

AMCOS

Conference and Tutorial on
Analysis and Modelling of Complex Oscillatory Systems

March 19-23, 2018
PRBB, Barcelona



Universitat
Pompeu Fabra
Barcelona



This is the short version of the booklet for print use. Full abstracts with all authors, references, and figures can be found in the electronic version at
<https://amcosconference.com/>

The open-source L^AT_EX template, AMCOS_booklet, used to generate this booklet is available at https://github.com/maximelucas/AMCOS_booklet

Contents

About	6
AMCOS	6
COSMOS	6
Organizing committee	6
Timetable	7
Tuesday, 20 of March	7
Wednesday, 21 of March	8
Thursday, 22 of March	9
List of Abstracts	10
Modeling of flow and mass transfer in virtual porous media <i>Aziz Mohammed, Harun Koku</i>	11
Orgu Kuantum Renk Dinamiginde Ω_{cc} Baryonunun Yarı-Leptonik Gecisinin İncelenmesi <i>Hüseyin Bahtiyar</i>	12
Study of Dilepton Spectrum with Machine Learning Approach at the LHC <i>Serpil Yalçın KUZU</i>	13
Preliminary Data Recognition on Collision Images at Large Hadron Collider with Machine Learning Techniques <i>İlkay Türk ÇAKIR^{1,2}, Sajad EINY³, Sinan KUDAY⁴</i>	14
Static and Dynamic Modeling of N-Methyl-Indole (N=1-6) in Water at the B3LYP/AMBER Level Using the COBRAMM Interface <i>Caglar KARACA¹, Fehmi BARDAK², Etem KOSE³, Ahmet ATAC²</i>	15
Ab-initio MD Investigation of Co-based Planar Molecular Catalyst Immersed in Water: H ₂ Production Mechanism <i>İpek GÜCLÜ, Yeliz GÜRDAL</i>	16
Theoretical Insight Into Hydrogen Evolution Mechanism of Pentadentate Molec- ular Catalyst Having Cobalt As Reaction Center <i>Ayas KİSER, Yeliz GÜRDAL</i>	17
Effect of Copper-Coated Storage Materials on Reaction Kinetics <i>Gamze ATALMIŞ¹, Serkan TOROS², Nebi YELEGEN¹, Yüksel KAPLAN¹</i>	18
Yapay zeka ile hızlandırılmış nano-malzeme keşfi <i>Şener ÖZÖNDER¹, H. Kübra KÜÇÜKKARTAL²</i>	19

Size dependent change of mean square displacement in gold nanocrystals : A molecular dynamics simulation <i>Merdan BATYROW¹, İlknur ERUÇAR², Hande ÖZTÜRK¹</i>	20
Aerodinamik Veritabanı Modellerinin Adaptif Deney Tasarım Yöntemi ile İyileştirilmesi ve Sürecin Hızlandırılması <i>Ertan DEMİRAL, Kivanç ARSLAN, Çağatay ŞAHİN</i>	21
Classification of Stochastic Processes with Topological Data Analysis <i>İsmail GÜZEL, Atabey KAYGUN</i>	22
Dağıtık Ortamda Derece İlintileri Bazlı Gerçekçi Çizge Üretilimi <i>Furkan ATAS, Mehmet Burak AKGÜN</i>	23
A Simplified Methodology For Rotor-Stator Interaction Problems With An Upwind Linearized Harmonic Solver <i>Arash KARSHENASS, Özgür Uğraş BARAN, Onur ATA</i>	24
Parallel Performance Comparison of GMRES Type Sparse Matrix Solvers for Inviscid Flux Schemes using Open-Source CFD Solver SU2 <i>Uğurtan DEMİRTAŞ, Nilay SEZER-UZOL</i>	25
Kimyasal tepkimeli türbülanslı akışlar için hesaplamalı akışkanlar dinamiği çözümüsü, lestr3d <i>Tamer ŞENER, Burakhan ŞÜKÜROĞLU, Ayse G. GUNGOR</i>	26
RANS and LES of a Turbulent Non-Premixed Flame Using OpenFOAM <i>Yunus Emre KARASU, Tugba ZAMAN, Ayse G. GUNGOR</i>	27
Kısmi Karışıklı bir Yanma Odası Tasarımında Girdap Etkilerinin İncelenmesi <i>Yunus Emre KARASU¹, Tuğba ZAMAN¹, Ayşe Gül GÜNGÖR¹, Dilay GÜLERYÜZ², Emre BÖNCÜ², Tahsin Berk KIYMAZ², Mehmet KARACA³, Barış YILMAZ⁴, Christophe ALLOUIS⁵, İskender GÖKALP⁵</i>	28
Parallel Aeroacoustic Computation of Unsteady Transonic Cavity Flow via Open CFD Source Codes <i>Ali Can FADIL, Bahar ZAFER</i>	29
Implementations of the Needleman-Wunsch Algorithm for GPU Architectures <i>Furkan KURT, Deniz Turgay ALTILAR, Ayşe Yilmazer METİN</i>	30
Performance Evaluation of CUDA Optimizations for Convolution Operations <i>Burak TOPÇU, Işıl Öz</i>	31
Accelerating Graph Embedding on a Single GPU Using Graph Reordering <i>Amro Alabsi ALJUNDI, Kamer KAYA</i>	32
GPU-accelerated floating random walk based transient heat conduction solver <i>Ersin YILDIZ, Altuğ Melik BAŞOL</i>	33
Feasibility Study of Adding GPU Support to SU2 with ILU(0) Preconditioner <i>Najeeb AHMAD¹, Bilge Kaan GÖRÜR², Uğurtan DEMİRTAŞ², Özgür ATEŞOĞLU², Didem UNAT¹</i>	34
Izometrik Kasılmada Aponevroz Ortusunun Rolu ve Seklinin Eniyileme Yöntemiyle Tahminine Yonelik Hesaplamalar <i>Şükrü Furkan TAŞDEMİR, Cevat Volkan KARADAĞ, Ali Fethi OKYAR</i>	35

SIMD Instructions for Ethereum Virtual Machine	
<i>Aykut Bozkurt, Can Özturan</i>	36
A Graph Transformation Strategy for Optimizing SpTRSV	
<i>Buse YILMAZ, Abdulkadir Furkan YILDIZ</i>	37
Pekistirmeli ogrenme ile 5G baz istasyonunun otomize olarak yapılandırılması	
<i>H. Tugrul ERDOĞAN, Adnan ÖZSOY</i>	38
Makine Öğrenmesi tabanlı Gerçek Zamanlı Hedef Tespiti için Güç Verimli Paralel Hesaplama	
<i>Alparslan FİŞNE¹, Faruk YAVUZ¹, Adnan OZSOY²</i>	39
Development of a Generic Neural Network Potential for IR-MOF Series	
<i>Ömer TAYFUROĞLU, Abdulkadir KOÇAK, Yunus ZORLU</i>	40
Tek Boyutlu, Sıralı, Büyük Ölçekli Veri Dizileri için Sıralı Örüntü Madenciliği Yaklaşımı	
<i>Ali Burak CAN¹, Meryem UZUN-PER^{1,2}, Mehmet S. AKTAŞ³</i>	41
Sensitivity Analysis of Federated Learning over Decentralized Data and Communication Rounds	
<i>Mustafa Barış ÇAMLI, İsmail ARI</i>	42
Çekirdek Sayısının Hesaplamlı Gemi Direnci Analiz Performansına Etkileri	
<i>Ali Can KOYUNCUOĞLU, Çağrı AYDIN, Uğur Oral ÜNAL, Barış BARLAS</i>	43
Kullanılan Çekirdek Sayısının Kapsama Alanı Haritası Çıkarılma Performansına Etkisi	
<i>Uğur ERBAŞ, Mehmet Barış TABAKCIOĞLU</i>	44
Efficient Thread-to-Core Mapping for Application-level Redundant Multithreading	
<i>Sanem ARSLAN¹, Osman UNSAL²</i>	45
COMDETECTIVE ⁺ : An Inter-Thread Communication Analyzer for AMD Multicores	
<i>Muhammad Aditya SASONGKO¹, Milind CHABB², Paul H. J. KELLY³, Didem UNAT¹</i>	46
Approximate Execution of Critical Sections for Performance-Accuracy Tradeoff	
<i>Zuhai ALTUNTAŞ, Sanem ARSLAN, Betül BOZ</i>	47
Paralel İşlerin Çizelgelemesinde İşlemci Tahsisi için Hippersezgisel Yaklaşım	
<i>Gülçin BOLAT, Fatih Erdoğan SEVİLGEN</i>	48
List of Participants	49
Useful Information	50
How to get to the PRBB?	50
Partner Institutions and Sponsors	52
Sponsors	52

About

This is a generic version of the real AMCOS conference booklet for which this L^AT_EX template was generated. All information about the use and distribution of this template, and all related codes, can be found at https://github.com/maximelucas/AMCOS_booklet.

AMCOS

The conference on Analysis and Modeling of Complex Oscillatory Systems (AMCOS) aims to bring together theoretical and experimental researchers working on the state of the art in the field of complex oscillatory systems.

The main topics of the conference comprise both (a) the modeling of complex systems and the emergence of collective behavior, as well as (b) the analysis of complex data sets in order to infer the underlying structure and functionality of networks. Particular focus will be put on oscillatory phenomena in neuroscience.

