

Ph.D. Students' Day (JDD 2021) Friday 18 June 2021















Climate Modeling & **Global Change**









ComputationalFluid Dynamics























09:30	Welcome speech: Olivier THUAL			
Session 1		Chair: Olivier Thual		
09:45	WINGEL Christopher	Unsteady modelling and analysis of the aerodynamics and aerothermal of a cooled turbine stage	p.4	CFD
09:50	DROZDA Luciano	Data-driven discretizations in fluid flow configurations	p.4	ALGO- COOP
09:55	WERNER Paul	Aerothermal LBM simulation of bore-cooling cavities of HP compressors	p.5	CFD
10:00	GALLARDO Victoria	Evolution of high-temperature extreme events in the Euro- Mediterranean region and their impact on aircraft take-off performance	p.5	GLOBC
10:05	ZAPATA José Félix	Surrogate models based on large eddy simulations for the multi- disciplinary design of reusable liquid rocket engines	p.6	CFD
10:10	LINÉ Aurélien	Mechanisms, predictability and uncertainty of temperature and precipitation over Europe in the near-term (2020-2040)	p.6	GLOBC
10:15	LAMELOISE Etienne	Modeling of soot formation in gas turbines taking into account the morphology of aggregates	p.7	CFD
10:20	LUMET Eliott	Data assimilation of microscale air pollutant dispersion using mobile sensors	p.7	GLOBC
10:30	1 h Coffee break and Poster Session n°1: Wingel, Drozda, Gallardo, Liné, Cellier, Lameloise			

Session 2		Chair: Bénédicte Cuenot		
11:30	MARCHAL Thomas	Extension of the Spectral Difference method to combustion	p.8	CFD
11:35	NONY Bastien	Metamodelling for micro-scale atmospheric pollutant dispersion large-eddy simulation	p.8	GLOBC
11:40	NGUYEN Minh	High-Fidelity Aerothermal simulations using the Lattice Boltzmann method	p.9	CFD
11:45	VILLARD Jean	Simulation of the combustion of metal particles	p.9	CFD
11:50	PEATIER Saloua	Quantification of uncertainties associated with climate projections	p.10	GLOBC
11:55	NAESS Thomas	Prediction of the production of pollutants in aeronautical engines	p.10	CFD
12:00	GENTIL Yann	Modeling of combustion noise in turbines	p.11	CFD
12:15	Lunch			



13:15	1 h Coffee break and Poster Session n°2: Marchal, Nguyen, Nony, Noun, Peatier, Suau				
Session 3		Chair: Pavanakumar Mohanamuraly			
14:15	ORDONEZ Ana	Scalable solvers for thermo-hydro-mechanical problems	p.11	ALGO-COOP	
14:20	MOCQUARD Clément	Simulation of afterburner in fighter aircraft engine	p.12	CFD	
14:25	HOK Jean-Jacques	Chemistry-turbulence interaction modeling for the large-eddy simulation of explosions	p.12	CFD	
14:30	FOUDAD Mohamed	Impact of climate change on clear-air turbulence for aviation	p.13	GLOBC	
14:35	GIOUD Thibault	Study of CH4-LOx combustion in subcritical, trans- and supercritical and super/subcritical transient conditions	p.13	CFD	
14:40	DURANTON Thibault	Advanced LES modelisation of multi-perforated plates for new generation aeronautical engines	p.14	CFD	
14:45	DEFONTAINE Théo	Flood predicting on the Garonne upstream of Toulouse by means of Machine Learning	p.14	GLOBC	
14:50	GIANOLI Thomas	Development of a Lattice-Boltzmann method for turbomachinery S- Duct simulations	p.15	CFD	
15:00		15 min Break			

