한국계산과학공학회
2025년 추계학술발표대회

2025 Fall Conference of Korean Society for Computational Sciences and Engineering

발표논문 초록집

2025년 9월 4일(목) 서울 삼성동 코엑스

주최 KISTI 한국과학기술정보연구원 주관 KISTI 국가슈퍼컴퓨팅본부 KSF 한국초고성능컴퓨팅부문 KSCSE 한국계산과학공학회

계산과학공학회 2025년도 추계학술대회 프로그램

- **일 시 : 2025년 9월 4일 목요일 (13:30~18:00)**
- **장 소 : 서울 삼성동 코엑스** (2F 아셈볼룸)

좌 장: 김종수 부회장 (KASI)

시 간	발표 논문	발표자(소속)
13:30~14:00	GPU-Accelerated Solver for Batched Block Tridiagonal Matrix Systems on Distributed Memory Architectures	김기하 (KISTI)
14:00~14:30	ab initio nuclear theory	김영만 (IBS)
14:30~15:00	An Efficient, High-Precision Self-Gravity Solver in Rotating Frames	김용휘 (KISTI)
15:00~15:30	Break Time	
15:30~16:00	Efficient Implementation of a GMRES Solver for Compressible Flow Simulations Using Python	김남형 (인하대학교)
16:00~16:30	Local Constraint Neural Operator for Discretization-Invariant Super-Resolution Turbulent Flow Prediction	허정원 (연세대학교)
16:30~17:00	An Adaptive Mesh Refinement for Relativistic Hydrodynamics Using a Finite Volume PredictorCorrector Scheme	김진호 (KASI)
17:00~17:30	Spin-Dependent Polaron Pair Charge Recombination and Singlet Exciton Yields of Blue Organic Light-Emitting Diode Materials	이영민 (KAIST)
(*) 포스터 발표 논문		
Design of ALU Based on Complex-base Numeral System: Performance Evaluation and Application Methods		권도한 (안동고등학교)

GPU-Accelerated Solver for Batched Block Tridiagonal Matrix Systems on Distributed Memory Architectures

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In this study, we present a domain-decomposed parallel solution method for batched block tridiagonal matrix systems on distributed memory architectures, incorporating GPU acceleration. Such systems frequently arise in the numerical solution of multidimensional partial differential equations, particularly when employing high-order finite difference schemes or nonlinear implicit techniques, and their efficient solution in large-scale batch-processing environments is a critical challenge in modern scientific computing. The proposed method extends the PaScaL_TDMA algorithm—originally developed for scalar tridiagonal matrix systems—to handle block matrices, adopting a modified block Thomas algorithm and minimizing inter-process communication through a two-step reduction and back-substitution strategy. The implementation is optimized for batched operations to maximize GPU computational efficiency. Performance evaluation on CPU platforms shows that, for block tridiagonal systems, the high computation-to-communication ratio of block matrix inversion can actually degrade performance compared to conventional all-to-all communication–based methods. In contrast, on GPUs, the substantial acceleration of computational kernels increases the relative impact of communication costs. Moreover, with increasing GPU counts, the proposed method demonstrates nearly ideal scaling performance, whereas existing methods achieve only about 35% scaling efficiency. This approach is well-suited for large-scale simulation applications requiring high throughput and parallel performance, and contributes both theoretically and practically to advancing domain partitioning strategies in scientific computing and high-performance computing (HPC) environments.

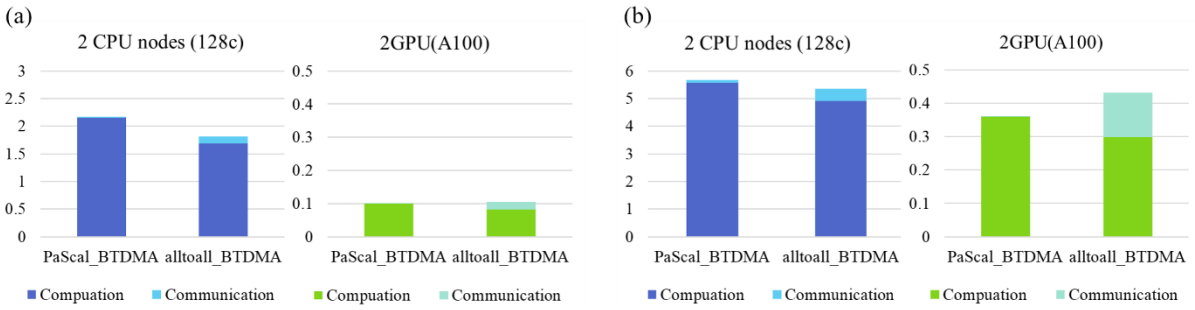

Figure 1 Computation and communication time breakdown for the PaScaL_BTDMA and alltoall_BTDMA methods on 2 CPU nodes and 2 GPUs: (a) block size = 2, (b) block size = 5.

