INTRODUCTION

A blue whirl, shown in Fig. 1A, is a small, soot-free blue flame that was discovered serendipitously while performing experimental studies of fire whirls burning liquid hydrocarbon fuels on a water base (1). Although fire whirls are dangerous, violent, turbulent eddies of fire, they can be created in (relatively) safe, confined conditions for laboratory study [e.g., (2–5)]. Because fire whirls burn at higher temperatures (6) with higher burning rates (3, 7, 8) than their nonwhirling counterparts, preliminary studies (1) were being performed to determine whether it would be beneficial to use controlled fire whirls for practical purposes, such as oil-spill remediation.

In the initial experiments (1), the blue whirl evolved spontaneously from a 1-m-high fire whirl in a few seconds, as the whirling flame transitioned through a series of intermediate states. The result was that a noisy, turbulent, yellow fire whirl changed into a quiet, laminar, blue spinning flame. When a stable blue whirl becomes unstable for a short time, as shown in Fig. 1B, a yellow bubble-like structure appears in the center of the cone. This change in color, indicating the appearance of soot, led us to think of soot as a flow diagnostic that could be a hint of the otherwise invisible internal structure of the blue whirl. This structure suggested that the complex reactive-flow system was subject to the fluid dynamics instability, vortex breakdown, which changes simple swirling flows into bubble, helical, or whirling structures (9, 10).

After these initial experiments that demonstrated the blue whirl’s existence, newer experiments have produced temperature maps (11, 12), chemiluminescence measurements (12), scaling laws (13), swirl levels (vane inclination angles) leading to a stable blue whirl (14), ways to stabilize the blue whirl (13), and ways to create the blue whirl more easily (14).

Experimental measurements have given us considerable information about the formation conditions and the final state of the blue whirl. There has, however, not been any clear theory or measurements that reveal the flame structure or dynamics, in particular, what is the mechanism by which it forms from a fire whirl. There was considerable speculation, including that made in (1), but no definitive answers.

There are two limits of laminar flames that are discussed quite separately in the literature. In a laminar premixed flame, the flame front passes through premixed fuel and oxidizer, leaving behind the reaction products. The flame front is driven by expansion because of heat release from the reactions and physical diffusion processes, such as thermal conduction, molecular diffusion, and radiation transport. There can be fuel-lean, stoichiometric, and fuel-rich premixed flames. This is to be contrasted to a laminar diffusion flame, in which the fuel and oxidizer are initially separated and mix by physical diffusion processes. In this case, the rates of reactions are controlled by diffusion and the flame is said to be “diffusion limited.”

Thus, a fundamental question for combustion theory that was posed by the blue whirl is the following: What is the flame structure of the blue whirl? Is it a premixed flame or a diffusion flame, or some combination? Only if we understand its structure can we tame it, scale it, and create it at will.

Parallel to experiments, there have been computational and theoretical efforts to simulate fire whirls and the evolution to a blue whirl. Because of difficulties in experimental diagnostics, the flow and flame structure are still not certainly defined. This led us to believe that numerical simulations would be needed to tell us what the blue whirl really is. Such a simulation capability could also be used with experiments to study fundamental questions, such as whether the blue whirl scales or how to create it more directly without going through the full, dangerous fire whirl state.
This paper presents the first results of unsteady, three-dimensional (3D) numerical simulations that examine vortex breakdown in a reactive flow that leads to a blue whirl. It reveals the flame and flow structure of the blue whirl through a series of numerical diagnostics, relates the results to previous experiments, and suggests a path forward for both future experiments and simulations to examine and potentially use this previously unknown, soot-free flame structure.

RESULTS
The simulation in this paper began with a whirling flame that went through several transitional stages, with the blue whirl emerging as the result of vortex breakdown. At the quasi–steady state, the blue whirl slightly meanders and tilts but remains stable through the duration of the simulation. To explain the dynamics of the blue whirl, and understand its relation to vortex breakdown and flame theory, we focus here on one time instance in a quasi-steady solution.