Ma thèse en 3 minutes		Chair: Matthieu Pouget		
15:15	CELLIER Antony	Simulation aux grandes échelles de feux de batteries Lithium-Ion pour le diagnostic de l'emballement thermique Large Eddy Simulation of Lithium-Ion Battery Fire for the diagnostic of Thermal Runaway	p.15	CFD
15:20	NOUN Mark	Prédiction et mitigation des instabilités de cavité issues de couplages fluide-structure Prediction and mitigation of cavity instabilities resulting from fluid structure interaction	p.16	CFD
15:25	SUAU Adrien	Implémentation d'une bibliothèque QBLAS pour accélérateur quantique Implementation of a QBLAS library for quantum accelerators	p.16	ALGO-COOP
15:30	BOGOPOLSKY Guillaume	<i>Modélisation d'un propulseur à effet Hall</i> Modelisation of a Hall thruster	p.17	CFD
15:35	LAFARGE Thomas	Investigation de l'utilisation des méthodes de Lattice Boltzmann sur réseaux appliquées aux écoulements multiphasiques Lattice Boltzmann methods applied to multiphase flows for the atomization of swirled injectors	p.17	CFD
15:45	Voting for best Poster and best "Ma thèse en 3 minutes" presentation			
16:00		Closing speech: Olivier THUAL		



Ma thèse en 3 minutes

Some students have chosen to do their presentation under the "Ma thèse en 3 minutes" format, which is a theatrical science communication exercise. They entered a specific training course given by Dr. Matthieu Pouget, who holds a PhD in Performing Arts from the Université de Toulouse and is a professor at the Conservatoire d'art dramatique de Toulouse. He guided them throughout the process of writing the script, creating their performance, and learning how to communicate their research subject to a wide audience in the format of the national competition "Ma thèse en 180 secondes".

The presentations will be in French. The participants who have prepared a poster will move on to a regular poster session in English.





Christopher Wingel

9:45 (poster 10:30)

Unsteady modelling and analysis of the aerodynamics and aerothermal of a cooled turbine stage

The continuous improvement of helicopter engines performances involves a more precise prediction and understanding of the physics in the high-pressure turbine since the flow is complex and turbulent. In fact, radial and azimuthal distortions at the stage inlet combined with curvature effects lead to a 3D flow. Moreover, blade-vane interactions are sources of unsteady phenomena. Finally, vanes must be protected from high temperatures by adopting

cooling. All these phenomena have an impact on the aerodynamics and aerothermal of the main vein, but above all introduce unsteadiness that are necessary to capture with numerical simulations. The objective of this PhD thesis is to evaluate the capacity of URANS methods to correctly predict the aerodynamics and aerothermal of a cooled turbine stage.



Luciano Drozda

9:50 (poster 10:30)

Data-driven discretizations in fluid flow configurations

In the context of the Data-Science strategic program, many topics are investigated at CERFACS in relation to machine learning and computational physics. They are structured in the Helios project, the cross-laboratory workgroup on machine learning with ISAE-SUPAERO.



The objective of this particular PhD is data-driven explore new to methodologies for the discretization of the Navier-Stokes equations. Recent work has shown the great potential of these approaches compared to traditional techniques, but much work is needed in this field to bring them to maturity for concrete CFD applications. We are currently focusing on data-driven discretizations, where a neural net learning to approximate spatial derivatives is included as a part of the CFD solver workflow.



Paul Werner

Aerothermal LBM simulation of bore-cooling cavities of HP compressors

Reduction in compressor blade clearance has improved engine efficiency in decades. However, it pertains directly to a meticulous control of the thermal dilatation of rotor disks, which is ensured by the bore-cooling system. It is composed of a cold, turbulent axial throughflow and consecutive rotating cavities where natural convection induced by centrifugal forces and large temperature gradients occur. The LBM is perfectly suited to such unsteady flow and complex geometry but lacks maturity in modeling rotating perfect gases.



The objectives are to extend the LBM in a rotating frame, validate the force terms implementation and model the ICAS-GT2 configuration. A major challenge is to correctly predict heat exchange through rotor disks, which may lead to optimized cooling techniques.

Victoria Gallardo

10:00 (poster 10:30)

9:55

Evolution of extreme hot temperature events in the Euro-Mediterranean region, and its impact on aircraft take-off performance

Global warming may negatively impact aircraft performances since they also depend on air temperature. In particular, increasing hot temperatures may overspeed the aircraft engine, increasing pollutant emissions. This thesis aims at assessing the future impact of hot temperatures on the aircraft engine performance during takeoff. In the first year, the analysis of trends of hot temperatures over the main Euro-Mediterranean airports was carried out.

Regional and global climate models were evaluated in the present period in order to select the most accurate tool to simulate extreme hot temperatures and their trends in future climate. Results show that regional models don't represent better the amplitude nor the trends of hot temperatures than global models, despite their higher spatial resolution.