COSMOS

The AMCOS Conference is organized by the Early Stage Researchers (ESRs) of the Marie Curie Initial Training Network led by Arkady Pikovsky of Potsdam University. COSMOS trains 15 ESRs at the interface between Physics, Applied Mathematics, and Life Sciences, integrating theoretical and data-driven methods, in 7 universities across Europe.

Organizing committee

Gloria Cecchini	Marco Faggian	Aleksandra Pidde
Rok Cestnik	R. Janis Goldschmidt	Bastian Pietras
Pau Clusella	Marc Grau Leguia	Eero Satuvuori
Nicolás Deschle	Maxime Lucas	Çağdaş Topçu
Federico Devalle	Irene Malvestio	Clément Zankoc

Timetable

CT: Contributed Talk, IS: Invited Speaker, KL: Keynote Lecture, IT: Invited Talk.

Tuesday, 20 of March

8:30–9:00	Registration		
9:00–9:10	Welcome remarks		
9:10–10:05	KL	Leon Tremblay Montreal, Canada	Title of a keynote lecture
10:05–10:30	CT	Marc Fournier Brussels, Belgium	Title of contributed talk
10:30–11:00	Coffee		
11:00–11:40	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
11:40–12:45	CT	Marc Smith Brussels, Belgium	Title of contributed talk with math and paragraphs
12:45–14:00	Lunch		
14:00–14:30	CT	Marc Rodriguez Barcelona, Spain	Title of contributed talk with math and references
14:30–15:05	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
15:05–15:30	Coffee		
15:30–16:00	CT	Marc Jansen Amsterdam, The Netherlands	Title of contributed talk and references and a figure
16:00–17:10	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
17:10–19:30	Poster session with Wine & Cheese		

Wednesday, 21 of March

9:00-9:40	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
9:40-10:10	CT	Marc Fournier Brussels, Belgium	Title of contributed talk
10:10–12:45	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
10:45–11:10	Coffee		
11:10–11:40	CT	Marc Jansen Amsterdam, The Netherlands	Title of contributed talk and references and a figure
11:40–12:10	CT	Marc Jansen Amsterdam, The Netherlands	Title of contributed talk and references and a figure
12:10–12:45	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
12:45–14:00	Lunch		
14:00–14:30	CT	Marc Fournier Brussels, Belgium	Title of contributed talk
14:30-15:00	CT	Marc Fournier Brussels, Belgium	Title of contributed talk
16:30–18:00	Excursion		
20:00	Conference Dinner		

Thursday, 22 of March

9:00 – 9:40	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
9:40–10:20	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
10:20–10:45	IT	Franck Schmidt Munich, Germany	A Special Talk about Diversity in Science
10:45–11:10	Coffee		
11:10-11:40	CT	Marc Jansen Amsterdam, The Netherlands	Title of contributed talk and references and a figure
11:40–12:35	KL	Leon Tremblay Montreal, Canada	Title of a keynote lecture
12:35–12:45	Poster Prize & Conclusion		
12:45–14:00	Lunch		

List of Abstracts

Modeling of flow and mass transfer in virtual porous media

Aziz Mohammed, Harun Koku

Middle East Technical University Department of Chemical Engineering - Ankara, Turkey

In this work we simulated flow and mass transfer in virtual porous media for a liquid chromatography application. The three-dimensional geometry was formed by a diffusion-limited aggregation approach. The velocity field was obtained using the lattice Boltzmann methodology (LBM) via the PALABOS open-source library with modification. For mass transfer, a tracer-based random walk particle tracking (RWPT) model was used to obtain pulse simulation results.

Keywords

Chromatography, Random Walk, Flow simulation, mass transfer.

Orgu Kuantum Renk Dinamiginde Ω_{cc} Baryonunun Yarı-Leptonik Gecisinin İncelenmesi

Hüseyin Bahtiyar

Mimar Sinan Güzel Sanatlar Üniversitesi Fizik Bölümü - İstanbul, Türkiye

Tılsımlı parçacıkların yarı leptonik bozunmalarını incelenmesi, standart modeli test etmede öne çıkan bir yöntemdir. Tılsımlı baryon sektörünün zayıf bozunmalarındaki son zamanlarda geliştirilen deneylerden gelen motivasyon ile 2+ 1 çeşnili örgüler üzerinde $\Omega_{cc}^+ \rightarrow \Omega_c^0 \ell^+ \nu$ geçişinin form faktörleri incelenmiştir. Öncelikte iki ve üç nokta fonksiyonları hesaplanmış, boyutsuz projeksiyonlu korelatörler çıkarılmış ve form faktörler oluşturulması için korelatörler birleştirilmiştir. Sıfır aktarılan momentum limitinde f_1 ve g_1 form faktörleri hesaplanmış diğer modellerle uyumlu olduğu gözlemlenmiştir.

Keywords

Tılsımlı baryonlar, yarıleptonik form faktörler, Orgu KRD

Study of Dilepton Spectrum with Machine Learning Approach at the LHC

Serpil Yalçın KUZU

Firat University Faculty of Science, Department of Physics - Elazig, Turkey

Machine learning (*ML*) application in diverse fields has been favored to elevate the performance of human endeavors due to its effectiveness in solving different types of real-world issues requiring intensive computation. In particle physics, the investigation of dimuons ($\mu^+\mu^-$) has an important role to understand various systems produced at high energy collisions. The absence of strong interaction makes these lepton pairs suitable to examine particles such as J/ψ , Υ and Z boson. Dimuons can be identified by sophisticated techniques depending on cut-based methods as other particle analyses. In this contribution, the implementation of Random Forest and Weighted Random Forest ML models for defining dimuon pairs produced in proton-proton collisions at 7TeV at the LHC are discussed.

Keywords

Dimuon, lepton pairs, particle analysis, random forest, weighted random forest, machine learning.

Preliminary Data Recognition on Collision Images at Large Hadron Collider with Machine Learning Techniques

İlkay Türk ÇAKIR^{1,2}, Sajad EINY³, Sinan KUDAY⁴

¹ Ankara University Faculty of Engineering, Department of Artificial Intelligence Data Engineering - Ankara, Turkey

² Giresun University Faculty of Engineering, Department of Energy Systems Engineering - Giresun, Turkey

³ İstanbul Aydin University, Faculty of Engineering, Department of Computer Engineering - İstanbul, Turkey

⁴ Ankara University, Faculty of Science, Department of Physics - Ankara, Turkey

A preliminary analysis have been implemented to distinguish good events in Monte Carlo (MC) data using image recognition tools. All images from MC simulations are created with DELPHES detector program with ATLAS detector card. The experimental dataset contains some of the signal events in three different forms: side front, and -plane. We increased the number of images to 600 with improving image resolution, and quality by utilizing Image Data Augmentation code from Keras (Python deep learning API). Furthermore, we utilized transfer learning from ImageNet database due to overfitting problems. Different types of well-known models are employed for classification task such as VGG16, VGG19, Resnet 50, MobileNetv2 and Xception.

Keywords

ATLAS, machine learning, deep learning algorithm, Delphes

Static and Dynamic Modeling of N-Methyl-Indole (N=1-6) in Water at the B3LYP/AMBER Level Using the COBRAMM Interface

Caglar KARACA¹, Fehmi BARDAK², Etem KOSE³, Ahmet ATAC²

¹ Manisa Celal Bayar University Applied Research Center - Manisa, Turkey

² Manisa Celal Bayar University Department of Physics - Manisa, Turkey

³ Manisa Celal Bayar University Technical Sciences Vocational School - Manisa, Turkey

Computational dynamic emission spectroscopy in rigid medium solvents is a highly difficult technique. In recent years, technological improvement makes realistic models capable of experimental observables is possible. In this study, we have improved a successful simulation strategy in excitation and emission energies using hybrid models. The selected high layer target molecules and low and mobile layer water molecules are optimized with together. The hybrid QM/MM level is a powerful tool to efficiently is described the interactions of a molecule with its solvent medium. In this context, we simulate static and dynamic excited and emission spectra using COBRAMM interface protocol at the B3LYP/AMBER for rigid solvent models, TIP3P models are used within the mobile MM layer up to 50 nanometers radius away, for methyl derivatives of indole to a room-temperature. The QM/MM optimization calculations give us reliable structures both ground and excited states. Energy fluctuation of systems involves four states starting on the S0-S3, computations have been carried out by the same level for 150 femtoseconds. These calculated processes in ultrafast time scale have been explained how the evolution of excited and emission spectra when solvent molecules are movable. S0 and S1 geometry optimization of molecule in water droplet consisting of 500 TIP3P water are computed B3LYP/6-311++G(d,p) basis set and all low and mobile layer data was obtained Amber GAFF force field. S1 state geometry is converged approximately within 120 optimization cycles while the S0 optimization cycle takes longer time because of librational movements of water. Because this librational motion causes chaos at the RMS/D value, the number of mobile molecules has been reduced from the optimization steps. The energy difference between the first excited and ground state has a fluctuating character. The distribution of these fluctuations has been analyzed to create Fluctuating Gap Distribution (FGD) which reveals the most appropriate excitation/emission wavelengths.

