Visualization of MFiX-Exa Codes for Chemical Looping Combustion

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Abstract

In the United States, fossil-fuel related industrial processes account for approximately half of all greenhouse gas emissions in the United States. Wide-scale implementation of Carbon-Capture Technologies such as Chemical Looping Reactors (CLRs) provide a promising path to reducing carbon emissions. However, scale-up and testing of these systems is expensive and time-consuming. In recent years, scientists have developed computational tools to simulate multiphase reactors to reduce scaling and testing costs by harnessing the power of HPC. In particular, understanding bubble dynamics in fluidized beds is important to scientists studying multiphase flows in order to design efficient, cost-effective chemical looping reactors. In our video, we highlight scientific use cases of the MFiX-Exa simulation for a general science audience and outline the importance of Los Alamos National Laboratory's (LANL) in situ statistical feature detection algorithm in identifying the features of interest in the MFiX-Exa data; and the use of LANL's Cinema visualization tool to create a novel post hoc workflow. In particular, we highlight MFiX-Exa, which provides new computing capabilities needed to combine CFD-DEM simulation with computing at the Exascale via an adaptive mesh refinement (AMReX) framework. Visualizations were run in ParaView and the rendering in our model visualizes bubble features as well as fluid velocity of fluid in the fluidized bed. Average rise velocities from the particle data were estimated and saved for comparison and overlayed in the background of the visualized bubbles to study fluid features. We discuss the influence of exascale computing in the future of CLR and Carbon capture technologies.

Keywords:
MFiX-Exa, Exascale Computing, Scientific Visualization, ParaView, Zero-emissions, Carbon Capture Technologies, Chemical Looping Reactors, Statistical Feature Detection.

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1. Introduction

Currently in the US, fossil-fuel related industrial processes are a major source of greenhouse gas emissions. Chemical looping reactors (CLRs) offer a viable path to help the US address climate change, reduce greenhouse gas emissions, and meet the DOE's goal to achieve net-zero emissions in the near future. Wide-scale implementation of Carbon-Capture Technologies like Chemical Looping Reactors (CLRs) provide a promising path to reducing carbon emissions. However scale-up and testing of these systems is very expensive and time-consuming. In recent years, scientists have developed MFiX-Exa, which provides new computing capabilities needed to combine CFD-DEM and the power of Exascale with an AMReX [1] framework as part of the Exascale Computing Project (ECP) [2]. Additionally, multiphase reactors play a key role in direct air capture systems that could be used to extract existing greenhouse gasses from the atmosphere [3]. In our video, we showcase a state of the art, integrated workflow combining in situ feature detection with a post hoc analysis, which is novel for addressing the science problems of interest to developers of MFiX-Exa [4]. We we demonstrate scientific use cases of the MFiX-Exa simulation, underscoring the capabilities for MFiX-Exa to combine CFD-DEM simulations with the power of computing at Exascale. This novel solution allows for a fully integrated workflow, from large scale computation to insitu processing, and finally to interactive post-hoc capabilities. Additionally, we produce engaging visuals to draw in the audience and emphasize the importance of the influence of Exascale Computing on a greater scope.

Currently, the National Energy Technology Laboratory (NETL) supports several Chemical Looping Combustion (CLC) projects in collaboration w/ industry, academia, and NETL's Research and Innovation Center (RIC), ranging from lab and bench-scale testing to evaluation of pilot-scale prototypes. Since oxygen carrier durability and production are the primary CLC operating cost, current CLC research efforts are focused on developing and refining oxygen carriers to improve oxygen carrying capacity and production cost. Additionally, developing effective solids circulation and separation techniques and overall system design and optimization are part of ongoing efforts to improve CLRs. Through the use of Exascale computing, the opportunity arises to greatly reduce scaleup and testing costs through accurate multi-phase simulation results.

