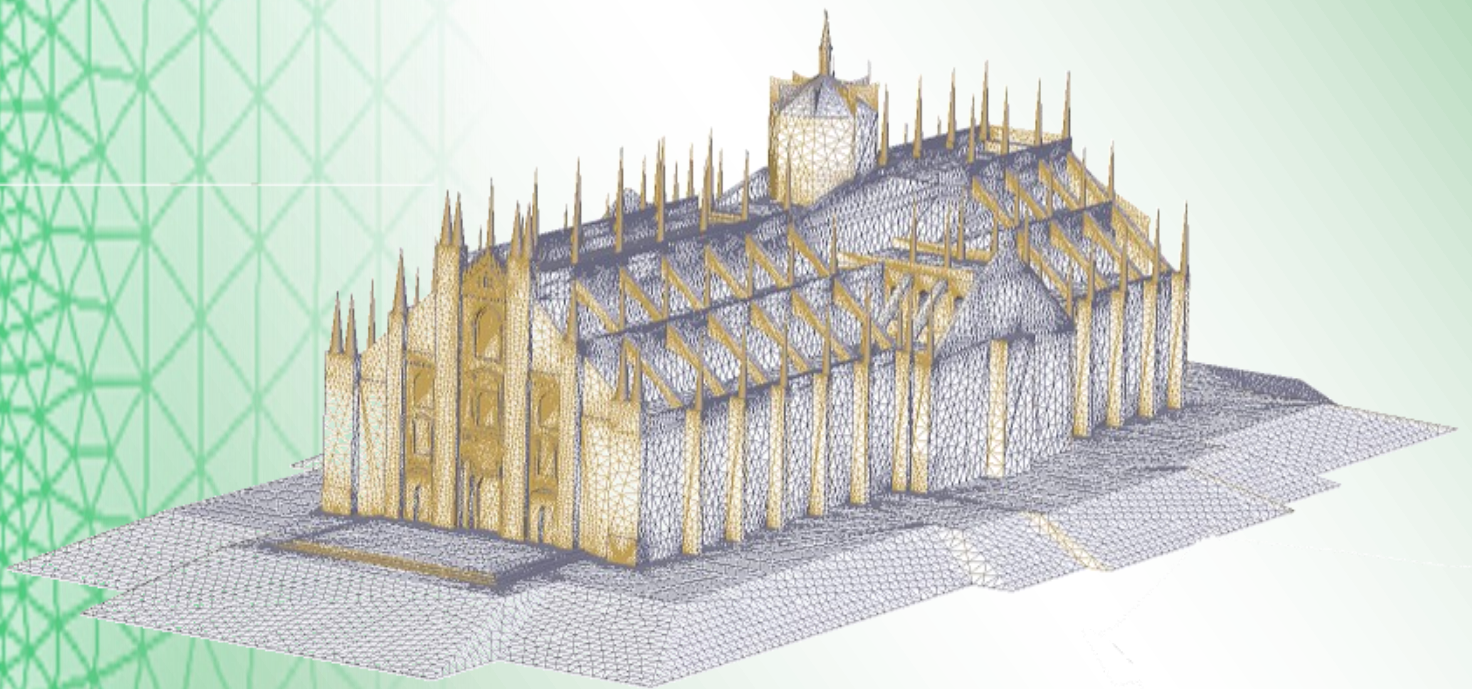




EUROPEAN COMMUNITY ON COMPUTATIONAL METHODS IN APPLIED SCIENCES

ECCOMAS NEWSLETTER



JANUARY 2017

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ECCOMAS NEWSLETTER — JANUARY 2017

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MESSAGE OF THE PRESIDENT

NEWSLETTER FOR ECCOMAS CONFERENCES IN 2017

The main purpose of the current ECCOMAS Newsletter is that it will be distributed in particular to all participants of ECCOMAS Conferences in **2017**. These are the 35 Thematic Conferences (TC) (<http://eccomas.cimne.com/vpage/1/14/2017>) and the ECCOMAS Young Investigators Conference YIC 2017, see below. The TCs cover the entire thematic spectrum of ECCOMAS from Computational Solid & Structural Mechanics (CSM), Fluid Dynamics (CFD), and Applied Mathematics (CAM) to Scientific Computing (SC); traditionally an emphasis lies on topics within CSM. Most of the meetings are part of a series of conferences which took place in several previous years before. One conference is in particular worth mentioning, namely the International Conference on Computational Plasticity (COMPLAS) which started 30 years ago, some time before ECCOMAS was founded. As some other TCs it has a strong intercontinental orientation

conferences of up to 450 participants still focused on a main topic. In 2015 over 3700 people attended the 25 Thematic Conferences. In 2017 we face the 7th edition with a substantial increase in number of conferences. It can be stated that the system of ECCOMAS Thematic Conferences taking place in odd years is really a success story.

FURTHER FUTURE CONFERENCES

For **2017** I again would like to refer to the ECCOMAS Young Investigators Conference YIC 2017 organized by the Polytechnic University of Milan 13-15 September 2017 (<https://www.eko.polimi.it/index.php/YIC2017/conf>). It is chaired by Massimiliano Cremonesi, Assistant Professor at POLIMI, and is the 4th edition of the series of YICs after those in Aveiro (Portugal), Bordeaux (France) and Aachen (Germany). YIC Conferences are exclusively organized in odd years and run by Young Investigators, or – as we used to say - “for young scientists from

young scientists”, i.e. the target groups are PhD students in all stages of their PhD programs, postdocs and young researchers from academia and industry under the age of 35.

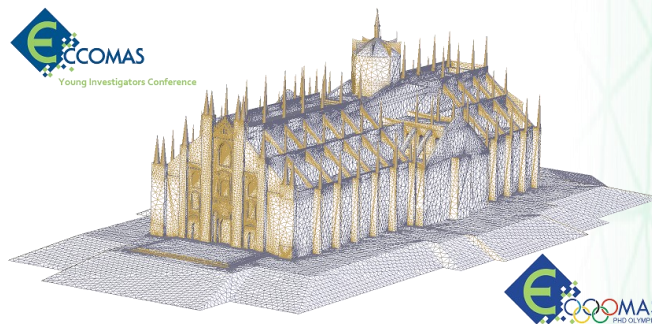
YIC 2017 comes along with the 7th ECCOMAS PhD Olympiad. In this event every Member Association is represented by a number of selected PhDs submitted for consideration for the two ECCOMAS PhD awards (<http://eccomas.cimne.com/vpage/1/18/RulesConditions>).

As known ECCOMAS organizes the European Conferences on Computational Mechanics (Solids, Structures and Coupled Problems) ECCM and on Computational Fluid Mechanics ECFD in even years, alternating with the ECCOMAS Congress; the last Congress took place in Crete 2016 with over 2200 participants. ECCOMAS decided again merging the two Conferences in **2018** under the condition that the two individual parts have equal rights and keep their own identity. This joint ECCM – ECFD 2018 Conference takes place in Glasgow (UK) 11-15 June 2018 (<http://www.eccmecfd2018.org/frontal/default.asp>). It is hosted by the University of Glasgow and the University of Edinburgh and organized in partnership with the UK



indicated by the label “IACM Special Interest Conference”.

Originally ECCOMAS Thematic Conferences were supposed to be small highly specialized meetings with up to 100 attendees. However it turned out that the format was also best suited for medium size





Association for Computational Mechanics in Engineering (UKACM). For ECCOMAS it is a very special conference because the Association celebrates its 25th anniversary during the meeting.

The calls for the Thematic Conferences as well as the YIC conference in 2019 have already been started end of last year. The final decisions on this issue are scheduled for the board meetings of ECCOMAS in May 2017.

Joining big conferences makes a lot of sense when clusters of big conferences in close thematic neighborhood take place in the same period of the respective year. This is true in 2018 and will be also the case in 2020. The International Association for Computational Mechanics (IACM) organizes their World Conference WCCM again in Europe. It was obvious that both organizations IACM and ECCOMAS decided merging again their main conference events in 2020, as it was successfully done previously. After a

joint call for tender leading to excellent proposals, and a secret selection procedure by their main boards both associations decided to choose Paris as the venue for the combined ECCOMAS Congress 2020 and the 14th World Conference on Computational Mechanics on 19-24 July, 2020.

ECCOMAS ADVANCED COURSES, SCHOOLS AND WORKSHOPS

ECCOMAS' Bylaws define among others the objective to stimulate and promote education in its field of operation. Following this objective the Managing Board decided in its meeting in Crete 2016 to launch a program for the organization of *ECCOMAS Advanced Courses, Schools and Workshops*, for simplicity denoted as ECCOMAS Advanced Courses (EAC). The project could be denoted a twin program to the successful series of Thematic Conferences.

Three different types of Advanced Courses can be distinguished:

1. Stand-alone courses not related to other ECCOMAS events or other scientific institutions, in arbitrary times and locations in Europe,
2. Courses in cooperation with other scientific institutions, as for example the CISM-ECCOMAS International Summer Schools,
3. Courses taking place in the framework of ECCOMAS events, such as ECCOMAS Congresses, ECCM and ECFD Conferences and ECCOMAS Thematic Conferences, as pre- or post-conference events.

Equivalent to the procedure for the TCs ECCOMAS will support each EAC by disseminating the event via entries in its website, through regular email announcements, on conferences and its newsletter. Further rules and conditions are defined on the website:

<http://eccomas.cimne.com/space/1/19/advanced-schools-and-courses>.

I would like to mention two very successful examples for EACs, the CISM-ECCOMAS International



Summer School 2016 on Fluid-Structure Interaction in Udine and the ECCOMAS Advanced School on Isogeometric Analysis in Crete in connection with the ECCOMAS Congress 2016.

As for the Thematic Conferences also the Advanced Courses should follow the ECCOMAS corporate visual identity; related brochure templates with a dual layout are given on the website. They allow enough flexibility for the individual layout of the respective event. For the homepages of courses see the examples for the TCs in the website.

The ECCOMAS community is encouraged to join this program which could and should be as successful as the TCs.

AWARDS

After conducting severe selection processes several ECCOMAS Awards could be presented during the ECCOMAS Congress 2016 in Crete. It is important to note that candidates for the ECCOMAS Medals as well as the young scientist awards can be nominated by every individual member of ECCOMAS or from the member associations. The awardees are selected by an award committee by secret voting.

The highest distinction, the Ritz-Galerkin Medal, was awarded to Franco Brezzi, Professor of Mathematics at the University of



Pavia, Italy, for his outstanding, sustained contributions in computational methods in applied sciences during a substantial portion of his professional life, so to speak as a “life time award”. Two distinguished scientists were honored for their brilliant work in a selected field: Professor Ferdinando Auricchio, U Pavia, for computational solid and structural mechanics by the Leonard Euler Medal, and Wolfgang A. Wall, TU Munich, for computational fluid dynamics by the Ludwig Prandtl Medal. The two awards for young scientists, the Lions Award in Computational Mathematics and the Zienkiewicz Award in Computational Engineering Sciences, were presented to Lourenco Beirão da Veiga, U Milano, and Antonio Javier Gil, U Swansea, respectively.

The best PhD thesis awards for the year 2015 were proposed by ECCOMAS Member Associations and selected by a PhD Awards Committee. The winners were Ursula Rasthofer, TU Munich, and

Federico Negri, EPFL Lausanne.

We from ECCOMAS congratulate all awardees for their excellent research.

RESUME

The four years term of the present administration ends in May 2017. An assessment of our work can and should only be done by the membership. We tried to improve the management for the association and consolidate existing building blocks, but also implement new structures. These elements are related to the efficiency of the three boards, General Assembly, Managing Board, and Executive Committee, the reactivation of the four ECCOMAS Technical Committees, and definition and refinement of rules and conditions for the major activities of our Association. I would like to refer to a few selected actions:

safeguarding the financial situation for the future, nomination and selection of awards, set up rules and

Ritz-Galerkin Medal



Franco Brezzi

Euler Medal



Ferdinando Auricchio

Prandtl Medal



Wolfgang A. Wall

Lions Award



Lourenco Beirão da Veiga

Zienkiewicz Award



Antonio Javier Gil

PhD Awards 2015



Ursula Rasthofer



Federico Negri



Ekkehard Ramm Ferdinando Auricchio



Pedro Diez Josef Eberhardsteiner



Rémi Abgrall Cristina Forace

THE OUTGOING TEAM

conditions for all conferences, proposal and selection of plenary and semi-plenary lecturers for the large ECCOMAS Conferences, improving the dissemination of ECCOMAS activities, update the content of the website, establish a new program for ECCOMAS Advanced Courses, Schools and Workshops (see above), renewal of the cooperation with the Centre for Mechanical Sciences (CISM) in Udine, etc. A particular important aspect was the reactivation of the ECCOMAS Young Investigator Committee (EYIC). It turned out that the group started with a new momentum coming up with a lot of novel ideas. I have to confess that this was a special highlight in my term as president.

Of course we also faced the one or the other difficulty in running such a scientific association like ECCOMAS, based on voluntary input and a lot of idealism of the acting members in the administration. We recognized that the information flow between us as the officers and members of boards and committees on the one hand and the individual members of the member associations on the other hand was by far not optimal. Having only national and regional associations as members of ECCOMAS and no direct link to their personal members is a situation which should be reconsidered in the future. Based on a suggestion of the Managing Board the Executive Committee recently started an intensive discussion how this

obstacle and some other difficulties can be overcome. Respective recommendations will be made for the next administration.

THANKS

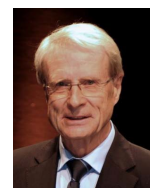
I would like to express my particular thanks to all who substantially supported our work in ECCOMAS. Let me start with Manolis Papadrakakis and his team in Athens for the perfect organization of the wonderful ECCOMAS Congress 2016 in Crete. It was a great success. Thanks also to Bert Sluys for preparing the present Newsletter as a guest editor together with Panagiota Kouniaki in Athens as technical editor in a perfect manner, and to all authors for their contributions.

The support by the officers in the Executive Committee (EC), in particular by both Vice-presidents Ferdinando Auricchio and Pedro Diez and the Treasurer Rémi Abgrall, is highly appreciated. Without the extraordinary assistance by the Secretary Josef Eberhardsteiner my work as President would have not been possible; thank you so much for the exchange of many ideas and initiatives over the entire time.

The commitment of the heads in our Barcelona office, Iztok Potokar and since March 2016 Cristina Forace, was and is of great value for all of us.

I am also grateful for the support by the members of the boards, in particular in the Managing Board (MB); I appreciate the constructive input and the positive working atmosphere. I would like to include the chairmen of the four Technical Committees and of the Young Investigator Committee for their assistance in many aspects of the daily work; it was a definite advantage including them as guest members in the EC and the MB.

