

Computational Methods in Applied Sciences

Pedro Diez · Pekka Neittaanmäki ·
Jacques Periaux · Tero Tuovinen ·
Jordi Pons-Prats *Editors*

Computation and Big Data for Transport

Digital Innovations in Surface and Air
Transport Systems



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This series publishes monographs and carefully edited books inspired by the thematic conferences of ECCOMAS, the European Committee on Computational Methods in Applied Sciences. As a consequence, these volumes cover the fields of Mathematical and Computational Methods and Modelling and their applications to major areas such as Fluid Dynamics, Structural Mechanics, Semiconductor Modelling, Electromagnetics and CAD/CAM. Multidisciplinary applications of these fields to critical societal and technological problems encountered in sectors like Aerospace, Car and Ship Industry, Electronics, Energy, Finance, Chemistry, Medicine, Biosciences, Environmental sciences are of particular interest. The intent is to exchange information and to promote the transfer between the research community and industry consistent with the development and applications of computational methods in science and technology.

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Foreword

People will pay any price for motion
—William Faulkner, *The Reivers*.

The world is in motion like never before. In the first quintile of the twenty-first century, we have witnessed a massive increase in the movement of materials, goods, and humans. Supply chains stretch across the globe, individuals are constantly traveling, and delivery times now are often estimated in hours or days as opposed to weeks or months.

Transportation is one the world's largest industry and central to the global economy. Its components include, railway, trucks and automobiles, planes, ships and barges, pipelines and warehouses as well logistics and distribution. Advances in computation now make it possible to gather, manage enormous data sets as well to utilize this data analysis for planning, recognition, and automatic decision-making. In the transportation and e-mobility sectors, information technology, data science, and artificial intelligence are playing a transformational role impacting all segments all sectors of the transportation sector, not only facilitating, operating, and managing transportation systems but also for the design and development of technology infrastructure to support these systems. Environmental concerns and sustainability that play a prominent role in the design and an efficient operation of transportation systems are a recurring theme within the context of this volume.

The present volume contains a compendium of papers presented at the ECCOMAS Thematic Conference CM3-2017: *Computation and Big Data for Transport—Digital Innovations in Surface and Air Transport Systems* held in Brussels, November 2017. The Brussels workshop is a sequel workshop to a workshop held at University of Jyväskylä in May 2015 that focused on big data modeling, logistics, distribution, and transportation. Both the Brussels workshop organizers and the participants recognized the paramount importance of cybersecurity for data driven, data operations, and control. For this reason, two papers on cybersecurity are added to the portion of the volume devoted to conference presentations.

Given the enormity transportation enterprise and the multiplicity of roles and potential role for data science and technology, a comprehensive survey would fill several library shelves. The present volume is only a small but hopefully

representative, sample. The contents subdivide into two parts: the first and larger portion is devoted to chapters of varying length and technical detail based on the presentations of the workshop and the second portion is the white paper. The workshop based material trifurcates in three thematic sections: Reviews and Perspectives, Computational Methods and Applications, and Translational Research. The bulk of the material focuses on selected sectors of transportation; included are contributions from the areas of urban mobility, logistics and distribution, maritime operations, aviation and railways. Environmental concerns and sustainability that play a prominent role in the design and an efficient operation of transportation systems are a recurring theme within the context of this volume. Conversely, neural networks and deep learning algorithms can be developed to assess environment quality from large data sets mounted on aerial platforms both manned and unmanned. The reliance of transportation systems in all sectors coupled internet connectivity render these systems vulnerable to cyberattack and there is the present concern (risk) of catastrophic software failure.

Although the modes of transportation are still same, much has changed since the beginning of the 21st century. Moreover, there is a heightened awareness of the necessity of addressing environment concerns and societal needs. The upcoming decade will present challenges in all sectors of transportation as well as we utilize computational science, data science, and artificial intelligence/deep learning technologies to design, implement, and operate more efficient, safer, and greener system that account for evolving societal needs. The volume's first section is a white position paper required by a team of DG Research and Innovation Policy officers from the European Commission, and coauthored by selected conference participants and outside experts, which provides input on these challenges.

