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EDITORIAL: BRIDGING THE SCIENCE AND TECHNOLOGY BY MODERN MATHEMATICAL METHODS AND HIGH PERFORMANCE COMPUTING

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Modern mathematical methods and algorithms associated with robotic, intelligent and high performance computing strategies have been intensively used and have shown powerful capabilities for understanding and solving numerous important, yet challenging, issues in science and technology. Latest research developments in this area include extended finite element method and discontinuous Galerkin technique for fluid-structure interactions with moving mesh configurations, effective high order hybrid approximations of fractional partial differential equations, asymptotic stability analysis for nonlinear systems of differential equations modeling, phase shifts of coral reef herbivores, accuracy-guaranteed numerical computations of large systems of linear equations on supercomputers and parallelized variational process to optimize 3D sensor placement in big data environments.

The aim of this special issue is to highlight new developments in aforementioned fields reported during the Third International Conference on Modern Mathematical Methods and High Performance Computing in Science and Technology (M3HPCST) held in Ghaziabad, India, January 2020. Five highly representative lectures have been selected within a very limited content. The guest editors of this special issue would encourage the readers, while enjoying the remarkable results presented in this special issue, to participate in various research activities in theory and applications, and to continue supporting and promoting the study of cutting-edge mathematical methods and high performance computing up to a much higher level in the near future.

Many important engineering processes involve the modeling, computations and simulations of interactions between moving structures and fluids, such as supercavitations under the sea level. However, corresponding numerical procedures can be extremely challenging, since the structures are frequently subject to large displacements and deformations. Delicate strategies are required to handle the movements of

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computational grids adaptively. Traditional Arbitrary Lagrangian-Eulerian (ALE) approaches may fail in such a case, since inverted fluid elements may appear, or lead to spurious solutions due to the presence of very stretched fluid elements. New classes of interface methods have emerged recently, including the immersed boundary method, fictitious domain schemes, fully Eulerian approach, extended finite element method (XFEM), cut-finite element method, and polygonal discontinuous Galerkin (DG) strategies. Hybrid algorithms combining an ALE and unfitted technology have also been proposed and tested. Nitsche's approaches are employed to weakly couple underlying fluid and solid at interfaces.

A state of the art of computational developments in the above field can be found in this special issue. A highly effective hybrid XFEM algorithm, mortared through discontinuous Galerkin platforms, is presented in detail. This new XFEM/DG method takes the advantage of simplicity of classical finite element methods while more accurate numerical treatments are achieved via fluid elements enriched throughout interfaces. Such a design not only takes care of discontinuities between multiple elements, but also preserves physical jumps in the numerical solution correctly. Consequently, fluids and structures at unfitted interfaces are handled precisely. Furthermore, penalization methods that characterize non-penetration conditions at the solid-solid interfaces are also investigated for contacts between immersed structures. Although only single penalty function is discussed for the contact model and no-slip conditions for fluid-structure interaction couplings for the simplicity in the initial study, extended investigations can be found in simulation experiments, in particular for situations where i) unfitted meshes are employed; ii) nonlinear governing equations are used for fluids while different constitutive laws are considered for solids; or iii) two-body contact cases are enforced.

On the other hand, Schrödinger equations have been playing a fundamental role in the description of the wave functions in quantum-mechanical systems. Their solutions are keys to understand underlying quantum phenomena. One of the cutting-edge topics in the research has been related with the latest fractional Schrödinger equations. Developments of higher order solution approximations have attracted researchers from computational science, quantum mechanics and precision engineering due to their profound applications in societies and high-tech industry.

This special issue provides the latest information in the literature. A sixth order hybrid method is presented and analyzed based on linearized $L1$-Galerkin finite element discretization reinforced through combined compact difference (CCD) technologies for fast numerical solutions of fractional Schrödinger equations in the Caputo sense, that is,

$$\mathrm{i}\frac{\partial^\gamma \psi}{\partial t^\gamma} + \alpha\frac{\partial^2 \psi}{\partial x^2} + \beta|\psi|^2\psi + v(x)\psi = f(x,t), \quad (x,t) \in \Omega \times (0,T],$$

where i is the imaginary unit, $0 < \gamma < 1$, $\alpha, \beta \in \mathbb{R}^+$, and Ω is a closed interval, together with suitable initial-boundary conditions. Rigorous numerical analysis is accomplished to ensure the numerical stability of the complex $L1$-CCD algorithm derived. It is proven that the hybrid finite element-finite difference scheme is stable unconditionally under the Von Neumann sense. The fast convergence of the numerical solution is further demonstrated.

