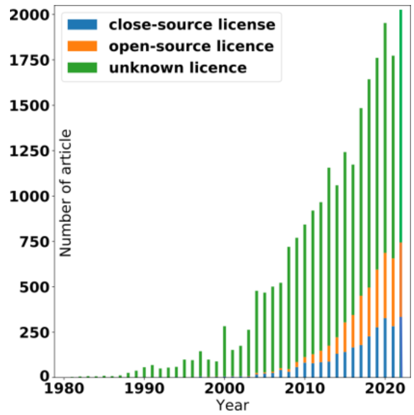
TECHNICAL ANNEX

1. S&T EXCELLENCE

1.1. SOUNDNESS OF THE CHALLENGE

1.1.1. DESCRIPTION OF THE STATE OF THE ART



The Discrete Element Method (DEM) is a class of numerical methods that solve the equations of motion of a huge number of particles simultaneously. These methods are applied to a wide range of problems which can be described in a discrete framework. It naturally includes the studies of bonded and unbonded granular media such as rocks, powders and sand-like materials, but also gases and bulk materials when the discrete nature of such media plays a crucial role. The figure on the right shows the evolution of the number of DEM-related articles since 1980 (extracted from SCOPUS on 15/10/2022). The use of DEM by the scientific community has grown exponentially with more than 2000 papers referenced for the first time in 2022. This interest is due to the specificity of this numerical method enabling it to tackle a class of problems that cannot be solved with classical continuum models such as the Finite Element Method (FEM). Currently, the most efficient DEM platforms are able to simulate ten to one hundred million spherical particles [1] and/or tens of thousands complex-shaped particles [2]. Despite this remarkable performance, a million particles (each 1 mm^3) would represent a volume of only 1 litre. This is many orders of magnitude smaller than the granular flows found in industry or the natural environment. To overcome such a limitation many strategies are applied, including:

- periodic boundary conditions and homogenization in a multi-scale approach [3],
- modelling complex shapes using spherical elements including sophisticated contact models [4],
- using the so-called "Coarse Grained Method" which is able to model an agglomerate of individual particles with a single numerical element (often used in fluidized bed simulation) [5].
- computational multi-scale methods where a cheaper continuum model is used (where appropriate) to speed up the simulations.

Another DEM limitation concerns the time scale. The time scale is always limited because DEM implements an explicit time integration scheme that requires very small time-steps to ensure the stability of the numerical solution. In such a case, DEM achieves physical times of one or more orders of magnitude lower than real processes. Again, simple strategies can be applied such as:

- the well-known mass/density scaling technique that reduces the time-step.
- time extrapolation strategies that take advantage of (pseudo) temporal periodicity patterns [6].

Overcoming these limitations is an active research area. Another part of the DEM development and implementation is focused on physics and particle interaction laws. Here, a strong dialogue between simulation, model and physical experiment is needed to ensure the relevance of the models. Adequate calibration is also paramount. By increasing the complexity of models and their number of parameters, the effort required for their calibration increases. Parameter calibration of complex contact models may also require the avoidance of ambiguous parameter combinations. From this perspective, use of optimisation, inference, Artificial Intelligence (AI) algorithms or surrogate modelling seems promising [7].

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The last reason for the growing interest in DEM simulation is the significant improvement of hardware efficiency combined with the wide availability of new DEM software solutions. Depending on the type of license and the availability of the source code, a distinction can be made between open-source software and proprietary software with limited access to source code. Open-source solutions are well adapted to research activities, promote the sharing of knowledge, reproducibility of results, versatility and prevent the “black box” problem when code review is not possible by peers. Currently, more than ten open-source software packages with a large number of users are available. Amongst them, many are supported and/or affiliated with European research teams. As shown in the figure above, the use of open-source solutions is increasing. Furthermore, the growing rate of open-source DEM related articles is higher than the proprietary ones. The collaborative and open nature of open-source yields to improvements between codes, and increases access to these codes. For these reasons, this Action entitled “Open Network on DEM (ON-DEM)” will place a strong emphasis on these open technologies.

1.1.2. DESCRIPTION OF THE CHALLENGE (MAIN AIM)

Nowadays, DEM is used in many academic fields such as geomechanics, civil engineering, material science, physics or chemistry covering a wide range of industrial and engineering applications including pharmaceutical processing, mining and tunnelling, powder processing, ceramic making, steel making, agriculture machining or landslides, amongst others. Each of these applications has particular needs regarding DEM. Special emphasis is required on different features such as computational performance, multi-physics coupling, model coupling, contact (or bonding) models, calibration, particle shapes, collision algorithms or the ability to deal with particle clustering and their fragmentation. To cover all these requirements, a large set of open-source DEM packages, coming from different scientific disciplines is available. These packages range from general solutions able to cover a wide range of applications, to very dedicated solutions able to solve particular problems with great accuracy. This heterogeneity, inside the DEM community, results in a kind of compartmentalisation of stakeholders and knowledge. The DEM community is often segmented around a particular DEM code, a particular academic discipline and/or a particular set of applications. This leads to diverse pocket users with strong expertise, but few global discussions beneficial for the entire DEM community. A simple analysis of DEM articles published in 2021 shows that they were distributed among 160 different journals. The top five journals capitalise on 17% of these publications. Furthermore, these top five journals are mainly focused on powder, granular media and geosciences. Only one has a strong emphasis on numerical methods. Also, 47% of the articles are related to engineering science, 32% to geosciences, 23% to chemical engineering, 14% to materials science and 14% to computer science. This analysis highlights the compartmentalisation of knowledge. The main aim of this Action is to unify this knowledge by bringing together people, from software developers to experienced users including stakeholder companies from a wide range of scientific disciplines. This will enable the Action to assess what can be achieved with DEM approaches, share and disseminate new developments to tackle current challenges and promote best practices in particle-based simulations. The research questions for this COST Action are: **Can the existing boundaries and capabilities of both DEM models and simulation tools be pushed by a joint effort by the existing and distinct DEM sub-communities? How can the community be unified, synergising the diverse knowledge and expertise such that more rapid advances in the field can be made?** This will set the foundation for solving the next generation of problems across disciplines, and set standards and training strategies for the future of DEM modelling.

For many years, particle-scale simulations considered almost exclusively rigid circular or spherical particles with linear/non-linear elastic contact models. In this case, no question remains about the accuracy of DEM simulations. However, more complex contact models now exist, and significant advances have been made in modelling non-spherical particles and simulating particle breakage. Considering soft and compressible particles is also possible now. What remains to be done is to increase the level of complexity/realism of DEM codes and ensuring their reliability. The ON-DEM Action will take benefit of the variety and large number of participants to carry out, on different open-source codes, a set of well-chosen and well documented problems that are validated in order to give reference results and benchmarking problems, maximising the potential benefits to the community. Recommendations will be given to assess the level of complexity required to effectively capture physical reality for different applications and share the understanding of how to implement and analyse these models.