José Félix Zapata

Surrogate models based on large eddy simulations for the multi-disciplinary design of reusable liquid rocket engines

Rocket propulsion systems design is under growing pressure of reducing development costs. CFD codes for the simulation of combustion chambers can provide a low-cost alternative to experiment-driven design. Nonetheless, a holistic approach for design optimization is not yet practical as the exploration of the entire engine design space through full-scale CFD evaluations is too expensive. Surrogate models may avoid this conundrum through fast

inference times, without significant accuracy loss.

The main goal of this thesis is the development of surrogate models of rocket combustion chamber а injectors plate, comprised of gaseous oxygen-methane shear-coaxial injectors. These are to be derived through the leveraging of machinetechniques, learning particularly deep learning, in combination with LES data of the target system.



Aurélien Liné

10:10 (poster 10:30)

10:05

Mechanisms, predictability and uncertainty of temperature and precipitation over Europe in the near-term (2020-2040)

It has been established that climate change is attributable to human activity. Greenhouse gas and aerosols emissions, and land cover play a predominant role in climate change, called forced variability. In order to make predictions on future climate, 4 socio-economic pathways have been proposed by the intergovernmental panel on climate change (IPCC). However,



internal variability of the climate system can modulate the future response. To study this variability, a grand ensemble of 30 members has been computed for each scenario with the CNRM-CM6-1 model developed by CNRM and Cerfacs. Climate possibilities are explored to better understand physical mechanisms controlling the next decade climate, especially for changes of temperature, precipitation, wind, surface radiation, and extreme events.



Étienne Lameloise

10:15 (poster 10:30)

10:20

Modeling of soot formation in gas turbines taking into account the morphology of aggregates

Soot is a known contributor to global warming as well as a public health problem. In their lifespan, soot aggregates undergo various processes affecting their morphology, which is known for playing a critical role in their interactions with the media and their harmfulness.

As such processes cannot be explored experimentally, modeling effort is forced towards an accurate prediction of the particles shape. While soot particles evolution and trajectories are modeled thanks to semi-determinist Lagrangian approaches, aggregates morphology modeling calls on cluster aggregation models, assuming Brownian or ballistic motion. The main objective of this thesis funded by the ANR ASTORIA is thus to couple both methods within an LES framework to accurately predict soot aggregates distribution and morphology.



Éliott Lumet

Data assimilation of microscale air pollutant dispersion using mobile sensors

A detailed understanding of atmospheric processes in the bottom part of the atmospheric boundary layer like air pollutant dispersion requires the development and evaluation of high-fidelity numerical models. However, simulating the microscale plume dynamics in complex geometry such as urban or mountainous areas remains challenging due to the strong atmosphere/surface interactions, the intrinsic variability of turbulent wind conditions and the

land surface heterogeneity.

The objective of this PhD is to design a data assimilation strategy to optimally combine large-eddy simulation predictions and UAV measurements to reconstruct the best possible plume representation. One of the main issues is to design an optimal sensor placement method so that the assimilated measurements can reduce as much as possible the modeling uncertainties.



7/17



Thomas Marchal

11:30 (poster 13:15)

Extension of the Spectral Difference method to combustion

The aim is to assess the potential of the Spectral Differences (SD) method for the simulation of turbulent combustion in aeronautical engines. The SD method is a high-order numerical discretization approach, which has the potential to increase the accuracy of solutions at no extra cost. This is crucial for the design of the new generation of combustors, which must reduce both fuel consumption and pollutant emissions. The SD method is implemented in the

code Jaguar, jointly developed with ONERA. The implementation of a combustion model will be first validated on simple test cases. The final objective is to perform the 3D calculation of the PRECCINSTA burner, and evaluate the gain in the tradeoff between accuracy and computational cost.



Bastien Nony

11:35 (poster 13:15)

Metamodeling for micro-scale atmospheric pollutant dispersion large-eddy simulation

In atmospheric dispersion problems, mapping pollutant concentrations within the first tens or hundreds of meters from the emission point source remains a modelling challenge. Computational fluid dynamics (CFD) approaches provide relevant insights into turbulent flow and pollutant concentration patterns in complex terrains such as urban areas. In such conditions, large-eddy simulations (LES) seem promising to assess public short-term exposures. The design of metamodels for multiple LES scenarios could help handling physical

uncertainties of an atmospheric pollutant dispersion case.

