Nek5000 User Meeting 2010

Argonne National Laboratory

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Flow Destabilization and Heat Transfer Augmentation using Transverse Surface Grooves

John Akerley University of Nevada

Experimental investigations and direct numerical simulations of passive flow destabilization and heat transfer augmentation have been performed in the past concerning transversely grooved channels with fully developed flow. These experiments and simulations have shown both unsteady flow effects and enhanced heat transfer with two-dimensional disturbance occurring at a Reynolds number of about 350 and three-dimensional disturbance occurring around a Reynolds number of 750. Two postulates have arisen: small grooves at the leading edge of a channel disrupting the boundary layer and intermittently grooved channels improving the combination of heat transfer/pumping power performance. Two and three-dimensional simulations will be performed with Nek5000 to design an experiment and limit the parameters, including the number of grooves, the growth of groove dimensions with boundary layer growth, and the length of the recovery region. An experiment will be designed based on the results of these simulations that will measure the heat transfer and pumping power performance and a final three-dimensional simulation will be used as a model in the goal of correctly predicting heat transfer and Reynolds-number-independent friction factor behavior.

Flow dynamics and heat transfer in turbines

Andrew Duggleby Michael Meador Texas A&M University

At the Fluids, Turbulence, and Fundamental Transport (FT2L) lab at Texas A&M, NEK5000 is primarily used for characterizing the flow dynamics and heat transfer in gas turbines. The overall goal is to provide realistic operating conditions such as large Reynolds numbers, length scales, combustor exit profiles, and density ratios such that the secondary flow structures that degrade performance may be investigated and then mitigated.

In part I of this talk (A. Duggleby) results of a low-pressure turbine (LPT), high-pressure turbine (HPT), and pin-fin heat transfer are shown. In the LPT the flow relaminarizes forming a separation bubble which reattaches downstream is examined. In the HTP examinations dynamics of the stagnating boundary-layer horseshoe vortex are shown. This vortex is responsible for 30% drag and a significant increase in endwall heat transfer. The pin-fin heat transfer (trailing edge

HPT internal cooling) simulations outline strategies for using Time-Orthogonal Decomposition for identifying and modifying flow structures to reduce drag and increase heat transfer.

Part II of this talk (M. Meador) we discuss current and future projects that involve developing models with very complex geometries. Results of a film-cooling conjugate heat transfer and HPT with film-cooling holes are shown. Future work on combustor simulations as well as inlet condition development and control will be discussed.

Complex Transport Phenomena

Alexandre Fabregat University of Ottawa

Nek5000 will be used to simulate complex transport phenomena in different flow configurations taking advantage of the high order accuracy of the underlying spectral element concept on which it has been based. Other approaches like the finite volume methods ensure local conservation of the transported quantities but they are often not suitable for complex geometries. On the other hand, spectral elements have been widely used under these scenarios becoming a reliable method to be used in configurations involving transitional flows, vortex shedding in airfoils, mesoscale meteorology and boundary layers. On the development side, we would like to implement the Discontinuous Galerkin approach to improve the local conservation using the numerical flux concept at the cell boundaries while keeping the same nek5000 algorithm that has demonstrated to be highly efficient on parallel architectures.

DNS of low Mach number combustion

Christos Frouzakis Swiss Federal Institute of Technology

Rayleigh-Taylor unstable, premixed flames: the transition towards turbulence

Elizabeth Hicks University of Chicago

A premixed flame moving against a sufficiently strong gravitational field becomes deformed and creates vorticity. If gravity is strong enough, this vorticity is shed and deposited behind the flame front. I will show two-dimensional simulations of this vortex shedding process and its effect on the flame front for various values of the gravitational force. The flame and its shed vortices go through the following stages as gravity is increased: no vorticity and a flat flame front; long vortices attached to a cusped flame front; instability of the attached vortices and vortex shedding (Hopf bifurcation); disruption of the flame front by the shed vortices, causing the flame to pulsate; loss of left/right symmetry (period doubling); dominance of Rayleigh-Taylor instability over burning (torus bifurcation); and, finally, complex interactions between the flame front and the vortices.