1.2. PROGRESS BEYOND THE STATE-OF-THE-ART

1.2.1. APPROACH TO THE CHALLENGE AND PROGRESS BEYOND THE STATE OF THE ART

To address the key challenge of **how to deal with larger, more complex/realistic simulations with more reliability**, the synergy of knowledge from many different disciplines is needed. Thus, the key aim of the ON-DEM Action is to bring together knowledge from diverse disciplines within the particle-scale simulation community to ensure rapid progress. This will require contributions from mathematics (to develop new algorithms), computer science (to develop faster codes), and other scientific disciplines that have experimental knowledge on how to deal with shape and multi-physics coupling, amongst others. An additional novelty in this approach is the involvement of the developers of open-source DEM codes. This will allow the rapid development and implementation of new algorithmic and modelling strategies. In addition, it will allow comparison of the proposed solutions to retain only the most relevant ones. Comparisons of results to be carried out between different DEM codes and verified by experimental observations will enhance the reliability of codes and appropriateness of models. With this perspective, the ON-DEM COST Action will also include experimentalists and experienced DEM users. Finally, the COST Action will also propose a standard file format to promote interoperability and sharing data that will enable work on common high-performance visualisation and post-processing tools.

Five main topics were identified as additional challenges. This Action will be managed in different Working Groups (WGs) to independently address these key challenges:

1. **Passing through time and space scales** for tackling real, and large-scale problems.
2. **Getting closer to physics** to take into account more complex phenomena.
3. **Processing big data and visualization** to better analyse and post-process results.
4. **Working with industry** for widening commercial utilisation of open-source DEM codes.
5. **Disseminating best practices** to promote interoperability and enforce robustness of results.

The output of these interdisciplinary WGs will be combined to set the foundations for the next generation of particle-scale simulations, capable of tackling real, large-scale geophysical, engineering and industrial problems. The numerical solutions, tools and procedures developed and implemented will be accessible to the whole community, through open and free access licences.

1.2.2. OBJECTIVES

1.2.2.1. Research Coordination Objectives

The goal of ON-DEM Action is to enhance the research efforts of different scientific fields which share the same numerical tool and method for tackling very different problems. To achieve this goal a pan-European network will be established which will bring together leading and young researchers in these diverse research fields with key non-academic and industrial stakeholders. Small spin-off companies, which are affiliated with universities and researchers that develop original open-source DEM software will be present. Some companies focusing on numerical solutions such as high-performance visualisation tools will also be associated with the Action. Similarly, companies that develop original characterization equipment, apparatus and protocols for granular media are also part of the Action. The main research coordination objectives of the Action corresponding to each of the challenges/WGs listed above:

1. To study, implement and develop new algorithms able to gain one or more orders of magnitude in terms of **time and space scales** with DEM based simulations. Such algorithms can be divided into two distinct categories. The first one concerns better exploitation of new hardware architectures while the second class of algorithms are based on physics by exploiting enriched contact models and/or taking advantage of time periodicity of a problem. Abundant literature is available concerning these topics which remains unclear as no definitive benchmarking study

exists. The main objectives of this Working Group are to (i) identify a list of the most promising solutions (ii) implement them in several DEM codes and (iii) benchmark them on a short list of “model” problems. At least four relevant problems (i.e. one per year) will be chosen for each of the research areas represented in the Action. The final objective involves establishing a comprehensive list of solutions, combined with recommendations on their usage context, while proposing implementations and documented test cases in different open-source DEM codes.

2. To develop and establish a comprehensive methodology for **accurately capturing the physics** of typical granular media. The different steps to reach this objective are (i) defining a short list of granular “model” materials with typical different physical properties, (ii) carrying out experimental characterization using equipment owned by industry and businesses associated to the Action, (iii), establishing a very well documented material database based on experiments and (iv) exploiting this database for proposing different modelling strategies and calibration methodologies on different DEM codes. As before the short list will consider at least four “model” materials of relevance to each of the research disciplines represented in the Action.
3. To enhance interoperability between DEM codes by proposing a common **output data format for post-processing and visualisation** is the main objective of this WG. Specifications about the proposed standardized format will be well documented and freely available. Such a standard format will open the possibility to work on common post-processing techniques and high-performance visualisation tools. A collaboration with dedicated companies that develop generalist scientific visualisation tools is already part of this Action. In such a way, this work will lead the way to DEM specific visualisation tools available for any code that implements the proposed standard file format. Again, such a proposition will benefit the whole scientific community, SMEs, as well as then next generation of leading DEM researchers. This objective requires significant discussion and agreement between scientific fields and as such it is expected that this objective will only be achieved by the last year of the Action.
4. To focus on **creating links with industry** stakeholders and facilitating commercial utilisation of the outputs of this Action. This WG will work directly with key industrial users of DEM to determine what are the current barriers to commercial utilisation and will input WG1, WG2 and WG4 in the form of “model” solutions and materials. The needs of industry are often quite different to academic users. Industrial focus is often on easy-of-use/setup, robustness, ‘quick’ results and how to calibrate the models for real industrial materials. Joint work with software houses and DEM consultancy firms will help develop the tools to overcome these barriers. In the last few years there is an increasing number of commercial software houses and consultancy companies that utilise/develop open-source solutions. These will be the focus of this WG.
5. To **disseminate the scientific and technological outcomes** provided by the ON-DEM Action: data, best-practices, algorithms and new developments. This WG will be in charge to maintain an overview of the other WGs in order to extract and keep available the related developments that present an interest for interested communities as well as the public. Special attention will be paid to providing smart communication support for science dissemination to the general public through smart videos and online events. This WG group will also ensure that all Action outputs are freely available making use of existing open access platforms and licences.

Note that WG1 to WG3 also focus on better processes for simulation quality control, validation and verification by developing guidelines on code testing. Whilst not an additional challenge there is also a WG on **normalisation and best practices (WG4)**. Also note that without international, multi-disciplinary coordination none of these objectives can be achieved.

