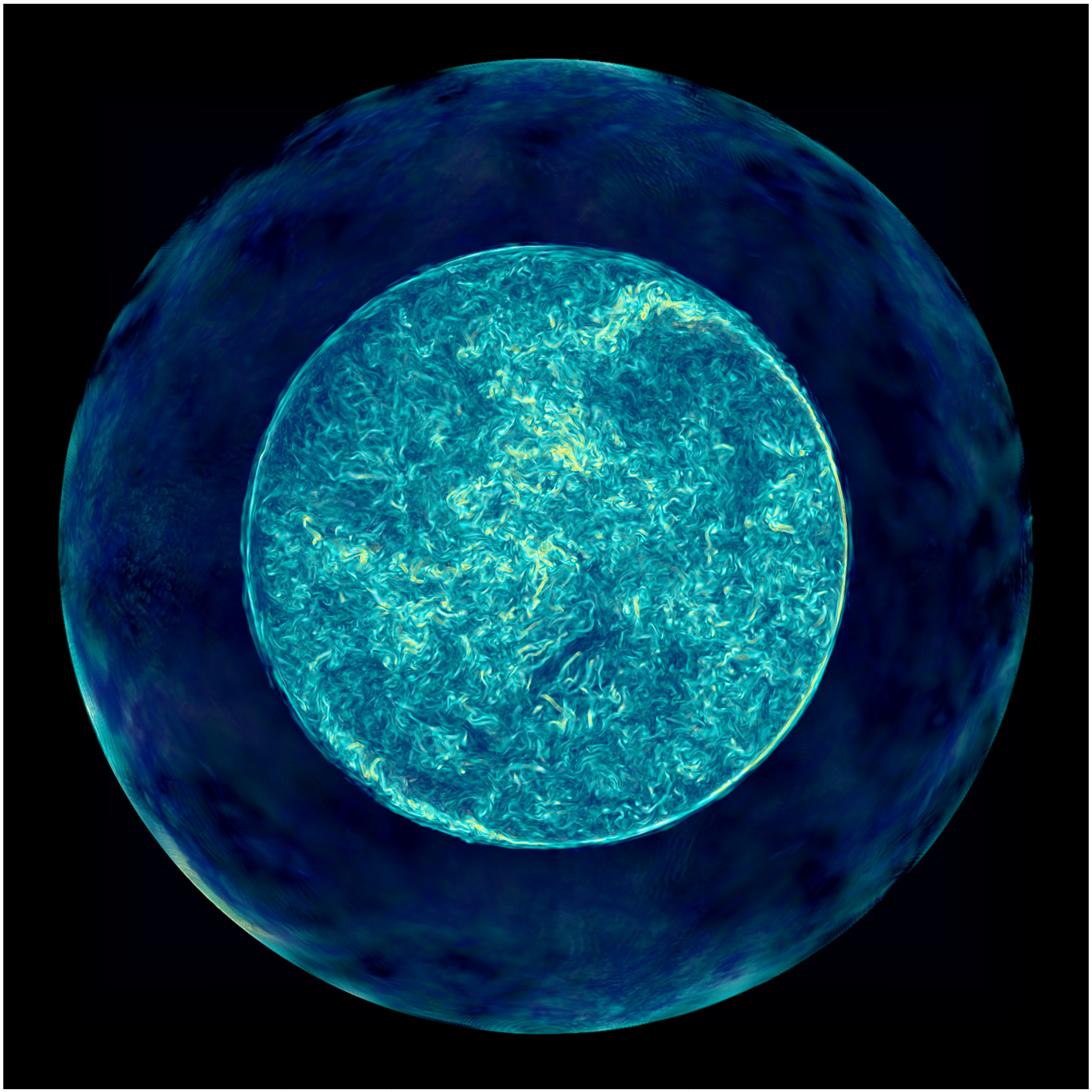

Figure 3 Vorticity shows how "curly" the flow is, and irregular patterns of vorticity in the core region show the high degree of turbulence that is captured by this high-resolution simulation.

