AmeriMech Symposium

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Interfaces and Mixing

Non-Equilibrium Transport Across the Scales

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AmeriMech Symposium

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Non-Equilibrium Tramsport Across the Scales

PROCEEDINGS

ABSTRACTS

18 - 19 November, 2017

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Abstracts of the Proceedings of the

AmeriMech Symposium

'Interfaces and Mixing – Non-Equlibrium Trasport Across the Scales'

18-19 November 2017; Denver, USA

Edited by Snezhana I. Abarzhi

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Preface

Interfacial mixing and transport control a broad variety of phenomena in fluids and materials, in nature and technology, over celestial to atomistic scales. Examples include fusion and supernovae, planetary convection and reactive and super-critical fluids, material transformation under impact, colloidal assembly, wetting and adhesion, and turbulence and turbulent mixing. 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 meso- and 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 flow diagnostics and control. Capturing properties of interfaces and mixing 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, laboratory experiments, and technology development. 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 experiment, theory and numerics. 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. Alternative energy sources, efficient use of non-renewable resources, purification of water and development of reliable diagnostics and therapeutics in medicine - addressing these challenges requires the in–depth understanding of non-equilibrium dynamics, and the strong interplay of ideas and approaches from the interdisciplinary areas of research.

The symposium is focused on mechanics and hydrodynamic aspects of interfacial transport and mixing that couples kinetic to macroscopic scales. It provides the opportunity to bring together

scientists from different areas of fluid dynamics, applied mathematics, statistics, chemistry and material science. The symposium is structured to encourage participants' interactions with experts from various fields to motivate the discussions of rigorous mathematical issues, theoretical approaches and state-of-the-art numerical simulations along with advanced experimental techniques and technological applications. Participants include experts and researchers at experienced and early stages of their careers from academia, national laboratories and industry, from national and international communities. The organizers expect the symposium 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 AmeriMech 'Interfaces and Mixing'

S.I. Abarzhi

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INTERFACES and MIXING – NON-EQUILIBRIUM TRANPOSRT ACROSS the SCALES

Presenter	Abarzhi SI
Affiliation	The University of Western Australia, AU
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Title	Stability of an accelerated hydrodynamic discontinuity
Author(s)	Ilyin DV (1); Fukumoto Y (2); Goddard III, WA (1); Abarzhi SI (3)
Affiliation(s)	California Institute of Technology, USA (1); Kyushu University, Japan (2); The University of Western Australia, Australia (3)
Abstract	While looking from a far field at the accelerated interface separating ideal fluids of different densities, we identify, for the first time to our knowledge, a new type of hydrodynamic instability that develops when the acceleration magnitude exceeds a critical value. The flow dynamics conserves the fluxes of mass, momentum and energy at the interface, has potential velocity fields in the fluid bulk, and is shear-free at the interface. The growth rate and the flow fields' structure of this unstable dynamics depart substantially from those of other interfacial hydrodynamic instabilities, thus suggesting new opportunities for stabilization, diagnostics, and control of the interfacial dynamics.
Supported by	The National Science Foundation, USA

Presenter	Adams NA
Affiliation	Technical University of Munich, Germany
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Title	Droplet breakup as multi-scale computing challenge
Author(s)	Adami S; Paula T; Hoppe N; Adams NA
Affiliation(s)	Technical University of Munich, Germany
Abstract	Improvements in numerical model development for multi-physics problems have enabled the research in fluid mechanics nowadays to consider very complex problems by high-performance computation. Such problems are characterized by nonlinear mechanisms that generate multiple temporal and spatial scales. Whereas turbulence is a broad-band phenomenon whose largest scales are determined by flow boundaries and exterior forcing, and whose smallest scales are determined by viscous dissipation length scales, singularities such as shocks and interfaces do not possess inherent length and time scales if considered in a continuum description. They generate small scales by instabilities, driven through their mutual interaction, and interact with broad-band flow structures, creating a scenario which is extremely complex for numerical flow modeling: high-resolution requirement of broad-band scales and instabilities, monotonic capturing of shocks and interface, tracking of interfaces without artificial diffusion and mass loss. In the talk we will discuss recent approaches towards efficient models and algorithms for sharp-interface representation that allow to en-force critical properties of the numerical discretization without compromising efficient computing strategies. Application scenario is the violent breakup of a water droplet driven by x-ray energy deposition. Consistent and conservative interface interaction is crucial for capturing the fast dynamics. For this purpose, a sharp interface-interaction model including phase change is proposed. Strategies for multi-resolution and efficient parallelization will be presented. Physical phenomena of the particular type of droplet breakup will be discussed.
Supported by	European Research Council Advanced Grant NANOSHOCK, EU