1.2.2.2. Capacity-building Objectives

The main objective of the proposed network is to bring together the stakeholders related to the open-source DEM community. It includes researchers from diverse research fields, companies that have direct use of DEM, and companies which have indirect interests in DEM. The originality of the Action is to promote synergy and discussion between developers, experienced users of DEM, companies, early career researchers, as well as experienced investigators. Extensive discussions between these different stakeholders (driven by each of the WGs above) should improve the quality of DEM simulations in order to provide both more realistic and more reliable results (one of the current limitations in DEM simulation). Specific capacity-building objectives of the Action are to:

1. Develop a large and well-identified pan-European network focusing on DEM that fosters knowledge exchange and acts as a stakeholder platform to enhance best-practices in DEM simulation. This is needed to increase the commercial utilisation of tools, processes and methods related to DEM. Particularly those within the context large-scale applications.
2. Bridge the separate research/industrial disciplines to achieve faster scientific and technological advances in DEM simulation to tackle more complex/realistic challenges.
3. Hold bi-annual online meetings for each WG and regular physical meetings, workshops and/or seminars. WG (online) meetings ensure the monitoring and achievement of research coordination objectives. Physical meetings favour the bridging between scientific disciplines and enable targeting underrepresented target groups.
4. Two major events associated with a well identified international conference cycle will be organised to (i) disseminate progress and outputs, (ii) discuss and identify new/existing challenges and (iii) reach to new audiences.
5. Ensure that the Management Committee (MC) and every WG is well represented in terms of research field, industrial interest, gender, experience, countries of affiliation, etc.

2. NETWORKING EXCELLENCE

2.1. ADDED VALUE OF NETWORKING IN S&T EXCELLENCE

2.1.1. ADDED VALUE IN RELATION TO EXISTING EFFORTS AT EUROPEAN AND/OR INTERNATIONAL LEVEL

Internationally, there are large numbers of publicly and privately funded research activities related to the use of DEM codes. The analysis discussed in Section 1.1.1 shows that in 2021 52% of DEM publications originated from China, and 11% from the United States. Considering Europe, 50% of European outputs are from the UK, Germany and France. Enhanced access to knowledge, equipment and networks is evidently needed across Europe. Particularly amongst Inclusiveness Target Countries (ITCS).

A word search at https://cordis.europa.eu/ using “granular materials” as a keyword (accessed on 19/10/2022) yields 628 results relating to EU funded research projects. Arguably, all of these projects would benefit from interacting with this ON-DEM COST Action, and vice-versa. More importantly, a quick look at these projects will rapidly conclude the obvious compartmentalisation of knowledge that this specific Action aims to solve. Most deal independently with calibration, specific granular characteristics (e.g. structural properties, polydispersity), constitutive relations, experimental approaches (e.g. features of mechanical behaviour (e.g. thermo-mechanics, energy dissipation) and/or specific training needs. There seems to be no efforts with a scope as wide and comprehensive as the one in this COST Action.

Due to the nature of the Action, comprising investigators across different scientific areas, as well as a diverse group of stakeholders, together with the need for scientific advancement toward large-scale realistic simulation, interaction with these existing efforts is unavoidable and welcome. A particular task of each Working Group is to perform horizon scanning exercises that enable providing true added value to all interested parties. This ACTION has an international reach and aims to bridge, for the first time, all these interested parties for mutual benefit.

2.2. ADDED VALUE OF NETWORKING IN IMPACT

2.2.1. SECURING THE CRITICAL MASS, EXPERTISE AND GEOGRAPHICAL BALANCE WITHIN THE COST MEMBERS AND BEYOND

This Action’s constitution provides the ideal critical mass required for the achievement of its objectives and in general terms, to address the challenge of providing general frameworks, procedures and advice to generate and analyse DEM data that so far has been compartmentalised to specific research areas. This COST Action involves 64 participants, including 19 COST Full Member countries, 10 of these being

ITCs. The geographical distribution of participants facilitates further dissemination of outputs at a more local level and includes three carefully chosen international partner countries (IPC) to fully achieve this in geographical terms (i.e. Colombia, United States, Iran, South Africa and Australia). Their main roles of these international partners is to contribute to horizon scanning exercises, dissemination activities and specific objectives of the Action. The inclusion of these partners adds mutual benefit. On one hand they enable the network of proposers to gain from their insight, experience and their close geographical contacts to enhance the reach of the Action. The IPCs will in turn, benefit from access to outputs, methods and contacts that the Action will provide and produce. In fact, DEM is used worldwide and the existing challenges are shared internationally.

Furthermore, participants have been chosen to cover a wide spectrum of research disciplines as required by the aim and objectives of this Action; 42.2% are civil engineers, 23.4% mechanical engineers, 10.9% physical scientists, 6.3% chemical engineers, 6.3% material engineers and the remaining 11.1% belong to other fields. The Action also engages with industrial stakeholders including software companies as well as those involved in experimental fields and validation. These represent 12.6% of the Action. The percentages above guarantee that all stakeholders will be fully represented in the Management Committee (MC) and each of the Working Groups (WGs).

There is an evident bias towards civil engineering that will be addressed in various ways. For example, (i) linking online meetings and physical events to other conferences related to underrepresented research areas, (ii) dissemination activities such as videos targeting on attraction of these under-represented groups and (iii) advertisement of the Action activities using social networks, websites, etc. Furthermore, while 48.4% of the network of proposers are under the age of 40, only 31.3% of them are identified as female. This is an important issue that the Action will aim to improve. The experience of many of the proposers indicates that DEM seminars organised by them (and so far largely discipline-specific) have been often over-subscribed. So there is confidence when stating these issues can be improved. A simple example to achieve this is by prioritising the registration of hackathon groups/teams including underrepresented genders.

2.2.2. INVOLVEMENT OF STAKEHOLDERS

There are many (European) SMEs relevant to this COST Action. Some of them are focused on the characterisation and calibration of particulates. Others use open-source DEM codes/tools to solve industrial problems and offer three-dimensional visualisation of complex datasets. These companies will be involved in the Action from the outset and will have direct input across several WGs. These include WP1 (in which a set of simulation examples are chosen), WP2 (where contact laws need to be validated experimentally and convincingly for industrial use), WP3 (where standardised and optimised datasets and plug-ins will be developed) as well as WP5 where best-practice and dissemination are considered. On the other hand, WP5 is specifically aimed to increase stakeholder involvement. Their involvement is however not limited to specific work packages. Company representatives will be actively engaged as Management Committee members providing continuous advice and input into the Action. Investigators of all genders, ages and origins with direct or indirect interest in using DEM are of course stakeholders targeted in this Action. They are also considered in the future constitution of the Management Committee and Working Groups as well as all the networking and research activities (e.g. PhD fora, initial/final conferences, seminars, and production of research outputs).

