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EDITORIAL

Editorial: In Memory of Mark Robbins

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Mark Robbins (1956 – 2020) (Photo: N.D. Spencer)

In this special issue, we remember Mark Robbins, who passed away, unexpectedly, on August 14, 2020. The many submissions by world-renowned scientists only provide a glimpse of the appreciation that he received for the unique way in which he used computer simulations to deepen our understanding of mechanical and thermal properties of condensed matter systems. He was a true giant in the field, while being as humble, warmhearted, and empathetic as a physicist can possibly be.

Mark received his BA and MA degrees from Harvard University. After 1 year as a Churchill Fellow at Cambridge University, he moved on to the University of California, Berkeley, where he obtained his Ph.D. in 1983. Following an interlude as a postdoctoral fellow at Exxon's Corporate Research Science Laboratory in New Jersey, he accepted an offer from Johns Hopkins University in 1986, where he spent his entire career as a professor in the Department of Physics & Astronomy. He became a Fellow of the American Physical Society in 2000 and of the American Association for the Advancement of Science in 2017. He was awarded Simons Fellowships in Theoretical Physics in 2012 and 2019. Mark served our community as organizer of more than a dozen conferences, symposia, and workshops including the KITP workshop, From the Atomic to the Tectonic: Friction, Fracture and Earthquake Physics in 2005, and the Gordon Research Conference on Tribology in 2010.

Mark's contributions to condensed-matter physics in general and to tribology in particular were as numerous as they were multi-faceted. Here, I describe some of them from a personal perspective, although messages that I received from former colleagues, collaborators, and his many friends and alumni confirmed and corroborated my deep admiration of him as both a scientist and a person.

When I first learned about Mark Robbins in 1997, I was a Postdoc in the Department of Chemistry at Columbia University and was concerned with what I thought was complicated mathematics that allowed us to push the borders of how water can be modeled realistically. My former Ph.D. supervisor, Kurt Binder, whom I could trust blindly, had recommended me to join Mark's group. Thus, I was in a state of shock when I realized that most of the things that Mark did boiled down to the use of something as archaic as bead-spring models, Lennard–Jones potentials, and the Verlet algorithm. However, I quickly learned why Mark was already famous at that time.

Mark had been invited to give a colloquium at Rockefeller University and he seized the opportunity to get to know me as his prospective postdoc. We had a pleasant chat in a small café on Broadway, which, in retrospect may have been the real interview, since Mark fell asleep during my official interview. He blamed this on his newly born son Thomas, though I feared it was my fault. In retrospect, I suspect that he pushed himself more than was good for him. The introduction of Mark at Rockefeller started as usual with the mentioning of his academic career and his official recognitions. But then came the sentence that still rings in my ears and best describes Mark's work: *Although Mark Robbins is a computational physicist, he does not produce numbers but insight*. There can be scarcely a greater compliment

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for a computational physicist and I cannot think of a single person who would deserve it more than Mark. Indeed, as his career progressed in lock-step with the vast advances in computing, his delight with the increased computing power was unmistakable and his scientific insight was never overshadowed by it.

After I had joined his group in 1997, Mark told me about the project that he wanted to pursue with me. He had agonized about an old and truly central question of tribology: What is the general, microscopic origin of frictional forces between solid surfaces? Coulomb had already argued, in one of his most ingenious and yet most overlooked sentences, that it can only be due to either the interlocking of surface asperities, which need to deform so that they can elevate one over the other, or because of surface molecules, which, due to their proximity, adopt a coherence that needs to be overcome to initiate sliding.

Mark had recognized that most surfaces should not interlock significantly on a local scale, because their surface corrugations have no reason to match and elasticity is a strong restoring force in three spatial dimensions. He appreciated that rare gas monolayers adsorbed on metals, and also, flat interfaces between copper showed superlubricity, i.e., predominantly small damping forces that are linear in velocity, unless the surfaces in contact miraculously happened to be commensurate. In later work on coarser scales, he also found pinning or static friction forces due to typical microscopic roughness to be rather minor. Mark proposed that loosely adsorbed molecules on surfaces should be a game changer. He introduced his idea to me with a sentence like, "If you have a polymer on a surface, say, an airborne hydrocarbon, then one end can connect to one surface and the other end to the other surface. If both ends of the polymer are bonded to opposite surfaces, then there can be a static friction force, even when the surfaces originally don't match." He thereby concretized Coulomb's idea about the importance of surface molecules from being part of the solids to being adsorbed onto surfaces and being squished into well-defined positions in response to the large pressures that typically exist at true microscopic contact.

Mark went on and mentioned that Gang He, an excellent Ph.D. student of his at Hopkins, had already run some simulations showing that macroscopic friction laws can also be observed locally, but that it wouldn't hurt to have more support to fully deliver the message and to identify the circumstances when Amontons and Coulomb's law even apply at the microscopic scale. I was surprised that such a fundamental issue like the origin of solid friction had not yet found a generally applicable answer and after a few second of silence, I responded: "I don't know if I buy your idea. But if it is correct, why do you need polymers, it should also work for monomers." Rather than being offended by my skepticism, he instantly responded with a big smile on his face: "This is a neat idea. I will test it right away." There are few people in the world, whose comment "this is a neat idea" would make me as proud as when Mark would utter it, in particular, as a much more frequent and justified response of him started with the words, "I did this 15 years ago and found that …" And, owing to his incredible memory, he equally often acknowledged the work of others.

His insight into the origin of solid friction is merely one of his many, many contributions. And just to set the record straight, Mark was able to use and develop tools that were much more complex than bead-spring models. He told me about having written a tight-binding code from scratch with which he had simulated tribo-chemical processes of hydrogen-terminated carbon, but that he never found the time to write things up. It took others, whom I also hold in the utmost high esteem, more than a decade to duplicate his results and to publish them prominently.

In general, Mark pioneered molecular simulation to unravel physical phenomena on the atomistic scale that are not captured by continuum theory but that still matter at macroscopic scales. For example, in collaboration with Kurt Kremer and Gary Grest, he found how and why the crystallization of colloidal suspensions is slowed down due to ordering in the liquid phase. Particularly successful was his work with his Ph.D. student Peter Thompson on the dynamics of fluids near solid interfaces. They demonstrated, among many other things, that sliding-induced melting and subsequent reordering of boundary lubricants are a frequent cause of stick–slip dynamics. Together with his Ph.D. student Binquan Luan, Mark established that atomic discreteness effects of just the very last layer and small variations of atomic heights can induce deviations of shear forces from continuum theory by an order of magnitude. In the field of contact mechanics, Mark's group joined forces with that of Jean-Francois Molinari to conduct the first (rigorous) multi-scale analysis of elasto-plastic contacts. They identified scaling relations for the distribution of contact stresses and contact morphologies that hold for different plasticity laws. His highly cited work on fluid invasion in porous media with Marek Cieplak, strain hardening of polymer glasses with Robert Hoy, cracks and crazes of polymer glasses with Jörg Rottler, the peculiarities of capillary adhesion at the nanometer scale with Shengfeng Chen, and the dynamics of colloidal systems with Mark Stevens as well as important contributions to the multi-scale/multi-physics modeling of fluids are only selected pinnacles of his work.

Mark's brilliance was also revealed during scientific discussions. Jim Belak noticed that you'd only have to explain an idea to Mark once. The students at Hopkins described his teaching with a clear "awesome". Judith Harrison, who met Mark at many tribology conferences over a time period of more than 30 years, wrote that she always thought of him as the smartest person in the room, no matter who else was in the room. If it weren't inappropriate, I would argue that this may be the reason why Mark never received a Tribology Award.

One of the reasons why Mark could relate his computer simulations so successfully to laboratory experiments may be that he benefited from discussions with his wife, Patty McGuiggan, who, herself, is a very thoughtful and productive scientist doing real tribology. Mark was very much aware and very appreciative of the support that he owed to his wife.

In addition to leaving traces in the annals of sciences, Mark cared for the personal lives of his friends and alumni. Our paths hadn't crossed for a few years. One day I received an e-mail out of the blue in which he told me that he had heard from someone that I wanted to return to Germany and that he had learned a few minutes ago about an open position in my native city. None of my life since 2009 would have unfolded in the way it did, if Mark had not thought of someone who only spent a year with him as a postdoctoral fellow. Many others, also non-alumni like Mehmet Baykara, have shared similar stories, in which Mark became active in their favor.

While Mark's caring personality put him on friendly terms with almost everyone in the field, he did have quite an intense feud with the other leader of theoretical tribology, Bo Persson, rather in the tradition of Feynman vs. Gell-Mann or Newton vs. Hook. Early editions of Bo's famous book on Sliding Friction testify the intensity of their debate. Together with Marek Cieplak and Elisabeth Smith, Mark had proposed that dissipation of adsorbed layers occurred through anharmonic coupling between phonon modes and substrate-induced deformations in the adsorbate. Bo argued that Jacqueline Krim's famous experiments of mono- or bi-layers of simple adsorbates on metals were better explained through a coupling to the electronic degrees of freedom in the metal. The controversy is not necessarily settled, but, as so often, the real question may be under what circumstances which of the mechanisms is dominant. Despite, or, perhaps because of their dispute, Mark invited Bo to his KITP workshop and was also an admirer of his contact-mechanics theory, both of which were ultimately at the root of a friendship between them and a deep mutual appreciation. This did not prevent them from starting a new, albeit friendly debate in the past few years on what explanation resolves the adhesion paradox. Together with Lars Pastweka, Mark had identified a criterion for when surfaces become (locally) sticky, while Bo was interested in the pull-off stress averaged over the nominal contact, which, of course, can be small even if individual meso-scale asperities are sticky.

In fact, identifying scaling relations, as for example, the stickiness criterion, was one of the Mark's trademarks. However, in contrast to the other half a dozen people at APS meetings sharing his ability, he would be the only one who also knew where to get the cool gadgets for his children at the science booths. And he'd be equally excited about both. Mark had many passions beyond science and his family, which he often talked about to friends. We both shared dance as a hobby, though he made it to off-Broadway stages. He was also completely infatuated with orchids. His basement was full of them and breeding new ones made him gain the Award of Merit from the American Orchid Society.

Mark was a realist and yet always optimistic, concerned about the planet but hoping for and thinking of solutions. He was a true patriot but the opposite of a nationalist. He cared for people no matter what was their background, their color of skin, their choice of partners, or their education. He could converse with anyone about anything and usually it would not take more than 10 min until his incomparable laughter would cut through the air. When he laughed at others, he would only do it if he could add "… and he is smart!!!" and then keep laughing twice as loudly. When he was taken from us, he was as active as he had ever been. He looked forward to spending more time with Patty after his retirement, although it is hard to imagine that he would have quit science altogether. He also leaves behind two just grown-up children, Thomas and Catherine. Two newly bred orchids carry their names.

We are still in shock and in sadness. If Mark had heard about someone passing like him, his comment might have been a deeply sighed "What a waste!".

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