

## **Stochastic modeling for systems without separation of scale**

D. Bernstein, A.J. Chorin, O.H. Hald, P. Stinis,  
Lawrence Berkeley National Laboratory

J.Barber, Los Alamos National Laboratory

**Summary: We have developed stochastic modeling methods for systems without separation of scale, such as the ones that occur in hydrodynamics, plasmas, geophysics, and neuronal networks.**

Most problems in science are too complicated for a full computer description- because there are too many variables, and/or there are not enough data, and/or the models are incomplete. Standard tools for dealing with such problems involve stochastic modeling- the replacement of the "less important" variables by random variables subject to statistical constraints. This is in general difficult, so earlier workers have focused on cases in which there is separation of scales - i.e., the variables that are modeled statistically are smaller and faster than that the ones that are actually computed. Under these assumptions one can show that the variables that are omitted can be modeled as white noise; this is the world of Langevin equations, Fokker-Planck equations, fully described in many standard textbooks. It is often said that there can be no stochastic modeling without separation of scales.

However, it has been known for many years that the assumption of separation of scale fails, and fails badly, for many important

cases; these cases include all hydrodynamic systems, including the weather system, as well as neuron dynamics in biology. Many of the failures in the modeling of such systems, including the difficulties of large eddy simulation in turbulence, can be ascribed to the use of separation of scale assumptions where such assumptions do not hold (and we have produced simple but dramatic examples demonstrating the point).

We have set out to rectify this situation and we have succeeded. Over a period of about 10 years we developed a general methodology and theory for making predictions on the basis of partial models and partial data ("optimal prediction"). The general formalism we have produced, based on a combination of probability and of methods borrowed from statistical mechanics, is in principle "optimal" in that it provides a solution which is best in a statistical sense. The formalism is however complicated and hard to use. The main difficulty is that solutions based on a partial description necessary involves a non-

---

\* Telephone Number, E-mail address

Markovian memory (as we have proved in great generality), and the determination of the kernel that represents this memory is very laborious. If one adds to our theory an assumption of separation of scale one sees that the memory becomes short, and one recovers the standard methods, with an occasional improvement in cases where the separation of scales is weak.

More important, using our general framework, we succeeded in deriving a new, unexpected, and simple, formalism for modeling underdefined systems where there is no separation of scale and where, as a consequence, the memory is long. We think that this is a major breakthrough which opens many new avenues for the computer modeling of complex systems. We have carried out a number of test calculations for problems whose solution is known to test the ideas in practice.

We have also carried out a number of real applications, in particular to finance and to molecular dynamics. The most dramatic, which is being written up now, is the numerical determination of the decay rates of homogeneous turbulence. Though this is not a full solution of the turbulence problem- the decay problem is a special case- yet it is, to our knowledge, the first numerical determination of a property of fully developed turbulence from first principles.

#### References:

A.Chorin, O. Hald, and R. Kupferman, Optimal prediction with memory. *Physica D* 166 (2002), pp. 239-257.

A.Chorin, Averaging and renormalization for the Korteweg-deVries-Burgers equation., *Proc. Nat. Acad. Sci. USA* 100 (2003), pp. 9674-9679.

A. Chorin and P. Stinis, Problem reduction, renormalization, and memory. *Comm. Appl. Math. Comp. Sc.* 1 (2005), pp. 1-27.

A. Chorin and O. Hald, *Stochastic Tools for Mathematics and Science*. Springer-Verlag, New York (2005).

A. Chorin, O. Hald, and R. Kupferman, Prediction from partial data, renormalization, and averaging, *J. Sci. Comput.* (2006, in press).

J. Barber, Application of optimal prediction to molecular dynamics, PhD thesis, UC Berkeley, 2004, and submitted for publication.

D. Bernstein, Application of optimal prediction to the Burgers equation, *Mult. Scal. Mod. Sim.* (2006, in press)

P. Okunev, Application of optimal prediction to spin systems and to finance, PhD thesis, UC Berkeley, 2006.

O. Hald and P. Stinis, Computation of the decay rate of turbulence in two and three dimensions through optimal prediction, in preparation.

**For further information on this subject contact:**

Dr. Anil Deane, Program Manager  
Mathematical, Information, and Computational  
Sciences Division  
Office of Advanced Scientific Computing Research  
Phone: 301-555-3691  
Federal.M.Ployee@science.doe.gov

---

\* Telephone Number, E-mail address