The objective of this PhD is to gather the turbulent flow information provided by multiple LES into one accurate and fast-computing metamodel. Applying this approach to realistic flow configurations could motivate the use of LES to alert of toxic pollution risks during major environmental disasters.





Minh Nguyen

11:40 (poster 13:15)

High-Fidelity Aerothermal simulations using the Lattice Boltzmann Method

The development of cooling systems for high pressure turbines requires rapid high-fidelity fluid simulation tools. The Lattice Boltzmann Method (LBM) is an interesting candidate due to its computational speed and rapid mesh generation, but it is typically limited to weakly compressible isothermal flows.

Although there have been many attempts to extend the LBM to fully compressible flows, these have largely been limited to simple academic test cases. The principal objective of this thesis is to develop a compressible LBM solver for complex turbulent flows and to investigate its ability to perform high fidelity simulations of turbine cooling systems at a reasonable computational cost.



Jean Villard

Simulation of the combustion of metal particles

Metal as a fuel has been used in the space and arms industry for many years for its high energy density and release. This type of flame is very complex to stabilize, experimentally and numerically. Therefore, very few numerical simulations exist in the literature. Recently, metal fuels have been considered as promising alternatives to fossil fuels due to their carbon free combustion process. Moreover, metal combustion products can be transformed back to fuel, effectively creating a clean battery. To use metal fuels, thermal machines will have to be

redesigned and a better understanding of the phenomenology is therefore mandatory. To do so, numerical simulation of these capricious, yet very promising flames will be playing a major role.



11:45



Saloua Peatier

11:50 (poster 13:15)

11:55

Quantification of uncertainties associated with climate projections

The global surface temperature response to CO_2 increasing has been persistently uncertain. Moreover, the parametric uncertainties are not well estimated in current climate models. Parameter calibration choices in General Circulation Models can greatly impact their sensitivity to greenhouse gases. Our objective is to quantify the uncertainties in current and future climate change projections by exploring the choices made in the parametrization of



climate models. We produce a Perturbed Physics Ensemble (simulations using slightly different parameter values within plausible ranges) of the CNRM-CM6-1 climate model and use machine learning techniques to explore the range of future global and regional responses to changes in greenhouse gas concentrations, consistent with past observations and physical understanding of processes.

Thomas Naess

Prediction of the production of pollutants in aeronautical engines

New aeronautical technologies must comply with international regulations and answer the public environmental concern about global warming and human health. In particular, focus is made on the emission of soot and NOx. Combustion in real engines implies chemistry, turbulence, and spray interaction in addition to pollutant emissions description. Reactive Large Eddy Simulation has been shown a powerful tool to understand these interactions, combining accurate chemistry (for fuel oxidation, NOx, and soot precursors) and a Lagrangian framework to describe both the fuel spray and the soot particles. This Ph.D. aims to predict NOx and soot emissions with a reasonable degree of confidence in real-like combustors. For that purpose, the confrontation of simulations with experimental measurements will assess the pollutants prediction accuracy.



Yann Gentil

Modeling of combustion noise in turbines

To meet environmental constraints, new generation of turboshaft engines will be more compact resulting in combustion noise to become one of the main noise sources. Therefore, it is essential for the design of these engines to rely on a computational methodology that enables the prediction of combustion noise. Nevertheless, computational cost of a complete engine is still prohibitive, which justifies the use of modeling. CERFACS has been working for



several years on the development of a computational methodology based on Large Eddy Simulation (LES) of combustion chambers coupled with analytical an method propagate noise to turbine. This through the analytical method still needs to be improved so that the models take into account the physics of new turboshaft engine architectures.

Z CERFACS

Ana Ordonez

Scalable solvers for thermo-hydro-mechanical problems

We are interested in the modelling of thermo-hydro-mechanical (THM) problems with a second gradient of dilation regularization, which describe the behaviour of a soil, represented as a porous medium in which a weakly compressible fluid evolves. This model is used for the evaluation of THM impact of highlevel activity radioactive waste. The parallel and scalable solution of the linearized equation systems is the objective of this work.



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In this talk, we shall present the definition and results of a block preconditioner for the fully coupled THM equations with second gradient regularization based on parameter-robust preconditioners. Numerical results reflect the good performance of the proposed preconditioner that shows to be independent of the matrix size.

