



Proceedings of the 35th Parallel Computational Fluid Dynamics International Conference 2024

Andreas Lintermann, Sohel Sebastian Herff and Jens Henrik Göbbert

IAS Series

Band / Volume 69

ISBN 978-3-95806-819-3

Forschungszentrum Jülich GmbH
Institute for Advanced Simulation (IAS)
Jülich Supercomputing Centre (JSC)

Proceedings of the 35th Parallel Computational Fluid Dynamics International Conference 2024

Andreas Lintermann,
Sohel Sebastian Herff
and Jens Henrik Göbbert

Schriften des Forschungszentrums Jülich
IAS Series

Band / Volume 69

ISSN 1868-8489

ISBN 978-3-95806-819-3

Contents

Preface	i
Sponsors	vii
Acknowledgements	ix
Invited Speakers and Keynotes	1
Mini-Symposium 1: Quantum Computing for CFD Applications	9
Quantum Annealing Computations to Obtain Converged Flow Solutions; <i>Kuya, Y. & Asaga, T.</i>	10
Strategies for the Application of Quantum Computers in Computational Fluid Dynamics; <i>Görtz, S. & Langer, S.</i>	13
Towards Large-Scale Computational Fluid Dynamics Solvers With Quantum Iterative Algorithms; <i>Williams, C. A., Gentile, A. A., Elfving, V. E., Berger, D., & Kyriienko, O.</i>	16
Solving Fluid Dynamics Equations With Differentiable Quantum Circuits; <i>Chaudhary, S., Tosti Balducci, G., Kyriienko, O., Barkoutsos, P. Kl., Cardarelli, L., & Gentile, A. A.</i>	20
A Practical Implementation of Quantum Lattice Boltzmann Algorithms; <i>Georgescu, C. A. & Möller, M.</i>	23
Mini-Symposium 2: Advances in Parallel Simulation of Reacting Flow	29
An Efficient Parallel Implementation of an Hybrid Method for the Advection of High Schmidt Scalars in Flows; <i>Santoso, S., Houzeaux, G., & Dosimont, D.</i>	30
Enhancing Insight Into Turbulent Lifted Hydrogen Jet Flames Using a Reynolds Stress, Stretched Flamelet Model; <i>Wu, C., Yang, J., & Gu, X.</i>	33
Parallel Adaptive High-Resolution Simulation of Rotating Detonation Engines in 3D; <i>Peng, H. & Deiterding, R.</i>	37
DNS of a Hydrogen Flame Interacting With Homogeneous Isotropic Turbulence Maintained by a Deterministic Force; <i>Xu, Y., Fang, J., Lu, Z., Gu, X., & Chen, Z. X.</i>	40
Computation of Transport and Chemistry for Combustion Applications in the Code Alya Using Accelerated Architectures; <i>Moure, Á., Daviña, A. L., Surapaneni, A., & Mira, D.</i>	44

