# Simulations of Flow and Transport: Modeling, Algorithms and Computation


Shuyu Sun[1[0000-0002-3078-864X]], Jiangguo Liu[2[0000-0002-2188-5157]] and Jingfa Li[1,3[0000-0002-5207-1156]]

[1] Computational Transport Phenomena Laboratory, Division of Physical Science and Engineering, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia
[2] Department of Mathematics, Colorado State University, Fort Collins, CO 80523-1874, USA
[3] School of Mechanical Engineering, Beijing Institute of Petrochemical Technology, Beijing 102617, China
shuyu.sun@kaust.edu.sa



**Abstract.** We first briefly discuss the significance of flow and transport simulation that motivates the international workshop on "Simulations of Flow and Transport: Modeling, Algorithms and Computation" within the International Conference on Computational Science. We then review various works published in the proceedings of our workshop in 2018. Based on the works presented in this workshop in recent years, we also offer our observations on the general trends of the research activities in flow and transport simulations. We discuss existing challenges, emerging techniques, and major progress.



**Keywords:** Algorithms, Flow and transport, Modeling, Numerical simulations


## 1 Introduction

Most processes in natural and engineered systems inherently involve flow and transport. Thus simulations of flow and transport are extremely important for a wide range of scientific and industrial applications at various spatial and temporal scales. In this year's international workshop on "Simulations of Flow and Transport: Modeling, Algorithms and Computation" (SOFTMAC) within International Conference on Computational Science (ICCS), we focus on the recent advances in mathematical modeling, numerical algorithms, scientific computation, and other computational aspects of flow and transport phenomena. We have received 26 active submissions from China, Japan, Russia, Saudi Arabia, Singapore, and United States of America. After a strict peer review process, a total of 19 papers in this SOFTMAC workshop have been accepted for publication in the Proceeding of ICCS 2018.

It is worth noting that the SOFTMAC workshop has been held within the ICCS for seven years since 2011. A brief overview of our workshop is presented in Table 1. As one of the important sessions within ICCS, it has successfully attracted attention from worldwide researchers and scientists in the field of flow and transport. The workshop provides a great platform for bringing together scholars in this field annually to report their research progresses in both theory and methods, to exchange new ideas for research, and to promote further collaborations.

**Table 1.** Overview of our international workshop within the ICCS

| NO. | Our Workshop | ICCS Theme | Time and Location |
|---|---|---|---|
| 1 | Flow and Transport: Computational Challenges | The Ascent of Computational Excellence | Nanyang Technological University, Singapore, 1-3 June, 2011 |
| 2 | Flow and Transport: Modeling, Simulations and Algorithms | Empowering Science through Computing | Omaha, Nebraska, USA, 4-6 June, 2012 |
| 3 | Flow and Transport: Modeling, Simulations and Algorithms | Computation at the Frontiers of Science | Barcelona, Spain, 5- 7 June, 2013 |
| 4 | Computational Flow and Transport: Modeling, Simulations and Algorithms | Computational Science at the Gates of Nature | Reykjavík, Iceland, 1-3 June, 2015 |
| 5 | Computational Flow and Transport: Modeling, Simulations and Algorithms | Data through the Computational Lens | San Diego, California, USA, 6-8 June, 2016 |
| 6 | Simulations of Flow and Transport: Modeling, Algorithms and Computation | The Art of Computational Science. Bridging Gaps – Forming Alloys | Zürich, Switzerland, 12-14 June, 2017 |
| 7 | Simulations of Flow and Transport: Modeling, Algorithms and Computation | Science at the Intersection of Data, Modelling and Computation | Wuxi, China, 11-13 June, 2018 |

## 2 Overview of Work Presented in This Workshop Proceeding

The list of papers published in this workshop covers state-of-the-art simulations of flow and transport problems. These papers represent ongoing research projects on various important topics relevant to the modeling, algorithms and computation of flow and transport. Here the workshop papers may be classified into five groups as follows.