3. IMPACT

3.1. IMPACT TO SCIENCE, SOCIETY AND COMPETITIVENESS, AND POTENTIAL FOR INNOVATION/BREAK-THROUGHS

3.1.1. SCIENTIFIC, TECHNOLOGICAL, AND/OR SOCIOECONOMIC IMPACTS (INCLUDING POTENTIAL INNOVATIONS AND/OR BREAKTHROUGHS)

Particle simulations are just getting to the stage where they are able to approach full scale industrial and engineering applications. However, there are many scientific and technological obstacles that must be overcome for particle simulations to realise their full potential impact. The ON-DEM Action will address many of the urgent challenges, enabling the necessary scientific, technological and socioeconomic breakthroughs to solve the next generation of problems and train the next generation of DEM users.

As mentioned before, particulates and their simulation are a truly trans-disciplinary problem but knowledge is often compartmentalised within specific disciplines. Therefore, one of the key short-term goals of the COST Action is to collate and disseminate the current-state-of-the-art, cross fertilising the different disciplines. Secondly, the area of particle simulations is rapidly advancing in areas like improved physical models and better and faster algorithms. This COST Action aims to reduce the barriers between fundamental and applied science/industry allowing the applied stakeholders to profiteer from these advances. The recent boom in open-source codes for particle simulations is leading the way in reducing these barriers; however, this COST Action will remove them further by:

- Introducing guidelines, best practices and worked examples allowing new users to rapidly apply these advanced methods (**WG5**).
- Creating the required calibration and validation protocols (**WG1** and **WG2**).
- Creating new universal and standardised analysis and visualisation tools to ensure interoperability between DEM codes (**WG4**).
- Developing new algorithms allowing larger problems to be considered (**WG1 and WG2**).
- Working with industry partners on commercial utilisation of DEM codes on developing new calibration techniques, developing user interfaces and cloud development, as well as using true-scale case-studies for benchmarking and validation (**WG5**).
- Creating online and downloadable central resources to disseminate the latest advances, which codes they are available in, and, how to use them, with worked examples (**WG6**).

From a scientific point of view, this Action will create new scientific advances, new technological development and expand the user groups of particle simulations by increasing awareness and usability of the current open-source solutions. This will lead to more advanced methods that can simulate phenomena and processes which have significant societal importance in Europe. These include (but are not limited to): static liquefaction, foundations for offshore wind turbines, scour around structures, conservation of historical structures, landslides, quality control and mixing in industry, transporting or conveying of granular materials, additive manufacturing, tabletting or steel making, amongst others.

From a direct economic point of view, this Action will also have a large impact. There are many (European) SMEs in this area, ranging from companies focused on the characterisation and calibration of particulates to companies utilising open-source codes/tools to solve industrial problems. The customers of these SMEs are often (European) multi-billion Euro businesses; however, at the moment, often projects are small proof-of-concept (TLR-5) style projects. Also companies that develop open-source scientific visualisation tools will benefit from this COST Action to enlarge their open-source solutions to DEM problems. Furthermore, this Action will create the knowledge and tools to enable these companies to move towards larger, more applied projects with more companies, helping stimulate their growth, future revenues and also giving their customer a competitive edge, potentially leading to substantial economic growth in Europe.

3.2. MEASURES TO MAXIMISE IMPACT

3.2.1. KNOWLEDGE CREATION, TRANSFER OF KNOWLEDGE AND CAREER DEVELOPMENT

There will be several interconnected activities that are designed to reach each of the different stakeholders to promote knowledge creation, transfer and career development:

- **Opening conference:** to launch the Action and promote its activities and programme of work. The main aim will be to bring together the researchers, open-source code developers and companies in an ‘ice-breaking’ event involving technical presentations and invited keynote speakers. The conference sessions will broadly match the themes of the Working Groups.
- **Training schools:** one training school will be held each year, targeting both early-career investigators and experienced researchers. The aim of the training school will be to transfer

state-of-the-art information, that is only available in a narrow discipline, to the wider simulation community. We will align at least two of the training schools with established international conferences (e.g. the PARTECH conference or the EGU annual meetings) to broaden the number of potential participants and increase the visibility of the Action.

- **Action-specific wiki (website):** A wiki will be created and developed during the COST Action. The wiki will serve several purposes:
  1. It will act as a central information point for companies and other researchers to see the outputs of the Action. This will facilitate the addition of new stakeholders.
  2. It will act as a gateway to repositories containing validation and other data.
  3. It will maintain lists of available resources for the community in terms of open-source codes, high-performance facilities and knowledge.
  4. It will show the current actions and progress of each Working Group. The wiki will have a dynamic website allowing members of each Working Group to continuously update the information. This will facilitate ease of communication for members of each Working Group that are geographically spread across Europe and beyond. Also it will enable each Working Group to keep up-to-date with the activities and outputs of the other groups allowing better and closer synergy between Working Groups.
  5. It will act as a central point to advertise jobs in the area of particle simulations both in academia and industry. Leading to both a consistent supply of skilled employees for both academia and SMEs and better career development opportunities for people within the field.
- **Working group meetings:** all Working Groups will meet face-to-face every six months to discuss progress, set priorities for the next six months, and take on new members. These meetings are designed to be a focusing event. The output and progress of the individual Working Groups will be disseminated on an ongoing basis via the wiki.
- **Management Committee (MC) meetings**: every six months the MC will meet to coordinate the actions of the whole Action for the next six months.
- **Workshops:** each workshop will be held in a different host region and priority given to ITC, for both capacity building and career development of young researchers in particular. At least two workshops will coincide with well-known international conference series. The primary aim of the workshops will be to transfer knowledge between the different Working Groups. The workshops will be open to all (including non-members of the COST Action) and will include invited external expert speakers. This will enable internal knowledge transfer between the different WGs and allow external stakeholders to be briefed on and contribute to the progress of the Action. These will also serve as a recruitment event for new members of the Action and individual WGs. A part of these workshops will be devoted to young researchers to create an amenable environment where they can freely discuss their research.
- **Short-term scientific missions**: these will take place between researchers involved in the COST Action. These will be targeted at early-career investigators and are designed to allow them to gain cutting-edge knowledge from multiple COST members. This will lead to the creation of a new generation of researchers with the broad interdisciplinary skill set required to take the discipline of particle simulations forward in the years after this Action is complete.
- **Closing conference:** To disseminate findings, highlight best practices and develop a plan to grow links and the field in the future.