Last but not least we all should be thankful for all personal members being engaged in the many activities of ECCOMAS, especially as conference and mini-symposium organizers, lecturers and participants. Their contributions make ECCOMAS a very successful scientific organization with a great promise for the future. For me as President it was a valuable experience. The best wishes go to the new administration!



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HOW APPLIED SCIENCES CAN ACCELERATE THE ENERGY REVOLUTION - A PLEADING FOR ENERGY AWARENESS IN SCIENTIFIC COMPUTING

1 INTRODUCTION

1.1 SCIENTIFIC COMPUTING CANNOT CONTINUE TO BE DONE THE WAY IT HAS BEEN

There is no denial that the transition from nuclear- and fossil-driven energy supplies to more sustainable options is one of the most challenging tasks of our time. While this transitioning is usually referred

to as 'the energy revolution' its basic pillars are not limited to alternative energy production but also are agreed to include better energy grids as well as more energy-efficient *consumers*. In this sense computing in general and particularly scientific computing as the basic tool for applied sciences contain a great deal of energy consumption since the computers (devices), compute clusters and data

-/compute centers do.

Recently the Semiconductor Industry Association (SIA) released a report where a prediction on the world's total energy production was made alongside an analogous prediction for the energy consumption of the world's computers [SIA 2015]. In order to demonstrate the urgency of what shall later be proposed here let us first summarize these findings. For this purpose consider Figure 1. Here the world's total energy production is extrapolated with a comparatively slow increase leveling out at approximately one Zettajoule in 2015. Speaking on these scales this value is not expected to increase much in this century. On the demand side energy consumption due to usage of computers is expected to increase much faster: Based on current technology (with today's (digital) computer technology and the way single devices are built and clustered to larger units) the total energy consumed (only by computing) will exceed the world's energy

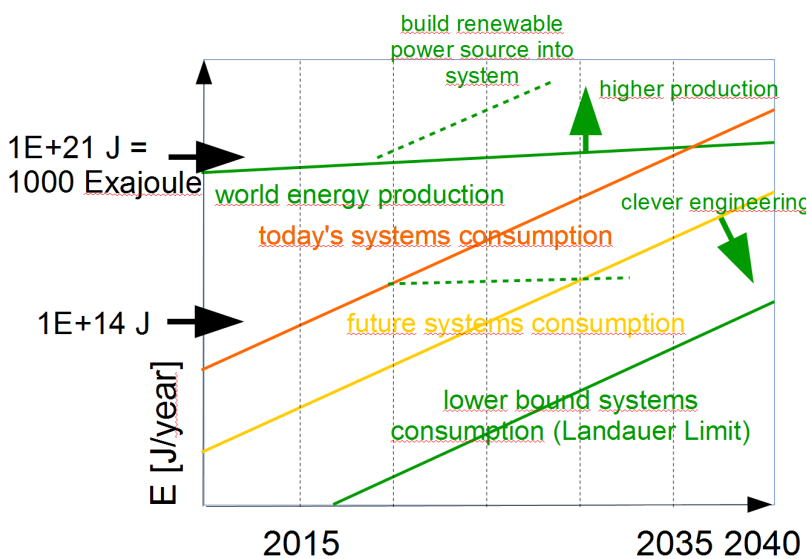


Figure 1. Prediction of world's total energy production and overall energy consumption by computing based on [SIA 2015]

production and supply by around 2040. Even based on extrapolating current technology to a hypothetical future technology level (mainly based on improved manufacturing processes leading to smaller transistors) this would lead to only an insignificant delay of this point in time. Consider this as the catastrophe that it is: No additional electrical device would be able to be plugged into the power grid any more. Applications on the other side are continuing to increase their hunger for ever more computational resources. Consider the lowest plot in Figure 1. It represents a theoretical lower bound for the energy consumption per year based on a hypothetical device that needs the minimum amount of energy to flip a bit of information. This limit is called the Landauer Limit. Due to an increasing demand for computational capacities this limit will also be increasing over time since more and more computers will be built. It is more or less increasing with the same rate as today's or close future's computer systems' consumption and such optimal computers would therefore also only postpone the inevitable.

1.2 HARDWARE AND SOFTWARE IN APPLIED SCIENCES ARE BLIND ON THE 'ENERGY EYE'

Today's compute and data centers mostly rely on massively parallel distributed memory clusters. The compute nodes are also multilevel parallel and heterogeneous. They usually comprise one or more high-end server CPUs based on the x86, Power, or SPARC architectures optionally accelerated by GPUs or other (accelerator) hardware. Large HPC sites of this type have substantial energy requirements so that the associated expenses over the lifetime of the system may

exceed the initial acquisition costs. In addition, the energy supply for supercomputers is not always an integral part of its overall design - consumers (such as the compute cluster, cooling, networking, management hardware) are often developed independently from the key technologies of the energy revolution, e.g. renewable energy sources, battery and power grid techniques. Taking a look at the largest supercomputers today it can be observed that as a consequence of decades of performance-centric hardware development there is a huge gap between pure performance and energy efficiency in these designs: The Top500 list's best performing HPC system (dissipating power in the 20 Megawatts range making a power supply by local solar farming for instance an impossible-to-achieve aim) is only ranked 84th on the corresponding Green500 list whereas the most energy-efficient system in place only performs 160th in the metric of raw floating point performance [Meuer et al. 2015; Feng et al. 2015]. It is well known [Schäppi et al. 2009] [Lawrence Berkeley National Laboratory 2006] that 40–60% of the energy consumption of an HPC site can be attributed to the compute nodes (processors and memories).

Using and developing scientific *software* on the other hand requires knowledge of the specific target hardware architecture which implies adjustments of numerical methods and their implementation. Otherwise efficiency losses are axiomatic and always imply too much energy spent. Therefore scientific software should not follow a hardware-oblivious design paradigm. In the resulting performance engineering studies for decades energy efficiency has been eclipsed by computational performance and only recently

power and energy metrics started being included into performance models for numerical software [Hager et al. 2014; Benner et al. 2013; Anzt and Quintana-Orti 2014; Malas et al. 2014]. This in-depth understanding of energy and power requirements of different classes of scientific applications is essential on two levels: First application developers and users must control the overall (energy) costs; second HPC site operators (such as data centers / universities) have to identify the most economical way to operate their computational facilities. Both levels are related since the application user is very much interested in efficient utilization of available computational resources whereas system operators are just as motivated that platform-optimized application codes are being used.

1.3 CONSEQUENCES AND PAPER CONTRIBUTION

From the previous section we can find two major facts: (1) With current knowledge and (digital) computer technology there is no instant solution available to a possible 'black out' situation in scientific computing: Providing better devices only leads to a global energy consumption converging to a theoretical limit that also ultimately leads to an energy shortage in the mid 21st century. Remember that these numbers are only for computer devices and do not even cover all other energy consumers. (2) For too many years performance engineering and hardware engineering has been eclipsed by the misdirected longing for ever more performance where *faster* seemed to be the only paradigm. A movement towards incorporation of power and energy into performance models gains momentum but resulting efforts are often limited to

simple, basic kernels and not very visible in applied sciences.

In the following sections we describe how the applied sciences community can contribute to tackle the fundamental problem of limited future energy supplies for (scientific) computing. This is achieved by presenting a simple course of action in scientific hardware usage and software development. This requires thinking more ‘out-of-the-box’ in two aspects: Application software usage and development as well as hardware usage and development.

2 WAYS TO TACKLE A FUTURE ENERGY CRISIS IN SCIENTIFIC COMPUTING

2.1 HARDWARE-ORIENTED NUMERICS REVISITED

The major aspect in performance engineering for energy efficiency is the numerical methods used in application and their implementation: (1) **‘Classical’ performance engineering can be applied to enhance the efficiency of the current method on the target hardware** and/or in many cases **numerical alternatives can be found that might better fit to the hardware in use** and/or (2) **other numerical methods can be found to improve the numerical efficiency**. Both are heavily interdependent: Overall tuning in (1) might have negative effects on the numerical scaling whereas improving in (2) often results in numerically stronger but slower/less hardware-efficient methods. Tuning both simultaneously is what we used to call *hardware-oriented numerics* [Turek et al. 2006; Turek et al. 2010; Geveler et al. 2013]. Now we plead for adding a new dimension to this former dualism of hardware and numerical efficiency: (3) energy-efficiency. Although tuning (1) and

(2) normally leads to improvements in (3) this is not always the case as we exemplify in the following section. In this example everything essentially breaks down to powering the memory interface. This is a very representative case for many simulation codes.

It also shows that for all improvements of application codes proper *performance modeling* is key. A performance model is intended to predict performance in some metric, i.e. number of floating point operations per time unit or its inverse: time to solution. The prediction can then be related to obtained measurements (for instance execution wall clock times) and the information one gains is how good a given code performs on the hardware compared to sustainable performance on that hardware. We demonstrate how such a model can be derived empirically that is, by taking a few time and power measurements.

2.2 TAKING CONTROL OF ENERGY CONSUMPTION ON THE APPLICATION LEVEL

The importance of modeling energy to solution in scientific codes can be illustrated by a simple example: Many performance-critical kernels of numerical partial differential equation (PDE) solvers involve stencil discretizations or large linear equation systems. Such applications tend to be memory bandwidth-bound that is the overall computational intensity is comparatively small. As a consequence any increase in the number of parallel cores reduces the core saturation resulting in poor parallel scaling i. e., there exists a certain number of cores N_{\max} for which adding another core produces marginal performance gains. From the user’s point of view (and even

from the classical performance-engineers’ point of view) running the application with N_{\max} or $N_{\max} + 1$ shouldn’t make a difference because there is no loss in performance.

Additional cores however usually dissipate the same power (for a short period of time) as fully saturated ones making the performance gains infinitely disproportional to energy consumption rises. In other words: With regard to the energy-efficiency there is an optimal number of cores N_{opt} that is usually smaller than the maximum number of available cores N_{cores} (because of the saturated memory interface). Since the majority of codes are still lacking reliable energy models running an application on N_{cores} is still a common choice. Although power signatures of sophisticated simulation codes as well as the hardware behavior on the specific workloads are very complex the measurement, modeling, tuning and prediction of the energy to solution can often be achieved quite easily. In recent work we have shown that this goal can be achieved by only a few power and time measurements on the system level resulting in a robust model that predicts energy consumption of a whole application class as well as prevents the user from choosing the wrong run time parameters such as – like in the scenario rendered above – launching a suboptimal amount of threads on a compute node [Geveler et al. 2016a].

In the following we show how to deduce a model that predicts the energy to solution E for a given CFD code. This model hence is simply an equation, that determines E when running the application with certain run time parameters. This model is given in Equation (1). Its construction requires empirical data – in this case, time and energy

measurements.

In order to deduce a model that incorporates the energy to solution as a metric for energy efficiency we consider the averaged time to solution for a time step to complete (T), the averaged power dissipation during that time (P), and the resulting energy to solution (E). For this type of application once a problem is big enough to saturate the memory interface its wall clock time can be used to make predictions for other problem sizes because the time to solution is expected to behave as

$$T(N) = (N / N_{measured}) T_{measured}.$$

All three T , P and thus E are then functions of the number of used cores, k . Additionally, we introduce variables ΔT for the total decrease in wall clock time and ΔP for the total increase in power dissipation

$$\Delta T = \Delta T(k) = T_{k-1} - T_k,$$

$$\Delta P = \Delta P(k) = P_k - P_{k-1}$$

We summarize some of the performance measurements that lead to the performance model described in the subsequent Equation (1) for a 3D PDE solver for the simulation of global ocean circulation on two different hardware architectures: the Intel Haswell [Intel Corp 2015a; Intel Corp 2015b] and the Cortex-A15, the CPU in an NVIDIA Tegra K1 [NVIDIA Corp 2014] SoC, in Table 1. With these results substantiating our hypothesis

k	T [s]	P [W]	E [J]	ΔT [s]	ΔP [W]
Haswell					
1	0.0768	65.6	5.038	-	-
2	0.0434	80.7	3.502	0.0334	15.1000
3	0.0352	91.4	3.217	0.0082	10.7000
4	0.0316	100.3	3.169	0.0036	8.9000
Cortex-A15					
1	0.477	7.5	3.577	-	-
2	0.249	10	2.49	0.228	2.5000
3	0.173	12	2.076	0.076	2.0000
4	0.170	13.9	2.363	0.003	1.9000

Table 1. Performance and power measurements and values of basic model variables

that we have in fact a memory bandwidth-bound situation here the expected solution time for this code (given the problem size and application parameters but independent from the hardware architecture) can be modeled as a super-linear function in the number of used threads with quickly decreasing slopes, that is, $\Delta T(k) = 0$ for moderate values of k . Power on the other hand behaves more linearly: First one can notice that when leaving the idle state a comparatively large power jump occurs which can be explained with the CPU being reconnected to the system clock or in other words, with all four cores being provided with a baseline power independent of the core workload denoted by P_{base} . Once at least one core is tasked with a job, i. e., $k \geq 1$, the chipset baseline power is increased by an additional constant power dissipation called P_{socket} . Second it can be seen that ΔP is roughly 10W for Haswell and ca. 2W for Tegra K1. Based on these findings power (and therefore energy) for this application can be modeled as a simple linear function in the number of used cores:

$$E(k) = P(k) T(k) = (P_{base} + P_{socket} + k\Delta P) T(k), k \geq 1 \quad (1)$$

The practical effects of this model can be understood better when the above values are displayed

differently in an energy / time chart like in Figure 2. Because of an *over-proportional power increase compared to performance increase* there is an optimal number of threads as described above: Using more than three threads is obviously not beneficial and – for one of the two hardware architectures – sometimes even comprises an energy efficiency penalty since energy to solution increases with no benefits for the execution time. For many codes this qualitative finding by simple means holds true for many different runs on many nodes of a local cluster or on a workstation offering a great source of energy savings.

Hence we propose a **rigorous performance measurement, modeling and engineering policy in the development of applied sciences codes.**

2.3 TAKING CONTROL OF THE HARDWARE TO TARGET

Let us reconsider Figure 2. Another aspect that is depicted here is that the hardware architectures used for scientific computing are fundamentally different: The two processors used there can be both considered multi-purpose processors with one (the Cortex-A15) not originating from the field of

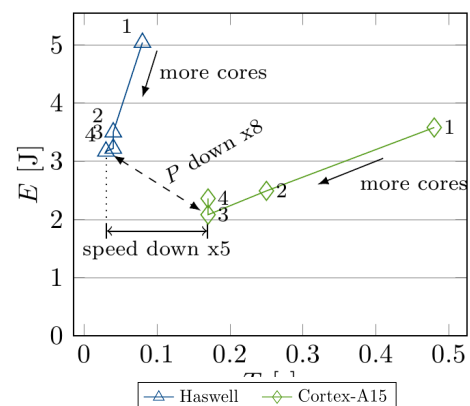


Figure 2. Energy and time to solution of a memory bandwidth-bound application on two different hardware architectures

computing. Recently a game-changing impulse regarding energy-efficient compute hardware comes from mobile/embedded computing with devices featuring a long history of being developed under one major aspect: they have had to be operated with a (limited) battery power supply. Hence as opposed to x86 and other commodity designs (with a focus on chipset compatibility and performance) the resulting energy efficiency advantage can be made accessible to the scientific community.