To conclude, we can assess the role of big data and associated data science and technology by returning to William Faulkner with the paraphrase The Reivers, *The future is not yet unborn, it is not even the future.*

September 2019

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Preface

Multidisciplinary Scientific Computing is now one of the powerful design technologies used in industry. This trend has been enhanced by the ever-increasing capabilities of computational technology, storing of information, and the decreasing cost of computer hardware. Analysis of Multidisciplinary Big Data is also becoming extremely important in process control, intelligent systems for surveillance and safety procedures.

In this edited volume, we have chosen contributors that will share their perspectives on the new societal challenges about greener, safer, and more digitalized Surface and Air Transport. In the book, we will debate on future software and methods needed to master new greener technologies. We have organized articles under three specific topics: Automotive/Mobility, Aeronautics and Marine/Maritime. Articles are summaries from panel discussions in which seniors experts from Industry, Governmental Organizations, and Academy have addressed current issues and trends in greener technologies. Aim is to establish an efficient software roadmap for the design of new intelligent multimodal products constrained by economical and societal imperatives. The target of this book is bringing together academic and small and large industries experts and knowledge in the fields of Computational Methods and Tools for Transport and its Applications.

The content of this volume is organized into three main sections with 12 contributions in the above disciplines classified as follows:

1. White paper
2. Reviews and Perspectives
3. Computational methods
4. Translational Research

The book begins with so-called White Paper, recommendations for decision-makers in the Europe. Second part is dedicated to overview articles. Third part contains more technical and methodological issues. Finally, in fourth part we introduce the chapter related translational research. The book is addressed to researchers and technology experts in the fields of “Greening Transport”, ranging from innovative

computational methods to software tools used for solving challenging industrial and societal problems in Transport.

The editors would like to thank Ms. Jaana Räisänen for helping in the technical editing of the book. We would also express our gratitude to Ms. Nathalie Jacobs and Ms. Anneke Pot from Springer publishing house and to Prof. E. Onate, CIMNE Director and Editor of the Series Lectures Notes in Numerical Methods in Engineering and Sciences for their fair patience in receiving the material of this volume.

This book is based on invited articles collected after the CM3 2017 Conference (Computational Multi physics, Multi Scales and Multi Big Data in Transport Modeling, Simulation and Optimization) which was the second of a series on European Conferences on Green Challenges in Transport which took place at Brussels, Belgium on November 22–23, 2017. The conference was organized by UPC/International Center for Numerical Methods in Engineering (CIMNE) with the University of Jyväskylä in association with the European Commission (EC) DG Research and Innovation. This series of Thematic Conferences on Transport was originally launched by the Industry Interest Group (IIG) of ECCOMAS with main following objectives: strengthening the industrial liaison and developing contacts between ECCOMAS and the different DGs of the European Commission.

Jyväskylä, Finland
September 2019

Pedro Diez
Pekka Neittaanmäki
Jacques Periaux
Tero Tuovinen
Jordi Pons-Prats

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Part I
White Paper

Chapter 1

Digital Technologies for Transport and Mobility: Challenges, Trends and Perspectives



Pedro Diez, Jacques Periaux, Tero Tuovinen, Jaana Räisänen, Martti Lehto, Adel Abbas, Carlo Poloni, Trond Kvamsdal and Chris Bronk

Abstract This white paper aims at presenting the ideas emerging from the different fields pertaining to transport and mobility, to describe the capacities of current state-of-the-art digital technologies and the perspectives that are expected to shape the future of transport and mobility.

Keywords Surface transport · Aeronautics and aviation · Cyber security · Logistics

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1.1 Introduction

Technologies for transport and mobility face incredible challenges created by globalization, the need of mitigating climate change, the change of social behavior (evolution of the demand toward more and more personalized services), and the full digitalization and automation (that is vulnerable to security breaches in the cyber space). Considerable efforts were performed in the last decades in improving the vehicle technologies, engineering optimization, and Information and Communication Technologies. All of them boosted by the amazing progress in data science and engineering. Such efforts ignite new and powerful computational methodologies that should be capable to cope with the complexity of decision-making in such a rapidly evolving arena. Particular attention is to be paid to the challenges and paradoxes prospected after the implementation of Autonomous Driving Systems in the different transport modes.

