ABSTRACT
Due to the high expense of running Computational Fluid Dynamics (CFD) simulation. CFD end users are constantly navigating a speed-vs-accuracy trade-off. The answer to the question of where to land in this trade-off is fluid and it changes based on the purpose of the simulation or the current position of the CFD end user in the entire simulation workflow. The required simulation accuracy could change even in successive iterations of the same simulation. The current approach of using literature studies and grid convergence studies to navigate the speed-vs-accuracy does not allow for the needed flexibility of adjusting the ideal grid resolution to meet constantly changing accuracy needs and results in simulations that are run using using constant accuracy levels. Our overall goal is to support the ever changing end user accuracy requirements of simulation applications by providing CFD end users with an insight error variance feedback measure as well as an insight slider user interface that allows simulation end users to change their speed-vs-accuracy trade-off requirements on demand, while making informed decisions when selecting ideal grid resolutions to speedup their simulations. This work contributes to this goal by modelling the impact of varying grid resolution on insight error variance. This model allows us to use insight error variance as feedback measure for CFD end users using grid resolution to speed up their simulations. Using a crowd study, we successfully model insight error in CFD applications are present the details of our model.

Modelling the Effect of Computation Sampling on Insight Error in Computational Fluid Dynamics Scientific Simulation

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ARTICLE HISTORY
Compiled August 10, 2020

1. Introduction

The human has been an afterthought in the collection and generation of big data. After these massive amounts of data have been collected and generated, humans are caught trying to figure out how to process them. There is a disconnect between human cognitive abilities and the high powered algorithms and computers used to produce and process this data. What is needed is a framework for data intensive computing applications like those of Computational Fluid Dynamics (CFD) scientific simulation and data mining, that puts the human front and center of all data related processes.

Given that it is the human who is the consumer of the data, human limitations and strengths need to be taken into consideration when developing data intensive computing applications. One approach that does just that is that of data visualization. For that reason, it is used in many data intensive computing applications like those of simulation, data intensive analytics, and data mining. However, data visualizations has its limitations. Limitations that include slow responsiveness, high overplotting and the inability to store and display entire big data sets highlight the inability of traditional visualization techniques to scale to massive amounts of data (Wang et al. 2015).

The accuracy of the CFD scientific simulation depends on the amount of calculations that are a function of the the grid resolution in addition to how well the selected solution scheme and modelling parameters effectively represent the underlying physics of the problem. The finer the grid resolution of the simulation, the longer the simulation runs. Simulations can take hours, days, weeks, or months given the intensive algebra and matrix operations required to solve the computational problem, in addition to frequency of disk writes for purposes of time series analysis and checkpointing. These long runtimes can be exacerbated by the iterative and exploratory nature of simulation as well as long wait times as jobs wait in the high performance computing (HPC) queue for resource allocation. Common work flows include executing simulation runs with different physical parameters and grid resolutions in order to decide on an adequate resolution, with these runs being interspaced with long queue wait times for resource allocation. Additional runs would then be executed in an attempt to find the solution to the simulation objective. A lot of these runs would then be discarded after looking at the postprocessing visualization, when it is determined that the input parameters

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for the simulation need to be altered.

In scenarios where software licensing fees are paid for per processor or core and the simulation is run on a high performance computer that uses large amounts of power and cooling, any discarded or excessive simulation runs are not only a waste of time, but they impact an organization's bottom line. Given that the results of the simulation are processed visually by humans to determine correctness, and in some cases convergence, any level of accuracy that exceeds the capabilities of humans to perceive in a visualization is not only a waste of time but a waste of money too.

Similar to our previous work, we define insight error (IE) as the difference between i) a human estimate of a sample statistic made after observing a visualization of a sample drawn from the population and ii) the ground truth, which is the actual population parameter. We define perception error (PE) as the error in the human estimate of the sample statistic made from viewing the visualization of the sample in comparison to the ground truth of the sample. When one visualizes a sample drawn from a population, the error between a sample statistic of that sample and the objective representation of that sample statistic calculated from that visualization is our visualization error. Sampling error (SE) is the error of the sample statistic of a sample drawn from a population in comparison to the ground truth of the actual population parameter.

In this work, we apply our IE framework to the postprocessing results of a two phase CFD simulation of interacting fluids in a tank as a step towards putting the human front and center of the loop of the simulation process. Using the quantification of insights gained from visualized results of CFD simulation, we model the relationship between insight and grid resolution. Using a case study, participants are asked to evaluate the results of the simulation. They are asked questions about the simulation and asked to provide any additional insights they have about the simulation. Using a ground truth calculated from the actual results of the simulation, error is calculated between the participants' responses and the ground truth. The variance of these errors is used to investigate the relationship between the level of insight and the grid resolution. This work makes the following contributions:

C 1. We conduct a crowd study that investigates the relationship between insight variance levels and grid resolution in a scientific simulation.

C 2. We provide a model for the relationship between insight and its component errors and the grid resolution in a scientific simulation.

C 3. We demonstrate the ability of our model to predict a grid resolution given an arbitrary insight variance level.

2. Background and Related Work

CFD turns computers into safe and timely virtual laboratories (Wang and Yan 2008). Due to the high expense associated with long CFD execution times, CFD end users use refining and coarsening of the grid resolution as a method for changing the amount of calculations that the simulation is doing and this causes a change in the amount of data produced, which in turn alters the run time of the simulation executions. CFD end users use the idea of reducing the number of elements used for simulation calculations or grid resolution coarsening to speed up simulation executions and total simulation workflows (Yahya et al. 2018). This can be thought of a form of spatial or systematic sampling. The effect of grid resolution coarsening is similar to that of sampling in that it results in a change of accuracy (Tu et al. 2018). Similar to sampling the benefits of refining the grid resolution diminish out after some threshold. The benefits of grid resolution refinement are also impacted by the underlying physics of the fluids being modelled (Ferziger et al. 2020).

Grid convergence study results allow CFD end users to understand the effects of grid resolution coarsening in terms of simulation wall clock savings and simulation accuracy, given an accurate numerical model of the physics being simulated (Krishnamurthy 2017). This work complements the approach of grid resolution coarsening to reduce simulation wall clock time. It provides a feedback metric that gives CFD end users additional insights on the effects of grid resolution coarsening on human cognitive insights in order to enable them to make an informed decision when managing the accuracy vs performance trade-off (Banks et al. 2018) that we refer to as the speed-vs-accuracy trade-off.

The viability of simulation including CFD depends on user trust. For example people would not use CFD even though it is shown to be faster and safer than an actual experiment if it has not been shown to produce accurate results. User trust is gained by showing that the simulation is either accurate or by accounting for any inaccuracy and informing the end users of any error or uncertainty resulting from the inaccuracy. Validation and verification are simulation steps concerned with gaining and maintaining end user trust (Stamou et al. 2018). Validation is concerned with determining the accuracy of a simulation in comparison to experimental results while verification is determined by comparing simulation results to those of a computational model (Oberkampf et al. 2004). A common approach to making the validation and verification results actionable for end users is that of uncertainty quantification (Wu et al. 2018) .

Bao et al learn the relationship between simulation error and the simulation physical features that are derived from the mesh size, model information and simulation parameters. They model this relationship and use the physical features to predict the simulation error in order to suggest the optimal mesh size for simulation end users given simulation physical features (Bao et al. 2019a). Bao et al also use historical simulation data to train a deep forward neural network to predict the simulation error given a grid resolution (Bao et al. 2019b). Similar to these works, we use machine learning to learn the relationship between grid resolution and simulation result uncertainty, which is calculated based on error.Wang, Wu and Kozlowski use simulation results as well as bayesian inference to provide uncertainty distributions for given simulation input parameters in order to show the necessity of quantifying uncertainty information in simulation applications (Wang et al. 2019).

Similar to our work these works base their approach on various sources of error that propagate through the simulation steps. However, our approaches differ in how we calculate the error. These works calculate error based on variable values within grid cells. Our approach calculates error based on measured human cognitive insight. We choose this approach because we believe that a human centered approach will result in more efficient simulations that do not produce or process data whose results exceed human cognitive capabilities.

Oberkampf and Barone present a confidence interval metric that is based on the mean response of the simulation system (Oberkampf and Barone 2006). Ferson, Oberkampf and Ginzburg introduce a validation metric and in the process discuss the need for validation metrics to consider entire uncertainty distributions as opposed to just the means of errors (Ferson et al. 2008). We agree with this observation and for that reason, we use the variance of errors to provide insight error feedback to simulation users on the impact of a selected grid resolution on the model accuracy. Our approach for providing feedback has similarities with the approaches mentioned above, but we have a major difference in the envisioned use of our feedback metric. Even though we also aim to present a feedback metric for the purpose of allowing CFD end users to find the ideal grid resolution to execute the simulation, we realize that the ideal grid resolution selection criteria is a fluid one that changes based on circumstances like the simulation budget and where in the total workflow simulation end users are. For that reason our feedback metric is designed to be provided with a slider that allows end users to change select varying insight error requirements based on their cognitive insight requirements as needed.

3. Experiment Methodology

Our ultimate goal is speeding up scientific simulation, particularly CFD by incorporating human limitations into the simulation process in a way that will result in the speedup of the simulation workflow. Our general research approach is based on visualization being the interface between the simulation results and the human. Our general research approach is also guided by the realization that CFD and other applications that process and visualize large amounts of data present a speed-vs-accuracy trade-off for and users of such applications. Sampling is a widely used method to allow for this trade-off. In case of CFD simulation, coarsening the simulation grid resolution in order to speedup the simulation is a form of spatial sampling. For that reason, the grid resolution in CFD simulation is synonymous with the sample size in other sampling applications. Coarser grid resolutions result in faster simulation, but they also result in less accurate simulations. Since humans get desired insights from the simulation via the visualization we model the insight extraction process in order to i) identify the bounds of human insights and ii) understand the relationship between insight variance levels and the amount of data sampling. This will allow us to use user provided insight requirements as parameters for the stimulation, which would put the human front and center of the simulation process and result in a simulation with little or no wasted processes beyond those required by the human.