In our example the CFD code shows higher energy efficiency on the mobile CPU than on the commodity CPU. This is possible because comparing the respective run on the two micro architectures the **power down is larger than the speed down**. Obviously this comes with a price: the execution time is larger when using the embedded processor. This exemplifies a general problem: Energy to solution is not only barely visible to the applied sciences community but also minimizing it is not an inherent goal of what is usually done and even worse: Using the most energy-efficient hardware penalizes the user with a slowdown. We shall demonstrate how to overcome this issue by scaling such unconventional

hardware resources and numerically scale the code, see below.

However in situations when it is possible in future times **energy efficiency should be favored over performance** and in this case a good knowledge of the energy-related hardware specifics is needed. Luckily the performance modeling described in the above section offers a good way to explore these. Devices of the family used in the above benchmarks are on the march and are more and more built into servers and data centers. Normally in a local data center in future times or even now there might be a variety of types of compute nodes available to the user or a department comprises several clusters and workstations of different kind. As a basic pattern to reduce the energy footprint of applied sciences work **the performance modeling allows for choosing the most energy-efficient hardware for a workload or application**.

To fortify our point here we demonstrate the performance and energy efficiency on the device level for very different hardware architectures and very different types of codes in Figures 3 and 4.

The results depict two very well known but often not addressed phenomena: (1) Performance and energy efficiency are functions of device hardware and (the operational intensity of) code; and (2) the hardware ecosystem is evolving very fast over time.

For (1) consider for example the top diagram in Figure 3. The purple plot marks performance for the same ARM Cortex-A15 CPU as in Figure 2. Note that this time for a compute-bound kernel (dense matrix multiply, GEMM) performance and energy efficiency are considerably higher when using commodity processors based on the x86 architecture. Hence over-generalized assumptions like 'ARM-based devices/computers are always more energy-efficient than x86 ones' are as wrong as they are futile. For (2) consider the bottom plot in Figure 3 where this time commodity and embedded GPUs of different hardware generations are compared. Here we examined the low power GPUs of the NVIDIA Tegra-K1 SoC [Geveler et al. 2016b]. Note how the low power GPU is able to beat desktop CPUs of their time as well as later generation desktop GPUs in terms of energy efficiency whereas same-generation compute GPUs (Tesla line) are the

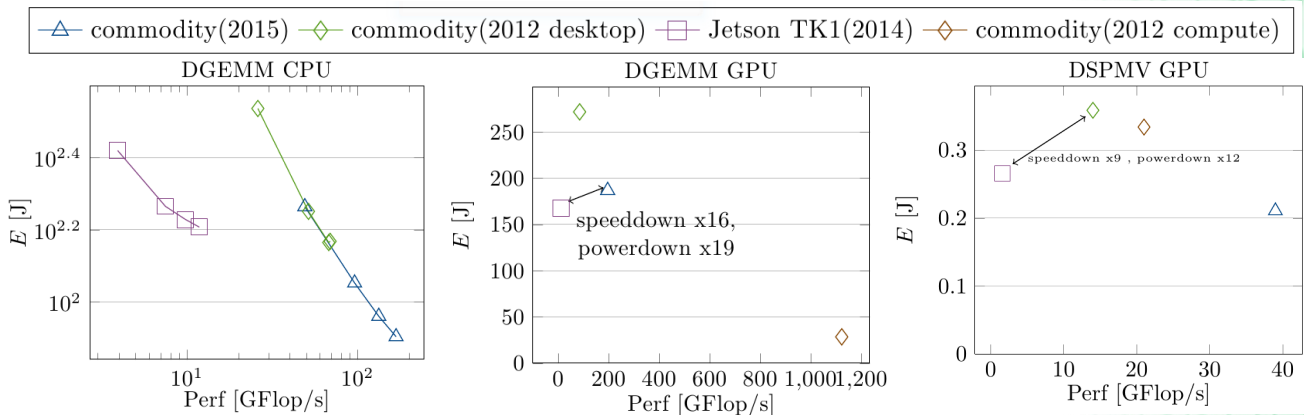


Figure 3. Energy and time to solution of compute-bound basic kernels on different hardware architectures

Figure 4. Energy and time to solution for memory bandwidth-bound basic kernels on different hardware architectures

most energy efficient floating point accelerators of that time. For a different type of kernel the picture is changing: In the memory bandwidth-bound case in Figure 4 (as with the sparse matrix vector multiply) powering memory interfaces is much more important and thus hardware generation determines the energy-efficiency due to the enhanced memory interface of the 2015 GPU. Also the embedded GPUs are evolving and the next generations (Tegra X1 and X2) may turn this picture upside down again. Hence continuous work regarding measurement and modeling energy for application codes and available hardware is crucial and nothing should be taken as carved in stone.

Another point here is that computing is not all about CPUs and memory interfaces. A compute node in a cluster may be a complex architecture which is then aggregated into an even more complex system with communication switches, storage and control hardware. This cluster is integrated into a housing with cooling systems. All these systems drain energy for the sake of computations. Let us now take a look at the cluster level where everything is scaled up. In Figure 5 we demonstrate results from a cluster of compute nodes consisting of single Tegra K1 SoCs which combine 4 Cortex- A15 CPU cores and a low power Kepler GPU. These results show that together with energy-efficient switches we can use a number of nodes comprising the ‘unconventional’ computer hardware to be both more energy-efficient as well as faster. Hence **we can scale the energy-efficiency bonuses by embedded hardware up to a point where the resulting cluster performs faster and uses less energy at the same time as compared to single commodity devices**. It is very important to

understand that this is only possible by **developing numerics that fit to the underlying hardware and are able to be scaled numerically and hardware efficiency-wisely to reach that point**.

Another aspect concerning hardware is that the energy revolution is not all about energy efficiency. Up to now we basically proposed to reduce energy by enhancing hardware or software energy efficiency on the scale of our own codes and hardware devices. This does not ease the problem that even with optimal devices the problem of too few energy supplies for future computing cannot be resolved – at least not with ‘standard’ computers. This kind of thinking led us to a system integration project where we **built a compute-cluster alongside with its power supply by renewable energies**, see Figure 6 for snapshots of the ICARUS project site [Geveler and Turek 2016]. This prototypical data and compute center comprises a great deal of theoretical peak performance (around 20 TFlop/s) provided by 60 Tegra K1 processors that all have a low power GPU on the SoC. By applying a 45 m² solar farm offering a 8 kWp power source alongside with a Lithium-Ion battery with a capacity of 8 kWh we can maintain operation of the 1 kW peak power dissipation computer even during nighttime for several hours. Even with comparatively cloudy weather and considerably large nightly workloads we can recharge the battery at day times while computing under full load. This computer has all its energy needs fed by renewables even the cooling system and it is not connected to the power grid at all.

The idea of the project is: If we cannot tackle the overall problem of energy demand increasing much faster than its supply why not build

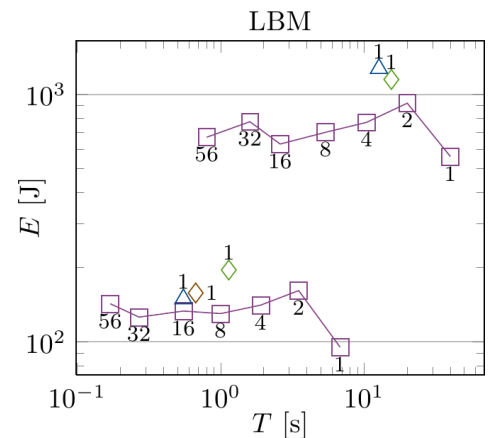


Figure 5. Energy and time to solution of a CFD application on a cluster of Tegra K1 SoCs and several workstations comprising commodity hardware

any new needed supply directly with the system? In recent work we proved that this is possible [Geveler et al. 2016b]. With this we come back to Figure 1. Note that finally building new renewable energy sources alongside with its demand in the model used by the SIA the supply curve would be parallel to the consumption. Higher energy efficiency is still needed because renewable energy sources such as photovoltaic units impose new constraints like area or initial cost that should be minimised. Building compute centers this way we could reduce the follow-up energy cost of a computational resource to zero.

3 CONCLUSION

Keep in mind that the system integration described in the previous section is only possible due to simple yet very effective performance modeling which allows for choosing hardware and numerics as well as tuning them properly. Therefore **hardware-oriented numerics is the central aspect here**: The approach is successful for a specific type of numerics that can be



Figure 6. Snapshots of the ICARUS cluster at TU Dortmund

scaled effectively i.e. numerically and in terms of hardware -and energy- efficiency. Hardware-oriented numerics therefore means:

(1) The extension of the original paradigm by the aspect of **energy-efficiency**. New methods in performance modeling have to be developed and applied and energy to solution has to be internalized into tuning efforts of software on the application level.

(2) The **selection of compute hardware should be based on these models**. In any decision and where necessary **energy efficiency should be favored over raw performance** although we have shown how this can be bypassed by clustering unconventional computer hardware and enhancing scalability properties of a given code.

(3) Furthermore **knowledge concerning energy efficient computing has to be spread in the applied science community**. A knowledge base should be installed that disseminates methods in power and energy measurement as well as profiling and benchmarking techniques in order to bring up sophisticated performance models for the application level, performance engineering for energy -efficiency, energy consumption of compute devices in local compute resources and energy consumption of compute clusters and whole data centers.

(4) After hardware selection many **hardware parameters have to be tuned during operation**. We demonstrated how to determine an optimal number of threads for a maximum of energy efficiency. Another good example here is finding an optimal preset core frequency. Although with Dynamic Frequency Scaling modern processors show very complex behavior for different workloads and especially during runs of complex applications, in many cases one can find an optimal frequency for a certain type of applications with similar sets of measurements like in our example.

(5) Finally, the development of the ICARUS system has been accompanied by a two semesters student project where the participants actively contributed to the system design. Here they learned how to co-develop hard- and software/numerics from scratch for computations being powered by renewables and batteries starting with performance modeling and hardware details up to integrating everything into a future-proof resource. It is **bringing sensitivity for energy efficiency and consumption into the peoples' minds which starts with being integrated into teaching** which is in the end maybe the most important thing one can do.

ACKNOWLEDGMENTS

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THE VIRTUAL ELEMENT METHOD: A NEW PARADIGM FOR THE APPROXIMATION OF PARTIAL DIFFERENTIAL EQUATION PROBLEMS

Foreword. The present note is not intended to provide an exhaustive account of the numerous research directions, results and applications developed by the various groups working on the Virtual Element Method. Instead, our aim is to concisely present the basic ideas of the method, and to mention only a few aspects which highlight the potential and the flexibility of this innovative approach.

The Virtual Element Method (VEM) is a new technology for the approximation of partial differential equation problems. VEM was born in 2012, see [6], as an evolution of modern mimetic schemes (see for instance [14, 5, 12]), which share the same variational background of the Finite Element Method (FEM). The initial motivation of VEM is the need to construct an accurate Galerkin scheme with the following two properties.

- The flexibility to deal with highly general polygonal/polyhedral meshes, including “hanging vertexes” and non-convex shapes. A couple of instances are depicted in Figures 1 and 2.

- The conformity of the method, i.e. the property to build an approximated solution which shares the same “natural” regularity as the analytical solution of the problem. In many interesting cases, this means that the discrete solution is *continuous across adjacent elements*.

When confining to polynomial local approximation, the two features above are severely conflicting, thus making the method design extremely difficult. The virtual element method overcomes the trouble by *abandoning the local polynomial approximation concept*, and use, instead, approximating functions which are solutions to suitable local partial differential equations (of course, connected with the original problem to solve). Therefore, in general, the discrete functions are not known pointwise, but a limited information of them are at disposal. However, the available information is sufficient for the formation of the stiffness matrix and the right-hand side: this can be accomplished by designing a *weakly* (not strongly!) consistent scheme;

strong consistency is imposed only for polynomials up to a suitable degree, but not for the whole approximating space. We remark that the strong consistency on polynomials essentially implies the fulfilment of the *patch test* relevant to the specific problem at hand.

In addition to the features mentioned above, we present some other interesting properties that make the virtual element method an attracting methodology:

- An accurate description of possible discontinuities in the data, especially when they occur in accordance with complex patterns (e.g. in reservoir simulation or crack propagation problem).
- For mesh adaptivity, the possibility to refine without the need to avoid hanging nodes/edges allows for more efficient refinement strategies. Moreover using polygonal/polyhedral meshes allow interesting de-refinement procedures in which groups of elements are coalesced into single ones.

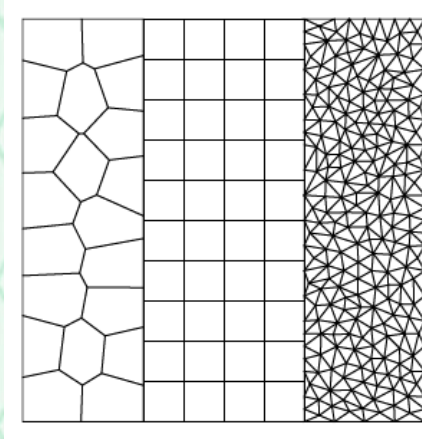


Figure 1. Example of 2D mesh that can be used in connection with VEM (courtesy of A. Russo).

- In topology optimization, the use of polygonal/polyhedral meshes may alleviate phenomena connected to preferred geometric directions, inevitably occurring with low-sided polygons/polyhedra.
- Surprisingly, the virtual element method can easily handle approximating spaces with *high order regularity*, such as C^1, C^2 or more. This property makes VEM very attractive when dealing with high-order partial differential equations, such as the Kirchhoff plate problem.
- VEM is generally more robust than traditional FEM with respect to mesh distortion or degeneration.
- For constrained problems, such as incompressible elasticity, the flexibility of VEM to choose the approximating spaces, opens the way to new schemes, where the constraint is *exactly satisfied*. In the FEM framework, instead, the exact satisfaction of the constraints is typically difficult to reach.

