

Digitalization in the Lab – Really a One-Way Towards More Sustainability?

Kerstin Hermuth-Kleinschmidt, PhD
 NIUB Sustainability Consulting, Germany

Executive Summary

Digitalization has entered our lives, and we've seen a big push in the last year with video-conferencing being the new normal. This is also true for the lab, where we get used more and more to electronic lab journals, the digital management of our samples, chemicals, and consumables, or connected devices. Lab 4.0 is on the rise – and with it the promise to more efficiency, less resource consumption, and more sustainability. But is it that simple? What are the advantages, but also the challenges? What do we need to pay attention to and where should we focus to build a digitalized and sustainable laboratory – so that we can benefit from both trends?



Digitalization, Sustainability & Green IT

Sustainability gets more and more important. The society realizes the need for changes which includes the lab environment as well.

These changes imply a rethinking of our behavior and habits as well as our current use of resources, but it does not mean turning back everything to green roots.

Rather, such a transformation process raises the questions of how to benefit from modern and future technologies to reduce the environmental, social, and financial load.

There is an emerging discussion in the scientific community how the sustainability trend can benefit from digitalization and related technologies.

These are not limited to the consumer world but also provide opportunities for the life science areas. For at least the last five years, there has been a clear trend to digitalize the

lab world, connect devices, and benefit from cloud-based data. We are on the way to Lab 4.0 where automatization and digitalization plays a key role. Hence, processes will become more efficient, and also contribute to a more sustainable lab.

The COVID-19 pandemic has brought a big push in digitalization throughout the entire business and private world. We all got used to video calls, online meetings and conferences as well as remote work. Also in science, digitalization has been accelerated:

During the pandemic, scientific congresses and meetings were transferred into online sessions. Scientists were forced to reduce their travel activities and as a consequence, they reduced their CO₂ emissions by a significant amount.

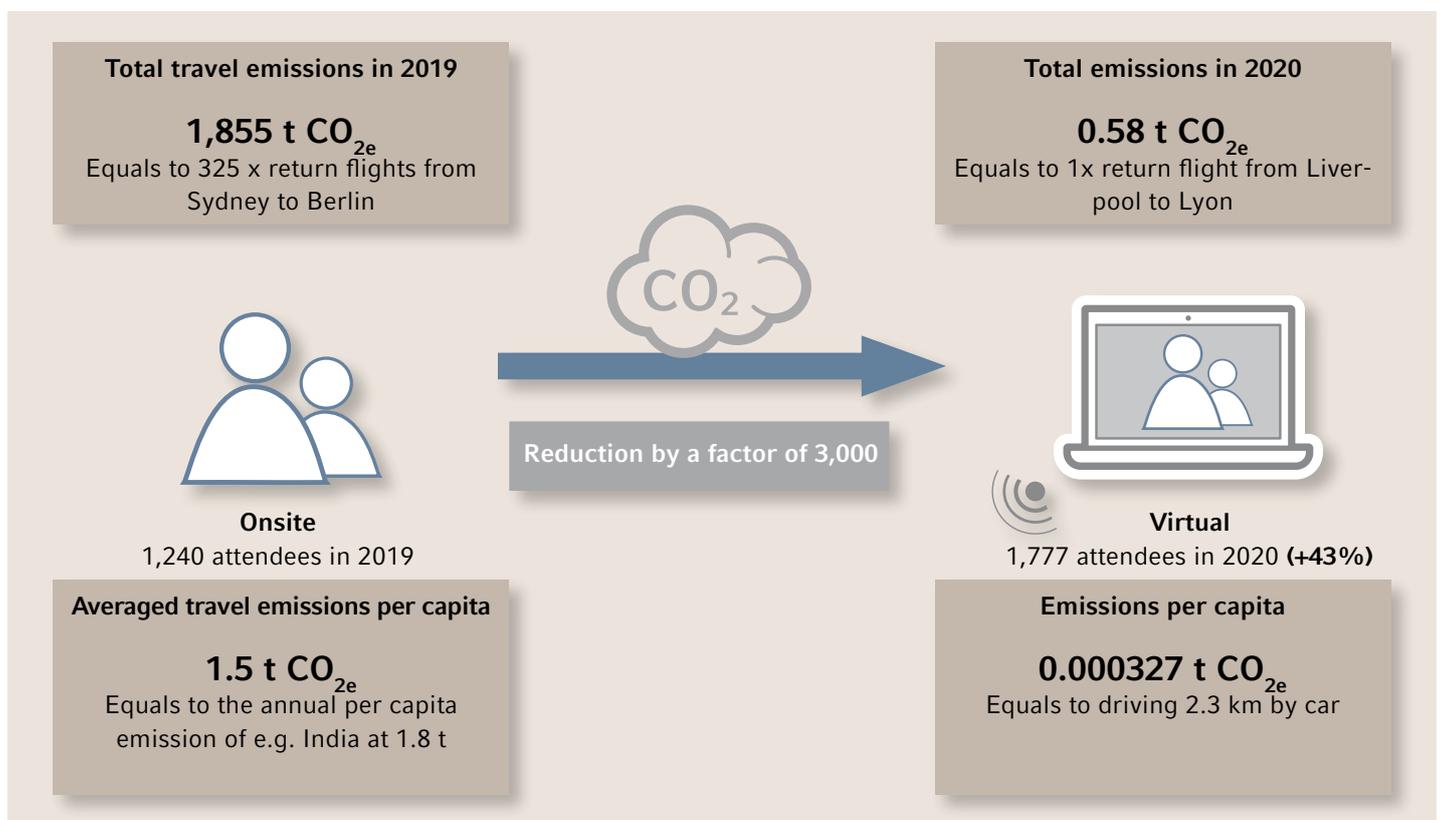
In other words, the environment had a direct benefit. But the use of the web and its infrastructure is a big thriver for energy consumption and associated greenhouse gas

