Matrix Program

Conservation Laws, Boundary Value Problems, Interfaces and Mixing – Non-Equilibrium Processes at Continuous and at Kinetic Scales

04-08 November 2019

Creswick, Australia

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PROCEEDINGS

ABSTRACTS

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Matrix Program: Conservation laws, boundary value problems, interfaces and mixing – non-equilibrium processes at continuous and at kinetic scales

Edited by Snezhana I. Abarzhi

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Preface

This Program of the Matrix - Mathematical Research Institute is focused on the 'Conservation laws, boundary value problems, interfaces and mixing – non-equilibrium processes at continuous and at kinetic scales' at the.

Interfacial mixing and transport control a broad variety of phenomena in fluids, plasmas and materials, in nature and technology, over celestial to atomistic scales. Examples include supernovae and fusion, planetary convection and reactive fluids, wetting and adhesion, turbulence and turbulent mixing, nano-fabrication and bio-technology. Addressing the societal challenges posed by alternative energy sources, efficient use of non-renewable resources, purification of water and development of reliable diagnostics and therapeutics in medicine, requires a better understanding of non-equilibrium dynamics.

Interfacial transport and mixing are non-equilibrium processes coupling kinetic to macroscopic scales. Their dynamics often involve sharp changes of vector and scalar fields, and may also include strong accelerations and shocks, radiation transport and chemical reactions, diffusion of species and electric charges, among other effects. Interfacial transport and mixing are inhomogeneous, anisotropic, non-local, and statistically unsteady. At macroscopic scales, their spectral and invariant properties differ substantially from those of canonical turbulence. At atomistic and meso-scales, the non-equilibrium dynamics depart dramatically from the standard scenario given by Gibbs ensemble averages and the quasi-static Boltzmann equation. At the same time, non-equilibrium transport may lead to self-organization and order, thus offering new opportunities for diagnostics and control. Capturing properties of interfaces and mixing, enabling their accurate description and conservative properties, solving the boundary value problems - can aid better understanding of the fundamental of Eulerian and Lagrangian dynamics, and developing methods of control of non-equilibrium transport in nature and technology.

Significant success has been recently achieved in understanding of interfacial transport and mixing on the sides of theoretical analysis, large-scale numerical simulations, and data analysis. This success opens new opportunities for studies of fundamentals of non-equilibrium dynamics across the scales, and for developing a unified description of particles and fields on the basis of synergy of theory, numeric and data. This is the right moment to apply the fundamentals of non-equilibrium transport for addressing contemporary challenges of modern science, technology and society, including energy, environment and health care. Addressing these challenges requires the in–depth understanding of non-equilibrium dynamics and the strong interplay of ideas and approaches from interdisciplinary research.

The Program is focused on fundamental properties of interfacial transport and mixing that couples kinetic to macroscopic scales, and on conservation laws and boundary value problems. It will provide the unique opportunity to bring together mathematicians and scientists from applied mathematics, applied analysis, dynamical and complex systems, stochastic processes and data analysis, dynamics of fluid and plasmas, industrial mathematics and material science. The Program will motivate the discussions of rigorous mathematical problems, theoretical approaches and state-of-the-art numerical simulations along with advanced data analysis techniques. The participants include leading experts and researchers at experienced and early stages of their carriers from Australia and from abroad.

The Program is expected to explore and assess the state-of-the-art in the non-equilibrium transport, and to chart new directions of the interdisciplinary research for the future.

The Book of Abstracts includes 19 contributions. They are sorted alphabetically by the last name of the presenter.

You are cordially invited to take a look at this Book for information on the frontiers of theoretical, numerical and experimental research and state-of-the-art technology.