Mini-Symposium 3: Convergence of Artificial Intelligence and High-Performance Computing for Computational Fluid Dynamics (AI + HPC4CFD PT. 3)	49
Hard Constraint Projection in a Physics Informed Neural Network; <i>Horne, M. J. S., Jimack, P. K., Khan, A., & Wang, H.</i>	50
Drag Correlations for Multiphase Flows Using Artificial Neural Networks; <i>Vorspohl, J., André, L., Rüttgers, M., & Schröder, W.</i>	54
HydroGym-GPU: From 2D to 3D Benchmark Environments for Reinforcement Learning in Fluid Flows; <i>Lagemann, C. Rüttgers, M., Gondrum, M., Meinke, M., Schröder, W., Lintermann, A., & Brunton, S.</i>	57
Super-Resolution and Parallel-In-Time Integration to Accelerate Simulations With the ICON-O Ocean Model; <i>Freese, P., Witte, M., Lapolli, F. R., Götschel, S., Korn, P., Kadow, C., & Ruprecht, D.</i>	64
Deep Reinforcement Learning Strategies for Optimizing Flow Control in Wings; <i>Montalà, R., Font, B., Suárez, P., Rabault, J., Lehmkuhl, O., Vinuesa, R., & Rodríguez, I.</i>	67
A Study on the Effect of the Number of Collocation Points in the Training of Physics-Informed Neural Networks for Unsteady Flows; <i>Onishi, J. & Tsubokura, M.</i>	72
Predicting Turbulent Boundary Layer Flows Using Transformers Coupled to the Multi-Physics Simulation Tool m-AIA; <i>Sarma, R., Hübenthal, F., Orland, F., Terboven, C., & Lintermann, A.</i>	76
Creating a Virtual Population of the Human Nasal Cavity for Velocity-Based Predictions of Respiratory Flow Features Using Graph Convolutional Neural Networks; <i>Calmet, H., Calafell, J., Sarma, R., Rüttgers, M., Lintermann, A., & Houzeaux, G.</i>	80
Evaluating Random Forest Classifiers to Optimize Load Balancing of Parallel Mesh Generation; <i>Gangopadhyay, A., Bartholomew, P., & Weiland, M.</i>	84
Investigating the Effects of Spanwise Transversal Traveling Waves on a Turbulent Compressible Flat Plate Flow With the Aid of a Deep Autoencoder Network; <i>Shao, X., Ayan, H. O., Hübenthal, F., Rüttgers, M., Lintermann, A., & Schröder, W.</i>	89
Predicting NOx Emissions From Porous Media Burners Using Physics-Informed Graph Neural Networks; <i>Puri, R., Stein, O. T., & Zirwes, T.</i>	94
Mini-Symposium 4: Modernizing CFD: Exploring CI/CD for Improved Software Development Life Cycle	99
Adapting the Development of a CFD Application Following the CI-CD Life Cycle and a DevOps Approach; <i>Dosimont, D. & Houzeaux, G.</i>	101
Verificarlo CI : Continuous Integration for Numerical Optimization and Debugging; <i>Delval, A., Coppens, F., Petit, E., Iakymchuk, R., & de Oliveira Castro, P.</i>	104
Assessing Computational Fluid Dynamics on GPU Using Portable Languages; <i>Faqir-Rhazoui, Y. & García Sánchez, C.</i>	108
Comparing Several HPC CFD Software Through Codemetrics: A Case Study; <i>Marzlin, T. & Dauplain, A.</i>	111

