ACCELERATING MULTIPHASE FLOW PREDICTIONS BY USING NOVEL ALGORITHMS AND PROCESSORS

Final Project Report

Erwin-Schroedinger Fellowship J 3072-N13, granted 2010-09-27

Report Period: November 15 2010 - December 15 2011(13 months)

Introduction

The ultimate goal of our project was to better understand multiphase flows (e.g., catalyst particles moving in gas) by using graphic processing units (GPUs). Therefore, we used a Lagrangian approach to track (i) physical particles, and (ii) surrogate particles ("parcels") that represent the particle population. To allow time-efficient simulations, we adapted and already existing computer code for particle tracking, and combined it with the open-source code "OpenFOAM".

The three main objectives of our project were (1) to explore the virtues, merits and limitations of the parcel-based approach (i.e., approach ii); (2) to demonstrate the capabilities of our code by simulating several millions of particles in a time-efficient manner; and (3) to use the code to gain a better understanding of granular flows.

Results

Theory for Particle-Phase Flow

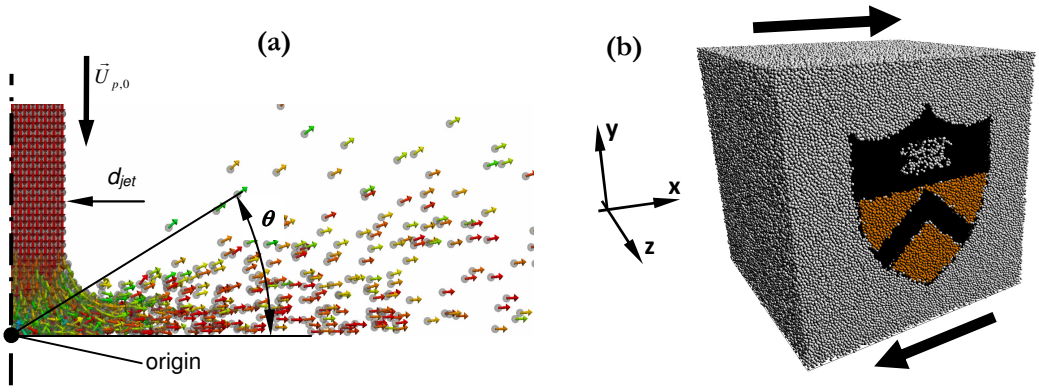

Figure 1. Granular jet impinging on a flat surface (a: we have used the scattering angle θ to validate our simulation runs), as well as simple shear flow of a particle assembly (b: shown is the logo of Princeton University that is used to visualize particle mixing).

After implementing the core routines of the parcel-based approach, we recognized that recently published models significantly mis-predict the particle-phase stress. Our efforts to improve the algorithm resulted in a significant improvement of the flow prediction (our model was awarded the 'Best Paper Award' at the CFD2011 conference in Trondheim).

Specifically, we investigated different granular flow setups (discharge from a hopper, jet flow, shear flow; free-flowing, as well as cohesive particles; see Figure 1) with our code, and validated the results with literature data.

Performance of the Gas-Particle Flow Code "r2d2"

Coupling the gas and particle-phase turned out to be relatively straight forward, and we managed to couple the gas and particle phase by only transferring pre-averaged data between CPU and GPU. Hence, there is little performance loss when using a gas-particle coupled simulation compared to a purely particle-based simulation (see Figure 2, "r2d2, DEM" is a purely particle-based simulation, "r2d2, CFD-DEM" is a gas-particle coupled simulation).

