

Proceedings of the 12th International Conference on
Computational Fluid Dynamics in the Oil & Gas,
Metallurgical and Process Industries

Progress in Applied CFD – CFD2017



SINTEF Proceedings

Editors:

Jan Erik Olsen and Stein Tore Johansen

Progress in Applied CFD – CFD2017

Proceedings of the 12th International Conference on Computational Fluid Dynamics
in the Oil & Gas, Metallurgical and Process Industries

SINTEF Academic Press

SINTEF Proceedings no 2

Editors: Jan Erik Olsen and Stein Tore Johansen

Progress in Applied CFD – CFD2017

Selected papers from 10th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries

Key words:

CFD, Flow, Modelling

Cover, illustration: Arun Kamath

ISSN 2387-4295 (online)

ISBN 978-82-536-1544-8 (pdf)

© Copyright SINTEF Academic Press 2017

The material in this publication is covered by the provisions of the Norwegian Copyright Act. Without any special agreement with SINTEF Academic Press, any copying and making available of the material is only allowed to the extent that this is permitted by law or allowed through an agreement with Kopinor, the Reproduction Rights Organisation for Norway. Any use contrary to legislation or an agreement may lead to a liability for damages and confiscation, and may be punished by fines or imprisonment

SINTEF Academic Press

Address: Forskningsveien 3 B
 PO Box 124 Blindern
 N-0314 OSLO

Tel: +47 73 59 30 00

Fax: +47 22 96 55 08

www.sintef.no/byggforsk

www.sintefbok.no

SINTEF Proceedings

SINTEF Proceedings is a serial publication for peer-reviewed conference proceedings on a variety of scientific topics.

The processes of peer-reviewing of papers published in SINTEF Proceedings are administered by the conference organizers and proceedings editors. Detailed procedures will vary according to custom and practice in each scientific community.

PREFACE

This book contains all manuscripts approved by the reviewers and the organizing committee of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in May/June 2017 and is also known as CFD2017 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focuses on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. In addition pragmatic modelling concepts and bio-mechanical applications have become an important part of the conference. The papers in this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are included in the proceedings. 108 contributions were presented at the conference together with six keynote presentations. A majority of these contributions are presented by their manuscript in this collection (a few were granted to present without an accompanying manuscript).

The organizing committee would like to thank everyone who has helped with review of manuscripts, all those who helped to promote the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: ANSYS, SFI Metal Production and NanoSim.

Stein Tore Johansen & Jan Erik Olsen



Organizing committee:

Conference chairman: Prof. Stein Tore Johansen

Conference coordinator: Dr. Jan Erik Olsen

Dr. Bernhard Müller

Dr. Sigrid Karstad Dahl

Dr. Shahriar Amini

Dr. Ernst Meese

Dr. Josip Zoric

Dr. Jannike Solsvik

Dr. Peter Witt

Scientific committee:

Stein Tore Johansen, SINTEF/NTNU

Bernhard Müller, NTNU

Phil Schwarz, CSIRO

Akio Tomiyama, Kobe University

Hans Kuipers, Eindhoven University of Technology

Jinghai Li, Chinese Academy of Science

Markus Braun, Ansys

Simon Lo, CD-adapco

Patrick Segers, Universiteit Gent

Jiyuan Tu, RMIT

Jos Derksen, University of Aberdeen

Dmitry Eskin, Schlumberger-Doll Research

Pär Jönsson, KTH

Stefan Pirker, Johannes Kepler University

Josip Zoric, SINTEF

CONTENTS

PRAGMATIC MODELLING	9
On pragmatism in industrial modeling. Part III: Application to operational drilling	11
CFD modeling of dynamic emulsion stability	23
Modelling of interaction between turbines and terrain wakes using pragmatic approach	29
FLUIDIZED BED	37
Simulation of chemical looping combustion process in a double looping fluidized bed reactor with cu-based oxygen carriers.....	39
Extremely fast simulations of heat transfer in fluidized beds.....	47
Mass transfer phenomena in fluidized beds with horizontally immersed membranes	53
A Two-Fluid model study of hydrogen production via water gas shift in fluidized bed membrane reactors	63
Effect of lift force on dense gas-fluidized beds of non-spherical particles	71
Experimental and numerical investigation of a bubbling dense gas-solid fluidized bed	81
Direct numerical simulation of the effective drag in gas-liquid-solid systems	89
A Lagrangian-Eulerian hybrid model for the simulation of direct reduction of iron ore in fluidized beds.....	97
High temperature fluidization - influence of inter-particle forces on fluidization behavior	107
Verification of filtered two fluid models for reactive gas-solid flows	115
BIOMECHANICS.....	123
A computational framework involving CFD and data mining tools for analyzing disease in carotid artery	125
Investigating the numerical parameter space for a stenosed patient-specific internal carotid artery model.....	133
Velocity profiles in a 2D model of the left ventricular outflow tract, pathological case study using PIV and CFD modeling.....	139
Oscillatory flow and mass transport in a coronary artery.....	147
Patient specific numerical simulation of flow in the human upper airways for assessing the effect of nasal surgery.....	153
CFD simulations of turbulent flow in the human upper airways	163
OIL & GAS APPLICATIONS	169
Estimation of flow rates and parameters in two-phase stratified and slug flow by an ensemble Kalman filter	171
Direct numerical simulation of proppant transport in a narrow channel for hydraulic fracturing application	179
Multiphase direct numerical simulations (DNS) of oil-water flows through homogeneous porous rocks	185
CFD erosion modelling of blind tees	191
Shape factors inclusion in a one-dimensional, transient two-fluid model for stratified and slug flow simulations in pipes	201
Gas-liquid two-phase flow behavior in terrain-inclined pipelines for wet natural gas transportation	207

NUMERICS, METHODS & CODE DEVELOPMENT	213
Innovative computing for industrially-relevant multiphase flows	215
Development of GPU parallel multiphase flow solver for turbulent slurry flows in cyclone.....	223
Immersed boundary method for the compressible Navier–Stokes equations using high order summation-by-parts difference operators	233
Direct numerical simulation of coupled heat and mass transfer in fluid-solid systems	243
A simulation concept for generic simulation of multi-material flow, using staggered Cartesian grids.....	253
A cartesian cut-cell method, based on formal volume averaging of mass, momentum equations.....	265
SOFT: a framework for semantic interoperability of scientific software	273
 POPULATION BALANCE	 279
Combined multifluid-population balance method for polydisperse multiphase flows	281
A multifluid-PBE model for a slurry bubble column with bubble size dependent velocity, weight fractions and temperature.....	285
CFD simulation of the droplet size distribution of liquid-liquid emulsions in stirred tank reactors	295
Towards a CFD model for boiling flows: validation of QMOM predictions with TOPFLOW experiments	301
Numerical simulations of turbulent liquid-liquid dispersions with quadrature-based moment methods.....	309
Simulation of dispersion of immiscible fluids in a turbulent couette flow	317
Simulation of gas-liquid flows in separators - a Lagrangian approach.....	325
CFD modelling to predict mass transfer in pulsed sieve plate extraction columns	335
 BREAKUP & COALESCENCE	 343
Experimental and numerical study on single droplet breakage in turbulent flow	345
Improved collision modelling for liquid metal droplets in a copper slag cleaning process	355
Modelling of bubble dynamics in slag during its hot stage engineering.....	365
Controlled coalescence with local front reconstruction method	373
 BUBBLY FLOWS	 381
Modelling of fluid dynamics, mass transfer and chemical reaction in bubbly flows	383
Stochastic DSMC model for large scale dense bubbly flows.....	391
On the surfacing mechanism of bubble plumes from subsea gas release.....	399
Bubble generated turbulence in two fluid simulation of bubbly flow	405
 HEAT TRANSFER	 413
CFD-simulation of boiling in a heated pipe including flow pattern transitions using a multi-field concept	415
The pear-shaped fate of an ice melting front	423
Flow dynamics studies for flexible operation of continuous casters (flow flex cc).....	431
An Euler-Euler model for gas-liquid flows in a coil wound heat exchanger.....	441
 NON-NEWTONIAN FLOWS.....	 449
Viscoelastic flow simulations in disordered porous media	451
Tire rubber extrudate swell simulation and verification with experiments	459
Front-tracking simulations of bubbles rising in non-Newtonian fluids.....	469
A 2D sediment bed morphodynamics model for turbulent, non-Newtonian, particle-loaded flows.....	479