Before presenting a concise but “precise” description of the method, we state that despite VEM was born very recently, a significant number of contributions have already appeared in literature. From the theoretical side, the analysis of VEM applied to several *linear* model problems have been developed. We cite here the works: [6, 9, 13, 17]. For *nonlinear problems*, the available theoretical results are still very limited, see [15, 2]. Regarding the application side, VEM is experiencing a growing interest from the engineering community. We mention a few (non exhaustive) list of applications where the VEM approach has shown or is showing promising results:

- *The Stokes problem.* In fluid-dynamics applications, the flexibility of VEM has been exploited to develop a highly regular (i.e. C^1) scheme based on a *stream function* formulation of the Stokes problem, see [1]. A different approach has been followed in [8], where the non-polynomial character of VEM is

used to design new *exactly divergence-free* schemes.

- *2D and 3D elasticity problems.* The classical elasticity problem, in the framework of the infinitesimal theory, has been addressed in the works [7, 16, 3], among others. Also in this case, VEM has proved to be a competitive alternative to the more traditional FEM procedures, especially when the problem requires a particularly flexible management of the geometry description.
- *Fracture problems.* For some fracture problems arising from reservoir applications, the VEM approach has been developed in [10].
- *Contact problems.* In [20], VEM is proved to provide an interesting methodology for contact problems. Here, the VEM ability to deal with glued *unrelated meshes* is greatly beneficial.
- *Inelastic problems.* In the papers [15, 4] VEMs are used for the analysis for inelastic phenomena

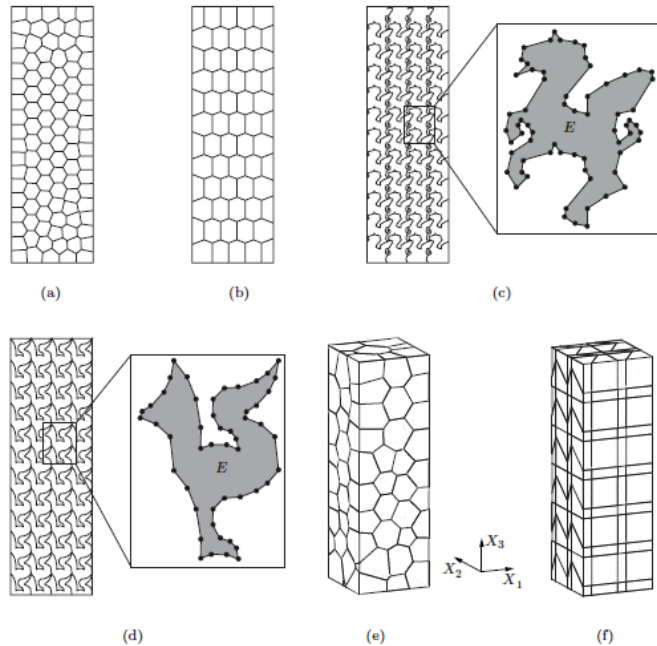


Figure 2. Example of 2D and 3D meshes that can be used in connection with VEM (courtesy of G.H. Paulino).

(such as plasticity, shape memory alloys and viscoelastic problems), modelled by the generalized standard material theory (see [11], for example). Among other results, it is proved that the VEM approach can be interfaced with a standard numerical treatment of the evolution flow rule governing the internal and history variables. Therefore, most of the technology already developed in the FEM framework for such problems, can be easily reused by the new paradigm.

- *Phase separation problems (the Cahn-Hilliard equation)*. For phase separation problems modelled by the Cahn-Hilliard equation, the VEM philosophy has been studied in [2], where the ability of designing highly regular (i.e. C^1) schemes is exploited.
- *The Helmholtz problem*. For the 2D Helmholtz equation with impedance boundary conditions, an application of VEM can be found in [18].

However, we remark that this new technology has been tested essentially on academic, though interesting, problems. So far, VEM has displayed a number of surprisingly interesting features. *It is now time to inject efforts towards the development, the assessment and the validation of the VEM paradigm when applied to real-life problems.*

A CONCISE PRESENTATION OF THE VIRTUAL ELEMENT METHOD

We here present the basic idea of the virtual element method by considering a very simple model problem: the Poisson problem. Accordingly, we are asked to find a function $u: \Omega \rightarrow \mathbb{R}$, solution to the following problem:

$$-\Delta u = f \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega. \quad (1)$$

It is well-known that a variation formulation of problem (1) reads:

$$\text{Find } u \in V \text{ such that:} \\ \alpha(u, v) = (f, v) \quad \forall v \in V, \quad (2)$$

where V is the trial/test space,

$$\alpha(u, v) := \int_{\Omega} \nabla u \cdot \nabla v, \\ \text{and } (f, v) := \int_{\Omega} f v.$$

The virtual element method falls in the category of Galerkin schemes for the approximation of the solution to problem (2):

Find $u_h \in V_h$ such that:

$$a_h(u_h, v_h) = F_h(v_h) \quad \forall v_h \in V_h. \quad (3)$$

Here above, V_h is the finite dimensional approximating space tailored to a given mesh Ω_h made by polygons E , $a_h(\cdot, \cdot)$ is the discrete bilinear form (leading to the method stiffness matrix), and $F_h(\cdot)$ is the discrete loading term.

DEFINITION OF THE APPROXIMATING SPACE V_h

The first problem we have to face is to find a finite dimensional space $V_h \subset V$, tailored to the mesh Ω_h . Similarly to the finite element approach, we would like to define V_h by gluing local approximation spaces V_E , one per each polygon $E \in \Omega_h$. The polynomial character of a typical $v_E \in V_E$ is abandoned, and v_E is instead defined as the solution of a particular partial differential equation problem in E . More precisely, we take

$$V_E = \{v_E: \Delta v_E = 0, v_E|_{\partial E} \in C^0(\partial E), v_E \text{ linear on every edge } e \in \partial E\}. \quad (4)$$

Therefore, the local degrees of freedom can be chosen as the vertex values of V_E . We notice that it obviously holds $\mathbb{P}_1(E) \subseteq V_E$, where $\mathbb{P}_1(E)$ denotes the space of linear polynomials defined on E . This property is one of the roots for the consistency of the method, and ultimately for the *satisfaction of the patch test*.

The approximating space V_h is then built by gluing together the local spaces V_E . Therefore, the global degrees of freedom are the values at the interior vertexes of the mesh Ω_h . We also notice that, when Ω_h is a triangular mesh, the space V_h is exactly the same as for the standard linear triangular finite element method.

DEFINITION OF THE DISCRETE BILINEAR FORM $a_h(\cdot, \cdot)$

At a first glance, definition (4) seems to hide an insurmountable obstacle: in general, the functions $v_E \in V_E$ are *not explicitly known, and of course, nor are the elements of a basis, say $\{\varphi_i\}$* . The observation that the local stiffness matrix is formed by the terms $\int_E \nabla \varphi_j \cdot \nabla \varphi_i$, seems to put

an end to the utility of definition (4) in designing a Galerkin scheme. We now show how to overcome this trouble.

First Step. For each polygon E , we introduce a projection operator $\Pi_E: V_E \rightarrow \mathbb{P}_1(E)$, thus taking values on the linear polynomial space. More precisely, we set:

$$\Pi_E v_E \in \mathbb{P}_1(E): a_E(\Pi_E v_E, q) = a_E(v_E, q) \\ \forall q \in \mathbb{P}_1(E); \quad \int_{\partial E} \Pi_E v_E = \int_{\partial E} v_E. \quad (5)$$

where $a_E(\cdot, \cdot)$ denotes the energy contribution computed on the polygon $E \in T_h$. We notice that:

$a_E(\Pi_E v_E, q) = a_E(v_E, q) \forall q \in \mathbb{P}_1(E)$ is a linear system of three equations in the unknowns, since $\dim(\mathbb{P}_1(E)) = 3$. However, taking $q = 1$ gives $0 = 0$, which means that there are only two independent equations. As a consequence, we need to add another independent equation to uniquely define $\Pi_E v_E \in \mathbb{P}_1(E)$: this is indeed embodied by the condition

$$\int_{\partial E} \Pi_E v_E = \int_{\partial E} v_E,$$

We also notice that Π_E is nothing but the *orthogonal projection operator onto the linear polynomials, with respect to the bilinear form $a_E(\cdot, \cdot)$* . But the crucial remark is that $\Pi_E v_E$ is *computable for every v_E , despite v_E is not explicitly known, in general*. For the details of such a fundamental property we refer to [6].

Second Step. Given $u_E, v_E \in V_E$, one can now write $u_E = \Pi_E u_E + (I - \Pi_E) u_E$ and $v_E = \Pi_E v_E + (I - \Pi_E) v_E$, and notice that they are orthogonal decompositions with respect to the bilinear form $a_E(\cdot, \cdot)$. As a consequence, it holds $a_E(u_E, v_E) = a_E(\Pi_E u_E, \Pi_E v_E) + a_E((I - \Pi_E) u_E, (I - \Pi_E) v_E)$. The first term at the right-hand side is computable, hence it can be retained *as it is* to design a Galerkin scheme. Instead, the second term at the right-hand side cannot be computed, hence it needs to be properly modified. The modification should mimic the original term as much as possible, but it must be computable for every $v_E \in V_E$. In particular, it must scale, with respect to the size of the polygon E , as $a_E(\cdot, \cdot)$ scales. A typical choice stems from the introduction of the bilinear form

$$s_E(u_E, v_E) = \sum_{p \in \text{Vertexes}(E)} u_E(p) v_E(p) \quad (6)$$

Then, we can set

$$a_E^h(u_E, v_E) := a_E(\Pi_E u_E, \Pi_E v_E) +$$

$$s_E((I - \Pi_E) u_E, (I - \Pi_E) v_E), \quad (7)$$

which turns out to be computable for every $u_E, v_E \in V_E$. We notice that the form in (7) is strongly consistent on linear polynomials, and it scales as the original bilinear form. These two features are indeed sufficient to design an effective method, and different stabilisation terms s_E might be accordingly designed.

Third Step. The global bilinear form $a^h(\cdot, \cdot)$ is simply defined by gluing the local contributions:

$$a^h(u_h, v_h) = \sum_{E \in \Omega_h} a_E^h(u_E, v_E)$$

where $u_E = u_{|E}$ and $v_E = v_{|E}$. (8)

DEFINITION OF THE RIGHT-HAND SIDE $F_h(\cdot)$

For the approximation of the right-hand side

$$\int_{\Omega} f v_h = \sum_{E \in \Omega_h} \int_E f v_E,$$

we first define a piecewise constant approximation $P_0^E f$ of $f|_E$. Then, we set

$$F_h(v_h) := \sum_{E \in \Omega_h} \text{Area}(E) (P_0^E f) \bar{v}_E, \quad (9)$$

where $\bar{v}_E := \frac{1}{n(E)} \sum_{p \in \text{Vertexes}(E)} v_E(p)$,

and $n(E)$ is the number of vertexes in E .

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ANDERSON LOCALIZATION IN A BALLASTED RAILWAY TRACK

1 INTRODUCTION

Although the annual funding for railway tracks construction and maintenance is high, a large part of track design and maintenance planning is still based on strongly empirical grounds. The passage of trains is the main source of damage on the track and hence contributes heavily to this budget. In the past years, with the increasing average velocity of the train passages, dynamical effects have been shown to accelerate track deterioration and cause heavier damage to neighbor buildings [5]. Understanding precisely the dynamical behavior of ballasted railway tracks (see Fig. 1) is therefore paramount to proposing improved design strategies and maintenance programs.

Experimental work on small granular samples indicates that the heterogeneity of the material constitutes the main reason for its peculiar dynamical behavior. In particular, it has been shown that the wave propagation velocity depends on the confining pressure through the complex assemblage of contacts [9]. In experiments of ultrasound wave propagation in granular media, the appearance of an incoherent coda behind the main pulse is also due to the heterogeneity of the medium [15]. Although at a different scale, the latter observation is classical in seismic wave propagation and has

also been attributed to the heterogeneity of the Earth crust [1].

Analytical models have been constructed to try and explain the influence of heterogeneity on the dynamical behavior of granular material, using in particular springs with random properties [19, 18] and winker-type springs [22, 21]. However, more realistic models are called for to discuss actual engineering systems. Two classes of numerical models are used to try and predict the behavior of these dynamical systems: (1) discrete approaches, in which each grain of the ballast is represented by a rigid body and interacts with its neighbors through nonlinear contact forces (using molecular dynamics or non-smooth contact dynamics); and (2) continuum approaches, in which the ballast is replaced by a homogenized

continuum and a Finite Element Method (FEM) is used to solve the problem. Although they are very efficient at representing complex nonlinear behaviors [4], the discrete approaches are today capable of solving only a few meters-length of ballast. The development of an efficient scheme for parallelization over large clusters of computers and the coupling with continuum models remains an open problems [24]. On the other hand, FEM [3] and Boundary Element methods [8], all based on continuum models, have been used to compute the dynamical behavior of ballasted railway tracks over large distances. Unfortunately, these models are all based on an assumption of homogeneity of the ballast layer. They hence cannot reproduce the typical behavior of granular materials.



Figure 1. Coarse crushed stones of the ballast layer under a railway track. Picture by LooiNL, licensed under the Creative Commons Attribution-Share Alike 3.0 Unported license

In a recent paper [6], we introduced a randomly-fluctuating heterogeneous continuum model of the ballast. The Young's modulus is modeled as a random field parameterized by its average, its variance and a correlation model representing non-interpenetrating spheres. Being continuous, a numerical model of the ballast and the surrounding soil can then be constructed based on an efficient implementation of an explicit spectral element solver on a large cluster of computers. Being heterogeneous, it is expected that the complex behavior of granular media can be better reproduced than with previous homogeneous continuum models.

2 RANDOMLY-FLUCTUATING HETEROGENEOUS CONTINUUM MODEL OF THE BALLAST

We recall in this section the randomly-fluctuating heterogeneous continuum model of the ballast [6]. Young's modulus E is the only parameter that is assumed to be heterogeneous, although more complex media could be considered, including anisotropic [23] or non-linear [14]. The correlation model of Young's modulus is constructed analytically and corresponds to that

of a dense packing of spheres with known diameter and packing density [25] (both quantities measurable on real ballast). The first-order marginal law is obtained by identification on Discrete Element simulations of granular samples. A gamma law is considered, with average $\mathbb{E}[E] = 95 \text{ MPa}$ and variance $\mathbb{E}[(E - \mathbb{E}[E])^2] = 135 \times 10^3 \text{ (MPa)}^2$. Note in particular that the coefficient of variation is extremely high, on the order of several times the average. As desired, the model therefore recreates the heterogeneity of the granular material, that has been shown to be influential on its dynamical behavior. However it does not capture its discrete character, and hence cannot take into account rearrangements or changes of topology that would occur in real granular samples.