In order to meet the objectives above, we collect data from humans as they generate insights from the visualized results of a CFD scientific simulation. We use a crowd study to recruit humans for this task because of the participant diversity and the rest of the reasons stated in our earlier work. We ask our participants to complete benchmark tasks due to the ease of quantifying and comparing human insights associated with such tasks (North 2006). However, due to the limitations of such tasks we also ask or participants to complete an open ended task. We hypothesize the behavior of our errors and proceed to quantify the insights provided by our crowd participants. We calculate IE and its component errors. We then use our framework to model the behaviors of our errors. Using our crowd responses and models from our framework, we test our hypotheses and use our results to validate our framework for the speedup of CFD applications.

4. Design of Experiment

We use a randomized between subjects experiment with blocking. Grid resolution is our independent variable while insight error is our dependent variable. Our experiment has

1 treatment factor with 5 levels. In case varying timestamps has an effect on insight variance levels, we block the responses by timestep. 150 Participants are randomly assigned to one of 5 groups and also randomly assigned to one of 5 blocks within a treatment Each treatment consists of an image of the visualization of the results from a given grid resolution and timestep. Each participant sees one treatment. Participants are asked to complete a benchmark and open ended task. Given that benchmark tasks constrain the insights that our participants can provide, while open ended tasks require more participant training and administrator expertise for coding and analyzing the response (North 2006), we provide tasks that take advantage of the benefits of both task types. Benchmark tasks allow us to guarantee that our participants provide insights that align with our study design. Our choice of simulation, which is based on an experiment that is easy for participants to understand, allows us to benefit from the advantages of open ended tasks without having to provide extended training to our participants. The open ended task also allows us to identify automated response from bots We use responses from all 150 participants in our analysis.

4.1. *Research Questions*

In this work we are interested in understanding how the choice of a grid resolution impacts the IE, PE, VE and SE. Given a uniform mesh and a two phase fluid CFD simulation, we answer the following research questions:

R 1. What is the relationship between grid resolution and the variance of IE?

R 2. What is the relationship between grid resolution and the variance of PE, VE and SE?

R 3. Can one use SE, VE and PE to predict the variance of IE in a scientific simulation?

R 4. Can one predict IE as a function of grid resolution?

4.2. *Assumptions*

In this work we assume the task of estimating the percentage volume is representative of a typical analysis task conducted on the results of CFD postprocessing. We also assume that the behaviour of the relationship between insight error and grid resolution in this task generalizes to other CFD postprocessing analysis tasks. We make these assumptions because CFD result analysis consists of reviewing animated results that consist of frames of images similar to those used in our experiments. CFD simulation end users generate insights from series of frames. Our insight framework and our experiment tasks allow us to determine how well people understand each of these frames.

4.3. *Hypotheses*

As done previously, in order to answer our research questions we create hypotheses that are aligned to our questions. Using the results from our crowd study, we test our hypotheses. The results of our hypothesis tests allow us to determine the answers to our research questions. Our hypotheses that assume a uniform grid and a two phase fluid CFD simulation as a starting point before addressing non-uniform grids and other multi-phase simulations are:

H 1. The variance of IE is high for coarse grid resolutions, reduces and finally grows again for large resolutions for insights generated from viewing CFD postprocessing visualizations.

H 2. The variances of the component errors of IE have an exponential decay, exponential decay and a U-shaped relationship with grid resolution for SE, VE and PE errors, respectively for insights generated from viewing CFD postprocessing visualizations.

H 3. The component errors of IE, SE, VE and PE, can be used to predict the IE for insights generated from viewing CFD postprocessing visualizations.

H 4. There is a non-linear relationship between grid resolution and the variance of IE and as a result, grid resolution can be used to predict the variance of IE for insights generated from viewing CFD postprocessing visualizations, using a higher order polynomial.

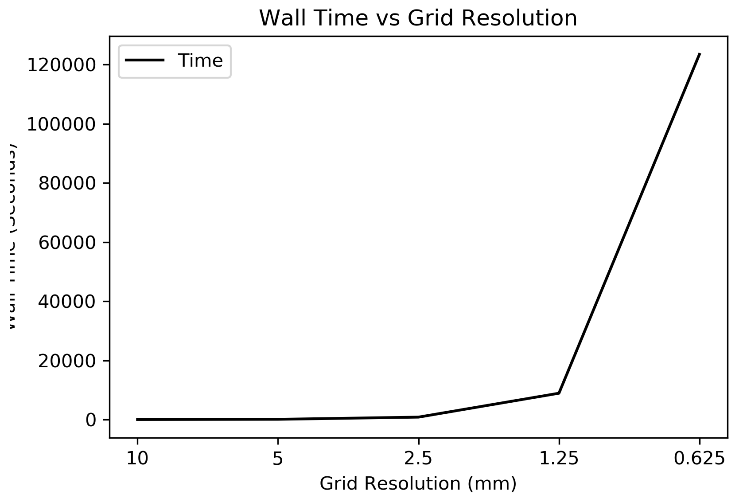

Figure 1. Simulation wall times in seconds as a function of grid resolution for the simulations run for our study. Simulations are run on a High Performance Computer using an Intel Xeon E5 2.1GHz processor with 16 cores and 32 threads and 128GB of memory.

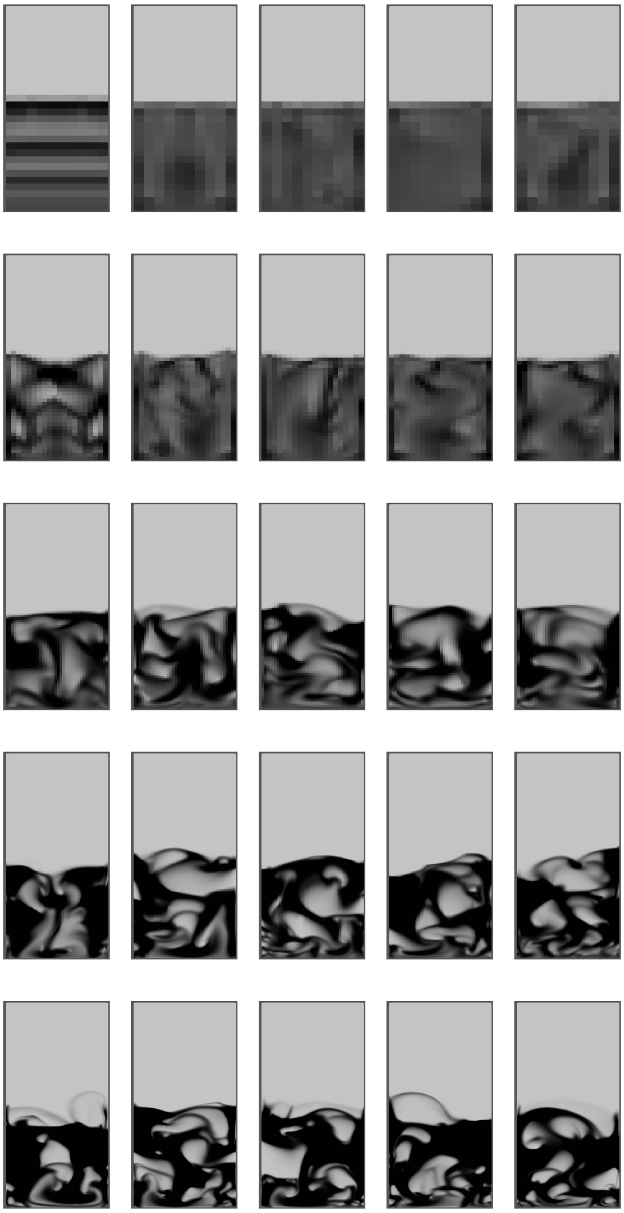

Figure 2. CFD simulation result images that our participants saw in the study. Visualization results are visualized using a gray color map that humans perceive linearly. Rows are order by increasing grid resolution refinement and columns are ordered by increasing timesteps.

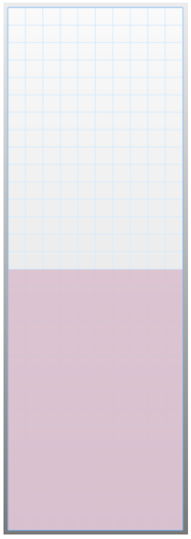

Figure 3. An image of our geometry showing the coarse grid cells and the water particles at the bottom of the 2 dimensional fluid bed.

5. Simulation Data

Our two phase simulation of water particles mixing with air particles using the MFix Two Fluid Model (MFix-TFM)[1] simulates water turbulence in a container. People care about this simulation because it allows observing otherwise harmful experiment conditions such as boiling temperatures and high turbulence in a safe computing environment. The MFix-TFM represents air as a fluid phase and the water particles as a solid pahse. Solid phases are represented using glass beads with physical properties such as diameter and density. Solid particles with the same physical properties are assumed to move collectively. Our geometry and initial conditions are based on those found in the two dimensional TFM tutorial and our geometry consists of a two dimensional 10cm x 30cm rectangular fluid bed (Figure 3). Our fluid particles have a diameter of 200 microns and a density of 2500kg/m^2. The initial conditions include a temperature and pressure of 298K and 101325Pa, respectively. The initial gas volume is set to 100% and the galss beads volume is set to 40%. Our boundary conditions include a mass inflow of 0.25m/s for our fluid velocity and an outlet region with a pressure of 101325Pa. We run our simulations with grid resolutions of 10, 5, 2.5, 1.25 and 0.625mm (Figure 1).