The first group consists of seven papers that devoting to various issues and applications in the area of fluid flow and heat transfer. P. Sun et al. studied a dynamic fluid-structure interaction (FSI) problem involving a rotational elastic turbine by using the arbitrary Lagrangian-Eulerian (ALE) approach in the paper entitled "*ALE method for a rotating structure immersed in the fluid and its application to the articial heart pump in hemodynamics*". S. Ishihara et al. investigated the influence of depth from the free surface of the fish and turning motion via the moving-grid finite volume method and moving computational domain method with free surface height function in the paper entitled "*Free Surface Flow Simulation of Fish Turning Motion*". In the paper entitled "*Circular Function-Based Gas-kinetic Scheme for Simulation of Viscous Compressible Flows*", Z. Meng et al. simplified the integral domain of Maxwellian distribution function and proposed a stable gas-kinetic scheme based on circular function for the simulation of viscous compressible flows. J. Li et al presented an N-parallel FENE-P constitutive model for viscoelastic incompressible non-Newtonian fluids based on the idea of multiple relaxation times in the paper entitled "*Study on an N-parallel FENE-P constitutive model based on multiple relaxation times for viscoelastic fluid*". Moreover, in another paper entitled "*LES study on high Reynolds turbulent drag-reducing flow of viscoelastic fluids based on multiple relaxation times constitutive model and mixed subgrid-scale model*", J. Li et al. further revealed the drag-reduction mechanism of high Reynolds viscoelastic turbulent flow and addressed the different phenomena occurring in high and low Reynolds turbulent drag-reducing flows. A coupled LBGK scheme, constituting of two independent distribution functions describing velocity and temperature respectively, was established by T. Zhang and S. Sun in the paper entitled "*A Compact and Efficient Lattice Boltzmann Scheme to Simulate Complex Thermal Fluid Flows*". The complex Rayleigh-Benard convection was studied and various correlations of thermal dynamic properties were illustrated. In the last paper of this group entitled "*A new edge stabilization method*", H. Duan and Y. Wei theoretically and numerically studied a new edge stabilization method for the finite element discretization of the convection-dominated diffusion-convection equations.

The second group of papers concerns the modeling and simulation of multiphase flow and the flow and transport in porous media. In the paper entitled "*A novel energy stable numerical scheme for Navier-Stokes-Cahn-Hilliard two-phase flow model with variable densities and viscosities*", X. Feng et al. constructed a novel numerical scheme for the simulation of coupled Cahn-Hilliard and Navier-Stokes equations considering the variable densities and viscosities. And the accuracy and robustness of this novel scheme were validated by the benchmark bubble rising problem. Z. He et al. studied linearly first and second order in time, uniquely solvable and unconditionally energy stable numerical schemes to approximate the phase field model of solid-state dewetting problems based on the novel scalar auxiliary variable (SAV) approach in the paper entitled "*Efficient Linearly and Unconditionally Energy Stable Schemes for the Phase Field Model of Solid-State Dewetting Problems*". Y. Wang et al in their paper "*Study on Numerical Methods for Gas Flow Simulation Using Double-Porosity Double-Permeability Model*" first investigated the numerical methods for gas flow simulation in dual-continuum porous media by using the mass balance technique and local linearization of the nonlinear source term. The paper of G. Harper et al., "*A Two-field Finite Element Solver for Poroelasticity on Quadrilateral Meshes*", focused on a finite element solver for linear poroelasticity problems on quadrilateral meshes based on the displacement-pressure two-field model. This new solver combined the Bernardi-Raugel element for linear elasticity and a weak Galerkin element for Darcy flow through the backward Euler temporal discretization. In the paper entitled "*Coupling multipoint flux mixed finite element methods with discontinuous Galerkin methods for incompressible miscible displacement equations in porous media*", J. Chen studied the numerical approximation of the incompressible miscible displacement equations on general quadrilateral grids in two dimensions with the multipoint flux mixed finite element method and discontinuous Galerkin method.

The third group is related to applications in petroleum engineering. In the paper entitled "*Computational Studies of an Underground Oil Recovery Model*", Y. Wang deeply studied the underground oil recovery model, and extended the second and third order classical central schemes for the hyperbolic conservation laws to solve the modified Buckley-Leverett (MBL) equation. J. Shi, et al. conducted the grand canonical Monte Carlo (GCMC) simulation to investigate the displacement of methane in shale by injection gases and employed the molecular dynamics (MD) simulation to investigate the adsorption occurrence behavior of methane in different pore size in the article entitled "*Molecular Simulation of Displacement of Methane by Injection Gases in Shale*". P. Wang et al. developed a pipeline network topology-based method to identify vulnerability sources of the natural gas pipeline network based on the network evaluation theory in the paper entitled "*Study on topology-based identification of sources of vulnerability for natural gas pipeline networks*".

The fourth group, which consists of two articles, is focusing on the traffic flow problems. In the first paper entitled "*Data Fault Identification and Repair Method of Traffic Detector*", X. Li et al. combined the wavelet packet energy analysis and principal component analysis (PCA) to achieve the traffic detector data fault identification. D. Liu et al. proposed three different methods for node importance measurement of urban road network based on a spatially weighted degree model, the Hansen Index and h-index in the paper entitled "*Method of Node Importance Measurement in Urban Road Network*". Moreover, the topological structure, geographic information and traffic flow characteristics of urban road network were considered.