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Ab initio nuclear theory

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Nuclei are fascinating quantum many-body systems that provide a solid testing ground for our understanding of the strong interaction at low energies. A central and challenging problem in nuclear physics is to fully understand how stable and radioactive nuclei emerge from protons and neutrons, whose interactions are governed primarily by the strong force.

Recent advances in high-performance supercomputing have opened up exciting opportunities for rigorous studies of nuclear structure and reactions using fundamental (or realistic) nuclear interactions derived from QCD.

The ultimate goal of ab initio nuclear theory is not only to describe nuclei with high precision from QCD or its effective theories, but also to uncover key features of the strong interaction at low energies through reliable many-body methods.

In this presentation, we will introduce nuclear lattice effective field theory as an example of such ab initio approaches, and present some recent achievements along with future research plans.

An Efficient, High-Precision Self-Gravity Solver in Rotating Frames

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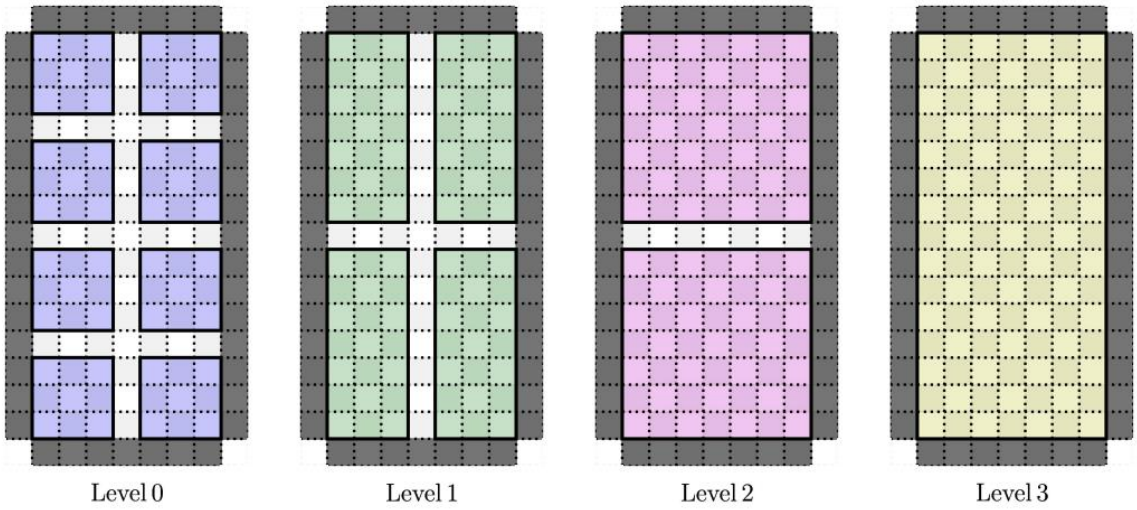
We present a fast and high-precision algorithm for solving the Poisson equation in spherical polar coordinates, designed for rotating astrophysical systems such as accretion disks. The method features a logarithmic radial grid with open boundary conditions and decomposes the computational domain hierarchically to efficiently manage varying spatial resolutions. Zero-boundary potentials are computed using James's algorithm and combined via matrix-vector operations with precomputed kernel matrices. The open-boundary correction is applied using a discrete Green's function approach. The solver achieves a computational complexity of O(N3 log(N)), ensuring scalability for high-resolution simulations. Implemented in the FARGO3D MHD code, the solver demonstrates second-order accuracy and robust performance in various test problems. This approach enables precise and efficient modeling of self-gravity in rotating, stratified systems, opening new opportunities for large-scale simulations in computational astrophysics.



[Figure 1] Illustration of our grid partitioning and level structure for adopting the developed Poisson solver in the case of a 7 x 15 grids. Connected colored cells form units at each level, while white cells represent intervening boundaries at the same level. The boundaries of the entire domain are shaded in gray.

