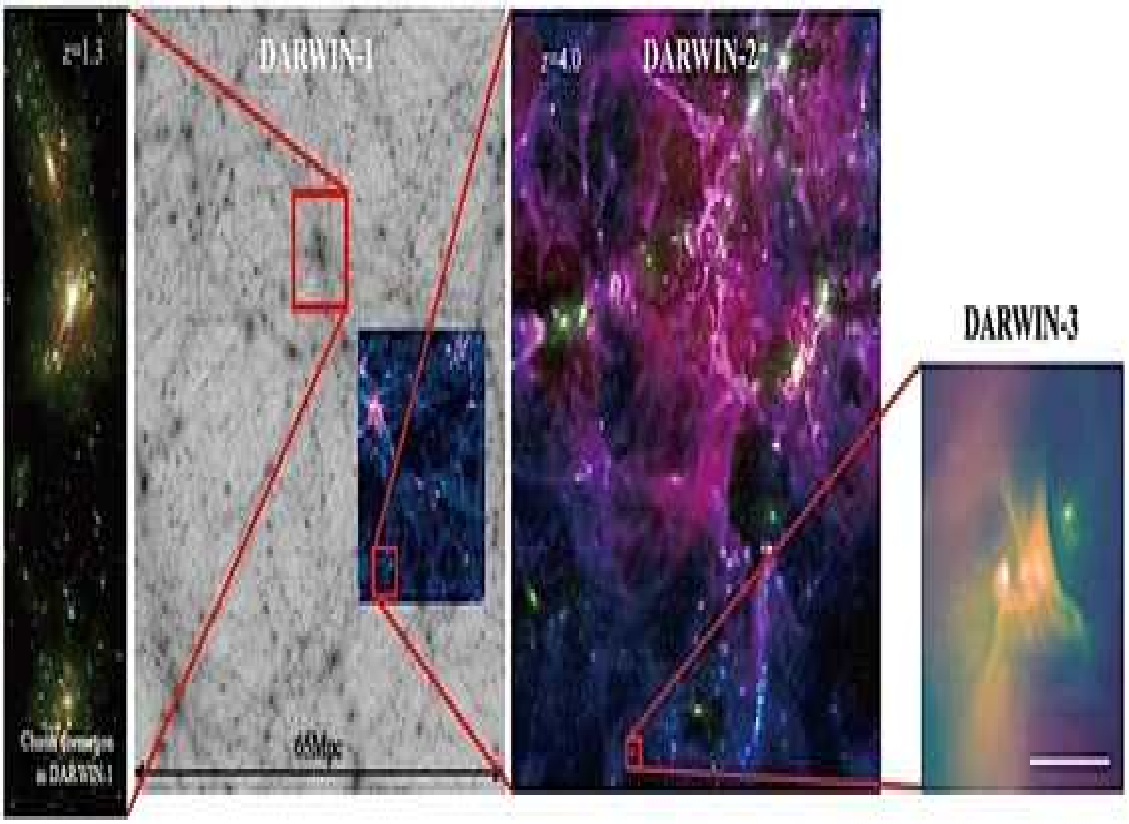
한국계산과학공학회

2026년 추계학술발표대회

2026 Fall Conference of Korean Society for Computational Sciences and Engineering



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한국계산과학공학회
Korean Society for Computational Sciences and Engineering

목 차

학술대회 정보

❑ 개요

❍ 행 사 명 : 2026년 한국계산과학공학회 추계학술대회
❍ 일　　시 : 2026년 9월 8일 (화요일) 13:30 ~ 18:00
❍ 장　　소 : 서울 스위스 그랜드 호텔 컨벤션센터 (4F Room B)

❑ 행사 안내

2026.9.8(화)~9(수) 서울 스위스 그랜드 호텔에서 2026한국슈퍼컴퓨팅 컨퍼런스가 개최될 예정이오며 (*홈페이지참조 www.ksc-hpc.kr), 사단법인 한국계산과학공학회에서는 2026.9.8(화) 13:30~18:00 에 2026년 추계학술발표대회를 진행할 예정입니다.