Presenter	W. David Arnett
Affiliation	University of Arizona, USA
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Title	Stellar evolution and turbulent mixing
Author(s)	Arnett WD, Meakin CA
Affiliation(s)	University of Arizona, USA
Abstract	Fully three-dimensional simulations of fluid flow in stars, with sufficient resolution to be fully turbulent, now allow far more realistic study of mixing processes, boundary layers, entrainment, and instabilities than previously possible (although von Neumann anticipated this novel use of computers). We will explore surprises and connections to related areas of physical science: solar physics, inertial confinement fusion, synthesis of the elements, and supernova observations.
Supported by	

Presenter	Danaila L
Affiliation	The University of Rouen, France
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Title	Generalized high-order scalar structure functions for decaying turbulence with mean scalar gradient
Author(s)	Danaila L; Gauding M
Affiliation(s)	University of Rouen, France
Abstract	Homogeneous isotropic decaying turbulence with a constant mean scalar gradient is studied from a self-preservation perspective by means of highly resolved direct numerical simulations (DNS). The analysis is based on a hierarchy of scale-by-scale budget equations for higher-order moments of the scalar increment. These equations involve a balance between unsteady effects, turbulent and molecular interscale transport, and production due to the mean gradient. Functional forms of these terms are introduced to study the conditions under which self-preservation can be satisfied. This approach provides a systematical framework for the analysis of self-preservation and the derivation of self-similarity scales. It is shown from DNS that self-preservation is only possible over a limited range of scales, depending on the choice of the similarity scales. The concept of similarity scales is extended to higher-order moments, by using analytical solutions of the scale-by-scale budget equations. Moreover, the effect of the imposed scalar mean gradient on the self-preservation is studied. The imposed mean gradient injects energy at the large scales and induces an anisotropy. The DNS reveals that the scalar mean gradient breaks self-preservation at the large scales.
Supported by	Labex EMC3, EU

Presenter	Dell ZR
Affiliation	Carnegie Mellon University, USA
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Title	Maximum initial growth-rate of strong-shock-driven Richtmyer-Meshkov instability
Author(s)	Dell ZR (1,2); Pandian A (1); Bhowmick AK (1); Swisher NC (1); Stanic M (3); Stellingwerf RF (4); Abarzhi SI (1,5)
Affiliation(s)	Carnegie Mellon University, USA (1); The Ohio State University, USA (2); FluiDyna GmbH, Germany (3); Stellingwerf Consulting, USA (4); The University of Western Australia, AU (1,5)
Abstract	We focus on classical problem of dependence on the initial conditions of the initial growth-rate of strong shocks driven Richtmyer-Meshkov instability (RMI) by developing a novel empirical model and by employing rigorous theories and Smoothed Particle Hydrodynamics (SPH) simulations to describe the simulations data with statistical confidence in a broad parameter regime. For given values of the shock strength, fluids' density ratio, and wavelength of the initial perturbation of the fluid interface, we find the maximum value of RMI initial growth-rate, the corresponding amplitude scale of the initial perturbation, and the maximum fraction of interfacial energy. This amplitude scale is independent of the shock strength and density ratio, and is characteristic quantity of RMI dynamics. We discover the exponential decay of the ratio of the initial and linear growth-rates of RMI with the initial perturbation amplitude that excellently agrees with available data.
Supported by	The National Science Foundation, USA

