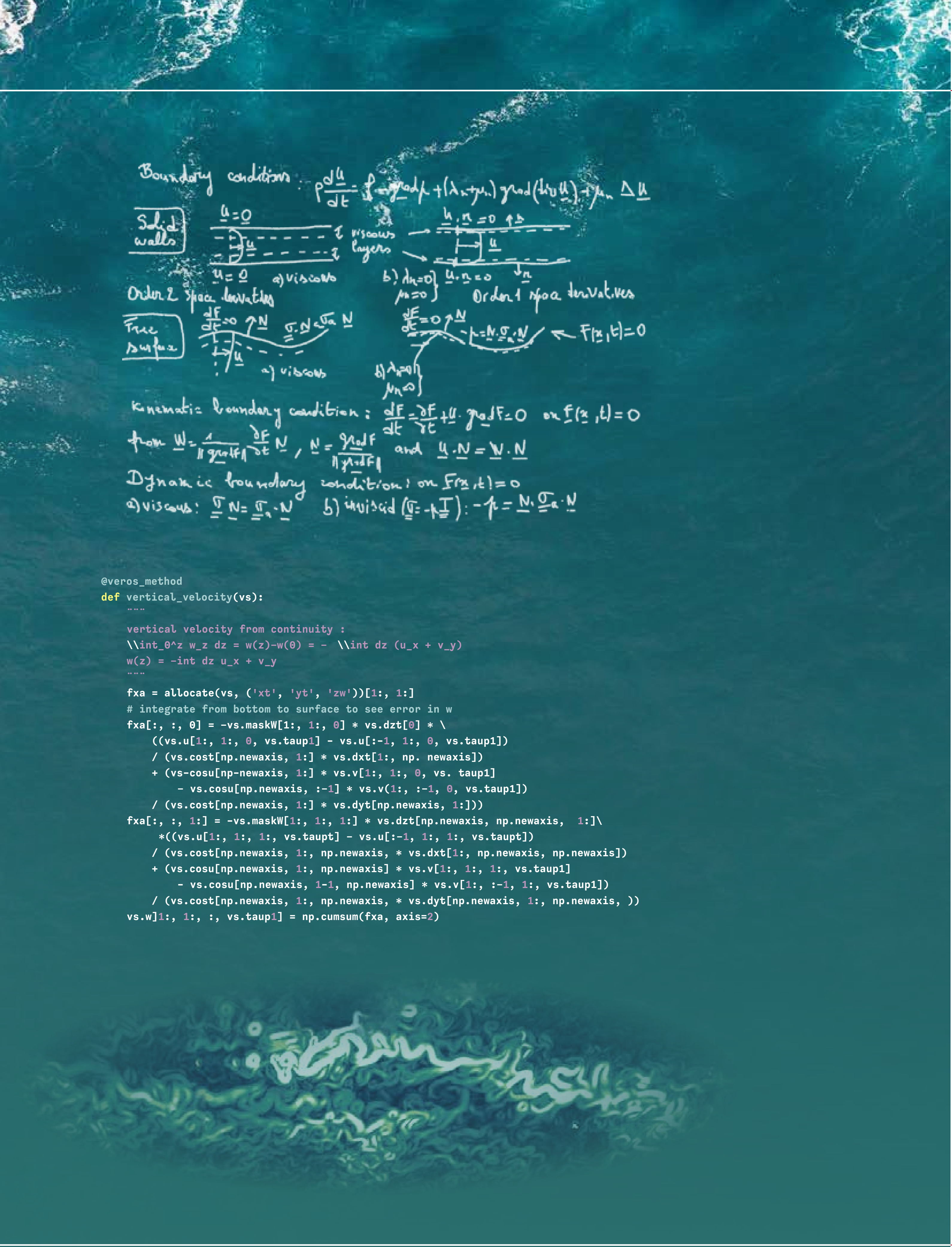
Digital Worlds

Rebuilding Life, Planets and Galaxies

UNIVERSITY OF
COPENHAGEN




```
@veros_method
def vertical_velocity(vs):
    """
    vertical velocity from continuity :
    \\int_0^z w_z dz = w(z)-w(0) = -  \\int dz (u_x + v_y)
    w(z) = -int dz u_x + v_y
    """
    fxa = allocate(vs, ('xt', 'yt', 'zw'))[1:, 1:]
    # integrate from bottom to surface to see error in w
    fxa[:, :, 0] = -vs.maskW[1:, 1:, 0] * vs.dzt[0] * \
        ((vs.u[1:, 1:, 0, vs.taup1] - vs.u[:-1, 1:, 0, vs.taup1])
        / (vs.cost[np.newaxis, 1:] * vs.dxt[1:, np. newaxis])
        + (vs-cosu[np-newaxis, 1:] * vs.v[1:, 1:, 0, vs. taup1]
            - vs.cosu[np.newaxis, :-1] * vs.v(1:, :-1, 0, vs.taup1])
        / (vs.cost[np.newaxis, 1:] * vs.dyt[np.newaxis, 1:]))
    fxa[:, :, 1:] = -vs.maskW[1:, 1:, 1:] * vs.dzt[np.newaxis, np.newaxis,  1:]\
         *((vs.u[1:, 1:, 1:, vs.taupt] - vs.u[:-1, 1:, 1:, vs.taupt])
        / (vs.cost[np.newaxis, 1:, np.newaxis, * vs.dxt[1:, np.newaxis, np.newaxis])
        + (vs.cosu[np.newaxis, 1:, np.newaxis] * vs.v[1:, 1:, 1:, vs.taup1]
            - vs.cosu[np.newaxis, 1-1, np.newaxis] * vs.v[1:, :-1, 1:, vs.taup1])
        / (vs.cost[np.newaxis, 1:, np.newaxis, * vs.dyt[np.newaxis, 1:, np.newaxis, ))
    vs.w]1:, 1:, :, vs.taup1] = np.cumsum(fxa, axis=2)
```


