CI²MA, Universidad de Concepción, January 16 and 17, 2025

An Oliver's approach to second-order MPRK schemes for some time-dependent hyperbolic equations

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Abstract

We are interested to study the variable coefficient Burgers' equation

 $u_t + f(x,t)uu_x + g(x,t)u_{xx} = h(x,t)$

focusing on Runge-Kutta second order schemes using Oliver's approach [3]. We want to to improve the accuracy of these schemes in the field of nonautonomous systems. The approach does not demand $\mathbf{Ae} = \mathbf{c}$ in the Butcher tableau $(\mathbf{A}, \mathbf{b}, \mathbf{c})$, where $\mathbf{e} = (1, \ldots, 1)^T$. We extended the second order generalized BBKS schemes defined in [1], considering different powers for the gradient modifier term depending on the negative terms in each stage of the RK schemes. Following the general analysis of MPRK schemes described in [2], positivity and mass conservation fundamental properties are proven and even conditions concerning the Patankar weights are given to get second order accuracy.

This presentation is based on joint research with Javier G. González, Universidad Central del Ecuador, Quito, Ecuador

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CI²MA, Universidad de Concepción, January 16 and 17, 2025

Invariant-region-preserving central WENO schemes for one-dimensional multispecies kinematic flow models

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Abstract

Multispecies kinematic flow models are defined by systems of N strongly coupled, nonlinear first-order conservation laws, where the solution is a vector of N partial volume fractions or densities. These models arise in various applications including multiclass vehicular traffic and sedimentation of polydisperse suspensions. The solution vector should take values in a set of physically relevant values (i.e., the components are nonnegative and sum up at most to a given maximum value). It is demonstrated that this set, the so-called invariant region, is preserved by numerical solutions produced by a new family of high-order finite volume numerical schemes adapted to this class of models. To achieve this property, and motivated by [3], a pair of linear scaling limiters is applied to a high-order central weighted essentially non-oscillatory (CWENO) polynomial reconstruction [2] to obtain invariant-region-preserving (IRP) high-order polynomial reconstructions. These reconstructions are combined with a local Lax-Friedrichs (LLF) or Harten-Lax-van Leer (HLL) numerical flux to obtain a high-order numerical scheme for the system of conservation laws. It is proved that this scheme satisfies an IRP property under a suitable Courant-Friedrichs-Lewy (CFL) condition. The theoretical analysis is corroborated with numerical simulations for models of multiclass traffic flow and polydisperse sedimentation.

This presentation is based on a joint work with Raimund Bürger (Universidad de Concepción, Chile), Pep Mulet (Universitat de València, Spain) and Luis Miguel Villada (Universidad del Bío-Bío, Chile).

- J. Barajas-Calonge, R. Bürger, P. Mulet and L.M. Villada, 'Invariant-region-preserving central WENO schemes for one-dimensional multispecies kinematic flow models', Preprint 2024-26, CI²MA, Universidad de Concepción.
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Hyperbolic and related problems in mineral processing and wastewater treatment

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CI²MA & Departamento de Ingeniería Matemática Universidad de Concepción

Abstract

This contribution is a survey on recent advances on the formulation, mathematical analysis, and numerical solution for models of solid-liquid or liquid gas multiphase flows in applications of mineral processing and wastewater treatment. These include batch and continuous sedimentation, countercurrent decantation, column flotation, and reactive settling. The models are based on balance equations of continuum mechanics followed by a dimensional analysis and further simplifications, and can in the widest sense be formulated as convection-diffusion-reaction partial differential equations. Typically, the sought unknowns are the volume fractions of components of a disperse phase that may either segregate and form areas of different composition (such as particles in a polydisperse suspensions that differ in size or density) or undergo reactions with other components (as occurs in reactive settling involving particles of biomass and various nutrients dissolved in the liquid). A characteristic property of most of the models developed is the reduction to one space dimension (aligned with gravity) and to a finite domain, as typical for unit operations. The latter restriction calls for the expression of boundary conditions by discontinuities of the governing flux, as well as the description of inlets through singular source terms. Some specific applications, and their respective main mathematical challenges that will be addressed include (1) batch and continuous sedimentation of flocculated suspensions in clarifier-thickeners, which are described by a conservation law with discontinuous flux and strongly degenerating diffusion term [8]; (2) polydisperse suspensions modelled first-order systems of conservation laws of arbitrary size for which results of hyperbolicity analysis [7, 9] have recently led to the formulation of invariant-region-preserving high-order WENO schemes [2, 10, 11, 12]; (3) models of reactive settling in wastewater treatment in secondary settling tanks (SSTs) and sequencing batch reactors (SBRs) that incorporate reaction terms and in the case of SBRs, call for incorporating moving boundaries [1, 4]; (4) models of froth flotation in columns that involve bubbles and particles and that are defined by systems of conservation laws with discontinuous flux, degenerate diffusion and triangular structure [5, 6]; and (5) settling with convection in an inclined channel described by a coupled flow-transport model [3].