Our finest grid resolution is 0.01mm smaller than the one used by Tricomi et al. in their 2D model sensitivity study for a similar CFD based experiment (Tricomi et al. 2017). Using a scaling factor of 2, we coarsen our grid resolution. Similar to the tutorial, our experiment simulates a 5 second process. We discretize our simulation runtime into 5 discrete timesteps that coincide with the 1s, 2s, 3s, 4s and 5s runtimes. We collect the cell data for each grid resolution and discrete timestep and use that for our SE analyses. We save screenshots of the postprocessing for each discrete timestep and use the pixel values for our VE analyses. We also use the images from the postprocessing for each timestep as the images that our crowd participants view to generate insights for our study results (Figure 2). Our simulation results are visualized using a gray color color scale that humans perceive linearly.

[1]https://mfix.netl.doe.gov/doc/mfix/19.1.4/about.html

6. Experiment Procedure

The experiment treatments are administered to 150 participants via an anonymous Qualtrics[2] survey. The study begins by providing participants with a high level overview of the study procedures, an explanation of the expectation of fair attempts to answer the questions and the need to complete the study and receive a study completion code in order to receive compensation for completing the study. Participants are paid $0.50 for about 5 minutes of work.

The initial overview is followed by a pre-study questionnaire with likert scale questions that ask about the participants experience with viewing and manipulating images on electronic devices and their comfort level with information visualization and computer graphics terminology used in the study like 'color maps', 'light colored pixels' and 'dark colored pixels'. This information is helpful for explaining unexpected trends or outlier responses. Participants are also asked about their sentiment of the study going into it. Participants go on to encounter detailed instructions for the tasks in the main questionnaire.

The main questionnaire consists of a simulation postprocessing image showing the interaction of turbulent water and air particles in rectangular container followed by the following two tasks: 1) 'Estimate the percentage of the image that is occupied by water particles'. 2) 'Describe in a sentence or two the behavior of the water and air pockets shown in the image'.

Participants are then presented with a post-study questionnaire before receiving a unique survey completion code that is used to differentiate the anonymous survey responses. The post survey questionnaire consists of questions related to the participants experience during the study like those asking if they were uncomfortable, if the instructions were clear, if they were out of their depth and resorted to guessing the responses, and if they would recommend the survey to a friend. This last question allows us to gauge their sentiment leaving the study and compare it to their sentiment going into it. The delta in sentiments gives more information if needed to understand any unexpected trends or outlier responses.

7. Results

In this section, we review the results of our main study as well as those of our pre- and post-study questionnaires. We also use our results to test our hypotheses in order to answer our research questions.

[2] https://www.qualtrics.com/

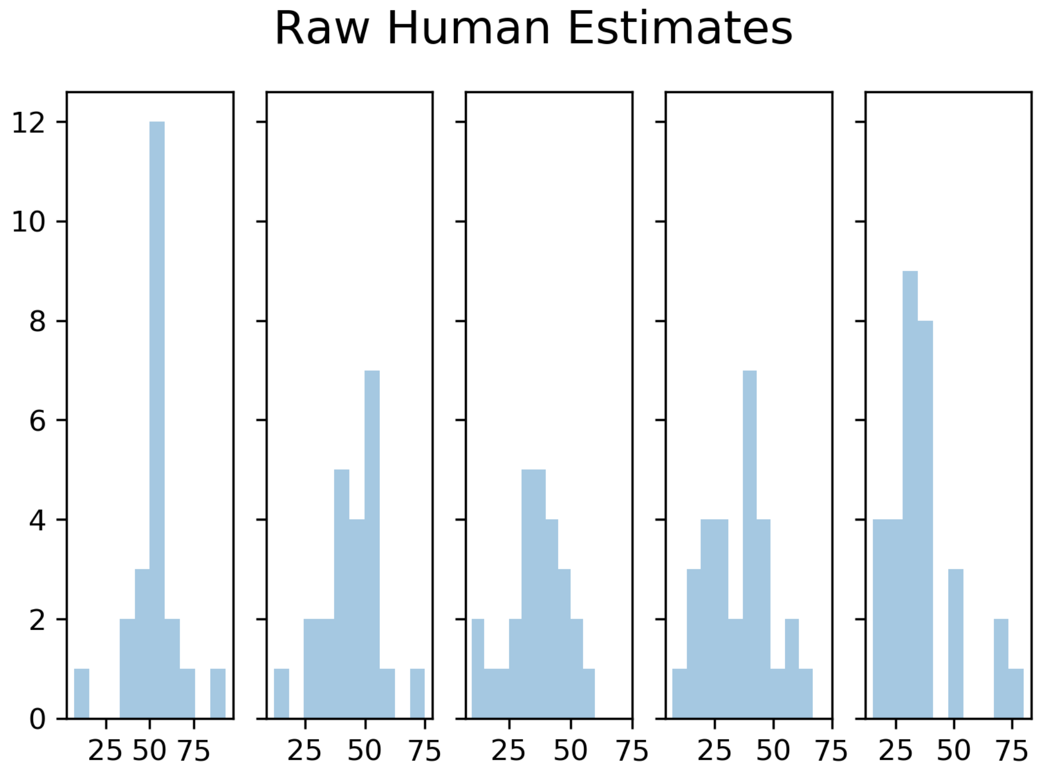

Figure 4. The distribution of raw estimates observed in our study.

7.1. *Calculating IE, PE VE and SE in CFD*

Using the estimates provided by our participants (Figure 4), we calculate our IE, PE VE and SE.

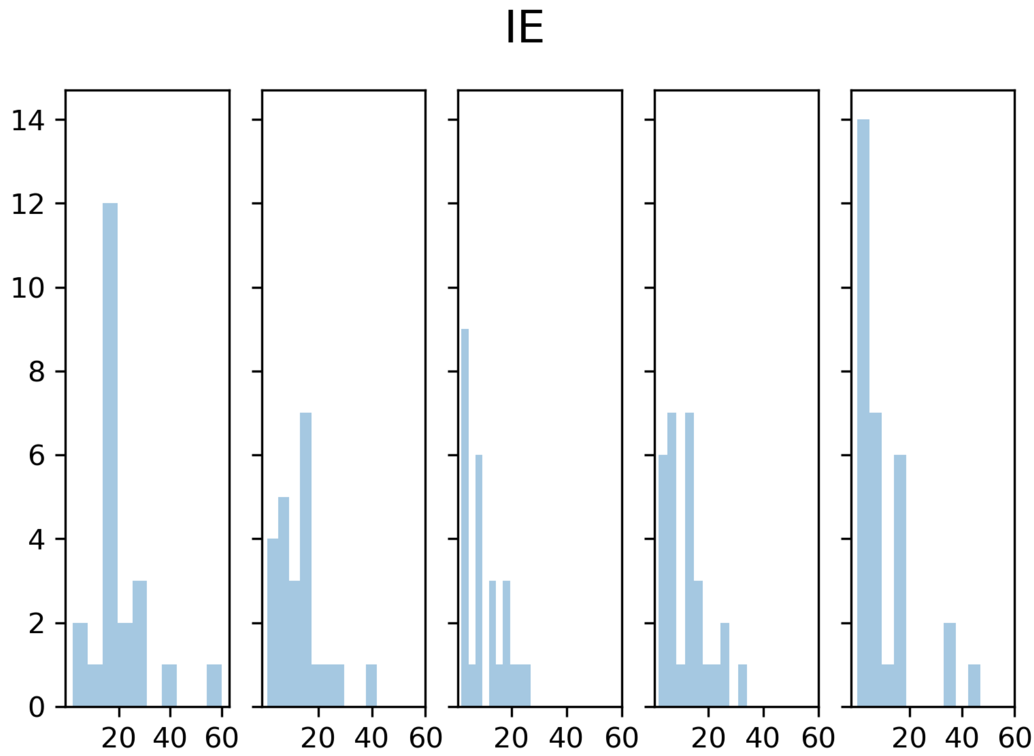

Figure 5. IE calculated from the ground truth and the human estimates observed in our study.

7.1.1. IE in CFD Calculation Sampling

For each human estimate of the volume of water in the simulation, we calculate the error of the estimate in comparison to the ground truth, which is the volume of water in the simulation using the finest mesh. We calculate the ground truth and the IE using the following equations:

$$pop_{gt} = \frac{\sum_{i=0}^{N} wv_i = \begin{cases} 1 & , \text{ if } cv_i <= 0.7 \\ 0 & , \text{ else} \end{cases}}{N} \tag{1}$$

The population ground truth (pop_{gt}) is calculated as the fraction of all particles (N) that are water particles (wv_i) in the simulation. Water particles are defined as the grid cells that have a value (cv_i) that is less than or equal to 0.7. 0.7 is our threshold that we use to determine if a grid cell value is categorized as water or air. We obtain this threshold value by clustering our grid cell values into 2 clusters and selecting the mid point between cluster centroids as our threshold.

$$IE = |pop_{gt} - hm_{est}| \tag{2}$$

IE is the absolute difference between the human estimate of the percentage of water in the simulation (hm_{est}) and the pop_{gt} (Figure 5).