Introducing
the digital physicist

Our universe, with its life, planets and galaxies, is governed by laws that have been uncovered painstakingly by generations of scientists through observation, experimentation and deduction. However, even a casual reading of advanced textbooks makes it obvious that while the governing laws are often of beautiful simplicity, they lead to staggering complexity in the real world.

This real world, the world that we live in, is full of randomness and complex interaction of multiple forces, remote and near – and almost impossible to analyze or predict with analytical methods. The recognition of this truth in the late 20th century led many to predict the end of science. Fortunately, it was at this junction in history that computers became powerful enough to become an epistemological tool, the third pillar of science next to experimentation and theory.

As envisioned by John von Neumann (1903-1957), the founding father of computing, we can now finally rebuild our universe as numerical simulacra that capture the complexity which arises when the fundamental equations evolve and interact! This computational experimentation not only vastly expands our knowledge, but it also allows us to predict phenomena as different as the majesty of supernovae and abyssal ocean currents, the quantum interactions that drive chemistry, or the evolution of life.

Scientists at the Niels Bohr Institute develop methods that merge physics and high-performance computing, to transcend reductionist textbook knowledge and understand our universe in all its beauty and complexity. I invite you to follow me through the next pages and share the joys my colleagues gain from building molecules, planets and galaxies!

Jan W. Thomsen
Professor, head of the Niels Bohr Institute

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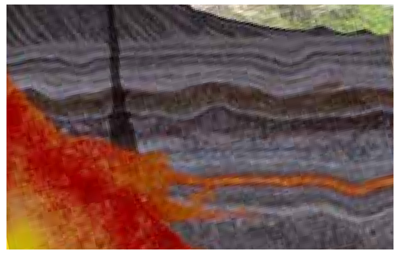
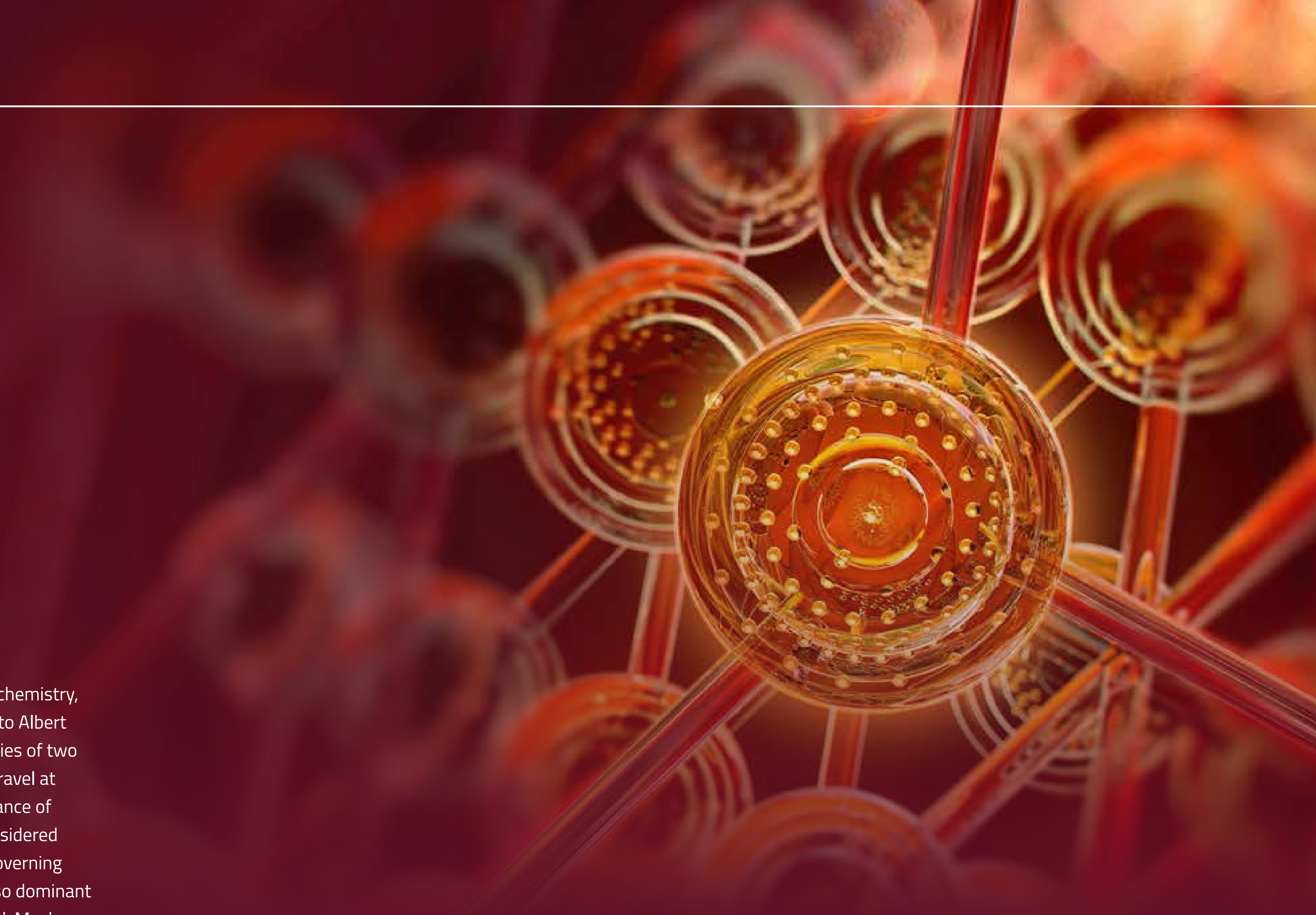