The generation of realizations of Gaussian random field is performed using a particular implementation of the spectral representation method that allows to generate realizations over very large clusters of processors. This is obtained by localizing the generation on each processor before merging at the interface to retrieve the desired correlation properties [20]. Fig. 2 presents one realization of the random field of Young's modulus for the ballast-soil system.

Numerical approximation of the solution in space and time are obtained with a solver based on the Spectral Element Method [16] (SEM). The SEM is a high-order FEM that uses a Gauss-Lobatto-Legendre quadrature rule for integration and Lagrange polynomials based on the nodes of that quadrature. Using under-integration, the mass matrix becomes naturally diagonal, which allows to use an explicit second-order finite-difference scheme in time. Even though the stability condition requires to use very small time steps, the construction of the solution at each time step is very easy because the inversion of the mass matrix is costless. Our implementation of the SEM has demonstrated scalability for more than 10'000 cores [11] while other implementations in the literature have even been shown to scale over 100'000 cores [16].

3 INFLUENCE OF THE HETEROGENEITY OF THE BALLAST LAYER ON THE WAVE FIELD INDUCED BY THE PASSAGE OF A TRAIN

To illustrate the difference between wave propagation in a homogeneous ballast and a

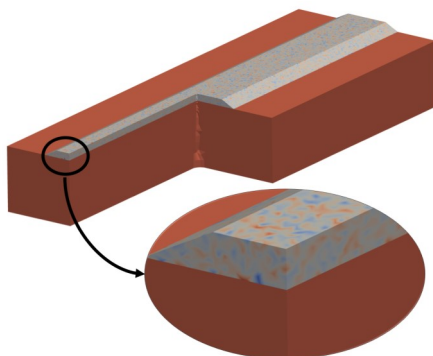


Figure 2. One realization of Young's modulus of the soil and heterogeneous ballast.

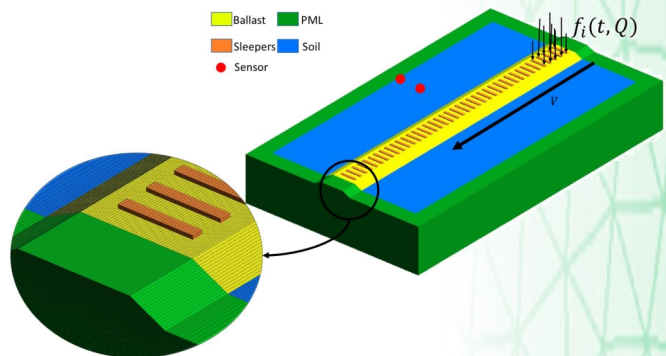


Figure 3. Geometry, loading, boundary conditions and mesh for the wave propagation analysis.

heterogeneous ballast, we consider the model depicted in Fig. 3. It is a 38 m-long one-way track segment, with a ballast (in yellow on Fig. 3) of height 48 cm and width between 3.9 m at the top and 5 m at the bottom. Below the track, the soil is numerically modeled on a width of 20 m and a depth of 5 m. The concrete sleepers have dimensions $20 \times 30 \times 200 \text{ cm}^3$, are separated by $d = 0.6 \text{ m}$, and are embedded in the soil on a height of 10 cm. In the simulated domain, the wave field is the solution of the wave equation:

$$\nabla \sigma - \rho \ddot{u} = 0 \quad (1)$$

where the material is assumed isotropic and linear, so that Hooke's law can be used to relate the strain and stress tensors. The density is denoted ρ , while the P-wave velocity and S-wave velocity are denoted V_p and V_s , respectively. The soil is assumed homogeneous in all simulations, with $V_s = 180 \text{ m/s}$, $V_p = 350 \text{ m/s}$, and $\rho = 1900 \text{ kg/m}^3$. The sleepers are assumed homogeneous in all simulations, with $V_s = 2500 \text{ m/s}$, $V_p = 4500 \text{ m/s}$, and $\rho = 2400 \text{ kg/m}^3$. In the simulations where the ballast is assumed homogeneous, we consider $V_s = 150 \text{ m/s}$, $V_p = 380 \text{ m/s}$, and $\rho = 1900 \text{ kg/m}^3$. In the simulations where the ballast is assumed heterogeneous, the random model of mechanical

properties is the one described above, with average values taken equal to those of the homogeneous case. A classical moving load is used to represent the influence of a train-rail system on the sleepers [10]. The mesh is discretized with 0.81 millions of hexahedral elements. High-order polynomials of order 7 are used in the spectral element solver, for a total of close to 500 millions of DOFs for the entire mesh. On the exterior of the soil box (green area in Fig. 3), a Perfectly Matched Layer [7] is added to absorb outgoing waves.

The displacement field at time $t=0.27 \text{ s}$ in the case when the ballast is homogeneous is plotted at the left of Fig. 4. The pattern is quite simple, with an energy clearly concentrated under the moving load. The largest displacements are close to the loading position, with rapid decrease both in depth and at distance from the track. There seems to be mainly a guided wave within the ballast layer, connecting with Rayleigh wave in the soil. At the right of Fig. 4, the same displacement field is plotted in the case of the heterogeneous ballast. The wave pattern is very different, with most of the energy remaining within the ballast, and not necessarily concentrated below the moving load. The energy seems to be trapped within the ballast layer,

and not moving forward as in the case of guided waves. Overall, the energy radiated in the soil seems to be smaller. This last statement is confirmed by the times histories (not shown here) at the sensors marked in Fig. 3, for which the maximum values are larger with a homogeneous ballast than with a heterogeneous one.

Using an array of sensors in the horizontal direction along the axis of the track, and performing Fourier transforms both in space and time, it is possible to construct dispersion curves from time simulations of the type described above (see [6] for details on this construction). We therefore construct such dispersion relations for a homogeneous ballast resting on a homogeneous soil (see the left of Fig. 5), and for a heterogeneous ballast resting on a homogeneous soil (see the right of Fig. 5).

For the homogeneous ballast, we observe the classical modal behavior of a waveguide [17]. Indeed, a series of thresholds appear, above which new dispersive modes appear, with velocities asymptotically approximating the S wave velocity in the ballast at high frequencies (indicated by a dashed line). Note also that, at lower frequencies, the velocity is intermediate between the shear wave velocities of the soil

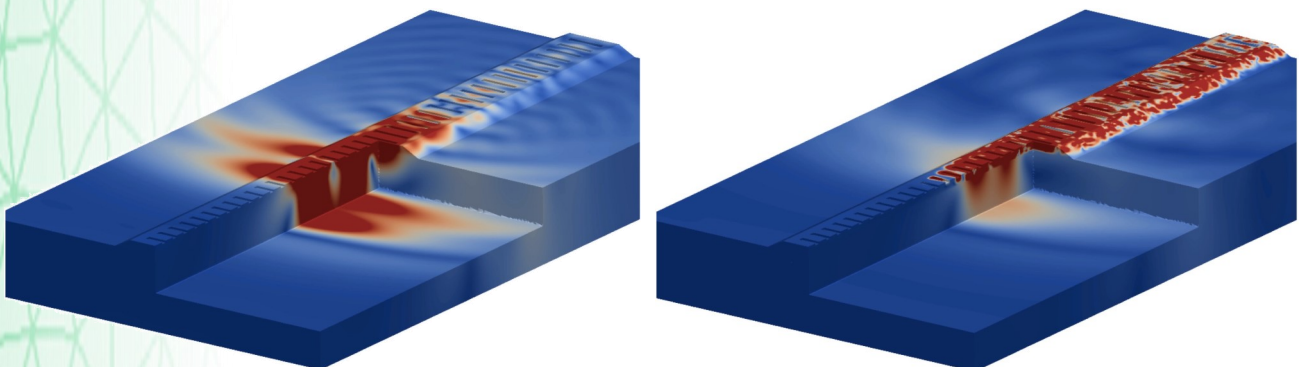


Figure 4. Displacement fields at time $t = 0.27 \text{ s}$ in a homogeneous ballast (left), and a heterogeneous ballast (right).

(indicated by a solid line) and the ballast, because the wavelength is larger than the ballast height, so that the soil is also mobilized by the wave.

For the heterogeneous ballast, two important effects can be observed: (i) the propagating behavior is dispersive in the low frequency range, with a very strong slowing down of the wave velocity at larger frequency, similar to that observed in the experimental work of [13] on unconsolidated granular packings; and (ii) the propagating behavior vanishes at higher frequencies. Note that the latter does not mean that there is no energy in the system, but only that the energy remains localized. This is confirmed by the observations in Fig. 4. Note that simulations considering a soil with the same average properties as the ballast (not shown here) have shown that the behavior observed here is mainly controlled by the heterogeneity within the ballast rather than the impedance contrast between the ballast and the soil.

4 CONCLUSIONS

A randomly-fluctuating heterogeneous continuum model of the ballast was introduced. The Young's modulus was modeled as a random field parameterized by its average, its variance and a correlation model representing non-interpenetrating spheres. Being heterogeneous, the complex behavior of granular media can be better reproduced than with previous homogeneous continuum models. Indeed, and although no dissipation was included in the model, we observe apparent damping due to a loss of coherence of the propagative wave. Part of the energy remains localized within the ballast, due to the heterogeneity of the ballast rather than due to the impedance mismatch between the soil and the ballast. This phenomenon is known as Anderson localization in the physics literature, and was described first to explain the transition from conductor to insulator of metals depending on the density of defects in the crystalline network [2]. It is more difficult to observe experimentally

for classical waves [12] than for the Schrödinger equation, because its effects are mixed with those of material dissipation. Computer simulations are a powerful tool here because material damping can be turned off to observe only the effects of Anderson localization.

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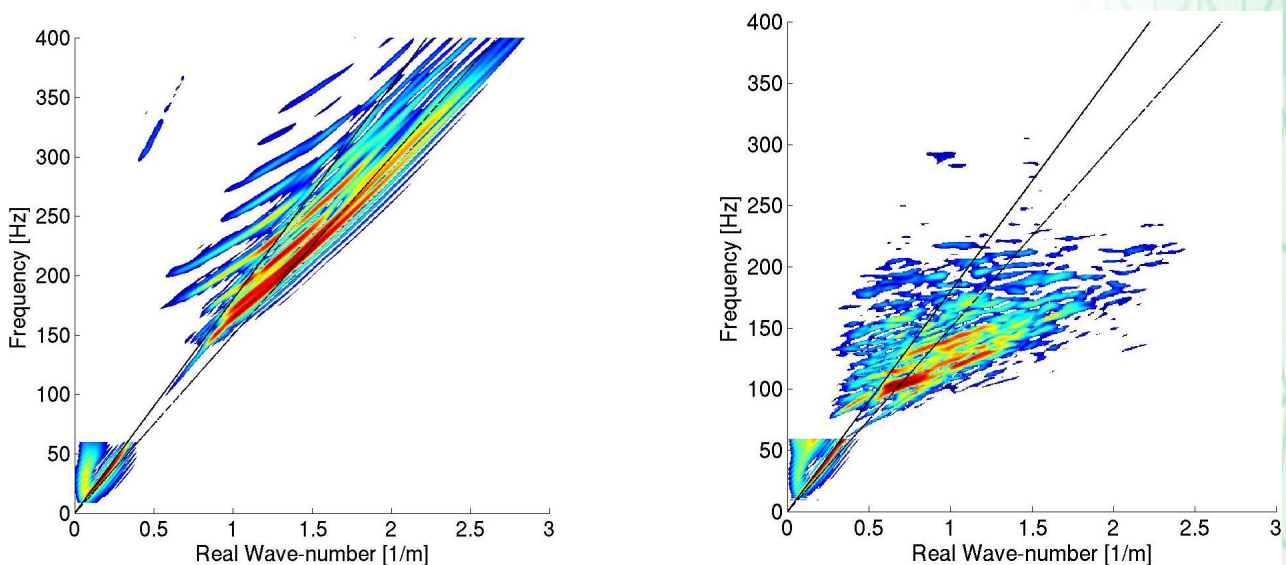


Figure 5. Dispersion curves for the homogeneous ballast (left), and the heterogeneous ballast (right). Dispersion relations for the ballast shear wave (black dashed line) and soil shear wave (black solid line) are also represented.

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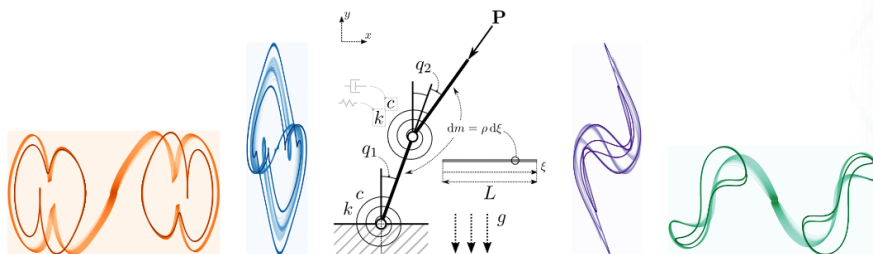
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GENERAL-PURPOSE CONTRAST-PRESERVING VISUALIZATION OF HIGH DYNAMIC RANGE DATA IN UNCERTAINTY QUANTIFICATION



1 INTRODUCTION

Humans are visual creatures; seeing is understanding. This point has been emphasized in statistics and data visualization at least since Tukey (1977), but not so much explored in the computational sciences. Data visualization design is important, because visualization is an essential part of the human - computer interface to the data - i.e. in the computational sciences, to the numerical results. Generally, the choice (Cleveland, 1993) and the quality (Tufte, 2001) of a data visualization determine whether patterns in the data are seen or lost.

Although numerical simulations themselves are free from measurement noise, its effects cannot be completely avoided, since most problem parameters are only known up to a tolerance. For robust simulation, it is crucial to consider input (problem parameter) and output (solution) sets instead

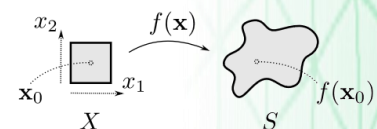
of single points in the input and output spaces. This leads to the need for uncertainty quantification (UQ).

In this short paper, we examine some qualitative aspects of a sample-based visual approach for UQ, and show some visualizations of high dynamic range (HDR) data generated by applying the approach to Ziegler's double pendulum with damping and a follower load (shown above). In order to be brief, we will just highlight the main points, and provide keywords and some selected references that can be used to find more information.

This double pendulum system, investigated by Ziegler (1952), is a classic counterexample that demonstrates there is no equivalent of the Kelvin-Tait-Chataev theorem (see e.g. Kirillov, 2013, p. 163) for non-conservative systems. Adding vanishingly small damping $c > 0$ into the ideal non-damped model causes the modified system to lose

stability already at a significantly lower value of the loading parameter than is the case for the ideal undamped system.