Large-eddy simulation of a horizontal microjet in backward-facing step flow

H. KanchiH. AbbassiF. MashayekUniversity of Illinois at Chicago

Clean and efficient energy conversion is critical for our economy, environment, and national security. Our group is investigating novel methods for low-emission and efficient combustion, which is one of the most common methods of energy conversion. We have explored the use of microjets in dump combustors as an effective means to improve combustor performance. Reynolds averaged Navier-Stokes (RANS) simulations were performed to evaluate combustor design. By adding four horizontal microjets in a backward-facing step combustor, it was shown that there was a significant increase in the heat release rate compared to the base case without microjets depending on microjet velocity. The finalized design using RANS simulations were used for experiments and the data collected from these experiments confirmed computational trends. In the next stage of our systematic investigation, large-eddy simulations (LES) need to be performed for a better understanding of the flow dynamics using Nek5000. LES studies of a reacting case with four microjets in a combustor will be too complex and computationally expensive. Hence, we begin with a case with only one microjet in the backward-facing step combustor and simulate a non-reacting case using Nek5000. Simultaneously, our group is working on developing Nek5000 to simulate reacting cases.

NekLBM: High-order Accurate Lattice Boltzmann Flow Solver with Spectral Element Discontinuous Galerkin Approximation

Taehun Lee City College of City University of New York Misun Min Argonne National Laboratory

The lattice Boltzmann method (LBM) is derived from the discrete Boltzmann equation by discretizing it on uniform rectangular mesh and usually comprises collision and streaming steps. While this greatly facilitates numerical procedure, it limits shapes of the computational domain that LBM can be applied to. This limitation could substantially increase computational effort for flows of boundary-layer type and in complex geometries. To overcome geometric constraint of LBM and to improve its numerical stability at high Reynolds number, we have recently proposed spectral element discontinuous Galerkin (SEDG) LBM, namely NekLBM. In this computational framework, LBM is regarded as a special space-time discretization of the discrete Boltzmann equation in the characteristic direction, and can be solved by higher-order accurate schemes on unstructured mesh. In this presentation, a brief introduction to the temporal and spatial discretizations of the discrete Boltzmann equation will be given, with emphasis on the SEDG approximation. Applications of NekLBM will be discussed in the simulations of shear layers and flow past an impulsively started cylinder. Planned work on NekLBM will be presented, which include extension to compressible flow, turbulent convection heat transfer, and liquid-vapor two phase flow.

Numerical Simulation of Biological Flows

Francis Loth University of Akron

Our group has been using Nek5000 to simulate biological flows for the past decade. We have simulated the hemodynamics of a stenosed carotid bifurcation and an arteriovenous graft. The goal for each simulation was to compute the biomechanical forces that the vessel experiences due to the complex flow pattern present within each of these geometries. Both simulations were based on human in vivo geometries and blood flow conditions. In both cases, transitional flow was observed. The numerical results of the arteriovenous graft were compared with experimental measurements using laser Doppler anemometry. Good agreement was obtained for both mean and RMS values of velocity. At present, we are conducting simulations of cerebrospinal fluid in the spinal canal to compute the hydrodynamic importance of a flow blockage in the spinal canal which can occur for a disease called Chiari Malformation. We hope to create an automated meshing scheme that will work well with Nek5000 in order to simulate patient specific cases rapidly for use in surgical planning.

Adaptive Spectral Elements

Catherine Mavriplis University of Ottawa

I will talk about adaptive Spectral Elements and my experience using high order methods, both spectral element and discontinuous Galerkin methods, in a variety of fields. We plan to write an adaptive high order discontinuous Galerkin code, so we look forward to your feedback about using nek5000. Grid generation is also of interest. Time permitting, I will also touch on comparisons we have done between spectral element and pseudospectral methods as well as discontinuous Galerkin with finnite difference and spectral difference.

Simulation of local phenomena for the flow in reactor cores and nuclear components

Elia Merzari Argonne National Laboratory

The accurate simulation of the flow in advanced and traditional nuclear reactors is of crucial importance to evaluate properly their design and safety margins. Such simulations are usually performed with mono-dimensional models, two-dimensional models or steady state CFD. To proper investigate the physics and validate such tools it is however often necessary to use higher fidelity techniques such as LES or DNS. These methodologies allow to investigate the physics of the flow in much bigger detail and to provide additional insight into the physics of the flows involved. In the present talk we will examine three examples: the flow in a counter-flow T-junction, the flow in a simplified geometry reminiscent of wire-wrappers and the flow in a rod-bundle with spacers.