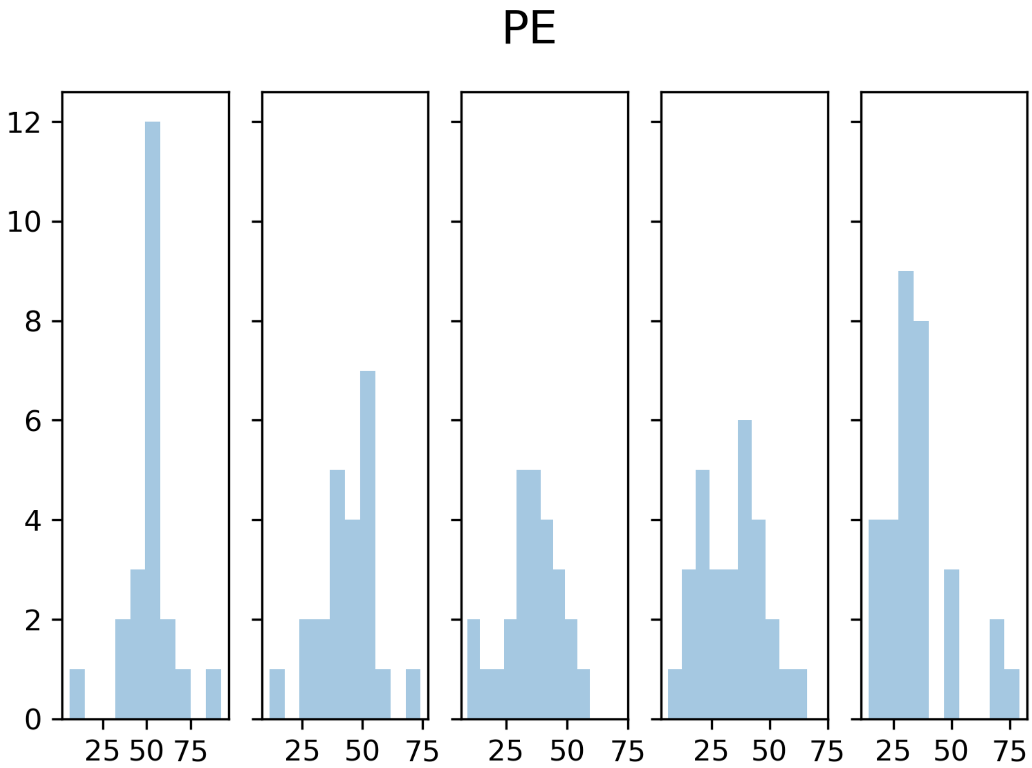

Figure 6. PE calculated from the visualization means and the human estimates observed in our study.

7.1.2. PE in CFD Calculation Sampling

$$viz_{gt} = \frac{\sum_{i=0}^{n} wp_i = \begin{cases} 1 & \text{, if } pv_i = 0 \\ 0 & \text{, else} \end{cases}}{n} \tag{3}$$

The visualization ground truth (viz_{gt}) is calculated by counting the fraction of water pixels (wp_i) out of the total pixels (n) in the visualized results of the simulation that our study participants see. The wp_i is calculated by counting the pixel values (pv_i) that are equal to zero in a black and white visualization where the 0.7 threshold is used to determine whether result visualization image pixels are black or white. We use the inverse thresholding feature of Python's OpenCV image processing library after mapping our 0.7 threshold to the 0-255 pixel value range to generate our black and white images of the simulation results.

$$PE = |viz_{gt} - hm_{est}| \tag{4}$$

PE is the absolute difference between the human estimate of the percentage of water in the simulation (hm_{est}) and the $sample_{gt}$ (Figure 6).

7.1.3. VE in CFD Calculation Sampling

$$sample_{gt} = \frac{\sum_{i=0}^{n} wv_i = \begin{cases} 1 & , \text{ if } cv_i <= 0.7 \\ 0 & , \text{ else} \end{cases}}{n} \tag{5}$$

The sample ground truth ($sample_{gt}$) is calculated as the fraction of all grid cell particles (n) that are water particles (wv_i) in the simulation. Water particles are defined as the grid cells that have a value (cv_i) that is less than or equal to 0.7.

$$VE = |sample_{gt} - viz_{gt}| \tag{6}$$

VE is calculated as the difference between the $sample_{gt}$ and viz_{gt}.

7.1.4. SE in CFD Calculation Sampling

$$SE = |pop_{gt} - sample_{gt}| \tag{7}$$

SE is calculated as the absolute difference between the pop_{gt} and the $sample_{gt}$.

7.2. *Models and Evaluation*

The models delivered in this work fall into the descriptive and inferential categories. Our descriptive models are concerned with describing what we have seen in our crowd study for the purpose of knowledge transfer and also for use justifying or making design decisions for future visualizations of similar CFD scientific simulation results. Our prediction model is concerned with making decisions for grid resolution vs insight variance level for grid resolutions that have not been studied. The idea is to produce models that generalize to unseen data so users of CFD simulations can make informed decisions on which grid resolutions to select in order speed up their simulations with a clear understanding of how their choice will impact their insight variance level. We test our descriptive models visually by determining how well the data fits a hypothesized curve, while we test our predictive models by determining how well the model performs when tested using data that the model has not seen in training. We use the R^2 value to test the performance of our predictive models.

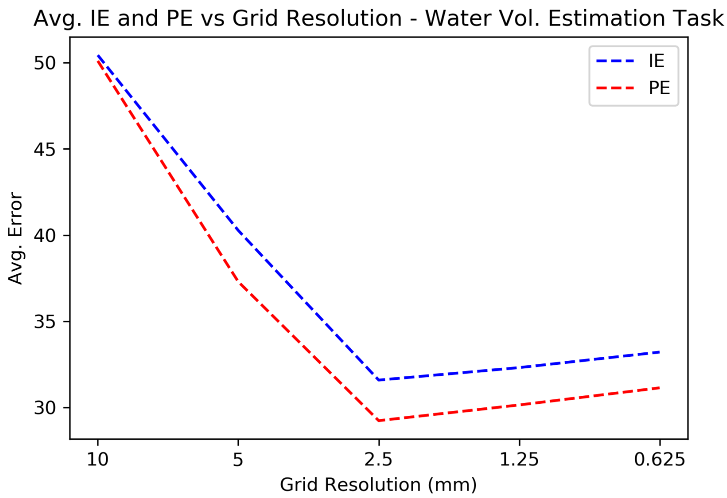

Figure 7. The avg IE and PE plotted along with the accompanying grid resolutions.

7.2.1. Insight Convergence in CFD

Currently, simulation end users navigate the speed-vs-accuracy trade-off using the results of mesh convergence studies or domain experience. Our approach provides an additional benefit to those of mesh convergence studies. Similar to mesh convergence studies were the accuracy of the results stops increasing with added grid resolution refinement after a certain grid resolution(Patil and Jeyakarthikeyan 2018), our results show that after a given grid resolution human insights stop improving. We see this by looking at the relationship between average insight error and the grid resolution. A visual inspection of the average insight levels provided by our participants shows that insight levels provided by our participants insight levels stop improving at the 2.5mm grid resolution (Figure 7). Tricomi et al's convergence study shows that the accuracy of the simulations stops improving at the 1.905mm grid resolution. This result is encouraging because it aligns with our intuition that human insight levels will stop improving before actual simulation convergence. If this is so, convergence studies based on human insight levels will lead to substantial time savings in the simulation workflow. Our approach shows similar benefits as a mesh convergence study but it provides those at a coarser grid resolution and this means faster simulation workflows.

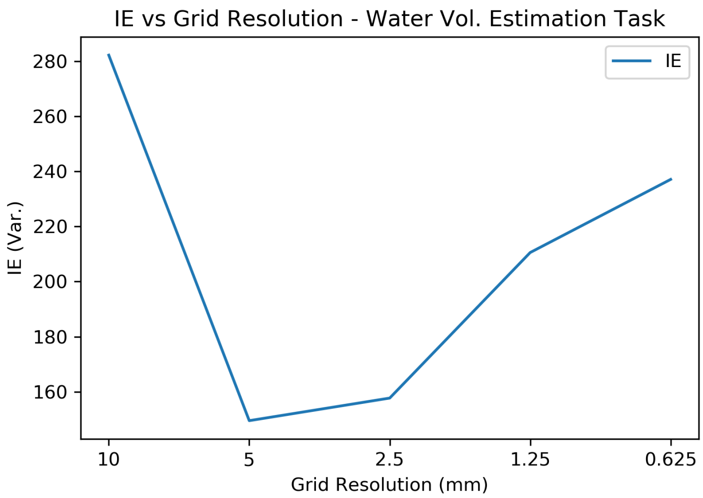

Figure 8. IE as a function of grid resolution observed from the benchmark tasks of our crowd study.

7.2.2. IE as a Function of Grid Resolution - Benchmark Task

As hypothesized (H1), the variance of IE is U-shaped as a function of grid resolution (Figure 8). IE variance is large for coarse grid resolutions and it drops with an increase in grid resolution refinement before increasing for the finest grid resolutions. This means that even though refining the grid resolution of a CFD simulation produces a more accurate result, this increase in accuracy not only comes at the expense of longer runtimes but it also negatively impacts insight. The lowest IE variance is observed from the results of the 5mm grid resolution, while the lowest IE is observed at 2.5mm. This means that human insight variance levels are minimized by running a simulation that takes between 98 and and 826 seconds.

From our study, we see that the most accurate insights are observed at the 2.5mm grid resolutions and the lowest IE variance is observed at the 5mm grid resolution. If one wants to run the simulation for highest accuracy without the results of our study or other previous knowledge like having run similar studies before, they could run the simulation at a grid resolution of 0.625mm. Our study shows that even though 0.625mm is the finest resolution, it does not provide the lowest IE (not IE variance). The lowest IE is seen at 2.5mm. However at the 2.5mm grid resolution, the IE variance is higher than it is at the 5mm grid resolution. A person using our study results to run this simulation could take both of these pieces of information into consideration when deciding on the best grid resolution for the most accurate simulation result. If they choose the 2.5mm grid resolution, they would get the result that provides the maximum insight level or lowest IE (not lowest IE variance) in 826 seconds. If they use a coarser grid resolution that does not exceed 5mm (because of the lowest IE variance at this resolution) they would bet a result in 98 seconds.