METALLURGICAL APPLICATIONS.....	491
Experimental modelling of metallurgical processes	493
State of the art: macroscopic modelling approaches for the description of multiphysics phenomena within the electroslag remelting process	499
LES-VOF simulation of turbulent interfacial flow in the continuous casting mold	507
CFD-DEM modelling of blast furnace tapping	515
Multiphase flow modelling of furnace tapholes	521
Numerical predictions of the shape and size of the raceway zone in a blast furnace.....	531
Modelling and measurements in the aluminium industry - Where are the obstacles?	541
Modelling of chemical reactions in metallurgical processes.....	549
Using CFD analysis to optimise top submerged lance furnace geometries	555
Numerical analysis of the temperature distribution in a martensic stainless steel strip during hardening.....	565
Validation of a rapid slag viscosity measurement by CFD.....	575
Solidification modeling with user defined function in ANSYS Fluent.....	583
Cleaning of polycyclic aromatic hydrocarbons (PAH) obtained from ferroalloys plant.....	587
Granular flow described by fictitious fluids: a suitable methodology for process simulations	593
A multiscale numerical approach of the dripping slag in the coke bed zone of a pilot scale Si-Mn furnace.....	599
INDUSTRIAL APPLICATIONS	605
Use of CFD as a design tool for a phosphoric acid plant cooling pond	607
Numerical evaluation of co-firing solid recovered fuel with petroleum coke in a cement rotary kiln: Influence of fuel moisture	613
Experimental and CFD investigation of fractal distributor on a novel plate and frame ion-exchanger	621
COMBUSTION	631
CFD modeling of a commercial-size circle-draft biomass gasifier.....	633
Numerical study of coal particle gasification up to Reynolds numbers of 1000.....	641
Modelling combustion of pulverized coal and alternative carbon materials in the blast furnace raceway	647
Combustion chamber scaling for energy recovery from furnace process gas: waste to value	657
PACKED BED.....	665
Comparison of particle-resolved direct numerical simulation and 1D modelling of catalytic reactions in a packed bed	667
Numerical investigation of particle types influence on packed bed adsorber behaviour	675
CFD based study of dense medium drum separation processes	683
A multi-domain 1D particle-reactor model for packed bed reactor applications.....	689
SPECIES TRANSPORT & INTERFACES	699
Modelling and numerical simulation of surface active species transport - reaction in welding processes	701
Multiscale approach to fully resolved boundary layers using adaptive grids.....	709
Implementation, demonstration and validation of a user-defined wall function for direct precipitation fouling in Ansys Fluent.....	717

FREE SURFACE FLOW & WAVES	727
Unresolved CFD-DEM in environmental engineering: submarine slope stability and other applications.....	729
Influence of the upstream cylinder and wave breaking point on the breaking wave forces on the downstream cylinder	735
Recent developments for the computation of the necessary submergence of pump intakes with free surfaces	743
Parallel multiphase flow software for solving the Navier-Stokes equations	752
 PARTICLE METHODS	 759
A numerical approach to model aggregate restructuring in shear flow using DEM in Lattice-Boltzmann simulations	761
Adaptive coarse-graining for large-scale DEM simulations.....	773
Novel efficient hybrid-DEM collision integration scheme.....	779
Implementing the kinetic theory of granular flows into the Lagrangian dense discrete phase model.....	785
Importance of the different fluid forces on particle dispersion in fluid phase resonance mixers	791
Large scale modelling of bubble formation and growth in a supersaturated liquid.....	798
 FUNDAMENTAL FLUID DYNAMICS	 807
Flow past a yawed cylinder of finite length using a fictitious domain method	809
A numerical evaluation of the effect of the electro-magnetic force on bubble flow in aluminium smelting process.....	819
A DNS study of droplet spreading and penetration on a porous medium.....	825
From linear to nonlinear: Transient growth in confined magnetohydrodynamic flows.....	831

DEVELOPMENT OF GPU PARALLEL MULTIPHASE FLOW SOLVER FOR TURBULENT SLURRY FLOWS IN CYCLONE

Kumar MAYANK^{1*}, Raja BANERJEE^{2†}, Narasimha MANGADODDY^{1‡}

¹IIT Hyderabad Department of Chemical Engineering, 502285 Medak, India

²IIT Hyderabad Department of Mechanical Engineering, 502285 Medak, India

* E-mail: ch15resch02001@iith.ac.in

† E-mail: rajabanerjee@iith.ac.in

‡ E-mail: narasimha@iith.ac.in

ABSTRACT

The development of GPU parallelized unstructured multiphase solver and its application in predicting turbulent swirling flow of slurries inside cyclones is presented. Algebraic slip mixture model (ASM) is modified with additional shear lift forces and slurry rheology is corrected with fines fraction. The modified ASM model coupled with LES is used to predict particle classification inside hydrocyclone. During hydrocyclone operation the residence time of the fluid is very small and hence there is insufficient time for the larger eddies to cascade into smaller eddies. LES can accurately resolve flow structures that are few times the Kolmogorov scale at an increased computational cost due to finer mesh requirement. Therefore, the solver has been parallelized using general purpose graphics processing units (GPGPUs). In the current solver, the Pressure Poisson equation has been parallelized with an algebraic multigrid solver on GPU architecture using CUDA programming language for unstructured grids. The single phase flow field predicted by LES shows good agreement with experimental results obtained from open literature. The turbulent flow fields, the size segregation and the particle efficiency curve obtained from multiphase simulations are presented. Additionally, computational speedup due to GPU parallelization is reported over its serial version of the solver.

Keywords: CFD, hydrodynamics, LES, GPU, ASM .

NOMENCLATURE

A complete list of symbols used, with dimensions, is required.

NOMENCLATURE

Greek Symbols

ρ_m Mixture density, [kg/m^3]
 μ_c viscosity of the continuous phase, [kg/ms].
 μ_m viscosity of the mixture, [kg/ms].
 α_k Volume fraction of phase.
 α_p Total particle volume fraction.
 α_{pm} Maximum packing fraction.
 ω_{mj} Vorticity vectors.
 ε_{ijk} Kronecker delta.

Other Symbols

p Pressure, [Pa].
 \mathbf{u}_m Mixture velocity, [m/s].

\mathbf{u}_{cp} Slip velocity for phase p, [m/s].
 d_p diameter of the particle, [m].
 Re_p Reynolds number of the particle.
 C_{lp} lift coefficient.
 S_f Face area vector.
 F_f mass flux through face f.

Sub/superscripts

i, j Spatial coordinate index .
 k Phase Index.
 f Face Index .