Interesting simulation experiments are carried out to illustrate the efficiency, accuracy, stability, and convergence of the $L1$-CCD method. Two standard testing problems from quantum mechanics are considered. It is found that the novel hybrid computational strategy ensures not only sixth order convergence in space, but also $2-\gamma$th order convergence in time.

Needless to say, hybrid $L1$-CCD simulations can be extended for solutions of multidimensional Schrödinger models, or other fractional order partial differential equations, including fractional Helmholtz equations at high wave numbers for electro-optical applications. Interested readers are encouraged to explore further the line of extremely rewarding research territories illustrated.

Coral reefs can undergo relatively rapid changes in the dominant biota, a phenomenon referred to as phase shift. Degradation of coral reefs is often associated with changes in community structure towards macroalgal dominated reef ecosystem due to the reduction in herbivory caused by overfishing. Let $P(t)$ and $C(t)$ be growing concentrations of the algae and corals at time t, respectively. Herbivorous parrotfish are growing in the natural system by feeding on algae as well as corals having concentration $X(t)$ at time t. Assume that the parrotfish are harvested at a density-dependent harvesting policy. Based on mathematical conservation principals H1–H4, an effective nonlinear system of modeling equations

$$\frac{\mathrm{d}\Phi}{\mathrm{d}t} \equiv F, \quad t > 0,$$

where $\Phi = (P, C, X)^\top$, $F = (F_1, F_2, F_3)^\top$, is derived and verified in this special issue. Boundedness and uniform persistence of the system are investigated and proven. It is observed that the system acquired possesses anticipated equilibria, that is, i) the organism-free equilibrium; ii) coral and fish-free equilibrium; iii) coral-free equilibrium; iv) macroalgae and fish-free equilibrium; and v) macroalgae-free equilibrium.

Poore's sufficient condition is employed in the study of the orbital stability of Hopf-bifurcating periodic solution of the nonlinear evolution system. Detailed calculations for supercritical and subcritical Hopf bifurcations are obtained and illustrated through numerical simulations, since such bifurcations may being evidence of oscillations of the system when the carrying capacity of macroalgae crosses some certain

thresholds. Extremely applicable conclusions are given for the shifts which can be utilized to qualitatively promote a healthy environment in coral systems.

Many scientific problems are boiled down to linear systems during discretization. Therefore, it is extremely important to solve those systems for accurate and reliable numerical solutions. On the other hand, the computational speed of supercomputers, such as floating-point operations per second (FLOPS), and the total amount of usable memory increase rapidly. Hence, the treatable problem sizes in scientific computing are getting larger. Since the larger the system's size, the more the number of FLOPS are needed, rounding errors have become more crucial nowadays. To see the impact, an evaluation algorithm is comprised in this special issue for accurate matrix-vector products and computations of linear system solutions over 1000K unknowns. FUJITSU FX100 supercomputer and parallelization are utilized. Answers are also given to following exploratory questions raised:

- ▷ Is a rounding error a problem? And is your accuracy assurance necessary?
- ▷ Is it possible to obtain accurate numerical results using iterative refinements?
- ▷ Is it possible to obtain a tight error bound for accurate numerical results?

Network sensor placement has been an optimization concern that has recently gained a tremendous amount of attentions. When a sensor location is optimally selected, the predictive model may greatly reduce its internal errors. A greedy-selection algorithm is often selected for locating optimal spatial locations from a numerically embedded space. In this special issue, for the first time in the field, a sensor placement model is developed for a 3D domain representing a real case scenario. Further, the model uses temporal sequences of data from fluid dynamic simulations. In the approach, a combination of deep learning, probabilistic frameworks and variational methods is considered for reducing the complexity associated with training, inferences and optimization. These have also enabled expected optimal placement results in a real case scenario. The complexity of novel new model is, in fact, only at the rate of $\mathcal{O}(klM^4)$ in operations, where k is the number of sensors, l is the number of iterations needed to optimize the sensor position, and M is an observatory parameter for which $M \ll N$ with N being the number of sides of a computational domain. A global extended strategy, mutual information-based optimization and fine-tuning of the selected optimal location are presented and discussed. A specially tailored parallelization procedure further reduces the computational costs and makes it possible to monitor real 3D spaces in real time.

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