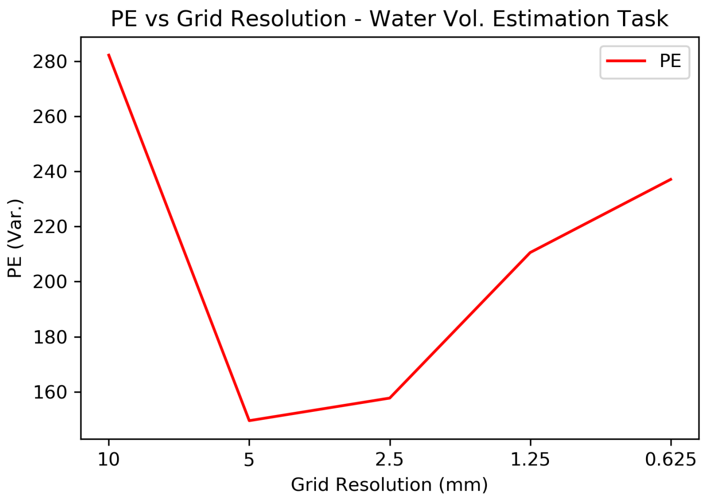

Figure 9. PE as a function of grid resolution observed from the benchmark tasks of our crowd study.

7.2.3. PE as a Function of Grid Resolution - Benchmark Task

Similar to what we saw in our previous work involving the measuring the relationship between insight level and sample size in spatial scatter plots using a fixed grid, PE behaves almost identical to IE in CFD simulation. This behavior that aligns with our hypothesized behavior (H2) is due to the relatively small VE in our simulation results. The VE is almost zero for the coarsest grid resolutions and for those resolutions PE is equal to IE. For the finer grid resolutions, VE grows and there is an apparent difference between IE and PE. However these differences are so small that they are almost negligible and this makes the IE and PE variance seem almost identical (Figure 7).

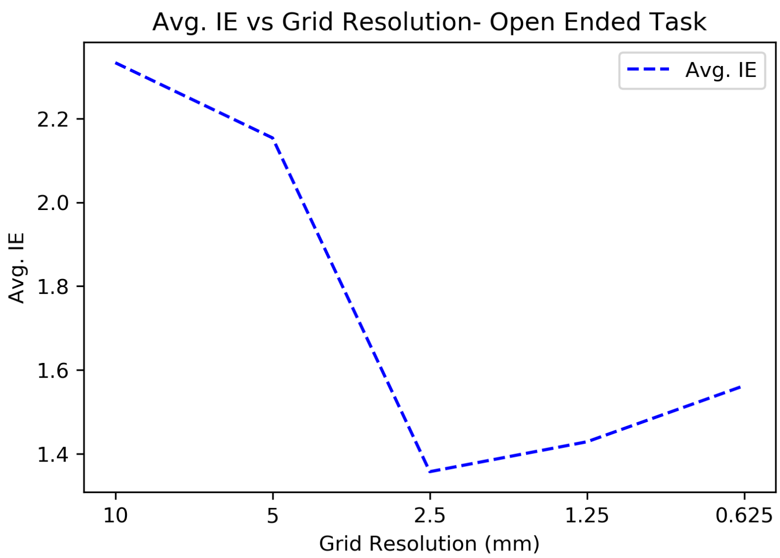

Figure 10. Average IE as a function of grid resolution as observed from the open ended tasks of our crowd study showing the same behavior as that seen in our water volume estimation task.

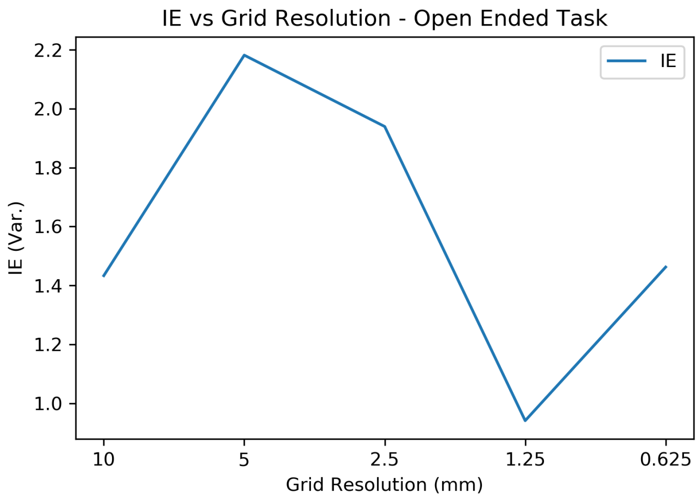

Figure 11. IE as a function of grid resolution as observed from the open ended tasks of our crowd study.

7.2.4. IE as a Function of Grid Resolution - Open Ended Task

In our open ended task we see the U-shaped behavior that we hypothesized seeing in the relationship between insight levels and grid size. Even though the average IE (Figure 10) behaves similar to that of our quantification task, we see an initial low variance (Figure 11). This is as a result of the skewed distribution of our participant responses. Small sample sizes result in insights that have low variance. We conclude this based an an analysis similar to our previous work by modelling our open ended insights as a random variable. As a result of not having a ground truth for our open ended tasks, we create one for the purpose of understanding this initial low IE that accompanies low sample sizes by scoring the participant insights using a rubric and assigning error to the insights..

Score	**Criteria**
0	Irrelevant or inapplicable insight(s)
1	Accurate simple description of the visualization
2	Multiple simple insights
3	More in depth insight(s) about the visualization
4	In depth insight(s) that includes domain knowledge not displayed in the visualization

Table 1. Open ended insight scoring rubric for insights received for our open ended task.

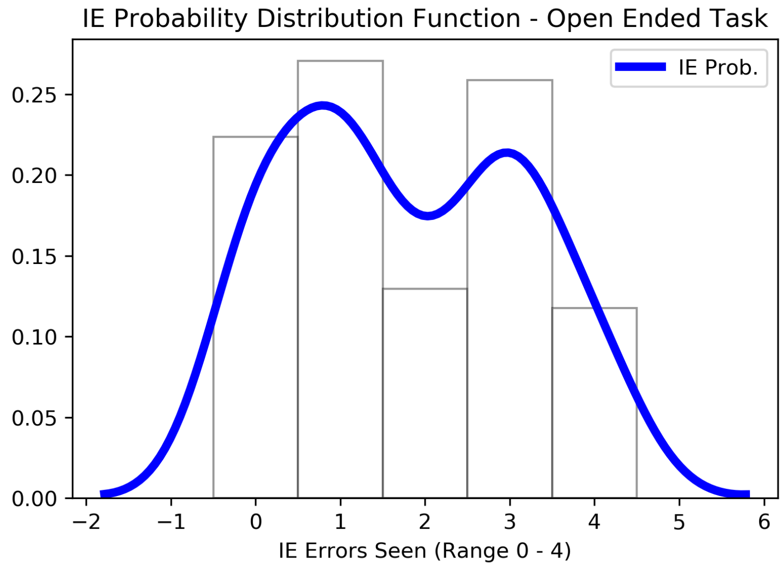

Figure 12. Probability Distribution Function for the IE errors seen in the open ended tasks of our crowd study.

When coding the insights submitted in our open ended task we assign them values ranging from 0 to 4, where 4 is the highest level of insight (Table 1). We assume that 4 is the ground truth and calculate the IE as the delta between a given insight and the ground truth. We then model our insight errors as a random variable and generate the probability distribution function of that variable to determine its distribution (Figure 12). Selecting a very small random sample is most likely to produce errors that have a small variance. Increasing the sample size would then increase range of the data and provide the variances of errors that we hypothesized to see. Removing the smallest sample sizes from the affected errors leaves us with a behavior of errors very similar to our hypothesized behavior. We expect the skewness of the underlying distribution combined with the characteristics of the task being performed to influence the sample size threshold needed to overcome this initial high accuracy that accompanies small sample sizes.

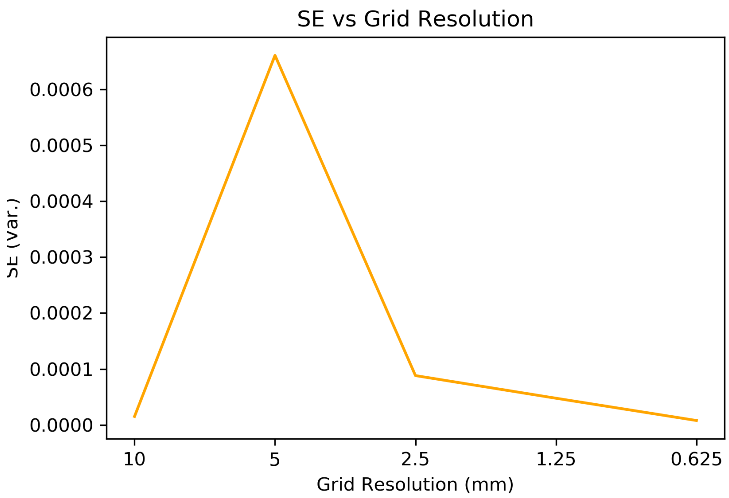

Figure 13. SE as a function of grid resolution for the data used in our study.

7.2.5. SE as a Function of Grid Resolution

Using the actual data from the simulation, we calculate the percent volume of the particles that represent the liquid in our simulation. We use the the average volume from 5 timesteps of the 0.625mm simulation as the ground truth and we calculate the SE as the delta between the percent volume of the liquid in the various timesteps and the ground truth (Equation 7). The volume of the continuous areas water particles is a continuous variable ranging from a low density of 0 to the highest density of 10.

The question that needed to be answered in order to determine the water volume ground truth was what of identifying the particle density threshold that determined the difference between the liquid and gas states in our 2 phase simulation. Using a histogram, we cluster our data into two clusters or bins and use the halfway point between our clusters as our threshold. Using that threshold we classify our particles into one of two states and calculate the water percent volume as the ratio of liquid particles to the total number of particles. We the plot the variance of our SE as a function of grid resolution. Excluding the negligible SE value for the coarsest grid resolution that occurs for same reasons listed in subsection above, SE behaves as hypothesized (H2).