INTRODUCTION

The use of computational fluid dynamics(CFD) for design exploration has been prevalent for the past couple of decades. Most of these studies have relied on RANS based approach to model the entire range of turbulence length scales in the flow. Though computationally efficient RANS based approach fail to account for the dynamic interactions between the large and small scales of motion, and has been observed to have limited predictive capabilities for decay of isotropic turbulence even in simpler configurations(Pope, 2004). With the availability of increased computational power recently, LES and DNS have been used extensively to model turbulence in complex flow configuration. While, DNS typically resolves all turbulence length scales down to the smallest Kolmogorov scale. LES uses a spatial filter to separate the larger scale motions from the smaller scales. The larger scales of motion are anisotropic and LES resolves all the scales above the specified cutoff length. While using a sub-grid scale model (Germano *et al.*, 1991; Lilly, 1992) to incorporate the effects of the small scale motions on the resolved scales. This feature makes LES much less computationally extensive as compared to DNS where even the universally isotropic smaller scales(Leonard, 1975) are resolved, requiring mesh resolution in the order of $Re^{9/4}$ for DNS computations. LES has been reported to have good turbulence predictive capabilities for channel flow (Deardorff, 1970; Moin and Kim, 1982), recirculating flows (Kobayashi, 1992) as well as in complex flow configuration such as in gas turbine combustion (Moin and Apte, 2006). LES has been used to simulate highly strained flows in complex geometries was first performed by (Slack *et al.*, 2000) and since has been used to predict flow dynamics inside hydrocyclones(Brennan, 2006) as well as predicting the cut size(Narasimha *et al.*, 2006).

The comparatively high mesh requirement for LES as compared to RANS based models is the major drawback that limits the scope of LES simulations for design exploration at realistic industrial configurations. Using general purpose GPU for parallelizing linear equation solvers was explored by (Sanders and Kandrot, 2010) and further development for method of parallelisation for unstructured and hybrid mesh solvers was presented in (Xu *et al.*, 2014) and for two phase flow problems in (Reddy and Banerjee, 2015). The massive parallel compute capability of the GPU allows conducting high fidelity LES simulations for industrial configurations computationally feasible.

The work presented in this study explains the development of a high fidelity LES multiphase solver using the algebraic slip model to study flow of poly dispersed slurry system. The solver was parallelized by porting the pressure poisson equation solver on the GPU. The single phase LES solver is validated against LDA measurements for cyclone flows reported in open literature. The multiphase code is tested for particle segregation inside a hydrocyclone. The cut point predicted by the multiphase code was found to be agreeable with the simulation results presented in literature. Finally the speed up obtained for parallel implementation over serial version is reported in the final section.

MODEL DESCRIPTION

The slurries consists of mixture of poly dispersed solid particles within a continuous phase mostly water. The governing equation for multiphase fluid flow following (Ishii 1975) notations is given by

Continuity equation

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m u_{mi}}{\partial x_i} = 0 \quad (1)$$

Momentum Equation

$$\frac{\partial \rho_m u_{mi}}{\partial t} + \frac{\partial \rho_m u_{mi} u_{mj}}{\partial x_j} = \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} (\tau_{\mu,ij} + \tau_{D,ij}) + \rho_m g_i \quad (2)$$

where the density and the velocity of the mixture is given by farve-averaged quantities explained in (Soo 1990).

$$\rho_m = \sum_{k=1}^n \alpha_k \rho_k \quad (3)$$

$$u_m = \frac{1}{\rho_m} \sum_{k=1}^n \alpha_k \rho_k u_k \quad (4)$$

Each dispersed phase is tracked using a scalar transport equation of the form

$$\frac{\partial}{\partial t} \alpha_k + \nabla \cdot (\alpha_k u_m) = -\nabla \cdot (\alpha_k u_{Mk}) \quad (5)$$

The viscous diffusive flux for the mixture ($\tau_{\mu,ij}$) is calculated using model by (Ishii-Mishima 1980) as

$$\mu_m = \mu_c \left(1 - \frac{\alpha_p}{\alpha_{pm}}\right)^{-2.5 \alpha_{pm}} \quad (6)$$

The extra term in the Eq. 2, ($\tau_{D,ij}$) is the diffusion flux arising due to phase slip and is given by

$$\tau_{D,ij} = - \sum_{k=1}^n \alpha_k \rho_k u_{mk} u_{mk} \quad (7)$$

The phase diffusion velocity u_{Mk} , is represented in terms of individual phase slip velocity as

$$u_{mp} = u_{cp} - \sum_{k=1}^n \alpha_k u_{ck} \quad (8)$$

The individual phase slip velocity using force balance on the particles experiencing drag was derived by (Manninen and Taivassalo, 1996) and extended to include the effects of lift forces by (Narasimha *et al.*, 2007) and is given by

$$u_{cpi} = \frac{d_p^2 (\rho_k - \rho_m)}{18 f_{Rep} \mu_c} \left(g_i - \frac{\partial}{\partial t} u_{mi} - u_{mj} \frac{\partial}{\partial x_j} u_{mi} + 0.75 \frac{\rho_c}{\rho_k - \rho_m} C_{lp} \epsilon_{ijk} \omega_{mj} u_{pck} \right) \quad (9)$$

Where the term f_{Rep} is given by

$$f_{Rep} = (1 + 0.15 Re_p^{0.687}) \alpha_p^{-4.65}$$

$$Re_p = \frac{d_p \rho_c |u_{cp}|}{\mu_m}$$

Numerical Implementation

The solver presented is capable of handling unstructured grid in CGNS format. Unstructured grids are preferred for industrial applications as the complex equipment geometry can be represented much easier as compared to structured grid arrangement. The implementation of numerical schemes for unstructured grids are complicated though, with increased and random inter-dependence of grid point variables. The geometric and neighbor data information of each cell is stored before the start of the solution. A collocated grid arrangement (Date, 2005) is used wherein all the solution variables are stored at the cell centers. Finite volume method is used to discretize the governing equation on the grid. A first order explicit scheme was used for the temporal term. A combination of first order and central difference scheme with the deferred correlation approach (Khosla and Rubin, 1974) was used to approximate the convective fluxes. Volumetric interpolation was used to calculate the face center values from the stored cell center variables. The diffusive fluxes and other terms are approximated in a similar method as followed by (Dalal *et al.*, 2008). The pressure correction method (Davidson, 1996) was used for the pressure velocity decoupling. The diffusive flux due to phase slip is implemented as a volumetric source term. The starting point of the solver is to initialize the grid points, initial and boundary conditions. In case of a velocity inlet both the primary phase and the secondary phase velocity as well as volume fraction for each secondary phases are specified. The solver then proceeds to calculate the density and mixture velocities at each boundary using eq. 3 and 4. These calculated mixture properties act as the actual boundary values for the solution. The mass flux for the mixture is calculated with the divergent field velocity obtained by solving the discrete form of eq. 2 without the pressure term. Then we solve the pressure poisson equation using the calculated mass flux value which is of the form.

$$\sum_f (\nabla p_f^{n+1}) \cdot S_f = \frac{\rho}{\Delta t} \sum_f F_f^* \quad (10)$$