The flame structure revealed
Figure 2A is a volume rendering of the heat release rate from the final result of the blue-whirl simulation effort. Figure 2B is a schematic diagram that summarizes the result. It is posed next to Fig. 2C, the observed blue whirl. We see now that the blue whirl is composed of four types of flames. The lower part of the blue whirl is a rich premixed flame, and the purple crown is a diffusion flame. What cannot be seen easily in the laboratory experiments is the lean premixed flame surrounding the purple haze, that is, the upper region just outside the diffusion flame. The bright blue ring is where the three types of flames meet, which is a triple flame. The interpretations presented in the schematic diagram in Fig. 2 are derived from data extracted from simulations in which an initial flow structure was given and allowed to evolve to a point where the basic blue-whirl structure no longer changed substantially in time.

The simulations consider a cubical enclosure with an open boundary at the top and no-slip walls at the lateral and bottom boundaries. Heptane vapor is injected at the center of the bottom wall with a constant velocity. Circulation is applied by forcing air through four gaps along the corners of the lateral walls. The details of the computational setup are described later in Methods.

Figure 3 is a comparison between the blue whirl experiment (12) and the simulation. The luminosity in Fig. 3A shows the experimental OH* concentration (12), which indicates the intensity of the reaction. For the simulation result, this is indicated by the 3D volume rendering of the heat release rate shown in Fig. 3B (now readjusted in gray scale in contrast with Fig. 2A). Bright regions indicate stronger reaction, and darker regions indicate weaker reaction. Both the experiment and simulation show that a significant amount of combustion occurs within the ring structure. The simulation result shown here agrees well with the experimental measurement in terms of curvature of the reaction regions and distribution of the reaction.

Figure 4A is a map of the flame index (15), \( I_f = \nabla Y_{\text{fuel}} \cdot \nabla Y_{\text{Ox}} \), where \( Y_{\text{fuel}} \) and \( Y_{\text{Ox}} \) are computed values of the mass fraction of fuel and oxidizer, respectively. \( I_f > 0 \) is a premixed flame and \( I_f < 0 \) is a diffusion flame. Figure 4B is the corresponding map of equivalence ratio, \( \phi \), and Fig. 4C shows temperature. Contours of heat release rate are superimposed on each figure to indicate reaction regions.

In Fig. 4A, region 1 has positive \( I_f \) and in Fig. 4B, region 1 has equivalence ratio larger than 1. Together, the heat release rate in region 1 corresponds to a premixed fuel-rich flame. By similar reasoning, the heat release rate in region 2 corresponds to a diffusion flame, because region 2 has negative \( I_f \) and an equivalence ratio of 1.

The heat release rate in region 3 corresponds to a premixed fuel lean premixed flame because region 3 has positive \( I_f \) and equivalence ratio less than 1. Region 4 is where the three flames meet and is the triple flame (or blue ring in the experiments). It has the most intense heat release, which is consistent with the OH* experimental measurements (12) as mentioned earlier. The temperature map, Fig. 4C, shows that the hottest regions are the diffusion flame in the purple crown, in agreement with the experimental measurements (11, 12), and the region at the bright blue ring (that could not be measured in the experiment). The peak temperature in the simulation is 2209 K. It is slightly higher than the peak temperature measured in the experiment, which is around 2000 K (11). The flame diameter at the ring is about 1.6 cm in Fig. 4, which is smaller than the diameter of 2 to 2.5 cm that was reported in the experiments (13).

Figure 4 shows a gap between the flame and bottom surface, which is consistent with the experimental observations (1). The gap in the simulation, however, is about 1.6 cm, which is larger than the gap observed in the experiments (1). Analysis of the composition of the data at the top of the computational grid shows that all of the fuel is consumed in the blue whirl and only hot product and air exit the computational domain.

Flow structure
The flow structure shown confirms and elaborates on experimental observations and replaces previous speculations. Figure 5 is a composite showing (A) streamlines, (B) tangential, and (C) axial velocities, again all with superimposed heat release rate as an indicator of the flame location, as well as (D) a profile of the tangential velocity...
through a slice below the blue whirl. The evolution to this structure from the initial conditions in the simulation shows the development of a whirling flame that undergoes vortex breakdown, leading to the typical bubble mode.