Enabling Lighter and Faster Simulations With Repeated Matrix Blocks; <i>Plana-Riu, J., Trias, F. X., Colomer, G., Alsalti-Baldellou, À., Álvarez-Farré, X., & Oliva, A.</i>	115
A Portable Algebraic Implementation for Reliable Overnight Industrial LES; <i>Mosqueda-Otero, M. F., Asalti-Baldellou, À., Álvarez Farré, X., Plana-Riu, J., Colomer Rey, G., Trias, F. X., & Oliva, A.</i>	119
Mini-Symposium 5: HPC Biomechanics and New Challenges	127
An Embedded Boundary Mesh Method for Simulating Rigid Heart Valves; <i>Samaniego, C., Vázquez, M., & Houzeaux, G.</i>	128
Parallel Mesh Developments to Prepare for Biosimulations; <i>Cullen, P., Moulinec, C., Gebbie-Rayet, J., Bonelle, J., & Fournier, Y.</i>	131
Comparison of Airflow and Particle Deposition in Different Acinus Geometries; <i>Eguzk-itza, A. B., Arnedo, C., Nasseti, F., Calderon, J., Muñoz, F., & Houzeaux, G.</i>	134
Lung Digital Twin COVID-19 Infection: A Multiphysics - Multiscale HPC-Modeling Based on CFPD and Agent Based Model Coupled Simulations; <i>Novell, A., Muñoz, F., Ntiniakou, T., Montagud, A., Houzeaux, G., & Eguzkitzza, A. B.</i>	147
Computational Modeling of Particles Fate in Nasal Drug Treatments; <i>Ceccacci, S., Vicente Porres, J. A., Rio Grela, N., Calmet, H., Gargallo Peiro, A., Rigaut, C., Haut, B., Houzeaux, G., & Eguzkitzza, A. B.</i>	154
Wet-Surface Modeling in Lattice-Boltzmann Simulations for Evaluating Surgery Impacts on the Humidity Transfer in Nasal Flows; <i>Ito, S., Rüttgers, M., Waldmann, M., & Lintermann, A.</i>	158
Fundamental Study on Fluid-Structure Interaction Models for Pulse Waveform Analysis Through Blood Vessels; <i>Kaneko, Y. & Fukui, T.</i>	163
GPU Accelerated Fem Based Lagrangian Particle Tracking Framework for Human Air Pathway; <i>Anandh, T. & Ganesan, S.</i>	166
Mini-Symposium 6: Mini-Symposium on Tool Support for Developing Highly-Parallel CFD Applications	175
Practical Empirical Performance Modeling for CFD Applications Using Extra-P; <i>Rothenberger, L., de Moraes, G., Geiß, A., & Wolf, F.</i>	176
On the Modeling and Improvement of Sub-Optimal Submission Patterns on HPC Workloads; <i>Larroque, A., Giraud, B., & Dauptain, A.</i>	180
Correctness and Performance Analysis of an Open-Source CFD Application; <i>Orland, F., Jenke, J., & Liem, R.</i>	185
Streamlining Performance Analysis Workflows Using Compiler-Assisted Instrumentation Selection; <i>Kreutzer, S., Arzt, P., & Bischof, C.</i>	188
Working Towards FAIRness in Performance Data; <i>Sander, M., Williams, W. R., & Wesarg, B.</i>	192
Mini-Symposium 7: Lattice Boltzmann Method-Based Computational Fluid Dynamics and its Application	197
On the Influence of the Blending Parameter σ in LBM WMLES With the HRR-BGK Collision Scheme; <i>Gericke, J., Masilamani, K., Klimach, H., & Spinelli, G.</i>	198

Numerical Simulation of the Effects of Internal and External Viscosity Contrast of a Red Blood Cell in a Non-newtonian Plasma on Its Motion and Suspension Rheology; <i>Morimoto, H. & Fukui, T.</i>	201
Mini-Symposium 8: Machine Learning-Based Reduced Order Models for Fluid Flow Emulators and Application to Design Optimization	205
Machine Learning Based Intelligent CFD Simulation for Interactive Design Exploration of Built Environments; <i>Adia, U., Khan, A., Sleigh, A., & Wang, H.</i>	207
A Surrogate Model Based Shape Optimization Framework for Compressible Flows; <i>Şenol, N., Akay, H. U., & Yiğit, Ş.</i>	213
Controllable Droplet Transport via Inverse Design of Substrate Heterogeneity; <i>Vrionis, P.-Y., Demou, A., & Savva, N.</i>	216
Data-Driven CFD-Based Design Optimization of Flow Pattern in a Gravitational Mixer Settler; <i>Khatir, Z.</i>	219
Mini-Symposium 9: Computational Fluid Dynamics with High-Order Spectral Element Methods on GPUs	225
Towards High-Fidelity Simulations of Urban Flows; <i>Duró, J. M., Muñoz, N., Mestres, E., Muela, J., Lehmkuhl, O., & Rodriguez, I.</i>	226
Parallel Performance and Communication Pattern Analysis on SOD2D: A CFD High-Order Spectral Element Code; <i>Muela, J., Gasparino, L., & Lehmkuhl, O.</i>	231
DNS of Intrinsically Unstable 3D Flames Using Deficient Reactant Thermochemistry: Validation and Scaling in nekRS; <i>Kavari, H., Lapenna, P. E., Bode, M., Mira, D., & Creta, F.</i>	235
Computational Investigation of the Atmospheric Boundary Layer in the GABLS Benchmark Problem Using the Spectral Element Code nekRS; <i>Konioris, D., Papageorgiou, D., Kavroulakis, I., Bode, M., Min, M., Fischer, P., & Tomboulides, A.</i> . .	238
In-Situ Visualization With Ascent and NekRS for Large-Scale CFD Problems on GPUs; <i>Göbber, J. H., Alvarez, D., Bode, M., Fischer, P., Frouzakis, C. E., Insley, J. A., Lan, Y.-H., Mateevitsi, V. A., Min, M., Papka, M. E., Rizzi, S., Samuel, R. J., & Schumacher, J.</i>	241
Unraveling Turbulent NH ₃ /H ₂ Flames Using High Performance GPU Computing: A Series of Spectral Element Method-Based High-Fidelity DNS; <i>Kaddar, D., Nicolai, H., Schuh, V., Bähr, A., Frouzakis, C. E., Bode, M., & Hasse, C.</i>	245
Unraveling the Boundary Layers of High Rayleigh Number Convection Through Direct Numerical Simulations; <i>Samuel, R. J., Shevkar, P. P., Bode, M., Scheel, J. D., Sreenivasan, K. R., & Schumacher, J.</i>	249
Portable Linear Solvers for High-Order Spectral Element Methods on GPUs; <i>Tsai, Y.-H. M.; Olenik, G., Herten, A., Bode, M., & Anzt, H.</i>	253
NekCRF: A Novel GPU-Accelerated Finite-Rate-Chemistry Solver and Application to Hydrogen; <i>Bode, M., Frouzakis, C. E., & Tomboulides, A.</i>	257
Large-Scale Engine Direct Numerical Simulations With NekRS: A Multi-Cycle Database; <i>Danciu, B. A., Frouzakis, C. E., & Bode, M.</i>	260
Other Topic 1: Academic Flows	265