DIGITAL MOLECULES:

In the quantum age, chemistry is physics

Future pharmaceutical drugs and improved photo-voltaic cells may not be found through trial-and-error experiments anymore. Scientists at NBI design molecular systems on their computers, paving the way for a new type of chemistry.

Why is gold yellow? Since gold is a metal, and other metals are greyish or silverish this is actually strange. The explanation lies in quantum theory and therefore was beyond our reach, until Niels Bohr and his fellow quantum pioneers opened the door to the understanding of nature at the atomic level a little more than 100 years ago.

Needless to say, gold is highly valuable in itself. Not just in jewelry. We talk about golden periods in painting and literature, award the best athletes with gold medals, and even today governments maintain national reserves of gold. Would all this be the same, if gold had the same color as, for example, iron? Certainly not. However, the explanation behind the phenomenon goes beyond the significance of gold itself. We have entered a new age, where the development of new materials is no longer a matter of mixing different substances to see what will happen. Merging chemistry with quantum theory, it will be possible to design new molecules on a computer.

Importantly, these new molecules may have just the right optical, conductive, or magnetic properties, for example to turn sunlight into energy or storing energy long-term, for designing new drugs, or for use in the nano-size electronics that drive modern society.

Fast electrons make gold yellow

Before going into the new field of digital chemistry, let us hear why gold is yellow. According to Albert Einstein's theory of relativity, the properties of two identical objects will be different if they travel at different speeds. Despite general acceptance of the theory, for many years it was not considered relevant in chemistry. The other forces governing chemical reactions were assumed to be so dominant that relativistic effects could be neglected. Much later, beginning in the 1970'ies, it dawned on some physicists that the electrons in many atoms – especially the heavier elements – were actually travelling so fast that relativistic effects had to be taken into account.

An example in support of this claim is indeed the color of gold. As described in quantum theory, electrons do not orbit the atomic nucleus randomly, but follow certain orbitals. In gold, electronic transition occurs in two orbitals – from the 5d orbital to the 6s orbital. Relativistic effects increase the 5d orbital's distance from the atom nucleus and decrease the 6s orbital's distance. The transition causes absorption of electromagnetic radiation at the wavelengths which appear blue to the human eye. Since yellow is complementary to blue, light with a lack of blue is perceived as yellow.

Daunting costs of computation

So, how can we take quantum effects into account in chemistry? It certainly makes things harder, that quantum mechanics rarely assign specific positions and properties to specific particles. Instead, quantum theory operates with sets of probabilities for a particle being in a given position and having certain properties. This makes matters so complex, that only a few trivial systems can be solved exactly: even a single atom with more than one electron has evaded exact solution. For anything but the simplest quantum systems, we instead numerically approximate solutions through enormous calculations.

Such computational experiments provide answers to many physics and chemistry questions. However, they are typically run at supercomputers, sometimes for many months. Thus, discovery is limited by the cost of computations, which grows at breakneck exponential rates with the number of electrons.

The eScience group at NBI designs new computational methods to tackle the daunting costs of studying quantum systems: to make computational experiments feasible without supercomputers, and more powerful with them. For example, the researchers use hyper-spherical harmonics to describe the high-dimensional geometry of quantum particle interaction to model small highly interacting systems, and a geometrical understanding of low-dimensional carbon structures to model large systems. This is a form of molecular origami that hopefully will make it possible to design new molecules with desirable properties in the future.

DIGITAL LIFE:

Fighting super-spreading through modeling

NBI researchers look for the universal mechanisms which govern the processes of life. As the COVID-19 pandemic hit, their work was applied in the national mitigation strategy.