emissions. So, let's have a more differentiated view on this topic and see what the increasing use of digital instruments means for the life sciences and digitalization in the lab.

Digitalization helps scientists to reduce CO₂ emissions

We as a scientific community stopped traveling and flying around the world in 2020/21. Sped up by the pandemic, meetings, congresses, and even large scientific conferences took place virtually. This saves carbon emissions but how much was really saved? The European Astronomical Society calculated the impact of "going virtual" by comparing two identical congresses of their organization, one taking place as an onsite conference in 2019 in Lyon, France, and the other which was held as a virtual event in 2020. By going virtual, the European Astronomical Society decreased the CO₂ emissions due to non-existent travels by a

factor of 3,000 [1]. This meant that they saved about 1,854 tons of CO₂. About 43% more scientists were able to join the online event. By this, the advantages of online events become obvious: Besides the environmental effect, it also saves time and financial resources as you do not travel to the event but you just can take part from wherever you are. Second, online events help people to participate who can hardly afford to join real sessions, to travel, due to budget or because of other reasons like lack of childcare [2]. Therefore, it is not only an environmental benefit but also a social benefit as more people can join online sessions.



Graphic 1: Calculation of the total and averaged individual carbon footprint for the annual meeting of the European Astronomical Society [1] which was performed onsite in 2019 and online in 2020

But there are also challenges: Especially in the early phase of a scientific career, networking and exchange are very important for young scientists to broaden their network, initiate projects, and get themselves known inside the community. But this is not limited to the young scientists. The social aspect of direct interaction is essential in science.

Suggestions to meet these challenges are, for example, to hold big international conferences biannually – one year in live and one year virtual. This would cut the emissions by half. Another idea out of the scientific community is to orga-

Digitalization helps scientists in the lab to be more efficient

Digitalization is not limited to scientific exchanges or travels. Now and even more in the future, the automated and digitalized Lab 4.0 will change the scientific work substantially. Some changes already happened, but others will come in the near future.