Finally the mass flux is corrected by subtracting the pressure gradient term from the initially calculated mass flux and the divergent free velocity is obtained for the new time step. The discrete form of the phase tracking eq. 5 is then solved and

density and viscosity values are updated using eq. 6. Slip velocity is calculated with the difference between the primary and secondary phase velocities as initial guess. We calculate the term f_{Rep} which is used to calculate the individual slip velocity using eq. 9 iteratively as long as the final value reaches the desired convergence criterion. The slip velocities are used to calculate the phase diffusion velocity using eq. 8. Finally the diffusion flux due to phase slip is calculated using eq. 7, gradient of which is stored as the source term for the next time step. The gradient of the volume flux of the scalar is stored to be as the source term for the scalar transport equation for the next time step. The algorithm of the solver is explained below

Initialization:

Initialize grid points, initial and boundary condition;

Calculate mixture velocity and density boundary values;

Solution:

while $T < Final\ Time$ **do**

Calculate mass velocity (u^*) and the mass flux for each face(F^*);
Solve pressure poisson equation using the mass flux(F^*);
Correct velocities (u^{n+1}) and flux(F^{n+1}) value using pressure correction;
Solve the phase tracking equations;
Update density and viscosity Calculate the slip velocities for each phase;
Calculate the source terms for the momentum and phase tracking equation for the next time step;

end

Algorithm 1: Algorithm of the solver

GPU PARALLELIZATION

A standard V-cycle algebraic multigrid (AMG) implementation was used for solving the pressure poisson equation. The equation is of the form $Au = f$ with the coefficient matrix(A) being a symmetric matrix with six dominant diagonals. Instead of working on one mesh AMG uses a hierarchy of mesh, which starts from the finest mesh and uses the coarsening algorithm suggested by (Haase *et al.*, 2010) to construct levels of coarser mesh. For each level the coefficient matrix(A_c), the prolongation matrix(P) and the restriction matrix(P^T) are populated. For a two level multigrid system which can be extended to multilevel system the algorithm can be summarized as

- Compute estimate u^* for u in $Au = f$;
- Compute the residual $r = f - Au^* = Ae$;
- Solve for e_c in the coarser system $A_c e_c = P^T r$;
- Correct $u^* \leftarrow u^* + Pe_c$.

CUDA programming module was used to implement the AMG solver on the GPU. The implementation is rather difficult for unstructured meshes as the interdependencies between the nodes are not in an ordered arrangement. The interdependencies of the nodes though irregular, remains constant for non deforming grids. Therefore, the neighbor element data is stored at the start of the solution. Greedy coloring scheme (Hege and Stuben, 1991) was used to identify set of independent nodes. Each independent set of nodes are

assigned a color class. The total number of color class was referred to as maximum degree. Which for tetrahedral element meshes comes out to be six independent sets. The nodes are updated in order of color class. Updating all the independent set of nodes simultaneously helps preventing any unrealistic solutions due to data race condition. The nodes are ordered in such a way that inter dependent nodes can be co located resulting in a coalesced memory access pattern thereby reducing the time required for the data transfer operations. Gauss Seidel method is used for the smoothening operation. In CUDA terminology, the CPU is referred to as the host and the GPU is referred to as the device. The device function is called a kernel and is identified by `__global__` identifier. The kernel is called, and the number of threads to be launched is specified from the host code. The number of threads to be launched is specified in terms of grids and blocks. For the current implementation we use grid size equal to the maximum degree and the block size is equal to the maximum number of cells within a color class. We use V-cycle multigrid, which is made up of a down cycle and up cycle. Down cycle is a sequence of smoothing and restriction operations performed alternately starting from finest grid till we reach coarsest grid. Up cycle is a combination of prolongation and smoothing operations performed alternately starting with the coarsest grid till we reach finest grid. The multigrid V-cycle is repeated till the desired convergence is reached. The algorithm for the parallelization code for the solution of the equation of the form $Ax = B$ is given in algorithm 2.

RESULTS

The parallel solver was tested for two cases. First is the single phase LES prediction for flow in industrial flow configuration within a gas cyclone. Second being the multiphase flow prediction of phase segregation under turbulent slurry flow conditions. The simulation setup and results are presented in the subsections below

Validation of LES solver

The single phase LES solver is tested for the flow configuration similar to the one presented in (Slack *et al.*, 2000). The dimensions of the geometry and the mesh used is given in the figure 1. Air with density 1.225 kg/m^3 and viscosity $1.78943 \times 10^{-5}\text{ kg.m}^{-1}\text{s}^{-1}$ was used to define the fluid properties. For the cyclone volume of 0.0203 m^3 around 6.5×10^5 hexahedral cells were used to discretize the flow domain. The inlet, overflow and the underflow are the boundary patches composed of quadrilateral cells. The inlet air flow rate was maintained at 0.08 kg/m^3 , the residence time at this flow rate was 0.25 s. The pressure at the overflow was specified as gauge pressure and the velocity was specified homogeneous neumann boundary condition, whereas the underflow was specified wall boundary condition. The time step size was 1×10^{-5} s. The mean velocity magnitude, axial velocity and tangential velocity profile along the central plane is given in figure 2. Velocity magnitude profile shows an increase in the magnitude as we proceed from the walls to the central axis, while the central core is the region of lowest magnitude. Typically fluid stream upon entering the cyclone moves along the outer wall while descending down, then accelerating due to the constriction of the area and reaches the bottom wall where the flow reversal happens and the stream moves towards the exit overflow. Vortex formation can be observed due to low dynamic pressure in the

Host Code:

Populate Coefficient matrix(A), Initial Guess pressure matrix(x) and RHS matrix(b) ;

Create levels of multigrid ;

for $i = 0; i < \text{number of levels} : i++$ **do**

 Calculate $A_p[i], P[i]$ and $P^T[i]$;

 Color the nodes using procedure explained by (Hege and Stuben, 1991);

 Rearrange the node for interdependent nodes to be collocated;

 Transfer data from the host to the device;

end

Device Code:

while $\text{residual} \geq \text{convergence criterion}$ **do**

for $\text{Numlevel} = 1; \text{Numlevel} < \text{MaxNumlevel};$

$\text{Numlevel}++$ **do**

 Calculate the residual for the finer mesh ($\text{NumLevel} - 1$) level using kernel `calculateResiduals()` ;

 Update the residual at the coarse level(NumLevel) using kernel `updateResiduals()`;

for $\text{ClrId} = 0; \text{ClrId} < \text{MaxDegree} - 1; \text{ClrId}++$ **do**

 Smooth the error on the coarse mesh level(NumLevel) for color class ClrId using `gaussSiedeliteration()` kernel;

end

end

for $\text{Numlevel} = \text{MaxNumlevel} - 2; \text{Numlevel} > 0;$

$\text{Numlevel} -$ **do**

 Update the pressure of the coarse mesh level($\text{Numlevel} + 1$) `updatepressure()` kernel;

for $\text{ClrId} = 0; \text{ClrId} < \text{MaxDegree} - 1; \text{ClrId}++$ **do**

 Smooth the error on the coarse mesh level(Numlevel) for the color class ClrId using `gaussSiedeliteration()` kernel;

end

end

for $\text{ClrId} = 0; \text{ClrId} < \text{MaxDegree} - 1; \text{ClrId}++$ **do**