Just three months in early 2020 was all it took for the COVID-19 virus to invade practically all countries in the world. The pandemic gave us all a firsthand demonstration of a phenomenon which most people only knew from math class: the power of exponential growth.

Thinking abstractly about the origins of the pandemic, the replicative success of the COVID-19 virus illustrates how a phenomenon on the nano length-scale – tiny alterations to the surface structure of a certain protein in the virus – can have vast consequences on a global scale.

Such a span in length scales from nano to global scale is difficult if not impossible to handle in traditional medical research. Epidemiological studies will address the population scale, clinical studies will look at the patient scale, and a combination of lab experiments and theoretical work may elucidate what goes on at the atomic level. But none of these can provide the full picture. This is where physicists and their silicon replicas of the involved life processes come to the rescue.

Part of the national mitigation strategy

Long before COVID-19 hit, biophysicists at NBI became engaged in developing digital models of fundamental life processes – including how certain diseases may disturb these processes. Building on methods from physics, the researchers look for the universal mechanisms which govern the processes of life.

Early on, these proposed mechanisms will be discussed with clinical doctors, biologists, epidemiologists and others. Why? Well, a model will most often propose a given condition – such as an illness – to cause a certain physical response in the body. However, in the complex world of biology this is seldom a one-way street. Often will the physical response in question trigger some kind of feedback which will influence the effect of the illness and possibly other bodily functions. This complexity can only be addressed through the involvement of domain experts, and these discussions will typically lead to modifications of the models.

So experienced is the group at NBI in this type of work, that the Danish health authorities (Statens Serum Institut) invited them to join the national COVID-19 pandemic mitigation efforts. Thus, the work at NBI around so-called super-spreaders soon became an integral part of the national COVID-19 management strategy. Acknowledging that different individuals have different capacity for transmitting the virus introduces an additional level of complexity. A model developed at NBI takes this phenomenon into account and is thus a valuable tool for instance in a situation where either introducing or phasing out lockdowns is considered.

Ready for future pandemics

Much like other digital worlds created at NBI, some of the models developed by the life physics researchers require significant computing resources, and applications for time at supercomputers are sent on a regular basis. Still, this is not always the case: the program which calculates super-spreading risks in a Danish context can be run at an ordinary laptop with a calculation time of just a few hours.

Thanks to a combination of lockdowns, massive testing and vaccinations, Denmark has managed to cope relatively well with the COVID-19 pandemic in comparison with many other countries. However, the virus is still around and not least the emergence of new variants warrants continuous attention and further modifications to the developed models.

Furthermore, we have to recognize that COVID-19 will surely not be the last pandemic that we see. There will be a next one, and another one. Each time, fast development and adaptation of an accurate digital model will be instrumental in addressing the situation, saving lives and mitigating societal costs.

"As humankind we are only able to spend a limited time on this planet. If we want to expand that time, we really need to understand the world around us."
Dion Häfner, PhD student in TeamOcean at NBI.

I feel I can bring something to the table

Age matters little as the NBI researchers create digital versions of the physical world. Often it will be the students who are able to teach their experienced professors a trick or two.

Academia has always had a tradition for open exchange of ideas, including between faculty and students. In a field where being born digital is a definite plus it can sometimes even be hard to tell who is teaching whom.

"One thing I did bring to the table was a new approach to testing various hypotheses against each other," says Dion Häfner, PhD student in the ocean dynamics group at NBI.

The group creates digital twins of oceans (as explained in the Digital Oceans chapter), mimicking currents and other processes of the real oceans.

"Creating these digital twins is really challenging and interesting. However, what interests me even more is how we can put these models into work once we have them," says Dion Häfner.

The computer does the boring work

Digital versions of the ocean can be utilized to obtain new knowledge by manipulating certain factors. What will for instance happen if the temperature increases or if a given current is weakened?

"The thing is, when we do this type of experiments and observe some results, different people will have different stories on what is going on in our complex climate system. Previously, people would just agree to disagree, but I don't think we should settle for that. That's why I am developing machine learning-based tools to test different hypotheses against each other in a principled, quantitative manner. This was a new approach to the group," explains Dion Häfner.

Asked what attracted him to the field, he replies:

"Right from the outset I liked the idea that I am able to leave a lot of the boring work to the computer. Just pushing a button and waiting for results to come in is really satisfying. Meanwhile, I can focus on what I find interesting."