separately in the code with high accuracy, and the mixing or entrainment can be seen in the rendering of the fractional volume of the envelope material shown in Figure 4. Our simulation reveals that the mass entrainment rate from the envelope into the core is two to three orders of magnitude higher compared to the mass that is available to be entrained over the lifetime of the core convection phase. This is obviously impossible and poses a serious conundrum. As the simulations were progressing we discussed possible mechanisms that could squelch this high entrainment rate. As we had worked the grid resolution up from low to medium and now high the entrainment rate did not change significantly, indicating that we have indeed reached numerical convergence on this simulation observable. Our discussions then zeroed in on the possible effect of rotation, which could break down the giant dipole mode and thereby supress some of the instability observed to be caused by the long and coherent boundary flows in the non-rotating case.

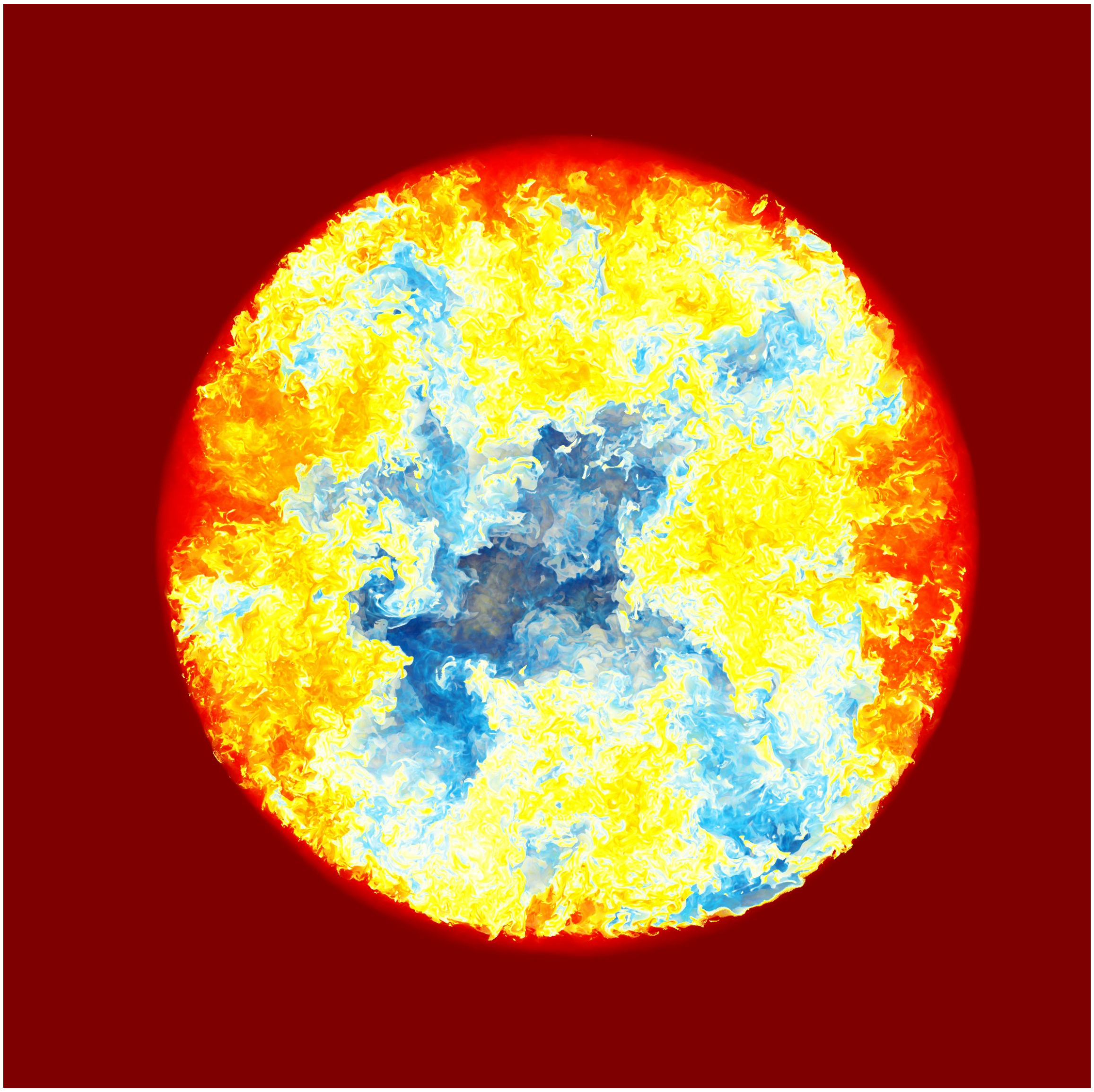

Figure 4 Concentration of the original star material in the stable layer that is initially located only above the convection zone (highest concentration is red and lower concentrations on a log scale are yellow, white, light blue and dark blue) and continuously mixed (or entrained) into the core region. The snapshot shows the simulation at 7.05 days star time.