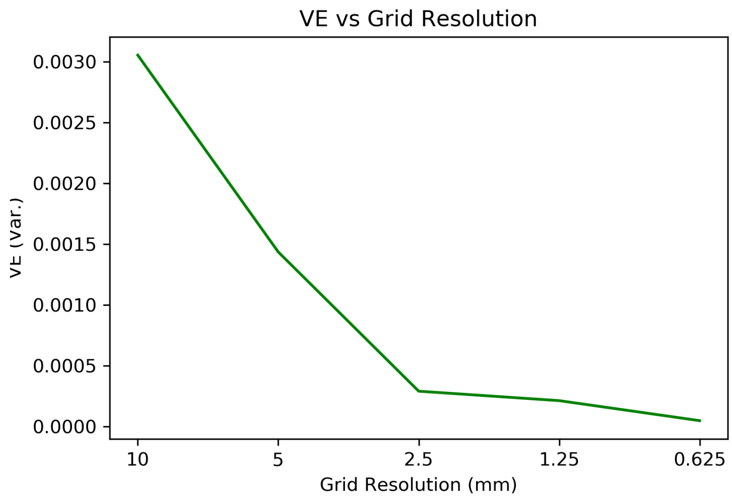

Figure 14. VE as a function of grid resolution for the data used in our crowd study.

7.2.6. VE as a Function of Grid Resolution

As stated earlier, we take snapshots of our CFD postprocessing visualization at discrete timesteps and use them as treatments in our crowd study. Using the same approach to determine the classification of a data point as either a liquid or gas particle, we classify the pixels in our images similarly. Using python's OpenCV library[3], we read the pixels in our images. The images used in our study are rendered using a gray scale color scheme that has a color map that humans perceive linearly. We map the range our pixel values to the 0 through 10 range and use our 0.7 threshold to differentiate the liquid particles from gas ones. The rationale for this approach is described above in the description of SE calculations. We proceed to convert our images to binary ones. We then count liquid particles and calculate the percent volume in our images. We proceed to calculate the VE as the delta between the percent volume calculated from the CFD simulation result data and that calculated from the corresponding postprocessing visualizations (Equation 6). The variance of VE is plotted as a function of grid resolution and it behaves as hypothesized (H2).

[3] https://pypi.org/project/opencv-python/

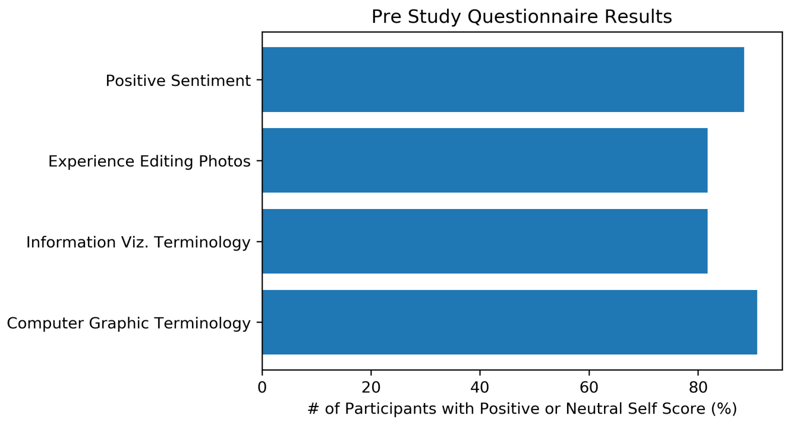

Figure 15. The results of our pre-study showing the percentage of participants that respond with a score of Strongly Agree, Somewhat Agree or Neutral to the questions asked.

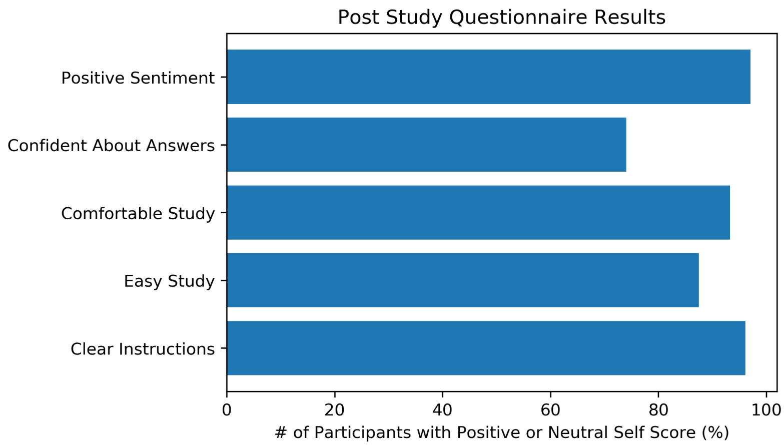

Figure 16. The results of our post-study showing the percentage of participants that respond with a score of Strongly Agree, Somewhat Agree or Neutral to the questions asked.

7.3. *Pre- and Post-study Result Analysis*

Major concerns going into the study were whether the tasks would be too difficult for participants and if they would understand the tasks they were being asked to complete. To address the first concern, we made an effort to design tasks that were both simple and allowed us to gain usable insights on the relationship between insight level and grid resolution in the context of CFD. To evaluate how well we accomplished this objective we measured the sentiment of the participants before and after the task and their confidence in their responses. The rationale being, if participants got overwhelmed by the tasks they would get frustrated and think poorly about the study. They would also answer the question asking if they had guessed the majority of the answers, with ‘Agree’ and ‘Strongly Agree’ responses. We see that the sentiment of our participants increased after taking the study from $88 - 97\%$ (Figures 15 and 16). We also see that 74% of our participants were confident about their responses, given that at least 25% of them saw images from very coarse grid resolution simulations. To evaluate our ability to mitigate our second major concern by providing clear easy to follow instructions, we ask the participants questions about the clarity of the instructions and ease of the study. With respect to whether the instructions were clear, if the study was easy, and if the participants were comfortable during the study, $98\%, 88\%, 93\%$ of participants provided a 'Strongly Agree', 'Agree' or 'Neutral' response, respectively.

8. Discussion

Even though we successfully model the relationship between grid resolution and IE and its component errors in simulation, we realize that more such models are needed for the various different types of simulations. We envision these models being created by various CFD users who would proceed to share these models with other members of the community of CFD users. In order to do that, we discuss some of the lessons learned from our study in the form of guidelines that anyone else can use to run similar studies using our IE framework.

8.1. *Beyond Grid Resolution*

Our study focuses on the relationship between grid resolution and the level of insights generated from looking at CFD postprocessing visualization results. To do so, we hypothesize a linear relationship between the obtained variance of insights for a given grid resolution and the grid resolution. The insight variance is our dependent variable and the grid resolution is the independent variable. The same approach is applicable to cases where one has a different input variable. In that case, one would run a similar study using CFD postprocessing visualizations generated using different levels of the input variable and measure the insight levels from each input level. The insight levels obtained can then be modelled as a function of the input parameter.

Even though we are mainly focused on the relationship between grid resolution and insight level because of the well understood time savings that can be obtained by varying the grid resolution. One might be interested in leveraging a similar relationship that is a function of more than one input variable. This work can also be extended to cases where the simulation has more than one input variable that determines simulation accuracy. For guidance, one could use the simple case in our previous work where we studied the relationship between the variance of insight as the dependent variable with sample size and marker filling status as the two independent variables in scatter chart visualizations. This would be similar to a turbulent flow CFD based experiment where insight variance is the dependent variable and grid resolution and the model type, e.g. Reynolds-averaged Navier-Stokes equations (RANS) or large eddy simulation equations (LES), are the independent variables.

If one has a small number of independent variables e.g. 2, and one of the predictors has a small number of categorical levels e.g. 2 or 3, one could build separate models for each of the independent variable's categorical levels. For example one could create a model for the relationship between insight level and grid resolution for the RANS turbulent flow case and a model for the LES turbulent flow case. End users needing to predict the insight level for a given grid resolution would then need to specify whether they are using RANS or LES modelling before making a prediction. In the case where one has a large number of independent variables or both variables are continuous or if they have a large number of levels then one could hypothesize a linear relationship between the dependent variable and the independent variables. One would then proceed to use multiple linear regression (MLR) to model this relationship based on the results of a user study where people are providing insights based on simulations run on different combinations of the various independent variable levels.

For cases where the relationship between the independent variable and a dependent variable is non linear, adding a non linear term to the MLR or a transformation to the independent variable should allow one to model this relationship. After modelling the relationship between the dependent variable and the independent variables, one would need to present it in an application with a slider that allows end users to view and use this relationship in their CFD simulations. In our work, we present our model in the form of a slider and a line chart. We have one dependent and one independent variable and this allows us to have one line chart. For the case where one has one dependent variable and multiple independent variables, they could show a single line chart for each independent variable with a slider for each variable. Moving each slider would show how each independent variable impacts the dependent variable.

8.2. *IE Framework Implementation Guidelines*

The goal of implementing the IE framework is to provide IE variance feedback for CFD end users trying to select the ideal grid resolution for their simulation. In order to achieve this goal, IE variance models need to be be grouped for similar simulation cases and stored in a database for access by any CFD end users (Figure **??**). To promote easy access and retrieval of IE variance models, they should be grouped by the simulation type e.g. single phase laminar flow, two phase turbulent flow, etc. IE variance models are also dependent on the type of visualizations that the CFD end users use to analyze the simulation results, e.g. heat map, line graph, etc. Different visualization type handle increases in data differently. Some aggregate data and result in lower IE with the addition of more data, while other suffer from overplotting and result in poor IE after a threshold of data volume has been exceeded.

General IE framework implementation steps consists of identifying the types of simulation and visualization to be analyzed as well as the people one intends to use in the IE study, designing and running the IE study and measuring and modelling IE and its component errors. We used complex benchmark tasks in our study that require that participants have a good overview of the simulation results. Participants in our study were asked to view static postprocessing visualizations and gain insights from those. Our benchmark tasks measure how well people understand the individual frames that make up the animated results of CFD simulation and for that reason we expect our results to be generalizable to other complex benchmark insight tasks because they too are based on how well people understand the overview of the simulation result. However, using simpler benchmark tasks could provide different results.