A deep connection with nature

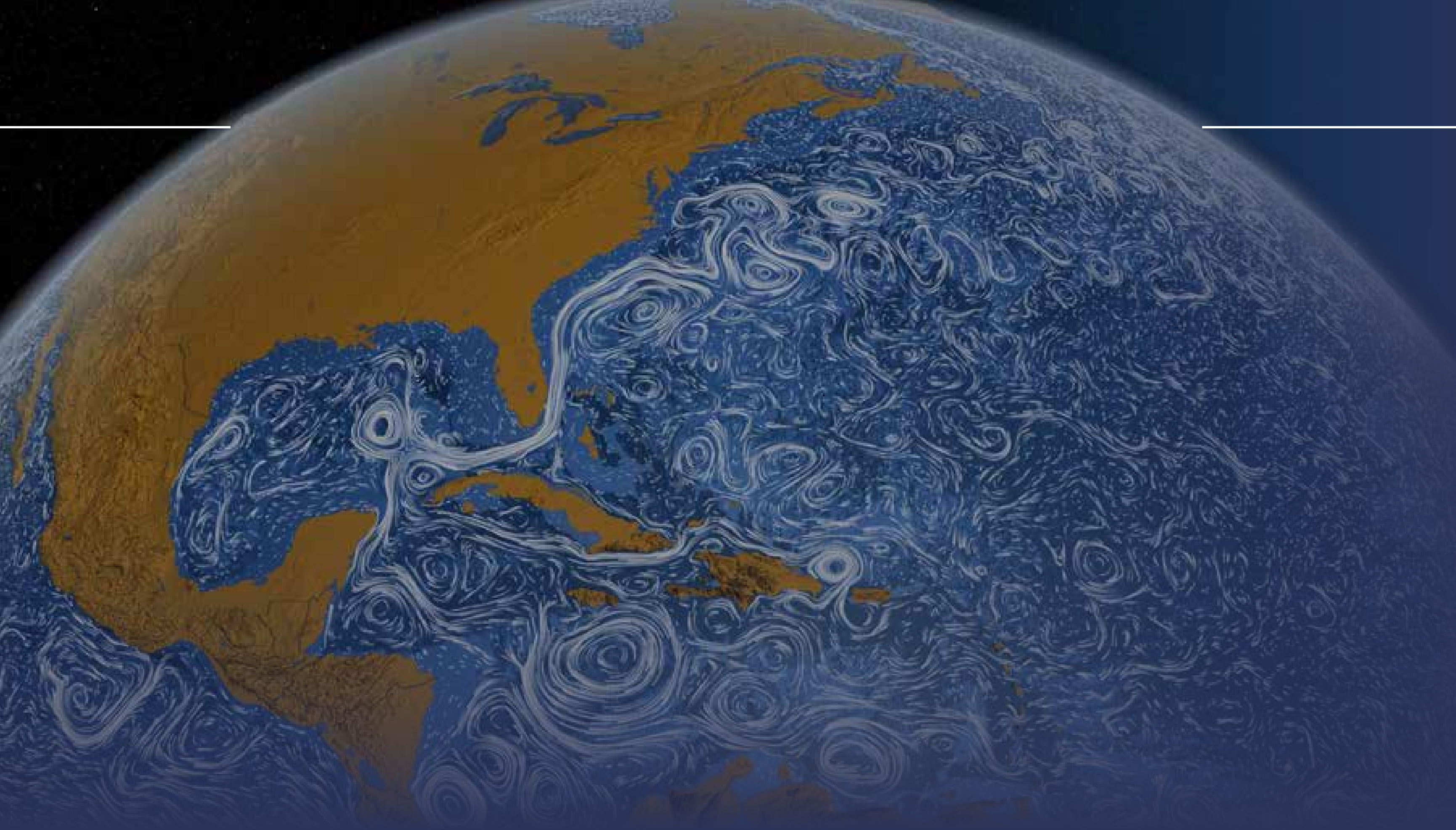
"Running an ocean model can almost feel like playing a computer game," Dion says with a smile, then adding on a serious note:

"But of course, this is not a game. What we create in our computers reflects what takes place in the outside world every day.

Sounds like you are motivated by mitigating climate change?

"In part, yes. Climate change is the most urgent challenge to us right now, but I am not only focused on that. Other changes in the Earth's climate will come after this one, and we need to understand our planet to handle them. Actually, I would say that the study of nature itself is my main motivation. Also, I am really fascinated by the technical details behind being able to build something as complex as our world inside a computer."

The computer is not the only way for Dion to study nature, he adds: "I feel a deep connection with nature – as most natural scientists do. Ironically though, considering that technically I am an oceanographer, I am not much of a boat person. I would probably just get sea-sick."



DIGITAL OCEANS:

Mysteries of The Big Blue

How will the world's oceans react to the warmer climate? This is just one of the many questions that can be addressed by building digital versions of the oceans.

We all know that the world is on route for a global warming of at least two degrees Celsius. However, this often-repeated figure is an average across the entire planet. Some locations will hardly see any difference, while others will really feel the heat has been turned on. The number one reason for the uneven distribution of the heat lies in the Big Blue – the world's oceans.

Huge ocean currents not only move massive amounts of water around, but also redistribute the heat received from the sun. In some places, the major currents have a cooling effect – possibly mitigating the effect of global warming – while other places they will enhance the warming.

Furthermore, we can expect that the distribution of the additional heat will not follow the same patterns that govern the ocean circulation today. In fact, it is likely that, as temperatures pass certain thresholds, some currents will vanish or reverse direction.

Building a silicon ocean

But how can we try and predict what will happen as the globe heats up over the coming decades? The ocean is opaque to light and radio waves and for a long time, most of what we know about it was wrestled from its abyssal depths in month-long expeditions, braving hurricanes, and icebergs. Unfortunately, the types of information obtained in this way did not easily translate into a description of the overall circulation governing the ocean currents.

