

## Nosé Shuichi, 17 June 1951→17 August 2005, In Memorium

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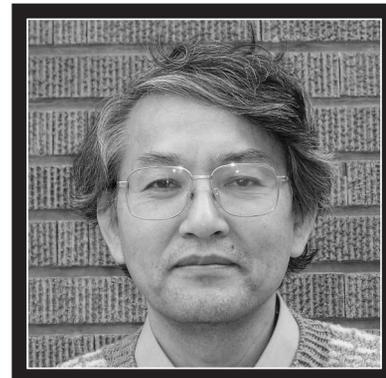
After his doctoral work at Kyoto, Shuichi Nosé travelled to faroff Canada for three years as a postdoctoral fellow. He worked in relative isolation, listening to Dvorák recordings, ice skating, and developing a new and fruitful approach to Gibbs' statistical mechanics. I was excited by the new ideas he described in his two fundamental papers of 1984.\*1 When I saw them, I immediately began to study and absorb the significance of this revolutionary approach to statistical mechanics. In the two papers, Nosé introduced and applied new algorithms for deterministic time-reversible simulations of isothermal systems. His new dynamics exactly reproduced Gibbs' canonical ensemble. This was an intellectual feat! For 100 years dynamics and statistics were regarded as two distinct approaches. Nosé united them. Today the applications of this development are well known, widespread, and far from exhausted.

That same year, 1984, I met Nosé for the first time, on a train platform in Paris—a real unplanned and unpredictable coincidence—my plane had been diverted to Orly from de Gaulle. While waiting at the airport's train platform I noticed a Japanese with "NOSE" lettered on his suitcase. Was he the same Shuichi Nosé whose work I had been studying? "Yes", he said, and we got acquainted. We were both in Paris to attend, several days later, a workshop on statistical mechanics and

simulation organized by an early fan of parallel processing, Carl Moser. Our hotels were both within an easy walk of Notre Dame, so Nosé and I arranged to meet there, and had several hours' discussions of his work on a bench in front of the cathedral. I learned enough from our Paris conversations to write a paper shortly thereafter (while visiting Philippe Choquard in Lausanne) stressing the importance of what is called the "Nosé-Hoover" version of his dynamical equations. Ever since 1984 I have worked hard to apply the new ideas to the understanding of both equilibrium and non-equilibrium systems.

I got to know Shuichi better in Japan, along with his charming wife Ibuki and (then) young son Atsushi (now a budding engineer). Shuichi had arranged for me to spend a sabbatical year with him at Keio University's Hiyoshi campus. My new wife Carol came too, and worked at Keio with Toshio Kawai and Taisuke Boku. Shortly after Carol and I were settled in Japan, we were invited to an elaborate dinner honoring Shuichi, sponsored by International Business Machines, which awarded him its Japan Science Prize in 1989. It was a great pleasure to see his parents enjoying their son's fame. We all watched a large-screen biographical video that IBM had made for this special occasion.

Nosé-san had arranged a very comfortable western-style apartment for us



at Nestle House, within walking distance of the Keio campus. The walk passed by the preschool where we often saw Atsushi at play. At the University, Nosé-san arranged for all the amenities, along with plenty of computer time and numerous conference invitations. Nosé's 1984 work changed my own research direction profoundly, toward exploring the nonequilibrium applications of Nosé-Hoover mechanics. The resulting interpretation of nonequilibrium distribution functions as zero-measure fractals, rather than smooth distributions, provided a fascinating explanation of irreversibility. Nosé's approach made analyses of such systems much simpler.

Nosé pursued a variety of topics, all related to computer simulation, after his revolutionary papers of 1984. His lasting legacy remains that early work together with the memories of those who knew him. I count myself fortunate to remember Shuichi. His early death is a shock for physics, and painful for his family and friends.

(2005年9月2日原稿受付)

本記事は追悼文であることを斟酌して、原文の雰囲気を活かすためあえて翻訳はしないで掲載しました。

会誌編集委員会

\*1 One in the Journal of Chemical Physics and one in Molecular Physics.