3.2.2. PLAN FOR DISSEMINATION AND/OR EXPLOITATION AND DIALOGUE WITH THE GENERAL PUBLIC OR POLICY

The five main sources and methods of dissemination of the results will be:

1. Wiki (website): as explained in detail above this website will consist of wiki-style pages and will be constantly updated. It is anticipated that the wiki will live beyond the lifetime of the COST network and remain an up-to-date and relevant central resource for knowledge, features and abilities of open-source codes, and best practices in particle simulations.
2. Creation of repositories of high quality test-data and well-documented benchmarks for validating and comparing particle simulation codes.

3. Workshops: a method for internal dissemination of the results and an access point for external persons (and new potential members) to observe the output of the Action.
4. Creation of best practices, worked examples and training material: A selection of representatives from each WG will construct a handbook of best practices. These practices will be freely available on the Wiki and as a book that will be published under the Creative Commons licence and/or using the newly established Open Research Europe (ORE) platform. A hard-copy will be developed in consultation with an academic publisher. Codes, data, examples, etc., will also be published under the General Public License (GPL).
5. Open access journal publications. It will be suggested that each WG publishes at least one peer-reviewed article per year specifically related with the Action's objectives.
6. Finally, SMEs participate in our COST Action, allowing them to exploit and benefit immediately from the advances created by it; advances can be rapidly tested in an industrial environment.

4. IMPLEMENTATION

4.1. COHERENCE AND EFFECTIVENESS OF THE WORK PLAN

4.1.1. DESCRIPTION OF WORKING GROUPS, TASKS AND ACTIVITIES

WORKING GROUP 1 – passing through time and space scales. This working group will focus on solutions to gain orders of magnitude for tackling simulations at scales which are relevant for real life applications. Two main strategies mentioned before are described here in more detail:

1. Using high-performance computing and taking benefits of new hardware architectures. Well-known solutions such as parallelization with both CPU and GPU will be investigated. The efficient use of these solutions in particular contexts is still challenging. For instance, simulating non-spherical particles with GPU-based algorithm, handling load balancing on CPU parallel architecture for simulations or parallelizing contact algorithms such as Voronoï based searching remains difficult and are still scientific barriers. The potential participation of hardware manufacturers will enable new insights for the optimisation of DEM algorithms.
2. Using model-based solutions such as enriched contact models, space periodicity, and/or time extrapolation strategies. The first approach consists in enriching the contact model in order to do more with fewer particles. The second and third approaches take advantage of temporal and spatial periodicities to use less particles or time steps. Of course, other promising solutions which are not listed here may be investigated.

To achieve this goal, this WG will first discuss a short list of typical simulations able to test different contexts such as particle number, grains distribution, dynamic or steady state problems. The most relevant solutions for enhancing performance will be implemented in several DEM codes in order to benchmark them and to provide a quantitative and comprehensive comparison though the simulations defined at the previous step. By enabling fruitful discussions, new disruptive solutions can potentially emerge to address this major problem.

WORKING GROUP 2 – going closer to physics. This Working Group will focus on actions to achieve more realistic numerical modelling of physical processes. These include (i) a better representation of particle shape in DEM simulations, (ii) enhancing existing contact laws (iii) strategies for monitoring energy, momentum and mass conservation. To achieve such objectives, this WG will carry out both experimental and numerical campaigns. Experiments will be conducted on a list of model materials that will be initially established by the WG.

First, the particle shape will be investigated as it is key in simulating real materials. Traditionally, DEM studies consider spherical particle shape for the sake of simplicity and computational efficiency as contact detection between spheres is trivial, and easily parallelisable. Different codes have different formulations to model non-spherical particles, all of which can benefit from an image-informed particle-shape strategy. This WG will provide an open-source database of particle shapes for different typical materials such as geo-materials, pharmaceutical powders and powders used in additive manufacturing.

In addition to particle shape, contact laws are a key feature in a DEM simulation describing different constitutive relationships of the materials in contact. Appropriate, experimentally derived contact laws that represent physical behaviour need to be implemented and validated across platforms to account for friction, rough surfaces and materials with visco-elastic properties. This WG will provide motivation for the interchange of algorithm implementation of contact laws across platforms.

The key outputs of this WG will be:

- image-informed strategy in simulating realistic particles,
- open-source database of model material properties under various conditions,
- implementation of complex physical laws (friction, surface roughness, viscoelasticity, plasticity),
- report demonstrating the ability of DEM codes to conserve energy, momentum and mass.

WORKING GROUP 3 – data processing and visualization. Discrete element models provide significant amounts of data which are unattainable using experimental and/or other numerical methods. These correspond to the physics of inter-particle interactions and include particle positions, velocities, accelerations, and normal and shear forces at particle contacts amongst others. The analysis of this data generally requires a mix of graphical, qualitative and quantitative methods. This Working Group proposes to produce a common standard output file format which may be used across different DEM open-source codes. The aim is to provide this in the form of an optimised file format (Open DEM format) that will enable faster post-processing and analysis of data across multiple common applications. This will at least include the most widely used contact models. Other objectives of this Working Group include:

- To generate a protocol in which data less commonly used contact models may be generated using the Open DEM format for the benefit of the community and interested stakeholders.
- To provide a set of visualisation tools that can work as plug-ins of open-source tools that are widely used. As expected, such plug-ins will be devised in such a way that they can efficiently interpret the files generated using the Open DEM format standard.

As a result of the objectives above, a set of the most common post-processing tools and algorithms will be produced for general use under a Creative Commons and/or General Public license and will be made available via the project's wiki. To this purpose, this Action aims to finalise the initial agreement made between various DEM code developers during the DEM8 conference with the same aim (to produce a common data format). The involvement of developers in this COST Action significantly facilitates the achievement of these objectives.

WORKING GROUP 4 – normalization and best practices. This Working Group will focus on the correct use of the DEM methods. It will look at issues around developing a particle-scale model of a physical system; considering appropriate parameters, including calibration to determine appropriate parameters, boundary conditions, sample size, time-step for numerical integration, etc. It will also provide simple cases-studies and (more complex) reference benchmarks for users to validate their simulation setups; in standardised file formats.

This WG will create guidelines and best practices for the following topics:

- how to correctly set boundary conditions to capture the process occurring,
- on calibration of particle simulations avoiding parameter ambiguity,
- on approaches to generate initial systems of particles (specimen / system generation),
- information on key issues such as quasi-static versus dynamic simulations,
- for creating models with non-spherical (more realistic) particle shapes and
- for documenting and developing new features within an open-source project.
- For packaging and deploying software on open-source-based operating systems.

This WG will also develop training materials and courses for young researchers and write a handbook on best practices that will be created towards the end of the Action. The training materials will be initially used at training schools given as part of this Action; however, all materials will be made freely and openly available under the Creative Commons license via the website.