Presenter	Goddard III WA
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Title	Complete reaction dynamics of complex chemical reactions: a machine learning grand challenge
Author(s)	Ilyin DV; Goddard III WA
Affiliation(s)	California Institute of Technology, USA
Abstract	We want to describe the reactions (products and rates) for the chemical processes involved in combustion, pyrolysis, and shock detonation. That is, we want to determine the rates at which various reactants and intermediates react and the products that they generate along with the energy released and the changes in temperature and pressure. Except for very simple dilute systems at low temperature experimental methods cannot generally provide the necessary information. Quantum mechanics (QM) can in principle describe the reaction processes, but they are limited to small systems (100s of atoms) and short times (10s of picoseconds), and the standard DFT methods have trouble describing bond breaking processes. An alternative is the ReaxFF reactive force field which can descriptions bond breaking/formation processes nearly as accurately as QM but can handle millions of atoms for 100s of nanoseconds. Here it is possible to catalog every reaction by observing when a new product occurs and tracing backward in time to determine which reactants lead to this product and their internal energies. But this leads to a big data problem of having the computer recognize these events while disentangling the multiple events and distinguishing true reactions from ephemeral complexes that form but do not react. We report here a general computational framework (Bimolecular Extracted Reaction Networks, BERN) for analysis of reaction dynamics of complex chemical systems that we apply here to the simple case of pyrolysis of hydrogen peroxide, HOOH. We find that there are only two important intermediates, HO, and HO2 and only two important products, O2 and H2O, although there are other long lived (100s of femtoseconds) intermediates. The net result is a set of two body reaction rates that are written in the Arrhenius form Rate(A+B→C+D) = P(A)P(B)(kT/h)exp[-δG(A,B,C,D, p, T)/kT], which we show reproduces the complex chemistries calculated. Analyzing these rates in terms standard quantities such as activation enthalpy and entropy, we find that the presence of vibrational and rotational energy in the reactants leads to systematic changes in the quantities that would be derived from simple adiabatic reaction pathways using QM and ReaxFF. The BERN computational framework is scalable and capable of application to complex combustion, pyrolysis, and detonation conditions.
Supported by	

Presenter	Grinstein FF
Affiliation	Los Alamos National Laboratory, USA
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Title	Coarse grained simulation and turbulent mixing predictability
Author(s)	Grinstein FF
Affiliation(s)	Los Alamos National Laboratory, USA
Abstract	Turbulent flow conditions cannot be reproduced with single laboratory or computational experiments, nor can they be fully simulated from first principles, and the impact of this inherent under-resolution on predictability of observable integral mixing consequences must be addressed. In coarse grained simulation (CGS) [1] – including classical and implicit large-eddy simulation, small-scales are presumed enslaved to the dynamics of the largest, and the spectral cascade rate of energy (the rate limiting step) is determined by the initial and boundary condition constrained large-scale dynamics. Beyond the complex multi-scale resolution difficulties of equilibrium turbulence, we must also address the challenging issues of unsteady non-equilibrium transitions dependent on initial conditions (IC). CGS predictability is examined for under-resolved mixing driven by under-resolved velocity fields, and then also in conjunction with under-resolved IC. We revisit evidence for small-scale enslavement of high Reynolds-number (Re) scalar mixing in isotropic forced turbulence and material mixing in shock-tube experiments. Turbulence metrics are used to show that a well-designed CGS can accurately capture the mixing transition and high-Re self-similar asymptotic behaviors, when suitable sub-grid scale realizability constraints are effectively built into the scalar mixing modeling. Robust CGS for dissipative turbulent phenomena can be achieved with large enough scale separation and well-resolved IC. However, late-time predictability for high-Re phenomena cannot be robust when coarse-grained (computational and laboratory) observations are constrained by characterization and modeling of their IC specifics. [1] F.F. Grinstein, Coarse Grained Simulation and Turbulent Mixing, Cambridge, 2016
Supported by	

Presenter	Haller G
Affiliation	ETH Zürich, Switzerland
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Title	Barriers and enhancers to diffusive and stochastic transport
Author(s)	Haller G; Karrasch D; Kogelbauer F
Affiliation(s)	ETH Zürich, Switzerland (1); Technische Universität München, Germany (2)
Abstract	We seek transport barriers and transport enhancers in a general, unsteady flow as material surfaces across which the transport of diffusive tracers is minimal and maximal, respectively. We find that such surfaces are extremizers of a universal, non-dimensional transport functional whose leading-order term can be computed directly from the flow velocity without diffusive simulations, as long as the diffusivity is small. This result extends to stochastic velocity fields and hence enables transport barrier and enhancer detection under uncertainties.
Supported by	Turbulent Superstructures priority program of the German National Science Foundation (DFG), Germany.