Already today, more and more scientists store their experimental data in an electronic lab notebook (ELN) or Laboratory Information Management System (LIMS) instead of using classic paper-based lab books. The switch to the digital format, including potential challenges in the beginning, has many advantages and finally saves time. It's far easier to retrace experiments, to identify potential sources of errors when an experiment failed, or to collaborate and

With VisioNize® Lab Suite, part of this future is already there...

Large instruments like ULT freezers, CO₂ incubators, shakers, and centrifuges as well as smaller devices like cyclers, thermomixers, microscopes, or pipettes can already be integrated today into the lab network [3,4]. You can control and monitor your devices remotely and the overall device performance is documented in detail. Especially 24/7 instruments like freezers are critical in the lab environment. In the worst case, a failure can result in a total loss of valuable samples. VisioNize Lab Suite notifies you if there's an irregularity, like exceeding a set temperature or an instrument failure and also reminds you of scheduled services and maintenance tasks. But digitalization is not limited to instruments' safety and performance – all your experimental data as well as pre-defined device protocols will be stored and can be accessed from everywhere.

nize regional hubs, which are available by public transport to exchange personally. The international exchange between the different regional hubs will then be online [1,2].

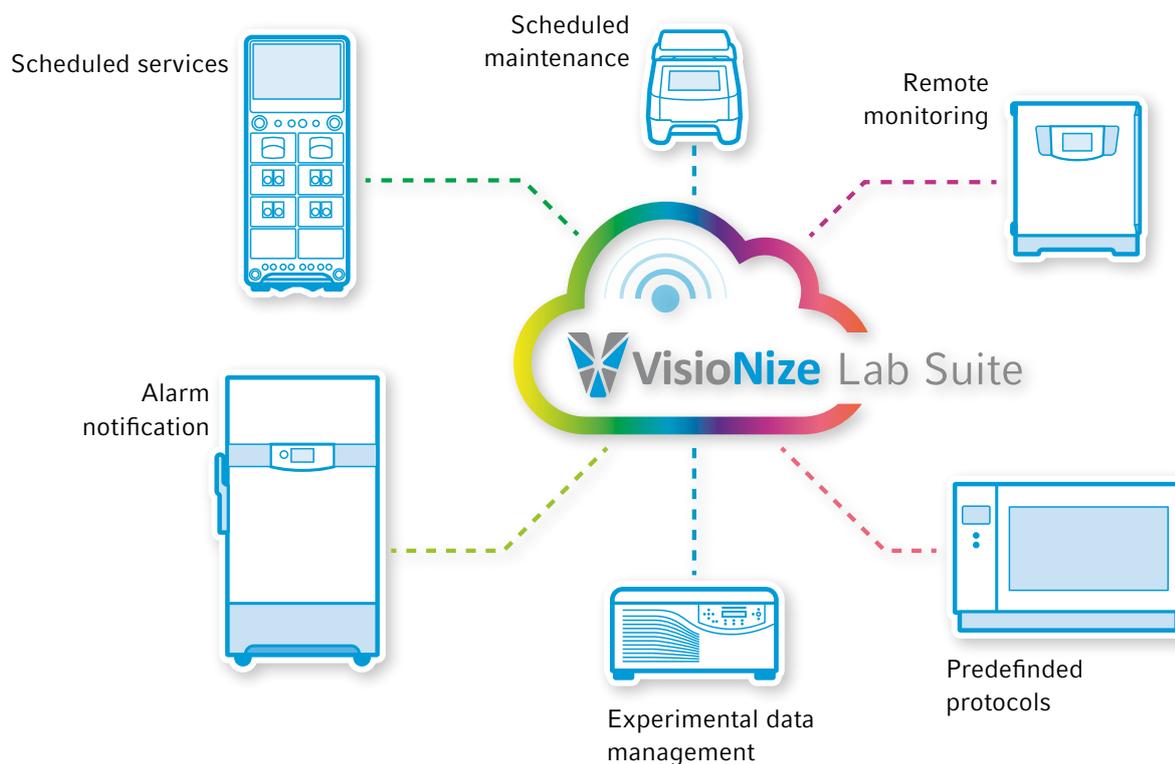
The growing digitalization also promotes and speeds up the digital and online exchange between researchers in their research area. Scientific results can be discussed and commented within the community. This can push research forward – instead of waiting several months until results are reviewed and published.