The key outputs of this WG will be:

- an open handbook containing all the best practices and guidelines,
- interactive training materials for learning particles simulations, use and analysis of software,
- simple case-studies for new users to learn from and to show the benefits of this approach to modelling, spanning spherical, non-spherical particles and including coupled simulations and,
- complex benchmarks which can be used for both training and comparison of different codes in a cross-comparison of different implementations for complex physical laws e.g. friction models.

WORKING GROUP 5: Industrial networking and commercial utilisation. This Working Group is explicitly focussed on creating/maintaining links with industry stakeholders and facilitating commercial utilisation of the achievements of this network. This WG will have two key aims: Firstly, to work directly with key industrial users of DEM to identify current barriers to commercial utilisation of DEM. Industry needs are often quite different to those for academic users. For industry the focus is more on easy-of-use/setup, robustness, 'quick' results and how to calibrate the models for real industrial materials. Secondly, to work with software houses and DEM consultancy firms in order to develop the tools to overcome these barriers. Here the use (G)UI/UX for codes, characterisation/calibration methodologies, cloud computing, etc. are of special interest. The outputs of these two aims will be combined via several industrial case studies that will synergise the fundamental knowledge from other WGs, software houses and industrial stakeholders.

The key outputs of this WG will be:
- the definition and standardisation of calibration methodologies,
- the design and implementations of UI/UXs for open-source codes,
- cloud deployment demonstration of codes (e.g. via Amazon Web Services),
- upscaling techniques for reducing simulation time (at small loss of accuracy),
- true industrial case-studies performed with stakeholders in academia, software houses/consultancy companies and industrial end-users.

WORKING GROUP 6 – communication and dissemination. The main outcome of each of the WGs 1-5 is information: data, best-practices, algorithms, etc. Therefore it is important that all this information is freely and easily available to the whole particle simulation community. To ensure that the dissemination of the information is given the status it deserves a dedicated WG will be formed. This WG will be responsible for unifying the output from each WG and finding the best and simplest format to present it in, both for experienced academics and young researchers. This WG will be responsible for setting up, maintaining and moderating the wiki-style website. The major outputs of this WG are listed below.

- Dynamic website: the website will be launched at the beginning of the Action and it will serve as the Action's principal communication and dissemination tool. It will publicise the Action's activities, objectives and members. The website will include links to repositories of data. It will function as an important source of state-of-the-art information for DEM simulation.
- Opening and closing conferences: the opening conference will launch the Action, advertise its activities and recruit new members. The closing conference will disseminate findings and highlight the key conclusions from each WG. The conference delegates will include researchers, commercial software developers and end users. One of the key aims of the opening conference is to build and create cross-disciplinary teams that will form the WG. The closing conference will advertise the newly created best-practice handbook (see WG4).
- Short-Term Scientific Missions (STSMs): four STSMs will be organised for early-career investigators per year. STSMs will be hosted in European centres of excellence and will situate early-career investigators within interdisciplinary research environments.
- Training Schools (TSs): one TS will be held per year, targeting both early-career investigators and experienced researchers. TSs will focus on key themes emerging from the WGs.
- Published Output: each WG will prepare an annual report on outputs that will be made freely available via the website. Also, a range of jointly written peer-reviewed articles and funding applications on each domain, will be produced over the Action's lifetime.
- Repository: a repository of validation resources will be developed. We will likely use the Zenodo research data repository (https://zenodo.org/), which has been developed as a repository for

EC funded research. However, alternative platforms will be discussed amongst the COST Action participants and include the Open Research Europe (ORE) platform.

- Video contest: this WG will also run a video contest once per year, which will encourage innovation in all areas including visualisations (WG-3).
- Coding workshops (Hackathons): Drop-in workshops will be run to bring together developers of open-source codes and potential new users. This allows developers to exchange ideas and tricks and expose new users to the possibility of open-source codes.

4.1.2. DESCRIPTION OF DELIVERABLES AND TIMEFRAME

The following major deliverables (**Dx.x**) are planned. Each of these will involve a short report.

WORKING GROUP 1 – passing through time and space scales

D1.1 – building a short list of academic reference problems (including their full definition in terms of initial configuration, boundary condition, time step, expected results, and/or analytical solutions, etc..)

Subgroup 1-1 – investigating hardware architecture-based solutions

- D1-1.1 – building a short list of potential solutions based on hardware algorithms able to handle the problems defined at D1.1
- D1-1.2 – implementing the algorithms defined in D1-1.1 on different DEM codes for reliability
- D1-1.3 – modelling the problems defined in D1-1.2, and post-processing the results

Subgroup 1-2 – investigating model-based solutions

- D1-2.1 – building a list of potential models able to handle the problems defined at D1.1
- D1-2.2 – implementing the models defined in D1-2.1 on different DEM codes for promoting better reliability of model implementations
- D1-2.3 –running and post-processing simulations of models defined in D1-2.2

D1.2 – running collective discussions about results given at the D1-1.3 and D1-2.3 steps in order to give a comprehensive comparison of the different investigated solutions defined at D1-1.2 and D1-2.2 and implemented at D1-1.3 and D1-2.3 and writing a conclusion report.
D1.3 – disseminating conclusions provided at D1.2 in collaboration with WG6

WORKING GROUP 2 – going closer to physics

D2.1 – building a short list of model materials with typical and academical physical properties (quasi-perfect spherical powders, polyhedral shapes, cohesiveness, etc...)

Subgroup 2-1 – managing experimental campaign

- D2-1.1 – making a full inventory of experimental apparatus available in the Action for running pertinent characterisation of the model materials defined at D2.1
- D2-1.2 – running experiments with the equipment inventoried at D2-1.1 with the model materials defined in D2.1. Here, STSMs will be conducted.
- D2-1.3 – collecting results provided at D2-1.2 and building an experimental database

·**Subgroup 2-2 – managing numerical campaign**

- D2-2.1 – building a list of contact models to simulate materials defined at D2.1
- D2-2.2 – building a list of typical shapes to simulate the model materials defined in D2.1
- D2-2.3 – implementing contact models defined in D2-2.1
- D2-2.4 – implementing collision detection algorithm for shapes defined at D2-2.2
- D2-2.5 – carrying out simulations on different DEM codes with the contact model defined at D2-2.1 and/or the shapes defined in D2-2.2 to reproduce the experimental results given at D2-1.3

D2.2 – running collective discussion about results provided at D2-1.3 and D2-2.3 for proposing the most adapted modelling strategies for each model material and writing a conclusion report
D2.3 – disseminating the conclusions provided at D2.2 in collaboration with the WG6