Woodward decided to implement a rotating initial state, and we were able to run several cases with different heating and rotation rates at medium resolution within the next days. We got a glimpse into a new research direction as rotation does indeed affect the convective flow substantially. The giant dipole mode is broken down by rotation, and Taylor column structures emerge. The entrainment rate is reduced by rotation, but only by a factor of about three, for typical rotation rates. Maybe this is the most important initial result of our simulations. We have found a new puzzle and a new question to investigate.

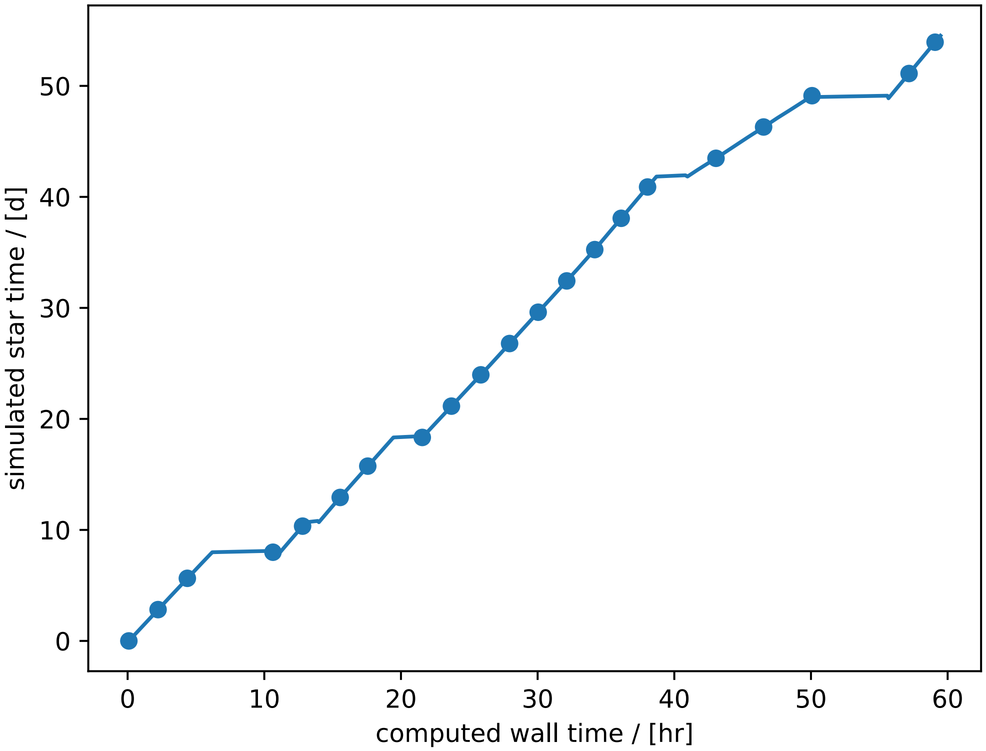

Figure 5: Simulated star time vs. time passed during the calculation according to the clock on the wall. Most parts were run on 1088 nodes, except a short section from hour 40 – 50 when we ran on 544 nodes and thus the rate of progress was reduced by a factor 2. Horizontal portions around 9, 20, 40 and 50-57 hrs indicate periods when the job was waiting in the queue between 8 hr jobs to proceed. Dots mark every 24th dump, which are written every 4126 time steps.

