한국계산과학공학회
2025년 춘계학술발표대회 및 총회

2025 Spring Conference and General Assembly of Korean Society for Computational Sciences and Engineering

발표논문 초록집

| 2025년 5월 14일(수) 대전 라마다호텔 |

주최 한국계산과학공학회 Korean Society for Computational Sciences and Engineering • KiSTi 한국과학기술정보연구원 Korea Institute of Science and Technology Information www.kisti.re.kr

- 초대의 글 -

회원 여러분께,

오는 2025년 5월 14일(수), 대전 라마다 호텔에서 계산과학공학회 춘계학술대회 및 총회가 개최됩니다. 이번 행사는 2025년 한국초고성능컴퓨팅포럼 정기총회 및 기술교류회와 같은 날 함께 열리며, 회원 여러분께서는 포럼 프로그램에도 적극적인 참여를 부탁드립니다.

이번 학술대회에서는 입자물리학, 하이브리드 양자-고전 컴퓨팅, 초고해상도 강수 예측, 생물정보학 기반의 단백질 분해 표적 탐색, 고성능 병렬 연산 기법 등 계산과학공학의 다양한 분야를 아우르는 최신 연구 성과들이 발표될 예정입니다.

계산과학공학회의 특성상 다양한 연구 분야의 전문가들이 참여하는 만큼, 발표자들께는 연구 내용을 가능한 한 쉽게 전달해 주시도록 부탁드렸습니다. 회원 여러분께서도 부디 많이 참석하시어, 각 분야의 연구 동향을 폭넓게 접하고 활발한 교류와 토론을 통해 뜻깊고 유익한 시간을 보내시기 바랍니다.

감사합니다.

회장 이식
부회장 김종수

계산과학공학회 2025년도 춘계학술대회 프로그램

2025년 5월 14일(수) 대전 라마다호텔

시 간	세션
10:00~11:00	한국초고성능컴퓨팅포럼 분과위원회 (3개분과별)
11:00~11:10	이동 및 정리
11:10~12:00	한국초고성능컴퓨팅포럼 정기총회
12:00~13:00	점심식사
13:00~15:00	**기조연설 세션** (2F 로얄볼룸홀)
13:00~13:15	환영 인사 및 축사
13:15~13:45	기조연설 Ⅰ : 우주분야 거대문제 해결을 위한 국가센터 초고성능컴퓨터 활용 (김주한 교수 : 고등과학원)
13:45~14:15	기조연설 Ⅱ : 범용인공지능(AGI)을 향한 여정과 딥시크 쇼크 (김현우 교수 : KAIST)
14:15~14:30	기조연설 Ⅲ : 국가센터 초고성능컴퓨터 6호기 도입 현황 (홍태영 센터장 : KISTI)
14:30~15:00	Break Time
15:00~17:30	**일반 세션** (3F 에메랄드홀) / **좌장 : 김종수** (KISTI)
15:00~15:15	Enhanced Deep Learning Framework for High-Resolution 6-Hour Precipitation Forecasting (박준, 이창훈 : 연세대학교)
15:15~15:30	Recent Advances and Trends in Hybrid Quantum-Classical Computing (이상민 : KISTI)
15:30~15:45	ELiAH-the atlas of E3 ligases in human tissues for targeted protein degradation with reduced off-target effect using supercomputer (백효정 : KISTI)
15:45~16:00	Particle physics in the KISTI-6 supercomputing era (조기현 : KISTI)
16:00~16:15	OpenMP-Parallel SymGS Variants for the 27-Point Stencil Problem on Many-Core Systems (Muhammad Rizwan, 최재영 : 숭실대학교)
16:15~16:30	Numerical methodology for complete transitional boundary layer simulation: receptivity calculation (김민우, 손일엽 : KISTI)
16:30~16:50	Break Time
16:50~17:30	**한국계산과학공학회 총회**
18:00~20:00	**만 찬**

Enhanced Deep Learning Framework for High-Resolution 6-Hour Precipitation Forecasting

