Dear Colleagues,

Computational Science and Discovery (CSD) was conceived to be a forum where scientific discovery in physics, chemistry, and biology achieved through computation could be reported fully and effectively. It was envisioned, and thereafter built into the definition and structure of CSD, that such breakthroughs would be achieved through multidisciplinary collaboration and that corroboration by other research groups, given the complexity of the systems considered, would be essential. CSD has provided a vehicle where multidisciplinary collaboration and authorship is encouraged and where all relevant simulation details can be provided, from the underlying numerical methods, details of the computer codes used, workflow management strategies, to scientific visualization and discovery. Moreover, given its electronic-only format, CSD is able to provide simulation data, simulation code, and other relevant “data” to its readers and the scientific user community in an effort to facilitate understanding of the scientific discoveries documented in its pages and the corroboration of these results by others after the fact.

We are happy to report that CSD continues to grow. The first two issues of articles, outlined here, comprise a collection of significant advances made in fields as diverse as lattice quantum chromodynamics, nuclear theory, nano- and materials science, combustion and fusion energy science, accelerator science, aeronautics, Earth and atmospheric science, and computational cosmology. CSD has also grown in another important respect. Its editorial board has nearly doubled in size since the launch, bringing both the breadth and the depth that will better enable CSD to ensure that all areas of physics, chemistry, and biology are well represented and are given the opportunity to use this new setting for their benefit. CSD’s breadth is unprecedented, and ensuring that such breadth is managed effectively has been an exciting challenge, one we continue to meet.

In the current collection, you will find articles devoted to the underlying numerical methods that will find application in future simulations, detailed descriptions of important community simulation codes that have played and will continue to play an important role in future computational advances, and scientific breakthroughs made through the use of high-performance and large-scale computing in many areas of physics, chemistry, and biology. You will also find review articles that capture the scientific state of the art, outline the numerical approaches adopted to date, and point to future challenges as greater complexity is considered.

I am particularly pleased to note that those who have published in CSD have enjoyed a substantial readership, as evidenced by significant downloads of articles in this collection, and have expressed their appreciation of the ability to include many, if not all, important aspects of their complex simulations in one place, together with the scientific discoveries made.

On behalf of its Editorial Board, I ask that you will allow CSD to serve as an effective tool in disseminating your next breakthroughs and in delineating the myriad components of your ever more complex simulations as we venture forth to the exascale.

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Plot of the the electrostatic potential isosurface for the dimer of a tetracyano substituted vinylbenzene monomer B G Sumpter et al 2008 Comput. Sci. Disc. 1 015006
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Iterative methods for overlap and twisted mass fermions

T Chiarappa, K Jansen, K I Nagai, M Papinutto, I Scorzato, A Shindler, C Urbach, U Wenger and I Wetzorke

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Abstract

We present a comparison of a number of iterative solvers of linear systems of equations for obtaining the fermion propagator in lattice quantum chromodynamics (QCD). In particular, we consider chirally invariant overlap and chirally improved Wilson (maximally) twisted mass (TM) fermions. The comparison of both formulations of lattice QCD is performed at four fixed values of the pion mass between 230 and 720MeV. For overlap fermions we address adaptive precision and low-mode preconditioning while for TM fermions we discuss even/odd preconditioning. Taking the best available algorithms in each case we find that calculations with the overlap operator are by a factor of 30–120 more expensive than with the TM operator.

Numerical ansatz for solving integro-differential equations with increasingly smooth memory kernels: spin-boson model and beyond

Michael Zwolak

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Abstract

We present an efficient and stable numerical ansatz for solving a class of integro-differential equations. We define the class as integro-differential equations with increasingly smooth memory kernels. The resulting algorithm reduces the computational cost from the usual $T^2$ to $TC(T)$, where $T$ is the total simulation time and $C(T)$ is some function. For instance, $C(T)$ is equal to $\ln T$ for polynomially decaying memory kernels. Due to the common occurrence of increasingly smooth memory kernels in physical, chemical and biological systems, the algorithm can be applied in quite a wide variety of situations. We demonstrate the performance of the algorithm by examining two cases. Firstly, we compare the algorithm to a typical numerical procedure for a simple integro-differential equation. Secondly, we solve the non-interacting blip approximation equations for the spin-boson model in real time.
Deterministic point inclusion methods for computational applications with complex geometry