This presentation is based on joint research with Fernando Betancourt and Lucas Romero (UdeC), Stefan Diehl (Lund University, Sweden), Juan Barajas-Calonge, Julio Careaga and Luis Miguel Villada (Universidad del Bío-Bío, Concepción), Pep Mulet and María del Carmen Martí (Universitat de València, Spain), and Yolanda Vásquez (Universidad Tecnológica de Panamá).

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Flux-vector splitting approach for the Shallow Water equation and applications

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Abstract

In this presentation we show a flux vector splitting approach to solve the shallow water equation in one and two spatial dimensions. The original ideas came from the work of Toro and Vázquez applied to the Euler equations [3]. The approach split the full system in two process called the advection and the pressure system and has been implemented to solve the Euler system with general equation of state[4], the Baer-Nunziato multiphase models [2] and shallow water equations [6] [1] [5] between others. The strategy originally developed for the Euler system does not apply directly to the Shallow Water system therefore a slightly different technique is used here.

After splitting the conservative flux into an advection and pressure flux (pressure flux name remains from Euler system) we construct a Riemann solver of the pressure system. This Riemann solver can be computed exactly with an inexpensive iterative process or approximately following a two rarefaction assumption for example. With this information the advection flux can be selected producing an exceedingly simple first order Godunov upwind method.

The presented scheme can be used as a building block for a high order numerical method. We use it in the framework of a Finite Volume high order ADER schemes on two dimension unstructured meshes.

We asses the numerical scheme on a suit of test problems with reference solution in one and two dimensions. For one dimension problems we consider classical initial value problems with exact solution and steady state solutions for transcritical flow over a bed bump. In two space dimensions we consider convergence problems with artificial source term, radially symmetric dam break problems and tsunami wave propagation in realistic bathymetry scenarios.

This presentation is based on joint research with Eleuterio F. Toro (Uni. Trento), Davide Vanzo (ETH Zurich) and Annunziato Siviglia (Uni. Trento).

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Trinidad Gatica

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1 Classifying acoustic cavitation with machine learning trained on multiple physical models

Acoustic cavitation refers to the formation and oscillation of microbubbles in a liquid exposed to acoustic waves. Depending on the properties of the liquid and the parameters of the acoustic waves, bubbles behave differently. The two main regimes of bubble dynamics are transient cavitation, where a bubble collapses violently, and stable cavitation, where a bubble undergoes periodic oscillations. Predicting these regimes under specific sonication conditions is important in biomedical ultrasound and sonochemistry. For these predictions to be helpful in practical settings, they must be precise and computationally efficient. In this study, we have used machine learning techniques to predict the cavitation regimes of air bubble nuclei in a liquid. The supervised machine learning was trained by solving three differential equations for bubble dynamics, namely the Rayleigh-Plesset, Keller-Miksis, and Gilmore equations. These equations were solved for a range of initial parameters, including temperature, bubble radius, acoustic pressure, and frequency. Four different classifiers were developed to label each simulation as either stable or transient cavitation. Subsequently, four different machine-learning strategies were designed to analyze the likelihood of transient or stable cavitation for a given set of acoustic and material parameters. Cross-validation on held-out test data shows a high accuracy of the machine learning predictions. The results indicate that machine learning models trained on physics-based simulations can reliably predict cavitation behavior across a wide range of conditions relevant to real-world applications. This approach can be employed to optimize device settings and protocols used in imaging, therapeutic ultrasound, and sonochemistry.

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ENO-ET reconstruction for finite volume methods applied to sediment transport in shallow water flows

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Abstract

The Shallow Water equations together with a mass balance law for the sediment bed load (Exner equation) forms the Saint Venant equations, of great utility in many areas such as fluid dynamics, hydraulic, geomorphology, environmental engineering, among others. The resulting systems of balance laws are hyperbolic with non-conservative terms [4][5], therefore it is interesting to develop appropriate high order schemes to solve and simulate the evolution of these flows accurately and eficiently. Furthermore, we are interested on schemes able to capture discontinuities and wave propagation. Nonlinear reconstructions play a key rol in the development of high order numerical methods, in particular the ENO type nonlinear interpolation [1][2] and its variants. In this work, we will explore the novel ENO-ET nonlinear interpolation [1][2] and its application to shallow water flows in conjunction with high order numerical schemes of ADER type [3] to solve the Saint Venant Exner system, and study possible extensions to two dimensions.