12:00

14:15



Clément Mocquard

Simulation of afterburner in fighter aircraft engine

The simulation of post-combustors is a useful tool during the design phase of an after-burner. Post-combustors imply several phenomena such as liquid jets atomization and evaporation in turbulent wakes of burnt gases at elevated pressure (~ 5 bars), two-phase combustion, and high frequency transverse thermo-acoustic instability known as "screech". Large Eddy Simulations is a method which has been proven able to capture complex flame/flow/acoustic interactions as well as gaseous/liquid phase interactions.



However, the coupling between these different phenomena is still an active field of research and some improvements are needed. In particular chemical schemes must reproduce accurately auto-ignition delays in an industrial context where ARC schemes are still very costly.

14:20

14:25

Jean-Jacques Hok

Chemistry-turbulence interaction modeling for the large-eddy simulation of explosions

The use of hydrogen for energy generation in combustion engines has become attractive to many industrials as it is decarbonated. However, this combustible exhibits wider flammability limits than usual fuels and the relatively small size of H2 molecules make leakages and explosions likelier. Part of the LEFEX (Large-Eddy Simulation for EXplosions) project, my PhD



thesis aims at providing a better understanding of the impact of H2 chemical properties on its combustion. particular, In attention is paid on the response of H2-air flames to stretch due to their non-unity Lewis number. Besides, my work will also analyze the formation mechanisms of flame front instabilities for lean hydrogen flames. Influence of both phenomena on flame acceleration will be assessed.



14:30

14:35

Mohamed Foudad

Impact of climate change on clear-air turbulence for aviation

Airplanes in flight can be subject to Clear-Air Turbulence (CAT) episodes, which can injure passengers, cause structural damage to planes and induce considerable economic loss. Recent studies have shown that the intensity and the frequency of CAT episodes could increase with the climate change. For this purpose, this PhD thesis aims at projecting changes in CAT episodes. The work will be realized in two stages. The first stage consists in analyzing recent climate scenarios performed with the CNRM-CM6-1 model in order to provide a comprehensive viewpoint of CAT changes.

The second stage will focus on designing a dynamical downscaling procedure through a coupling of different atmospheric models to characterize changes in severe CAT episodes at finer scales.



Thibault Gioud

Study of CH4-LOx combustion in subcritical, trans- and supercritical and super/subcritical transient conditions

Combustion in cryogenic rocket engines is a complex phenomenon, involving either liquid or super-critical fluids at high pressure and high turbulence intensity. Up to now, for liquid rocket engines, most of Large Eddy Simulations did not compute the liquid core but modelized it with analytical correlations, and ignored primary atomization. However, primary atomization is the main driver of the liquid spray structure and consequently of the resulting flame. On the other hand, extreme conditions make experimental measurements difficult and rare. Thereby, there is a need for accurate liquid injection models and simulations.

Based on recent progress made at Cerfacs on two-phase flow modelling using the diffuse

interface concept, the purpose of this PhD thesis is to develop a methodology to model and compute liquid injection in rocket engines, accounting for both the liquid core and the primary atomization, at an affordable cost.



13/17



Thibault Duranton

14:40

Advanced LES modelisation of multi-perforated plates for new generation aeronautical engines

Aeronautical combustion chambers generate high temperature gases and combustion instabilities. To deal with such conditions, thousands of submilimetric holes are drilled between the flame tube and the casing, acting both as a cooling system for the wall, and as an acoustic damper.



However, to fulfill their goals and in the context of the next generation of low NOx lean combustors, optimization of the multiperforated liner is required. Typically, the non uniform pressure drop field across the plate holes is now to be taken into account to properly reproduce the different mass flow repartition and the associated acoustic damping.

Théo Defontaine

14:45

Flood predicting on the Garonne upstream of Toulouse by means of Machine Learning

Flood prediction is still nowadays a thorny problem to assess. Hydrologic simulation techniques have proven their usefulness when the topology of the field is well defined. But, when the work to implement such models requires too much calibration, other simpler

empirical lag and route models are used. The Toulouse's Garonne basin is in such a case. Those models have limitations when new unseen floods happen. The aim of this PhD Thesis is to extend the discharge forecasting lead time of the lag and route models used in Toulouse by means of Machine Learning models or Deep Learning models. The case is a challenge to learning techniques due to the low number of floods events in the Toulouse basin.