The bubble mode of vortex breakdown is revealed by the streamlines in Fig. 5A. It shows that the recirculation zones are inside the flame, and in particular, the vortex rim is inside what we see as the blue ring. This is in qualitative agreement with the experimental results shown in Fig. 1B, where the recirculation zone illuminated by the soot pattern is inside the blue rim. The tangential velocity map in Fig. 5B shows that, below the flame, the peak tangential velocity is high and the vortex core is narrow. This is more easily seen in the tangential velocity profile shown in Fig. 5D, which is extracted along the white dashed line in Fig. 5B. The peak tangential velocity is approximately 2.3 m/s, and the vortex core is 0.6 cm measured from the positive and negative tangential velocity. The peak tangential velocity is higher and the vortex core is narrower compared to the initial whirling flame stage, at which the peak tangential velocity is around 1.8 m/s and the vortex core is about 1.2 cm. The upper portion of the tangential velocity map shows the flow recovering the vortex structure as it leaves the bubble. The axial velocity map in Fig. 5C shows a jet-like velocity profile below the flame with a maximum axial velocity of 4.5 m/s. Within the lower part of the flame, there is a negative axial velocity region, and together with the streamlines in Fig. 5A, we again see the characteristics of a vortex breakdown bubble inside the flame. The minimum negative axial velocity oscillates between around −0.65 m/s and −0.55 m/s at the quasi–steady state. In the upper portion of the flame, above the bubble, the flow is accelerating in the axial direction as shown in the axial velocity map. This acceleration is an upward-moving jet of hot product gas caused by the volumetric expansion from the flame and buoyancy effects. The resulting shear layer forms roll-ups, as seen in Fig. 5C, which show that it is beginning to go unstable. This instability has not, however, transitioned to turbulence and the flow structure remains laminar above the flame.

### Boundary-layer diagnostics

Last, we use information from the flow streamlines in Fig. 6 superimposed on a 3D map of heat release rate (yellow structure in the figure) to show how air from the boundary layer is introduced into the flame. The streamlines are colored by the local temperature of the flow. The four streamlines start at 5 cm away from the center of fuel injection on an x-y plane. The streamlines in Fig. 6 (A and B) originate at two different heights above the lower boundary, 0.5 mm and 2.0 mm, respectively.

First, from Fig. 6B, we see that air from the higher portion of the boundary layer maintains a low temperature of 300 K even after moving around the flame. This shows that air from the upper part of the boundary layer is not involved in the combustion process. (This is also consistent with the experiments in which you can put your hand right up to the flame on the sides and it does not feel hot.)

The story is different, however, with air from the lower part of the boundary layer, shown in Fig. 6A, depending on the height at which the flow reaches the upward draft and is pulled into the flame. Air from very close to the bottom boundary, as shown here, first encounters the heptane vapor and is mixed because of the strong circulation below the bubble. This forms the rich premixed flame conditions seen at the bottom of the bubble. Then, most of the residual, unburned fuel and product are pulled into the bubble. This region inside the bubble creates the fuel-rich region that feeds the diffusion flame in the crown.

Meanwhile and simultaneously, air from higher in the boundary layer, here between the bottom (e.g., the 0.5-mm height) and the 2.0-mm height, is drawn upward and flows around the entire structure. Outside air and the residual fuel from inside the bubble set up a diffusion flame bordering the crown. A small amount of fuel also leaks outside the bubble and burns with the outside air to form a very

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**Fig. 3. Comparison of the experiment and the simulation.** (A) Experimental OH* concentration measurement [taken from figure 8A in (12)]. (B) 3D volume rendering of heat release rate in the simulation. The volume rendering is taken from the side view.

**Fig. 4. Slices through the center of the computational domain and parameters selected for combustion diagnostics.** (A) Flame index. (B) Equivalence ratio. (C) Temperature. Contours of heat release rate are superimposed on top to indicate reaction regions. Slices are shown for a zoomed-in region that is 8 cm wide.
fire whirl with several intermediate stages that involve changes in the state. There are several elements of the physical results that should be discussed before the numerical model is described in more detail.

The formation of the blue whirl is sensitive to the inflow boundary conditions. We know, however, that it is more easily formed when the blue whirl does not depend on the external shape of the container. Thus, we know that the blue whirl only occurs within a very narrow range of boundary conditions (i.e., tangential velocity and heat release rate) and the flame structure is sensitive to these boundary conditions. There have been, however, no detailed measurements of the boundary conditions that can be applied directly to the numerical simulations. Therefore, we took the approach to numerically finding the blue whirl by exploring the effects of varying the boundary conditions. The 3D unsteady numerical simulation described in this paper is one of many simulations carried out in which boundary and fuel inflow conditions were successively varied until a flame structure appeared that was in qualitative and even quantitative agreement with the observed blue whirl. Many computations with variations in geometrical, physical, and computational parameters were required to find this solution shown above. Critical elements in finding the solutions consisted of determining the appropriate air and fuel inflow geometry and the inflow rate of air and fuel to allow vortex breakdown to occur, the flame to lift away from the bottom surface, and the blue whirl to form. The details of the path leading to the solutions in this paper are described in Methods.