Presenter	Ilyin DV
Affiliation	California Institute of Technology, USA
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Title	Stability and fields' structure in a flow with a hydrodynamic discontinuity
Author(s)	Ilyin DV (1); Fukumoto Y (2); Goddard III, WA (1); Abarzhi SI (3)
Affiliation(s)	California Institute of Technology, USA (1); Kyushu University, Japan (2); The University of Western Australia, Australia (3)
Abstract	We consider from a far field the evolution of a hydrodynamic discontinuity separating incompressible ideal fluids of different densities, with mass flow across this interface. By solving the boundary value problem and finding fundamental solutions of linearized dynamics, we directly link interface stability to structure of the flow fields. We find that the classic Landau system of equations for the Landau-Darrieus instability has a degenerate and singular character. Eliminating this degeneracy leads to appearance of a neutrally stable solution whose vortical field can seed the instability. We further find that the interface is stable if the flux of energy fluctuations produced by the perturbed interface is small compared to the flux of specific kinetic energy across the planar interface. The interface is unstable if the energy fluctuations flux is large compared to the kinetic energy flux. Landau's solution is consistent with the latter case.
Supported by	The National Science Foundation, USA

Presenter	Kais S
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Title	The coherence lifetime-borrowing effect in vibronically coupled molecular aggregates under non-perturbative system-environment interactions
Author(s)	Yeh S-H (1,2); Hoehnb RD (2); Engel GS (1); Kais S (2,3)
Affiliation(s)	The University of Chicago, USA (1); Purdue University, USA (2); Hamad Bin Khalifa University, Qatar (3)
Abstract	Recently it has been suggested that the long-lived coherences in some photosynthetic pigment-protein systems, such as the FennaMatthews-Olson complex, could be attributed to the mixing of the pigments' electronic and vibrational degrees of freedom. In order to verify whether this is the case and to understand its underlying mechanism, a theoretical model capable of including both the electronic excitations and intramolecular vibrational modes of the pigments is necessary. Our model simultaneously considers the electronic and vibrational degrees of freedom, treating the system environment interactions non-perturbatively by implementing the hierarchical equations of motion approach. Here we report the simulated two-dimensional electronic spectra of vibronically coupled molecular dimers to demonstrate how the electronic coherence lifetimes can be extended by borrowing the lifetime from the vibrational coherences
Supported by	Qatar National Research Foundation, Qatar

Presenter	Mahalov A
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Title	Local ensemble transform Kalman filter for ionospheric data assimilation: observation influence analysis during a geomagnetic storm event
Author(s)	Durazo J; Kostelich E; Mahalov A
Affiliation(s)	Arizona State University, USA
Abstract	We present a targeted observation strategy, based on the influence matrix diagnostic that optimally selects where additional observations may be placed to improve ionospheric forecasts. This strategy is applied in data assimilation observing system experiments, where synthetic electron density vertical profiles, which represent those of Constellation Observing System for Meteorology, Ionosphere, and Climate/Formosa satellite 3, are assimilated into the Thermosphere-Ionosphere-Electrodynamics. General Circulation Model using the local ensemble transform Kalman filter during the 26 September 2011 geomagnetic storm. During each analysis step, the observation vector is augmented with five synthetic vertical profiles optimally placed to target electron density errors, using our targeted observation strategy. Forecast improvement due to assimilation of augmented vertical profiles is measured with the root-mean-square error (RMSE) of analyzed electron density, averaged over 600 km regions centered around the augmented vertical profile locations. Our results demonstrate that targeted strategy can improve data assimilation efforts during extreme events by detecting regions where additional observations would provide the largest benefit to the forecast. J. Geophys. Res. Space Physics, 122, doi:10.1002/2017JA024274, 2017.
Supported by	AFOSR, USA; NSF, USA

Presenter	Meakin CA
Affiliation	Karagozian & Case, Inc., USA
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Title	Turbulent mixing and nuclear burning in stellar interiors
Author(s)	Meakin CA (1,2,3); Mocak M (2), Arnett WD (3); Campbell S (4)
Affiliation(s)	Karagozian & Case, Inc., USA (1); Los Alamos National Laboratory, USA (2); University of Arizona, USA (3); (4) Monash University, AU (4)
Abstract	In this talk, I will summarize several aspects of turbulent mixing and nuclear burning that play a central role in shaping the structure and evolution of stars and yet lack robust or predictive models. These processes will be discussed in light of current 3D simulations and associated Reynolds-averaged Navier-Stokes (RANS) analysis. An emphasis will be placed on (1) the identification of the physical mechanisms operating at convective boundaries; and (2) the associated issue of numerical convergence when modeling these phenomena with 3D simulation codes.
Supported by	Karagozian & Case, Inc., USA; University of Arizona, USA; Australian Research Council, AU