In the era of Big Data, modern decision makers in transport and logistics must be able to deal with enormous amounts of information and a variety of heterogeneous data sources. New vehicles with electric or hybrid engines will soon access the road network introducing totally new problems and opportunities. Decisions have largely widened their scope moving toward large scale and integrated time horizons in which several components of the supply chain or transport planning are jointly considered, allowing for increased efficiency and robustness of the solutions. These continuously changing scenarios thus will require innovative paradigms both to predict short-term events and long-term trends and to draw optimized decision patterns considering analysis of data variability and richness.

The attention to environmental sustainability in the recent years has attracted a huge attention of the researchers and of the industry, motivated by the fast growth in Greenhouse Gas emissions produced by transport modes over the last decades. To mitigate this trend, several technologies have been developed. On the technological side, carbon intensity can be lowered through the introduction of biofuels and alternative energy carriers (electricity and hydrogen). Today, the diffusion of electronic vehicles is modest, mainly due to the higher costs and limits in travel autonomy with respect to the traditional vehicles. From the optimization and management point of view, electric and hybrid vehicles will present new and complex challenges for which the study is still at an early stage. On the behavioral side of transport, Green House Gas (GHG) emissions will be reduced through policy choices that help decision makers selecting transportation options lowering GHG emissions.

The modal share of passenger mobility and freight transport will be shifted from carbon intensive options (air, passenger cars, and trucks) to fewer intensive ones (public transport and non-motorized modes for passengers; rails and inland water-

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ways for freight). Car-sharing systems will become increasingly environmentally friendly electric vehicles.

The generalized impact (including the extremely sensitive environmental issues) and cost of transport will be decreased by a more efficient organization and allocation of transport movements and its efficiency will be boosted by the introduction of radically new design of distribution networks. This is a tremendous change in the structure of future freight distribution and transportation, which need substantial investments in shared infrastructures and new handling and packaging technologies.

To answer to these changes, new digitalized software will strongly require the design of fast and accurate optimization algorithms that will synchronize and plan all transportations activities. Such new tools must incorporate Big Data predictive methods capable of anticipating the dynamic evolution of traffic conditions and shipment progress.

The remainder of the white paper is structured as follows. Three different thematic areas or disciplines are treated in separate sections:

- Surface Transport,
- Aeronautics and Aviation and
- Cyber Security.

Each of these sections has the same structure, consisting in three subsections:

- **Current situation and challenges.** Aims at presenting the state-of-the-art methodologies and the current challenges of digital technologies in the fields pertaining to applications to transport and mobility.
- **Trends.** Current methodological trends are described. The presentation is structured in terms of the digital tools and algorithms used in every sector.
- **Perspectives/Recommendations.** Draws a short summary of the technologies expected to play a significant role in the digitalization of transport and mobility, as identified in the previous section.

1.2 Surface Transport

1.2.1 *Current Situation and Challenges*

In surface transport (including Automotive, Railway and Maritime transport modes), the Computational Science and Engineering (CSE) (based upon Mathematical and Computational Modeling (MCM)) is currently driving design and development processes (and many others). Actually, CSE generates an “application pull” (i.e. advances within a given application area increasingly depend on the availability of numerical techniques). It is itself driven by a “technology push” (i.e. its development depends on a market for applications).

The Digital Twin concept is seen as an enabling technology for developing new paradigms for energy efficiency, safety and product lifecycle.

The automotive industry faces challenges in which a full digital development process is required. These challenges affect the following areas of application:

- Safety: in particular Human Body Modelling (HBM) and Full-body vehicle crash.
- Environmental impact: in particular Computational Fluid Dynamics (CFD) and Lightweight structures.
- Comfort

Urban mobility challenges are to deal with new disruptive transport services and changes in travel behaviors in the “Mobility as a Service” (MaaS) context... Accordingly, car industry has started diversifying its portfolio, from selling vehicles to selling services.

Statistical models are now more sophisticated (increase in computation power and amount of data available). This allows evolving from trip-based models to activity-based models.

Hybrid Analytics/Hybrid Modelling is defined as a modelling approach that combines the interpretability, robust foundation and understanding of a physics-based approach with the accuracy, efficiency, and automatic pattern identification capabilities of advanced data-driven machine learning and artificial intelligence algorithms. Although the why and what of hybrid modelling/analytics is reasonably understood, more focused research is required to develop innovative methods of combining the domain knowledge, physics based and data driven models.