 Smooth the error on the finest mesh level(0) using `gaussSiedeliteration()` kernel;

end

 Calculate the residuals for the finest mesh level(0);

end

Algorithm 2: Parallelization of standard V cycle algebraic multigrid solver

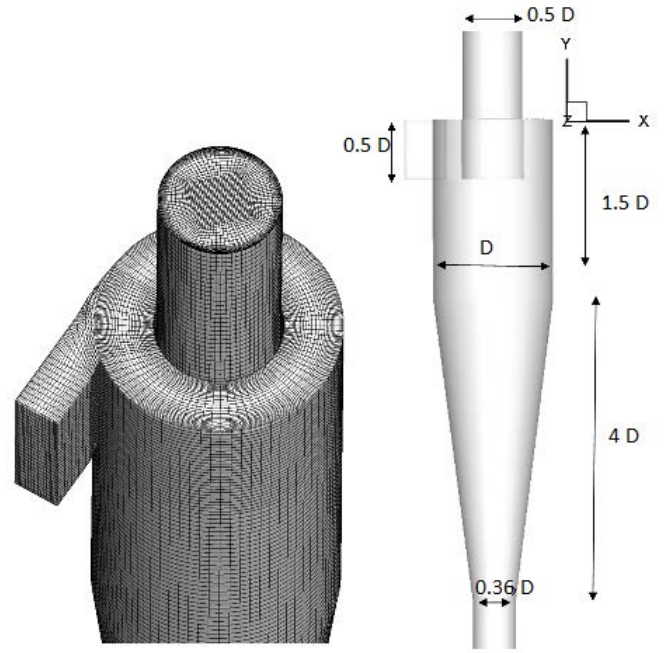


Figure 1: Geometry specifications and unstructured mesh of the stairmand cyclone(Slack *et al.*, 2000)

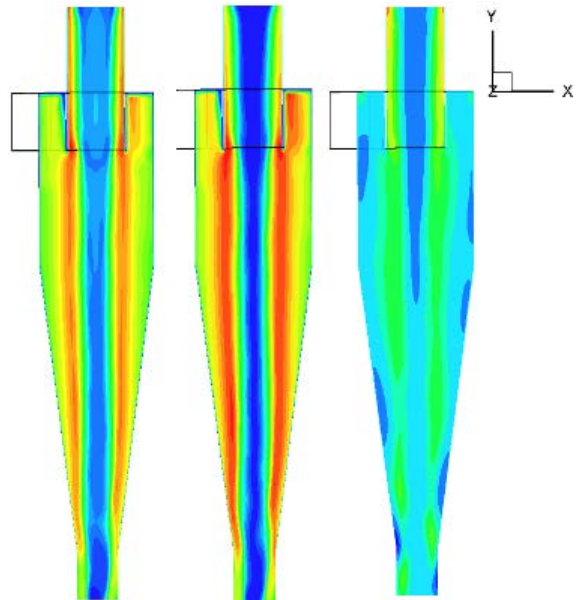


Figure 2: Contours of Left:Mean velocity magnitude(red is 40 m/s or higher and blue is 1 m/s or lower), Center: Mean tangential velocity (red is 36 m/s or higher and blue is 1m/s or lower) Right: Mean axial velocity (red is 20m/s or higher and blue is -10 m/s or lower)

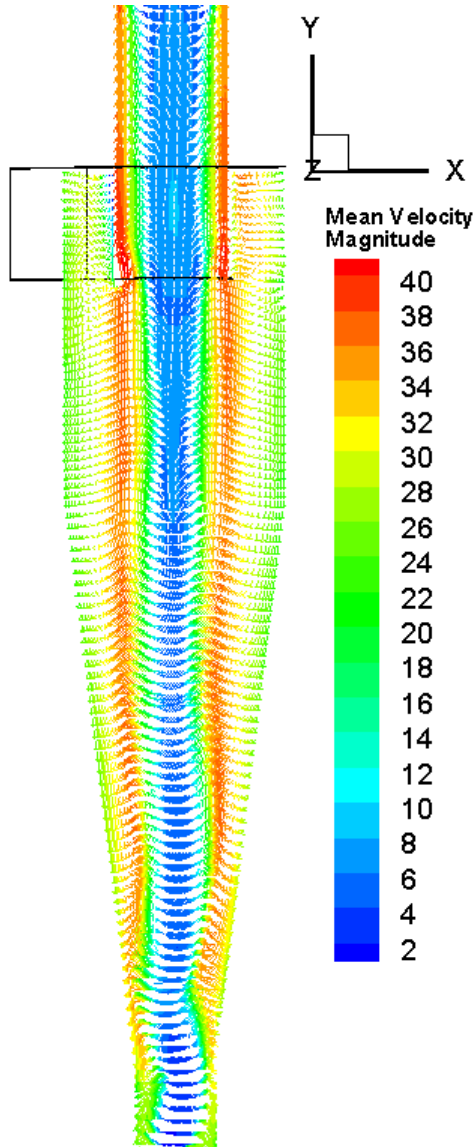


Figure 3: Velocity vectors for cyclone flow at feed air flow rate of 0.0203m^3 colored by velocity magnitude

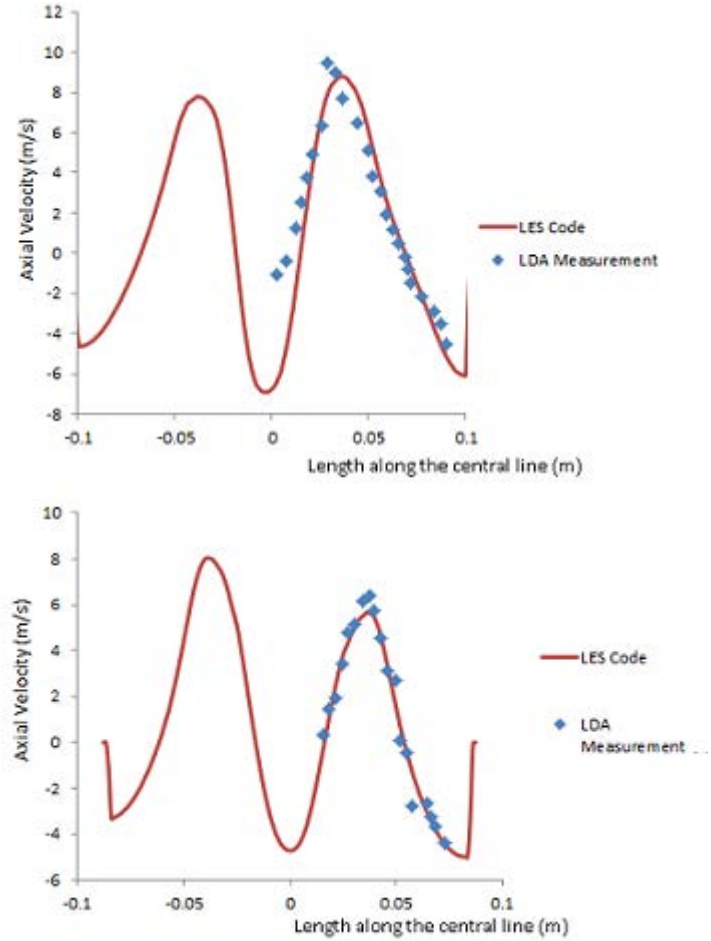


Figure 4: Comparison of axial velocity with LDA measurements from (Slack *et al.*, 2000) at left:0.38 m from top of the overflow and right: 0.59m from the top of the overflow

central core regions for such highly strained flows. The axial velocity profile show flow reversals near the central core region. Where the central core has downward flow towards the underflow while the region outside the central core has predominantly upward flow except near the walls where the flow is downwards towards the underflow. Similarly the tangential velocity also shows an increase in magnitude as we proceed from the walls towards the center reaching a maximum at a region where flow reversal start to take place and the tangential component reduces to a minimum value close to zero near the center. The comparison of the mean axial velocity and tangential velocity along the center line with the LDA measurements reported in (Slack *et al.*, 2000) for two different axial location are given in figure 4 and 5 respectively. Good quantitative comparison for the two velocity components at stations located at 0.38 m from the top and at 0.59 m from the top can be observed between the LES simulated value and the experimental results.