❑ 초록 모집

이번 행사에서는 다양한 프로그램을 구성하여 회원 여러분들에게 연구 교류의 기회의 장을 제공하고자 합니다. 더불어, 성공적인 행사를 위하여 회원 여러분들의 적극적인 초록 제출과 함께 많은 관심과 참여를 부탁드립니다.

❑ 사전 등록 및 초록 제출

❍ 사전 등록 기간 : 2026년 8월 4일(화)부터 ~ 2026년 9월 4일(금)까지
❍ 사전 등록 방법 : 온라인 등록 링크 (온라인 등록 불가 시, 학회 당일 현장 결제 가능함)
• 학회 홈페이지 www.cse.or.kr 접속 후 로그인(회원 가입 필요)
> 상단 학술대회&워크숍 > 프로그램결제 > 프로그램 선택 후 결제
❍ 초록 제출 기간 : 2026년 8월 28일(금)까지
❍ 초록 제출 방법 : 이메일 제출 kscseoffice@gmail.com
※ 학회 회원들의 다양한 전공분야 특성을 고려해 주시고 발표 내용을 가능한 이해하기 쉽게 준비해 주시기를 부탁드립니다.

❑ 초록 제출 분야 *기타(계산과학공학관련 분야)

- 인공지능
- 거대 시뮬레이션
- 수치 알고리즘
- BigData
- 유체역학 시뮬레이션
- 고성능컴퓨팅 아키텍처
- 물리기반시뮬레이션
- 구조해석 시뮬레이션
- 미분방정식의 수치알고리즘

❑ 참가 자격

한국계산과학공학회 회원 및 계산과학/공학 분야에 종사하는 자

❑ 기타 안내사항

- 문의 : 한국계산과학공학회 사무국 (02-966-6600, kscseoffice@gmail.com)
- 등록비 :

	일　　반	학　　생
정회원	100,000원	50,000원
비회원	150,000원	60,000원

학술대회 프로그램

시 간	발표 논문	발표자(소속)
13:30~13:40	**환영 인사 및 학회 운영 방안**	김종수 (회장)
1부	**좌장 : 김종수 회장**	
13:40~14:05	Simulating the Formation and Evolution of Dwarf Galaxies on a Next-Generation National Supercomputer	김용휘 (KISTI)
14:05~14:30	Effects of Rain-Gauge Network Variability on CycleGAN-Based Precipitation Estimation	김효진 (KISTI)
14:30~14:55	Fichera-corner First-passage Algorithm	이재호 (GIST)
14:55~15:20	Artificial Intelligence-Fokker-Planck Equation Hybrid for Optimal Descriptor Identification and Prognosis of Patient Fate Dynamics	정인춘 (중앙대학교)
15:20~15:50	**Break Time / 포스터 관람**	
2부	**좌장 : 이영민 수석 부회장**	
15:50~16:15	Test Vector Generator for the ALMA Wideband Sensitivity Upgrade: Application of NVIDIA DOCA GPUNetIO	김종수 (KASI)
16:15~16:40	Size-dependent free energy of micelles extracted from their size distribution and development of novel, efficient free energy calculation method	박진원 (중앙대학교)
16:40~17:05	Toward Multimodal AI for Drug Discovery: From ADMET Prediction and Molecular Generation to Foundation Models	한혜림 (나무ICT)
17:05~17:30	Q-CAR: A Noise and Congestion-Aware Deployment Scheme for Quantum Job Scheduling on Slurm Clusters	하지원 (서울대학교)
(*) 포스터 논문		
DeepKinomeWeb: a Quantitative, Panel-Level Platform for Kinase Inhibitor Screening and Selectivity Profiling		나현수 (KRIBB)
pH-dependent membrane insertion and folding of the Caveolin-3-derived peptide Cav3(7-26): an all-atom molecular dynamics study		양승훈 (KRIBB)
Virtual Screening of Covalent Inhibitors Targeting PNPLA3-I148M		김애진 (KRIBB)
Computational modeling of the AAVX-AAVR complex from Cryo-EM density map		전홍욱 (KRIBB)
EpiSearch: Identifying Disease-Specific Leading Search Indicators Using Wastewater Surveillance Data in Korea		강서진 (KISTI)