1.2.2 Trends

- Simulation and data assimilation: data-driven models.
- Optimization and Uncertainty Quantification
- Decision-making support based on data: model-driven data.

The novel trends in Computational Mechanics applied to the car industry consist in using Big Data tools and AI to speed up the computational process. The complexity of the computations (CFD, crashworthiness...) preclude doing standard parametric analysis when the design has a large dimension (the number of parameters is large: in realistic case it is huge). Facing this challenge (it is day-to-day business because it arises from optimization, uncertainty quantification, and data model updating) requires combining Big Data techniques and Artificial Intelligence (to standardize input data and to reduce the number of active parameters) with Reduced Order Models (ROM, allowing to build a computational vademecum from previous computation that turns new computations into a simple post-processing).

Focus should also be on developing methods to bound the errors, and uncertainties and proving the stability of the algorithms. Innovative methods, standards and guidelines are required to process data with appropriate security and to handle IPR, if possible, based on open data platforms.

Digital Twins targeting Industry 4.0 are specially well suited to assimilate data into the model. This requires combining

- Machine Learning (or Artificial Intelligence) techniques to analyze data, eliminate redundancies, convert data into information and eventually reduce the number of parameters that describe the system to be analyzed.
- Reduced Order Models to drastically increase the efficiency of the numerical models (multiple and extremely fast queries to the model are required).
- High Performance Computing to implement in a realistic manner both Machine Learning strategies and Reduced Order Models (ROM).

In the context of Urban mobility, the models are drastically evolving because they have to account for social, demographical, mobility and environmental aspects (here mobility refers to the transport modes themselves and the environmental aspects are mostly related with urban or built domains). This requires incorporating in the model variables that pertain and are able to represent perceptions, attitudes and lifestyle for all the social groups. It is of particular interest the so-called millennials because their mobility pattern is disruptive with respect to the previous generations and it is expected to be the dominant behavior in the near future.

The models that are used in the context of Urban Mobility are evolving from the classical aggregated models (in which travel demand is specified as aggregated transport flow between zones) to agent-based models that maintain travel demand at the level of individuals throughout the model. In fact, models based on individual level data sources improve aggregate level models in terms of policy appraisal. This result in the trend of integrating Activity-Based models and Agent-Based models to simulate complex mobility systems in large cities with intricated multimodal transport, with public (or mass) transport systems overlapped to individual transport means. Moreover, both are evolving rapidly and a stable configuration is far of being reached.

1.2.3 Perspectives/Recommendations

From the perspective of simulation and data assimilation, in the very next future, transport technologies will generate an enormous amount of heterogeneous data from sensors (in every discipline of transport and mobility). This opens the way to incorporate data into the models. Keywords like “*Sensor data fusion*”, “*Hybrid Modelling*”, and “*Big data Cybernetics*” pertain to the ideas of using real-time acquired data to update, improve, correct and validate the models leading to a more informed decision making.

- There is a genuine concern from the sector to
 - Deal with data provided by an enormous quantity of sensors in order to incorporate them to the models and allow making better decisions.
 - Reduce the computational burden of the simulations, making use of previous numerical experiments (snapshots) and to build a ROM using techniques like Proper Orthogonal Decomposition (POD) and Proper Generalized Decomposition (PGD).
 - Use data to improve models (data assimilation, parameter identification, model updating...)
 - Use models to qualify, select and understand data.
- These inquietudes may be formulated as a necessity of work in developing both
 - Data Driven Models: it referred originally to constitutive models based on data rather than on physical laws. Currently is a more flexible concept allowing to incorporate in the model information (that is, data treated using Machine Learning) and minimize the mismatch between the model and its observed outcomes.
 - Model Driven Data: this new concept refers to the necessity of using models in the data interpretation, filtering and postprocessing. In practice, it introduces Mathematical and Computational Modelling in the Machine Learning process. In other words, the intelligence of the models (physical laws, balance equations, thermodynamics...) is supporting the Artificial Intelligence algorithms that are initially conceived as a data crunching machine. Not all the information is contained in the data.