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Modelling biofilm in slow sand filters: one- and two-dimensional models

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Abstract

This presentation will consist of a brief overview of recent work on modelling slow sand filtration systems for drinking water treatment, with an emphasis on the physical modelling and some discussion on the numerical difficulties of the resulting equations.

In [2], a one-dimensional multi-phase model for the evolution of slow sand filters was introduced, with an emphasis on the growth of the biofilm volume fraction $\phi_{\rm b}$. The model consists of mass balances on a domain comprised of a supernatant water region (depth z < 0) on top of a sand bed (depth z > 0). The biofilm velocity $v_{\rm b}$ presents a spatial discontinuity at depth z = 0. In the sand bed, $v_{\rm b}$ is assumed to be 0, whereas in the supernatant water it is understood as the flux of a Cahn–Hilliard type equation with $v_{\rm b} = v_{\rm b}(\partial_z^3\phi_{\rm b},\partial_z\phi_{\rm b})$. In order to preserve positivity, a finite-difference discretization is used for the Cahn–Hilliard system coupled with an upwind scheme for which a CFL condition could be derived.

Recently, [1] introduced a positivity-preserving discontinuous Galerkin scheme for the homogeneous convective Cahn–Hilliard equation. Using this work as a basis, we are interested in developing two-dimensional positivity-preserving schemes for solving the mass balances modelling the growth of biofilm purely in the supernatant water.

This presentation is based on joint research with Stefan Diehl and Julio Careaga.

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A universal scheme for hyperbolic PDE in both conservative and non-conservative form

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Abstract

One dimensional partial differential equations of hyperbolic type have a wide range of applications, they normally describe propagation phenomena where physical constitutive laws are involved. Even these laws are based on conservation of physical quantities as momentum or mass, derived model can be non-conservative in the sense of [1], where no physical flux can be identified as an inverse operator of product between sate variables. On the other hand, conservative systems are desirable from theoretical and numerical issues, for instance properties as entropy, well balance and stability are mainly associated to conservative formulations. The method of path conservative proposed by Parés in [2], allows to define weak solution and a notion of entropy which allows to extend the definition of Riemann problems to non-conservative systems.

Riemann problems are the key to build the family of high-order finite volume schemes named ADER [3, 4]. In which the combination of non-linear interpolations, called reconstructions and the solver of Riemann problems allows a high-order approximation of fluxes at cell interfaces and the computation of source terms, if present.

We are interested on finite volume schemes able to solve accurately non-conservative systems. Furthermore, we are looking for a scheme which can be employed to solve conservative models expressed as quasilinear form, in such a case the system must reproduce an equivalent flux at cell interfaces, without any modification of the code, this is the so called universal property. This is achieved by the use of the path conservative strategy in the frame of the ADER approach, as reported in [6]. The resulting scheme can solve efficiently, hyperbolic balance laws in both conservative and non-conservative form. Furthermore, this verifies the well-balanced property and an empirical convergence rate assessment shows that the expected theoretical orders of accuracy are achieved up to the fifth order.

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Numerical methods for the compressible Cahn-Hilliard-Navier-Stokes equations

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Abstract

In [5] D. Siano reports a layering phenomenon in experiments of sedimentations of monodisperse colloidal particles and conjectures that a spinodal decomposition, governed by the Cahn-Hilliard equation [2], is the underlying mechanism that explains the layering phenomenon.

Since the Cahn-Hilliard equation cannot explain this phenomenon by itself, the gravitational force is introduced into the model by means of conservation of mass and momentum, which, together with conservation of individual species and ignoring temperature changes, yields a system of equation, the isentropic compressible Navier-Stokes-Cahn-Hilliard equations [3, 1], which are a system of fourth-order partial differential equations that model the evolution of mixtures of binary fluids under gravitational effects.

We consider the compressible case for the evolution of, e.g. foams, solidification processes, fluid-gas interface, although incompressible models for these equations might be more suitable for explaining the cited layering phenomenon.

The goal of this contribution [4] is the design of implicit-explicit time-stepping schemes to avoid the severe restriction posed by the high order terms for the efficient numerical solution of boundary-initial problems with these equations.

We show some two-dimensional experiments to assess the possibilities of obtaining efficient algorithms.