To simulate the carbon capture process, we can use innovative strategies to distribute particle work and fluid work across

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system resources allowing efficient use of the hardware. One of the features of AMReX is to use dual grids, allowing fluid and particle work to be managed separately and combined later. The dual grid gives us the ability to redistribute the particle work so that the amount of particle work per-GPU remains mostly constant, evenly distributing computing load in regions of dense particle buildup or regions needed larger than usual computing power [5, 6]. MFiX-Exa is currently being developed at NETL as a solution to this problem as part of the U.S. Department of Energy's Exascale Computing Project (ECP). The MFiX-Exa project goal presents the challenge of multi-flow, multi-phase reactions. The variety of flow regimes in loop and local particle concentrations vary greatly in space and time and present a challenge for multi-phase and DEM solvers [7]. For example, dense flow with sustained particle contacts in the fuel reactor are merged with less dense air reactor components, and both clustering and bubbling instabilities make the problem difficult to solve with a typical CFD-solver. The dual-grid approach considers reactions, phase changes, and heat transfer across particle-mesh boundaries [8]. Additionally, MFiX-Exa is set to harness the power of Exascale computing which will allow it to be run on a variety of supercomputing platforms including individual workstations, many-core HPC platforms and supercomputers such as OLCF Frontier. This is achieved by taking advantage of AMReX computing architectures which provide various features that enable MFiX-Exa and other CFD codes to run on different architectures without substantial code modification. Particularly, our emphasis is on the Bubble dynamics in the fluidized bed of the Chemical Looping Reactor. Visualizations were run in ParaView and the rendering in our model visualizes bubble features as well as fluid velocity of fluid in the fluidized bed [9]. Understanding bubble dynamics is an important way to determine the efficiency of the reactor [4]. In our video, we demonstrate MFiX-Exa's ability to model bubble dynamics and produce an expert-specified, interactive dataset for visualizing and interpreting results. The workflow uses Paraview and Cinema explorer in the post-hoc analysis and data processed in situ, selectively reducing the size of the output and allowing for interactive capabilities like tracking individual bubbles, selecting for key bubble features and timesteps, as well as layering of selection criteria. In our visualizations, simulated average particle rise velocities were overlaid on top of the bubbles to study velocity dynamics of the particles around the bubble regions.

2. Model Description, Analysis, and Visualization

2.1. Physics Model: Chemical Looping Combustion

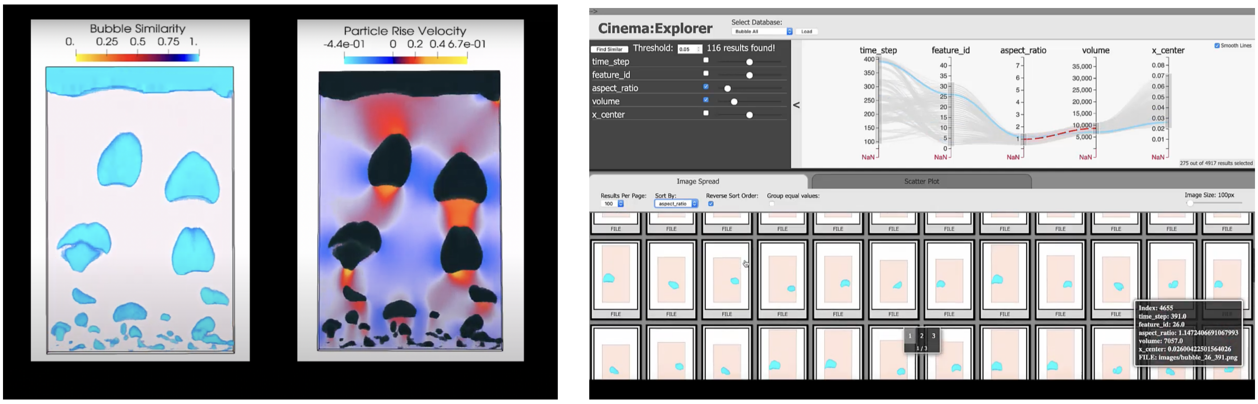
In a Chemical Looping Reactor, fuel reacts with oxygen in a solid carrier to produce CO_2 and H_2O which are easy to separate such that the CO_2 can be stored or recycled. The CLR approach is effective because fuel reacts to the oxide rather than directly with the air, producing more condensed and controllable outflow of CO_2 for capture. In the fuel reactor, a metal oxide or other oxygen carrier is reduced, subsequently being sent to the air reactor where it is reoxidized. In the air reactor, a hot spent gas stream is produced, generating power and the oxygen carrier is returned to the fuel reactor, re-starting the reduction-oxidation cycle, thus ultimately preventing the fuel from directly contacting the air. In the fluidized beds, large numbers of bubbles can form, causing poor gas/solids mixing and lowering conversion efficiency. Smaller bubbles at the bottom of the fluidized bed allow for sufficient mixing before bubbles merge and split as they rise through the fluidization zone, finally bursting out at the top [10, 11, 12]. Because formation of bubble regions in the fluidized bed is a strong predictor of overall reactor efficiency, we focus our work on the the bubble dynamics of the fluidized bed reactor [4].

