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Advanced coal gasifier designs using large-scale simulations

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Abstract. Porting of the legacy code MFIX to a high performance computer (HPC) and the use of high resolution simulations for the design of a coal gasifier are described here. MFIX is based on a continuum multiphase flow model that considers gas and solids to form interpenetrating continua. Low resolution simulations of a commercial scale gasifier with a validated MFIX model revealed interesting physical phenomena with implications on the gasifier design, which prompted the study reported here. To be predictive, the simulations need to model the spatiotemporal variations in gas and solids volume fractions, velocities, temperatures with any associated phase change and chemical reactions. These processes occur at various time- and length-scales requiring very high spatial resolution and large number of iterations with small time-steps. We were able to perform perhaps the largest known simulations of gas-solids reacting flows, providing detailed information about the gas-solids flow structure and the pressure, temperature and species distribution in the gasifier. One key finding is the new features of the coal jet trajectory revealed with the high spatial resolution, which provides information on the accuracy of the lower resolution simulations. Methodologies for effectively combining high and low resolution simulations for design studies must be developed. From a computational science perspective, we found that global communication has to be reduced to achieve scalability to 1000s of cores, hybrid parallelization is required to effectively utilize the multicore chips, and the wait time in the batch queue significantly increases the actual time-to-solution. From our experience, development is required in the following areas: efficient solvers for heterogeneous, massively parallel systems; data analysis tools to extract information from large data sets; and programming environments for easily porting legacy codes to HPC.

1. Introduction
Integrated Gasification Combined Cycle (IGCC) is a promising technology for meeting the growing demand for power using fossil fuel resources, while economically controlling the emission of CO₂ and other pollutants. A National Energy Technology Laboratory (NETL) study has shown that IGCC systems with carbon capture and storage (CCS) can generate power at efficiencies of 32%, compared to 25% for a conventional pulverized coal (PC) plant, and at a cost of electricity of 10.6 cents/kWh, compared to 11.9 cents/kWh for a PC plant [1]. The centerpiece of an IGCC system is the gasifier, which converts coal or other carbonaceous materials such as biomass into syngas, a mixture of CO and H₂. The syngas can be used for the production of liquid fuels and chemicals or for power generation.
In an IGCC system the syngas is shift converted into a mixture of CO$_2$ and H$_2$. CO$_2$ is captured and stored, and H$_2$ is used for power generation.

A reliable gasifier is critical for the commercial viability of IGCC. An advanced gasifier technology based on a transport gasifier is being developed at the Power Systems Development Facility (PSDF) in Wilsonville, Alabama, a joint project between the U.S. Department of Energy (DOE), Southern Company, and Kellogg Brown and Root (KBR). The gas-solids multiphase flow such as occurring in the transport gasifier is known to make the design of commercial-scale units using traditional scale-up methods unreliable [2]. Multiphase computational fluid dynamic (CFD) models are being developed at NETL to address that challenge, and this paper discusses the potential for using large-scale CFD simulations for gasifier design.

The validation of the NETL gasifier model with data from the PSDF pilot-scale facility has been reported before [3]. The results of the validation simulations were frequently communicated with the design engineers, and the acceptance of the results dramatically improved when simulations showed unexpected physical phenomena that were subsequently validated with experimental data. For example, the simulations showed that oxygen reached the upper region of the mixing section in the transport gasifier, whereas the engineers had expected that all the oxygen would be consumed in the lower region where the air is mixed with the hot, recycled char. This prediction was later verified when sampling probes were installed in the mixing section and the oxygen concentration in its upper region was measured. In another instance, the calculations showed high concentration of CO and solids near the top of the riser section of the transport gasifier. This prediction was also later validated with experimental data. These validated predictions showed that the model does not merely reproduce what is already known, but could provide information on unobserved phenomena that could be exploited for improving the gasifier design.