Welcome to the Matrix Program 'Conservation laws, Interfaces and Mixing'

S.I. Abarzhi

CONTENTS

CONSERVATION LAWS, BOUNDARY VALUE PROBLEMS, INTERFACES AND MIXING – NON-EQUILIBRIUM PROCESSES AT CONTINUOUS AND AT KINETIC SCALES

Presenter	Abarzhi SI
Affiliation	The University of Western Australia, AUS
Email	snezhana.abarzhi@gmail.com
Title	Interface dynamics: new mechanisms of stabilization and destabilization and structure of flow fields
Author(s)	Abarzhi SI
Affiliation(s)	The University of Western Australia, AUS
Abstract	Interfacial mixing and transport are nonequilibrium processes coupling kinetic to macroscopic scales. They occur in fluids, plasmas, and materials over celestial events to atoms. Grasping their fundamentals can advance a broad range of disciplines in science, mathematics, and engineering. This work focuses on the long-standing classic problem of stability of a phase boundary - a fluid interface that has a mass flow across it. We briefly review the recent advances and challenges in theoretical and experimental studies, develop the general theoretical framework directly linking the microscopic interfacial transport to the macroscopic flow fields, discover the new mechanisms of interface stabilization and destabilization that have not been discussed before for both inertial and accelerated dynamics, and chart perspectives for future research.

Presenter	Abarzhi SI
Affiliation	The University of Western Australia, AUS
Email	snezhana.abarzhi@gmail.com
Title	High energy density plasmas, fluid instabilities and interfacial mixing
Author(s)	Abarzhi SI
Affiliation(s)	The University of Western Australia, AUS
Abstract	Rayleigh-Taylor instability (RTI) and Rayleigh-Taylor (RT) mixing are common to occur in high energy density plasmas at astrophysical and at atomic scale. Examples include the RTI that quenches ignition in inertial confinement fusion; blast wave induced RT mixing in core-collapse supernova that creates conditions for synthesis of heavy mass elements; the RTI that governs material transformation of under impact in nano-electronics. By analyzing symmetries of RT dynamics in high energy density plasma and by focusing on certain patterns of variable acceleration, we discover a special class of self-similar solutions and identify their scaling, correlations and spectra. We find that dynamics of RT mixing can vary from super-ballistic to subdiffusive depending on the acceleration and retain memory of deterministic conditions for any acceleration. These rich dynamic properties considerably impact the understanding and control of RT relevant phenomena in high energy density plasmas. Particularly, they reveal the new mechanism for energy accumulation and transport at small scales in supernova, via energy localization and trapping.

Presenter	Agrawal T
Affiliation	The University of Melbourne, AUS
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Title	Estimation of mixing in a lock-exchange flow using molecular tagging velocimetry and thermometry
Author(s)	Agrawal T, Philip J, Klewicki J
Affiliation(s)	The University of Melbourne, AUS
Abstract	Gravity currents produced by a lock-exchange experiment are studied using the single-component version of molecular tagging velocimetry (MTV) in conjunction with its thermal counterpart, molecular tagging thermometry (MTT). The experiments are conducted in a Perspex tank of 2.0 m x 0.2 m x 0.2 m where the lock is located mid-way. Therefore, the current is studied only during the slumping phase and there are no transitions associated with the end-wall reflection. For these experiments, the initial density difference is created by introducing a thermal inhomogeneity on either side of the lock as compared to the general experimental practice of dissolving a salt on one side. The flow is first visualized by mixing a dye on the heavier side to establish the experimental parameters. Subsequently, MTV/MTT images are acquired that contain approximately 1000 data points distributed across the interface of hot and cold fluid. This high-resolution velocity and temperature data is then used to quantify the mixing being taken place at the interface. Specifically, background potential energy of the flow is evaluated over time to estimate the extent of irreversible mixing while an equivalent Thorpe scale is calculated to estimate the size of overturning eddies.

Presenter	Fukumoto Y
Affiliation	Kyushu University, Japan
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Title	Effect of compressibility in the reaction zone of a premixed flame and its implication to the Darrieus-Landau instability
Author(s)	Fukumoto Y
Affiliation(s)	Kyushu University, Japan
Abstract	The effect of compressibility on a premixed flame front is investigated by use of the method of M^2 expansions for small Mach numbers. We study the inner structure of the reaction layer, by applying the method of matched asymptotic expansions to an overall one-step irreversible chemical reaction expressed by the Arrhenius law. The temperature distribution is greatly influenced by the compressibility effect which originates from the material derivative of the pressure in the source term of the heat-conduction equation. This effect naturally embodies the volumetric heat loss, without having to include any artificial sink term, by decreasing the temperature, with the Mach number, on the burned side of the reaction zone, accompanied by the overshoot of the temperature in the midway of the reaction layer. An analysis of the burning-rate eigenvalue shows that the laminar flame speed can sensitively drops down by the compressibility effect. This implies that the compressibility acts to reduce the growth rate of the Darrieus-Landau instability. The relevance of our result to the Mallard-Le Le Chatelier theory is discussed.