Notable differences between the experiments reported and the simulations include fuel injection versus fuel evaporation, the shape of the external container, and self-determining inflow boundary conditions versus forced air inflow. The primary difference in physical conditions from the reported experiments is that the process of heptane evaporation was bypassed by assuming a small forced inflow of pure heptane gas (here 371 K) at the bottom of the domain. Recent experiments have shown the blue whirl can be obtained from gaseous fuel injection, which verifies our approach of not including fuel evaporation. Prescribing an inflow velocity for the fuel, however, adds upward momentum to the flow. Therefore, the simulation shows a larger lift-off height of the flame above the bottom boundary when compared with the experiments. The equivalent liquid fuel flow rate in the simulation is 0.35 ml/min, which is smaller than 0.5 ml/min measured in experiments. This results in a smaller flame width in the simulation. Experiments performed in square containers have been reported to produce blue whirls. Thus, we know that the blue whirl does not depend on the external shape of the container. The formation of the blue whirl is sensitive to the inflow boundary conditions. We know, however, that it is more easily formed when the inflow conditions are as smooth and laminar as possible.
The blue whirl is at least a curious phenomenon that has many intriguing aspects. The most curious aspect is that it evolves spontaneously and presents itself as a stable state persisting until all of the fuel is burned. The second curiosity was that it is laminar and burning soot free, whereas the initial state was sooty, turbulent, and noisy. A third curiosity was that, in the experiments, it was not burning a gas, but a liquid hydrocarbon sitting on a water surface. Further experimentation revealed more features, such as its averaged temperature profile and its sensitivity to the boundary layer. Added to all of this was that it was very beautiful, both in its stable state, as a spinning blue top-like flame, and when it went slightly unstable, perhaps revealing some of its inner structure. The route to its formation and its transient unstable states implied its relation to the fluid phenomenon of vortex breakdown and the various states that evolve from this instability.

A recurring question, however, was whether the blue whirl could be useful in any way for efficient combustion with no soot formation. This involves questions such as: Can it be formed under controlled conditions more directly and without going through the fire whirl state? Can the size be controlled? Can it be made larger or smaller? Is there a scaling that can be used? Other, perhaps more far out questions, were: Can it be made without the confining walls? Can multiple blue whirls be made and work together? Could it be part of a combustor or a propulsion device? The lure of being able to burn any liquid hydrocarbon efficiently and cleanly is extremely attractive.

None of these questions can be answered easily until we at least understand the structure and dynamics of the flame and have a tool through which we can easily explore some of these questions. This paper describes a first step: a tool that can be used to explore and test the phenomenon, and how it has been used to reveal the blue whirl structure.

**METHODS**

**Approach to the problem**

Simulating a realistic fire whirl is expensive computationally because of the very wide range of space and time scales involved. Simulating a blue whirl would mean either simulating a fire whirl subject to vortex breakdown or finding a way to go more directly to blue-whirl conditions. At the beginning of the simulation effort, we did not know which approach or whether a combined approach would work best. This leads us to a computational “hunt” for the blue whirl, in which we first developed the numerical method and then used the simulations to explore the effects of varying the controlling parameters, for example, fuel and air inlet sizes and velocities.

We took the approach to creating the simulations by first simulating vortex breakdown in a nonreactive gas to observe the modes induced by vortex breakdown as they evolve in a gaseous reactive flow. This led to the development of the low–Mach number algorithm (16) described in more detail in the next section. Then, we developed a chemical diffusion model (CDM) that reproduces features of a diffusion flame as well as a premixed flame and found parameters for it suitable for n-heptane (17) used as the fuel in the original experiments. The next step we took is simulating a fire whirl and ensuring that the resulting flow and properties are consistent with experimental observations. This required generalizing the low–Mach number algorithm so that it is able to simulate reactive flow, with energy release and species conversion (18). Then, we simulated reactive vortex breakdown (19), as it would occur when the swirling gas consists of an ignited mixture of fuel and air. The conditions should be similar to those that produced the experimentally observed blue whirl. Last, we used the recently developed numerical model and the general initial conditions of the experiment to reproduce the blue whirl numerically.