NekCEM: Performance and Scalability for Electromagnetic Modeling

Misun Min Argonne National Laboratory

NekCEM is a massively paralell, scalable high-order electromagnetic solver that uses the core structure of Nek5000. NekCEM is built for simulation-based investigations to understand the fundamental optical properties and predict optimal designs of advanced nanomaterials and next-generation accelerator devices. I will present performance and and scalability of NekCEM on the IBM BG/P for time-domain electromagnetic simulations based on spectral-element discontinuous Galerkin discretizations.

Magneto-Hydrodynamics with Nek5000

Aleks Obabko Argonne National Laboratory

We will describe how to setup Nek5000 to solve magneto-hydrodynamical (MHD) equations and provide an example test case based on dynamo flows by Galloway and Proctor.

Ocean Modeling Applications

Tamay Ozgokmen University of Miami

Grid Overlapping Capabilities in NEK 5000

Yulia Peet Argonne National Laboratory

It is well known that grid overlapping methods represent a powerful tool for simulating engineering problems in complex geometries, since they alleviate mesh generation process, provide a convenient way of resolution control and even allow for modeling different physics in multiphysics systems. Spectral element method is an excellent basis for grid overlapping procedure due to a high (spectral) accuracy of grid-to-grid interpolation, usually a weak point in conventional composite grid methods using finite-difference schemes. In the current talk, we will present the grid overlapping capabilities which were introduced into the NEK5000, describe the numerical methodology, comment on some interesting stability properties, and highlight a variety of problems which open up for investigation with the grid overlapping strategy. Finally, we will show an example of calculations performed with this method to simulate turbulent heat transfer in a model wire-wrapped fuel pin configuration.

A comparison of Nek5000 and OpenFOAM for DNS of turbulent channel flow

Michael Sprague Matthew Churchfield Avi Purkayastha Patrick Moriarty Sang Lee *National Renewable Energy Laboratory*

In this work we compare the performance of a high-order spectral finite-element code (Nek5000) with a low-order finite-volume code (OpenFOAM) for direct numerical simulation of incompressible turbulent channel flow. The channel-flow test problem is that described by Kim, Moin, and Moser (JFM 1987). The two codes are examined in terms of accuracy and wall-clock solution time for given spatial-refinement levels. We examined friction velocity and profiles for mean velocity and r.m.s. of velocity fluctuations. Strong-scaling performance was examined with 10-million-grid-point models on 32 to 2048 cores.

Transport in a Chaotic Flow Field

Himanshu Tiwari Mark Paul Virginia Tech

We study the transport of a scalar species in the flow field of Rayleigh-Bénard convection that is exhibiting spatiotemporal chaos. Recent work has quantified the passive transport of a scalar species in a spiral defect chaos flow field to yield enhanced diffusion. In this work we are interested in allowing the scalar species to also undergo active transport. For example, the combustion of premixed gases where the scalar quantity can react, or the motion of microorganisms in bioconvection where the scalar quantity can swim in some preferential direction.

We intend to present the details of the numerical set-up for the simulations to be run using Nekton and discuss some of the challenges. It is anticipated that these simulations will provide new physical insights into reaction-diffusion phenomena such as combustion of pre-mixed gases, convection of phytoplankton in rivers and oceans, and forecasting weather and climate, to name a few.

Conjugate Heat Transfer in LMFBR Fuel Pins

Justin Walker Argonne National Laboratory

Understanding the problem of heat transfer from fuel pins to liquid metal coolant is critical for the design of safe and efficient thermal hydraulic systems of SFR. The complex geometry of 271-pin sub-assemblies provides challenges in computing the temperature profile. Mean field calculations have been done with sub-channel or, more recently, RANS codes. Advances in computing power and algorithms allow us to now tackle this problem with LES and, potentially, DNS codes. I will

discuss the results of Nek5000 simulations I have run of the CHT problem with a single fuel pin without the wire wrapped spacer. I will conclude with a discussion of the setup of a single wire wrapped pin.