WORKING GROUP 3 – data processing and visualization

Subgroup 3-1 – building a common open DEM file format

- D3-1.1 – selecting the data to be saved in a common DEM file covering a range of applications

- D3-1.2 – writing the specifications of an optimized file format (Open DEM format)
- D3-1.3 – implementing the Open DEM format described in D3-1.2 in different DEM code

Subgroup 3-2 – going through a common visualisation and post-process tool(s)

- D3-2.1 – inventorying open-source high performance visualisation tools capable to receive specific developments through plugins mechanism
- D3-2.2 – developing specific plugins for the software defined in D3-2.1
- D3-2.3 – defining a list of the most common DEM post-processors and data analyses
- D3-2.4 – enriching visualisation tools defined at D3-2.D3.1 – communicating about these new features in collaboration with WG6

<u>WORKING GROUP 4 – normalization and best practices</u>

Subgroup 4-1 – providing simple reference benchmarks

- D4-1.1 – building a list of features to monitor (e.g. contact algorithms, contact models, etc.)
- D4-1.2 – building a list of very simple test case-studies which can provide reference for D4-1.1
- D4-1.3 – running the test cases defined in D4-1.2 on several DEM code
- D4-1.4 – collecting results given in D4-1.3 to build an open-access database of benchmarks

Subgroup 4-2 – investigating better calibration procedures

- D4-2.1 – organizing a contest for retro-fitting given test cases on different DEM codes
- D4-2.2 – comparing approaches implemented at D4-2.1 to determine the best ones

Subgroup 4-3 – investigating contact models versus particle shapes

- D4-3.1 – building a list of physical phenomena attributed to particle shape such as grain interlocking, sliding friction, rolling friction, etc.
- D4-3.2 – building a list of simple test cases to highlight the phenomena listed at D4-3.1
- D4-3.3 – running simulation defined at D4-3.2 with the two different approaches: simple contact laws with complex shapes versus complex contact laws with simple shapes
- D4-3.4 – discussing and collecting results given in D4-3.3 to propose recommendations

Subgroup 4-4 – optimizing initial domain generation algorithms

- D4-4.1 – organising a contest for the quickest and most accurate algorithm able to converge toward a quasi-perfect stable compact domain with negligible interpenetration
- D4-4.2 – discussing and collecting results given in D4-4.1 to propose recommendations

Subgroup 4-5 – enhancing coding & software development

- D4-5.1 – organising seminars related to programming performance, memory management, collaborative developments, documentation, valuation and business model solutions for DEM

D4.1 – writing reports through the collaborative website (wiki) in collaboration with WG6
D4.2 – writing a handbook based on the collaborative work provided at D4.1

<u>WORKING GROUP 5 - industrial networking and commercial utilisation.</u>

Subgroup 5-1– liaising with industrial partners

- D5-1.1 – maintaining regular communication with industrial partners
- D5-1.2 – providing feedback to other WGs regarding benchmarking and validation

Subgroup 5-2– identifying barriers to commercial utilisation of DEM codes

- D5-2.1 – arranging focus groups with industrial stakeholders
- D5-2.2 –assessment of difficulties experienced by users when using open-source DEM codes.

Subgroup 5-3– developing tools to improve to commercial utilisation of DEM codes

- D5-3.1 – select benchmarking and validation problems of true industrial-scale
- D5-3.2 – development and implementation of user interfaces for relevant applications
- D5-3.3 – creation of cloud deployment examples and upscaling techniques

<u>WORKING GROUP 6 – communication and dissemination</u>

Subgroup 6-1– ensuring the technical administration of the website

- D6-1.1 – designing and publishing a static website presenting the COST Action
- D6-1.2 – designing and publishing a dynamic (blank) collaborative website (wiki)

- D6-1.3 – implementing an open data management system to package the data generated
- D6-1.4 – ensuring continuous maintenance and survey of the whole website

Subgroup 6-2 – feeding the website content

- D6-2.1 – building a list of referent persons in each WG
- D6-2.2 – feeding the website with relevant content

Subgroup 6-3 – promoting general public communication

- D6-3.1 – organizing continuous social networking activities
- D6-3.2 – organizing recurrent large public events such as smart video contests
- D6-3.3 – exploiting results provided at D5-3.2 to enhance communication activities

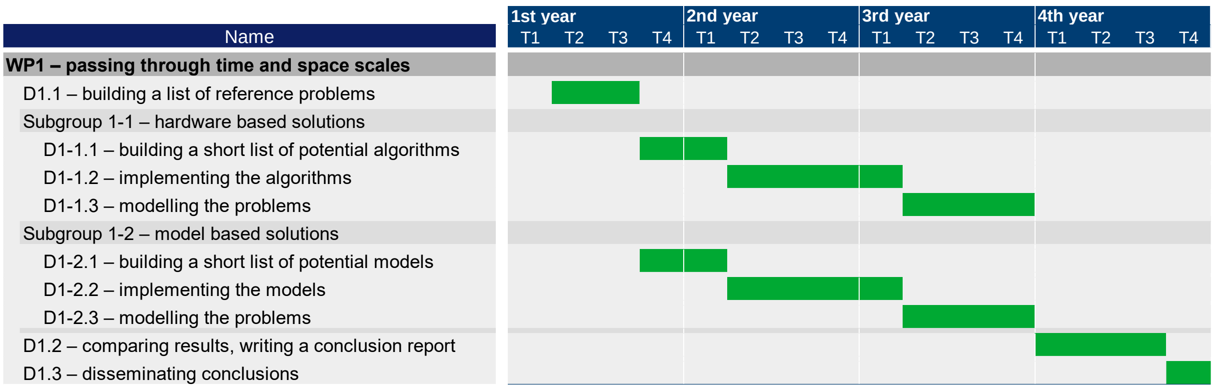
Subgroup 6-4 – ensuring technical and scientific communications