Following the previous study Jeronen (2011), we consider a numerical model as a deterministic, non-linear black-box function f , which maps each point x in the parameter space X into a point $f(x)$ in the solution space S :



The input to the model is characterized by the joint probability distribution of the problem parameters x_k , considered statistically independent. We consider only the case where the domain of the input distribution is bounded (indicated by the rectangle above). Feeding the input probability distribution through the model, we obtain an output

probability distribution, representing the quantity or quantities of interest. We further consider only the case where the output distribution has no singularities.

Let us consider the problem of visualizing the output probability distribution, given a model and the input probability distribution. This is useful in exploratory analysis, to facilitate intuitive understanding of the behaviour of a given system.

Using a sample-based approach, three steps are needed. First, the input probability distribution is sampled.

Then an ensemble simulation is run using the sampled input points. Finally, the density of the obtained discrete solution set is estimated in order to construct a numerical approximation of the output probability distribution: Figure 1.

The output density typically has a high dynamic range (HDR), and thus cannot be directly visualized on conventional (low dynamic range, LDR) media such as screen or print. In order to obtain an LDR rendering that preserves contrast, and thus visual detail, we apply a method designed for 3D computer graphics and HDR photography.

For simplicity, we have chosen to ignore the (sometimes prohibitive) computational expense of the ensemble simulation. If needed,

reduced order modelling techniques can be applied to remedy this.

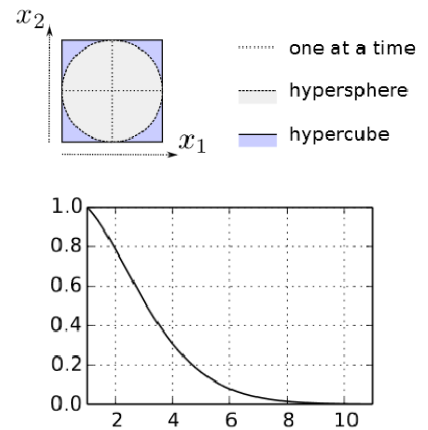
2 SAMPLE-BASED UNCERTAINTY QUANTIFICATION

Since we consider the model under study as a classical function, deterministically mapping each point in the parameter space onto a point in the solution space, it is clear that actual randomness (or actual pseudo-randomness) of the input sample is not required if our goal is to visualize the output.

In fact, classical Monte Carlo sampling tends to lead to undesired clustering and voids in the generated set of points. If we instead discretize the input probability distribution in a deterministic manner, we obtain a set of points whose local density, for small sample sizes, much more closely follows the original continuous probability distribution. This guarantees that all regions of the admissible parameter set will be represented in the sample; in the literature on sampling methods, this property is called *stratification*.

For a general nonlinear black-box model, it is not sufficient for uncertainty quantification to vary each uncertain parameter alone while keeping the others fixed to their reference values. In the d -

dimensional parameter space, where d is the number of problem parameters, this would probe a cross-shaped region, which is enclosed by a d -dimensional hypersphere, which in turn is enclosed by a d -dimensional coordinate axis aligned hypercube. Visualizing for $d=2$:



As the dimension d increases, the hypervolume fraction of the hypercube occupied by the hypersphere (see figure above) quickly approaches zero. Already at $d=3$, the corner regions represent about half of all admissible inputs.

Because we require the problem parameters to be independent, their joint distribution has the structure of a tensor product of one-dimensional marginal distributions. Furthermore, since any one-dimensional distribution can be obtained from a uniform

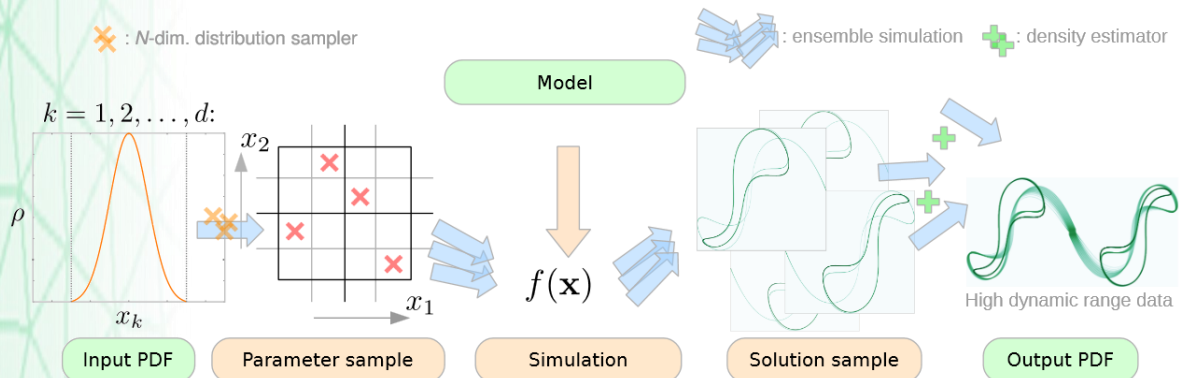


Figure 1

distribution via inverse mapping by its cumulative distribution function (CDF), it is sufficient to look at stratified sampling of a hypercube with a uniform distribution on each axis.

To discretize the d -dimensional hypercube representing the input set, we divide it into n bins along each axis (choosing n appropriately), and represent each bin by the point at its center. We obtain a set of n^d points, each representing one combination of values of the problem parameters x_k .

The remaining problem is to choose, out of this set of n^d points, a subset of m points (where, preferably, $m \ll n^d$) such that the distribution of the selected points in the large hypercube is as uniform as possible. The inverse mapping (on the left), and the bin division and the sampling (in the middle) are illustrated at Figure 2.

Because the model inputs were assumed statistically independent, we would like to have no statistical correlation between the variables in the generated set of points. In other words, if the generated points (**observations**) $x_k = (x_1^{(k)}, x_2^{(k)}, \dots, x_d^{(k)})$ are placed onto the rows of a matrix X , the Pearson product-moment correlation coefficient for each pair of columns $(j, k), j \neq k$, of X should be as close to zero as possible.

There are several families of methods for constructing stratified samples. The trivial method, usable only for very small n and d , is **combinatorial sampling**, where we simply take all n^d points as the input sample. Also for very small samples with suitably chosen n , it is possible to use **orthogonal arrays** (such as in **Taguchi methods**).

Many methods for stratified sampling have arisen in the context of improving the convergence rate of Monte Carlo numerical integration. One family of methods, based on deterministic low-**discrepancy sequences** (such as Sobol sequences), are collectively known as **quasi Monte Carlo (QMC)** methods. Another popular family are **Latin Hypercube Sampling (LHS)** methods. Especially high-quality samples can be produced via methods based on generating LHS from orthogonal arrays (Owen, 1992; Tang, 1993; Ye, 1998), and via the Improved Distributed Latin Hypercube Sampling (IHS) of Beachkofski and Grandhi (2002), which is based on distance maximization.

On the output side, in order to construct the output probability density function to be visualized, the density of the output set must be estimated. A useful family of (in the statistical sense) non-parametric methods is **kernel density estimation**. The idea is to simply place a copies of a function,

called a **kernel**, on each of the samples, and then sum the contributions at each point where the result is to be computed. The sample-centered approach eliminates the main drawback of histogramming, i.e. the very high sensitivity on the choice of the bin boundaries.

It is easily seen by testing that for large sample sizes, the shape of the kernel does not matter much; much more important is its rate of falloff as a function of distance, usually expressed in terms of **bandwidth**. The methods differ mainly in how to choose the bandwidth for a given sample, different methods providing different optimality criteria. The figure below (on the right) illustrates kernel density estimation for an artificial one-dimensional sample containing six points, using a Gaussian kernel and the method of Sheather and Jones (1991).

3 HIGH DYNAMIC RANGE PLOTTING

The resulting output density field will typically have a very large dynamic range. However, in a typical computer screen using 8-bit colour channels, the available intensity range (which is perceptually linear) is only [1, 255], which corresponds to a dynamic range of $B = 48.1\text{dB}$ on the intensity

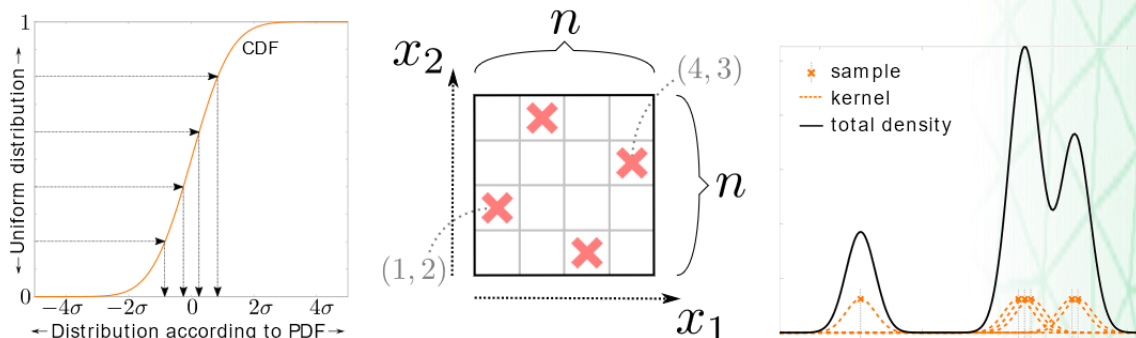


Figure 2

scale $[B = 20 \log (I/I_0)]$. In print, the available dynamic range is typically even smaller.

To overcome this, we introduce **tone mapping**, from HDR photography and realistic 3D computer graphics. Tone mapping is a type of dynamic range compression, which attenuates large contrasts, so that the compressed image becomes representable on a conventional computer screen or in print. This works, because the human visual system is sensitive to differences in light intensity, but not to absolute intensities (e.g. Larson et al., 1997).

The reproduction of HDR mathematical functions and HDR photographs differs in one important respect: for a photograph, it is sufficient to look good subjectively, while a mathematical function must have a global scale, of graph height or colour, that remains the same across the whole picture. Thus, **global tone reproduction operators** (global TROs) are the appropriate class to consider in the context of plotting.

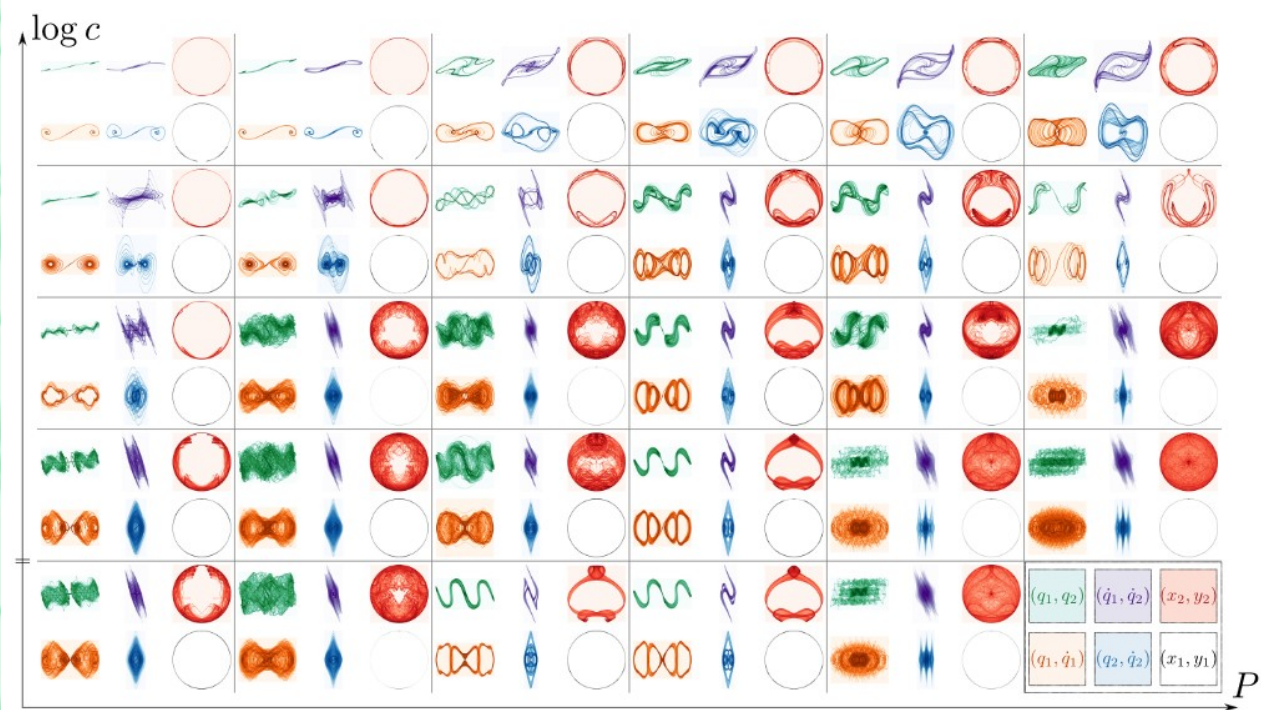
In the previous study Jeronen (2013), the simple saturating histogram equalizer of Larson et al. (1997) was found to work especially well; we refer the reader to these sources for details. The method allocates the display intensity scale in a data-adaptive manner such that as much detail is shown as possible, and the saturation prevents the exaggeration of small contrasts that is a well-known drawback of classical histogram equalization.

HDR plots produced using a global TRO typically visually reveal much more of the structure of the HDR data than classical linear or logarithmic scalings. In Jeronen (2013) it was found that global TROs work well at least up to $B = 100\text{dB}$ (linear range $[1, 10^5]$). At the extreme, the TRO chosen here is usable at least up to $B = 300\text{dB}$ ($[1, 10^{15}]$), albeit at some cost to legibility. Nevertheless, it is perfectly possible to see the actual result and very small numerical artifacts in the same picture, while using a single colour scale. See the original study for pictures.

4 APPLICATION EXAMPLE

The figure above illustrates a parametric study of Ziegler's double pendulum for different values of the problem parameters, each time starting from rest. The stiffness k is fixed; the damping parameter c and the magnitude of the follower load P are varied. The state of the system is fully described by the four-dimensional vector $(q_1, \dot{q}_1, q_2, \dot{q}_2)$. Time integration of the nonlinear ordinary differential equation system is performed using quadratic time-discontinuous Galerkin (dG(2)). The time coordinate is then discarded, and the resulting density in the state space is visualized, using different two-dimensional projections. This density is proportional to the fraction of time the system spends at a particular region of the state space.

For stability analysis purposes, the initial angles of the rods, q_1 and q_2 at time $t = 0$, are taken as uncertain parameters, both having a uniform distribution centered around the origin. For simplicity, and because this particular model is



computationally very light, combinatorial sampling is used. As discussed above, the ensemble simulation results are superposed onto the same picture. This readily captures both attractors in a pair (symmetric around the origin) into the same visualization, highlighting the symmetry in an intuitive manner.