Another criticism that the design engineers often have is that the computational time is much larger than the physical time simulated. For example, typical validation simulations took over a million seconds of computational time (on 32-64 parallel processors) for simulating around fifteen seconds of gasifier operation. But the computational time is much smaller than the time taken to make geometric changes in the physical gasifier and the computational cost, significantly smaller. In some cases those are more useful comparisons. This was well illustrated when NETL researchers completed the simulation of the transport gasifier with certain design modifications in less than two weeks at a cost of about $10 K, whereas the physical modification of the gasifier took around fourteen weeks at a cost of around $6 M. The simulation predicted a significant increase in CO concentration in the syngas, which was found to agree well with data from the modified gasifier. The simulation had the added advantage that the results could be interrogated to explain why the CO concentration would increase [2]. This showed that the computations could be completed much faster (~10 times faster) than the physical modifications and required only a small fraction of the cost of modifications (~< 0.2%).

The validated model was then used to study the impact of the exit geometry on syngas composition, the effect of reactor height on CO concentration, the coal trajectory within the gasifier, the gas temperature profiles in the gasifier, and the effect increasing the pressure. Later the model was used to help with the design of a Clean Coal Power Initiative (CCPI) gasifier (285 MW electric), which was scaled up from the pilot-scale gasifier (13 MW thermal), representing a factor of 50 scale-up. The multiphase CFD simulations were used to study the effect of pressure, the height to diameter ratio, coal feed rate, coal feed nozzle operation, solids circulation rate, and the effect of recycled syngas. Several sets of parametric evaluations showed an unexpected dependence of the gas species concentrations and solids temperature upon the coal jet penetration. Temperature dependency on the coal feed can impact the thermal decomposition of the coal, produce unwanted agglomeration, and could have a significant economic impact due to material degradation.

This result created interest in conducting simulations of the CCPI gasifier at greater grid resolutions. The rule-of-thumb for grid independence in gas-solids simulations is that the grid size should be of the order of 10 particle size [4]. This meant that the CCPI gasifier needed to be simulated with about 100 billion cells. This resolution would require well over three million compute cores and
result in file sizes on the order of 745 GB for a single time record for each scalar tracked in the simulation. This was certainly beyond the computational capability available at NETL and, in fact, even at the fastest HPC platforms. However, the INCITE grant is allowing the group to conduct CCPI gasifier simulations at greater grid resolution than was previously possible. This paper describes how the model was improved to run on HPC platforms and presents some of the preliminary computational results.

2. Coal gasifier model

2.1. The multiphase CFD model

Gasifiers contain a reacting mixture of coal (or other solids) flowing with the gas. In the continuum modeling approach used in this study the coal particles are represented as a granular phase, which co-locates with the gas phase to form a multiphase mixture, the volume fraction \( \varepsilon_m \) giving the amount of phase \( m \) at each spatial location. The multiphase CFD model consists of the mass, momentum, energy, and species-mass balances for each phase, gas (\( m = g \)) or solids (\( m = s \)):

\[
\frac{\partial}{\partial t} (\varepsilon_m \rho_m) + \nabla \cdot (\varepsilon_m \rho_m \tilde{v}_m) = \sum_{l=1}^{N_m} R_{ml}
\]

\[
\frac{\partial}{\partial t} (\varepsilon_m \rho_m \tilde{v}_m) + \nabla \cdot (\varepsilon_m \rho_m \tilde{v}_m \tilde{v}_m) = \nabla \cdot \tilde{S}_m + \varepsilon_m \rho_m \tilde{g} + \sum_n \tilde{J}_{mn}
\]

\[
\frac{3}{2} \varepsilon_m \rho_m \left( \frac{\partial \Theta_m}{\partial t} + \tilde{v}_m \cdot \nabla \Theta_m \right) = \nabla \cdot \tilde{q}_{\Theta_m} + \tilde{S}_m : \nabla \tilde{v}_m - \varepsilon_m \rho_m J_m + \Pi_{\Theta_m} \quad (m \neq g)
\]

\[
\varepsilon_m \rho_m C_{pm} \left( \frac{\partial T_m}{\partial t} + \tilde{v}_m \cdot \nabla T_m \right) = -\nabla \cdot \tilde{q}_m + \sum_n \gamma_{mn} (T_n - T_m) - \Delta H_{rm}
\]