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Interaction of jamitons in second-order macroscopic traffic models

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Abstract

Jamitons are self-sustained traveling wave solutions that arise in certain second-order macroscopic models of vehicular traffic. A necessary condition for a jamiton to appear is that the local traffic density breaks the so-called sub-characteristic condition. This condition states that the characteristic velocity of the corresponding first-order Lighthill-Whitham-Richards (LWR) model formed with the same desired speed function is enclosed by the characteristic speeds of the corresponding second-order model. The phenomenon of collision of jamitons in secondorder models of traffic flow is studied analytically and numerically for the particular case of the second-order Aw-Rascle-Zhang (ARZ) traffic model [1, 3]. A compatibility condition is first defined to select jamitons that can collide each other. The collision of jamitons produces a new jamiton with a velocity different from the initial ones. It is observed that the exit velocities smooth out the velocity of the test jamiton and the initial velocities of the jamitons that collide. Other properties such as the amplitude of the exit jamitons, lengths, and maximum density are also explored. In the cases of the amplitude and maximum exit density it turns out that over a wide range of sonic densities, the exit values exceed or equal the input values. On the other hand, the resulting jamiton has a greater length than the incoming ones. Finally, the behavior for various driver reaction times is explored. It is obtained that some properties do not depend on that time, such as the amplitude, exit velocity, or maximum density, while the exit length does depend on driver reaction time.

This presentation is based on joint research [2] with Raimund Bürger (Universidad de Concepción) and Sebastián Tapia (Universidad de Chile).

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A new two-dimensional blood flow model with arbitrary cross-sections

Cesar Alberto Rosales-Alcantar * CIMAT Mérida (CONAHCYT) & IMATE Juriquilla (UNAM)

Abstract

In this contribution, a new two-dimensional model for blood flow in arteries with arbitrary cross sections is derived [1]. The domain consists of a narrow, large vessel that extends along an axial direction, with cross sections described by radial and angular coordinates. The model consists of a system of balance laws for conservation of mass and balance of momentum in the axial and angular directions. The equations are derived by applying asymptotic analysis to the incompressible Navier-Stokes equations in a moving domain with an elastic membrane, and integrating in the radial direction in each cross section. The resulting model is a system of hyperbolic balance laws with source terms. The main properties of the system are discussed and a positivity-preserving well-balanced central-upwind scheme is presented. The merits of the scheme will be tested in a variety of scenarios. In particular, simulations using an idealized aorta model are shown. We analyze the time evolution of the blood flow under different initial conditions such as perturbations to steady states, which parametrizes a bulging in a vessel's wall. We consider different situations given by distinct variations in the vessel's elasticity. This presentation is based on joint research with Gerardo Hernández-Dueñas (IMATE Juriquilla).

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Symplectic Hamiltonian Hybridizable Discontinuous Galerkin Methods for shallow-water equations

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Abstract

We propose a new hybridizable discontinuous Galerkin method for approximating the linearized shallow-water equations. The discretization aims to preserve relevant physical quantities such as mass, vorticity, and energy. Specifically, we reformulate the system of equations in a Hamiltonian form, employing Hybridizable Discontinuous Galerkin Methods (HDG) for spatial discretization and obtaining a semi-discrete scheme written in Hamiltonian form. By leveraging on the inherent Hamiltonian structure of the numerical method and implementing symplectic time-marching schemes, we ensure the conservation properties of the fully discrete system of equations. We discuss the fundamental properties of our analysis and present numerical experiments to validate its performance.

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Well-posedness and numerical analysis of an elapsed time model with strongly coupled neural networks

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Abstract

The elapsed time equation is an age-structured model that describes dynamics of interconnected spiking neurons through the elapsed time since the last discharge, leading to many interesting questions on the evolution of the system from a mathematical and biological point of view. In this work, we first deal with the case when transmission after a spike is instantaneous and the case when there exists a distributed delay that depends on previous history of the system, which is a more realistic assumption. Then we study the well-posedness and the numerical analysis of the elapsed time models. For existence and uniqueness we improve the previous works by relaxing some hypothesis on the non-linearity, including the strongly excitatory case, while for the numerical analysis we prove that the approximation given by the explicit upwind scheme converges to the solution of the non-linear problem. We also show some numerical simulations to compare the behavior of the system in the case of instantaneous transmission with the case of distributed delay under different parameters, leading to solutions with different asymptotic profiles.

This presentation is based on joint research with Nicolás Torres (Universidad de Granada, Spain) and Luis Miguel Villada (Universidad del Bío-Bío, Concepción).

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Foam front dynamics in improved oil recovery: comparing pressure-driven growth with Darcy flow

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Abstract

The foam improved oil recovery process is analyzed, focusing on computing the propagating foam front location in two-dimensions. Two approaches are used, namely the pressure-driven growth model [1], and a two phase Darcy's model coupled with fractional flow theory for water/gas mass conservation [2]. In the pressure-driven growth model, the foam front is considered to be contained in a region of extent ϵ relative to overall gas displacement [3]. Within this region, the foam exhibits a finely-textured structure causing the foamed gas mobility to be orders of magnitude lower than that of a pure gas or pure liquid [4]. Although pressure-driven growth usually assumes ϵ to be a small fraction of the distance travelled by the foam [1, 3, 5], a recent study suggests that ϵ is actually close to unity [6]. In order to determine whether the foam front location can be predicted accurately using the pressure-driven growth model, despite ϵ being larger than expected, predictions are compared with the aforementioned Darcy model. In addition to the foam resistance at the front, to match Darcy's predictions, it is necessary to account for the liquid resistance downstream of the front, and the fact that Darcy's predictions access liquid saturations with lower mobilities than the pressure-driven growth model considers by construction via following fractional flow theory. To achieve agreement between the models, the foamed gas mobility in pressure-driven growth model is treated as a fitting parameter, which indirectly modifies the relative resistance of the liquid phase downstream. Consequently, adjustments to the foamed gas mobility are necessary for different horizontal extents of the solution domain to ensure model compatibility and accurate foam front prediction.

This presentation is based on joint research with P. Grassia (TU Eindhoven), J. Hernández-Montelongo (UCTemuco), Y. Boakye-Ansah (UENR) and P. Zuñiga (UCTemuco).

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Finite volumes scheme for a Kawahara equation with time-delayed boundary control.

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Abstract

This talk is devoted to the proposal and study of a finite volumes scheme for a Kawahara equation with a delay term as one of the boundary conditions. In particular, we will consider the following problem for $(x, t) \in \Omega \times \mathbb{R}^+$, for $\Omega := (0, L), L > 0$:

$$\begin{cases} \partial_t u(x,t) + \gamma_1 \partial_x u(x,t) + \gamma_2 \partial_x^3 u(x,t) - \partial_x^5 u(x,t) + u^p(x,t) \partial_x u(x,t) = 0, & (x,t) \in \Omega \times \mathbb{R}^+ \\ u(t,0) = u(t,L) = \partial_x u(t,0) = \partial_x (t,L) = 0, & t > 0, \\ \partial_x^2 u(t,L) = \mathcal{F}(t,h), & t > 0, \\ \partial_x^2 u(t,0) = z_0(t), & t \in (-h,0), \\ u(0,x) = u_0(x), & x \in \Omega, \end{cases}$$

where $\gamma_1 > 0$ and $\gamma_2 > 0$ are physical parameters, $p \in [1, 2]$, and $\mathcal{F}(t, h)$ is defined as

$$\mathcal{F}(t,h) = \alpha \partial_x^2 u(t,0) + \beta \partial_x^2 u(t-h,0),$$

for h > 0 and α , β are such that $|\alpha| + |\beta| < 1$. From [2] it is known that this problem is exponentially stable under a specific condition for the length L of the domain. Our main objective is to propose a numerical scheme that replicates this behavior, which takes ideas from [1], [3] and [4]. Computational examples are provided.

This is a work in progress, and is a joint research with Roberto Capistrano-Filho and Víctor Hugo G. Martínez (Universidade Federal de Pernambuco, Brazil).

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Well-posedness of a nonlocal reaction traffic flow model with on-off ramps

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Abstract

Models of conservation laws with nonlocal flux describe several phenomena such as slow erosion of granular flow, synchronization, sedimentation, crowd dynamics, navigation processes and traffic flow. In particular, non-local traffic models describe the behaviour of drivers that adapt their velocity with respect to what happens to the cars in front of them. In this type of models, the flux function depends on a downstream convolution term between the density of vehicles and a kernel function with support on the positive axis [2, 3]. In this talk we present a non-local version of a scalar balance law modeling traffic flow with on-ramps and off-ramps [1]. The source term is used to describe the traffic flow over the on-ramp and off-ramps. We approximate the problem using an upwind-type numerical scheme and we provide \mathbf{L}^{∞} and \mathbf{BV} estimates for the sequence of approximate solutions. Together with a discrete entropy inequality, we also show the well-posedness of the considered class of scalar balance laws. Some numerical simulations illustrate the behaviour of solutions in sample cases.

This presentation is based on joint research with Harold Contreras (USS-Chile) and Felisia Chiarello (L'Aquila University, Italy).

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