Our benchmark tasks rely on people viewing visualizations that have enough information to introduce uncertainty into the process of gaining cognitive insights from the results as a result of human cognitive differences that become apparent as people estimate the overview of such visualizations. These uncertainty levels are also influenced by the amount of computational sampling that is applied to the simulation process. These uncertainties lead to variation in human cognitive insight that forms the basis of our IE variance measure. Benchmark tasks that are simple and involve small ranges of possible responses like those searching for an individual object, tasks with boolean responses or those involving small quantities of data that allow people to gain insights as a result of counting small finite quantities will result in little or no variance. For example asking people to determine if there are any water particles present in a visualization of CFD simulation results will result in low variance results even for inaccurate simulations because of the low uncertainty associated with such a task. The following steps provide guidance for anyone implementing an IE study to measure IE variance using our IE framework.

8.2.1. 1. Identify the Simulation and Visualization Type

In order to promote knowledge sharing and avoid replication of effort one should identify the of simulation type as well as the visualization type that one is going to study. This information will be used to index the results of the study in a database for future retrieval by anyone studying the same problem. One approach of identifying the simulation and visualization type is by posing the study objective in the form of a question. For example asking "How does changing grid resolution impact IE variance from studying heat map visualizations of the multi phase turbulent flow of water and oil mixing in a container?" highlights a multi phase turbulent flow simulation type and a heat map visualization type. Anyone else in the future who needs to answer a similar question can use that simulation and visualization type to retrieve the results of the study.

Proceed to hypothesize the behavior of insight levels for the simulation and visualization types being analyzed. This will allow one to gain some intuition that will expose unexpected study results or highlight any problems with the study. Answering and analyzing the responses o the following questions will provide some guidance for hypothesizing this behavior: How accurate will the simulation be? How much detail will there be in the results of the simulation? How much visual clutter will the simulation produce? For grid resolution results with low accuracy and not a lot of visual detail, the variance of IE and PE are likely to be high. However, grid resolutions results with high visual detail are also likely to have high IE and PE, but these levels of IE and PE can be moderated by high simulation accuracy and lower amounts of visual detail. On the other hand, grid resolution results with high accuracy, high visual detail and low to moderate visual clutter are likely to have low IE and PE.

8.2.2. 2. Identify the IE Study Participants

Generate a list of types of insights that CFD end users should be able to draw from the simulation and visualizations type being studied. Identify participants for the study that have the capability to draw such insights. For example crowd workers, college students or domain expert participants. One should avoid using people familiar with the study design in order to avoid demand characteristics (McCambridge et al. 2012). One should also attempt to get participants that are similar to the typical users of the simulation type being studied.

8.2.3. 3. Design the Study

The IE framework study should involve two types of tasks: i) benchmark and ii) open ended. Benchmark tasks are those that ask precise questions or tasks with an objective ground truth e.g. 'How many blobs can you identify in the image?' or 'Estimate the volume percent of water in the image'.If participants are experts, ask them for insights that are typical of those often sought from the data. However, if they are crowd workers, simplify the task while still asking for insights that are pertinent for current simulation end users. For example decompose tasks into smaller tasks or simplify the terminology such that the common person can understand the task. Open ended tasks are those without predefined steps known to lead to a solution (Terry and Mynatt 2002). Figure

17 shows a sample question that we used in our study.

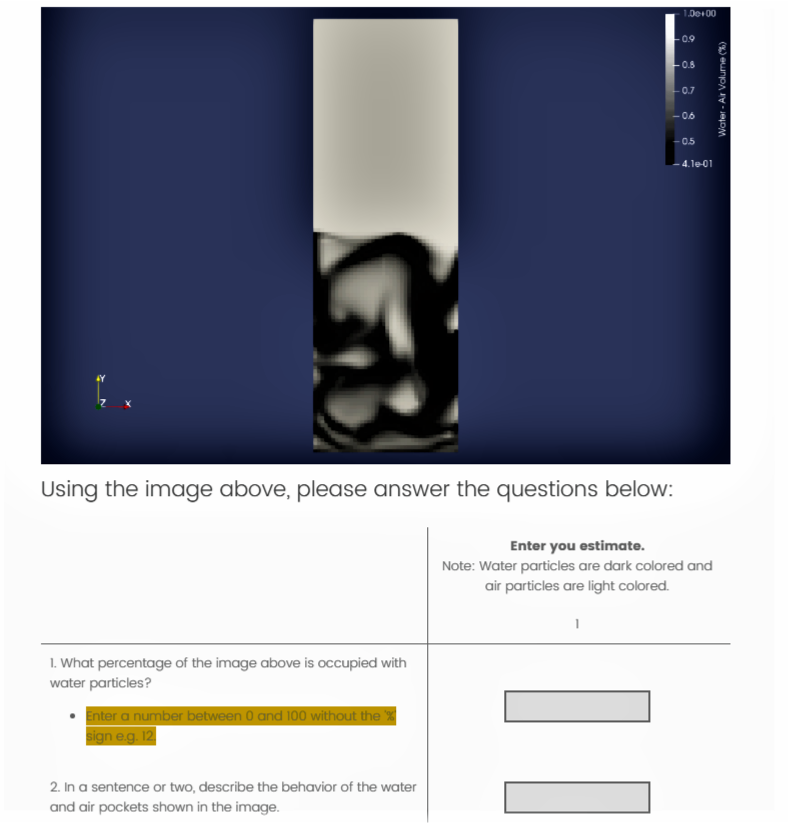

Figure 17. Sample question questions from our crowd study showing an image that participants saw in addition to the questions they were asked about the image.

8.2.4. 4. Run the Study in a Plausible Environment

When running an IE study with domain expert participants, conduct the study in their normal work environment. This is because increasing the participants' comfort level can reduce anxiety and stress that can impact insight and perception capability (Rosen et al. 2014). We also know that participants being tested can alter their behavior (Thomas 2019). For that reason too, we recommend conducting the test in as normal an environment as possible.

8.2.5. 5. Avoid Crowd Study Pitfalls

Crowd studies should have clear instructions for the expected level of work quality required for payment. Crowd studies provide a large diverse pool of participants but the pay for work environment attracts bad players that will provide poor quality work or no work in exchange for payment. One approach is through the use of automated scripting algorithms that pose as humans also known as Bots. Bot responses can contaminate the results of the study. An open ended free text question to identify and filter out such responses. Bot responses can be identified by being low quality or containing information irrelevant to the asked question.

8.2.6. 6. Measure participant sentiment before and after the study

Provide objectively measurable questions like likert scale questions asking for how comfortable or confident participants feel about taking the study before taking the study and how confident they feel about their responses or how comfortable they were in the study, after the study. This allows you to determine how engaged the participants were during the study. Significant level drop-offs could signal a participant who stopped trying or signal problems with the study design or a participant who was out of their depth. Figures 18 and 19 showing sample pre and post study questionnaires showing likert and open ended questions used in our study.

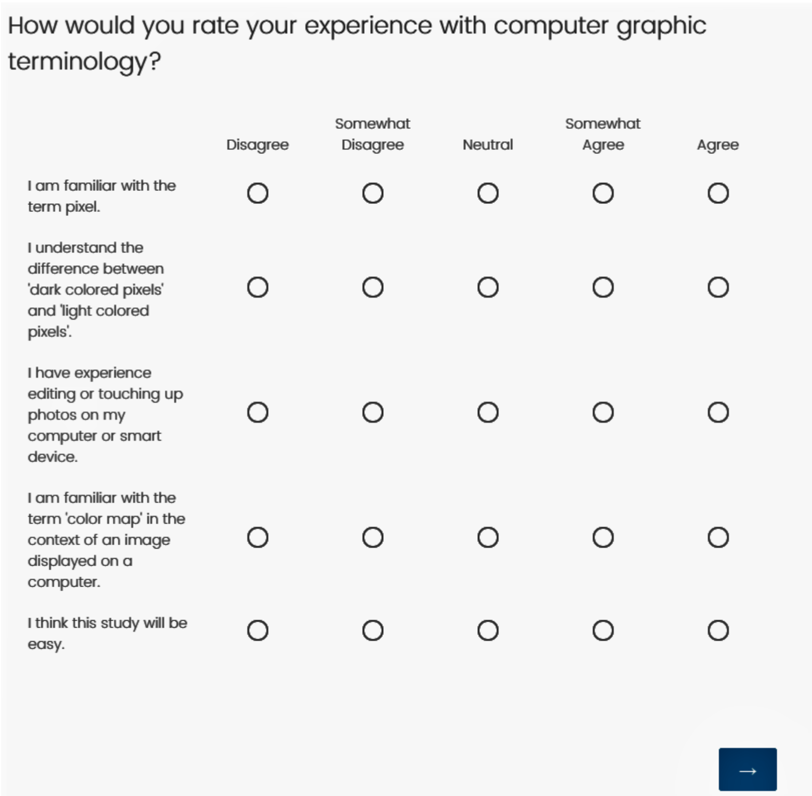

Figure 18. Sample pre-study questionnaire questions from our crowd study showing likert scale questions

8.2.7. 7. Follow Study Content Best Practises

- Provide simple but adequate training. Untrained IE study participants could provide unusable data as a result of not understanding the IE study tasks. Training can mitigate this risk, but too much training can be overwhelming and this could impact the quality of participant responses. Provide training if needed and either have a subgroup of potential participants review and provide feedback on the training or provide questions at the end of the training that test the effectiveness of the training. Our study tasks were designed to be intuitive, so training was not needed. Figure 20 and 21 shows sample instructions used in our study.
- Have simple clear instructions about what participants are referring to e.g. if the simulation results are in video format discretize them into well labelled image snapshots and use such images in the study in lieu of the the video results