Presenter	Hutchinson A
Affiliation	University of the Witwatersrand, ZA
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Title	Application of a modified Prandtl mixing length model to the turbulent classical far wake with a variable mainstream flow
Author(s)	Hutchinson A
Affiliation(s)	University of the Witwatersrand, ZA
Abstract	In this work, a modified Prandtl mixing length model that includes the kinematic viscosity is applied to the two-dimensional turbulent classical far wake with a variable mainstream flow. Mainstream flows that are constant, accelerating, and decelerating are examined and compared. Far downstream, the flow is divided into three interacting regions: the turbulent wake, the ideal slip-flow, and the mainstream flow. By integrating the momentum equation in the turbulent wake region over the width of the wake, and using the appropriate interface conditions, it is shown that the power is conserved. Lie point symmetry methods and conservation laws prove to provide a very powerful and robust method that allows for an expression for the mixing length to be obtained. The mixing length is shown to depend on the ideal slip-flow velocity just outside the wake boundary. Velocity profiles corresponding to constant, accelerating, and decelerating mainstream flows are plotted and compared. The effect of the mainstream flow on the expression obtained for the mixing length, the width of the wake, and the natural tendency of a wake to thicken with downstream distance is investigated.

Presenter	Hutchinson A
Affiliation	University of the Witwatersrand, ZA
Email	hutchinson.ash@gmail.com
Title	Comparison of algebraic closure models applied to the two-dimensional turbulent classical far wake
Author(s)	Hutchinson A
Affiliation(s)	University of the Witwatersrand, ZA
Abstract	The aim of this research is to compare the velocity profiles for the two-dimensional turbulent classical wake when various closure models are applied. Three closure models are considered. The first model, Prandtl's mixing length model, has been used extensively in turbulent wake flows. Despite the simplicity of this model, it contains mathematical and physical limitations. In particular, this model results in a poor estimate of the flow on the center-line and at the wake boundary. Prandtl constructed an improved model, which will be referred to as the revised mixing length model, in an attempt to address many of the inherent limitations of the original model. However, he was unable to fully resolve these limitations. One such problem involves the need to specify the form of the mixing length. It is shown that by using a modified version of Prandtl's mixing length model which includes the kinematic viscosity, an expression for the mixing length can be derived. Many of the other problematic mathematical and physical properties of the original models are addressed. In this work, the three models are compared. Similarity solutions that leave both the governing equations and the conserved quantity invariant are calculated. The governing partial differential equation is reduced to an ordinary differential equation. The ordinary differential equation cannot be solved analytically and thus a double-shooting method is developed to solve for the velocity of the flow.

Presenter	Khan AA
Affiliation	RMIT University, AUS
Email	kfamash@optusnet.com.au
Title	Determination of a transient shape of a sludge blanket in an anaerobic lagoon
Author(s)	Khan AA, Ding Y
Affiliation(s)	RMIT University, AUS
Abstract	In the Western Treatment Plant in Melbourne, as part of the waste processing in a settling lagoon of large size, a blanket of sludge settles under turbulent non-Newtonian manner under gravity. It leaves a clear layer on top which may be recycled. In this project we model the transient profiles of the sludge layer of various solid concentrations and examine the comparison with a real plant using a two dimensional computation fluid dynamic approach. The results are found to be useful in determination of the time taken to reach steady-state.