**Numerical algorithms**

To be able to compute the blue whirl, algorithms for low–Mach number reactive flows were developed, refined, and implemented into a computational fluid dynamics code, which solves the unsteady, compressible, reactive NS equations. The underlying concept of the low–Mach number algorithm is based on BIC–FCT, the barely implicit correction to flux–corrected transport, and is referred to here by the same name (20). The exact procedure is described in (16), and the extensions to reactive flows, with physical diffusion effects, chemical energy release, and species conversion have been reported in (17, 18, 21).

The underlying fluid solver of BIC–FCT is based on fourth-order FCT (22–24). The solution is modified by a pressure correction term $\delta P$ to filter out high frequencies of the sound–wave spectrum, thus removing the computational restriction imposed by sound waves, thereby removing the numerical expense of explicitly integrating the NS equations in a low–Mach number flow. The BIC–FCT algorithm enables large computational time steps while maintaining certain compressibility effects. One result of this large time step, however, is that the effects of nonsimultaneity in the various parts of the solution are exacerbated. To deal with these, a conservative monotone filter was applied to damp unphysical fluctuations as they arose. A number of 1D, 2D, and 3D accuracy and resolution tests were applied to a series of test flows (16). The code is stable, robust, and capable of solving problems with many types of boundary conditions (16, 25).

The effects of diffusion and chemical reactions with heat release for heptane and air mixtures were incorporated into the solver using the CDM (26, 27). The CDM is a way to represent chemical reactions and heat release by minimizing the number of species and reactions that are required to compute bulk combustion properties, for example, the flame speed, thickness, and temperature. The CDM differs from detailed chemical models in that it considers three species (fuel, air, and product) and does not include multiple reaction pathways. By
doing this, it reduces the computational cost of complex, 3D computations and therefore makes them more affordable. A mathematical expression, such as a polynomial or Arrhenius exponential, is used by the CDM to regulate the conversion of fuel and air to product. The mathematical form has constants that are fit to maintain constraints that come from the bulk combustion properties. The constants are found from an iterative calibration procedure that incorporates fundamental principles of combustion and diffusion processes. The values of the constraints can come from experiments or detailed chemical mechanisms. In the case here for heptane, we calibrated the CDM using the flame and diffusion properties from a more detailed chemical mechanism representing heptane-air combustion (28). Further details of the calibration and test problems for the version of the CDM used here can be found in (17, 27).

Computational setup
The computational setup for the simulation in this paper, including the mesh and the initial and boundary conditions, is shown in Fig. 7. The domain is a cube with sides that are 30 cm long. The upper boundary is an outflow condition, and all other boundaries are non-slip, adiabatic walls. Heptane vapor is injected within a specified diameter at the center of the bottom wall with a constant velocity of 5.8 cm/s and at the evaporation temperature of heptane at 1 atm, 371 K. The fuel inlet diameter varied from 2.54 cm to 0.9 cm during the simulation, which is explained in detail in the next section. Circulation is applied by forcing air through the four corners with a speed of 40 cm/s along slits that are 5 cm wide. Radial inflow is introduced by forcing air with a velocity of 60 cm/s through a 1.4-cm-high and 11-cm-wide region along the lower portion of the walls. The interior domain is initialized with quiescent air at 1 atm and 298 K with a column of hot product gas that is 1 cm in diameter and 10 cm high just above the fuel inflow for ignition.

As shown in Fig. 7B, the simulations were performed on a 3D mesh that concentrated a fine grid along the center to cover the region of a blue whirl. The fine grid region is 10 cm in width, 10 cm in depth, and 10 cm in height. For the results shown, the width of the finest cell size in the center region was 0.01465 cm, corresponding to five levels of refinement from the coarsest cells at the edge of the domain. During the entire simulation, however, the mesh was slowly refined from two levels to five levels. This is explained in detail in the next section.