Phase segregation in a hydrocyclone

The multiphase code is tested for a poly dispersed slurry flow problem and study the phase segregation within the cyclone. As the algebraic slip mixture multiphase solver has not been successfully tested for higher density ratio, air core free design from (Vakamalla *et al.*, 2017) having a rod along the central core is chosen for the study. The geometry and the unstructured grid containing around 5×10^5 hexahedral cells is shown in figure 6.

Water with density 998.1 kg/m^3 and viscosity 0.00103 kg .

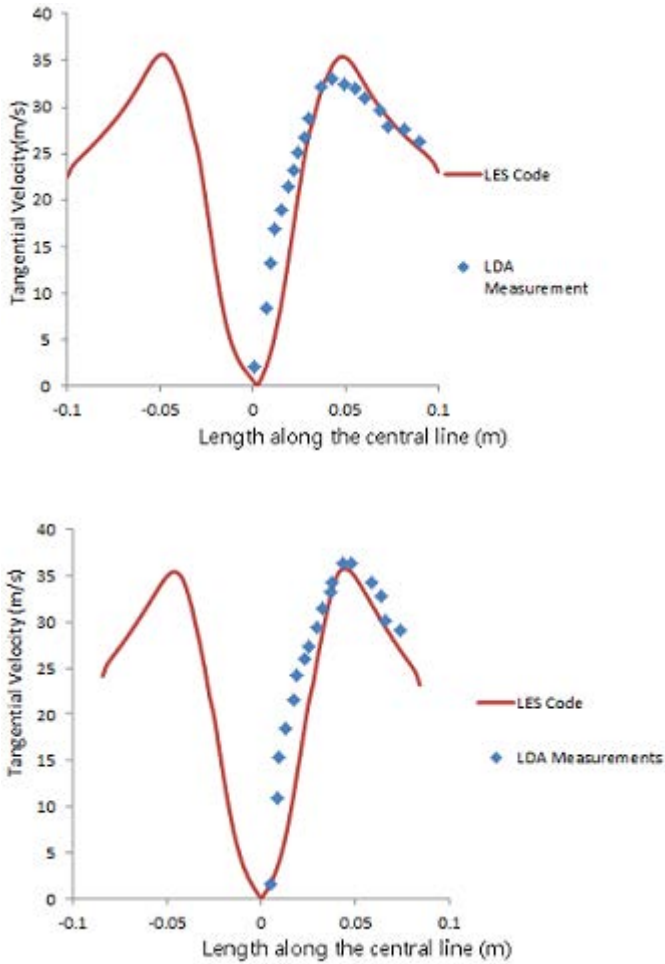


Figure 5: Comparison of tangential velocity with LDA measurements from (Slack *et al.*, 2000) at left: 0.38 m from top of the overflow and right: 0.59m from the top of the overflow

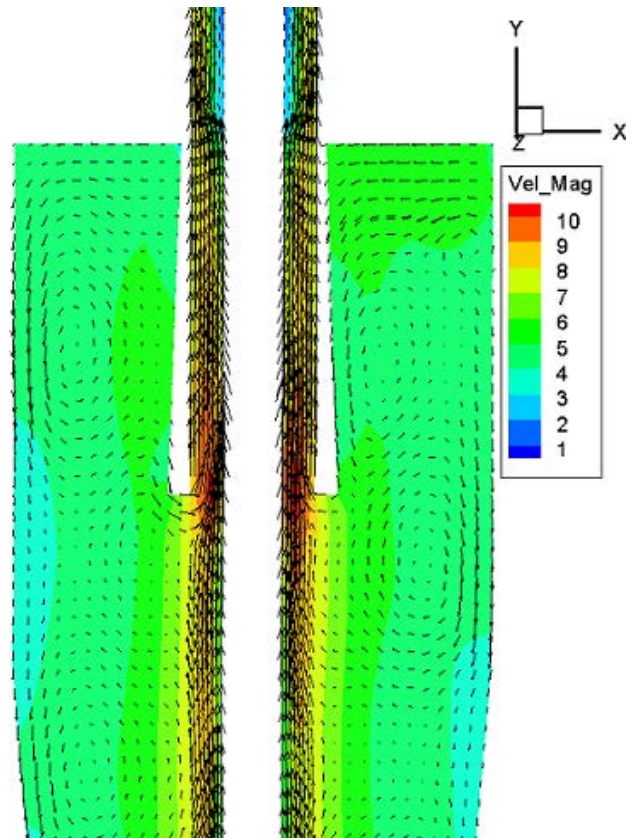


Figure 7: Vector plot for the slurry flow

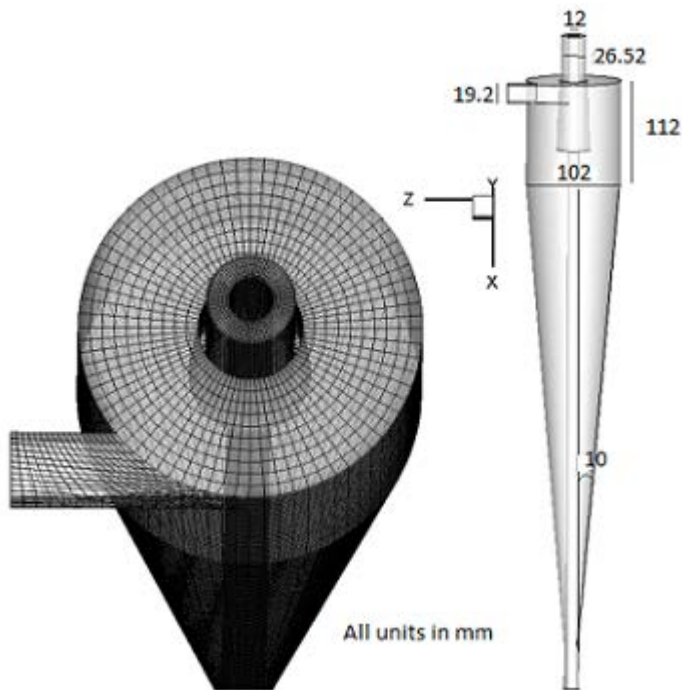


Figure 6: Geometry specifications and unstructured mesh prepared for the cyclone similar to (Vakamalla *et al.*, 2017)



Figure 8: Iso surface for contour level 0.005 volume fraction for phases left to right: phase 6 to phase 1



Figure 9: Iso surface for contour level 0.01 volume fraction for phases left to right: phase 6 to phase 1

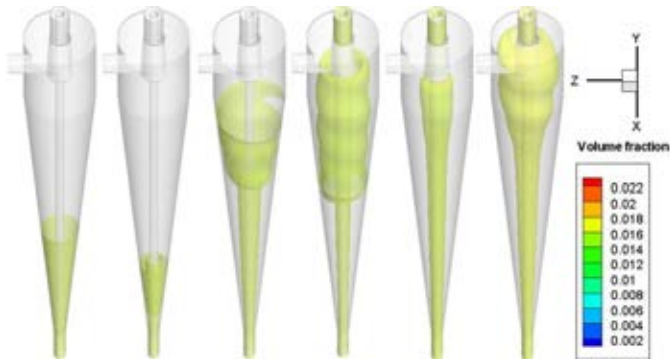


Figure 10: Iso surface for contour level 0.015 volume fraction for phases left to right: phase 6 to phase 1