Simulating the Formation and Evolution of Dwarf Galaxies on a Next-Generation National Supercomputer

Yonghwi Kim[1*], and DARWIN Collaboration

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Dwarf galaxies present a profound challenge for numerical simulations. Their shallow potential wells are highly susceptible to stellar feedback, necessitating that kiloparsec-scale outcomes be modeled alongside parsec-scale physics. Bridging this gap requires a spatial dynamic range of six orders of magnitude— a major computational and astrophysical challenge. This effort is timely, as dwarf galaxies are a primary observational target for upcoming next-generation telescopes.

We report the status of DARWIN (DAzzling Realization of dWarf galaxies In the Next generation of cosmological HD simulations), a 3-step cosmological simulation campaign achieving this dynamic range via nested refinement. The framework couples adaptive mesh refinement hydrodynamics with particle-mesh gravity, multi-band radiative transfer, and stiff thermochemical networks tracking over 12 species. Thus, computational costs are dominated by operator coupling and load imbalances inherent to this multi-physics system. DARWIN-1 evolves a 65 Mpc volume at 0.5 kpc, reproducing observed scaling relations across stellar mass, halo mass, chemical abundances, and central black hole mass. In DARWIN-2, 24 sub-regions were resimulated at 62.5–125 pc, yielding 243 dwarf galaxies and demonstrating environmental regulation on gas accretion: chemically pristine systems decrease tenfold near massive neighbors. DARWIN-3 reaches a 3.9 pc resolution across 16 zoom-in targets, resolving early star formation and gas stripping.

Since each stage incurs a computational cost 500 times greater than its predecessor, standard CPU-only architectures cannot sustain this scaling. Future progress necessitates utilizing the KISTI-6 national flagship supercomputer, HANGANG, and its accelerated solver, serving as the primary motivation for the numerical work presented separately at this conference.

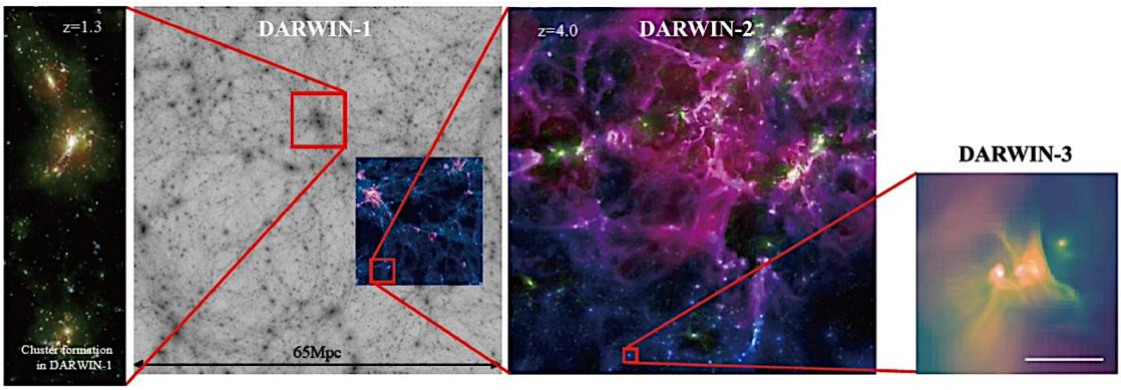

Figure 1 3-Steps of DARWIN Simulations

Acknowledgments This research was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2022M3K3A1097104), carried out at the Korea Institute of Science and Technology Information (KISTI) under project No. N25NM024-26.