Keywords

QM/MM md, Absorption and Emission, Lineer Response Theory

Ab-initio MD Investigation of Co-based Planar Molecular Catalyst Immersed in Water: H₂ Production Mechanism

İpek GÜÇLÜ, Yeliz GÜRDAL

Adana Alparslan Türkeş Science and Technology University Bioengineering Department - Adana, Turkey

The common use of hydrogen as a renewable energy source has been one of today's challenge which if solved can replace dependence on fossil fuels. One of the sustainable way of H₂ production is photo-catalytic water reduction reaction catalyzed by molecules having transition metals as reaction centers. In this work, we theoretically investigate water reduction mechanism of planar Cobalt based catalyst by employing Ab-initio Molecular Dynamics (AIMD) and Metadynamics (MTD) simulations. We model the first electron injection intermediate step of the ECEC reaction mechanism of the water reduction reaction. We identify the solvent response following the electron injection.

Keywords

Ab-initio Molecular Dynamics, Density Functional Theory, Cobalt-Bipyridine-Based Catalysts, Water Reduction

Theoretical Insight Into Hydrogen Evolution Mechanism of Pentadentate Molecular Catalyst Having Cobalt As Reaction Center

Ayas KİSER, Yeliz GÜRDAL

Adana Alparslan Türkeş Science and Technology University Bioengineering Department - Adana, Turkey

Hydrogen (H_2) molecule is a significant carrier of energy that is found naturally in biomass, water, and hydrocarbon. In this study, by applying Abinitio Molecular Dynamics simulations, we theoretically investigate water reduction mechanism of Co-based poly-pyridyl catalyst having octahedral coordination. For the hydrogen production cycle, ECEC mechanism is utilized and each intermediate step is simulated in order to determine the allowed spin states as well as solvent response around the reaction center. We demonstrate that, following the first electron injection, it is more likely for the catalyst to continue to the first protonation intermediate step with singlet multiplicity. Subsequently, following the first protonation step, Co center gains the required proton from the water molecule in the first solvation shell. Along the simulation, fast rotation of the nearest water molecule certifies the efficiency of the $CoPy_5$ for the water reduction reaction.

Keywords

Ab-initio molecular dynamics, H_2 production, water reduction

Effect of Copper-Coated Storage Materials on Reaction Kinetics

Gamze ATALMIŞ¹, Serkan TOROS², Nebi YELEGEN¹, Yüksel KAPLAN¹

¹ Niğde Ömer Halisdemir University Mechanical Engineering Department, Prof. Dr. T. Nejat Veziroglu Clean Energy Research Center - Nigde, Turkey

² Niğde Ömer Halisdemir University - Nigde, Turkey

In this study, hydrogen storage in metal hydride reactors was investigated numerically. A mathematical model including complex heat and mass transfer, which considers the flow occurring during the hydrogen charge/discharge process in metal hydride reactors, has been developed. In the experimental study, the thermal conductivity of the storage material, which was coated with copper and turned into pellets, was improved by 500-750 percent in order to accelerate the hydrogen charge/discharge processes and to get the needed hydrogen in a short time and at the desired flow rates. The developed macro modeling was solved numerically with the help of the COMSOL Multiphysics® software package. A two-dimensional axisymmetric model was developed to study the hydrogen absorption reaction. Simulation studies have shown that permeability of the metal hydride to be used in the study and thermal conductivity are essential for the optimization design of the metal hydride tank.

Keywords

hydrogen storage, metal hydride, two-dimensional axisymmetric.

Yapay zeka ile hızlandırılmış nano-malzeme keşfi

Şener ÖZÖNDER¹, H. Kübra KÜÇÜKKARTAL²

¹ İstinye Üniversitesi Elektrik-Elektronik Mühendisliği - İstanbul, Türkiye

² Eskişehir Osmangazi Üniversitesi Bilgisayar Mühendisliği - Eskişehir, Türkiye

Kimyasallar, ilaçlar, biyomalzemeler ve alaşımalar gibi malzemelerin çalışılması uzun yıllara yayılan süreçler gerektirmektedir. Ayrıca bu malzemelerin bulunan fiziksel ve kimyasal özellikleri pratik uygulamalar için aranan özelliklerle aynı olmayabilir. Bu uzun süreç yeni yapay zeka ve optimizasyon yöntemleriyle tersine çevrilebilir. Bir malzemeyi ve onun yapısal olarak yakın türevlerini sağlamak yerine, o malzemenin tüm olası türevlerini içeren kimyasal veya yapısal parametre uzayı hızlı ve akıllı bir şekilde taranarak istenilen fiziksel veya kimyasal özelliğe sahip malzeme yapısı bulunabilir. Bu amaçla Bayes optimizasyonu, Gauss regresyonu ve yapay sinir ağları hem laboratuvara sentez ile hem de bilgisayar ortamında simülasyonlar ile malzeme keşfini hızlandırmak için kullanılabilir.

Keywords

malzeme keşfi, makine öğrenmesi, yapay zeka, Bayes optimizasyonu, Gauss regresyonu, yapay sinir ağları, grafen.

Size dependent change of mean square displacement in gold nanocrystals : A molecular dynamics simulation

Merdan BATYROW¹, İlknur ERUÇAR², Hande ÖZTÜRK¹

¹ Özyegin University Dept. of Mechanical Engineering - İstanbul, Turkey

² Özyegin University Dept. of Natural and Mathematical Sciences - İstanbul, Turkey

Mean square displacements (MSDs) of 5, 10, 15, 20, and 30 nm diameter spherical gold nanocrystals were studied with Molecular Dynamics (MD) simulations at room temperature and below. Our analyses show that there is a strong size and temperature dependency of the MSD of spherical gold nanocrystals. Moreover, these displacements increase radially from the center of the nanocrystals and reach a maximum at the surface layers due to the presence of undercoordinated surface atoms and their relatively unrestricted motions. Results of this work will be useful to understand the effect of nanocrystal size on quantifying the amplitude of atomic vibrations and their effects on measured intensities from their x-ray diffraction data.

Keywords

Molecular dynamics simulations, gold nanocrystal, mean square displacement, x-ray diffraction, Debye-Waller factor.

Aerodinamik Veritabanı Modellerinin Adaptif Deney Tasarım Yöntemi ile İyileştirilmesi ve Sürecin Hızlandırılması

Ertan DEMİRAL, Kivanç ARSLAN, Çağatay ŞAHİN

ROKETSAN A.Ş. Aerodinamik Teknoloji Geliştirme Birimi - Ankara, Türkiye

Aerodinamik veritabanı modellerinin doğruluk seviyesi uçuş mekaniği çalışmalarının başarımı açısından kritik öneme sahiptir. Yüksek doğruluklu veritabanı modeli oluşturulması hem aerodinamik analiz yöntemine hem de analizlerin gerçekleştirileceği uçuş koşullarının doğru belirlenmesine bağlıdır. Bu çalışmada, aerodinamik veritabanı analizleri uçuş koşullarının adaptif deney tasarım yöntemi ile belirlenmesi amaçlanmıştır. Yapılan çalışmaların sonuçlarına göre, adaptif deney tasarım yöntemi örneklendirmeleri ile oluşturulan sürüklendirme katsayıları modelinin doğruluk seviyesi statik deney tasarım yöntemi örneklendirmeleri ile oluşturulan modele göre iyileştirilmiştir. Bununla beraber, adaptif deney tasarım çalışmaları grafik işlemci birimi sistemleri üzerinde yürütüllererek süreç hızlandırılmıştır.

Keywords

adaptif deney tasarım, aktif öğrenme, gauss süreci, aerodinamik

Classification of Stochastic Processes with Topological Data Analysis

Ismail GÜZEL, Atabey KAYGUN

İstanbul Technical University Mathematical Engineering - İstanbul, Türkiye

In this study, we examine if engineered topological features can distinguish time series sampled from different stochastic processes with different noise characteristics, in both balanced and unbalanced sampling schemes. We compare our classification results against the results of the same classification tasks built on statistical and raw features. We conclude that in classification tasks of time series, different machine learning models built on engineered topological features perform consistently better than those built on standard statistical and raw features.

Keywords

persistent homology, stochastic process, machine learning, feature engineering

Dağıtık Ortamda Derece İlintileri Bazlı Gerçekçi Çizge Üretilimi

Furkan ATAS, Mehmet Burak AKGÜN

TOBB Ekonomi ve Teknoloji Üniversitesi Bilgisayar Mühendisliği - Ankara, Türkiye

Çizge üreteçleri, yeni geliştirilen topolojik algoritmaları test etmek için kullanılan araçlardır. Algoritmalar gerçek sistemler üzerinde çalıştırılmadan önce, yapay çizgeler üzerinde performansları değerlendirilir. Bu testlerin sonucuna göre algoritmada gerekli düzenlemeler yapılır ve tekrar test edilir. Bu döngü, algoritmanın performansı istekleri karşılayacak seviyeye gelinceye kadar devam eder. Fakat algoritmanın test edildiği yapay çizgenin ait olduğu alanın çizge özelliklerini taşıyıp taşımaması, test sonuçlarının gerçeğe yakınlığında doğrudan etkin bir role sahiptir. Örneğin, yeni tasarılanan bir ağ protokolünü test etmek için bir sosyal ağ kullanmak, araştırmacıların ağ protokolünün gerçek performansını görmesine engel olacaktır. Dolayısıyla yapay olarak üretilen çizgenin mümkün olduğunda gerçekçi olması gereklidir. Rastgele üretilen bir çizgenin ait olduğu alana dair karakteristik özelliklerini korumak için gerçek bir çizgeyi kopyalamak en iyi yoldan biridir. Derece ilintileri bazlı yaklaşımlar çizgenin farklı derecelerdeki kenar-düğüm olasılıklarını kullanarak, verilen bir çizgeyi kopyalar. Günümüzde, internet erişiminin hem insanlar hem de cihazlar için kolaylaşmasıyla, üretilen veri hızla arttı. Büyük veri bir çok alanda kaçınılmaz hale geldi. Çizge verilerinin de büyük bir kısmı büyük veri seviyelerine geldi. Geleneksel tek makineli veri analitik çözümleri geniş ölçekli veriyi işlemek için yetersiz kaldı. Bu problemleri birleştirdiğimizde, büyük veri seviyesinde gerçekçi çizge üretimi problemi ortaya çıkmıştır. Bu çalışmada, Dk serisi kullanarak ölçülebilir algoritmaların tasarımları dağıtık olarak çalıştırılması gerçekleştirilmiştir.