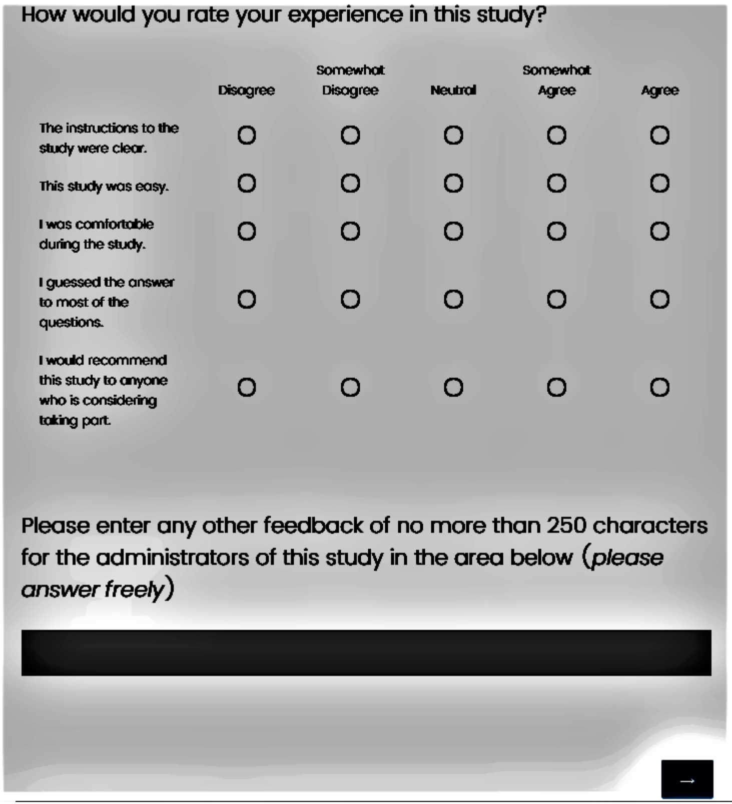

Figure 19. Sample post-study questionnaire questions from our crowd study showing likert scale questions.

- Overlay a grid or provide a well understood naming convention for areas in the image. Using images with an overlaid labeled grid instead of videos helps make sure that the identification of areas within the result under review image is easy to identify and understand.
- Provide response validation using the IE study interface if possible. For example use the study software controls to make sure that only numeric responses are provided in fields requiring numerical responses. This helps prevent data entry mistakes that can contaminate otherwise good results.
- Provide at least one open ended question either in the study, pre-study or post-study. This will allow the study to capture more complicated insights and help filter automated bot responses.
- Providing an extremely easy question can also help with data quality by highlighting participants that are not applying themselves. For example, a question could be added asking participants to count an easy to identify number of items in the simulation results. Anyone providing an incorrect number can be assumed to be paying very little attention to the task or instructions and their results need to be excluded from the analysis.
- Provide a free text question to collect participant feedback.
- Run a pilot study if possible, using similar but not identical questions to those used in the actual study. Looking at the pilot study results can help show if participants are having any issues with any part of the study. Prevent pilot study participants from participating in the actual study if possible or allow all participants to participate in the pilot study in order to prevent some participants

Instructions:

- You will see 1 image of turbulent water in a container
- The bottom of the image contains mostly water
- The top of the image contains mostly air
- The pixels in the image represent either air or water particles depending on their color
  - Water particles have a dark color
  - Air particles have a lighter color
- The turbulent water at the bottom of the image contains air pockets
- Our image has a color scale on the top right
  - Water particles have a value of 0.7 and below
  - Air particles have a value greater than 0.7

Figure 20. Sample instructions from our crowd study showing simple succinct instructions

having an advantage from having conducted the tasks before.

- Consider and measure all possible sources of variation in participant responses. For example in our study we considered individual result timesteps to be possible sources of variation. We did not find a difference in the insight levels provided by participants viewing results for different timesteps within the same grid resolution. However if this could be a source of variation in your particular study, you can factor this into your analysis and either study all relevant timesteps or limit your study to the most salient timestep.

8.2.8. 8. Measure IE and IE Component Errors

- **Measuring IE**. Our insight and perception metrics are error variance. For that reason, one needs to know the ground truth in order to implement our framework. This ground truth can either be calculated objectively from the data of the simulation that is run using the finest grid resolution or provided by domain experts who have analyzed responses to a given insight question question in the context of the simulation being studied. For example, in the case of a benchmark task like 'Estimate the volume percent of water in the container' one could run the simulation at the finest grid resolution, export the result data for the value of the fluid state of each particle and calculate the percentage of water particles and use this value as the ground truth. The difference between each response and the ground truth would be the IE. In the case of open ended tasks, domain experts can code each response and assign an IE value to each provided response. The relationship between each grid resolution used in the study and the corresponding variance of IE could then be modeled by fitting a curve to that data. From our study, we concluded that IE and PE were the same. For that reason anyone implementing our framework only needs to study the IE.
- **Measuring PE**. In order to measure PE, one needs to calculate an objective value being portrayed by the visualization. For example where a visualization is portraying a liquid and gas in a container and one is simulating the interaction of these two fluids, and the user task is estimating the volume of the liquid, one could binarize the result image being used in the study and use the pixel values

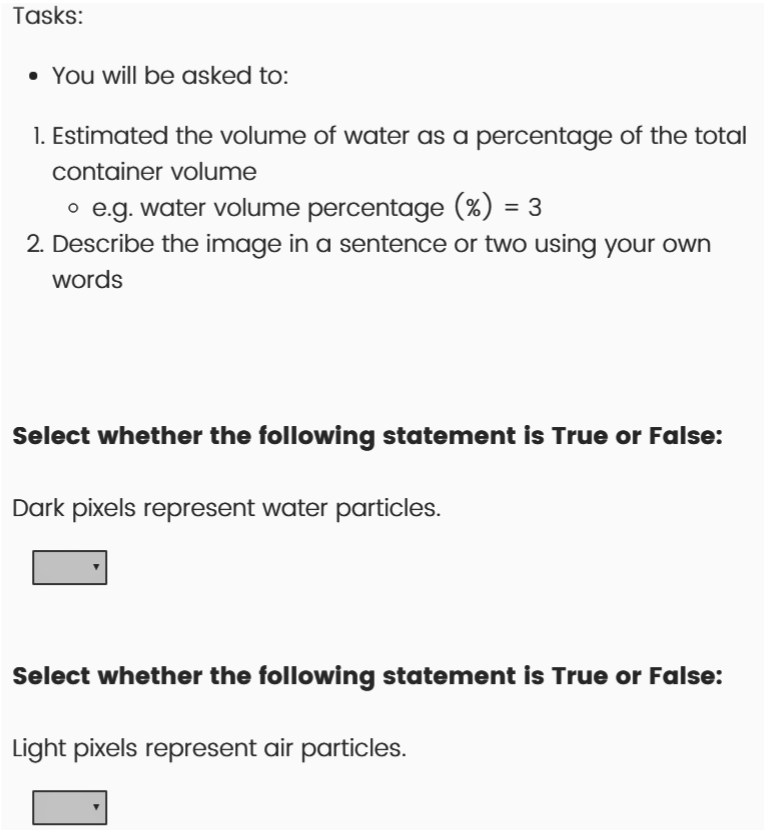

Figure 21. Sample instructions from our crowd study showing showing simple test questions to reinforce instruction materials.

to determine the volume of the liquid pixels. One could then use the difference between human provided estimates and the percentage calculated from the image as the measure of the PE. The relationship between each grid resolution used in the study and the corresponding variance of PE could then be modeled by fitting a curve to that data.

- **Measuring VE**. In order to measure the VE, one needs to calculate the measure being investigated for each sample. For example in the case where participants are being asked to estimate the volume percent of liquid in a container, the volume of the liquid in each sample needs to be calculated. In our guidelines for measuring IE we provide guidance on doing this. The difference between the value for the measure being investigated calculated from the sample and that calculated from the corresponding visualization is the VE. Guidance for calculating the measure being investigated portrayed in a visualization is provided in our guidance for measuring PE subsection above. The relationship between each grid resolution used in the study and the corresponding variance of VE could then be modeled by fitting a curve to that data.
- **Measuring SE**. SE is measured as the difference between the measure being investigated calculated from each sample and the measure being investigated calculated from the largest sample for the simulation running at the finest grid resolution is the SE. The relationship between each grid resolution used in the study and the corresponding variance of SE could then be modeled by fitting a curve to that data.

8.2.9. 9. Make Data Based Decision

Plotting the variance of IE on the y-axis against the grid resolution on the x-axis makes it possible to understand the impact of changing the grid resolution on IE variance. An additional plot of average IE on the y-axis against grid resolution on the x-axis gives further insight on the impact of changing grid resolution on IE. The former that is based on grid variance is more generalizable to similar simulation and visualization types due to it being variance based, while the latter may not be as generalizable due to it being based on absolute quantities. For example if one is comparing IE from two CFD simulations where the insight being measured or quantity of interest is the height of a fluid in a container at a given time during the simulation. The latter plot for two containers that have differing average IE will have differing y-values, while the former plot will show similar IE variance. The latter plot however can be used similar to the results of grid converge studies and both plots can be used in addition to other simulation literature data to help CFD end users make an informed decision on the ideal grid resolution for their simulation.

9. Conclusion

In this chapter, we use a crowd study based experiment to investigate the relationship between grid resolution and IE and PE error in CFD. Using CFD simulation postprocessing results, we measure the accuracy of insights that our participants generate for the results. We also measure the insight levels that participants provide based on an open ended task. We evaluate these insights in terms of the error between provided insights and an ideal ground truth of insights that we define as being of the highest level. We find that the variances of IE and PE have a U-shaped relationship with grid resolution, that similar to our previously studied visualization applications, our IE framework is valid for insights generated from CFD results and grid resolution can be used to predict the variance of IE resulting from observing CFD postprocessing results.

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