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Effects of Rain-Gauge Network Variability on CycleGAN-Based Precipitation Estimation

Hyojin Kim [1*], Wonsu Kim[1], Haenggon Lee[1]

[1] *Korea Institute of Science and Technology Information, Daejeon 34141, Republic of Korea*

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Accurate reconstruction of spatial rainfall patterns from sparsely distributed ground observations remains challenging. To address this problem, a CycleGAN-based approach was developed to learn spatial precipitation characteristics from radar data while retaining rainfall information observed at rain gauges. The effects of changes in the available gauge network were further investigated by evaluating model performance under varying rain-gauge network configurations. Rain-gauge precipitation and a station-location mask were used as inputs. The model generally achieved higher CSI values than radar and IMERG at gauges excluded from the input. Model performance deteriorated as the number of input gauges decreased below that used during training, particularly for intense precipitation. To improve applicability to different observation environments, diverse gauge configurations were incorporated during training. This strategy reduced performance degradation in a new region with a sparse gauge network and achieved performance comparable to a model trained directly on the target region. These results suggest that considering diverse gauge-network configurations during model training is important for practical application.

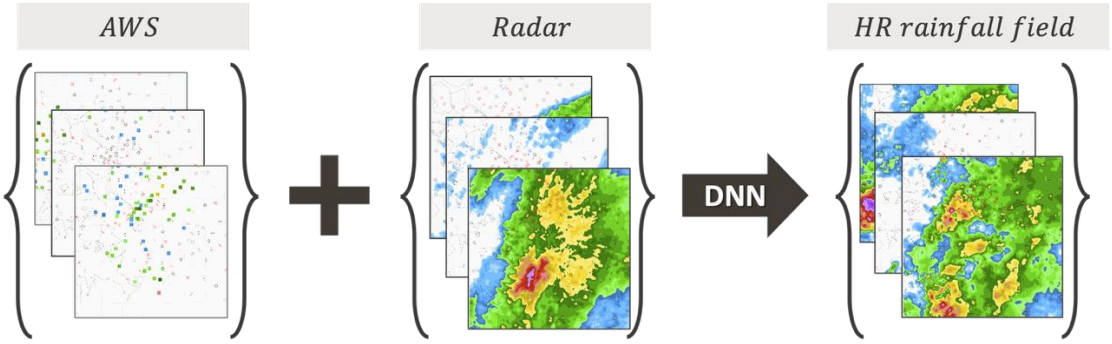

Figure 1 Schematic of high-resolution rainfall field generation from AWS and radar data

Acknowledgments This work was supported by the Korea Institute of Science and Technology Information (K26L4M1C1).

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Fichera-corner First-passage Algorithm

Jae-ho Lee[2], Sungwon Cho[3], Geonho Hwang[1*], and Chi-Ok Hwang[1†]

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In Diffusion Monte Carlo simulations, the “Walk-on-Spheres” (WOS) algorithm requires an absorption ϵ-layer to terminate diffusion near boundaries, inevitably inducing artificial truncation errors. This inefficiency is especially magnified near complex geometries like edges and corners. Exploiting the electrostatic-diffusion isomorphism, exact boundary-specific algorithms like Walk- on-Plane and Walk-on-Infinite-L-shaped (WOIL) have been developed. Extending this approach, we introduce a novel Walk-on-Infinite-Fichera-Corner (WOIFC) first-passage algorithm. By deriv- ing the exact first-passage probability distribution on an infinite Fichera-corner (cubic trihedral) boundary, we developed an acceptance-rejection sampling method for exact random walk jumps. To demonstrate this, an application combining WOIFC with WOS and WOIL to sample first-passage collision points within a finite cube is currently in progress.