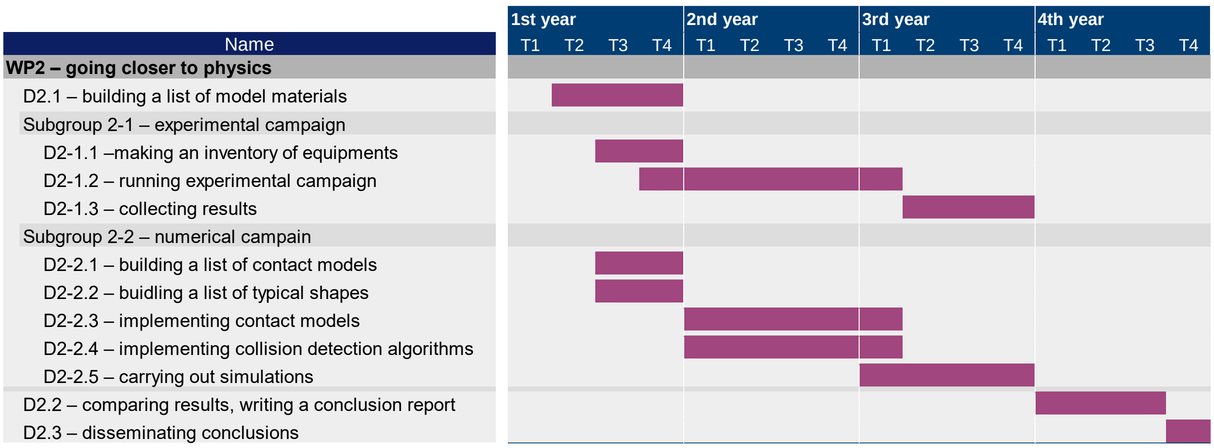
- D6-4.1 – organizing open and closing conferences
- D6-4.2 – organizing Short-Term Scientific Missions (STSMs)
- D6-4.3 – organizing one training school per year for young researchers and investigators
- D6-4.4 – organizing hackathon as part of training schools defined at D6-4.3

4.1.3. RISK ANALYSIS AND CONTINGENCY PLANS

The main risks in relation to the work plan are *delayed or unaccomplished deliverables; ineffective interdisciplinary working; and poor linkages between WGs*. Possible causes for delays may include collision between teaching, admin and research loads of the Action participants, illness, difficulties in relation to transportation and attendance, as well as lack of time to develop objectives and outputs. The solution to all of these problems is at the core, having a large number of members and good management. **Delayed and unaccomplished deliverables** will be avoided by ensuring that each working group has a person dedicated to tracking the progress of objectives. **Interdisciplinarity issues** will be addressed from the outset during the creation of the Management Committee (MC) and Working Groups (WGs). **WG Linkage Issues** may be avoided by developing personal links between participants in the WGs. WG meetings shall therefore coincide in terms of location and/or mode of delivery.

4.1.4. GANTT DIAGRAM





Name	1st year				2nd year				3rd year				4th year			
	T1	T2	T3	T4	T1	T2	T3	T4	T1	T2	T3	T4	T1	T2	T3	T4
WP3 – data processing and visualisation																
Subgroup 3-1 – common DEM file format																
D3-1.1 – enumerating data to save		X	X	X	X											
D3-1.2 – writing the file format specifications						X	X	X	X							
D3-1.3 – implementing the format										X	X	X	X	X		
Subgroup 3-2 – visualisation and post-process tool																
D3-2.1 – inventorying the avalaible tools		X	X	X												
D3-2.2 – developing plugins to read the file format										X	X	X	X	X	X	
D3-2.3 – defining a list of post-treatment					X	X	X									
D3-2.4 – implementing post-treatments plugins								X	X	X	X	X	X	X	X	
D3.2 – communicating about these new features														X	X	X

Name	1st year				2nd year				3rd year				4th year			
	T1	T2	T3	T4	T1	T2	T3	T4	T1	T2	T3	T4	T1	T2	T3	T4
WP4 – normalisation and best practices																
Subgroup 4-1 – reference benchmarks																
D4-1.1 – building a list of feature to monitor		X	X													
D4-1.2 – building a list of simple test cases-studies				X	X											
D4-1.3 – running test cases						X	X	X	X	X						
D4-1.4 – building database of reference results										X	X	X	X			
Subgroup 4-2 – calibration procedures																
D4-2.1 – organizing retro-fitting contests		X	X	X	X	X	X	X								
D4-2.2 – comparing the approaches								X	X	X	X	X	X			
Subgroup 4-3 – contact models vs particle shapes																
D4-3.1 – building a list of physical phenomena		X	X													
D4-3.2 – building a list of test cases-studies				X	X											
D4-3.3 – running test cases-studies						X	X	X	X	X						
D4-3.4 – comparing results										X	X	X	X			
Subgroup 4-4 – domain generation algorithms																
D4-4.1 – organizing contests		X	X	X	X	X	X	X								
D4-4.2 – discussing and comparing results								X	X	X	X	X	X			
Subgroup 4-5 – coding & software development																
D4-5.1 – organising seminars			X				X				X				X	
D4.1 – writing reports in the wiki website					X	X	X	X	X	X	X	X	X	X	X	X
D4.2 – writing handbook(s)													X	X	X	X

Name	1st year				2nd year				3rd year				4th year			
	T1	T2	T3	T4	T1	T2	T3	T4	T1	T2	T3	T4	T1	T2	T3	T4
WP5 – industrial links and commercial utilisation																
Subgroup 5-1 – liaising with industrial partners																
D5-1.1 – regular communication with partners	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
D5-1.2 – feedback to other WGS				X				X				X				X
Subgroup 5-2 – identifying barriers to utilisation																
D5-2.1 – arranging focus groups	X				X				X				X			
D5-2.2 – eassessment of (user) difficulties		X	X			X	X			X	X			X	X	
Subgroup 5-3 – general public communication																
D5-3.1 - select benchmarking and validation problems	X				X				X				X			
D5-3.2 – development of user interfaces		X	X			X	X			X	X			X	X	
D5-3.3 - cloud deployment examples				X				X				X				X

Name	1st year				2nd year				3rd year				4th year			
	T1	T2	T3	T4	T1	T2	T3	T4	T1	T2	T3	T4	T1	T2	T3	T4
WP6 – communication and dissemination																
Subgroup 6-1 – technical administration of website																
D6-1.1 – publishing a static website		X	X													
D6-1.2 – publishing a blank wiki			X	X												
D6-1.3 – creating a data management system				X	X	X	X	X								
D6-1.4 – ensuring maintenance		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
Subgroup 6-2 – feed the website content																
D6-2.1 – building a list of referent in each WP		X	X													
D6-2.2 – ensuring a continuous survey of WP				X	X	X	X	X	X	X	X	X	X	X	X	X
Subgroup 6-3 – general public communication																
D6-3.1 - organizing social networking		X	X		X	X			X	X			X	X		
D6-3.2 – organizing smart video contests		X				X				X				X		
D6-3.3, exploiting videos to communicate			X				X				X				X	
Subgroup 6-4 – technical and scientific communication																
D6-4.1 – organizing open and closing conferences				X												X
D6-4.2 – organizing STSMs					X	X			X	X			X	X		
D6-4.3 – organizing training schools				X				X				X				X
D6-4.4 – organizing coding marathon contests				X				X				X				X