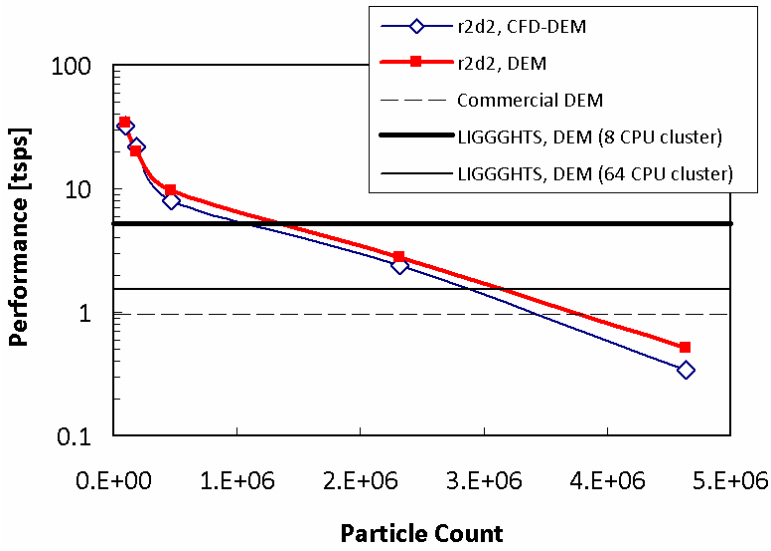

Figure 2. Single-Core performance (in terms of time steps per second, tsps) for the developed code as a function of problem size ("Commercial DEM" and "LIGGGHTS" refer to data for a simulation with 10^5 particles provided by [1] and is based on a single CPU; "*r2d2*" is data from the code developed in this project based on 1 GPU, "CFD-DEM" refers to the coupled gas-particle solver, and "DEM" is the particle solver only).

We compared the performance of our code "r2d2" with results from *LIGGGHTS* [1], a state-of-the-art CFD-DEM solver based on the well-known code *LAMMPS,*[1] as well as a commercial code, for which performance data for a moderately large system involving 10^5 particles was available [1]. As can be seen from Figure 2, our code "*r2d2*" is approximately 34 times faster than the commercial code (dashed line in Figure 2) running on a single CPU. Comparing our code with the latest (optimized) version of *LIGGGHTS* running on an 8 CPU cluster, we see that "r2d2" is 6.5 faster than a computation on a single CPU. However, the true advantage of our code becomes apparent when comparing "r2d2" with the

[1] http://lammps.sandia.gov

performance of a single CPU in a larger cluster (see results for *LIGGGHTS* on a 64 CPU cluster). It is well known that in such CPU clusters message passage becomes the limiting factor. Consequently, *r2d2* is 22 times faster than a single CPU, i.e., we can replace ~20 CPUs with one GPU. Figure 2 can be also interpreted from the perspective of the maximum feasible problem size to be handled in a certain amount of time. Thus, currently commercial codes (dashed line in Figure 2) are limited to ~10^5 particles in single CPU mode (based on 12 days maximum allowable computation time, and 10^6 time steps to be performed, 1 [tsps] is treated as "feasible"). **Our code can handle a system consisting of ~3.5 Mio. particles in the same amount of time**.

Parameter Studies for Dense Gas-Particle Flow

Thanks to the computational resources that were provided by the group in Princeton, we were able to perform a large set of sedimentation simulations in a periodic box. Example results of such a simulation are shown in Figure 3. The results of these simulations were key to quantify the effect of cluster formation on the (average) slip velocity $\mathbf{u}_{slip,av}$ between the two phases. For example, we could show that the drag law on the particle scale as well as the spatial resolution of the gas phase has relatively little effect on $\mathbf{u}_{slip,av}$. This is an extremely interesting result, since at the same time our group in Princeton showed that simulations based on the two fluid model (TFM; the particle-phase is treated as a fluid) are more sensitive to the spatial resolution in certain situations (e.g., if applied to reactive flows). This questions the results previously obtained with TFM. Motivated by our result, we started TFM-based simulations that aim on quantifying this grid dependency in very detail. Also, we implemented a filtered drag model into an existing TFM solver, to highlight the importance of filtered drag models on the flow prediction. Such filtered drag models can be extracted from our CFD-DEM simulations.

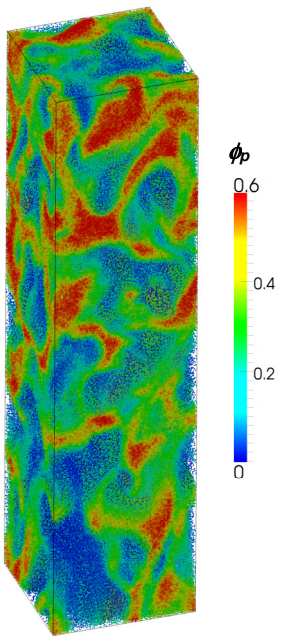

Figure 3. Clustering predicted by our code (this simulation involved 2.3· 10^6 particles).

Development of a Filtered Drag Models for Parcels

Since the group was very active in developing a "filtered drag model" for TFM in the past, we aimed on developing a similar model for our parcel approach. The idea behind this filtered model is to take cluster formation into account, such that simulations are more accurate on coarser computational grids. This approach is similar to so-called "a priori"

filtering of single-phase turbulent flow. Figure 4 shows the results for such a filtered drag coefficient $\overline{\beta}_p$, which has been normalized with the "microscopic" drag coefficient (i.e., the drag coefficient of a single particle in a suspension, we adopted the model of Beetstra et al. [2]). Clearly, our results show that the normalized filtered drag coefficient is significantly smaller than unity for moderately dense to dense gas-particle flows. While this effect has been recognized already ten years ago in connection to TFMs, we are the first that provide a systematic study that show that such a drag correction is also necessary for parcel-based methods.