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Abstract

A fundamental problem in computation is finding practical and efficient algorithms for determining if a query point is contained within a model of a three-dimensional solid. The solid is modeled using a general boundary representation that can contain polygonal elements and/or parametric patches. We have developed two such algorithms: the first is based on a global closest feature query, and the second is based on a local intersection query. Both algorithms work for two- and three-dimensional objects. This paper presents both algorithms, as well as the spatial data structures and queries required for efficient implementation of the algorithms. Applications for these algorithms include computational geometry, mesh generation, particle simulation, multiphysics coupling, and computer graphics. These methods are deterministic in that they do not involve random perturbations of diagnostic rays cast from the query point in order to avoid ‘unclean’ or ‘singular’ intersections of the rays with the geometry. Avoiding the necessity of such random perturbations will become increasingly important as geometries become more convoluted and complex.

The RAGE radiation-hydrodynamic code

Michael Gittings¹, Robert Weaver¹, Michael Clover¹, Thomas Betlach¹, Nelson Byrne¹, Robert Coker², Edward Dendy², Robert Hueckstaedt², Kim New², W Rob Oakes², Dale Ranta¹ and Ryan Stefan³

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Abstract

We describe RAGE, the ‘radiation adaptive grid Eulerian’ radiation-hydrodynamics code, including its data structures, its parallelization strategy and performance, its hydrodynamic algorithm(s), its (gray) radiation diffusion algorithm, and some of the considerable amount of verification and validation efforts. The hydrodynamics is a basic Godunov solver, to which we have made significant improvements to increase the advection algorithm’s robustness and to converge stiffnesses in the equation of state. Similarly, the radiation transport is a basic gray diffusion, but our treatment of the radiation–material coupling, wherein we converge nonlinearities in a novel manner to allow larger timesteps and more robust behavior, can be applied to any multi-group transport algorithm.

Exploded multi-material hybrid volume mesh on a spherical-like geometry.

Double Mach reflection test problem, blown up in the vicinity of the Mach stem, showing the effect of the tensor artificial viscosity on the vortical flow.
A combined theoretical and experimental study of the polymer inter-chain structure in poly (phenylene vinylene) derivatives

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Abstract
The structures and photophysical properties of single molecule MEh-PPV (2-methoxy-5-(2-ethyl-hexyloxy)-p-phenylenevinylene) and CN-PPV (2,5,2',5'-tetrahexyloxy-7,8'-dicyano-p-phenylenevinylene) nanoparticles are investigated using electronic structure theory and high resolution fluorescence experiments. It is shown that electron withdrawing substituents, such as CN, on the vinyl group of the PPV polymer backbone cause substantial change in the \( \pi \) electronic structure which subsequently decreases the inter-chain distance. Not only does CN-PPV have a smaller inter-chain separation compared to MEh-PPV, but also an increased binding energy and more efficient charge transport (carrier mobility) due to larger electronic coupling (charge transfer integrals). These changes help explain the enhanced luminescence quantum yield, photo-stability, and lifetime for CN-PPV versus MEh-PPV observed in experimental high resolution fluorescence imaging of individual single molecule nanoparticles.

Computational aspects of nuclear coupled-cluster theory

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Abstract
Coupled-cluster (CC) theory represents an important theoretical tool that we use to solve the quantum many-body problem. CC theory also lends itself to computation in a parallel computing environment. In this paper, we present selected results from \( \textit{ab initio} \) studies of stable and weakly bound nuclei utilizing computational techniques that we employ to solve CC theory. We also outline several perspectives for future research directions in this area.