share data inside and outside the lab. These tools like the Eppendorf eLabNext™ help to trace and track your samples and, in combination with an inventory management system, support to manage your consumables, chemicals, and solvents. The use of efficient lab data management and inventory management will even expand as more and more lab devices become connectable. An intelligent booking system supports a more efficient device usage but could also help to decrease the number of instruments in the lab as they could be shared institution-wide. In case of an instrument failure, online troubleshooting could help instantly and even support via Livestream to detect the failure cause as fast as possible. The next logical step will be online predictive maintenance to prevent failures as far as possible.

VisioNize Pipette Manager



Instead of adjusting your pipette volumes manually, you can define them in advance for all your connected pipettes and start immediately with your experiment. The integrated liquid manager in the software instructs you when working with liquids that differ in viscosity, volatility, surface tension, or are foam-forming liquids.



Graphic 2: Connectivity of lab devices is already possible today. You can use central software solutions like VisioNize Lab Suite to monitor and manage your instruments in the lab

... but this is just the beginning

With the ever-growing computing power and the enhancement of Virtual Reality and Artificial Intelligence, scientists will have far more possibilities to get more and more data – and to make them visible. Imagine, you look into complex structures, like cells, to explore its three-dimensional structure. You examine it from several angles or even dissect it layer by layer? Instead of looking on a big screen, you use VR glasses and get the feeling to be inside the cell. Although this still sounds fictional, first attempts have already been made. [5]

Artificial Intelligence and machine learning already help today in processing the big data which we get out of our experiments. In the future, AI will help modelling systems and even propose (and finally decide?) on the next steps in an experimental design [6]. Intelligent sensors allow real-time monitoring of our experiments, they will also be able to self-monitor, self-regulate or even interact with other components in the process environment to adapt to new experimental conditions at any time.

The ongoing automation of processes and experiments in the laboratory improves already today the reproducibility of experiments, diminishes the need to repeat them, and increases the safety of the users. In the future, the productivity in a lab could become higher when routine tasks are taken over by robotic systems providing scientists the role to think about experimental designs and strategies instead of working at the bench [6].