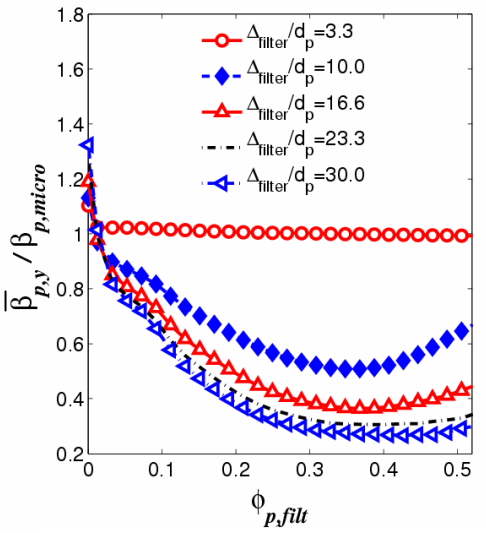

Figure 4. Filtered drag coefficient for parcels vs. the filtered particle volume fraction.

Liquid-Fluidized Beds

In order to validate the use of our code for liquid-fluidized beds, we have performed simulations of a small system previously analyzed by our group in Princeton [3]. Specifically, this previous work was done using simulations using a Lattice-Boltzmann (LB) code, which allowed a full resolution of the fluid flow around individual particles (Figure 5b). However, these previous LB studies were computationally extremely demanding. We showed that it is possible to predict wave formation in liquid-fluidized beds, as well as to accurately calculate (i.e., within a few percent) the speed of the wave using our code *without* resolving the

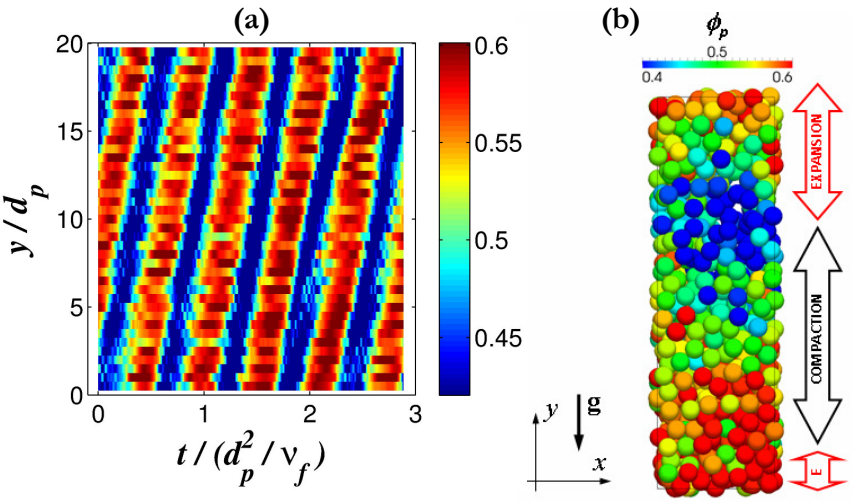

Figure 5. (a) Space-time plot of a 1D wave in a liquid-fluidized bed (d_p = 685 µm particles fluidized with water, ν_f is the fluid's kinematic viscosity); (b) particle arrangement and local particle volume distribution in the fluidized bed.

details of the fluid flow around the particles. The wave obtained with our code as shown in Figure 5a has a wave speed that is within 2% of the wave speed calculated by [3]. This is a very encouraging result for us to apply our code to the flow of dense suspensions, as well as to the more difficult motion of bubbles in liquids.

Relevance for Chemical Engineering as a Scientific Discipline

We identified the calculation of the particle fluctuation velocities ($\mathbf{u}_p$') in parcel-based approaches as a critical factor. The correct prediction of $\mathbf{u}_p$' is key for the future application of our code such as the investigation of particle mixing, or the prediction of liquid spreading in wet particle systems (e.g., relevant for granulation, as well as petro-chemical processes). Prof. Sundaresan's group was able to acquire a new project focusing on the latter aspect, and a PhD student (Matthew Girardi) will work on this project during the next 4 years. Because wet particulate systems tend to agglomerate, and currently available theories cannot properly handle this process, we expect a breakthrough in this field induced by our method. The results of liquid spreading in wet particulate systems are especially interesting also for pharmaceutical applications, and hence there is broad interest of the research group around Prof. Khinast in Graz (see "Development of Collaborations" in Appendix A).