However, by the late 1990'ies affordable large-scale computing entered the scene. By now, we can do numerical simulations which realistically represent ocean physics and dynamics: we can build a "digital twin" of the ocean, which can then be used to study what happens if the ocean warms or becomes more acidic.

Interaction at different length scales

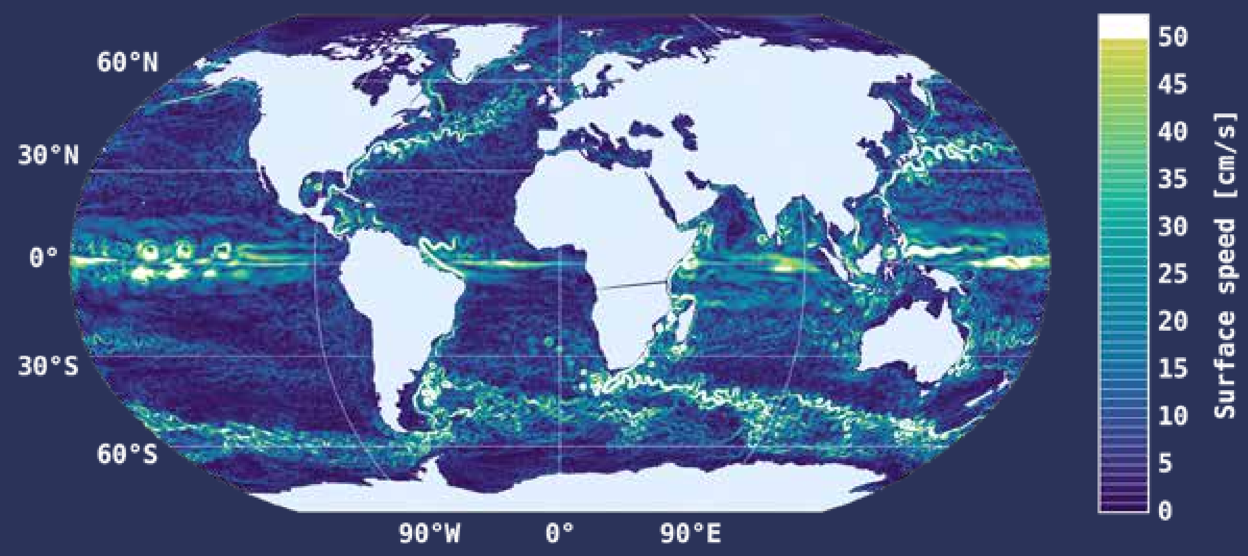
As a science, physical oceanography faces two fundamental challenges: the turbulence closure problem, and complexity. The former refers to the fact that the structure of the largest currents depends sensitively on the properties of turbulence on the millimeter scale. The latter results from the interaction of processes on the same scale; for example, the Kuroshio – the Pacific's equivalent of the Gulf Stream – has two different states, and each state can be maintained for several years in a row.

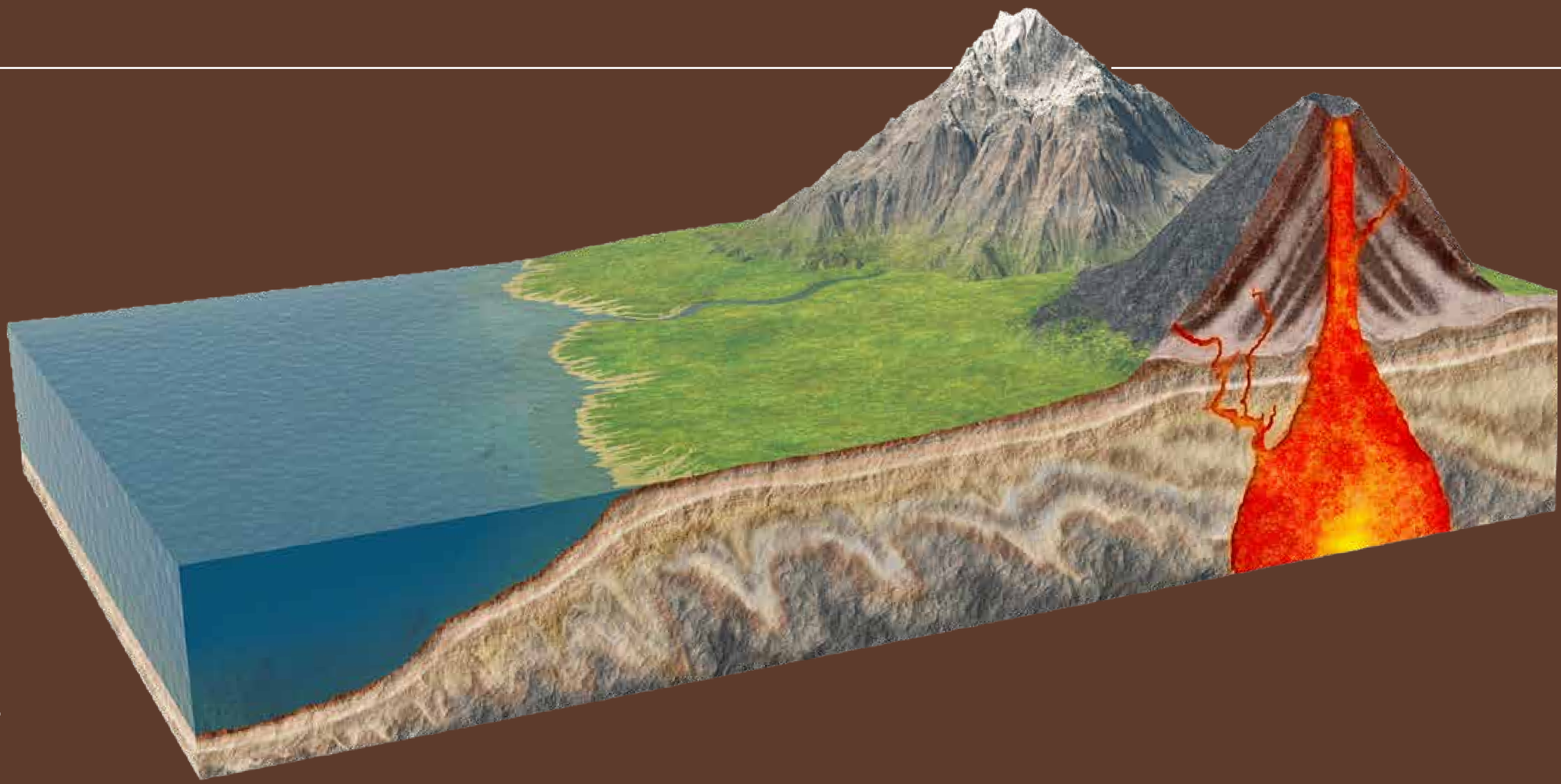
We will now be able to study a range of features which we previously could only poorly quantify, or maybe did not even know of, like abyssal storms, rogue waves or maelstroms. Not to mention the vast consequences for fisheries which almost any changes in the ocean will have.

As in the atmosphere, much of the heat in the ocean is not transported by currents or jets, but by storms or turbulence. The picture shows the instantaneous surface speed of the ocean in the NBI ocean model. Bright wiggles are ocean storms. These storms are most prominent around Antarctica, and it turns out that these storms contribute to the rapid melting of the Antarctic ice sheet from below.

The simulations of TeamOcean at NBI have finally allowed to determine the strength of these storms as a function of Earth's climate (Poulsen et al 2018), and the storms' contribution to ice sheet melt. In the model, the ocean is represented by 100,000,000 points. The simulations required continuous use for two years of 5,000 processors of one of the world's biggest supercomputers.

DIGITAL OCEANS AT NIELS BOHR INSTITUTE





DIGITAL EARTH:

Journey to the Center of the Earth; digital

Understanding what goes on in the deep underground has applications in geothermal energy, finding groundwater reservoirs, deposition of CO2, and prediction of earthquakes.

Which child hasn't at some point wondered what would happen if you were to dig a hole all the way to the opposite side of the Earth? The famous French novelist Jules Verne (1828-1905), by many considered the founder of the science fiction genre, took things a step further as he let his imagination send a crew on a "Journey to the Center of the Earth".

Today, we know well that such a mission wouldn't get far. We understand that below our planet's relatively thin solid crust, hot streams of fluid stone and metal make direct human exploration suicidal. Still, we cannot stop speculating about the conditions in the deep underground. Not only are we born curious, but developments in the underground influence our life in many ways. Millions of people live in areas that are subject to earthquake hazards, and knowledge about where to find groundwater resources is key to sustain living conditions in many areas.

A relatively young field is exploitation of geothermal energy. Due to the elevated temperatures in the deep underground, there is plenty of energy to be harvested. Moreover, geothermal energy does not produce CO2 nor pollute. Identifying the best geological sites for geothermal energy is a discipline of growing interest. Another emerging field is identifying geological structures which are suited for CO2 storage. Given the urgency of the climate crisis, increasingly more governments opt for capturing CO2 from energy production and industrial plants and store it underground.

Seismic waves travel the underground

How do we investigate all these topics, when we cannot send neither humans nor robots into the deep underground? The answer is to go there digitally. This is the scope of the Solid Earth and Computational Geoscience group at NBI.

Unlike Jules Verne, who could leave things to his rich imagination, the researchers need to be sure that their visualizations reflect the true conditions. And since, again, it is not possible to probe these conditions with on-location sensors, scientists have to make do with so-called seismic investigations. Investigators will send acoustic waves through the geological layers, or initiate controlled explosions which cause shock waves to travel the underground. The way these seismic waves are distributed will yield information about the geological formations.

For many years, the fundamental equations were not able to directly predict local phenomena – such as for instance earthquakes – in a highly complex system like the Earth. However, the advent of high-performance computing and new algorithms for efficient data analysis has provided a turning point. The digital representation of local Earth properties allows accurate simulation of complex wave forms in Earth's interior.