\[
\frac{\partial}{\partial t} (\varepsilon_m \rho_m X_{ml}) + \nabla \cdot (\varepsilon_m \rho_m X_{ml} \tilde{v}_m) = R_{ml}
\]

where subscript \( m \) and \( n \) stands for phases and \( l \) for a species in a phase and \( C_{pm} \), heat capacity at constant pressure; \( \Delta H_{rm} \) is the heat of reaction; \( \tilde{J}_{mn} \), momentum exchange between phases \( m \) and \( n \); \( J_m \), collisional dissipation of granular energy; \( \tilde{g} \), gravitational acceleration; \( \tilde{q}_{\Theta_m} \), heat flux; \( \tilde{q}_m \), granular heat flux; \( R_{ml} \), chemical reaction rate of the \( l \)th species of the \( m \)th phase; \( \tilde{S}_m \), stress tensor; \( T_m \), temperature; \( \tilde{v}_m \), velocity vector; \( X_{ml} \), mass fraction of the \( l \)th species in the \( m \)th phase; \( \gamma_{mn} \), coefficient of heat transfer between phases \( m \) and \( n \); \( \varepsilon_m \), volume fraction; \( \Pi_{\Theta_m} \), dissipation of granular energy due to interaction with gas; \( \rho_m \), density; and \( \Theta_m \), granular temperature or one-third the mean square of particle velocity fluctuations. These equations must be closed with constitutive relations for the momentum and energy exchange, and the phasic stresses, heat capacities, and heat fluxes. These equations are solved using a finite volume technique available in the open source code MFIX (http://mfix.netl.doe.gov) [5]. The gas phase pressure gradient multiplied by \( \varepsilon_m \) appears in all the momentum equations, the term accounting for a buoyancy force in the solids momentum equation. In addition, the solids momentum equation also contains a pressure term that is a function of the granular temperature and gas-phase volume fraction.

For modeling coal gasifiers, the chemical reaction rates and heats of reaction must be supplied, which is available through the module carbonaceous chemistry for continuum modeling (C3M) developed at NETL. C3M represents the gas phase composition with eight species (O2, CO, CO2, CH4, H2, H2O, N2, and tar) and the solids phase (coal) composition with four pseudo-species (fixed carbon, volatile matter, moisture, and ash). Ash does not take part in any reactions, moisture is released in an
initial stage reaction, and the volatile matter produces several gas-phase species through devolitization. The gas phase reactions are tar decomposition, water gas shift reaction, and combustion reactions for H₂, CH₄, CO. The heterogeneous reactions are char combustion and gasification. All the reaction schemes are shown in Figure 1 [6]. (The sorbent reactions shown in the figure were not included in the simulations reported here.)

2.2. Computational challenges
The multiphase CFD model of coal gasifier poses enormous computational challenges, primarily stemming from the gas-solids hydrodynamics, complicated by the homogeneous and heterogeneous chemical reactions. Gas-solids flows are in general unsteady – the volume fraction, stress, and energy typically fluctuating spatially and temporally with amplitudes comparable to the mean – and no reliable, time-averaged (turbulence like) equations are available for describing their stationary state behaviour. Therefore, the multiphase CFD approach involves computing the transient solution for a sufficiently long time to reach a statistically stationary state, from which a time-averaged solution is extracted to evaluate the reactor performance. The transient calculations usually require small time-steps, necessitated by rapid changes in the physics: The solids volume fraction can vary by several orders of magnitude over short length or time scales, a variation reminiscent of a single-phase flow transitioning from hypersonic to incompressible. When the solids volume fraction increases beyond a certain value (~0.5), the solids-phase undergoes a phase change, similar to glass transition, necessitating a drastic change in the solids-phase constitutive relations. The coupling terms between the gas and the solids phases dominate the momentum and energy equations, introducing small relaxation time-scales that vary with the solids volume fraction.

