

Constructive Methods of Invariant Manifolds for Kinetic Problems

Alexander N. Gorban^{1,2,3*}, Iliya V. Karlin^{1,2**},
and Andrei Yu. Zinovyev^{2,3***}

¹ ETH-Zentrum, Department of Materials, Institute of Polymers,
Sonneggstr. 3, ML J19, CH-8092 Zürich, Switzerland;

² Institute of Computational Modeling SB RAS,
Akademgorodok, Krasnoyarsk 660036, Russia;

³ Institut des Hautes Etudes Scientifiques,
Le Bois-Marie, 35, route de Chartres, F-91440, Bures-sur-Yvette, France

We present the Constructive Methods of Invariant Manifolds for model reduction in physical and chemical kinetics, developed during last two decades. The physical problem of reduced description is studied in a most general form as a problem of constructing the slow invariant manifold. The invariance conditions are formulated as the differential equation for a manifold immersed in the phase space (*the invariance equation*). The equation of motion for immersed manifolds is obtained (*the film extension of the dynamics*). Invariant manifolds are fixed points for this equation, and slow invariant manifolds are Lyapunov stable fixed points, thus *slowness is presented as stability*. A collection of methods for construction of slow invariant manifolds is presented, in particular, the Newton method subject to incomplete linearization is the analogue of *KAM methods for dissipative systems*. The systematic use of thermodynamics structures and of the quasi-chemical representation allow to construct approximations which are in concordance with physical restrictions. We systematically consider a discrete analogue of the slow (stable) positively invariant manifolds for dissipative systems, *invariant grids*. Dynamic and static *postprocessing procedures* give us the opportunity to estimate the accuracy of obtained approximations, and to improve this accuracy significantly.

The following examples of applications are presented: Nonperturbative deviation of physically consistent hydrodynamics from the Boltzmann equation and from the reversible dynamics, for Knudsen numbers $Kn \sim 1$; construction of the moment equations for nonequilibrium media and their dynamical correction (instead of extension of list of variables) to gain more accuracy in description of highly nonequilibrium flows; determination of molecules dimension (as diameters of equivalent hard spheres) from experimental viscosity data; invariant grids for a two-dimensional catalytic reaction and a four-dimensional oxidation reaction (six species, two balances); universal continuous media description of

*agorban@mat.ethz.ch, **ikarlin@mat.ethz.ch, ***zinovyev@ihes.fr

dilute polymeric solution; the limits of macroscopic description for polymer molecules, etc.

Keywords: Model Reduction; Invariant Manifold; Entropy; Kinetics; Boltzmann Equation; Fokker–Planck Equation; Postprocessing.

The full text is available online:

Preprint M03-50, Institut des Hautes études Scientifiques (IHES; France), Link:

<http://www.ihes.fr/PREPRINTS/M03/Resu/resu-M03-50.htm>

Preprint mp_arc 03-335, Link:

http://mpej.unige.ch/mp_arc/c/03/03-335.pdf

Home-links:

<http://agorban.fatal.ru/kinetics/pdf/cmimpro.pdf> or

http://owl.ethz.ch/d-werk/oettinger/MK_DIR/pag9/paper.pdf