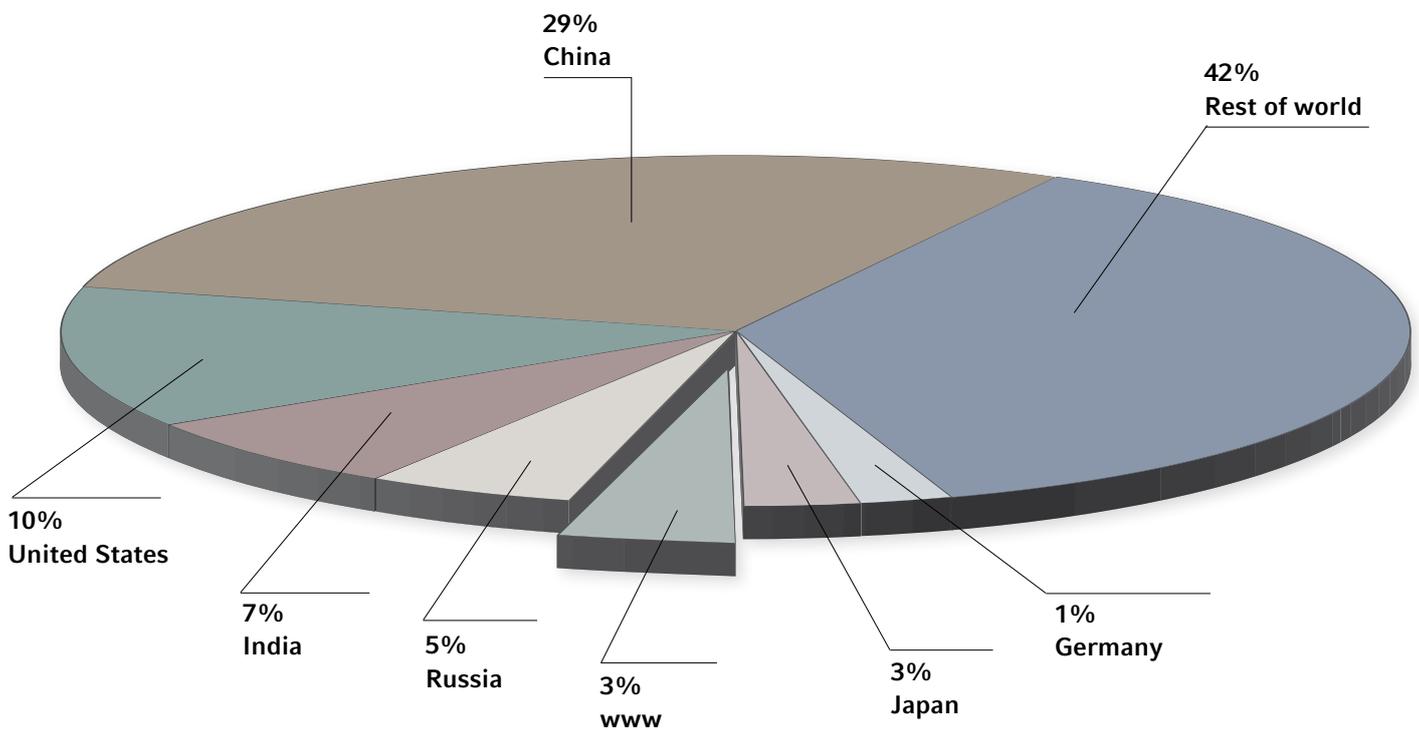
All this goes in combination with the third big trend in the context of automatization and digitalization: the miniaturization in analytics and experimental designs [6]. With the help of miniaturized instruments, applications can be developed in ever-smaller spaces while at the same time achieving ever higher throughputs.

These trends are in line with sustainability, as the monitoring of processes and experiments, as well as miniaturization, are three important principles of green chemistry [7] and green analytical chemistry [8].

The challenges of digitalization

We do not see the emissions which we cause when we google a scientific question, search for a definition or perform a protein BLAST search. But the use of the internet, its infrastructure, and Information Communication Technology (ICT) is a big thriver for energy consumption and greenhouse gas emissions (approx. 3,119 TWh - 3,834 TWh alone in 2020 [9]). Approximately 1,300 - 1,600 megatons of

greenhouse gas emissions are due to the use of web, servers, information and communication technology (including CO₂ emissions in the life cycle) [9]. Estimated, this is between 1.8% - 3.2% of the global greenhouse gas emissions [10]. If the Internet is seen as a country, it would rank 6th in terms of its greenhouse gas emissions.



Graphic 3: 52,400 Mt of greenhouse gases were emitted in 2019. Projecting emissions for 2020, the distribution per country shows, that the ICT usage is responsible for about 3% of the global greenhouse gas emissions.

Sources for estimation:

- https://www.pbl.nl/sites/default/files/downloads/pbl-2020-trends-in-global-co2-and_total-greenhouse-gas-emissions-2020-report_4331.pdf
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- https://www.bitkom.org/sites/default/files/2020-05/2020-05_bitkom_klimastudie_digitalisierung.pdf

Hence, what about researchers as they generate a lot of data, compare them in databases, or create compute-intensive models? This is a thriver of CO₂ emissions we should not underestimate. The Max Planck Institute of Astronomy in Heidelberg calculated its contribution in more detail and did an in-depth analysis. They realized that 3.75 t – 4.5 t of CO₂ emissions per researcher are related to computing resources [11]. This equals approximately to the CO₂ per capita emission in Switzerland with 4.19 tons [12].

