Turbulent Mixing and Beyond

Second International Conference and

Advanced School

ROUND TABLES

27 July - 7 August, 2009

The Abdus Salam International Centre for

Theoretical Physics

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Organizing Committee

- Snezhana I. Abarzhi (chairperson, University of Chicago, USA)
- Malcolm J. Andrews (Los Alamos National Laboratory, USA)
- Sergei I. Anisimov (Landau Institute for Theoretical Physics, Russia)
- Hiroshi Azechi (Institute for Laser Engineering, Osaka, Japan)
- Serge Gauthier (Commissariat à l'Energie Atomique, France)
- Christopher J. Keane (Lawrence Livermore National Laboratory, USA)
- Robert Rosner (Argonne National Laboratory, USA)
- Katepalli R. Sreenivasan (International Centre for Theoretical Physics, Italy)
- Alexander L. Velikovich (Naval Research Laboratory, USA)

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- Photron (Europe) Ltd., UK

Local Organizers at ICTP

- Joseph J. Niemela
- Katepalli R. Sreenivasan

Participants of Round Tables

Round Tables have been held in Oppenheimer Room at the Abdus Salam International Center for Theoretical Physics, Trieste, Italy on 30 July 2009 and 06 August 2009.
Round Table I united 30 participants, and Round Table II united 25 participants.

- Abarzhi, Snezhana I. (moderator, University of Chicago, USA)
- Andrews, Malcolm (Los Alamos National Laboratory, USA)
- Belotserkovskii, Oleg (Inst. Computer Aided Design of Academy of Sciences, Russia)
- Bershadskii, Alexander (ICAR, Israel)
- Brandenburg, Axel (Nordita, Denmark)
- Chumakov, Sergei (Stanford University, USA)
- Desai, Tara (University of Milano-Bicocca, Italy)
- Galperin, Boris (University of South Florida, USA)
- Gauthier, Serge (Commissariat à l'Energie Atomique, France)
- Gekelman, Walter (University of California - Los Angeles, USA)
- Gibson, Carl (University of California - San Diego, USA)
- Goddard III, William A. (California Institute of Technology, USA)
- Grinstein, Fernando (Los Alamos National Laboratory, USA)
- Gupta, Anupam (Indian Institute of Science, India)
- Hazak, Giora (Nuclear Research Center -Negev, Israel)
- Jayakumar, J. S. (Bhabha Atomic Research Centre, India)
- Kaneda, Yukio (Nagoya University, Japan)
- Klimenko, Alexander Y. (University of Queensland, Australia)
- Krommes, John A. (Princeton University, USA)
- Lvov, Victor (Weizmann Institute of Science, Israel)
- Meshram, Mayoordhwaj (Rashtrasant Tukadoji Maharaj Nagpur University, India)
- Minnini, Pablo (University of Buenos Aires, Argentina)
- Mukund, Vasudevan (Jawaharlal Nehru Centre for Adv Scientific Research, India)
- Nadiga, Balu (Los Alamos National Laboratory, USA)
- Nepomnyaschy, Alexander (Technion, Israel)
- Niemela, Joseph J. (International Centre for Theoretical Physics, Trieste, Italy)
- Nishihara, Katsunobu (Institute for Laser Engineering, Osaka University, Japan)
- Orlov, Sergei S. (Stanford University, USA)
- Petrosyan, Arakel (Space Research Institute of the Academy of Sciences, Russia)
- Pouquet, Annick (National Center for Atmospheric Research, USA)
- Procaccia, Itamar (Weizmann Institute of Science, Israel)
- Pudritz, Ralph E. (McMaster University, Canada)
- Pullin, Dale (California Institute of Technology, Israel)
- Sreenivasan, Katepalli R. (Int. Centre for Theoretical Physics, Trieste, Italy)
- Sukoriansky, Semion (Ben-Gurion University of the Negev, Israel)
- Thornber, B (Cranfield University, UK)
- van Duin, Adri (Pennsylvania State University, USA)
- Velikovich, Alexander (Naval Research Laboratory, USA)
- Williams, Robin (Atomic Weapons Establishment, UK)
- Youngs, David L. (Atomic Weapons Establishment, UK)
- Zweibel, Ellen (University of Wisconsin - Madison, USA)