Presenter	Klewicki J
Affiliation	University of Melbourne, AUS
Email	klewicki@unimelb.edu.au
Title	Structure of passive scalar transport in turbulent channel flow
Author(s)	Klewicki J, Zhou a
Affiliation(s)	University of Melbourne, AUS
Abstract	Multi-scale analysis of the mean equation for passive scalar transport is used to investigate the asymptotic scaling structure of fully developed turbulent channel flow subjected to uniform heat generation. Unlike previous studies of channel flow heat transport with fixed surface temperature or constant inward surface flux, the present flow has a constant outward wall flux that accommodates for volumetrically uniform heat generation.This configuration has distinct advantages relative to precisely elucidating the underlying self-similar structure admitted by the analytical treatment of the mean transport equation.The present analyses are advanced using direct numerical simulations (Pirozzoli, Bernardini and Orlandi 2016 J.Fluid Mech., 788) that cover friction Reynolds numbers up to 4088 and Prandtl numbers ranging from 0.2 to 1.0. The leading balances of terms in the mean equation are determined empirically and then analytically described. Consistent with its asymptotic universality, the logarithmic mean temperature profile is shown analytically to arise as a similarity solution to the mean scalar equation, with this solution emerging on an interior domain where molecular diffusion effects become negligible. In addition to clarifying the Reynolds and Prandtl number influences on the von Karman constant for temperature, the present theory also provides a couple of self-consistent ways to estimate this constant. The reasons for the noted differences between the von Karman constant for velocity are clarified through comparative analysis of the transport equations for the scalar variance and streamwise velocity variance.

Presenter	Klimenko A
Affiliation	University of Queensland, AUS
Email	a.klimenko@uq.edu.au
Title	Entropy, mixing and the direction of time
Author(s)	Klimenko A
Affiliation(s)	University of Queensland, AUS
Abstract	This presentation reviews the understanding of the direction of time introduced by Hans Reichenbach and advanced by Stephen Hawking, including the fundamental relation of the perceived flow of time to the second law of thermodynamics (i.e. the Boltzmann time hypothesis), and the principle of parallelism of entropy increase. A general discussion is supplemented by an example of a mixing process with quantum effects, which points to the existence of a presently unknown mechanism that reflects global conditions prevailing in the universe and enacts the direction of time locally (i.e. the ”time primer”)

Presenter	Klimenko A
Affiliation	University of Queensland, AUS
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Title	Thermodynamics and kinetics of antisymmetric extension of the second law to
Author(s)	Klimenko A
Affiliation(s)	University of Queensland, AUS
Abstract	This is more detailed and specific presentation that explores implications of the Boltzmann time hypothesis: thermodynamics can be extended from matter to anitimatter in two possible mutually excluding ways: symmetric (which is conventionally implied in most publications) and antisymmetric. We explore implications of these differences including implications for kinetic equations, leading to two forms of the Pauli master equation, symmetric and antisymmetric (which correspond to symmetric and antisymmetric extensions of thermodynamics). Considering quantum mixing we show (by demanding consistency with the Einstein theory of radiation). that matter is always decohers, antimatter can either decohere or recohere, while radiation must stay decoherence-neutral.

Presenter	Li X
Affiliation	SUNY Stony Brook, USA
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Title	Lagrangian front tracking and applications to conservation law, fluid mixing, and phase transition problems
Author(s)	Li X
Affiliation(s)	SUNY Stony Brook, USA
Abstract	In this talk, I will review the history of the Lagrangian front tracking method and the computational platform built on this methodology. I will review the front tracking in the study of fluid interface instabilities, including Rayleigh-Taylor instability, Richtmyer Meshkov instability and fluid mixing induced by these instabilities. I will also introduce the fully conservative front tracking method and its application in the phase transition problem.

Presenter	Li X
Affiliation	SUNY Stony Brook, USA
Email	xiaolin.li@stonybrook.edu
Title	Modeling of fabric surface through front tracking with application to parachute inflation
Author(s)	Li X
Affiliation(s)	SUNY Stony Brook, USA
Abstract	In this talk, I will introduce a mesoscale dual-stress spring-mass model based on Rayleigh-Ritz analysis to mimic the fabric surface as an elastic membrane using the front tracking data and function structures. Our model is coupled with both incompressible and compressible fluid solvers through the immersed boundary and impulse method. We apply this method to the simulation of parachute inflation. I will discuss both the numerical and physical aspects of this project, including numerical stability, verification and validation study, porosity modeling, and coupling with turbulent flow in the simulation.