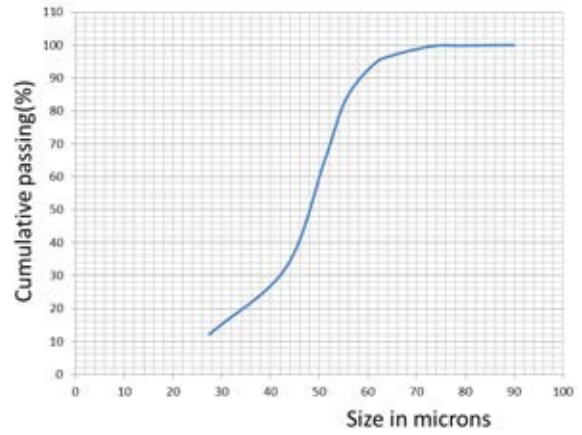


Figure 12: Particle classification curve for the air core free hydro-cyclone design for water flow rate of 1.665 kg/m^3

$\text{m}^{-1} \text{s}^{-1}$ is used as the continuous phase fluid. Varying sizes of silica powder with density 2650 kg/m^3 was used to specify the different secondary phases properties. The different phase size and volume fraction at the inlet is given in the table 1. Inlet flow rate of water was maintained at 1.664

Table 1: Phase size and distribution.

Phase	Diameter ($\mu \text{ m}$)	Feed Volume fraction
Phase 1	3.35	0.0174
Phase 2	10.25	0.0124
Phase 3	19.37	0.01158
Phase 4	28.27	0.00509
Phase 5	38	0.01329
Phase 6	68	0.00252

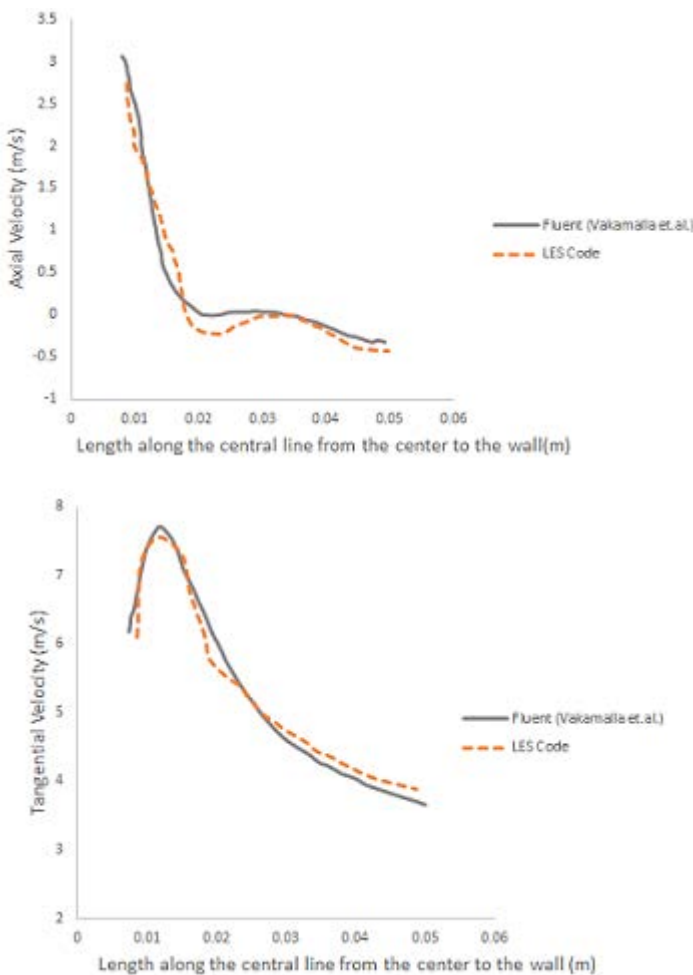


Figure 11: Comparison of left: Axial velocity and right: Tangential velocity at the mid plane along the line at the intersection of the conical and cylindrical sections

kg/s . Both the overflow and the underflow are specified gauge pressure values and the velocities and phase fractions were specified homogeneous neumann boundary conditions. The central rod was specified with no slip wall boundary condition. The secondary phase was introduced after the steady state velocity profile for the single phase water flow is obtained. The velocity magnitude profile at the mid plane for the single phase flow and the comparison of results with the fluent simulation performed in the study(Vakamalla *et al.*, 2017) is presented in the figure 11. The slurry flow patterns can be visualized using the vector plots given in figure 7 along the mid plane parallel to the inlet flow direction. Plots show the central region of positive axial velocity towards the overflow while minor circulations near in the central region. The phase segregation is studied using the iso contour for three different concentration. The low concentration contour at volume fraction value 0.005 is given in figure 8. The contour show that the smallest size fraction is more evenly distributed with very small regions near the overflow having smaller concentration. The regions of low concentration for the larger phases changes from the central rod region to regions near the wall as the size increases. The medium and high concentration iso contour at level 0.01 and 0.015 are given in figure 9,10 respectively. The smallest phase medium concentration regions are still the central core region while similar trend of segregation towards the walls for larger sizes can be observed. The largest phase fraction is located mainly near the walls and the underflow. The high concentration iso contour plots show the evenly distributed

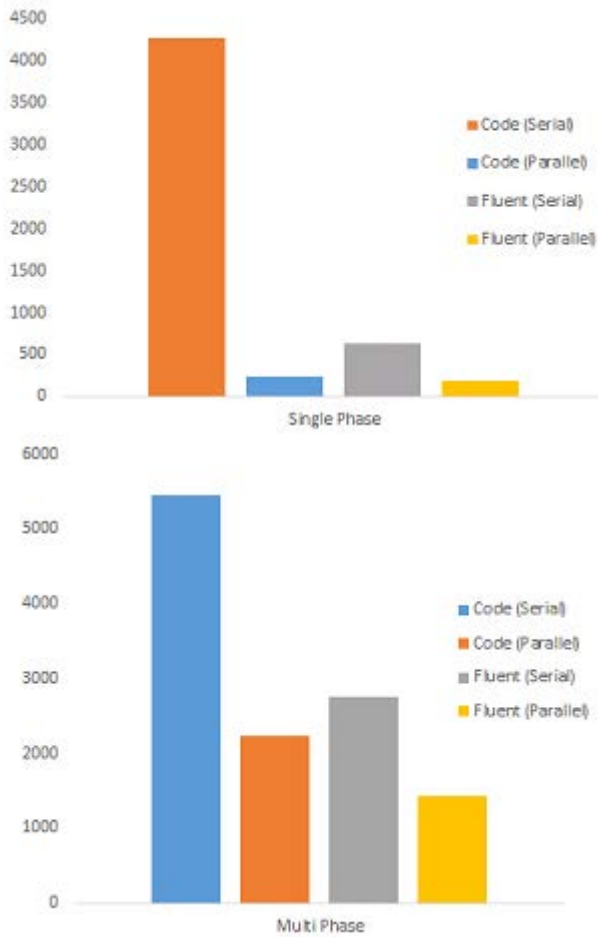


Figure 13: Comparison of time required in seconds for 100 timesteps of simulation

smallest size fraction. The cut-point for the said design was calculated using the particle efficiency curve given in figure 12, which comes out to be $48.1 \mu\text{m}$

Speed up obtained

The comparison of time required for the completion of 100 time steps of transient simulations due to the parallel GPU implementation with the serial implementation of the code along with the serial and parallel versions of commercial code Fluent is given in figure 13. The single phase parallel implementation reported speed up of around 11.3X over the serial code implementation. Compared to the serial version of fluent the speed up obtained is around 2.75 X. The code performs slower as compared to the parallel version of fluent using 4 cores where a speed up of 1.6X is recorded for fluent parallel implementation over the parallel code. While for the multiphase implementation a speed up of 2.3X is obtained for the parallel implementation of the code over the serial one. Whereas, the speed up obtained over fluent serial implementation is 1.25X. The multiphase parallel implementation also performs slower as compared to the parallel implementation of fluent. Where the parallel fluent solver is reported to be 1.9 X faster than the parallel code implementation. This slower operation of the multiphase code as compared to the single phase solver is due to the amount of time expended on solving the phase tracking equations which is done on the CPU. The parallelisation of the solver for the phase tracking equation and the validation of the multiphase solver is the scope of the future work.