Keywords: Monte Carlo, First-passage, Fichera-corner, Acceptance-rejection sampling

Artificial Intelligence-Fokker-Planck Equation Hybrid for Optimal Descriptor Identification and Prognosis of Patient Fate Dynamics

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Sepsis is a life-threatening critical illness that poses formidable clinical challenges. Its abrupt onset and heterogeneous pathophysiology impede early diagnosis and timely therapeutic intervention. In the absence of a gold standard for early sepsis diagnosis, deep learning (DL) approaches have been widely explored for both diagnosis and prognosis; however, a unified artificial intelligence (AI) framework that delivers accurate diagnostic and prognostic predictions for sepsis patients remains lacking. In this talk, we introduce an artificial intelligence-Fokker-Planck Equation (AI-FPE) hybrid framework for the construction of an effective descriptor characterizing a patient's clinical state and the prediction of clinical outcomes based on the probabilistic dynamics of this descriptor. From the AI module of this framework, we derive the Septic Infection-Related Risk Index (SIRRI), an interpretable descriptor that effectively represents the pathological severity of sepsis patients. The Fokker-Planck Equation-based prognostic module further predicts the temporal evolution of SIRRI distributions, time-dependent mortality and recovery rates across different clinical stages. Improving this framework, we are currently developing AI-based multidimensional representations of patient state, where distinct dimensions encode complementary aspects of the pathological state and disease progression of patients. This project requires systematic exploration of large-scale clinical datasets and diverse model architectures, integration with transcriptome analyses to establish biological relevance, and rigorous validation across independent external cohorts.

Test Vector Generator for the ALMA Wideband Sensitivity Upgrade: Application of NVIDIA DOCA GPUNetIO

Jongsoo Kim
Korea Astronomy and Space Science Institute

The Atacama Large Millimeter/submillimeter Array (ALMA) is undergoing its Wideband Sensitivity Upgrade (WSU) to significantly enhance its scientific observing capabilities. In the upgraded system, each antenna produces four high-speed digital data streams. Digitized at an ultra-high rate of 40 Giga-samples per second with 6-bit resolution, each stream generates a payload data rate of 240 Gbps (40 GSPS x 6 bits/sample), totaling nearly 1 Tbps per antenna. Developing and validating the downstream GPU-based real-time processing pipelines requires realistic input signal streams; however, relying on physical telescope digitizers or dedicated hardware fixtures during development is inflexible and cost-prohibitive.

To solve this challenge, we developed the Test Vector Generator (TVG)—an autonomous, software-defined signal generation system implemented on the NVIDIA GH200 Grace Hopper Superchip using NVIDIA DOCA GPUNetIO. TVG synthesizes realistic astronomical noise signals, encapsulates standard network packets directly within GPU High Bandwidth Memory, and streams them over 400 Gbps Ethernet links with zero host CPU involvement. By leveraging GPU-initiated transmission and hardware burst pacing on the NVIDIA ConnectX-7 network adapter, the system eliminates operating system jitter and delivers deterministic, line-rate packet streaming with nanosecond precision.

Benchmarking on the GH200 demonstrates that TVG achieves sustained generation and transmission speeds exceeding 270 Gbps per stream (accounting for protocol overhead) with substantial real-time safety margins. TVG provides a versatile, cost-effective test platform that successfully verifies high-throughput astronomical signal processing pipelines without specialized hardware.

Size-dependent free energy of micelles extracted from their size distribution and development of novel, efficient free energy calculation method

jinwon Park[1,2], Minho Lee[1,2], Donghee Kim[1,2], Ji-Hyun Kim[1,2] and Jaeyoung Sung[1,2]*

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Micelles are widely used as membrane-mimetic systems for structural and functional studies of membrane proteins [1]. Micellar assemblies have also been extensively investigated as carriers for therapeutic drugs. As their size can significantly affect drug accumulation, tissue penetration, and therapeutic efficacy [2], understanding and controlling the micelle size distribution is important for both fundamental studies and practical applications. Recently, a statistical-thermodynamic theory for mesoscopic nucleation systems was developed, which successfully explains the equilibrium size distributions of nanoparticles and biological condensates [3]. However, corresponding understanding and prediction of the micelle size distribution have yet to be achieved for lack of accurate information about the size-dependent free energy of micelles. In this talk, we will introduce a new method to extract the size-dependent free energy and chemical potentials of micelles from the experiments or large-scale simulation results for the equilibrium size distribution of micelles. