

**Breakup of a water droplet in air** upon the impact of a compression shock – Nikolaus Adams analyses such discontinuities in the fluid state.

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# Spotlight on Shock Waves

An abrupt change in the density, pressure and temperature of a flow as opposed to a gradual increase is known as a shock wave – a phenomenon that could prove promising for a wide range of applications in industry and medicine. However, this would first require significantly greater understanding of the occurrence and impact of these shocks. Prof. Nikolaus Adams intends to devote the next five years to intensive research into their potential for biomedicine and nanotechnology – supported by an ERC Advanced Grant of EUR 2.4 million.



Shock wave expanding in gas: A bubble in a mixture of hydrogen, oxygen and xenon is exposed to a strong pressure wave, which swirls and ignites the gas mixture. A front of flames is created, which propagates through the mixture.

#### Gitta Rohling

## Verdichtungsstöße – technisch gezielt einsetzbar?

Die Moleküle in einem Fluid streben nach einem Gleichgewichtszustand. Ändern sich Strömungszustände aber sprunghaft über sehr kleine Distanzen, entsteht ein thermodynamisches Ungleichgewicht in Form eines Verdichtungsstoßes. Ein typisches Beispiel ist der Knall, den der Mensch beim Überflug eines überschallschnellen Flugzeuges wahrnimmt. Die Moleküle der Luft müssen dem Flugzeug so schnell ausweichen, dass dies nicht mehr im thermodynamischen Gleichgewicht möglich ist. Es entsteht ein Verdichtungsstoß, der sich mit dem Flugzeug mitbewegt und den der Mensch als Knall wahrnimmt, wenn die sprunghafte Druckzunahme über ihn streicht. Mechanismen und Eigenschaften dieser Verdichtungsstöße wird Prof. Dr.-Ing. Nikolaus Adams in den nächsten fünf Jahren intensiv erforschen, gefördert durch einen mit 2,4 Millionen Euro dotierten ERC Advanced Grant. Verdichtungsstöße könnten für vielfältige Anwendungen in der Industrie und der Medizin interessant sein - beispielsweise für die Krebstherapie. Adams entwirft folgendes Szenario: "Nahe einer kranken Zelle werden winzige Dampfblasen erzeugt, die dann implodieren. Die so erzeugte Stoßwelle perforiert die Zellwände, sodass dank der nachlaufenden Strömung Medikamente schnell in die Zelle einströmen können. Ist die Perforierung klein genug, kann sich die Zellwand danach wieder schließen." Das wäre eine Therapie, die gezielt eingesetzt werden kann und die Dosierung von Medikamenten und damit auch die Nebenwirkungen deutlich reduziert.

Um solche Anwendungen zu ermöglichen, gilt es zunächst, das Verständnis über dieses Phänomen deutlich zu erhöhen. Adams interessiert ganz besonders, wie maßgeschneiderte Stöße erzeugt werden können und wie Stöße mit Phasengrenzen und Nanopartikeln interagieren. "Quantitativ und detailliert lassen sich diese Phänomene nur mit der numerischen Computersimulation untersuchen, die wir durch ausgewählte Experimente unterstützen werden." Einzelphänomene können die Wissenschaftler bereits gut simulieren; die Herausforderung liegt darin, mehrstufige Wechselwirkungen in komplexen Umgebungen nachzustellen - wie etwa in lebenden Organismen. "Oder ist die Komplexität so hoch, dass die Entstehung und die Auswirkungen der Verdichtungsstöße nicht vorhersagbar sind und diese sich daher nicht für die technische Beherrschung eignen?", formuliert Adams die Frage, die ihn umtreibt. Erst wenn sich diese Frage verneinen lässt, können die Wissenschaftler untersuchen, welche Mechanismen und Eigenschaften eine kontrollierte Bildung von Stößen ermöglichen und wie sie sich auswirken. □

olecules in a gas or liquid seek equilibrium. If the density, pressure and temperature of a fluid changes, the molecules usually have enough time to reach equilibrium – but not in the event of a shock wave. "In that case, the molecules cannot spontaneously achieve equilibrium. Instead, they are in a state of thermodynamic non-equilibrium," explains Prof. Adams, Chair of the Institute of Aerodynamics and Fluid Mechanics at TUM.

Shock waves are sudden changes in flow states across very short distances. A typical example is the sonic boom we hear when an aircraft flies overhead faster than the speed of sound. The air molecules are forced out of the path of the aircraft so quickly that maintaining thermodynamic equilibrium is no longer possible. A shock wave forms that moves with the aircraft and is perceived as a boom by people on the ground when the sharp rise in pressure passes over them.

The formation, impact and potential for targeting shock waves is the focus of Adams' research efforts, which he will now pursue intensively in a five-year project. This is facilitated by an ERC Advanced Grant – one of Europe's most prestigious sources of research funding. The European Research Council awards these grants, endowed with EUR 2.4 million, to scientists who already have an outstanding track record and intend to pursue ambitious, pioneering and unconventional research.

### From industry to medicine – of potential interest to a wide range of applications

Both the spatial localization and strength of shock waves means they hold potential for a wide range of applications. Direct fuel injection for diesel engines is a case in point. The automotive industry is keen to increase injection pressure as this would enable engineers to also reduce harmful emissions. However, extreme injection pressures result in extreme tensions in liquid fuel, which then evaporates without heating. Vapor bubbles, known as cavitation bubbles, form in the fuel and suddenly collapse (implode). This creates shock waves that are so strong, they can even damage hardened metals in fuel injector components on impact. This phenom"These phenomena are so tiny and fast that they are still largely unresearched and obtaining experimental data is a major challenge. Quantitative and detailed investigation is only possible by computer, using numerical simulation."

Nikolaus Adams



Dicture credit: ediundsepp (Source TUM)

When a fluid containing vapor bubbles is exposed to higher pressure the vapor condenses and emits a strong shock wave upon final bubble collapse.

enon is called cavitation erosion and is also a familiar problem in the operation of marine propellers and water turbines. Yet what is a downside in engine technology could prove a benefit in medicine. "A fundamental problem in cancer treatment is that diffusion is a relatively slow process, so it takes time for drugs to reach the cancer cells, which have a higher internal pressure than healthy cells," describes Adams. In contrast to diffusion, shock waves are rapid processes and could be used to accelerate drug uptake significantly. Adams envisages the following scenario: "Tiny vapor bubbles are produced – for instance by ultrasound – in the vicinity of a diseased cell and then collapse. The shock wave this generates perforates the cell walls, with the subsequent flow allowing a rapid influx of drugs into the cell. As long as the perforation is small enough, the cell wall can close again afterwards." This would be a therapy that could be precisely targeted, substantially reducing the amount of medication required and thus also the side effects.

#### Mastering complexity through simulation

But before this type of scenario can become reality, scientists first need to improve their understanding of the physical processes involved. Adams is particularly interested in ways of generating tailored shock waves and how shocks interact with phase boundaries and nanoparticles: "These phenomena are so tiny and fast that they are still largely unresearched and obtaining experimental data is a major challenge. Quantitative and detailed investigation is only possible by computer, using numerical simulation."

In numerical simulation, scientists first formulate the basic properties of shock waves by means of physical and mathematical models, then implement these in dedicated programs on high-performance supercomputers. The decisive factor here is the number of degrees of freedom – that is, the number of variable data describing the flow. "The more degrees of freedom, the more accurate the simulation," Adams emphasizes. So this entails processing huge volumes of data. Thanks to improved processing power, the possibilities of numerical flow simulation have grown enormously over



## "The ERC Advanced Grant gives us the freedom to redirect our research if unexpected results come up."

Nikolaus Adams



#### Prof. Nikolaus Adams

#### **Research as a vocation**

Inside Prof. Nikolaus Adams' office at the Department of Mechanical Engineering in Garching, near Munich, hangs a poster of aviation pioneer Otto Lilienthal with one of his flying machines. On it are printed three short phrases: "To know. To understand. To do." As far as Adams is concerned, Lilienthal represents the epitome of an engineer who acquires and analyzes knowledge to make it technically useful. "Lilienthal developed his flying machines without the possibility to rely on existing scientific knowledge, deriving knowledge and understanding from his observations of birds and his ability to turn those observations into technical solutions," recounts Adams, clearly impressed.

His ideal scientist, on the other hand, is Werner Heisenberg – due to the pursuit of scientific perfection that earned the physicist and founder of quantum mechanics his Nobel Prize in 1932. Heisenberg devoted himself to exploring the interplay between various findings in physics – such as the theory of relativity and quantum theory. As he recounted in 1970 in his talk" The Meaning of Beauty in the Exact Sciences": "In both cases, after years of vain effort at understanding, a bewildering plethora of details has been almost suddenly reduced to order by the appearance of a connection [...]."

Adams uses similar terms to describe his fascination with numerical simulation – the computational process that allows exploration of complex physical flows and has thus become one of the most important tools in fluid mechanics today: "To carry out the simulation, we define a model in the form of a numerical algorithm, which serves as our working hypothesis. This involves reducing reality to the essentials based on assumptions and simplifications. I find that a fascinating form of research – we're trying to recreate reality, albeit well aware of the shortcomings of this approach. But that's the only way to understand what is actually happening."

Adams has been fascinated by this topic since his studies in aerospace engineering at the University of Stuttgart – making his path into research a matter of course. "Anyone wanting to improve our understanding of fluid physics essentially needs to work as a researcher. In industry the pressure for practical applications is high, which doesn't really allow for deeper examination of approaches and methods," he explains. Having received his doctorate with honors, he then took up a postdoctoral fellowship at the Center for Turbulence Research in Stanford, California. He went on to work as a scientist and lecturer at ETH Zurich and as a professor at the Dresden University of Technology, before transferring to TUM's Institute of Aerodynamics and Fluid Mechanics in 2004.

According to Adams, you know instinctively whether you would be well suited to research: "It's a vocation." As far as he is concerned, people who primarily view work as an obligation are not cut out for research careers. "But if you feel called to it and come equipped with the right skills, you'll make your way forward," he concludes with conviction.

the last few years. However, for large-scale simulations, the processes call for a lot more computational power – another area Adams is focusing on. As part of a team of researchers, he received the Gordon Bell Prize in 2013 for a flow simulation of a cavitation bubble cloud with 13 trillion degrees of freedom – the largest and most efficient ever performed at that time. The researchers simulated the simultaneous collapse of 15,000 gas bubbles within a liquid. To accomplish this, they used one of the world's fastest supercomputers, reaching a processing speed of 14 petaflops. That equates to 14 quadrillion (14,000,000,000,000,000) computer operations per second.

## The burning question: can they be technically controlled?

The ERC Advanced Grant is crucial to Adams' ambitious research endeavors. Thanks to this funding, he is now able to extend an excellent research group by four doctoral students and one postdoc. Adams is particularly pleased to receive such "stable support over an unusually long period" and explains that, as a rule, grants tend to be smaller, shorter and thus more suited to incremental project proposals. In particular, the ERC Advanced Grant allows the scientists a fairly high degree of research freedom. "Disruptive research also becomes possible - we can redirect our efforts to pursue a new avenue if unexpected results come up," confirms Adams. The scientists will now start by using their simulations to address the burning question, namely can tailored shock waves be generated in complex environments such as living organisms? "We are already well able to simulate individual phenomena - the challenge lies in managing the complex interactions between them." clarifies Adams. Or. as he frames the question that drives him: "Is the level of complexity so great that the formation and impact of shock waves simply cannot be predicted, which means they cannot be controlled technically?" Only if he and his team succeed in managing this complexity can they then turn to investigating the mechanisms and properties that enable controlled formation of shock waves and their possible impacts - to the benefit of applications in industry and medicine. Gitta Rohling

In the future, shock waves could help get medication exactly where it is needed: With the help of ultrasound, we could produce tiny vapor bubbles in the vicinity of a diseased cell and then collapse the bubble. The subsequent shock wave would perforate the cell walls, allowing a rapid influx of drugs into the cell.