The movies of these three quantities accessible via the links provided at the bottom of this document provide the best impression of the time-dependent nature of core convection as revealed in these simulations.

About the simulations

Our team has been performing large-scale hydrodynamic simulations with the PPMstar code designed and written by Paul Woodward, based on decades of research on effective and highly scalable code design. Our team has in recent years mostly done the large runs on the NCSA Bluewaters machine on over 12,000 32-core nodes. The Niagara early access opportunity came fortuitously at the time when a major rewrite and redesign of the PPMstar code had been completed, and we were ready to try out the new PPMstar2.0 code at scale. All simulations on Niagara were computed with the new code. The simulations are performed on a Cartesian 3D grid and essentially solve the mass, momentum and energy conservation equations for stellar conditions. We typically distinguish between three grids. The 384^3 grid is used for tests. 768^3 grid is a medium resolution that gives good results for most applications. Occasionally high-resolution runs are needed to establish convergence properties and demonstrate that medium-grid runs provide sufficient resolving power for the relevant hydrodynamic instabilities to fully develop.

On Niagara we started with a number of low- and medium-resolution runs to establish the optimal configuration for the new code on the new machine. Adapting to the new platform was overall straightforward using the standard Intel compiler including MPI and OpenMP to deliver the hybrid parallelism the PPMstar code deploys. However, we were glad to be useful early users and able to point the SciNet team to some relatively minor setup issues with the scheduler that were quickly resolved. After doing initial runs with 68 or 144 nodes we eventually advanced to our big run.

We ran a H-core convection simulation for a 25 solar mass star on a 1536^3 grid for 2.02 million time steps to cover 57.69 days of star time. The simulation ran for the most part on 1088 nodes with 2176 ranks, 2 ranks per node and 40 threads per rank, taking advantage of the Intel hyperthreading capability that provides for our code a performance boost of approximately 25%. We increased the driving stellar luminosity by a factor 1000 to have convective velocities that are 10 times higher than in the real star. Figure 5 shows how the simulation progressed in terms of the simulated star time as a function of wall clock time of the computation.

What does Niagara mean for our research?

Our team has extensive experience running on among the largest supercomputers available. In the past we could run 768^3-grid simulations on the WestGrid orcinus computer in Canada, but only with the intervention of the admins to set up a reservation. Even then, such a run would take almost 2 weeks to complete, while using about ¼ of that machine. Now we can do such runs in one or two 8-hour jobs on 288 nodes on Niagara. In the past we were not able to run high-resolution simulations with acceptable run times in Canada. Our team is now, for the first time, able to perform simulations that are second to none internationally, in our own research area. This opens up entirely new research directions for our team in Canada. It also motivates us to invest more effort in Canada to improve and develop code capabilities for large-scale parallel simulations that are needed for more difficult problems, as we are now confident that we will have platforms in the future that will deliver scientific return on such capabilities investment.

About the team

Our team consists of two groups. The *Computational Stellar Astrophysics* group at the University of Victoria is led by Prof Falk Herwig. In his group CITA National Fellow Dr Robert Andrassy and PhD candidate Mrs Ondrea Clarkson were directly involved in the simulations performed on Niagara. Herwig and his group are investigating how the elements are formed in stars. Specifically they focus on how stellar convection, nuclear reactions and element formation processes play together in the final stages of the lives of stars. The Laboratory of Computational Science and

Engineering (LCSE) is led by Prof Paul Woodward at the University of Minnesota. Woodward has designed and implemented the PPMstar simulation code that we have been using on Niagara, and he is also directly involved in performing and analysing the simulations. He has a long track record of performing the largest hydrodynamic simulations on cutting edge hardware.

Media content and URLs

- YouTube playlist *core convection*: https://bit.ly/2HzTKtw
- Vimeo compilation *Core convection*: https://vimeo.com/album/5138161
- URL browser viewing/download, movies and still images original format: http://astrowww.phys.uvic.ca/~fherwig/Niagara
- Computational stellar astrophysics group at the University of Victoria: http://csa.phys.uvic.ca
- Laboratory of Computational science and engineering: http://www.lcse.umn.edu

Credits

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