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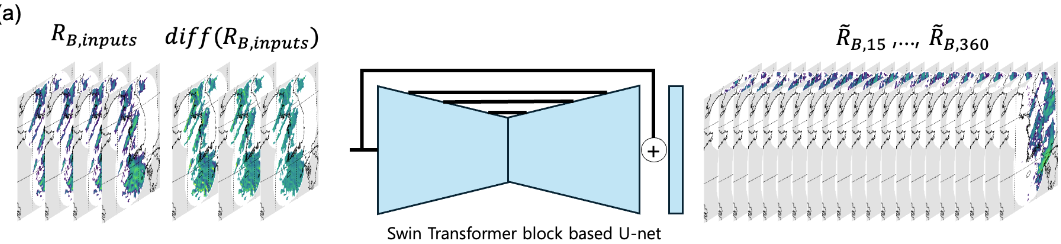
This study introduces a deep learning-based model for 6-hour precipitation prediction, addressing the limitations of traditional numerical weather prediction (NWP) models-such as long computation times and coarse grid resolutions compared to radar observations[1]. We preprocess 500 m radar data into multiple resolutions (1–32 km) and train models at 4, 8, 16, and 32 km scales. To optimize forecast skill, we compare various loss functions, including Balanced Mean Square Error (BMSE)[2], SoftCSI[3,5], and Wasserstein loss[4]. Our model, running on a single GPU, achieves substantial improvements: CSI for ≥1 mm/h precipitation is enhanced by 77% over persistence, and Critical Success Index(CSI) for ≥8 mm/h by 130%, outperforming previous models like DEEPRANE[5,6]. This demonstrates the effectiveness of high-resolution data and tailored loss functions for operational precipitation forecasting.

(a)



$$R_{B,inputs} = \{R_{B,-15}, R_{B,-10}, R_{B,-5}, R_{B,0}\}$$

$$diff(R_{B,inputs}) = \{R_{B,-15} - R_{B,0}, R_{B,-10} - R_{B,0}, R_{B,-5} - R_{B,0}\}$$

(b)

Model	Loss function	Data sources	Precipitation rates	CSI improvement over the persistence baseline [%] on average
DEEPRANE	SC	2020 Radar (summer)	≥ 1mm	34
	SC	2020 Radar (summer)	≥ 10mm	89
Ours. (Filtersize 4km)	BMSE, SC	2024 Radar (summer)	≥ 1mm/h	**77**
	BMSE, SC	2024 Radar (summer)	≥ 8mm/h	**130**

Figure 1 (a) Schematic diagram of the proposed model. *R_B* represents the rainfall value converted to decibels, and the adjacent number indicates the time difference in minutes from the present moment. (b) Comparative table of model performance, showing the improvement in CSI over persistence baseline for different precipitation rates.

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Recent Advances and Trends in Hybrid Quantum-Classical Computing

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Hybrid quantum−classical computing (HQCC) offers a practical approach to harnessing the complementary strengths of quantum and classical processors, particularly in the NISQ (Noisy Intermediate-Scale Quantum) era where fault-tolerant quantum hardware is not yet available. This review outlines the theoretical foundations and enabling technologies of HQCC, examining hardware architectures that integrate quantum processors with classical systems and cloud-based platforms supporting hybrid execution. Key software frameworks are introduced for their role in building and managing hybrid algorithms. Core methods such as the Variational Quantum Eigensolver (VQE), Quantum Approximate Optimization Algorithm (QAOA), and quantum kernel approaches are discussed, with emphasis on the interaction between quantum subroutines and classical optimization. Applications in quantum chemistry, optimization, and quantum machine learning highlight HQCC's practical utility. Key challenges such as noise, limited qubit scalability, and optimization barriers like barren plateaus are outlined, followed by future directions in error mitigation, tailored algorithms, and routes to quantum advantage.

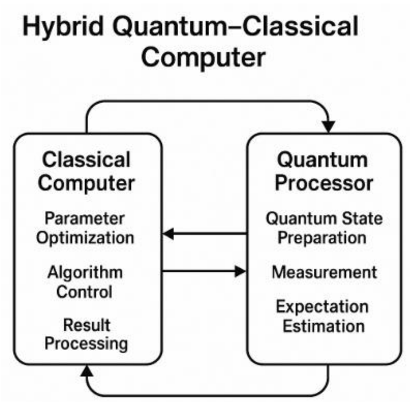

Figure 1. Conceptual diagram for HQCC

Acknowledgments This work has been carried under the support of Korea Institute of Science and Technology Information (KISTI).

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ELiAH: the atlas of E3 ligases in human tissues for targeted protein degradation with reduced off-target effect using supercomputer

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Targeted protein degradation (TPD), an emerging drug modality, utilizes bispecific molecules to direct specific proteins to E3 ligases for proteasome degradation. Unlike traditional drugs, this method catalytically degrades targets, enhancing efficacy and sustainability with lower dosages. However, consideration of prioritization at the transcriptomics level in conventional TPD design is still overlooked.