New strategies in urban mobility for data collection, accounting for multimodality. Prediction of behavior of complex systems using Machine Learning generated surrogate models.

1.3 Aeronautics and Aviation

1.3.1 *Current Situation and Challenges*

In air transport new capabilities will be essential in exploring new concepts including alternative configurations, engine integration, flow control technologies, laminar flow designs, and other new approaches enabling the necessary step change in performance on which the industry is relying. Designs employing numerical optimization simulation technologies are and will be also considered to ultimately provide capabilities that can underpin future aircraft design processes.

Aircraft design is a very competitive and demanding field. Highly optimized design with the objective of lower fuel consumption, lighter, quieter, safer, good

performance and handling qualities involves a large number of different disciplines (aerodynamics, structure, system, vibration, acoustic, etc.) in the design process.

An advanced toolset acting as a virtual facility, providing full information about design status, is the target of the European Aircraft industry. Numerical simulation tool is an essential target for every company involved in aeronautics. Unfortunately, such a tool or toolset does not exist today, however there is an evidence that such a capability needs to be put in place, if the aerospace industry is to meet future performance and environmental targets. Industrial numerical optimization simulation tools are still suffering two main drawbacks that prevent their full industrial deployment for massive applications.

1.3.2 Challenges for Improved Aircraft Design

Detailed aerodynamic analysis is used to judge on progress with respect to aerodynamic and overall aircraft performance.

Although fast strategies to find the optimum for multi-disciplinary design in 3D are still under development, the aircraft industry already uses optimization algorithms for detailed design tasks. However, there is a need to further explore available multidisciplinary design techniques since they represent a significant potential in enhancing design. For today's aircraft designs it has been achieved about 46% aerodynamically more efficient aircraft design compared to the first Airbus A300.

This multidisciplinary design process involves three different areas of actuations offering large number of opportunities for improved aircraft design:

- Search for lower engine fuel consumption;
- Aircraft primary structure weight reduction technologies;
- Drag reduction technologies.

Viscous drag currently is the area with largest potential for drag reduction. The ultimate challenge in the aircraft multidisciplinary design process on one side is to successfully integrate the right technologies into an optimal configuration that balances conflicting design objectives and meets the numerous design constraints present in real world design problems (i.e. operations, manufacturing...)

On the other side, the need for robust and sufficiently accurate prediction (numerical simulation technology) and trading capabilities to understand the main drivers and technologies that are essential to the delivery of a good overall product.

Further industrial needs require extending demands on aerodynamics shape optimization and highlight the needs for:

- Faster and more comprehensive Aero data production capability
- More efficient aerodynamic data production capability— increased data set containing steps into nodal data delivery

New and advanced technology steps require:

- Reliable and efficient simulation of mounted rotating prop-fan engines properly validated, including unsteady and flexibility effects.
- Reliable validated laminar/turbulent transition prediction capability Proven simulation capability for alternative high lift solutions (e.g. Krüger).
- Much faster aerodynamic data production capability,
- Most accurate physical modelling of flow control devices (active and passive).
- Aerodynamic data on surface level, as a complete electronic model.

1.3.3 Trends

Role of Numerical Simulation in Aircraft Design

On top of the objectives to improve aircraft design performance, another major objective is the reduction of aircraft development lead-time and the provision of robust optimal multidisciplinary designs. It is important to exploit any opportunity provided by enhanced or new classes of numerical simulation tools, in particular high fidelity multidisciplinary Computational Fluid Dynamics (CFD) and powerful High Performance Computing capabilities.

Presently, numerical simulation is regularly used in the design chain, by most (if not all) of aircraft industries (Airbus, Boeing, Dassault Aviation...) reducing the number of design options to be tested in wind tunnel. This trend, in spite of its current limitations, will continue to grow over the next decade. Progress in HPC will essentially contribute to achieve this goal.

Maximum accuracy is obtained by the direct numerical integration of the Navier–Stokes equations, however, the existing computational resources or the way we manage these resources, is still not enough to capture the small scales present in turbulence.