Scope of Themes

- **Canonical turbulence and turbulent mixing:**

invariant, scaling, spectral properties, scalar transports, convection

- **Wall-bounded flows:**

structure and fundamentals, non-canonical turbulent boundary layers, including unsteady, transitional flows, supersonic & hypersonic flows, shock-boundary layer interactions

- **Non-equilibrium processes:**

unsteady, multiphase and shock-driven turbulent flows, anisotropic non-local dynamics, connection of continuous description at macro-scales to kinetic processes at atomistic scales

- **Interfacial dynamics:**

instabilities of Rayleigh-Taylor, Kelvin-Helmholtz, Richtmyer-Meshkov, Landau-Darrieus, Saffman-Taylor

- **High energy density physics:**

inertial confinement and heavy-ion fusion, Z-pinches, light-matter and laser-plasma interactions, non-equilibrium heat transfer

- **Material science:**

material transformation under high strain rates, equation of state, impact dynamics, mixing at nano- and micro-scales

- **Astrophysics:**

supernovae, interstellar medium, star formation, stellar interiors, early Universe, cosmic-microwave background, accretion disks

- **Magneto-hydrodynamics:**

magnetic fusion and magnetically confined plasmas, magneto-convection, magneto-rotational instability, dynamo

- **Canonical plasmas:**

coupled plasmas, anomalous resistance, ionosphere

- **Physics of atmosphere:**

environmental fluid dynamics, weather forecasting, turbulent flows in stratified media and atmosphere, non-Boussinesq convection

- **Geophysics and Earth science:**

mantle-lithosphere tectonics, oceanography, turbulent convection under rotation, planetary interiors

- **Combustion:**

dynamics of flames and fires, deflagration-to-detonation transition, blast waves and explosions, flows with chemical reactions, flows in jet engines

- **Mathematical aspects of non-equilibrium dynamics:**

vortex dynamics, singularities, discontinuities, asymptotic dynamics, weak solutions, well- and ill-posedness, continuous transports out of thermodynamic equilibrium

- **Stochastic processes and probabilistic description:**

long-tail distributions and anomalous diffusion, data assimilation and processing methodologies, error estimate and uncertainty quantification, statistically unsteady processes

- **Advanced numerical simulations:**

continuous DNS/LES/RANS, Molecular dynamics, Monte-Carlo, predictive modeling, validation and verification of numerical models

- **Experimental diagnostics:**

model experiments in high energy density and low energy density regimes, plasma diagnostics, fluid flow visualizations and control, opto-fluidics, novel optical methods, holography, advanced technologies

- **High-performance computing and cyber-infrastructure:**

cyber-infrastructures, data annotation, visualization, storage and transfer, grid computing and high-performance computing systems, next-generation cyber-tools

Key issues suggested for discussion at the Round Tables

Based of survey and suggestions of invited speakers and lecturers and members of the Scientific Advisory Committee of the 2nd International Conference and Advanced School "Turbulent Mixing and Beyond," Round Tables were focused on the following key issues:

- What are "canonical" and "non-canonical" (non-equilibrium) turbulent flows, including similarity and distinctions and connections of TMB-related problems to problems in other well-established fields?
- What are the model scientific problems [deep enough and specific enough] to be considered and to be useful in a wide variety of TMB-related themes?
- What are the quantitative criteria for the estimate of the quality and information capacity of experimental and numerical data sets and for evaluation of predictive capabilities of theories and models?
- What cyber-infrastructure is required for TMB community, including collaborative computing environment and opportunities offered by modern technologies for data sharing, annotation, transfer, analysis, visualization?

Within the framework of these issues, the following specific topics questions have been discussed by the participants.

Outline of discussions held at the Round Tables

- **For canonical (local, isotropic and homogeneous) turbulent flows corrections to Kolmogorov theory are essential to account for**.

Upon intense discussions, participants of the Round Table have agreed that it is still unclear if canonical Kolmogorov turbulence is an observable physical phenomenon or a mathematical model. Several definitions of canonical turbulence have been considered. It was noticed that in a vast variety of realistic problems (under high and low energy density conditions, from micro- to astrophysical scales) the flow conditions depart from the assumptions of Kolmogorov theory. It is uncertain whether these distinctions can be completely accounted for with some corrections to Kolmogorov theory, whether these corrections are "continuous" or "discontinuous", and what is their quantitative influence on the values of observables in a given parameter regime. In experiments on canonical turbulence the conditions of isotropy, locality and homogeneity are hard to achieve. Numerical simulations open exciting avenues for accurate studies of fundamental theoretical issues provided there is a substantial accuracy and dynamic range (i.e. required computations of peta-scale and higher level).

