OAK RIDGE National Laboratory

An Adaptive Spacetime Wavelet Method for Multiscale Problems in Fluid and Solid Mechanics

Presented by:

Dr. Karel Matouš

University of Notre Dame

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Abstract: Modern computational science and engineering applications are inherently multiphysics and multiscale. Therefore, novel algorithms are required to solve nonlinear partial differential equations (PDEs) with features evolving over a wide range of spatial and temporal scales. In this work, Dr. Karel Matouš proposes a wavelet-based method that is ideally suited for problems developing localized structures, which might occur intermittently anywhere in the computational domain or change their location and scales in space and time. Wavelets have generated tremendous interest in both theoretical and applied areas as they allow for efficient multiscale decomposition and large data compression. Moreover, wavelets have localization properties in physical and wave number spaces and algorithmically possess operational complexity. Wavelet-based numerical methods are efficient for modeling multiscale and multiphysics problems because they provide spatial adaptivity using multiresolution basis functions. In this work, Dr. Matouš uses the Multiresolution Wavelet Toolkit (MRWT) he developed, which requires far fewer unknowns than other algorithms when applied to problems with a great range of spatial and temporal scales. In addition, the computational grid can be refined locally, and the *a priori* error estimates safeguard the accuracy of the numerical solution. MRWT is implemented as a hybrid Message Passing Interface (MPI) + Open Multi-Processing (OpenMP) parallel framework using modern C++ to execute in a hybrid central processing unit/graphics processing unit (CPU/GPU) parallel environment, and it scales favorably on ~10^3–10^4 cores. Consequently, MRWT provides high-fidelity simulations with significant data compression. Dr. Matouš explains how this technique uses differentiable wavelet basis functions and second-generation wavelets to solve nonlinear PDEs on finite domains. Moreover, he provides *a priori* error estimates for the wavelet representation of fields, their derivatives, and

the aliasing errors associated with the nonlinear terms in PDEs. Then, by projecting fields and spatial derivative operators onto the wavelet basis, his estimates are used to construct a sparse multiresolution spatial and temporal discretization that maintains the prescribed accuracy for each field. Additionally, MRWT utilizes a predictor-corrector procedure within the time advancement loop to dynamically adapt the computational grid, retaining the prescribed accuracy of the solutions of the PDEs as they evolve. First, Dr. Matouš employs an embedded Runge-Kutta (RK) integration scheme to control the temporal accuracy as the solution of the PDE advances. Second, he also presents a novel spacetime method and solves the full spacetime problem using adaptive wavelets. The preliminary spacetime results on dense grids show promise for the development of sparse spacetime wavelet schemes. Rigorous verification of the MRWT algorithm is shown for both time marching (RK integration) and spacetime problems, demonstrating mathematical correctness and physics simulation capabilities. Furthermore, he shows that special convergence is achieved at a rate that agrees with *a priori* estimates. Whereas traditional numerical techniques require a sequence of solutions on multiple grids (i.e., solution verification), this adaptive wavelet method provides self-verification from a single simulation. Finally, MRWT is applied to problems with shocks in gases using compressible Navier-Stokes equations and to high-strain rate damage nucleation and propagation in nonlinear solids using Eulerian-Lagrangian dynamic damage modeling.

Speaker's Bio: Dr. Matouš is a Professor of Aerospace and Mechanical Engineering at the University of Notre Dame. He received his Master of Science and Ph.D. in Theoretical & Applied Mechanics from the Czech Technical University in Prague. Dr. Matouš served as the Director of the Center for Shock Wave-processing of Advanced Reactive Materials (C-SWARM), which was established as one of the six National Nuclear Security Administration (NNSA) centers of excellence whose primary focus had been on the emerging field of predictive science. In 2016, he held a visiting professor position at the Department of Mechanical Engineering at the Eindhoven University of Technology. Dr. Matouš's interests are in predictive computational science and engineering at multiple spatial and temporal scales, including multi-physics interactions, the development of advanced numerical methods, and high-performance parallel computing. His research focuses on the interplay between applied mathematics, computer/computational science, and physics/materials science. Moreover, he leads a research program in image-based (data-driven) modeling of heterogeneous systems, focusing on co-designed simulations and experiments based on statistical analysis, computational mathematics, and artificial intelligence/machine learning. He has authored or co-authored more than 200 journal and/or conference proceedings articles and abstracts. He is involved in several interdisciplinary research programs with funding from various agencies and private companies. In 2022, Dr. Matouš received the *Rev. Edmund P. Joyce, C.S.C., Award* for Excellence in Undergraduate Teaching from the University of Notre Dame. Moreover, Dr. Matouš received the Rector's Award for the best Ph.D. students from the Czech Technical University in Prague. Several articles from Dr. Matouš's group have been featured on the Web of Science's highly cited list. One of his papers appeared as the cover article in *Proceedings of the Royal Society A*. He is a member of American Society of Mechanical Engineers (ASME), Society of Engineering Science, U.S. Association for Computational Mechanics, European Mechanics Society, and International Association for Computational Mechanics. Dr. Matouš is a fellow of ASME. Dr. Matouš serves as an Associate Editor of the *Journal of Computational Physics* and *International Journal for Multiscale Computational Engineering*.