Presenter	Nepomnyashchy A
Affiliation	Technion - Israel Institute of Technology, Israel
Email	nepom@technion.ac.il
Title	Excitation and control of interfacial instabilities
Author(s)	Nepomnyashchy A
Affiliation(s)	Technion - Israel Institute of Technology, Israel
Abstract	Instabilities of interfaces between fluids are widespread in nature and engineering. It is not sufficient to describe the development of instabilities 'in a natural way'. One has to control the instabilities, i.e., either eliminate them or support definite patterns. We discuss different ways of control, including temporal modulation of parameters, spatial modulation of parameters, and feedback control.

Presenter	Nepomnyashchy A
Affiliation	Technion - Israel Institute of Technology, Israel
Email	nepom@technion.ac.il
Title	Longwave oscillatory instabilities
Author(s)	Nepomnyashchy A
Affiliation(s)	Technion - Israel Institute of Technology, Israel
Abstract	The longwave instabilities are inherent to a variety of systems in fluid dynamics, geophysics, electrodynamics, and biophysics. In many cases, the nonlinear development of instabilities is governed by the universal complex Ginzburg-Landau equation. However, that equation is not valid in the presence of a conservation law preventing the growth of spatially homogeneous disturbances. We present a basic classification of the types of instabilities and corresponding nonlinear amplitude equations. We consider a number of examples of longwave interfacial instabilities, among them waves in a viscous layer flowing on inclined plane and Marangoni waves in thin films. Different ways of instability control are discussed.

Presenter	Roberts A
Affiliation	The University of Adelaide, AUS
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Title	Rigorous modelling determines both a macroscale model and its boundary conditions
Author(s)	Roberts A
Affiliation(s)	The University of Adelaide, AUS
Abstract	A slowly-varying or thin-layer assumption empowers macroscale understanding of many physical scenarios from dispersion in pipes and rivers, including beams, shells, and the modulation of nonlinear waves, to homogenisation of micro-structures: here we explore cases when the microscale is highly heterogeneous. We rigorously analyse the dynamics local to each cross-section, expressed in the local moments of the microscale heterogeneity. Centre manifold theory supports the local modelling of the system's dynamics with coupling to neighbouring locales as a non-autonomous forcing. The union over all cross-sections then provides powerful new support for the existence and emergence of a macroscale model global in the large, finite-sized, domain. The approach quantifies the accuracy of known approximations, extends such approximations to mixed order modelling, and opens previously intractable issues to new insights. In particular, such models of spatio-temporal dynamics require boundary conditions at the edge of the spatial domain. We consider the evolution near boundaries of the macroscale domain of models such as the advection-diffusion PDE. By interchanging the roles of space and time, centre manifold theory resolves how boundary layers transition into the smooth interior solutions. This resolution then provides boundary conditions for such PDE models---albeit with complicated details. This generic approach forms a solid foundation for accurate macroscale boundary conditions.

Presenter	Sato M
Affiliation	Kyushu University, Japan
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Title	Effect of magnetic field on Darrieus-Landau instability of a flame front
Author(s)	Sato M, Fukumoto Y
Affiliation(s)	Kyushu University, Japan
Abstract	Combustions are phenomena commonly occurring not only on the earth but also on astrophysical objects. We explore the effect of magnetic field on the Darrieus-Landau instability (DLI), the linear instability of a planar front of a premixed flame, to pursue a possibility for suppressing the DLI. An externally imposed magnetic field is parallel to the flame front. We find that the magnetic field acts to reduce the growth rate of the DLI and even could suppress it when the wavenumber-vector of disturbance field is parallel and near-parallel to the external magnetic field, but that this is not the case for disturbances with their wavenumber-vectors perpendicular to the magnetic field. Although, for astrophysical plasmas, the value of the magnetic permeability is usually taken to be uniform, with the value of the vacuum, we take account of the discrepancy of their values between the unburned and the burned regions. We show that the discrepancy has a significant influence on the DLI, depending on paramagnetism or diamagnetism of the fuel material. For instance, the supernova is thought to be diamagnetic. In addition, the Markstein effect, the effect of front curvature on the laminar flame speed, is revisited, which may not have properly included in a previous investigation.