![Figure 1. Schematic representation of chemical reactions in C3M Module.](image)

The inclusion of the coal gasification and combustion chemistry aggravates the computational challenge. The computational burden increases simply from the addition of twelve partial differential equations for tracking the species mass fractions, which more than doubles the total number of equations solved. The chemical reaction rates vary from the slow gasification reactions to very fast devolatilization and combustion reactions. Although the fast reactions are confined to small regions of the gasifier, they may control the size of the time-steps. Also the net reaction rates introduce coupling terms between the phasic continuity equations, which may reduce the rate of convergence of the non-linear iterations.
2.3. Porting the model to HPC

The model described in the previous section was developed at NETL over many years and was recently ported to HPC platforms. Figure 2 shows examples of multiphase flow reactor simulations, the computational cell count, the number of processors or cores, and the parallelization methods used over the years. In less than twenty years the cell count has grown by four orders of magnitude, necessitating the use of parallel computational platforms with a similar increase in the number of cores. The last two points on the graph labeled “CCPI gasifier” correspond to the simulations performed under the INCITE grant on the HPC platforms Cray XT4 and XT5. The results presented in this paper are from those simulations.

Extensive profiling of MFIX was conducted on HPC platforms using standard benchmark cases that scaled up to 10 million cells on 6032 cores, to determine the computational bottlenecks. Based on the profiling information and the experience in running on HPC platforms, MFIX was improved in several phases:

- Phase I: The compiler flags and MPI parameters were tuned to improve the scaling.
- Phase II: The global collective operations become very expensive as the number of processors is increased because a small amount of data is transferred between the processors and the data transfer speed becomes limited by the latency. It was found that successive over relaxation (SOR) could be used for all the variables, except the gas pressure and solids volume fraction. SOR was found to scale well as it does not require global collective operations (e.g., dot-product). Furthermore, the BiCGStab linear equation solver used for the gas pressure and solids volume fraction was improved by decreasing the number of global collective operations. One iteration of the standard BiCGStab [7] involves 6 vector-vector dot products, two of which are for residual checks. An intermediate residual check was eliminated, and the frequency of the final check was reduced. The last two dot products are independent and they were combined into one collective operation on the two vectors. This reduced the number of dot products to ~3 per iteration, thus reducing the cost associated with dot products by 50%. The change of compiler from Portland Group to PathScale also substantially contributed to the improvements obtained in Phase II.

- Phase III: Currently work is ongoing to conduct hybrid mode operation of MFIX to take advantage of multicore platforms with MPI and OpenMP. Although MFIX includes OpenMP directives for most of the loops, enabling multithreading for all the loops degrades the performance on a large number of processors. An extensive profiling study was performed to determine the loops that will most benefit from multithreading. As a result of this study, multithreading for several subroutines

![Figure 2. Size of the coal gasifier simulations over the years and the number of cores used to solve the problem.](image-url)
(e.g., linear equation solver routine, \texttt{leq\_msolve}) were enabled. Identification of other subroutines that could improve the time-to-solution performance of MFIX is still under progress.

- **Phase IV:** Current MFIX I/O is not equipped to handle such high resolution runs for long transient periods and post-processing becomes a challenge. For example, when one of the 11 output files storing nearly 5 s of data reaches a size of 95 GB, the automated script for storing the data on the tape archival utility (HPSS at NCCS) fails because of the large file size. The large file size is a peculiarity of how data sets are stored in MFIX output files, all time-records of a group of variables being stored in a single file. The storage format is being improved by using netCDF/pnetCDF formats.

- **Phase V:** Currently we have plans to integrate MFIX with highly scalable and tuned solver library such as Trilinos.