CONCLUSION

The development of an unstructured LES multiphase solver was presented for simulating highly strained slurry flows. Algebraic slip model was used to model the poly-dispersed slurry system. Where local velocity fields cause phase segregation due to varying inter phase momentum exchange due to drag and lift based on size of the particle. The solver is tested for single phase cyclone flows and validated against LDA measurements provided in (Slack *et al.*, 2000). The multiphase implementation was tested for particle classification with hydrocyclone geometry suggested in (Vakamalla *et al.*, 2017). The velocity profiles and the cut point obtained from the predicted particle separation curve was similar to the one obtained using the same design in the reference. Implementation of GPU parallelization for the compute intensive LES methodology is presented and the speed up obtained for the parallel implementation is reported. The parallel solver makes it computationally feasible to conduct design explorations even at industrial configuration.

REFERENCES

- BRENNAN, M.S. (2006). "CFD Simulations of Hydrocyclones with an Air Core: Comparison Between Large Eddy Simulations and a Second Moment Closure". *Chemical Engineering Research and Design*, **84**(6), 495–505.
- DALAL, A., ESWARAN, V. and BISWAS, G. (2008). "A Finite-Volume Method for Navier-Stokes Equations on Unstructured Meshes". *Numerical Heat Transfer, Part B: Fundamentals*, **54**(3), 238–259.
- DATE, A.W. (2005). "Solution of transport equations on unstructured meshes with cell-centered colocated variables. Part I: Discretization". *International Journal of Heat and Mass Transfer*, **48**, 1117–1127.
- DAVIDSON, L. (1996). "A Pressure Correction Method for Unstructured Meshes with Arbitrary Control Volumes". *International Journal for Numerical Methods in Fluids*, **22**, 265–281. URL [http://doi.wiley.com/10.1002/\(SICI\)1097-0363\(19960229\)22:4{ }3C265::AID-FLD359{ }3E3.0.CO;2-J](http://doi.wiley.com/10.1002/(SICI)1097-0363(19960229)22:4{ }3C265::AID-FLD359{ }3E3.0.CO;2-J).
- DEARDORFF, J.W. (1970). "A numerical study of three-dimensional turbulent channel flow at large Reynolds numbers". *Journal of Fluid Mechanics*, **41**(1970), 453. URL <http://www.journals.cambridge.org/abstract{ }S0022112070000691>.
- GERMANO, M., PIOMELLI, U., MOIN, P. and CABOT, W.H. (1991). "A dynamic subgrid-scale eddy viscosity model". *Phys. Fluids A Fluid Dyn.*, **3**(7), 1760. URL <http://scitation.aip.org/content/aip/journal/pofa/3/7/10.1063/1.857955>.
- HAASE, G., LIEBMANN, M., DOUGLAS, C.C. and PLANK, G. (2010). "A parallel algebraic multigrid solver on graphics processing units". *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*, **5938 LNCS**, 38–47.
- HEGE, H.C. and STUBEN, H. (1991). "Vectorization and parallelization of irregular problems via graph colouring". *Proceedings of the 5th International Conference on Supercomputing*, 47–56.
- KHOSLA, P.K. and RUBIN, S.G. (1974). "A diagonally dominant second-order accurate implicit scheme". *Computers and Fluids*, **2**(2), 207–209.
- KOBAYASHI, T. (1992). "Large eddy simulation of backward-facing step flow". *Communications in applied numerical methods*, **8**(October 1991), 431–441.
- LEONARD, A. (1975). "Energy Cascade in Large-Eddy Simulations of Turbulent Fluid Flows". *Turbulent Diffusion in Environmental Pollution Proceedings of a Symposium held at Charlottesville, Volume 18*, 237–248. URL <http://www.sciencedirect.com/science/article/pii/S0065268708604641>.
- LILLY, D.K. (1992). "A proposed modification of the Germano subgrid-scale closure method". *Physics of Fluids A: Fluid Dynamics*, **4**(3), 633.
- MANNINEN, M. and TAIVASSALO, V. (1996). "On the mixture model for multiphase flow".
- MOIN, P. and APTE, V. (2006). "Large-Eddy Simulation of Realistic Gas Turbine Combustors". *AIAA Journal*, **44**(4), 698–708.
- MOIN, P. and KIM, J. (1982). "Numerical investigation of turbulent channel flow". *Journal of Fluid Mechanics*, **118**, 341–377.
- NARASIMHA, M., BRENNAN, M. and HOLTHAM, P. (2006). "Large eddy simulation of hydrocyclone prediction of air-core diameter and shape". *International Journal of Mineral Processing*, **80**(1), 1–14. URL <http://linkinghub.elsevier.com/retrieve/pii/S0301751606000032>.
- NARASIMHA, M., BRENNAN, M., HOLTHAM, P. and NAPIER-MUNN, T. (2007). "A comprehensive CFD model of dense medium cyclone performance". *Minerals Engineering*, **20**(4), 414–426. URL <http://www.sciencedirect.com/science/article/pii/S0892687506002494>.
- POPE, S.B. (2004). "Ten questions concerning the large-eddy simulation". *New Journal of Physics*, **6**(1), 35.
- REDDY, R. and BANERJEE, R. (2015). "Computers & Fluids GPU accelerated VOF based multiphase flow solver and its application to sprays". *COMPUTERS AND FLUIDS*, **117**, 287–303. URL <http://dx.doi.org/10.1016/j.compfluid.2015.05.013>.
- SANDERS, J. and KANDROT, E. (2010). *CUDA by Example*, vol. 54. arXiv:1011.1669v3, URL <http://wwwzb.fz-juelich.de/contentenrichment/inhaltsverzeichnisse/2010/9780131387683.pdf>.
- SLACK, M., PRASAD, R., BAKKER, A. and BOSYAN, F. (2000). "Advances in cyclone modelling using unstructured grids". *Chemical Engineering Research and Design*, **78**(November), 1098–1104.
- VAKAMALLA, T.R., KORUPROLU, V.B.R., ARUGONDA, R. and MANGADODDY, N. (2017). "Development of novel hydrocyclone designs for improved fines classification using multiphase CFD model". *Separation and Purification Technology*, **175**, 481–497.
- XU, C., DENG, X., ZHANG, L., FANG, J., WANG, G., JIANG, Y., CAO, W., CHE, Y., WANG, Y., WANG, Z., LIU, W. and CHENG, X. (2014). "Collaborating CPU and GPU for large-scale high-order CFD simulations with complex grids on the TianHe-1A supercomputer". *Journal of Computational Physics*, **278**, 275–297. URL <http://www.sciencedirect.com/science/article/pii/S0021999114005786>.