Simulating nonlinear neutrino flavor evolution

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Abstract
We discuss a new kind of astrophysical transport problem: the coherent evolution of neutrino flavor in core collapse supernovae. Solution of this problem requires a numerical approach which can simulate accurately the quantum mechanical coupling of intersecting neutrino trajectories and the associated nonlinearity which characterizes neutrino flavor conversion. We describe here the two codes developed to attack this problem. We also describe the surprising phenomena revealed by these numerical calculations. Chief among these is the nonlinearity in the problem can engineer neutrino flavor transformation which is dramatically different to that in standard Mikheyev–Smirnov–Wolfenstein treatments. This happens even though the neutrino mass-squared differences are measured to be small, and even when neutrino self-coupling is sub-dominant. Our numerical work has revealed potential signatures which, if detected in the neutrino burst from a Galactic core collapse event, could reveal heretofore unmeasurable properties of the neutrinos, such as the mass hierarchy and vacuum mixing angle \( \theta_{13} \).
The nuclear force from Monte Carlo simulations of lattice quantum chromodynamics

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Abstract
The nuclear force acting between protons and neutrons is studied in the Monte Carlo simulations of the fundamental theory of strong interaction, the quantum chromodynamics defined on the hypercubic space-time lattice. After a brief summary of the empirical nucleon–nucleon (NN) potentials that can fit the NN scattering experiments in high precision, we outline the basic formulation for deriving the potential between the extended objects such as the nucleons composed of quarks. The equal-time Bethe–Salpeter (BS) amplitude is a key ingredient for defining the NN potential on the lattice. We show the results of the numerical simulations on a 32^4 lattice with lattice spacing a ≈ 0.137 fm (lattice volume (4.4 fm)^4) in the quenched approximation. The calculation was carried out using the massively parallel computer Blue Gene/L at the High Energy Accelerator Research Organization (KEK). We found that the calculated NN potential at low energy has the basic features expected from the empirical NN potentials: attraction at long and medium distances, and the repulsive core at short distances. Various future directions along this line of research are also summarized.

Nonlinear turbulent transport in magnetic fusion plasmas

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Abstract
For more than a decade, the study of microturbulence driven by ion temperature gradient (ITG) drift instabilities in tokamak devices has been an active area of research in magnetic fusion science for both experimentalists and theorists alike. An important impetus for this avenue of research was the discovery of the radial streamers associated with the ITG modes in the early 1990s using the particle-in-cell (PIC) simulation method. Subsequently, ITG simulations using codes with increasing realism have been made possible by the dramatic increase in computing power. Notable examples were the demonstration of the importance of nonlinearly generated zonal flows in regulating ion thermal transport and the transition from Bohm to gyroBohm scaling with increased device size. In this paper, we will describe an interesting nonlinear physical process, as well as the resulting turbulent transport, that is associated with the interactions between the nonlinear parallel acceleration of the ions and the zonal flow modes. This study was carried out by utilizing a fully parallelized three dimensional PIC code in global toroidal geometry on the most advanced, modern, massively parallel supercomputers.

Topical review: Multiscale methods in turbulent combustion: strategies and computational challenges

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2009 Computational Science & Discovery 2 013001

Abstract
A principal challenge in modeling turbulent combustion flows is associated with their complex, multiscale nature. Traditional paradigms in the modeling of these flows have attempted to address this nature through different strategies, including exploiting the separation of turbulence and combustion scales and a reduced description of the composition space. The resulting moment-based methods often yield reasonable predictions of flow and reactive scalars’ statistics under certain conditions. However, these methods must constantly evolve to address combustion at different regimes, modes or with dominant chemistries. In recent years, alternative multiscale strategies have emerged, which although in part inspired by the traditional approaches, also draw upon basic tools from computational science, applied mathematics and the increasing availability of powerful computational resources. This review presents a general overview of different strategies adopted for multiscale solutions of turbulent combustion flows. Within these strategies, some specific models are discussed or outlined to illustrate their capabilities and underlying assumptions. These strategies may be classified under four different classes, including (i) closure models for atomistic processes, (ii) multigrid and multiresolution strategies, (iii) flame-embedding strategies and (iv) hybrid large-eddy simulation–low-dimensional strategies. A combination of these strategies and models can potentially represent a robust alternative strategy to moment-based models; but a significant challenge remains in the development of computational frameworks for these approaches as well as their underlying theories.
Terascale direct numerical simulations of turbulent combustion using S3D