Presenter	Tanveer S
Affiliation	Technion - Israel Institute of Technology, Israel
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Title	Analysis of two fluid Couette flows
Author(s)	Tanveer S
Affiliation(s)	Ohio State University, USA
Abstract	We will be concerned with analysis and computations of a non-local thin film model developed in Kalogirou & Papageorgiou (J. Fluid Mech. 802, 5–36, 2016) for a perturbed two-layer Couette flow when the thickness of the more viscous fluid layer next to the stationary wall is small compared to the thickness of the less viscous fluid. Travelling wave solutions and their stability are determined numerically, and secondary bifurcation points are identified in the process. We also determine regions in parameter space where bistability is observed with two branches being linearly stable at the same time. The travelling wave solutions are mathematically justified through a quasi-solution analysis in a neighbourhood of an empirically constructed approximate solution. This relies in part on precise asymptotics of integrals of Airy functions for large wave numbers. The primary bifurcation about the trivial state is shown rigorously to be supercritical, and the dependence of bifurcation points, as a function of Reynolds number R and the primary wavelength 2 pi ν^(−1/2) of the disturbance, is determined analytically. We also discuss Hopf-bifurcation results.

Presenter	Williams K
Affiliations	The University of Western Australia, AUS
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Title	Mixing and dissipation processes in rotating stratified turbulence
Author(s)	Williams K. Hill DL, Abarzhi SI
Affiliation(s)	The University of Western Australia, AUS
Abstract	Rayleigh Taylor Instability is a fluid instability that develops when fluids of different densities are accelerated against their density gradient. Its applications include inertial confinement fusion, supernovae explosion, fossil fuel extraction and nano fabrication. We study Rayleigh-Taylor instability developing at the interface with a spatially periodic perturbation under a time varying acceleration using group theoretic methods. For the first time, to our knowledge, both regular and singular nonlinear solutions are found, which correspond to the structure of bubbles and spikes emerging at the interface. We find that the dynamics of bubbles is regular, and the dynamics of spikes is singular, and the singularity is a nite time. The parameters affecting the behaviour of both bubble and spikes are discussed, including the inter-facial shear, which is shown to have a profound effect. The applications of these findings in benchmarking numerical simulations and experiment design are also discussed.

Presenter	Wright C
Affiliation	The University of Western Australia, AUS
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Title	Shock-driven instabilities in convergent geometry
Author(s)	Wright C, Abarzhi SI
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Abstract	Richtmyer-Meshkov Instability (RMI) is an instability that develops in the interface between fluids of distinct values of the acoustic impedance when impacted by a shock wave. Its applications include inertial confinement fusion, supernovae explosions, and the evolution of blast waves. We systematically study the effect of the adiabatic index of the fluids on the dynamics of strong-shock driven flows, particularly the amount of shock energy available for interfacial mixing. Only limited information is currently available about the dynamic properties of matter at these extreme regimes. Smooth Particle Hydrodynamics simulations are employed to ensure accurate shock capturing and interface tracking. A range of adiabatic indexes is considered, approaching limits which, to the best of the author's knowledge, have never been considered before. We analyse the effect of the adiabatic indexes on the interface speed, interface morphology, and on the perturbed interface amplitude immediately after the shock passage. The simulation results are compared, wherever possible, with rigorous theories and with experiments, achieving good quantitative and qualitative agreement. We find that the more challenging cases for simulations arise where the adiabatic indexes are further apart, and that the initial growth rate is a non-monotone function of the initial per-turbation amplitude, which holds across all adiabatic indexes of the fluids considered. We also observe and quantify the flattening of the interface. The applications of these findings on experiment design are discussed.

NOTES