Presenter	Nepomnyashchy AA
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Title	Anomalies of transport in steady plane laminar flows
Author(s)	Zaks MA (1); Poeschke P (1); Sokolov IM (1); Nepomnyashchy AA (2,3)
Affiliation(s)	Humboldt University of Berlin, Germany (1); Technion - Israel Institute of Technology, Israel (2); Northwestern University, USA (3)
Abstract	Advection of passive tracers on large spatial temporal scales in turbulent, chaotic or random fluid flows is usually viewed as a normal diffusion process. It is known that in random but strongly correlated velocity fields, as well as in spatially regular velocity fields that share the property of Lagrangian chaos, the transport processes can display anomalies. Remarkably, anomalous transport can be also encountered in the absence of chaos and fluctuations: in the laminar setup of steady two-dimensional viscous flows. Here, we present two examples of such transport anomalies. The first case concerns deterministic advection in plane time-independent spatially periodic flows past stagnation points or solid obstacles. In such flow patterns, the passage time for tracers carried along certain streamlines is unbounded. We derive the large time asymptotics of dispersion with the help of the tool from ergodic theory: the special flow construction. Depending on the type of the passage time singularity, dispersion turns out to be subdiffusive or superdiffusive. Explicit estimates of the transport exponents are matched by results of extensive numerical simulations. The second case refers to transport on intermediate time scales in diffusion-advection problem for spatially periodic, steady plane flow patterns that include closed cells, with a possibility of separation by jets. Intermediate anomalies of dispersion are predicted and confirmed by direct simulations. On larger time scales these transport regimes are superseded by normal diffusion. We also discuss the peculiar aging properties of dispersion in such flow patterns.
Supported by	German-Israeli Foundation Grant, Germany & Israel

Presenter	Pouquet A
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Title	Mixing and dissipation processes in rotating stratified turbulence
Author(s)	Pouquet A (1); Rosenerg D (2); Marino R (3); Herber C (4)t
Affiliation(s)	NCAR, USA (1); NOAA, USA (2); LMFA, France (3); ENS, France (4)
Abstract	We present a simple model for the scaling properties of mixing in stratified and weakly rotating flows characterized by their Rossby, Froude and Reynolds numbers, Ro, Fr, Re. It is based on equipartition between kinetic and potential modes, sub-dominant vertical velocity w, and lessening of the small-scale energy transfer as measured by the dissipation efficiency $\beta = \varepsilon/\varepsilon_d$, with $\varepsilon = -D_t E$ the kinetic energy dissipation rate and $\varepsilon_d = u_{rms}^3/L$ its dimensional expression. We determine the domain of validity of such laws by analyzing a parametric study of the unforced Boussinesq equations on grids of 1024^3 points, using direct numerical simulations, with an emphasis on atmospheric and oceanic parameters and with mostly constant $Re \sim 10^4$; the Prandtl number is one, initial conditions are isotropic and at large scale for the velocity, and zero for the temperature fluctuations θ. Three regimes in Froude number, as for stratified flows, are observed: dominant waves, eddy-wave interactions and strong turbulence. We find that both β and the Ellison scale grow linearly with Froude number in the intermediate regime, $0.01 < Fr < 0.2$, and the flux Richardson number R_f transitions for roughly the same parameter values. With $\Gamma_f = R_f/[1 - R_f]$ the mixing efficiency, putting together the three relationships of the model allows for the prediction of the scaling $\Gamma_f \sim Fr^{-2}$ in the low and intermediate regimes for high Reynolds number, whereas for higher Froude, $\Gamma_f \sim Fr^{-1} \sim R_B^{-1/2}$, as already observed: as turbulence strengthens, $\beta \sim 1$, $w \sim u_{rms}$, and smaller buoyancy fluxes altogether correspond to a decoupling of velocity and temperature fluctuations which become passive.
Supported by	NCAR and the Laboratory for Atmospheric and Space Physics, USA