The instability of the trivial equilibrium position at the origin and the resulting behaviour are clearly seen in the pictures. In cases exhibiting limit cycles, despite the fact that almost all of the output data lies on the limit cycle (leading to very high state density), the full history of the simulations is also visible.

The small multiples format, albeit very useful for parametric studies, leads to individual plots being rather small. The figure at the beginning of this article displays one particular case at a larger size. There, from left to right, the subfigures respectively represent (q_1, \dot{q}_1) , (q_2, \dot{q}_2) , (\dot{q}_1, \dot{q}_2) , and (q_1, q_2) . The grid formed by the combinatorial sample in the initial state can be seen in the (q_1, q_2) plot, in its center. The same plot also suggests that only the initial sign of q_2 matters as to which of the two attractors the system will pick in this particular case.

5 CONCLUSION

In this short paper, we looked at some qualitative aspects of a visual approach to sample-based uncertainty quantification, which often leads to probability density functions with a high dynamic range (HDR).

The visualization of HDR data on conventional media requires dynamic range compression. This is achieved in a data-adaptive manner by applying a global tone mapping operator originally developed for

realistic 3D computer graphics and HDR photography. The operator renders the data into a low dynamic range representation that preserves contrast and thus visual detail, improving upon classical linear or logarithmic scalings.

Graphical representations with a high level of visual detail, such as those obtained, are especially useful for exploratory analysis of numerical models.

ACKNOWLEDGEMENT

The author was financially supported by the Jenny and Antti Wihuri Foundation.

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VII ECCOMAS CONGRESS

CRETE, JUNE 2016

The VII European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS Congress 2016) was held in Crete, Greece, on June 5-10, 2016. It was organized by the Institute of Structural Analysis and Antiseismic Research of the National Technical University of Athens with the support of the Greek Association of Computational Mechanics (GRACM).

The event was hosted at the Creta Maris Convention Centre - one of the biggest Convention Centres in the Mediterranean - located near the city of Heraklion. Fifty eight countries were represented by over 2.250 participants.

The main objective of ECCOMAS Congress series is to provide a forum for presentation and discussion of state-of-the-art advances in computational methods in applied sciences and engineering, including basic methodologies, scientific developments and industrial applications and to serve as a platform for establishing links between research groups of academia and industry with common as well as complementary activities.

Almost 70% of the participants who attended the ECCOMAS Congress 2016 can be considered as young investigators, while the percentage of the postgraduate and PhD students who registered was 35% among all participants. This is the most important message, not only to the European but also to the International Scientific Community; that Computational Methods in Applied Science and Engineering is a fast growing and very dynamic scientific field with great future at the forefront of technological progress worldwide.

SCIENTIFIC PROGRAMME

More than 2.600 abstracts related to all areas of computational methods in applied sciences and engineering were submitted, out of which 2.111 were accepted for presentation following the review process, while 667 full-length papers were accepted and have been indexed in SCOPUS database.



The organization team of the Congress: From left to right: Irimi Diakomanoli, Jenny Mitsoura, Fotini Chrystofilli, Manolis Papadrakakis, Panagiota Kouniaki, Eva Konti



Participants during the Welcome Reception



Opening Session in the Zeus Hall

The Scientific Programme consisted of 8 plenary lectures, 27 semi-plenary lectures, 162 minisymposia, 8 special technological sessions, one minisymposium dedicated to the Young Investigators Committee of ECCOMAS. Furthermore, the 6th ECCOMAS Olympiad was hosted by the Congress during which, the best PhD theses approved by a university or research organization in Europe for the year 2015 were presented.

Opening Session: Theodosios Tasios (Greece)

Plenary Speakers: Alexandre Ern (France), Charbel Farhat (USA), Gerhard A. Holzapfel (Austria), Antonio Huerta (Spain), Thomas J.R. Hughes (USA), Alfio Quarteroni (Italy), Ole Sigmund (Denmark)



Opening Session head table, from left to right: Manolis Papadrakakis (Chairman of ECCOMAS Congress), Ekkehard Ramm (President of ECCOMAS and Honorary Chairman of ECCOMAS Congress), Wing Kam Liu (President of IACM)



From left to right: Professors Theodosios Tasios, addressing the Opening Session, Alexandre Ern, Charbel Farhat, Gerhard A. Holzapfel, Antonio Huerta, Thomas J.R. Hughes, Alfio Quarteroni, Ole Sigmund, addressing the Plenary Sessions

Semi-Plenary Speakers: Assyr Abdulle (Switzerland), Olivier Allix (France), Lourenco Beirao da Veiga (Italy), Andreas G. Boudouvis (Greece), Annalisa Buffa (Italy), Ramon Codina (Spain), Laura De Lorenzis (Germany), Bernard Geurts (The Netherlands), Kyriakos Giannakoglou (Greece), Antonio J. Gil (United Kingdom), Dan Givoli (Israel), Anthony Gravouil (France), George Karniadakis (USA), Mats G. Larson (Sweden), Kim Meow Liew (Hong Kong), Wing Kam Liu (USA), Federico Negri (Switzerland), Shinji Nishiwaki (Japan), Ursula Rasthofer (Germany), Ernst Rank (Germany), Cord-Christian Rossow (Germany), Giancarlo Sangalli (Italy), Jörg Schröder (Germany), Bert Sluys (The Netherlands), Christian Soize (France), Roberto Verzicco (Italy), Barbara Wohlmuth (Germany)

EXHIBITION

The technical program was complemented by an exhibition, strategically located at the center of the daily activities of the congress to facilitate the interaction of participants interested in viewing and discussing publications, software, hardware, and other materials related to computational mechanics.



AWARDS

The President of ECCOMAS Ekkehard Ramm delivered the ECCOMAS Awards for 2016:

- Ritz-Galerkin Medal: **Franco Brezzi**
- Leonhard Euler Medal: **Ferdinando Auricchio**
- Ludwig Prandtl Medal: **Wolfgang A. Wall**
- Jacques Louis Lions Award for young Scientists in Computational Mathematics: **Lourenco Beirão da Veiga**
- Olgierd Cecil Zienkiewicz Award for young Scientists in Computational Engineering Sciences: **Antonio J. Gil**
- ECCOMAS Awards for the best PhD theses of 2015 on Computational Methods in Applied Sciences and Engineering: **Ursula Rasthofer, Federico Negri**
- Two best Olympiad Oral Presentation Awards: **Konrad Perzyński, Konstantinos Panagiotou**



From left to right: Franco Brezzi, Ferdinando Auricchio, Wolfgang A. Wall, Lourenco Beirão da Veiga, Antonio J. Gil, Ursula Rasthofer, Federico Negri

THE CONGRESS IN FIGURES

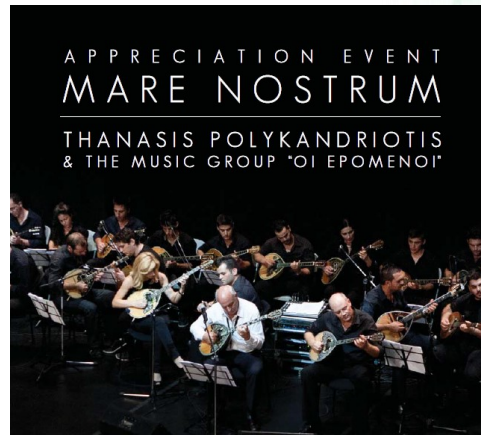
As a response to the call for abstracts, more than 2.600 contributions were received and went through the review process. In the end, 2.111 abstracts were presented in the Scientific Programme.

Registered participants: 2.259 from 58 countries
 Abstracts : 2.111
 Minisymposia: 162
 Contributed sessions: 33
 Papers indexed in SCOPUS: 667

Germany	423	Portugal	33	Croatia	8	Slovenia	3
France	285	Czech Republic	24	India	8	Belarus	2
Italy	173	Norway	22	Slovakia	7	Egypt	2
United States	154	Brazil	21	Saudi Arabia	6	Latvia	2
United Kingdom	151	Finland	19	Argentina	5	Thailand	2
Spain	99	Denmark	15	Colombia	4	Bahrain	1
Greece	77	Luxembourg	15	Lebanon	4	Bangladesh	1
Russian Federation	77	Canada	14	Mexico	4	Bulgaria	1
Belgium	75	Israel	13	New Zealand	4	Iceland	1
Japan	71	Cyprus	12	Romania	4	Kazakhstan	1
Poland	69	Turkey	11	Taiwan	4	Reunion	1
China	60	Korea (South)	10	Algeria	3	Ukraine	1
Netherlands	60	Serbia	9	Hong Kong	3	United Arab Emirates	1
Sweden	52	South Africa	9	Hungary	3		
Switzerland	50	Australia	8	Iran	3		
Austria	48	Chile	8	Singapore	3		



Antonis Martsakis and his group playing traditional Cretan music at the Welcome Reception



Thanasis Polykandriotis and his group provided an anthology of Greek folk music based on the Bouzouki instrument

SOCIAL PROGRAMME

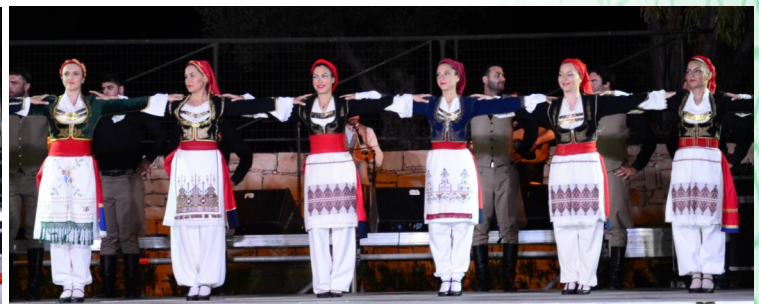
ECCOMAS Congress 2016 had apart from its advanced scientific perspective, a strong cultural and social dimension. In this context, a number of events took place during the course of the Congress which complemented the Scientific Programme of the Congress. The Opening Speech by Theodosios Tasios, illustrated the achievements of the four great engineers of the Hellenistic era: Ctesibius, Archimides, Philon and Heron, which among other engineering achievements invented a fully operational automata and the first prerequisite for the analog computer, i.e. the Antikythera Mechanism. During the Welcome Reception, Antonis Martsakis and his group entertained the participants with traditional Cretan music played by violin, Cretan lyra and lagotho. At the Appreciation Event, honoring the invited speakers and those who contributed to the organization of the Minisymposia, Thanasis Polykandriotis' music group "OI EPOMENOI", which performed at the Opening Ceremony of the XXVIII Olympic Games "Athens 2004", provided an anthology of Greek folk music based on the Bouzouki instrument. At the Congress Banquet, Cretan dancers showed their artistry in performing traditional folk dances of Crete which depict the brave heroism, dynamism and rebellious character of the Cretan people.



Appreciation Event



Congress Banquet



Cretan dancers showing their artistry in performing traditional folk dances of Crete

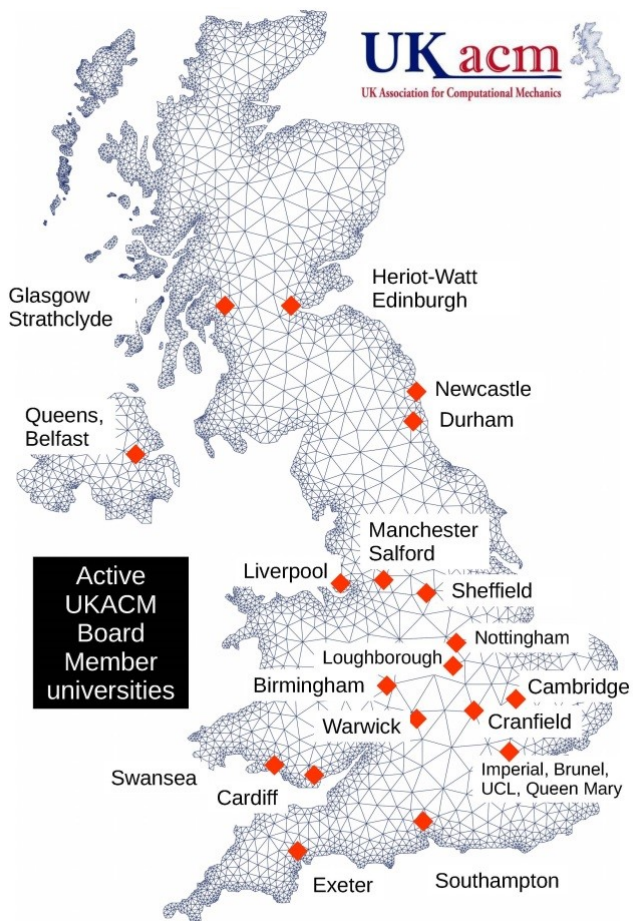
WHO REPRESENTS COMPUTATIONAL MECHANICS RESEARCH IN THE UK?

U.K.A.C.M.

The United Kingdom Association for Computational Mechanics (UKACM) was formed in March 1992 to promote research in computational mechanics in the UK, and to establish formal links with similar organisations in Europe, and worldwide. We were initially named “ACME” (Association of Computational Mechanics in Engineering) but from 2016 we became UKACM. The UKACM is managed by a small Executive Committee and a larger Board, the latter comprising representatives from universities active in computational mechanics.

UKACM Conferences and “Schools”

The principal activity of the Association is the organisation of an annual two day conference on computational mechanics: developments and research trends. The conference provides an opportunity for researchers of all vintages (PhDs to Professors) to present and defend their research in computational mechanics, in a welcoming but challenging forum. Since 2011, each annual conference has been preceded by a “School” aimed at PhD students. This is an afternoon of lectures on a particular topic or theme in computational mechanics. The topics covered to date include meshless methods, isogeometric approaches, high order methods and multiscale modelling. Our 25th conference in 2017 is in the city of Birmingham and, while it is a UKACM conference, it is open to all from Europe and beyond.





Attendees of the 1st conference of the Association, Swansea, 1993. In the centre is Prof. Olgierd Zienkiewicz, the Association's first president.

Looking ahead

The 2018 UKACM conference will be incorporated into the 2018 ECCM-ECFD conference in Glasgow (which you can read about elsewhere in this issue) Scotland still being part of the UK at the time of writing!

A key goal of the Association for the coming years is to improve our representation of activity in computational fluid mechanics and applied mathematics and to encourage the involvement of younger researchers from diverse backgrounds.

For more information on UKACM, our 2017 conference and much more, visit www.ukacm.org

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Attendees of the 24th Conference, Cardiff, 2016

BELGIAN NATIONAL COMMITTEE FOR THEORETICAL AND APPLIED MECHANICS

BNCTAM is the Belgian *National Committee* for Theoretical and Applied Mechanics. It is a part of RASAB, the *Royal Academies for Sciences and the Arts of Belgium* (<http://www.rasab.be/index.php?lang=en>). The association is headquartered in the former stables of the Palace of the Academies in Brussels.