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Abstract
Computational science is paramount to the understanding of underlying processes in internal combustion engines of the future that will utilize non-petroleum-based alternative fuels, including carbon-neutral biofuels, and burn in new combustion regimes that will attain high efficiency while minimizing emissions of particulates and nitrogen oxides. Next-generation engines will likely operate at higher pressures, with greater amounts of dilution and utilize alternative fuels that exhibit a wide range of chemical and physical properties. Therefore, there is a significant role for high-fidelity simulations, direct numerical simulations (DNS), specifically designed to capture key turbulence-chemistry interactions in these relatively uncharted combustion regimes, and in particular, that can discriminate the effects of differences in fuel properties. In DNS, all of the relevant turbulence and flame scales are resolved numerically using high-order accurate numerical algorithms. As a consequence terascale DNS are computationally intensive, require massive amounts of computing power and generate tens of terabytes of data. Recent results from terascale DNS of turbulent flames are presented here, illustrating its role in elucidating flame stabilization mechanisms in a lifted turbulent hydrogen/air jet flame in a hot air coflow, and the flame structure of a fuel-lean turbulent premixed jet flame. Computing at this scale requires close collaborations between computer and combustion scientists to provide optimized scaleable algorithms and software for terascale simulations, efficient collective parallel I/O, tools for volume visualization of multiscale, multivariate data and automating the combustion workflow. The enabling computer science, applied to combustion science, is also required in many other terascale physics and engineering simulations. In particular, performance monitoring is used to identify the performance of key kernels in the DNS code, S3D and especially memory intensive loops in the code. Through the careful application of loop transformations, data reuse in cache is exploited thereby reducing memory bandwidth needs, and hence, improving S3D’s nodal performance. To enhance collective parallel I/O in S3D, an MPI/I/O caching design is used to construct a two-stage write-behind method for improving the performance of write-only operations. The simulations generate tens of terabytes of data requiring analysis. Interactive exploration of the simulation data is enabled by multivariate time-varying volume visualization. The visualization highlights spatial and temporal correlations between multiple reactive scalar fields using an intuitive user interface based on parallel coordinates and time histogram. Finally, an automated combustion workflow is designed using Kepler to manage large-scale data movement, data morphing, and archival and to provide a graphical display of run-time diagnostics.

SURPRISES: when ab initio meets statistics in extended systems

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Abstract
The surface photoelectron and inner shell electron spectroscopy (SURPRISES) program suite performs ab initio calculations of photoionization and non-radiative decay spectra in nanoclusters and solid state systems by using a space-energy similarity procedure to reproduce the band-like part of the spectra. This approach provides an extension of Fano resonant multichannel scattering theory dealing with the complexity arising from condensed matter calculations at a computational cost comparable to that of molecules. The bottleneck of electron spectroscopy ab initio calculations in condensed matter is the size of the Hilbert space where the wavefunctions are expanded and the increase in number of final decay states in comparison to that of atoms and molecules. In particular, the diagonalization of the interchannel interaction to take into account the correlation between the double ion and the escaping electron is impracticable when hole delocalization on valence bands and electronic excitations are included in the model. To overcome this problem SURPRISES uses a ‘space-energy similarity’ approach, which allows the spreading of the Auger probability over the bands without tuning semi-empirical parameters. Furthermore, a completely new feature in the landscape of ab initio resonant decay processes calculations is represented by including energy loss through a statistical approach. Using the calculated lineshape as electron source, a Monte Carlo routine simulates the effect of inelastic losses on the original lineshape. In this process, the computed spectrum can be directly compared with acquired experimental spectra, thus avoiding background subtraction, a procedure not free from uncertainty. The program can exploit the symmetry of the system under investigation to reduce the calculation scaling and may compute photoemission and Auger decay angular
High performance parallel computing of flows in complex geometries: I. Methods

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Abstract

Efficient numerical tools coupled with high-performance computers, have become a key element of the design process in the fields of energy supply and transportation. However flow phenomena that occur in complex systems such as gas turbines and aircrafts are still not understood mainly because of the models that are needed. In fact, most computational fluid dynamics (CFD) predictions as found today in industry focus on a reduced or simplified version of the real system (such as a periodic sector) and are usually solved with a steady-state assumption. This paper shows how to overcome such barriers and how such a new challenge can be addressed by developing flow solvers running on high-end computing platforms, using thousands of computing cores. Parallel strategies used by modern flow solvers are discussed with particular emphases on mesh-partitioning, load balancing and communication. Two examples are used to illustrate these concepts: a multi-block structured code and an unstructured code. Parallel computing strategies used with both flow solvers are detailed and compared. This comparison indicates that mesh-partitioning and load balancing are more straightforward with unstructured grids than with multi-block structured meshes. However, the mesh-partitioning stage can be challenging for unstructured grids, mainly due to memory limitations of the newly developed massively parallel architectures. Finally, detailed investigations show that the impact of mesh-partitioning on the numerical CFD solutions, due to rounding errors and block splitting, may be of importance and should be accurately addressed before qualifying massively parallel CFD tools for a routine industrial use.