Thomas Gianoli

Development of a Lattice-Boltzmann method for turbomachinery S-Duct simulations

The continuous improvement of the propulsion efficiency of aircraft engines has led to optimizing every component of an engine to avoid all possible losses. For performance issues, the bypass ratio has increased, thus, forcing the radial offset between the Low-Compressor Pressure and the High-Pressure Compressor to get higher. However, these two parts are connected via an annular S-shaped duct which can be described as an aerodynamic passage used to redirect the fluid from one radial position to another and that is becoming more aggressive in design. The goal of this thesis consists of developing a Lattice-Boltzmann method suited to run turbomachinery simulations of the S-duct and to evaluate the main physical phenomena creating pressure losses inside the duct.



3だ Antony Cellier

15:15 (poster 10:30)

14:50

Large Eddy Simulation of Lithium-Ion Battery Fire for the diagnostic of Thermal Runaway

The metamorphosis of the energy mix to come raises interrogations about the production and the storage of greener forms of power. The fraction of this mix taken by electricity is on the verge to drastically increase. Storage devices are thus to be studied in order to guarantee high efficiency without sacrificing the safety of the users. Recent developments of Lithium-ion cells

present interesting power-toweight specifications but can be subject to critical events such as Thermal Runaway, causing battery fire. A multiphysics Large Eddy Simulation is needed to capture the transient phenomena initiating such fires which propagate from cell to cell. The long-term aim is then to increase the safety and operability when designing new Li-ion battery packs.



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15/17



3 Mark Noun

15:20 (poster 13:15)

Prediction and mitigation of cavity instabilities resulting from fluid structure interaction

Different complex unsteady phenomena can appear in rotor/stator cavities whether at the these cavities or the surrounding structure can generate major risks for the operation of the turbopump. The objective of this PhD is to improve the understanding of unsteady phenomena in these rotor/stator cavities by the use of Large Eddy Simulation and global linear stability analysis with the aim of considering the multi-physical aspect of fluid-structure type



of instability. A fluid-structure coupled global linear stability analysis tool will therefore be developed to identify the multi-physical modes. Such a solution will allow the analysis of these instabilities and, above all, to propose mitigation solutions whether at the fluid or structural level.

3 Adrien Suau

15:25 (poster 13:15)

Implementation of a QBLAS library for quantum accelerators

The thesis goal is to investigate the potential of quantum computing in the field of scientific computing, more specifically in the resolution of PDEs, by building a library of core algorithms that can be re-used by researchers to implement efficiently their own algorithms.

Given the currently limited quantum variational hardware, quantum algorithms are targeted, as they are believed to be real contenders for a quantum speed-up on useful tasks. In order to increase the efficiency of these algorithms, automatic differentiation of quantum programs and hardware-inspired optimisations have been considered.





3. Guillaume Bogopolsky

15:30

15:35

Modelisation of a Hall thruster

Hall thrusters for spacecraft propulsion are becoming more widely used nowadays, notably for space exploration and satellite constellation (e.g. SpaceX). However, their physics is far from being well understood: many instabilities of different frequencies and origins are observed, and their influence on the plasma and the thruster behaviour is not clear yet.

Computer simulation seems to be the best way to understand and predict the behaviour of those thrusters. Such simulations are performed with the in-house code AVIP, which has both Eulerian and Lagrangian formulations. The objective of the thesis work is to establish the best formulation -Lagrangian, Eulerian or hybrid – for the fast, accurate and robust prediction of Hall thrusters. It will also be used to study the azimuthal instability characteristic of such systems.



3 Thomas Lafarge

Lattice Boltzmann methods applied to multiphase flows for the atomization of swirled injectors

The work of this thesis focuses on the simulation of multiphasic flows through Lattice Boltzmann methods. The Lattice Boltzmann methods are generally divided into four different methods: The gradient-color, the pseudo-potential method, the free energy and the mean-



field methods. Our thesis works mainly consist in a theoretical analysis of the different methods. We showed why the gradient-color method's recoloration step were equivalent to resolving the Allen-Cahn equation for the order parameter. We also investigated the use of Stiffened gas equation of state in the Lattice-Boltzmann framework, that allows to fixe one the main issue of gradient color method: spurious compressibility.