The Royal Academies were founded by empress Maria-Theresia in the 18th century, with the aim of promoting the sciences and the arts in Belgium. To meet this demand, the Academies organize scientific and cultural activities. They try to stimulate cooperation between universities in Belgium, they assure Belgian representation in international organizations and forums, they attract foreign researchers, they give recommendations and advice to government, industry, education and research institutions and they give prizes to talented researchers and artists.

RASAB is also responsible for coordinating the activities carried out at national as well as international level by different *National Committees* such as BNCTAM.

The main specific activities of BNCTAM are:

- The promotion of Mechanics in a broad sense.

- The organization of GRASMECH, the (Belgian) GRADuate School on Mechanics (<http://www.grasmech.frs-fnrs.be/index.html>). The purpose of the Graduate School is to organize courses in the field of Computational and Experimental Mechanics, on a third cycle level, to all Belgian graduate students, to stimulate the cooperation between universities and favor exchanges of researchers.
- The representation of Belgium in scientific international organizations, such as IUTAM, EUROMECH, EURASEM, IACM and ECCOMAS.
- The organization of scientific events.

Another important mission of BNCTAM is to elect the best Belgian PhD Thesis of the year in Mechanics and to propose the winner as a candidate to the ECCOMAS best thesis Award. To elect the best thesis, we have recently launched a new procedure in two steps. In a first round, a selection is made on classical criteria to establish a short list of candidates. Then the candidates in the short list have about one month to prepare a short movie where the applicant explains why his/her thesis is outstanding. There is no further indication/recommendation about this movie except that its maximum duration is

10 minutes. Based on both the manuscript and the movie, the Executive Committee then decides who will be the recipient. As recent examples, the movies from Katrien Van Nimmen, Award 2015 (<https://www.youtube.com/watch?v=D7ZOTtv-Gsk>) and from Pieter Coulier, Award 2014 (<https://www.youtube.com/watch?v=DMW6nYCp6t0>) are both available on Youtube. Pieter Coulier was also awarded for the ECCOMAS Award for the Two Best PhD Theses in 2014 for the thesis "*The numerical solution of large scale dynamic soil-structure interaction problems*".

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6th European Conference on
Computational Mechanics
(Solids, Structures and Coupled Problems)
- ECCM 6

7th European Conference on
Computational Fluid Dynamics
- ECFD 7

ECCM - ECFD 2018

ECCM 6 & ECFD 7 will be held in Glasgow, UK on June 11-15, 2018. The Congress is being hosted by The University of Glasgow, The University of Edinburgh and UKACM

Conference Venue

The Scottish Exhibition and Conference Centre (SECC) is Scotland's largest exhibition centre, located in the popular district of Finnieston on the bank of the River Clyde. It is an iconic landmark venue and business tourism destination with facilities which are second to none. The Welcome Reception, hosted by The Lord Provost, will take place across the River at the Glasgow Science Centre.

Important Deadlines

31 March 2017

Submission of minisymposia proposals

Early September 2017

Presenting a one page abstract

Early February 2018

Final contribution and early payment

Programme

Six Invited Plenary and 18 Semi-Plenary lectures on topics of broad interest to the ECCM and ECFD communities will be given by experts in each field. The programme will also include Minisymposia dealing with exciting current topics.



THE UNIVERSITY
of EDINBURGH



info@eccm-ecfd2018.org www.eccm-ecfd2018.org

ECCOMAS THEMATIC CONFERENCES 2017

Acronym	ECCOMAS Thematic Conference	Location	Date
KomPlas Tech	Conference on Computer Methods in Materials Technology	Zakopane, Poland	Jan 15 - 18
HONOM	European Workshop on High Order Nonlinear Numerical Methods for Evolutionary PDEs: Theory and Applications	Stuttgart, Germany	Mar 27 - 31
SYMCOMP	International Conference on Numerical and Symbolic Computation: Developments and Applications	Guimarães, Minho, Portugal	Apr 6 - 7
EURO:TUN	Computational Methods in Tunnelling	Innsbruck, Austria	Apr 18 - 20
MARINE	VII International Conference on Computational Methods in Marine Engineering	Nantes, France	May 15 - 17
MultiBioMe	Multiscale Problems in Biomechanics and Mechanobiology	Cargese, Corsica (France)	May 15 - 17
CM3	Computational and Big Data Transport Research solving Societal and Industrial Challenges in Aeronautics, Automotive, Logistics, Maritime and Railways	Brussels, Belgium	May 22-24
CompWood	Computational Methods in Wood Mechanics - from Material Properties to Timber Structures	Vienna, Austria	May 29 - 31
IPM	4th International Conference on Inverse Problems in Mechanics of Structures and Materials	Kraczyzn, Poland	May 31 - Jun 2
SMART	8th Conference on Smart Structures and Materials	Madrid, Spain	Jun 5 - 8
COUPLED PROBLEMS	VII International Conference on Coupled Problems in Science and Engineering	Rhodes, Greece	Jun 12 - 14
CFRAC	Fifth International Conference on Computational Modeling of Fracture and Failure of Materials and Structures	Nantes, France	Jun 14 - 16
COMPDMN	6th International Conference on Computational Methods in Structural Dynamics and Earthquake Engineering	Rhodes, Greece	June 15 - 17
UNCECOMP	International Conference on Uncertainty Quantification in Computational Sciences and Engineering	Rhodes, Greece	June 15 - 17
X-DMS	eXtended Discretization MethodS	Umeå Univ., Sweden	June 19 - 21
ICTE	5th International Conference on Tissue Engineering	Manchester, UK	June 22 - 24
ADMOS	VIII International Conference on Adaptive Modeling and Simulation	Verbania, Italy	Jun 26 - 28

Acronym	ECCOMAS Thematic Conference	Location	Date
MULTIBODY	Multibody Dynamics	Prague, Czech Republic	Jun 26 - 29
ICCCM	International Conference on Computational Contact Mechanics	Lecce, Italy	Jul 5 - 7
M-FET	Modern Finite Element Technologies - Mathematical and Mechanical Aspects	Bad Honnef, Germany	Aug 21 - 23
COMPLAS	XIV International Conference on Computational Plasticity	Barcelona, Spain	Sept 5 - 7
IGA	V International Conference on Isogeometric Analysis	Pavia, Italy	Sept 11 - 13
	Computational Modelling of Multi-Uncertainty and Multi-Scale Problems 2017	Porto, Portugal	Sept 12 - 15
EUROGEN	12th International Conference on Evolutionary and Deterministic Methods for Design, Optimization and Control with Applications to Industrial and Societal Problems	Madrid, Spain	Sept 13 - 15
CompHPC	Computational Methods and Algorithms on HPC Platforms and Accelerators	Athens, Greece	Sept 18 - 20
COMPOSITES	VI Conference on Mechanical Response of Composites	Eindhoven, Netherlands	Sept 20 - 22
ECCOMAS MSF	3rd International Conference on Computational Methods for Solids and Fluids.	Ljubljana, Slovenia	Sept 20-22
PARTICLES	V International Conference on Particle-based Methods	Hannover, Germany	Sept 26 - 28
STRUCTURAL MEMBRANES	VIII Internacional Conference on Textile Composites and Inflatable Structures	Munich, Germany	Oct 9 - 11
Sim-AM	Simulation for Additive Manufacturing	Munich, Germany	Oct 11 - 13
VipIMAGE	VI Conference on Computational Vision and Medical Image Processing	Porto, Portugal	Oct 18 - 20
ICBT	III International Conference on Biomedical Technology	Hannover, Germany	Nov 6 - 8
CMCS	Computational Modeling of Complex Materials Across the Scales	Paris, France	Nov 7 - 9
MORTech	4th International Workshop on Reduced Basis, POD and PGD Model Reduction Techniques	Seville, Spain	Nov 8 - 10
CORASS	International Conference on Rehabilitation and Sustainability of Structures – Advanced structural models, materials and applications	Coimbra, Portugal	Nov 21 - 22

OTHER ECCOMAS CONFERENCES 2017

YIC	ECCOMAS Young Investigators Conference 2017	Milan, Italy	Sept 13 - 15
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ECCOMAS YOUNG INVESTIGATORS CORNER

NEW CHAIRPERSONS AND CORE GROUP OF THE ECCOMAS YOUNG INVESTIGATORS COMMITTEE ELECTED

On 8 June 2016, at the ECCOMAS Congress in Crete, Alexander Popp (Munich, Germany) and Stefanie Elgeti (Aachen, Germany) were elected as new chairpersons of the ECCOMAS Young Investigators Committee (EYIC). Together with 21 young researchers representing the different national and regional associations within ECCOMAS, the new EYIC spokespersons will do their best to continue the great work that has been started in the last years by the first EYIC chairman Alessandro Reali (Pavia, Italy) and all other former committee members. The EYIC has been created in order to promote the main goals of ECCOMAS among young researchers and to encourage activities of young ECCOMAS members. With the number of young investigators working on computational methods in applied sciences having significantly increased over the last years, the EYIC has become a very active and dedicated coalition of young researchers as could be witnessed during several innovative activities at the ECCOMAS Congress 2016 (see report below). The next milestone for the young investigator activities within ECCOMAS will undoubtedly be the 4th ECCOMAS Young Investigators Conference to be hosted at Politecnico di Milano (Italy) on 13-15 September 2017, which will continue the tradition of bringing together young researchers working in the field of computational science and engineering.

EYIC website: <http://www.eccomas.org/vpage/1/0/Committees/YIC-General>

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Stefanie Elgeti – elgeti@cats.rwth-aachen.de
ECCOMAS Young Investigators Committee



Speakers of the Young Investigators Minisymposium together with the ECCOMAS YIC members J. Baiges, A. Popp and J.-W. Simon

FIRST YOUNG INVESTIGATORS MINISYMPOSIUM AT THE ECCOMAS CONGRESS 2016 IN CRETE A GREAT SUCCESS

A new type of scientific sessions at ECCOMAS events, the so-called “*Young Investigators Minisymposium*”, took place for the first time at the European Congress on Computational Methods in Applied Sciences and Engineering, which was held in Crete on 5-10 June 2016. The Young Investigators Minisymposium was organized by members of the Young Investigators Committee of ECCOMAS, a group of young academics that was formed in order to promote the main goals of ECCOMAS among young researchers, with a special emphasis on encouraging activities of young ECCOMAS members. The minisymposium was themed

“By Young Investigators For Young Investigators”

and consisted of a total of nine presentations, which were prepared in two different formats: first, so-called “*presentations in pairs*”, where two presenters prepared and submitted their abstract together. By also giving the scientific talk as a team of two, this format allowed the audience to view research topics from two different perspectives and gain a broader understanding than usual. Second, the minisymposium also featured presentations of “*things that did not work (as expected)*” focusing on research lines that led to different outcomes than initially intended, which gave many unexpected and most helpful insights into the long, rocky road towards scientific progress.

Both of these formats resulted in very dynamic minisymposium sessions with a great deal of interaction between presenters and audience, which strongly encourages the organizers to reproduce and extend these and other innovative ideas within dedicated Young Investigators Minisymposia at future ECCOMAS conferences.

Joan Baiges – jbaiges@cimne.upc.edu
Alexander Popp – popp@lnm.mw.tum.de
Jaan-Willem Simon – jaan.simon@rwth-aachen.de
ECCOMAS Young Investigators Committee



“Presentations in pairs” was one of two new scientific talk formats tested within the Young Investigators Minisymposium

4TH ECCOMAS YOUNG INVESTIGATORS CONFERENCE 2017

ECCOMAS PHD OLYMPIAD 2017

We would like to invite you to join us for the **Young Investigators Conference 2017 (YIC 2017)**, which will take place **from 13rd to 15th September 2017** in Milan, Italy. The conference will be hosted by the Department of Civil and Environmental Engineering of Politecnico di Milano.

YIC 2017 will be the fourth meeting organized by ECCOMAS (European Community of Computational Methods in Applied Sciences) specifically conceived for young researchers.

The conference is planned to extend over three days. Each day will start with an invited plenary lecture, which will present the state-of-the-art of the research in computational science and technology. The conference will be organized in parallel sessions. At the end of each session, enough time for discussion will be arranged. **A special section will be devoted to the presentations of the finalists of the PhD Olympiad.**

As proposed in the previous Young Investigator Conferences, new formats, closer to young investigators interests, will be introduced.

To favor the informal discussion between participants, **round-tables** will be organized to discuss on the recent trends of the computational sciences and engineering.

Special sections, called **problem solving**, will be proposed. In this particular section, young researchers can present their problem to a team of experts through a brief presentation. After that, the team of experts will provide advice, suggestions or new insights to the specific problem.

Hope to see you in Milan in 2017.

Conference Chairman:

Massimiliano Cremonesi
Department of Civil and Environmental Engineering
Politecnico di Milano (Italy)
massimiliano.cremonesi@polimi.it

website: www.yic2017.polimi.it

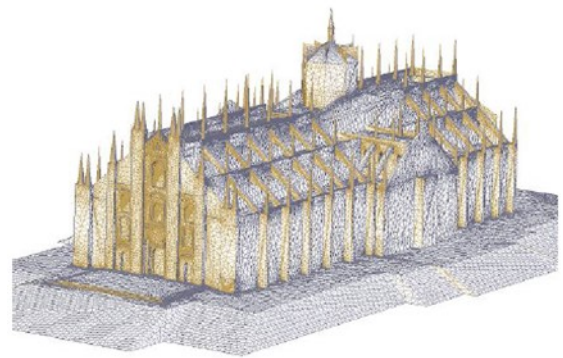
contact: yic2017-dica@polimi.it



YIC 2017

4th ECCOMAS
Young Investigators Conference
and PhD Olympiad 2017

13 - 15 September 2017, Milano, Italy



www.yic2017.polimi.it

Organized by
Politecnico di Milano



Important Dates

Abstract submission: January 31, 2017

Notification of acceptance: March 3, 2017

Early payment: April 3, 2017

*Welcome to Paris,
ECCOMAS Congress 2020*

*XIVth World Congress of
Computational Mechanics*

19-24 July 2020



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ECCOMAS
European Community on
Computational Methods
in Applied Sciences

6th European Conference on Computational Mechanics
(Solids, Structures and Coupled Problems) - ECCM 6

7th European Conference on Computational Fluid Mechanics - ECFD 7

11 – 15 JUNE 2018, GLASGOW, UK

A collage of images showing the Glasgow Science Centre and the SSE Hydro stadium at night, illuminated with green and blue lights, set against a background of a blue and green grid pattern.

25th Anniversary of ECCOMAS
ECCM - ECFD 2018
Glasgow

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