The last group addresses some numerical issues to tackle challenges in flow and transport simulations. A method to calculate intersections of two admissible general quadrilateral mesh of the same logically structure in a planar domain was presented by X. Xu and S. Zhu in the paper entitled "*Symmetric Sweeping Algorithms for overlaps of Two Quadrilateral Mesh of the same connectivity*". G. Jr. et al. improved the efficiency of preprocessing phase of the ALT algorithm through parallelization technique which could cut the landmark generation time significantly in the paper entitled "*Preprocessing parallelization for the ALT-algorithm*".

## 3 Observations of General Trends in Flow and Transport Simulations

The past decade has seen remarkable advances in the simulations of flow and transport phenomena because of its significance to understand, predict, and optimize various scientific and industrial flow and transport processes. Nevertheless, accurate, efficient and robust numerical simulations of flow and transport still remain challenging. Below we give a brief overview on the general trend of flow and transport simulations.

(1) *"Multi"-modeling*: With the increased complexity of the flow and transport phenomena, the modeling tends to be more complex. For instance, multiphase flow especially in porous media and with the partial miscibility of different phases provides more challenges and opportunities now. Multicomponent transport with reaction, such as computational thermodynamics of fluids, especially hydrocarbon and other oil reservoir fluids, and its interaction with flow and transport still remain to be further explored. From the aspect of computational scale, coupling of flow and transport in different scales is also a research hotspot, such as transport in molecular scale, pore scale, lab scale, and field scale, flow from Darcy scale to pore-scale, etc.

(2) *Advanced "multi"-algorithms*: The increasing complexity of flow and transport simulations demands the algorithms to be multi-scale, multi-domain, multi-physics and multi-numerics. For the complex flow and transport phenomena, the mathematical models usually with possibly rough and discontinuous coefficients, and the solutions are often singular and discontinuous. Thus, the advanced discretization methods should be applied to discretize the governing equations. Local mass conservation and compatibility of numerical schemes are often necessary to obtain physical meaningful solutions. In addition, the design of fast and accurate solvers for the large-scale algebraic equation systems should be addressed. Solution techniques of interest include mesh adaptation, model reduction (such as MsFEM, upscaling, POD, etc.), multiscale algorithms (such as coupling of LBM and MD, etc.), parallel algorithms (such as CPU parallel, GPU parallel, etc.), and others.

(3) *Heterogeneous parallel computing with "multi"-hardware:* Today flow and transport simulations are becoming more and more computationally demanding, more than one kind of processors or cores are preferred to be used to gain a better computational performance or energy efficiency. Thus the "multi"-hardware for the heterogeneous parallel computing is a clear trend. Especially the heterogeneous parallel computing coupled with tensor processing unit (TPU), graphics processing unit (GPU) and cloud computing should be paid more attentions. The TPU parallel, GPU parallel and cloud computing provide completely new possibilities for significant cost savings because simulation time can be reduced on hardware that is often less expensive than server-class CPUs.

(4) *"Multi"-application*: The interaction of flow and transport with other physical, chemical, biological, and sociological processes, etc. is gaining more attentions from the global researchers and scientists, and application areas of flow and transport have been widened largely in recent years. It includes but not limited to the fields of earth sciences (such as groundwater contamination, carbon sequestration, petroleum exploration and recovery, etc.), atmospheric science (such as air pollution, weather prediction, etc.), chemical engineering (such as chemical separation processes, drug delivery, etc.), biological processes (such as biotransport, intracellular protein trafficking, etc.), traffic flow (such as traffic networks, material flow in supply chain networks, etc.), material design, natural disaster assessments, information flow and many others.

## 4 Concluding Remarks

In conclusion, this workshop proceeding presents and highlights new applications and new (or existing) challenges in five different important research areas of flow and transport mainly from the aspects of modeling, algorithms and computation. The workshop proceeding is not intended to be an exhaustive collection nor a survey of all of the current trends in flow and transport research. Many additional significant research areas of flow and transport still exist and remain to be explored further, but “multi”-modeling, advanced “multi”-algorithms, heterogeneous parallel computing with “multi”-hardware and “multi”-application are clear trends.

## Acknowledgments

The authors would like to thank all the participants of this workshop for their inspiring contributions and the anonymous reviewers for their diligent work, which led to the high quality of the workshop proceeding. The authors also express their sincere gratitude to the ICCS organizers for providing a wonderful opportunity to hold this workshop. The workshop chair S. Sun and co-chair J. Li would like to acknowledge the research funding from King Abdullah University of Science and Technology (KAUST) through the grants BAS/1/1351-01, URF/1/2993-01 and REP/1/2879-01. J. Liu would like to acknowledge the funding support from US National Science Foundation (NSF) under grant DMS-1419077.