Keywords

dağıtık hesaplama, yapay çizge üretimi, derece ilintileri, dk serisi

A Simplified Methodology For Rotor-Stator Interaction Problems With An Upwind Linearized Harmonic Solver

Arash KARSHENASS, Özgür Uğraş BARAN, Onur ATA

Middle East Technical University Mechanical Engineering Department - Ankara, Turkey

The family of harmonic techniques for flow problems is an approach for solving unsteady but temporally periodic problems. These problems are often found in industrial applications such as turbomachinery, helicopter, aeromechanic, noise generation. Time-accurate solutions to such problems are computationally expensive. The harmonic methods are preferred in such problems as they benefit the temporal periodicity for solving the time-independent governing equations in the frequency domain. The linearized harmonic method (LH) is the less sophisticated member of the family of harmonic flow solvers. LH methods allow the mean and perturbed flowfield to be solved separately and in sequence. Simplifications lead to the LH method allow solutions with less computational cost than more advanced harmonic methods. In this study, we assess the performance of a new LH method in turbomachinery flows. For this purpose, inviscid, ideal gas is considered as the working fluid with a novel upwind flux discretization scheme. An explicit multistage Runge-Kutta method is applied for solving LH equations for compressible flow within a compressor stage where shocks are present within the channel. LH model is developed with Loci framework and coupled with a modified version of flowPsi open-source CFD solver. The test case involves the flowfield within the NASA rotor-stator37 stage. For simplicity, it is assumed that generated disturbance waves only affect the stator domain and hence, only unsteady flowfield in the stator is investigated. The model can be extended to take the rotor domain also into account. Comparing LH results to those from time-accurate shows that LH resulted in over-amplification of unsteady effect, but much sharper discontinuities can be captured compared to the time-accurate solver.

Keywords

unsteady, turbomachine, stage37, rotor-stator, harmonic, linearized, Steger-Warming, upwind

Parallel Performance Comparison of GMRES Type Sparse Matrix Solvers for Inviscid Flux Schemes using Open-Source CFD Solver SU2

Uğurtan DEMİRTAŞ, Nilay SEZER-UZOL

Middle East Technical University Dept. of Aerospace Engineering - Ankara, Turkey

Computational Fluid Dynamics (CFD) is used in aerospace engineering design and analysis for aerodynamic database generation, investigation of wing/control surface interactions and aerodynamic stability analysis. Due to the need for lower computational times in design, implicit solvers are generally used in many CFD flow solvers. Implicit solvers being stable allow to use higher CFL (Courant-Friedrich-Lowy) numbers, larger than unity, to increase convergence for both steady and dual time stepping unsteady CFD cases. This comes with a price of solving block type sparse matrices that must be constructed and solved at each iteration on a CFD run. Since the nonlinearity of coupled Navier Stokes equations are stemmed from inviscid flux terms as in Euler equations which has no diffusion term unlike Navier Stokes equations, the condition number of block matrices are affected by the inviscid flux scheme used as well as Mach number in the domain. In this study, the effects of the inviscid flux scheme over the parallel performance of GMRES (General Minimizing RESidual) solvers used in open source CFD code SU2 are investigated.

Keywords

CFD, Parallel Computing, Sparse Matrix Solvers, SU2

Kimyasal tepkimeli türbülanslı akışlar için hesaplamalı akışkanlar dinamiği çözümü, lestr3d

Tamer ŞENER, Burakhan ŞÜKÜROĞLU, Ayse G. GUNGOR

İstanbul Teknik Üniversitesi Uçak ve Uzay Bilimleri Fakültesi - İstanbul, Türkiye

Tepkime sonucunda olusacak türler ile taze, yanmamış gazların karışılmasını sağlamak üzere yanma odalarında genellikle türbülanslı akış tercih edilir. Bu gibi problemlerde, kimyasal tepkime ile türbülansın etkilesimi sebebiyle ortaya çıkan akış yapılarının zaman ve uzay ölçekleri oldukça küçülür ve bu yapıların zengin fizигini modelleyebilmek üzere yüksek başarımı hesaplama ihtiyacı doğar. Kullanılan yazılımin ise yüksek başarımı hesaplama platformlarında kullanılan çekirdek sayısı artışı ile hesaplama hızında artış gözlemlenmeli ve bu yazılım platformdan bağımsız olmalıdır. Bu sebeple bu çalışmada, türbülanslı yanma benzetimleri için geliştirilen paralel akış çözümü lestr3d, yüksek başarımı platformlarda test edilmiş ve bu yazılımin ölçeklenebilir olduğu gösterilmiştir. Ayrıca, çekirdek sayısı ile hızlanma performansı tür deklemlerinin çözülmESİ ve çözülmemesi durumunda test edilmiştir. Bununla beraber bu yazılım farklı platformlarda, UHeM ve TRUBA, çalıştırılarak aynı sonucu verdiği ve platformdan bağımsız olduğu gösterilmiştir. Bunlara ek olarak akış çözümü lestr3d'nin türbülanslı küt bir cisim etrafındaki akış benzetimi sonuçları deneysel sonuçlar ile kıyaslanmış ve bu sonuçların birbiri ile uyumlu olduğu gösterilmiştir.

Keywords

Türbülanslı akışlar, Yanma, Yüksek Başarımı Hesaplama, Paralel Programlama, Büyük Girdap Benzetimi

RANS and LES of a Turbulent Non-Premixed Flame Using OpenFOAM

Yunus Emre KARASU, Tugba ZAMAN, Ayse G. GUNGOR

Istanbul Technical University Faculty of Aeronautics and Astronautics - Istanbul, Turkey

This paper presents numerical simulations of non-premixed methane-air diffusion flame, Sandia Flame D. The numerical simulations are performed with OpenFOAM. Reynolds averaged Navier–Stokes (RANS) approach is employed with different combustion and radiation models, and chemistry mechanisms. The results are compared with each other and against experimental data. It is found that the partially stirred reactor (PaSR) combustion model gives accurate results considering its computational cost and numerical accuracy with reduced GRI-Mech 3.0 and P1 radiation heat transfer model. RANS results are in reasonable agreement with experimental data and computationally affordable. Subsequently, large eddy simulation (LES) approach is employed. LES gives very good predictions of temperature profiles and species mixing. Although LES approach comes with increased CPU cost, it is required for simulating time-dependent flow characteristics and dynamics of the flame alongside enhanced numerical accuracy of mean profiles.

Keywords

Turbulent combustion, methane-air flame, RANS, LES, high performance computing.

Kısmi Karışıklı bir Yanma Odası Tasarımında Girdap Etkilerinin İncelenmesi

**Yunus Emre KARASU¹, Tuğba ZAMAN¹, Ayşe Gül GÜNGÖR¹, Dilay GÜLERYÜZ²,
Emre BÖNCÜ², Tahsin Berk KIYMAZ², Mehmet KARACA³, Barış YILMAZ⁴,
Christophe ALLOUIS⁵, İskender GÖKALP⁵**

¹ İstanbul Teknik Üniversitesi Uçak ve Uzay Bilimleri Fakültesi - İstanbul, Türkiye

² Orta Doğu Teknik Üniversitesi Makina Mühendisliği Bölümü - Ankara, Türkiye

³ Orta Doğu Teknik Üniversitesi Havacılık ve Uzay Mühendisliği Bölümü - Ankara, Türkiye

⁴ Marmara Üniversitesi Makina Mühendisliği Bölümü - İstanbul, Türkiye

⁵ Orta Doğu Teknik Üniversitesi Makina Mühendisliği Bölümü - Ankara, Türkiye

Bu çalışmada, kanatçıklı bir geometriye sahip, on karışısız bir yanma odasının soguk akış analizleri üç farklı model için gerçekleştirilmştir. Sayısal olarak kanatçıkları modellemek yüksek hesaplama maliyetlerini de beraberinde getirdiği için kanatçık geometrisi kullanılmadan akısa girdap etkisi kazandırmayı hedefleyen iki farklı model geliştirilmştir. Üçüncü modelde yanma odası kanatçık ile birlikte modellenmiştir. Tüm modeller ile elde edilen sonuçlar deneyel veriler ile kıyaslanmıştır.

Giriste girdap etkisi kazandırılmış olan kanatçiksız model, eksenel ve tegetsel hızlarda deneye yakın sonuçlar elde etmistir. Merkezi sirkulasyon bölgesinin yakalanmasında yalnızca kanatçık geometrisi dahil edilen model deneye yakınsamaktadır.