Acknowledgments This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (RS-2025-00517264), and by Korea Institute of Science and Technology Information (KISTI) under the institutional R&D project (K25L2M2C3).

References

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Efficient Implementation of a GMRES Solver for Compressible Flow Simulations Using Python

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In steady-state flow analysis, the objective is to reach a steady solution rapidly; accordingly, implicit time-integration schemes that permit large time steps are commonly employed. With implicit time discretization, one must solve a system of linear equations at each time step. Among many methods for solving linear systems, Krylov subspace methods support efficient computation in flow analysis because the system matrix is extremely large and sparse. Especially GMRES, a member of the Krylov subspace family, is applicable to nonsymmetric matrices therefore numerous research has been conducted in computational fluid dynamics.

However, unlike most flow solvers which use compiler-based languages such as C/C++ for their execution speed, Python is an interpreter-based language that executes code line by line. Consequently, iterative loop phrases tend to be slow, which is especially detrimental for basic linear-algebra operations that access matrix and vector entries sequentially. Because GMRES is dominated by such linear-algebra kernels, additional optimization strategies are required when implementing GMRES in Python to mitigate this issue.

This study compares and analyzes a range of optimization techniques available in Python for the efficient implementation of GMRES in flow analysis. We first implement a baseline GMRES code using standard Python syntax and perform a bottleneck analysis, then evaluate performance improvements by applying several optimization methods to the compute-intensive functions. In addition, through the Roofline model, how closely each optimization method approaches the theoretical performance is assessed.

The results show that for the sparse matrix–vector multiplication (SpMV), the Block Sparse Row (BSR) format combined with the Intel Math Kernel Library (MKL) implementation via Foreign Function Interface (FFI) delivers the best performance, while for the vector–vector inner product and *daxpy* operations the differences among optimizing methods are modest except Numpy. Considering the computational performance with code consistency and simplicity, it is recommended to apply the Just-In-Time (JIT) compilation using Numba package by default and invoking Intel MKL through FFI if applicable.

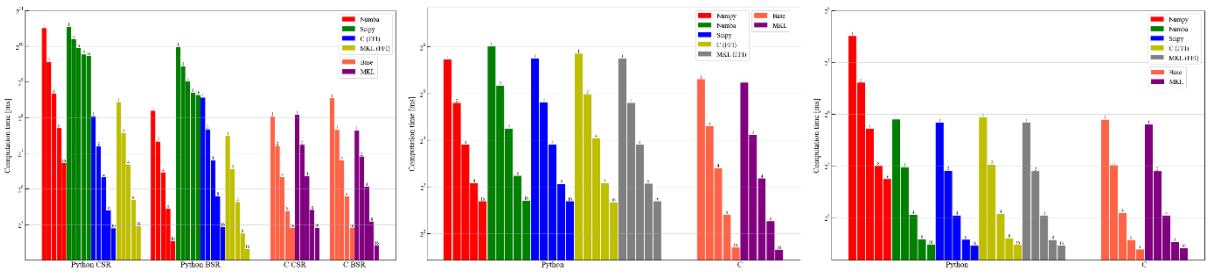

Figure 1 Performance comparison results for basic linear algebra operations with reference to the various optimization methods

Acknowledgments This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korean government (MSIT) (No. RS-2023-00282764).

Local Constraint Neural Operator for Discretization-Invariant Super-Resolution Turbulent Flow Prediction

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Resolving small-scale turbulence through fine-grid Direct Numerical Simulation (DNS) remains computationally expensive, making coarse-grid models such as Large-Eddy Simulation (LES) and RANS the practical alternative. However, in highly turbulent regimes, these model approaches exhibit significant large error from DNS results. Recent studies have explored machine learning methods to overcome such limitation. Among them, Fourier Neural Operator (FNO)[1] offers the discretization invariant framework, that can, in theory, extrapolate from coarse grid training data to finer grid test predictions within bounded error. However, in practice, FNO suffers from spectral bias, over fitting large scales while under-predicting small scales and its computational cost grows rapidly with increasing resolution.