Presenter	Samtaney R
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Title	Shock-driven instabilities in convergent geometry
Author(s)	Bakhsh A (1); Bond D (2); Li Y (1); Mostert W (3); Pullin D (3); Samtaney R (1); Wheatley V (2)
Affiliation(s)	King Abdullah University of Science and Technology, SA (1); University of Queensland, AU (2); California Institute of Technology, USA (3)
Abstract	Shock-driven instabilities such as the Richtmyer-Meshkov instability (RMI) arise in fluids when an interface is impulsively accelerated, usually by a shock wave. RMI studies are mostly motivated by inertial confinement fusion (ICF) in which it plays a rather detrimental role. We present our work on linear and nonlinear simulations of RMI in convergent geometries especially focusing on suppression of the RMI in the presence of a magnetic field using magnetohydrodynamics (MHD). In convergent geometry, the RMI is usually followed by a Rayleigh-Taylor (RT) phase. Linear hydrodynamic simulations indicate that the RMI phase is short-lived, followed by RTI, whereas linear MHD simulations show partial suppression of the instabilities. Depending upon the wavenumber and the magnetic field strength, the instabilities are suppressed but this comes at the price of the loss of implosion symmetry. To mitigate the loss of symmetry, we have proposed a novel octahedral field configuration. A discussion of converging RMI/RTI is somewhat incomplete without a discussion of a purely radially converging MHD shock. This is of historical significance going back to the work of Guderley who showed that radially symmetric convergence of strong shocks in a neutral gas is described by a power-law, Mach-number-radius profile. We show the existence of different Mach-number-radius regimes for a radially collapsing MHD shock, in the presence of an azimuthal field produced by a line current at the origin. The single-fluid MHD model of for plasma does not account for charge separation, finite plasma length scales and self-consistently generated electromagenetic fields. We propose to use a two-fluid plasma model that includes electrons and ion dynamics coupled via the complete set of Maxwell's equations. Finally, we will present some results from simulations of two-fluid plasma and compare and contrast the RMI between the single- and two-fluid models.
Supported by	KAUST Office of Sponsored Research, SA; The Australian Research Councils, AU

Presenter	Schilling O
Affiliation	Lawrence Livermore National Laboratory, USA
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Title	Reynolds-averaged modeling of reshocked Richtmyer−Meshkov turbulent mixing: progress and challenges
Author(s)	Schilling O
Affiliation(s)	Lawrence Livermore National Laboratory, USA
Abstract	Recent progress and challenges in modeling reshocked Richtmyer−Meshkov instability-induced turbulent mixing experiments using Reynolds-averaged turbulence models are reviewed. This includes efforts to use an advanced, multicomponent K−ε model that incorporates terms generally neglected in other models. Applications of this model to a variety of experiments with different shock Mach numbers, times of reshock, and Atwood numbers are presented and discussed. In an application to the Ma = 1.50 Vetter−Sturtevant and Ma = 1.45 Poggi et al. experiments, it is shown that other turbulence models based on a turbulent lengthscale and on transport equations for the shock production terms (rather than an algebraic closure) give very similar predictions, which are largely within the uncertainties in the experiments. Some of the important challenges facing this modeling approach are also briefly discussed, including model calibration to data, ambiguities in the choice of initial conditions, modeling sharp and diffuse interfaces, and numerical convergence behavior.
Supported by	Department of Energy, USA

Presenter	Schlossman ML
Affiliation	University of Illinois at Chicago, USA
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Title	A nanoscale view of assisted ion transport through the liquid-liquid interface
Author(s)	Schlossman ML
Affiliation(s)	University of Illinois at Chicago, USA
Abstract	The selective separation of targeted metal ions is utilized for environmental remediation, mining of rare earth and base metals, as well as the separation and isolation of long-lived radionuclides from nuclear waste. During solvent extraction, amphiphilic extractants assist the transport of target metal ions across the liquid-liquid interface between an aqueous ionic solution and an organic solvent. Investigations of the role of the interface in the ion transport challenge our ability to probe fast molecular processes at liquid-liquid interfaces on nanometer length scales. Recent development of a thermal switch for solvent extraction has addressed this challenge, which has led to the characterization by X-ray surface scattering of interfacial intermediate states in the extraction process. We find that trivalent rare earth ions, Y(III) and Er(III), combine with DHDP extractants to form inverted bilayer structures at the interface; these appear to be condensed phases of small ion-extractant complexes. The stability of this unconventional interfacial structure is verified by molecular dynamics simulations. The ion-extractant complexes at the interface are an intermediate state in the extraction process, characterizing the moment in which ions have been transported across the aqueous-organic interface, but have not yet been dispersed in the organic phase. In contrast, divalent Sr(II) forms an ion-extractant complex with DHDP that leaves it exposed to the water phase; this result implies that a second process that transports Sr(II) across the interface has yet to be observed. Calculations demonstrate that the budding of reverse micelles formed from the interfacial Sr(II) ion-extractant complexes could transport Sr(II) across the interface. These results suggest a role for interfacial dynamical processes in the extraction.
Supported by	Department of Energy, USA