The adequacy of the numerical resolution was tested by increasing the levels of refinement in the blue-whirl region until there were no changes to the flow and flame structure. Refinement required for a premixed flame is reported in (26). In this computation, there are enough computational cells within the flame thickness to give at most an 8% difference between the flame speed computed by BIC-FCT and the ideal value computed by chemical equilibrium software (28, 29). In the rich and lean flame regions, this difference is smaller because there are more cells within the flame thickness since non-stoichiometric flames are thicker. The resolution in this simulation is also enough to resolve a diffusion flame, for which a cell size of 0.07 cm or smaller is required, determined by solving 2D counterflow diffusion flames.

Simulation pathway
The computational search for the blue whirl took its lead from the experiments. We started the simulation with air and fuel flow rates close to the experimental measurements, which are an air inflow of 40 cm/s at the corner gaps and 60 cm/s at the lower gaps along the bottom boundary and the equivalent liquid fuel volumetric flow rate of 0.4 ml/min (13). The global equivalence ratio \( \phi \) started as 0.00241, which is calculated according to Eq. 1

\[
\phi = \frac{m_{\text{fuel}}}{m_{\text{air}}} \cdot \frac{FA_{\text{stoich}}}{\text{stoich}}
\]

Here, \( m_{\text{fuel}} \) is the mass flow rate of fuel entering the domain, \( m_{\text{air}} \) is the mass flow rate of air entering the domain, and \( FA_{\text{stoich}} \) is the stoichiometric fuel to air mass ratio that is approximately 0.066 for heptane-air. We successively varied the boundary conditions and mesh in five steps to reach the quasi–steady state presented in this paper. Details of the flow development at each step are shown in figure 2 of (30). Here, we summarize the changes made and the state of the solution at each step.

We started with specifying the fuel inlet diameter as 2.54 cm. The resulting gaseous fuel inlet velocity is 0.9 cm/s. We used two levels of mesh refinement with the coarsest mesh described in the previous section. The initial transient development, the flow reached a quasi–steady state with a whirling flame attached to the bottom boundary and no negative axial velocity. The average flame width was 1.7 cm, and the average flame height was 10 cm.

Then, in the second step, the fuel inlet diameter was decreased to 0.9 cm and the equivalent liquid fuel volumetric flow rate was decreased to 0.35 ml/min. All other conditions were kept the same. The resulting fuel inlet velocity is 5.8 cm/s. The global equivalence ratio decreased slightly to 0.00211, calculated by Eq. 1. After the flow reached the new quasi–steady state, the flame lifted from the bottom boundary, but there was still no negative axial velocity and, hence, no sign of vortex breakdown. The flame was approximately 1.1 cm wide, 3 cm tall, and lifted by 0.7 cm.

In the third step, the mesh refinement was increased to three levels and the flame remained lifted and stable, but a recirculation zone was observed inside the flame, which indicated vortex breakdown. The flame was approximately 1.2 cm wide, 5 cm tall, and lifted by 0.9 cm. The flame was relatively long and slender compared with the observed blue whirl. The minimum axial velocity was approximately −27 cm/s.

In the fourth step, the mesh was further refined to four levels. The flame became more lifted and the reversed flow became stronger. After the flow reached a quasi–steady state, the flame became flatter and wider and the blue whirl structure appeared. The flame was approximately 1.4 cm wide, 2.5 cm tall, and lifted by 1.1 cm. The minimum axial velocity oscillated between approximately −90 cm/s and −70 cm/s.

Last, the mesh was refined to five levels. The structure of the blue whirl was maintained, and the flame is approximately 1.6 cm wide, 1.5 cm tall, and lifted by 1.6 cm. The minimum axial velocity oscillated between approximately −65 cm/s and −55 cm/s. There was no major change in the flow and flame structures. We consider the solution to be well resolved, and the result shown in this paper is one time instance taken from the calculation at this stage.

Computational resources required
With two levels of mesh refinement, this computation covered 12 s of physical time, and with three levels of refinement, the computation covered another 3 s of physical time. The computation covered another 0.6 s of physical time in total with four and five levels of...
refinement, 0.3 s each. The final mesh with five levels of refinement contains 410 million cells. The computation overall took about 600,000 central processing unit (CPU) hours on 40 Dell PowerEdge C8220 nodes using dual Intel Ivy Bridge E5-2680v2 processors running at 2.80 GHz with 20 cores per node.

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