Our simulation is a model of fluidized bed (0.15 × 0.0032 × 0.0508 m3) where a constant density (1.205 kg/m3), constant viscosity (1.8 × 10-5 Pa-sec) gas is used for fluidizing spherical particles of constant size (148 × 10-6 m diameter) and density (1300 kg/m3). A constant velocity gas inlet with a value of 0.0342 m/sec is introduced at the bottom while a pressure outflow is kept at the top. The domain of our simulation test case contains around 3.6 million particles and a single timestep of it outputs particle fields with particle ID, location, velocity, and other key fluid variables. As the simulation progresses, the particles interact with each other under the influence of gas inlet and gravity and gradually start forming bubbles. The data was generated on the National Energy Research Scientific Computing Center's (NERSC) Cori computer. Cori is a Cray XC40 system, capable of achieving a peak performance of about 30 petaflops.

For a high fidelity model of MFiX-Exa, it aims to run with several billions of particles to model a full-scale chemical looping reactor. For our visualization prototype, first the particle data is processed in situ, during the simulation run, to produce summarized bubble specific data sets that are significantly smaller compared to the raw particle output [4].

2.2. Bubble Extraction and Particle Rise Velocity Field Generation

Before visualization, raw unstructured particle data is converted to a particle density field. A Gaussian distribution is estimated from the particle density values of a user-selected 3D bubble region and then statistically similar regions can be identified from the data to produce a statistical bubble similarity field. Here, the 3D region is selected by domain experts and identified to be a known-bubble region. Values in the bubble similarity field ranges from 0 to 1 and is an indication of how much each region statistically similar to that of the user selected bubble region. From the similarity field, a threshold value for bubble similarity can be determined and used to extract and then track bubbles. Along with the bubbles, domain experts take interest in the velocity profile of the surrounding fluid as well as that of individual bubbles. To achieve this, we compute a particle rise velocity scalar field from the raw particle velocities and is used in the visualization. Average particle rise velocities from the particle data were estimated using a spatial 3D histogram and saved as a regular scalar field along with the particle density field for comparative study and overlayed in the background of the bubble visualization to study bubble and fluid interaction. We can observe the changes in fluid velocity



Select Database: Bubble All
Threshold: 0.05 116 results found!
275 out of 4917 results selected
Results Per Page: 100
Sort By: aspect_ratio
Reverse Sort Order: ☑
Group equal values: ☐
Image Size: 100px

Index: 4655
time_step: 391.0
feature_id: 26.0
aspect_ratio: 1.1472406691067993
volume: 7057.0
x_center: 0.02600422501564026
FILE: images/bubble_26_391.png

Figure 1: Feature Similarity and Upward Fluid Velocity field rendering. Bubble features can be tracked for post hoc analysis [4] and viewed in CinemaExplorer [13] (right sub-figure).

as bubbles rise upward, move laterally, and combine to form new bubbles. A higher value in the particle rise velocity scalar field indicated fluid regions with a high velocity in the positive X (upward) direction.

2.3. *Visualization Set Up*

ParaView [9] offers several options to visualize particles from particle data. One example is the `Surface` representation which we can use to obtain a quick overview of the simulation results. We can also apply either the `Point Gaussian` representation or the `Glyph` filter to plot particles as spheres with sizes defined by the smoothing length. However, we use a more effective volume rendering in ParaView to represent the continuum with particles, modifying the opacity array of the fluid to highlight bubble features and visualize fluid velocity. Through the graphical user interface (GUI), a user can set the bounding box of the particle dataset and configure the *xyz*-dimensions, origin, and spacing for the uniform grid. Users can visualize the in situ derived attributes, for example, statistical feature similarity data, and fluid velocity data, etc., interactively. High valued regions in the feature similarity field indicates bubbles and separate colormaps were used for highlighting bubble regions and fluid velocity field around the bubbles in ParaView. To show both the information, we used overlayed volume rendering of two scalar fields in ParaView where the particle rise velocity field works as a context for the bubbles.