The high CO₂ emission is not limited to astronomy. A recent study estimates the CO₂ emissions generated through bio-informatics: A genome-wide association analysis (GWAS) which is used to identify genetic variants across the genome could emit 4.7 kg CO₂ to 17.3 kg CO₂ for a single trait GWAS, depending on which software version is used [13]. As comparison, a passenger car emits about 14.3 kg CO₂ per 100 kilometers [14].

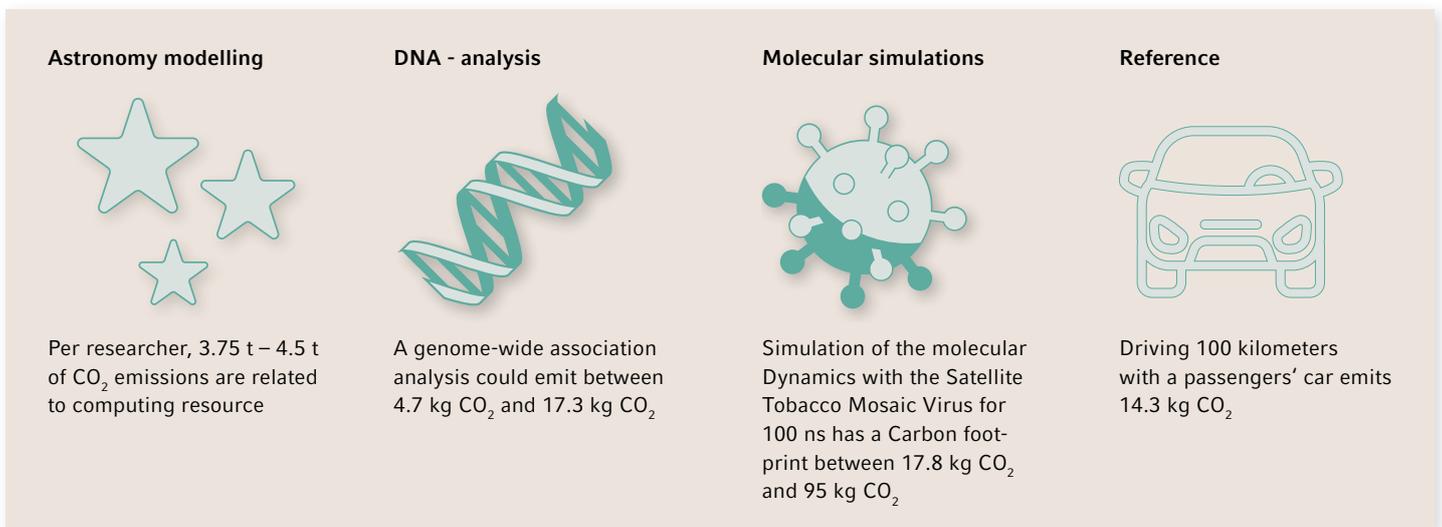


Figure 4: Research work results in different amounts of CO₂ emissions

If the contribution of research to CO₂ emissions is already high today, how will it grow with more data generation and the computing power which VR and AI require?

What about the data and virtual applications combined with the digitalized lab with all its connected devices? Required resources go beyond energy and CO₂. With more and more connected devices in the lab, each device has more electronics inside – from the pipette up to the big instruments. More electronics make these devices more vulnerable and failure-prone. Repair is not so easy anymore and a newer version might have a better performance and could also be seen as the better economic choice compared to fixing the failed device. But even if an “older” instrument may still work, the software version could be outdated, not updat-

able, or be not integrable in the lab network. Here’s the next challenge: Every device should be connected and “speak” with each other. But if there is no common standard, the smart lab could hardly become reality. This is a much-discussed issue and the lab world is working on it preferring two standards at the moment: the open-source SiLA and the industry-proven OPC UA standard. We will see which standard will prevail.