Keywords

Girdap etkisi, büyük girdap benzesimi, numerik analiz, OpenFOAM

Parallel Aeroacoustic Computation of Unsteady Transonic Cavity Flow via Open CFD Source Codes

Ali Can FADIL, Bahar ZAFER

İstanbul Technical University Department of Aeronautical Engineering and Astronautical Engineering - İstanbul, Turkey

Cavity flow research has been ongoing experimentally since the 1940 s, especially for weapon bay use in fighter aircraft. With the development of technology, experimental studies have begun to be simulated. With the emergence of High-Performance Clusters, the success of these simulations has increased and simulation studies have begun to replace experimental studies. In this paper, an open rectangular, unsteady transonic cavity with a length to depth ratio of 5 , Mach number 0.85 and Reynolds number of approximately 6.5×10^6 was simulated using High-Performance Cluster. Likewise cavity doors were used to model a real weapon bay. Detached Eddy Simulation was used to resolve turbulent properties in the flow domain. Results compatible with experimental results were obtained with OpenFOAM® , an open-source CFD code based on the finite volume method.

Keywords

Cavity Flow, OpenFOAM, Aeroacoustics, Parallel CFD

Implementations of the Needleman-Wunsch Algorithm for GPU Architectures

Furkan KURT, Deniz Turgay ALTILAR, Ayşe Yılmazer METİN

Istanbul Technical University Department of Computer Engineering - Istanbul, Turkey

Abstract-Similarity search is a fundamental yet timeconsuming algorithm in bioinformatics. Many dynamic programming-based and heuristic algorithms are proposed to solve alignment problems. The Needleman-Wunsch algorithm is a well-known dynamic programming-based algorithm for global sequence alignments. The algorithm has $O(n^2)$ time and space complexity. The quadratic complexity limits the use of the algorithm with relatively smaller sequences. Various parallel and distributed methods were proposed to overcome the quadratic complexity of the algorithm.

In this paper, we describe a graphics processing unit(GPU) kernel to parallelize and reduce the execution time of the algorithm. We propose a new data partitioning method representation to increase the data transfer throughput between the GPU and the host. We implemented the serial approach of the algorithm and various parallel CUDA methods. We also used CUDA Cooperative Groups for the first time in Needleman-Wunsch algorithm parallelization. The evaluation shows that the new implementation is increased the performance of the algorithm 60 times for similarity score calculations, and 17 times for the alignment calculations.

Keywords

parallel computing, sequence alignment, bioinformatics

Performance Evaluation of CUDA Optimizations for Convolution Operations

Burak TOPÇU, İşıl Öz

İzmir Institute of Technology Computer Engineering Department - İzmir, Turkey

Convolution operations are important for image processing and deep learning applications. With a large amount of data and independent computations, the execution time of convolutions can be reduced substantially by GPU acceleration. CUDA programming model offers architecture-aware performance optimizations for programs running on GPL devices by employing software techniques. In this work, we perform a set of CUDA optimizations for multidimensional convolution operations implemented in the Polybench benchmark suite. Specifically, we utilize constant memory, shared memory, CUDA streams, and their combinations. We systematically apply the optimizations and present the results by comparing both execution time and resource utilization. Our results demonstrate that combined optimizations achieve up to 1.6 times speedup compared to the baseline implementations.

Keywords

Convolution, CUDA, Optimization

Accelerating Graph Embedding on a Single GPU Using Graph Reordering

Amro Alabsi ALJUNDI, Kamer KAYA

Sabancı University Faculty of Engineering and Natural Sciences
VERİM, Center of Excellence in Data Analytics - Istanbul, Turkey

Abstract-Graph embedding is the process of converting the irregular connectivity information of a graph into a structured, d -dimensional latent vector representation. This representation enables utilizing decades of existing machine learning models for graph-specific tasks such as link prediction and node classification. The excellent performance of graph embedding comes at the cost of memory and time, and the ever-increasing size of real-world graphs only exasperates these costs. Numerous algorithms accelerate graph embedding both on the CPU and on memory-limited GPUs. To alleviate the memory burden of graph embedding on GPUs, many of these algorithms will partition the parameter space of the problem into evenly sized parts that fit the GPU memory. In this work, we show that reordering graphs as a pre-processing step can substantially improve the speed of partition-based graph embedding algorithms.

Keywords

Graph embedding, GPU programming, reordering, high-performance computing

GPU-accelerated floating random walk based transient heat conduction solver

Ersin YILDIZ, Altuğ Melik BAŞOL

Özyegin University Department of Mechanical Engineering - İstanbul, Turkey

Solving diffusion processes with random walk Monte Carlo methods offers certain advantages over the discretization-based methods. One of the main advantages of these types of methods is that they can solve for the temperature at only selected points as opposed to the other discretization-based methods that require solving for the entire physical domain even though the temperature at a single physical point is of interest. In this study, a floating random walk (FRW) method, a type of meshless random walk method, has been implemented on graphics processors. In this method, the integral representing the analytical solution at a local point is evaluated by the statistical sampling from the possible random paths between the point and the domain boundaries. The implementation has been verified on two test problems with analytical solutions. The standard deviations in the results were quantified running the test problems with the increasing number of particles. Except for a deficient number of particles, the GPU-accelerated solver showed a clear speed advantage over the serial code running on the CPU. Running the solver with 105 particles resulted in an x100 speed-up on a gaming-level graphics card. Finally, the implemented solver was also tested on a more realistic transient heat conduction problem and the results were compared with laplacianFoam, an implicit finite volume based transient heat conduction solver available in OpenFOAM. It was found that the GPU-accelerated solver with 106 particles runs about x10 faster in comparison to laplacianFoam running in serial on CPU. It is anticipated that a further increase in the speed-up could be reached by parallelizing the algorithm on multiple graphics processors.

Keywords

heat conduction, random walk, floating random walk, Monte Carlo, graphics processing unit, GPU

Feasibility Study of Adding GPU Support to SU2 with ILU(0) Preconditioner

Najeeb AHMAD¹, Bilge Kaan GÖRÜR², Uğurtan DEMİRTAŞ², Özgür ATEŞOĞLU², Didem UNAT¹

¹ Koç University - İstanbul, Turkey

² Roketsan Missiles, Inc. - Ankara, Turkey

The open source computational analysis tool SU2 employs various linear solvers and preconditioners, all of which are currently written for commodity CPUs. Incomplete LU (ILU) is one such important preconditioner available in SU2, often used in linear solvers such as GMRES. In this work, we implement GPU-based ILU(0) preconditioner in SU2 using NVIDIA cuSPARSE library, evaluate its execution time on an NVIDIA Tesla V100 GPU for two input mesh sizes and compare its performance with state-of-the-art multicore AMD Epyc and Intel Cascade Lake CPUs. The implementation shows 22% (8M mesh size) and 30% (13M mesh size) speedups against AMD Epyc while slowdowns of 26%(8M mesh) and 11%(13M mesh) against Intel Cascade Lake CPU. We observe that while the cuSPARSE triangular solve (compute phase) takes lesser time for both mesh sizes than it takes on the CPU, the matrix update and cuSPARSE ILU(0) factorization (build phase) overshadows this gain on Intel Cascade Lake and results in a slowdown. In conclusion, it is important to have efficient implementations of both the build and compute phases for a significant overall performance gain on the GPU versus CPU for ILU(0) preconditioning in SU2.

Keywords

SU2, ILU Preconditioner, CUDA, cuSparse

Izometrik Kasılmada Aponevroz Ortusunun Rolu ve Seklinin Eniyileme Yontemiyle Tahminine Yonelik Hesaplama

Şükrü Furkan TAŞDEMİR, Cevat Volkan KARADAĞ, Ali Fethi OKYAR

Yeditepe Üniversitesi Mühendislik Fakültesi Makine Mühendisliği Bölümü - İstanbul, Turkey

Bu çalışmada sayısal olarak modellenmiş kurbaga gastrocnemius (*plantaris longus*) kasının sonlu elemanlar yontemiyle yapılan kasılma benzetimi (simülasyon) ile üzerinde tasıldığı ince bir zar olan aponevroz ortusunun geometrisinin bulunmasına çalışılmıştır. Her bir örnek için çözüm üretilmesi standart bir ofis bilgisayarında ortalama 200 saniyelik işlem süresi gereklidir. Ortalama geometrisinin tanımlanmasında gereken parametrelerin fazlalığı, çok yüksek sayıda yerel minimum değerlerinin eliminasyonu gerekliliği ve belirli bir karar uzayında en iyinin bulunması gereklidir. Genetik algoritma kullanılarak yapılması hedeflenen ortalama geometrisinin eniyileme süreci için yaklaşık 20 bin işlemci-saat ihtiyacı basgostermektedir. Bu ihtiyaç göz önüne alınarak Ulusal Hesaplama Merkezi'ne (UHEM) proje başvurusunda bulunulmuş ve çalışmaların devamı orada yapılmıştır. UHEM'de MATLAB-FEAP paralel işlem senaryosu oluşturulmuştur. Olusturulan bu senaryo ile oncelikle parametre uzayının taraması ve ardından aponevroz ortalama geometrisinin bulunması çalışması başarı ile tamamlanmıştır. Sonuç olarak, elde edilen aponevroz ortusunun fizyolojik ve mekanik bulguları irdelenmiştir.