In previous, we introduce the Atlas of E3 Ligase in Human Tissues (ELiAH), which can explore E3 ligase expression across ten human tissues by analyzing 2,292 transcription profiles selected from the Genotype-Tissue Expression (GTEx). Tissue-specific association of 933,830 E 3-target gene pairs (Bonferroni adjusted p-value < 0.05) was predicted using ARACNe-AP, a gene regulatory network estimator based on mutual information. Here, we further developed ELiAH2 by adding over 1400 samples covering 24 of human tissues. By analyzing the transcriptional association and abundance between these gene pairs, users can assess the potential drugability of E3 ligase-target gene pairs in each tissue and anticipate potential drug side effects in unexpected organs. Narrowing down these gene pair candidates in this manner can accelerate the cost-effective development of TPD therapies. Moreover, the binding affinity between E3-target gene pairs is provided through the docking scores of binding structures predicted with RosettaDock and supercomputer. In this version, we also included the binding simulation results using known linkers of TPD. This enables the prediction of intrinsic degradation effects that might occur without TPD drug intervention. In conclusion, ELiAH2 presents more comprehensive exploration of the research repertoire of E3 ligases suitable for TPD-based drug development. Anyone can easily query their genes of interest on a user-friendly website to explore the comprehensive expressional characterization of each E3 ligase-target gene pair. ELiAH is freely available at the following URL: https://eliahdb.org

Particle physics in the KISTI-6 supercomputing era

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Supercomputers have enabled us to challenge previously unimaginable computational science. In the area of particle physics, various research methods and tools have been attempted to understand the origin of matter and its interactions [1]. Using the KISTI-5 supercomputer with 25.7 PFLOPS (floating point operations per second) from the Korea Institute of Science and Technology Information (KISTI), we have conducted a large-scale challenge program using 1500 nodes in particle physics. We present several research experiences on machine learning using the world's largest KNL supercomputer in the LHC-CMS experiment, effective theory of nucleating for exploring the secret of generating cosmic elements, neutron drip lines, and RAON accelerator beam simulations [2].

However, since large-scale science requires deep learning and big data processing, the architecture of supercomputer requires heterogeneous GPU computing in traditional CPU evolutionary computing. In 2025, heterogeneous computing's KISTI-6 supercomputer will be installed at the KISTI. Particle physics is an experimental-theory-simulation convergent study [3]. Therefore, utilizing KISTI-6 supercomputers can bring about maximization of research as they require deep learning and big data processing. Examples show nuclear lattice effective field theory, neutron star cluster-level dynamic properties, and high-speed simulation of particle-to-material interaction [2]. Ultimately, the KISTI-6 supercomputer can expect further discoveries in particle physics.

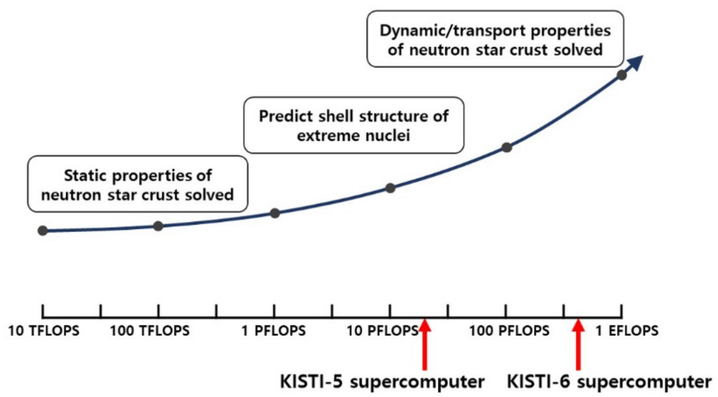

Figure 1 The status and future of particle physics with high-performance computing [2].

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OpenMP-Parallel SymGS Variants for the 27-Point Stencil Problem on Many-Core Systems

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The increasing complexity of scientific computing tasks, especially those represented by sparse linear systems, has revealed the performance constraints of conventional iterative techniques on contemporary many-core architectures. This work systematically explores and implements various OpenMP-parallelized variants of the Symmetric Gauss-Seidel (SymGS), designed for high order 27-point stencil problem in the High-Performance Conjugate Gradient (HPCG) benchmark. Previous techniques focused on lower-order stencil problems, except for multi-coloring and level scheduling.

We present and evaluate temporal blocking, wavefront scheduling, hybrid Jacobi-GS, and over-relaxation variants that preserve the core forward-backward structure of SymGS while enabling parallelism. The over-relaxation method achieves up to 7x and 10x improvement on KNL and SKL platforms, respectively, while temporal blocking significantly reduces iteration counts without compromising numerical stability. We also validate our optimized SymGS by solving large-scale problems (n = 160^3 on KNL and 288^3 on SKL) in multi-node MPI+OpenMP environments, achieving an average 1.4x improvement in HPCG performance over the native implementation in both KNL and SKL multi-nodes setup. Our optimized parallelized SymGS variant enables parallel execution and proves to be simpler and more efficient than multi–coloring based dependency resolution.