### 3. Results of scaling study

Table 1 shows the results obtained from the actual production runs for the 10 million cell transport gasifier model on 2064 cores [8]. A sampling size of eight batch job run sessions were used to obtain the average simulated time per session (last column). The duration for each batch job session was 12 h of wall clock time, the maximum permitted for the requested number of cores. As seen from the results, runs employing 1032 MPI processes and 2 threads per process (in linear equation solver routines only) performed nearly 2.5 times better than those employing 2064 cores of MPI processes with a single thread. On average the simulation progressed for 0.18 s at the end of 12 hour run for 2064 cores of MPI processes only, whereas the simulation running in hybrid mode progresses 0.47 s at the end of the same duration.

| Mode Of Operation | Number of MPI cores | Number of Threads | Average simulated time (s) / 12 h job |
|-------------------|---------------------|-------------------|-------------------------------------|
| MPI only          | 2064                | 1                 | 0.18                                |
| MPI + OpenMP      | 1032                | 2                 | 0.47                                |

A continuous improvement cycle to monitor and improve execution performance of MFIX with the deployment of new HPC platforms is a critical component in utilizing these resources effectively for advanced coal gasifier designs and reduce time-to-solution. For this purpose a new benchmarking study to investigate the performance of MFIX on the new Cray XT5 platform at NCCS with quad cores was started. Preliminary results indicate that MFIX performance degrades if all eight cores are used for MPI processes (without any multithreading) possibly due to memory contention issues [8]. For example, for the standard 10M cell benchmarking case where time to solution is measured for integrating over 100 steps of 2.5x10^{-4} s, running a 516 processor job shows that requesting only 4 cores per node (remaining cores being idle) versus all 8 cores in a node results in 40 % reduction of time-to-solution.

The next improvement task was to investigate the effect of hybrid mode execution (i.e., MPI + OpenMP) on Cray XT5 with more than 2 threads per node. The results of the performance analysis conducted with CrayPAT tool show that boundary condition setup routine, \texttt{bc\_phi} was the most time consuming routine after MPI and linear equation solver subroutine \texttt{leq\_msolve}. Figure 3 shows the comparison for employing multithreading only in \texttt{leq\_msolve} routine versus both \texttt{leq\_msolve} and \texttt{bc\_phi} subroutines by varying across 1 to 8 threads. Although enabling multithreading in \texttt{bc\_phi} didn’t improve time-to-solution as much as the \texttt{leq\_msolve} subroutine, additional benchmarking needs to be conducted to replicate the runs to reduce the impact of variability due to operating system noise and to determine the optimal number of cores for MPI and OpenMP threads on Cray XT5 for the given configuration of the gasifier simulations.
For using large-scale simulations for design, the practical issue of achieving a desirable time-to-solution must be considered. For large-scale computations on HPC, the time-to-solution is dependent upon factors beyond the computational challenges described previously. A target time-to-solution is 12 h for simulating a fully-resolved 25 MW unit, which is to be achieved by the year 2015 [2]; that is, the designers would like to get the results after an overnight simulation. To reach a stationary state in one of our large-scale simulations, it must be carried out for around 15 s (the residence time being typically 1–3 s for gas and 3–5 s for solids) and the time-average of the last 5 s are used for further analysis. Although an adaptive time-step algorithm is employed, on the average the time-step is $10^{-4}$ s, requiring around 150,000 time-steps for each calculation. For a 10 million cell case (285 MW unit) on 2064 processors (MPI only operation mode), the total run time on a Cray XT4 (Jaguar system at NCCS) is around 19 days. But the actual time-to-solution is significantly longer, when the factors such as wait time in the batch queue, system downtime, and job termination due to intermittent node failure are considered. Because of the long duration of the transient simulations, it is necessary to have high availability of a large number of processors for a long duration. At a shared resource center like National Center for Computational Sciences (NCCS) the runs are constrained by the throughput of the batch queue; for example, 2064-core jobs depending on the system status typically wait for 2–4 days in the queue for every 12 h compute session, which simulates 0.35–0.45 s of physical time (if employing hybrid mode of operation with MPI and OpenMP). This is equivalent to about 112 days to complete a calculation for 15 s simulation of physical time. We also need to consider the additional time required for analyzing the results, a challenge complicated by the much larger output files generated by the high resolution simulations conducted on HPC.