SIMD Instructions for Ethereum Virtual Machine

Aykut Bozkurt, Can Özturan

25

Recently, Ethereum and its smart contracts have become very popular. Hence, there is an urgent need for higher transaction throughput on Ethereum blockchains. Ethereum Virtual Machine (EVM) is a Turing-complete computer which executes Ethereum bytecode-encoded instructions for smart contracts. Every instruction uses 256-bit wide stack items as input and output operands. They pop the required inputs from the stack and push the result onto it after an execution. A gas consumption cost is assigned to them relative to the complexity of the instruction as it prevents halting problem. Consumed gas multiplied by gas price is charged as transaction fee by the transaction sender to mitigate Denial of Service (DoS) attacks can be avoided. The current supported instruction set has some weaknesses. Firstly, transactions containing large sized vector operations require excessive amount of gas cost. Secondly, transaction throughput is limited because of no parallelism in execution. Therefore, we extend the EVM instruction set by Single Instruction Multiple Data (SIMD) operations in order to benefit from data-level parallelism based on Ethereum improvement proposal EIP-616. We show how EVM can benefit from SIMD instructions by lowering gas consumption and increasing transaction throughput.

Keywords

Computer Society, IEEE, ethereum, EVM

A Graph Transformation Strategy for Optimizing SpTRSV

Buse YILMAZ, Abdulkadir Furkan YILDIZ

Istinye University Dept. of Software Engineering - Istanbul, Turkey

Sparse triangular solve (SpTRSV) is an extensively studied computational kernel. An important obstacle in parallel SpTRSV implementations is that in some parts of a sparse matrix the computation is serial. By transforming the dependency graph, it is possible to increase the parallelism of the parts that lack it. In this work, we present an approach to increase the parallelism degree of a sparse matrix, discuss its limitations and possible improvements, and we compare it to a previous manual approach. The results provide several hints on how to craft a collection of strategies to transform a dependency graph.

Keywords

Sparse Triangle Solve, spTRSV, sparse matrix, graph transformation, parallel computing

Pekistirmeli öğrenme ile 5G baz istasyonunun otomize olarak yapılandırılması

H. Tugrul ERDOĞAN, Adnan ÖZSOY

Hacettepe Üniversitesi Bilgisayar Mühendisliği Bölümü - Ankara, Türkiye

Halihazırda iletişim teknolojilerini yaygın olarak kullanmaktadır. Yakın gelecekte ise 5G teknolojileri ile iletişim teknolojilerinin sunacağı yeni kapasite ve olanaklar ile de daha farklı alanlarda da telekomünikasyon teknolojilerinin kullanıldığını görmek hiç de şaşırtıcı olmaz. 5G teknolojilerinin ise; sektördeki büyük beklenilere cevap olarak, yenilikçi tasarım ve altyapı farklılıklarını ile konumlanacağı şimdiden görülmektedir. Bu yenilikçi tasarım ve altyapı farklılıklarını, var olan problemleri çözerken aslında henüz karşılaşmadığımız yeni problemleri de bugüne taşıyacaktır. Bu çalışma ile 5G altyapısı ile potansiyel problemlerden birisi olarak kendisini göstermeye başlayan baz istasyonu kaynak paylaşım problemini yapay zeka yöntemleri ile çözmeye çalıştık.

Makine Öğrenmesi tabanlı Gerçek Zamanlı Hedef Tespiti için Güç Verimli Paralel Hesaplama

Alparslan FİŞNE¹, Faruk YAVUZ¹, Adnan OZSOY²

¹ ASELSAN A.Ş. Aselsan Araştırma Merkezi - Ankara, Türkiye

² Hacettepe Üniversitesi Bilgisayar Mühendisliği - Ankara, Türkiye

Bu çalışmada, eşik tabanlı Sabit Yanlış Alarm Oranı (SYAO) radar hedef tespit yöntemine göre daha yüksek doğruluk sunan makine öğrenmesi tabanlı radar hedef tespiti için güç-verimli ve gerçek zamanlı hesaplama tasarımları anlatılmaktadır. SYAO yöntemine benzer şekilde iki boyutlu (2B) tarama yaparak hedef varlığını kontrol eden makine öğrenmesi uygulaması, Evrişimsel Sinir Ağı (Convolutional Neural Network, CNN) modeli içermektedir. CNN modelinin taramalı hesaplama yapısından dolayı tekraren veriler işlemeye alındığı için hesaplama kaybı gerçekleşmektedir. Önerilen katman optimizasyonları sayesinde taramalı yöntem kaldırılarak ve paralel hesaplama yapılarak gerçek zamanlı hesaplama sağlanmıştır. Güç-verimli bir hesaplama mimarisi için Jetson AGX Xavier GPGPU birimiyle 15 W ve 30 W güç modlarında Intel Xeon W-2123 CPU biriminden sırasıyla 1.2x ve 2x hızlanma sağlanmış olup düşük güç tüketimi ile gerçek zamanlı tespit uygulaması başarıyla gerçekleştirılmıştır.

Keywords

Makine öğrenmesi, radar hedef tespiti, katman optimizasyonu, enerji verimli hesaplama, GPGPU.

Development of a Generic Neural Network Potential for IR-MOF Series

Ömer TAYFUROĞLU, Abdulkadir KOÇAK, Yunus ZORLU

Gebze Technical University Department of Chemistry - Gebze, Kocaeli, Turkey

Abstract-Metalorganic frameworks (MOFs) with their exceptional porous and organized structures have been subject of numerous applications. Predicting macroscopic properties from atomistic simulations require the most accurate force fields, which is still a major problem due to MOFs' hybrid structures governed by covalent, ionic and dispersion forces. Application of ab-initio molecular dynamics to such large periodic systems are thus beyond the current computational power. Therefore, alternative strategies must be developed to reduce computational cost without losing reliability. In this work, we describe the construction of a generic neural network potential (NNP) for IRMOFn series ($n = 1, 4, 7, 10$) trained by PBE-D4/def2-TZVP reference data of MOF fragments. We validated the resulting NNP on both fragments and bulk MOF structures by prediction of properties such as equilibrium lattice constants, phonon density of states and linker orientation. The energy and force RMSE values for the fragments are only 0.0017 eV/atom and 0.15eV/, respectively. The NNP predicted equilibrium lattice constants of bulk structures, which are not included in training, are off by only 0.2-2.4% from experimental results. Moreover, our fragment trained NNP greatly predicts phenylene ring torsional energy barrier, equilibrium bond distances and vibrational density of states of bulk MOFs. The publicly available pre-trained model opens the door to investigate different aspects of IRMOFs at the first principle level accuracy.

Keywords

Machine learning, Metal-organic framework, Neutral network potential, DFT

Tek Boyutlu, Sıralı, Büyük Ölçekli Veri Dizileri için Sıralı Örüntü Madenciliği Yaklaşımı

Ali Burak CAN¹, Meryem UZUN-PER^{1,2}, Mehmet S. AKTAŞ³

¹ BiletBank Research and Development Center, Akdeniz PE-TUR A.S - Istanbul, Turkey

² Istanbul Health and Technology University Computer Engineering Department- Istanbul, Turkey

³ Computer Engineering Department, Yıldız Technical University - Istanbul, TurkeyYıldız Technical University Computer Engineering Department - Istanbul, Turkey

Sıralı örüntü madenciliği algoritmaları, belirli bir sıraya dayalı olarak bir araya gelmiş sıralandırılmış veri dizileri (içinde bir ya da birden fazla eleman bulunan veri dizileri - 1-sequence, n-sequence) üzerinde, sıralı örüntülerin bulunmasını sağlayan gözetimsiz makine öğrenmesi algoritmalarıdır. Literatürde, bu kategoride yer alan algoritmaları inceledigimizde; bu algoritmaların, uzunluğu birden fazla olan sıralı veri dizileri (n-sequences) için optimize edildikleri görülmektedir. Buradan yola çıkarak, genom dizisi verileri gibi, tek eleman içeren (1-sequence) sıralı veri dizilerinden oluşan veri setlerine yönelik optimize edilmiş sıralı örüntü tespiti algoritmalarına ihtiyaç olduğu görülmektedir. Bu araştırma kapsamında, tek elemanlı sıralı veri dizileri (1-sequence) içeren veri setleri üzerinde, sıralı örüntülerin yüksek performanslı bir şekilde tespit edilebilecek bir algoritmanın tasarılanması ve geliştirilmesi problemi üzerinde çalışılmaktadır. Yine bu araştırma kapsamında, tek bir bilgisayarın veri saklama ortamlarında (bellek ve fiziksel disk) tutulamayacak büyülüklükte olan veri setleri üzerinde, sıralı örüntülerin tespitine olanak verecek bir sıralı örüntü madenciliği algoritması üzerinde çalışılmaktadır. Önerilen algoritmanın çalışırken ihtiyaç duyduğu zaman ve bellek gereksinimleri deneysel olarak irdelenmiştir. Elde edilen sonuçlar, önerilen algoritmanın literatürde yer alan benzer kategorideki algoritmalarla, aynı doğruluk derecesine ulaşırken, daha az çalışma süresine sahip olduğunu göstermektedir. Elde edilen sonuçlar umit vericidir.

Keywords

Sıralı Örüntü Madenciliği, GSP, PrefixSpan, Spark

Sensitivity Analysis of Federated Learning over Decentralized Data and Communication Rounds

Mustafa Barış ÇAMLI, İsmail ARI

Ozyegin University - İstanbul, Turkey

Federated Learning (FL) refers to distributed learning via exchange of model metadata instead of raw data among the clients servers in a centralized architecture or among peers in a decentralized architecture. It is quickly becoming the defacto standard in Machine Learning (ML) due to its network efficiency and privacy-preservation. However, there are several issues that need to be resolved, which require a sensitivity analysis of FL techniques to decentralized data and federation parameters. In this paper, we focus on federated learning with a client-server architecture. The clients train neural network (NN) models with their local data while the server takes weighted average of all models exchanged in periodic communication rounds. A Convolutional Neural Network (CNN) model is trained in a federated way over different image classification benchmark datasets. Our results demonstrate the effects of (1) datasets having independent identically distributed (IID) vs. non-IID as well as balanced vs. unbalanced distributions, (2) number of communication rounds between clients and the server, and (3) the initial model selection in the distributed setting. In near future, we plan to extend our analysis to peer-to-peer architectures.