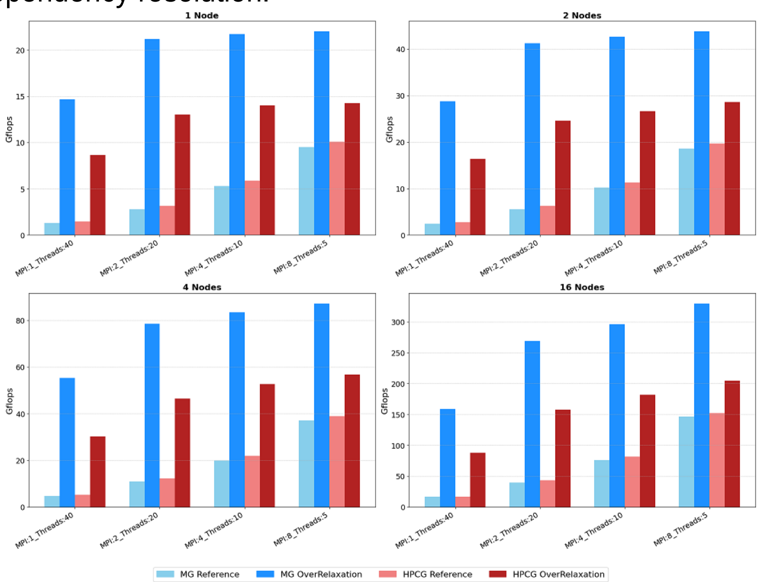

Figure 1 Performance of MG (Multigrid) and HPCG for a problem size of 288^3 using different MPI+OpenMP configurations across multiple SKL nodes.

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Numerical methodology for complete transitional boundary layer simulation: receptivity calculation

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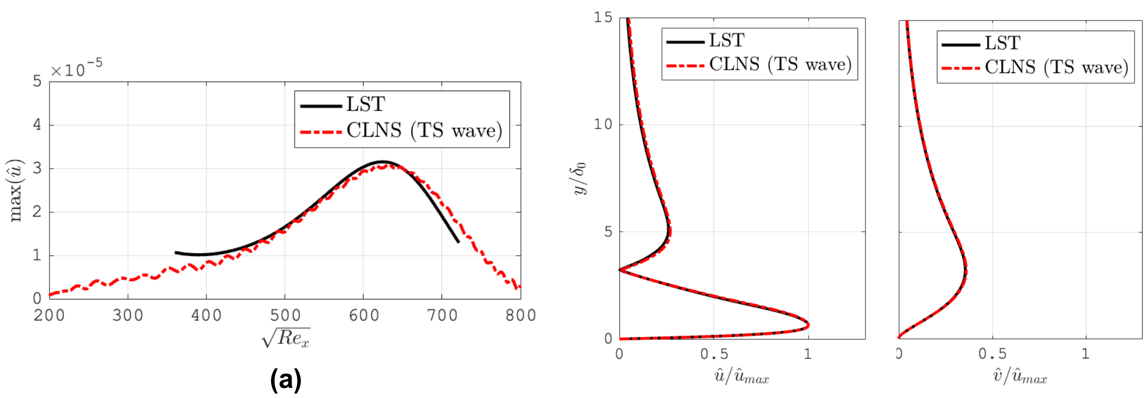
Turbulent transition significantly influences drag and heat transfer on aircraft surfaces. Despite research over five decades, it is not fully understood due to its complexity, such as the coalescence of minute fluctuations in the laminar boundary layer into the thick turbulent boundary layer. Common numerical approaches for turbulent transition are stability analysis and high-fidelity simulations, e.g., direct numerical simulation (DNS). However, these methods have limited application due to their own assumptions in governing equations or unaffordable computational cost. Therefore, the present study suggests the efficient and high-fidelity method to simulate transitional boundary layer. DNS combined with stability analysis has been widely used to calculate controlled transition. However, it cannot reproduce actual natural transition scenario because the computational domain should be in linear region of transition process, thus receptivity process, the first stage of transition process, is inevitably ignored. To address this limitation, the current study integrates compressible linearized Navier-Stokes equations (CLNS) with DNS. CLNS can provide absolute instability, and it means that the propsed combining method can handle the realistic natural transition scenario rather than controlled transition process. As the first step, receptivity process for Tollmien-Schilichting wave (TS wave), the key instability mode in subsonic boundary layer, is computed using CLNS. Receptivity occurs through linear mechanism so that CLNS provides DNS-like accuracy with dramatically low computational cost. The computational results of CLNS are comparable to stability analysis data and previous studies (selected results are shown in Figure 1). As future work, after clear validation and verification of CLNS, the entire natural transition simulation will subsequently be carried out.



(a) (b)

Figure 1. CLNS results for TS wave. (a) Amplitude growth of streamwise velocity fluctuations and (b) mode shapes at $\sqrt{Re_x} = 600$.

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