Presenter	Abarzhi SI
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Title	On the fundamentals of Rayleigh-Taylor mixing driven by variable acceleration
Author(s)	Sreenivasan KR (1); Abarzhi SI (2)
Affiliation(s)	New York University, USA (1); The University of Western Australia, AU (2)
Abstract	Rayleigh-Taylor (RT) mixing occurs in a variety of natural and man-made phenomena. In most instances, RT flows are driven by variable acceleration, whereas the bulk of existing studies have considered only steady and constant acceleration. Here, we analyze certain patterns of variable accelerations and discuss the symmetries and invariants of RT mixing, by assuming that the dynamics of a fluid parcel is driven by the gain and loss of specific momenta. Analytical solutions in the balanced and imbalanced cases show the existence of two regimes -- the acceleration-driven regime and the non-universal, dissipation-driven regime. We find that the scaling, correlations, fluctuations spectra of RT mixing depart substantially from those of the canonical cases of Kolmogorov turbulence and of the self-similar blast waves of the first (Sedov-Taylor) and second (Guderley-Stanyukovich) kind. The RT mixing exhibits greater order in comparison to homogeneous isotropic turbulence, and greater disorder in comparison with self-similar blast-waves.
Supported by	The National Science Foundation, USA

Presenter	Thornber B
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Title	Transitional and self-similar Richtmyer-Meshkov instability
Author(s)	Groom M; Thornber B
Affiliation(s)	University of Sydney, AU
Abstract	The Richtmyer-Meshkov instability occurs when a perturbed interface between two fluids is impulsively accelerated, depositing vorticity in the region of the interface which causes a linear growth of any initial perturbations. The instability develops from linear, through to nonlinear saturation, growth of secondary instabilities leading to a transitional turbulent flow through to quasi self-similar turbulent mixing. Simulations of Inertial Confinement Fusion capsules undertaken at the National Ignition Facility indicate that the mixing layer may not have sufficient time during the implosion to achieve self-similarity, thus there is interest in understanding the complete transition process. Gaining experimental data, particularly on mixing, is challenging during the transitional regime. Large Eddy Simulation (LES) may be employed to probe the fully turbulent limit, however the transitional process requires accurate modelling of non-turbulent, yet high Reynolds number, mixing, as the layer is stretched in the initial linear and non-linear phases. Thus LES is not appropriate at this stage, and Direct Numerical Simulation must be employed. This paper summarises the current understanding of the transition process, and presents some recent results on algorithms and Direct Numerical Simulations aiming to understand the transitional region between linear growth and the self-similar mixing layer.
Supported by	Australian Research Council, AU

Presenter	Vasilyev OV
Affiliation	Skolkovo Institute of Science and Technology, Russia
Email	O.Vasilyev@skoltech.ru
Title	Adaptive wavelet methods for simulation of interfacial transport and mixing
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Abstract	Accurate simulation of the dynamics of interfacial mixing and transport require the development of computational approaches that can efficiently handle not only a vast range of scales, but also a variety of flow physics, which may include voritcal generation and interactions, accelerating and decelerating interfaces, sharp interfacial transitions, acoustic and shock waves, strong stratification, and many other localized and long-range phenomena. In this talk we describe a relatively young, yet promising dynamically adaptive wavelet-based computational approach for simulation of interfacial transport and mixing. What distinguishes wavelet methods from traditional approaches is their ability to unambiguously identify and isolate localized dynamically dominant flow structures such as shocks, sharp fronts or vortices and to track these structures on adaptive computational meshes, ultimately leading to substantial reduction in the computational cost, while resolving dynamically dominant flow structures. This lecture will give a general overview of wavelet-based approaches for solution of the Navier-Stokes and Euler equations in adaptive wavelet bases as well as provide examples of using Adaptive Wavelet Collocation Method for simulation of interfacial mixing. Recent developments such as hybrid stabilized conservative level set/adaptive wavelet collocation method and adaptive-anisotropic wavelet collocation method will be also discussed.
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