Nevertheless, within such a scenario of devices be relatively quickly outdated or incompatible with the network, the overall resource consumption will go up and overcompensate possible savings. As a problematic add-on, the use of rare elements which are essential in a wide range of electronic applications will also grow.

Green IT and sustainable digitalization

Digitalization is a challenge, but wisely used, it also has enormous potential and can contribute to reducing CO₂ emissions. According to a study, Germany can save about 33% to 49% of its CO₂ emissions by 2030, depending on the degree of digitization achieved [15]. The biggest reduction potentials are available in industrial manufacturing, followed by mobility, energy, and buildings. For example, a pharma company could reduce its energy- and CO₂ emissions by 80% by using a digital twin in the production of drugs [15].

How can digitalization unfold its full potential?

Digitalization is based on servers. These huge data centers produce about 90% of their total greenhouse gas emissions during their use phase. By using central servers, which are operated more energy efficient than smaller local servers, and the operation with green energy, the environmental impact can be reduced significantly.

The source of power as well as the server location (environmental conditions may require active cooling) have a significant impact:

A server in Switzerland emits about 20 g CO₂ per kWh whereas a server located in Australia emits more than 800 g CO₂ per kWh [16]:

Software development should consider resource consumption and efficiency. As the software controls the hardware, the controlling should be as efficient as possible to reduce energy consumption as much as possible. The choice of the programming language already impacts energy consumption [17,18]. As this is only for the specialists, it is good to know for everyone, to keep it in mind and to ask also about this aspect before deciding for or against a software.

The analysis of big data or modelling uses a lot of energy. Often, these analyses run in parallel over multiple processing cores to reduce analysis time. But this also enhances energy consumption. Nobody could wait for hours until all the data is processed. But one has to know that there's a critical balance where marginal improvements in running time mean an enormous increase in CO₂ emissions. Switching to a newer software version normally implies an increase in efficiency and thus energy-saving. By using a newer software version to run a GWAS analysis a user could save 12.6 kg CO₂.

Finally, let's have a look at the hardware. Electronic devices generate over 50% of its greenhouse gas emissions during the production phase [10]. By extending the use phase, we could reduce CO₂ emissions the most. Before buying new devices, the repair, the upgrading, or the refitting devices