- **Realistic turbulent processes depart from classical scenarios.**

Upon intense discussions, participants of the Round Table have agreed that realistic turbulent processes are characterized by non-equilibrium heat and mass transports, sharp gradients of pressure and density, and may be subject to spatially varying and time-dependent acceleration and rotation and shocks. Their sensitivity to details and transient character of the dynamics impose constraints on the accuracy and spatio-temporal resolution of the measurements of the flow quantities as well as on data acquisition rate. It has been emphasized that theoretical, experimental and numerical descriptions of non-equilibrium turbulent processes require innovative approaches going well beyond classical statistically steady considerations.

- **TMB-related problems, from atomistic to astrophysical scales, under high and low energy density conditions, have in common a set of outstanding scientific problems. Their solution has a potential to provide paradigm-shifting advances in a variety of disciplines in science, technology and mathematics.**

Participants of Round Table have discussed at length a set of characteristic problems that would be deep enough and specific enough to represent a variety of TMB themes. Among others, examples included hydrodynamic instabilities [Kelvin-Helmholtz, Rayleigh-Taylor, Richtmyer-Meshkov, Landau-Darrieus, Magneto-Rotational, etc, in plasmas, fluids and astrophysics]; interactions of eddies and structures with waves and relation between discrete and continuous spectra [especially for astrophysical and geophysical flows and atmosphere]; dynamics of plasmas and magneto-hydrodynamics [high and low energy density conditions]; connection of kinetic processes to dynamics of continuous media under non-equilibrium conditions [from atomistic to macro scales beyond the limits of quasi-static Boltzmann equation with emphasis on reactive flows and material science] and Lagrangian versus Eulerian descriptions [flow-particle interactions, environmental problems]; flows in unsteady and multi-phase flows in aeronautics and aerodynamics [non-canonical boundary layers, hypersonic and supersonic flows]; and mathematical aspects [modeling of statistically unsteady processes, partial differential equations with discontinuities]. Participants of Round Table have emphasized a necessity to focus on the quality of research and to maintain the information flux in TMB community

- **Connection between experiments and simulations has been discussed at length.**

Participants of Round Table have discussed qualitative differences between experimental and numerical data sets. Experimental data are more informative about physical processes, whereas simulations only sample from a model requiring validation. At the same time, simulations can track all of the predetermined field quantities, and experiments can only measure some. Participants of Round Tables have noticed that experiments and simulations complement one another in research process. Substantial part of modern era discoveries is provided by experiments, including "qualitative" (exploration of novel parameter regimes) and "quantitative" experiments (enhancements in diagnostics) and the state of the art experimental capabilities in plasmas, optics, astrophysics and technologies. Advances in numerical simulations (peta-scale level and higher) enabled studies of phenomena previously inaccessible for research (for instance, in astrophysics, geophysics, combustion and material science) and provided community with invaluable expertise on how to operate, process, analyze and interpret massive data sets as well as with opportunities to test theoretical hypotheses and explore parameter regimes. It has been emphasized a necessity to share across the disciplines the information on novel experimental and computational approaches, and on data visualization and data processing methodologies.

- **Further development and organization of TMB community is required.**

Participants have agreed that further development of TMB community is in demand. They have emphasized that collaboration effort is required to achieve success in solution of the highly fascinating problem of non-equilibrium dynamics. The strong sides of TMB community are that it is interdisciplinary and international, it is focused on high quality fundamental research and may provide an impact on technology (from nuclear fusion to optical telecommunications). Participants have requested the Organizing Committee to contact National Academies of Sciences (USA, Russia, Japan, Canada, Australia, European

Union and India) and national funding agencies with an inquiry to launch a decade of study. Two suggestions have been made: 1) identify what might be a single representative problem "attractive to mankind" (TMB "black hole") and, more importantly, 2) outline what TMB community, that has already demonstrated high quality results and strong potential for innovative research, can suggest to scientific community in broad sense and "mankind." The Organizing Committee has also been requested to launch and develop collaborative computing environment for sharing data and methods of their analysis in TMB community. The goal of the environment is provide an infrastructure and serve for elaboration of quantitative criteria for the estimates of the quality and information capacity of experimental and numerical data sets and for evaluation of predictive capabilities of theories and models.