Keywords

Federated learning, neural networks, model training, communication round, IID, unbalanced, decentralized.

Çekirdek Sayısının Hesaplama Gemi Direnci Analiz Performansına Etkileri

Ali Can KOYUNCUOĞLU, Çağrı AYDIN, Uğur Oral ÜNAL, Barış BARLAS

İstanbul Teknik Üniversitesi Gemi İnşaatı ve Deniz Bilimleri Fakültesi Gemi İnşaatı ve Gemi Makineleri Mühendisliği - İstanbul, Türkiye

Bu çalışmada Hesaplama Akışkanlar Dinamiği vasıtasyyla bir açık deniz destek gemisi modelinin dalgalı su koşullarında iki serbestlik dereceli akış simülasyonları İstanbul Teknik Üniversitesi bünyesinde bulunan Ulusal Yüksek Başarımlı Hesaplama Merkezi imkanlarından faydalananarak gerçekleştirilmiştir. Yüksek işlem gücü gerektiren çalışmada gemi modelinin ek dalga direncinin yanısıra farklı çekirdek sayılarının hesaplama sistemi performansına olan etkisi incelenmiştir. Hesaplama üç boyutlu, sıkıştırılabilir RANS denklemlerinin SST $k-\omega$ modeli ile birlikte çözümünü içermektedir. Serbest su yüzeyi VoF metodu kullanılarak modellenmiştir. Ağ örgüsü hücre sayısının performansa etkisinin anlaşılması maksadıyla iki farklı ağ yoğunluğu uygulanmıştır. Simülasyonlarda 128 çekirdek sayısına sahip 4 hesaplama sunucusu kullanılmıştır. Çekirdek sayısı sistematik olarak artırılarak temel performans parametrelerindeki değişim gözlenmiştir.

Keywords

gemi direnci, ek dalga direnci, HAD, çekirdek, paralel hesaplama

Kullanılan Çekirdek Sayısının Kapsama Alanı Haritası Çıkarılma Performansına Etkisi

Uğur ERBAŞ, Mehmet Barış TABAKCIOĞLU

Bursa Teknik Üniversitesi Elektrik-Elektronik Mühendisliği - Bursa, Türkiye

Son zamanlarda iletişim teknolojisinin gelişmesi ve nüfusun artmasıyla birlikte baz istasyonlarına olan ihtiyaç da artmıştır. Bunun yanında yeni gelişen 5G teknolojisinde çok sayıda baz istasyonuna ihtiyaç duyulacağı tahmin edilmektedir. Bu çalışmada küçük bir bölgenin 3 boyutlu dijital verileri kullanılmıştır. İlk olarak MATLAB programında 3 boyutlu yeryüzü haritası çıkarılmıştır. Ardından iki farklı nokta seçilmiş ve kısa çizgilerle 2 boyutlu haritalar oluşturulmuştur. Baz istasyonlarının doğru pozisyonlara yerleştirilebilmesi için elektrik alanlarını doğru tahmin etmek ve kapsama alanı belirlemek çok önemlidir. Bu nedenle işin izleme algoritması ile yansyan, direkt ve kırınan tüm işinler belirlenmiştir. Kapsama alanlarının belirlenebilmesi için elektrik alanlarının hesaplanması gerekmektedir. Bu çalışmada Uniform Kırınım Teorisi (UKT) ve Geometrik Optik (GO) modeliyle elektrik alanlar hesaplanmış; bir merkez noktası seçilmiş, 3000 metre için elektrik alanları hesaplanmış ve kapsama alanı haritası çizilmiştir. Kapsama alanı haritalarına bakıldığından girişimlerden kaynaklı dalgalanmaların olduğu ve merkez noktadan uzaklaşıkça elektrik alanlarının azaldığı görülmektedir. Yüksek başarılı hesaplama teknikleri kullanılarak kapsama alanı haritası oluşturmak için gerekli çözüm süreleri çekirdek sayısına bağlı olarak karşılaştırılmıştır. Genel olarak kullanılan çekirdek sayısı arttıkça çözüm süresi azalmıştır.

Keywords

Baz istasyonu konuşlandırması, Kapsama alanı haritası, İşin izleme tekniği, Geometrik optik, UKT.

Efficient Thread-to-Core Mapping for Application-level Redundant Multithreading

Sanem ARSLAN¹, Osman UNSAL²

¹ Marmara University Computer Engineering Department - İstanbul, Turkey

² Barcelona Supercomputing Center - Barcelona, Spain

Redundant multithreading (RMT) is an effective thread-level replication method to improve the reliability requirements of applications. Although it significantly improves the robustness of applications, it comes with additional performance overhead since the redundant threads might share the same core resources. In our previous study [1], we presented an efficient software-level RMT approach, where we execute the most critical code regions with three threads to correct errors. In this study, we focus on further improving the performance of our software-level RMT method by presenting a set of different thread-to-core mapping alternatives. We provide different static mapping methods, which require preliminary information about the applications, such as execution time or cache usage behaviors, and a dynamic mapping method, which maps threads to cores dynamically at runtime without requiring any prior information. Experimental results show that the dynamic mapping method outperforms all static methods in addition to our baseline model, where the thread-to-core mappings are left to the operating system, by 8%, 7%, and 20% based on average speedup, harmonic speedup, and mean slowdown metrics.

Keywords

[1] S. Arslan and O. Unsal, "Efficient selective replication of critical code regions for sdc mitigation leveraging redundant multithreading," *The Journal of Supercomputing*, vol. 77, p. 14130 – 14160, 2021.

COMDETECTIVE +: An Inter-Thread Communication Analyzer for AMD Multicores

Muhammad Aditya SASONGKO¹, Milind CHABBI², Paul H. J. KELLY³, Didem UNAT¹

¹ Koç University - İstanbul, Turkey

² Scalable Machines Research - California, USA

³ Imperial College - London, UK

Abstract-AMD Processors have become more widely used in recent years due to the high performance yet low power consumption of the Ryzen series. Along with the increasing popularity of this processor series, there is also a rising need for profiling tools that can identify performance bottlenecks with low overheads in these machines. One common source of performance bottlenecks in multithreaded programs running on multicore systems is inter-thread communication.

We propose ComDETECTIVE +, an inter-thread communication analyzer that leverages the existing hardware features in AMD processors to support low-overhead detection of communications. It employs the instruction-based sampling (IBS) facility available in current AMD CPU cores to sample memory accesses, and debug registers to intercept communications involving the sampled memory accesses. In addition to detecting communications, COMDETECTIVE + also differentiates the communications into true sharing and false sharing, and attributes the communications to their locations in source code. We perform an experimental study to evaluate the accuracy, time, and memory overheads of this tool. Our tool exhibits high accuracy while introducing 2.8× runtime and 1.92× memory overheads, which are much lower than the overheads of existing cycle-accurate simulators and code instrumentation-based tools.

Keywords

PMUs, performance analysis, multicore

Approximate Execution of Critical Sections for Performance-Accuracy Tradeoff

Zuhal ALTUNTAS, Sanem ARSLAN, Betül BOZ

Marmara University Computer Engineering Department - İstanbul, Turkey

Approximate computing enhances performance and energy efficiency of applications, while still achieving acceptable accuracy. Some of the multithreaded applications can tolerate the accuracy loss when critical sections are approximately executed, which in turn will eliminate the synchronization overhead of these applications and increase their performance. In this study, our objective is to explore the behavior of the critical sections and selectively skip the ones yielding performance improvements with an acceptable accuracy loss. We have observed the behaviour of 49 critical sections of 2 selected applications. Our experimental study indicates that skipping 76% of the critical sections offers 2.5x performance gain with 16% accuracy loss for Raytrace whereas 1.4x performance improvement with 17% accuracy loss is obtained for Radiosity on the average when 36% of the critical sections are skipped.

Keywords

approximate computing, multithreaded application, critical section, performance, accuracy

Paralel İşlerin Çizelgelemesinde İşlemci Tahsisi İçin Hipersezgisel Yaklaşım

Gülçin BOLAT, Fatih Erdoğan SEVİLGEN

Gebze Teknik Üniversitesi Bilgisayar Mühendisliği Bölümü - Kocaeli, Türkiye

Paralel bilimsel uygulamaların çizelgelenmesi kaynakların verimli kullanılması ve işlemlerin tamamlanma süresinin azaltılması için oldukça önemlidir. Paralel uygulamalar veri paralelliği ve işlem paralelliği içerir. Çoklu işlemcili sistemlerde sadece işlem paralelliği içeren uygulamaların çizelgelenmesi probleminin NP-Tam problem olduğu bilinmektedir. Veri paralel işlemlerinde eklenmesi ile problem daha da zorlaşmaktadır. Yapılan çalışmalarda problemin işlemci tahsisi ve çizelgeleme aşaması için çeşitli algoritmalar önerilmiştir. Bu çalışmada işlemci tahsisi süreci için çeşitli sezgisel algoritmalar ve genetik algoritma birlikte kullanılarak özgün bir hipersezgisel yaklaşım sunulmaktadır. Deneysel sonuçlar, algoritmanın açgözülü algoritmalar ile karşılaştırıldığında daha iyi performans sonuçları sunduğunu göstermektedir.