Also, we want to continue our work with respect to drag models for parcel-based simulations. Specifically, we have started to look at systems with higher particle Reynolds numbers. Also, the recent results of the group in Princeton for bidisperse systems [4] show that there is significant room for improvement of methods for dense, polydisperse gas-particle flows. Our code will enable elaborate studies of these systems, without the need for complicated theories. This might be the key for numerous industrial applications, like the prediction of particle segregation in pharmaceutical production lines, dust formation in particle handling applications, or particle transport in geophysical applications (e.g., sand transport in deserts).

Finally, our results for wave formation in liquid-fluidized beds might be useful for the pulp & paper industry, since a lot of processes in this branch involve dense suspensions. Specifically, it would be interesting whether one can predict flocculation using our method, or even attempt to develop models to describe flotation (i.e., liquid-particle-bubble) processes based on first principles.

Deviations from Project Plan

During the first six month we focused more on the treatment of the particle phase, and already ran a significant number of simulations that were scheduled for the latter project phases. Therefore, we needed to postpone the implementation of the gas-particle interaction code, which was finished by End of April.

Another deviation is that we did not focus on an industrial-scale reference flow problem with our code (planned for work package V), but used an already existing two-fluid model solver for this purpose. The reason for this decision was that we focused on the development of a filtered drag model, which turned out to be critical for successful demonstration on an industrial-scale flow problem. However, the demonstration on an industrial-scale flow problem with our parcel-approach will be done during the implementation phase in Graz after finalizing the filtered drag model for parcels.

Comment on the Host Institution

The host institution supported me with two new GPU-based computers (in total 10 GPUs), as well as access to the group's computer cluster *hema* (~120 CPU cores). These computational resources exceeded my expectations, and hence we were able to run a significant amount of simulations during the project (we performed ~50 runs for the granular jet, ~250 for simple shear flow, and ~70 for fluidized beds). Also, the group financed my trip to the APS meeting in Baltimore.

The support of Prof. Sundaresan was outstanding, and he allocated between 1 and 5 hours per week for personal discussions. Prof. Sundaresan's group supported me in an outstanding manner, both with respect to science (thanks to post-doc Kapil Agrawal, numerous PhD students, as well as a high-school student that helped in programming) as well as with respect to administrative tasks (especially the administration of the GPU computers).

In summary, the scientific community at Princeton University was "open door", extremely helpful, generous, and eager to advance science without penalizing the personal development of individual researchers or group members.

Relevance for Other Branches of Science

Besides chemical engineering, the results of the project seem to be especially relevant for suspension physics, as well as could be interesting for astro-physics. For example we found that a similar methodology called Smoothed Particle Hydrodynamics (SPH), widely applied in astro-physics, shares common features with our parcel-approach.

For example, in the area of geophysical flows, the prediction of saltation (i.e., the often unwanted transport of particles by a fluid; e.g., transport of gravel in rivers, erosion in desserts, or snow transport in the Arctic) is an active field of research. We think that our simulation code might be useful for this purpose. This is because recently interesting studies on drag and lift forces in such systems have been performed [5]. Incorporating such sophisticated force models in our code could significantly increase the reliability of the prediction of saltation.

Broader Impact

The results of our work have certainly important consequences for plant engineering (especially for environmental technology, such as incineration of waste in fluidized beds, biomass gasification, carbon capture technology, or numerous petrochemical applications). More reliable computational models will help to better design and operate those plants.

References

[1] N. N, LIGGGHTS Performance Evaluation. (2012).

[2] R. Beetstra, M.A.V.D. Hoef, and J.A.M. Kuipers, Drag Force of Intermediate Reynolds Number Flow Past Mono- and Bidisperse Arrays of Spheres. AIChE J. 53 (2007) 489-501.

[3] J.J. Derksen and S. Sundaresan, Direct numerical simulations of dense suspensions: wave instabilities in liquid-fluidized beds. J. Fluid Mech. 587 (2007) 303-336.

[4] W. Holloway, S. Benyahia, C.M. Hrenya, and S. Sundaresan, Meso-scale structures of bidisperse mixtures of particles fluidized by a gas. Chem. Eng. Sci. 66 (2011) 4403-4420.

[5] J.J. Derksen and R. a. Larsen, Drag and lift forces on random assemblies of wall-attached spheres in low-Reynolds-number shear flow. J. Fluid Mech. 673 (2011) 548-573.