In this study, we propose a constraint based local operator layer that embeds convolutional kernels within the FNO architecture, enforcing locality and retaining the spectral generalization mapping. Our method enables more accurate reconstruction of unseen high frequency components during super resolution, despite training on coarse grids. We conducted intensive turbulence statistics evaluation including energy spectra on isotropic turbulence (periodic boundaries) and Rayleigh–Bénard convection (non periodic boundaries) datasets[2]. Our study shows that the discretization invariant property of neural operators can be practically applied for turbulence super-resolution, enabling high-resolution reconstructions without additional training.

Acknowledgments

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An Adaptive Mesh Refinement for Relativistic Hydrodynamics Using a Finite Volume Predictor–Corrector Scheme

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This study aims to develop a highly accurate numerical scheme for relativistic hydrodynamics (RHD) simulations. We construct a computational framework that combines the conservative finite volume method (FVM) with a predictor–corrector algorithm on top of the adaptive mesh refinement (AMR) technique. The proposed method is designed to capture nonlinear dynamics such as shock waves, steep density gradients, and relativistic flows with high resolution and numerical stability under extreme conditions. This approach enables accurate modeling of high-energy astrophysical phenomena, including accretion disks around black holes, neutron star mergers, and relativistic jets. By implementing an RHD simulation software fully developed in Korea, this work contributes to securing independent core technology and establishing a foundation for large-scale computational astrophysics. The developed framework is expected to be applicable to a wide range of astrophysical simulations and to contribute to producing internationally competitive research outcomes.

Spin-Dependent Polaron Pair Charge Recombination and Singlet Exciton Yields of Blue Organic Light-Emitting Diode Materials

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Recently, hot excitonic materials have been suggested toward improving the efficiency of fluorescent organic light-emitting diode (OLED) materials. The improvements are achieved by harvesting triplet excitons via high-lying reverse inter-system crossing (hRISC), which requires suppression of internal conversion (IC) within triplet state manifolds. This violates Kasha's rule and, in fact, there is no direct evidence that triplet ICs are really suppressed. Here, we propose spin conversion in polaron pairs (PPs) as an alternative channel that can explain such hRISC. In our model, spin states can be converted to each other via hyperfine coupling, and the singlet exciton yield can be affected by the relative rates of charge recombination of singlet and triplet PPs. We investigate the variations of singlet exciton yields by calculating rate constants for charge recombination, IC, and (hR)ISC processes for hot excitonic molecules together with a kinetic picture through the kinetic master equation.

Acknowledgments This work was in part supported by Samsung Display Company (SDC).

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2025년 한국계산과학공학회 추계학술대회

복소수 진법 체계 기반 ALU 설계: 성능 평가 및 응용 방안

(Design of ALU Based on Complex-base Numeral System: Performance Evaluation and Application Methods)

권도한[1]

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초 록

1960년 Donald Knuth가 처음 제안한 복소수 진법(An Imaginary Number System, DOI: 10.1145/367177.367233)은 복소수를 기수(radix)로 사용하는 새로운 수 체계로, 기수로 어떤 복소수를 선택하느냐에 따라 숫자 집합과 표현법이 달라진다. 복소수 진법의 장점은 실수부와 허수부를 분리해 계산하지 않고 하나의 수로써 복소수 연산을 수행할 수 있다는 점이며, 이는 복소수 연산의 처리 속도 향상에 기여할 수 있다. 이후 연구에서는 다양한 기수를 탐구하면서 모든 복소수를 표현할 수 있는 체계를 확립하였고, 표현에 0과 1만을 사용하는 체계를 CBNS(Complex Binary Number System)로 정의하여 이진수와 유사한 표현을 갖게 되면서 컴퓨터 과학적 응용 가능성이 확대되었다. 본 논문은 국내에서 상대적으로 연구가 활발하지 않은 복소수 진법을 대상으로 수학적 이론을 정리하고, 복소수 연산에 특화된 ALU 설계 및 하드웨어 구현 방안을 제시한다. 설계한 ALU의 성능을 기존 방법과 비교·평가하고, 복소수 진법의 특성을 활용한 응용 사례들을 논의한다. 특히 특정 기수를 사용하는 복소수 진법에서 소수부를 복소평면에 나타냈을 때 생성되는 프랙탈 구조를 영상 손실 압축 기법에 적용하는 가능성을 탐색한다.

키워드— 복소수 진법, 논리회로, ALU, 프랙털, 양자컴퓨팅, 영상 손실압축, AI

| 오시는 길 |

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