Numerical Simulation/Optimization State-of-the-Art

It is clear that design flaws have to be avoided at any cost, as their correction late in the process requires substantial economic cost and time and is in many cases even impossible to correct. Numerical simulation/optimization is one of the most important means to realize this objective.

There are at least two ways to perform such design optimization process, which ideally would happen on an almost “real time” basis: Flying by the equations and Flying through the database. The former consists of the definition of the overall aircraft model, which will ultimately translate into between 500 million to 1 billion nonlinear equations which have to be resolved during each reiteration in a time-accurate manner. The latter exists of the modeling of hundreds of pre-computed solutions throughout the flight envelope which will form a proper basis for interpolation to represent the whole mission range.

Airbus, and others European aeronautical industries, has a vast interest in the further evolution of this field, and so is actively pursuing advanced research in this area, in most cases in formalized programs looking for the cooperation with partners from recognized R&D institutes and universities active in this area with the ultimate objective to make aforementioned vision a reality. Major areas of interest among others are: High fidelity flow Simulation capability; Parametric aircraft—shapes and aero data model; Highly efficient numerical simulation & optimization; High performance computing, latest processor and hardware architecture.

Generally, planned activities target the radically improvement of existing simulation capability on two main aspects:

- Accuracy (physical modeling and algorithms)
- Efficiency (numerical algorithms and advanced computing)

Technology Streams for Improving Accuracy

Apart from physical modeling (turbulence modeling), on the numerical side the way to solve this problem has been focusing mainly on local preconditioning methods.

Other important line of research is focusing on the development of new numerical methods/new schemes better adapted to stiff problems.

The correct simulation of flow separation onset is quite challenging. It is characterized by the limit between steady and unsteady solutions, with coexistence of compressible and incompressible flows. The correct prediction of flow separation is important for the industry, since it has a very strong impact on the design of high-lift devices and buffet on set determination.

Technologies Streams for Improving Numerical Efficiency

Preliminary estimations amount in 10⁵ the number of simulations required in a design optimization process. A speed-up factor estimate for a typical computational requirement of around 10⁶ compared to current computational capabilities. MPI or pure threaded applications will be replaced by hybrid MPI-threaded (Open MP, CUDA, Open CL, etc.).

The question is: are the current simulation solvers mature enough to take full advantage of these technologies? The answer is yes, but at a modest degree. Aeronautical industry is aware of this; the development of fully new code from scratch requires billions of Euros worth of investments and consumes multiple years. On the other side, update of exiting industrial solvers is a slow process. Numerical algorithms need to face substantial developments in order to cope with these new technologies.

Innovative Procedures for Improved Scalability

Today, the parallelization of numerical simulation/optimization solvers used in the European aeronautical industry is based on domain decomposition and MPI communication.

In order to reduce the overhead of the domain decomposition approach a hybrid parallelization strategy can be applied by using MPI parallelization between compute nodes and shared-memory parallelization. This additional level of parallelism is of importance for increasing number of cores which can be supported by heterogeneous hardware using accelerators, such as GPUs.

1.3.4 Perspectives

Algorithms for Improved Efficiency

CFD solvers used by the aeronautical industry in Europe are mainly finite-volumes based methods, with central or upwind discretization. In general, solution algorithms for the Navier–Stokes equations are based on iterative algorithms with explicit (Runge–Kutta) or implicit (Newton) formulas to solve the residuals.

Another potential area for improved efficiency is parallel grid manipulation algorithms. On this line, Chimera techniques adapted to parallel architectures with focus on efficiency as well as on improved accuracy in data transfer between meshes will be of great interest.

Grids

Geometrical modelling is necessary to allow the designer to construct and modify aircraft components and shapes. There is still a lack of automatic assembly due to imperfections of the CAD systems, non-conformal use of those tools by the designers and too strict requirements of the follow-on numerical mesh generation process.

Mesh related problem is not only confined to geometrical description, but mesh has also strong impact on accuracy and efficiency of the numerical solver. Different ways to obtain the error of the solution and use this information to adapt the meshes are under study such as: adjoint or local error estimation.

Another possibility will be to use mixed (hybrid) meshes techniques, i.e. an integrated combination of structured, unstructured and chimera mesh discretization's. Hybrid meshing technology has recently reached a high degree of sophistication however many issues are still unsolved and require further research.