Keywords

Statik Çizelgeleme, Veri Paralelliği, İşlemci Tahsisi, Genetik Algoritma

List of Participants

John1 Doe1	Barcelona, Spain
John2 Doe2	Barcelona, Spain
John3 Doe3	Barcelona, Spain
John4 Doe4	Barcelona, Spain
John5 Doe5	Barcelona, Spain
John6 Doe6	Barcelona, Spain
John7 Doe7	Barcelona, Spain
John8 Doe8	Barcelona, Spain
John9 Doe9	Barcelona, Spain
John10 Doe10	Barcelona, Spain
John11 Doe11	Barcelona, Spain
John12 Doe12	Barcelona, Spain
John13 Doe13	Barcelona, Spain
John14 Doe14	Barcelona, Spain
John15 Doe15	Barcelona, Spain
John16 Doe16	Barcelona, Spain
John17 Doe17	Barcelona, Spain
John18 Doe18	Barcelona, Spain
John19 Doe19	Barcelona, Spain
John20 Doe20	Barcelona, Spain
John21 Doe21	Barcelona, Spain
John22 Doe22	Barcelona, Spain
John23 Doe23	Barcelona, Spain
John24 Doe24	Barcelona, Spain
John25 Doe25	Barcelona, Spain
John26 Doe26	Barcelona, Spain
John27 Doe27	Barcelona, Spain
John28 Doe28	Barcelona, Spain
John29 Doe29	Barcelona, Spain

Useful Information

Talks will be held at the **Conference Hall-Auditorium** of PRBB. It is situated on the first floor of the central courtyard and has independent access from the rest of the building (through stairs located at the ground floor, main entrance of PRBB).

Coffee breaks and lunches will be offered in the half-covered terrace in front of the main entrance of the conference hall.

The **poster session** will be held on Tuesday and Wednesday night on the **ground floor** of the PRBB.

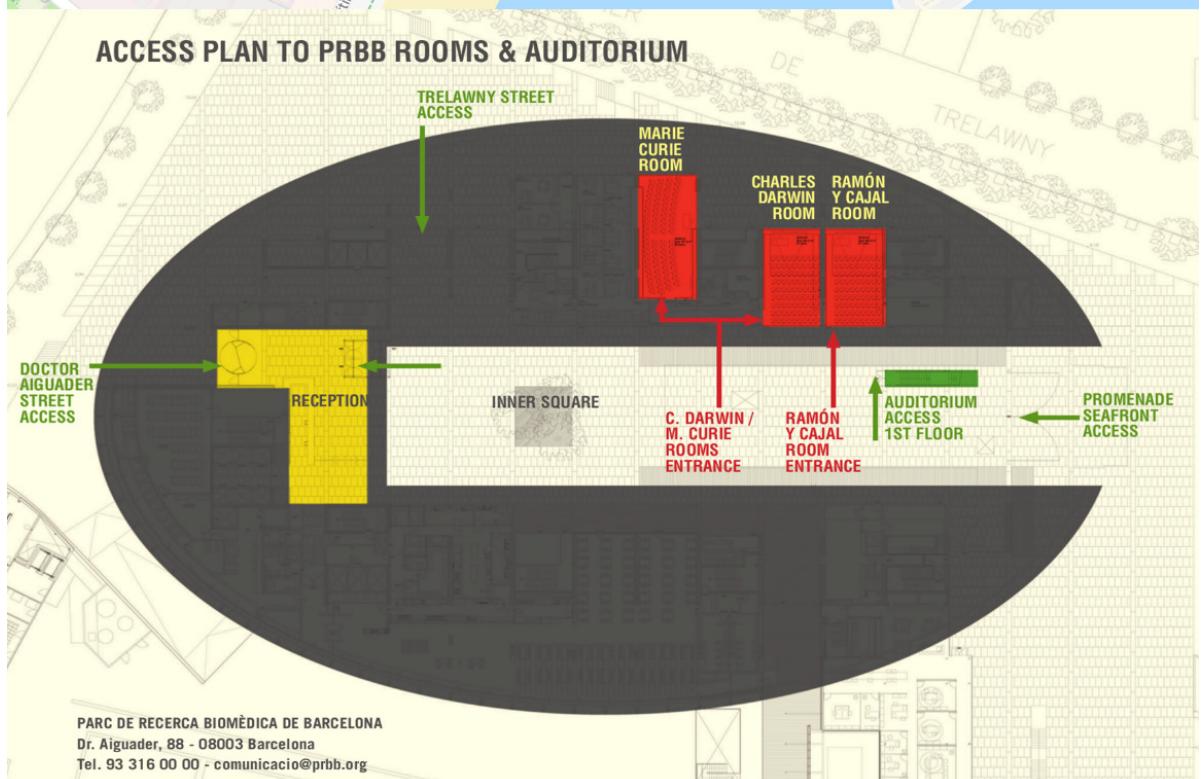
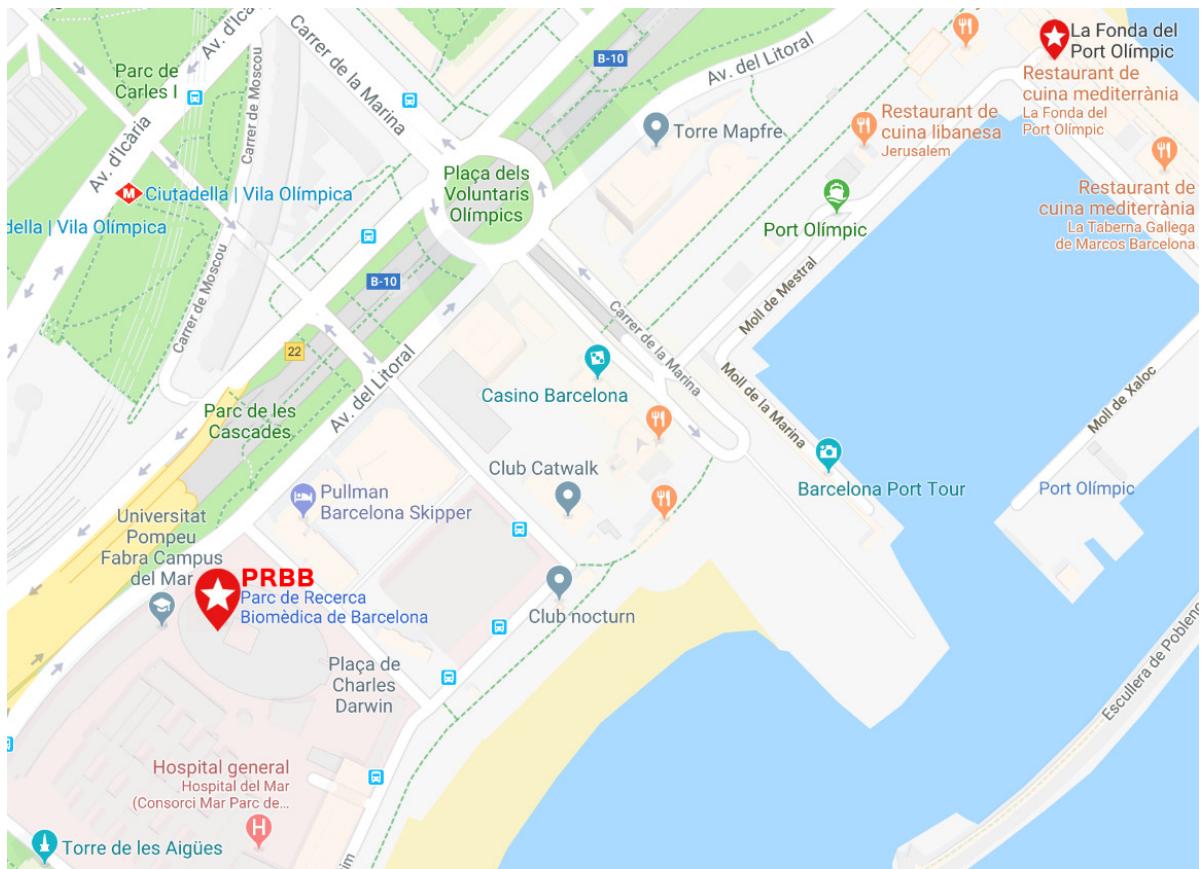
Wi-Fi will be available during the conference. The PRBB also provides access to an eduroam network.

The **conference dinner** will be held at the "The best restaurant", at Some Street, 39, Barcelona.

How to get to the PRBB?

The PRBB building overlooks the Ronda del Litoral and is next to the twin towers of the Olympic Village: Torre Mapfre and Arts Hotel. The address is Carrer del Dr. Aiguader, 88, 08003 Barcelona, Spain. and can be reached by:

- **Subway:** yellow line, L4, station Ciutadella/Vila Olímpica,
- **Bus:** lines V21, 14, 36, 41, 45, 59, 71, 92, D20,
- **Tram:** line 4, stop Vila Olímpica.



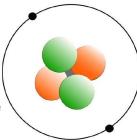
Partner Institutions and Sponsors

The AMCOS conference is part of the COSMOS project, funded by the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 642563.

Sponsors

Lancaster Helium Ltd

Purveyors of Isotopically Purified ${}^4\text{He}$



images/logos/Partnerlogos/springer.pdf