4. Results of high resolution simulation

Preliminary results of a high resolution simulation (10 million cells) conducted through the INCITE award are compared with the results of a low resolution simulation (~1 million cells) previously conducted at NETL clusters (typically taking 2 weeks on 24 cores). Figures 4 and 5 show the gas temperature (in Kelvin), and, the carbon mass fraction and the volatile mass fraction in the solids-phase in the bottom section of the gasifier at a typical instance in time. They also include a horizontal clip plane, showing the mass fractions of O\(_2\), CO, and CO\(_2\). Not surprisingly, the higher-resolution results show greater structure in the field variable distributions. These preliminary results also show a difference in the value of the gas temperature, the high resolution simulation producing overall lower gas temperatures, especially near the coal jets (located just above the horizontal clip plane). The carbon and volatile mass fractions show that the bulk of the coal as it enters the gasifier tends to move away from the wall to a greater extent in the high resolution case than in the low resolution case. The high-resolution simulation shows (in the clip plane of the middle frame) much higher CO concentration coming up into the coal jet region from the lower portion of the gasifier. These higher levels of CO indicate better mixing of the recycled material in the lower portion of the gasifier with the burner air resulting in greater consumption of the carbon in the recycled stream entering the gasifier from below.

Figure 3. Comparison of time-to-solution after enabling multithreading across 1 to 8 cores on Cray XT5 for different subroutines.
Figures 6 and 7 compare the high and low resolution simulations zooming into the coal jet region of the gasifier. The coal jet entering the gasifier is shown by plotting the isosurfaces for five values of the void fraction \( \varepsilon_g = 1 - \varepsilon_s \). The three horizontal clip planes are located where the coal jets enter the gasifier and show the gas temperature. The boundary conditions imposed on the coal jets set the flow of coal in a 45 degree downward direction. The high-resolution plots show that the isosurfaces go below the clip planes, predicting that the coal jets flow downward after entering the gasifier, turn around, and then move upward. Perhaps the upward turning movement causes the jet to move away from the wall. The low resolution simulation, however, shows that the coal jet quickly turns upward with little or no downward movement and takes an upward trajectory closer to the wall.

The differences in the simulation results at the two resolutions have practical implications for the gasifier design. For example, the trajectory of the coal jet could have significant effect on the gasifier reliability. A coal jet trajectory closer to the wall could lead to greater erosion of the refractory. So the low resolution simulation would predict a shorter refractory life than the high resolution simulation. Given that it is not currently feasible to conduct high resolution simulations for all the design cases, it remains to be determined how a few high resolution simulations could be combined with a large number of low resolution simulations to help with the design.
5. Conclusions
Computational gas-solids flows such as occurring in coal gasifiers are one of the highly non-linear processes observed in natural and man-made devices. To be predictive, the simulations need to model the spatiotemporal variations in gas and solids volume fractions, velocities, temperatures with any associated phase change and corresponding chemical reactions. These processes occur at various time- and length-scales requiring very high spatial resolution and large number of iterations with small time-steps. To solve these stiff set of non-linear partial differential equations at high spatial resolution, large-scale computer resources are required, and with the INCITE allocation, we were able to perform perhaps the largest known simulations of gas-solids reacting flows, providing detailed information about the gas-solids flow structure and the pressure, temperature and species distribution in the gasifier. One key finding is the new features of the coal jet trajectory revealed with the higher spatial resolution, which provides information on the accuracy of the lower resolution simulations. Methodologies for effectively combining high and low resolution simulations for design studies must be developed. Further analysis has to be performed to understand the causality relationships between the hydrodynamics, heat and mass transfer, and chemical reactions.

From a computational science perspective, we have found that global communication has to be reduced to achieve scalability to 1000s of cores. In addition, we have to employ hybrid parallelization to effectively utilize the multicore chips. We also find that the factors such as wait time in the batch queue could significantly increase the time-to-solution. From our experience, developments have to be
made in the following areas to efficiently use large petascale resources and enable computational discovery:

- Efficient solvers for heterogeneous, massively parallel systems
- Data analysis tools to extract information from large data sets
- Programming environments for easily porting legacy codes to HPC platforms

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