Solving inverse problems

Further important advances have been made in a related field. Seismic information is indirect information. Often different geological structures could, in principle, cause the observed patterns. In science, this is known as the inverse problem: the Earth's structure is calculated backwards from the observed seismograms.

The group at NBI has contributed to solving inverse problem challenges in recent years, culminating in 2021 with the development of the first computational method for high-speed calculation of Earth models with more than 1,000,000 unknown parameters, and at the same time quantifying the uncertainties of the solutions.

The method will enable us to generate high-resolution images of the deep Earth, while also contributing to a range of important practical applications: Mapping of sub-surface reservoirs for geothermal energy, discovery of groundwater reservoirs, and search for geological layers suitable for deposition of CO2.

DIGITAL GALAXY:

How stars are born

Wouldn't it be wonderful if we could – like in a science fiction movie – travel the universe to observe stars and planets from different angles? By creating galaxies in the computer, this is now possible!

The scientific method involves observations, hypothesis, experiments to test the hypothesis, and finally conclusions. In astrophysics, the time and length scales involved makes this procedure challenging. We can only passively observe the Universe and observations only give us two-dimensional projections of the three-dimensional Universe from a fixed vantage point, and are taken as snapshots in time. Furthermore, the resolution is limited by our instruments because of the tremendous distances and the inability to move objects closer. While it would be amazing, we cannot build planets, stars, and much less galaxies in our laboratories, and therefore controlled experiments, the bedrock of most sciences, are out of reach for astrophysics.

For centuries, we have built new mathematical models to describe nature, and this has allowed us to obtain new insights into the workings of the heavens. An example of such success stories are stellar models: stars are enormous balls of gas, and the attractive force of gravity makes them approximately spherical. This allowed astronomers to build the first precise models already a century ago by assuming spherical symmetry and solving the structural equations from the center of a star to the surface.

Like a spoon mixing milk in coffee

Today, the frontier in astrophysics is understanding how stars, gas, and dust interact in galaxies to create new stars, and how, around new-born stars, planets are formed. This is part of what is called the star-gas life cycle. In galaxies, gas is found in many different forms, from extremely hot and tenuous gas reaching 100 million degrees to cold and dense molecular clouds. The dynamics is driven by the differential rotation of the galaxies, that works like a spoon mixing milk in a coffee, and feedback from massive stars exploding as supernova and producing copious amounts of high energy radiation. The end result is a complex, turbulent, filamentary gas structure. Stars are formed in the dense, cold regions: when the density is high enough, the attractive force of gravity wins over the constant changing turbulent flows, and a star is born.

Our basic model of gas flows are the equations of magnetized fluid dynamics. They describe how matter is transported under the forces from magnetic fields, gravity, and radiation. Fluid dynamics is non-linear, (ie.; the acceleration of a fluid depends on its speed), and in some fluids this non-linearity can be damped by friction (a prime example is honey that flows very slowly and steadily due to friction). However, in the Universe densities are very low, and friction is almost non-existent. This combination of the non-linear nature of fluid dynamics, the low densities of the gas, and the enormous velocities imparted by exploding stars is what gives the interstellar gas its complex structure.

Molecular clouds give birth to stars

In astrophysics, computer simulations that solve the equations of fluid dynamics have emerged as an indispensable tool and substitute for carrying out laboratory experiments, to understand and interpret our observations. Simulations that solve the equations numerically are not only used to reproduce observations. Computational astrophysics is becoming the primary pillar of modern theoretical astrophysics because once we are able to reproduce observations, we investigate what are the most important forces at work, and that allow us to guide theory and test the validity of our models.

The Niels Bohr Institute has traditionally been at the forefront of computational astrophysics, and we have the last 40 years been developing new numerical codes and using the largest supercomputers world-wide to understand the Universe. Today, we are developing a new unique tool, DISPATCH, which will make it possible to execute our models of up to a billion computer cores simultaneously, reaching so-called exa-scale levels of performance to show how stars are born in molecular clouds when dust and gas contract under their own gravity, and how they die explosively in supernovas.

Early users of new supercomputer

To understand the life cycle of stars and gas in galaxies with a volume that contains enough material for tens of thousands of stars to be born has to be modelled, as massive stars are very rare. This requires enormous computational resources and algorithms that are capable to span a dynamical range of more than 100 million in space and time, i.e., from seconds to billions of years, from millimeters to lightyears.

Early next year a new European supercomputer, LUMI, will open and be in the top five of supercomputers world-wide. Researchers at NBI have been selected as one of a select few teams of early users. The combination of the new DISPATCH tool and the enormous power of the LUMI computer will make it possible to evolve a piece of the Milky Way in silicio over time scales of hundreds of millions of years allowing us to test our theories about the interaction between stars and matter in the Milky Way to better understand how stars are born and how galaxies evolve. These models will be the most realistic ever of star-forming areas, and in close collaboration with astronomers from the Niels Bohr Institute, data will be compared with observations from the large European ALMA telescope.

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