3. Results

In our workflow, the bubble similarity field and the particle rise velocity field are output from the in situ algorithm and become the input for the post hoc analysis, which is interactive and easy to visualize for the domain scientist. The post hoc analysis uses CinemaExplorer, a LANL developed interactive multipurpose visualization tool, to show tracking of bubbles and their attributes such as volume, velocity, aspect ratio, and position [14]. This allows the domain scientists to flexibly study the bubble dynamics and track merge and split events. The analysis method enables tracking of single bubbles as well as all the bubbles from a user selected timestep of interest.

Results of the visualization of bubbles based on the feature similarity can be seen in Figure 1. It shows the Feature Similarity and Upward velocity render. The Feature similarity ranges from 0 to 1 and regions with a higher similarity value are more statistically similar to the user-selected known bubble region. We observe negative (downward directional) particle velocities for regions in blue and positive (upward) particle velocities on top of the bubbles, indicated by reddish yellow. The particle rise velocity field indicates a high velocity above and below the bubbles. As bubbles increase in velocity, they rise and merge forming large regions of low particle density.

The bubble similarity threshold of 0.92 was applied to segment all timesteps for consistent results [4]. Our analysis method enables tracking of a single bubble as well as all the bubbles selected from a specific timestep by the user. From the left sub-figure of Figure 1, we see that fluid around the bubbles move downward, consistent with the existing literature [15]. Fluid surrounding the bubble can moves downward towards regions of low density in the wake of the upward-moving bubble. The region immediately behind the bubble is seen as a red-to-yellow region, where fluid is moving fastest in the upward direction. Generally, particle velocities above and below bubbles are high, and the velocity is observed to be higher underneath the bubbles than above bubbles which is seen from the yellow regions. This distribution of low-velocity fluid next to the bubbles and high-velocity particles above and below each bubble generates a circular flow, causing the bubbles to rise [4].

4. Conclusion

The MFiX-Exa project goal presents the challenge of multiflow, multi-phase reactions. In our video, we highlight real life scientific use cases of MFiX-Exa simulation and the importance of creating a workflow encompassing an in situ analysis and feature detection algorithm that supports a post hoc workflow. The video demonstrates the use of highly summarized data sets, processed in-situ to produce interactive post hoc visualizations of bubble dynamics. LANL's in situ statistical feature detection algorithm addresses the domain science problem of identifying voids in a fluidized bed while decreasing the size of the data.

We underscore the novel capabilities for MFiX-Exa to combine CFD-DEM simulations with the power of supercomputing and visualize a fluidizeed bed of a CLR using ParaView and Cinema Explorer. The post hoc Cinema-based analysis allows the scientist to explore bubble dynamics in a real-time analysis tool, relevant to the domain scientist.

The influence of Exascale Computing in the future of CLR and Carbon capture technologies is extremely promising. Further, CLRs offer a viable path to tangibly address climate change and reduce greenhouse gas emissions significantly in the US with the ultimate goal of achieving net-zero emissions. With OLCF's Frontier now coming online, even larger simulations are on the horizon. By harnessing the power of HPC, we can greatly optimize the bandwidth of our computational power, significantly reducing the extremely high physical testing and scale-up costs.

Acknowledgments

This research was supported by the Exascale Computing Project (17-SC-20-SC), a joint project of the U.S. Department of Energy's Office of Science and National Nuclear Security Administration, responsible for delivering a capable exascale ecosystem, including software, applications, and hardware technology, to support the nation's exascale computing imperative. This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under Contract No. DE-AC02-05CH11231 using NERSC award ASCR-ERCAP0019934. The authors would like to thank the MFiX-Exa team, especially Jordan Musser and Ann Almgren, for the opportunity to use their code and data. Released under LA-UR-22-27922.

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