Three-Dimensional Parallel Simulations of the Scour Around Multiple Cylinders; <i>Uh Zapata, M., Itzá Balam, R., & Pham Van Bang, D.</i>	266
Hypersonic Flow Past an Open Cavity Using HPC and Open-Source Software; <i>Emerson, D. R., Fang, J., & John, B.</i>	271
Other Topic 2: Aerospace	277
Application of the HEMLAB Algorithm to a Delta Wing Geometry and a 5 th Generation Fighter Model; <i>Akgun, H. & Sahin, M.</i>	278
Application of the HEMLAB Algorithm to a Case from the 7 th AIAA CFD Drag Prediction Workshop; <i>Asar, I. & Sahin, M.</i>	282
Other Topic 3: Numerical Methods	287
Comparison of Eddy-Viscosity Models in Modeling a Simplified Reactor Vessel Auxiliary Cooling System; <i>Wang, W., Liu, B., Cartland-Glover, G., He, J., Moulinec, C., Rolfo, S., & He, S.</i>	288
Multigrid Accelerated Projection Method on GPU; <i>Chiu, T.-H. & Lin, C.-A.</i>	292
Parallel Unstructured Conservative Level-Set (UCLS) Method for Liquid-Vapour Phase Change Phenomena; <i>Balcazar-Arciniega, N., Rigola, J., & Oliva, A.</i>	295
A Parallel-In-Time Spectral Deferred Correction Method for the Incompressible Navier-Stokes Equations; <i>Ouardghi, A. & Speck, R.</i>	299
Other Topic 4: Scalable Solvers	303
An In-House Overset Supersonic Solver With Grid Refinement Capability on Parallel Environment; <i>El Hajj Ali Barada, M. & Çelik, B.</i>	304
Roadmap for Extreme-Scale Simulations: On the Evolution of Poisson Solvers; <i>Trias, F. X., Alsalti-Baldellou, À., & Oliva, A.</i>	309
Domain Decomposition Method for Equivalent Sources Method in Aeroacoustic; <i>Débit, N., Denis, R., Fabrege, B., & Tromeur-Dervout, D.</i>	313
Epilogue	319
Advertisement	321

IAS Series
Band / Volume 69
ISBN 978-3-95806-819-3