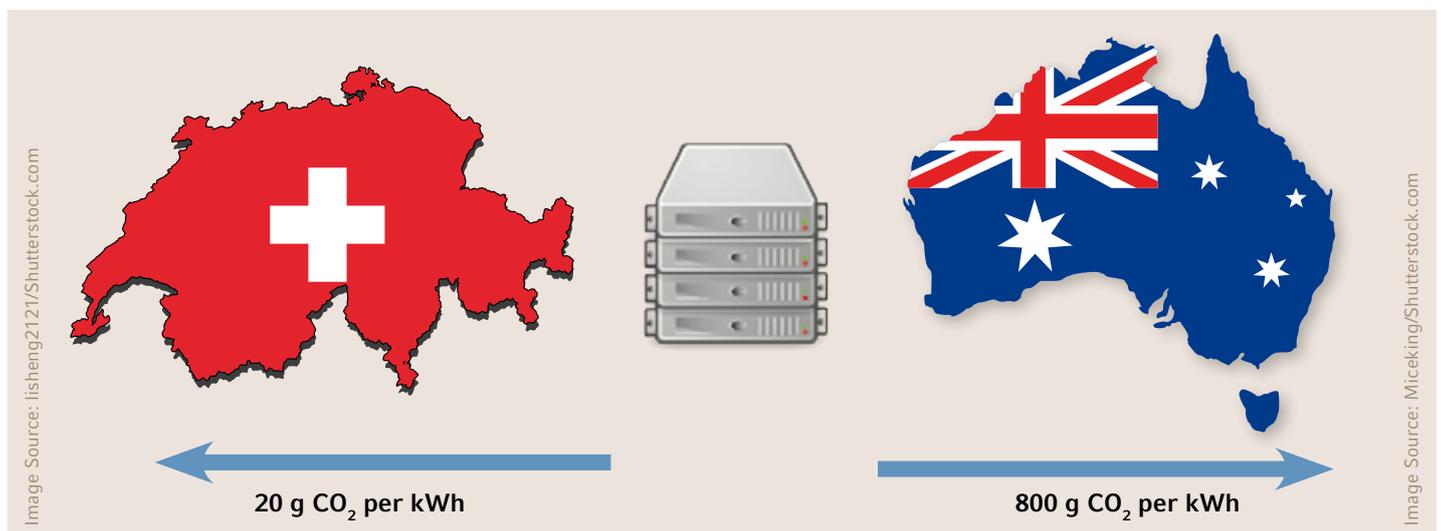


Figure 5: The location as well as the power source of a server have a significant impact on the CO₂ footprint of digital work [16]

shall have priority. To reach these goals and extend an instruments' lifetime, manufacturers have to focus on longer availability of critical spare part and the upgradability of their software.

The last point focuses on the end of a life of an electronic device. Proper recycling is key but as the recycling rate for electronic devices in the EU is less than 40%, there is still a

lot of work to do. Politics is aware of these specific problems and the EU has launched a Circular Electronics Initiative for electronics and ICT [19] that will feed into the EU Industrial Strategy. This initiative includes inter alia the demand of an energy-efficient design as well as to consider the aspects of the durability of an electronic device, of its reparability and upgradability. To fulfil the last two aspects, the EU also

added the right to repair and the right to update obsolete software for consumers. Of course, it also includes the aspects of maintenance, reuse, and recycling. Therefore, the collection and treatment of electrical waste and electronic equipment should also be improved.

This initiative is still limited to consumer products but it would sense to expand it to the professional areas (B-2-B) as well.

Using the best of two worlds...

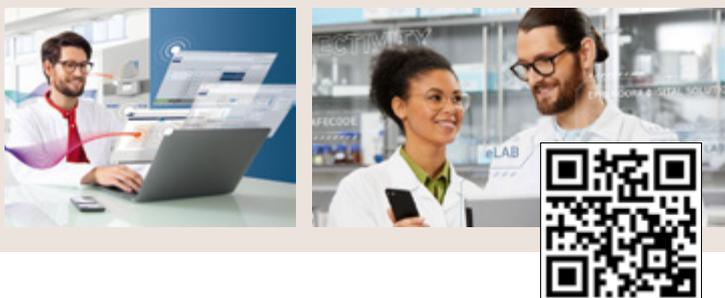
Digitalization and Green IT can be a big thriver for sustainability. The potentials are enormous, not only in terms of efficiency but also in terms of resource reduction and cutting CO₂ emissions. But to take full advantage of these opportunities, everyone needs to be aware of the carbon emissions associated with the web usage and related digitization.

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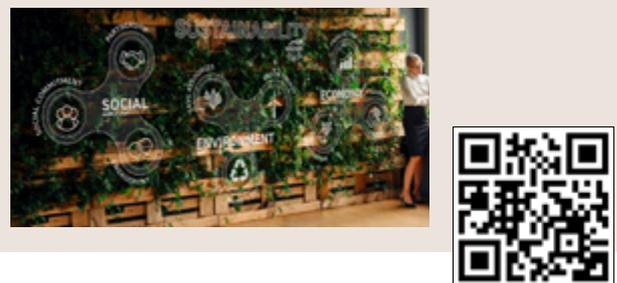
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