High performance parallel computing of flows in complex geometries: II. Applications

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Abstract

Present regulations in terms of pollutant emissions, noise and economical constraints, require new approaches and designs in the fields of energy supply and transportation. It is now well established that the next breakthrough will come from a better understanding of unsteady flow effects and by considering the entire system and not only isolated components. However, these aspects are still not well taken into account by the numerical approaches or understood whatever the design stage considered. The main challenge is essentially due to the computational requirements inferred by such complex systems if it is to be simulated by use of supercomputers. This paper shows how new challenges can be addressed by using parallel computing platforms for distinct elements of a more complex systems as encountered in aeronautical applications. Based on numerical simulations performed with modern aerodynamic and reactive flow solvers, this work underlines the interest of high-performance computing for solving flow in complex industrial configurations such as aircrafts, combustion chambers and turbomachines. Performance indicators related to parallel computing efficiency are presented, showing that establishing fair criterions is a difficult task for complex industrial applications. Examples of numerical simulations performed in industrial systems are also described with a particular interest for the computational time and the potential design improvements obtained with high-fidelity and multi-physics computing methods. These simulations use either unsteady Reynolds-averaged Navier–Stokes methods or large eddy simulation and deal with turbulent unsteady flows, such as coupled flow phenomena (thermo-acoustic instabilities, buffet, etc). Some examples of the difficulties with grid generation and data analysis are also presented when dealing with these complex industrial applications.

Simulation of aero-elastic effects in a whole generic long range aircraft performed with eA-- instantaneous solution of total pressure.
Virtual materials design using databases of calculated materials properties

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Abstract

Materials design is most commonly carried out by experimental trial and error techniques. Current trends indicate that the increased complexity of newly developed materials, the exponential growth of the available computational power, and the constantly improving algorithms for solving the electronic structure problem, will continue to increase the relative importance of computational methods in the design of new materials. One possibility for utilizing electronic structure theory in the design of new materials is to create large databases of materials properties, and subsequently screen these for new potential candidates satisfying given design criteria. We utilize a database of more than 81 000 electronic structure calculations. This alloy database is combined with other published materials properties to form the foundation of a virtual materials design framework (VMDf). The VMDf offers a flexible collection of materials databases, filters, analysis tools and visualization methods, which are particularly useful in the design of new functional materials and surface structures. The applicability of the VMDf is illustrated by two examples. One is the determination of the Pareto-optimal set of binary alloy methanation catalysts with respect to catalytic activity and alloy stability; the other is the search for new alloy mercury absorbers.

Macro–micro interlocked simulation algorithm: an exemplification for aurora arc evolution

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Abstract

Using an innovative holistic simulation algorithm that can self-consistently treat a system that evolves as cooperation between macroscopic and microscopic processes, the evolution of a colorful aurora arc is beautifully reproduced as the result of cooperation between the global field-aligned feedback instability of the coupled magnetosphere–ionosphere system and the ensuing microscopic ion-acoustic instability that generates electric double layers and accelerates aurora electrons. These results are in agreement with rocket and satellite observations. This shows that the proposed holistic algorithm could be a reliable tool to reveal complex real dramatic events and become, in the near future, a viable scientifically secure prediction tool for natural disasters such as earthquakes, landslides and floods caused by typhoons.

An anisotropic preconditioning for the Wilson fermion matrix on the lattice

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Abstract

A preconditioning for the Wilson fermion matrix on the lattice is defined, which is particularly suited to the case when the temporal lattice spacing is much smaller than the spatial one. Details on the implementation of the scheme are given. The method is tested in numerical studies of quantum chromodynamics on anisotropic lattices.
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