Specific important aspects for TMB-related problems

- **Numerical simulations:**

- It has been emphasized that one of important directions for future numerical simulations is the development of the sub-grid-scale models that not only accommodate assumptions of canonical approaches but also reflects most recent advances in theory, rigorous mathematical description and experimental studies of fundamental properties of non-equilibrium turbulent dynamics. Proper sub-grid-scale models may help to capture the coupling of multi-scale and multi-physics processes in a system with a proper level of coarseness (i.e. quantities measured on coarse and fine grids).
- It has been outlined a necessity to performing a "hero" direct numerical simulation, governed by advanced theory, of the Rayleigh-Taylor instability for a variety of Schmidt numbers as well as that f the Richtmyer-Meshkov instability.

- **Experiments:**

- The role of experiments in modern day research has been discussed in depth. Role of experiments is seen by participants in (1) exploration of new parameter regimes and in (2) advancements of diagnostics. It has been mentioned that in a carefully designed experiment detailed space-time measurements of a number of quantities (flow, magnetic fields, currents, etc.) now are possible and thus enabling and encouraging direct collaboration between experimental, simulations and theory.
- Regarding diagnostic approaches, a necessity to develop methods capable of monitoring "fields" (currently - linear tracers or snapshot images) have be strengthened.

- **Theory and fundamentals:**

- It has been discussed a necessity to understand connection of continuous dynamics to transport processes at atomistic and molecular scales under conditions of non-equilibrium. Participants have agreed that understanding limitations of Navier-Stokes and Euler equations and Physical Kinetics as well as comprehension of links between these descriptions are missing crucial points requiring intense research.
- A set of important problems have been outlined by participants and a necessity to further interact with the community regarding these problems has been emphasized. The problem of shock-turbulence interactions has been added to the list of problems discussed earlier (i.e. rotation, eddies and waves, MHD, astrophysical applications, Rayleigh-Taylor instabilities, etc)

- **Data to Knowledge:**

- An important issue raised was that how the problems that we are dealing with can be useful to other fields and communities. The development and sharing of research tools and TMB extensive expertise was considered by participants as a required part of research.
- Participants of Round Table agreed that for non-equilibrium processes, complexity and simplicity are "mixed" due to their non-locality and statistical unsteadiness. Participants have emphasized a necessity to strengthen collaborations between experiments, simulations and theories and to augment these collaborations with modern approaches in statistics, stochastic processes and data analysis.
- Participants have noticed that TMB community has proven record of first-rate expertise in solving formidable and long-standing scientific problems. Participants have discussed at length on how to turn this expertise in educational programs for graduate and professional education in science, mathematics and technology, and in other community outreach programs.

Action Items for Organizing Committee

Participants of Round Tables have agreed on the following action items.

- Non-canonical turbulent processes are most representative processes in natural and artificial systems. These processes are characterized by non-equilibrium heat and mass transports, strong gradients of pressure and density, subjected to acceleration and rotation and are statistically unsteady. These flows are crucial to study in order to understand and extend the range of applicability of traditional statistically steady approaches, and to capture essentials of a wide range of phenomena from atomistic to astrophysical scales, under both high and low energy density conditions.
- In close interaction with participants of TMB-2007 and TMB-2009, the Organizing Committee is kindly requested to finalize a list of a few [1-3-5] representative problems [deep enough and specific enough] to consider [for the proposal submission] and to be useful for a variety of TMB-related themes.
- It is recommended for the Organizing Committee to organize a collaborative computing environment to maintain the information flux in the community, to share research tools, methodologies and data, including application of modern computational approaches for data sharing, annotation, transfer, analysis, and visualization. The goal of the environment is provide an infrastructure and to serve for elaboration of quantitative criteria for the estimate of quality and information capacity of experimental and numerical data sets and for the evaluation of predictive capabilities of theories and models.
- Members of the Organizing Committee are recommended to contact funding agencies with a pre-proposal (white paper) for the community project and national academies of sciences with a proposal to launching a decade of study of non-equilibrium turbulent processes.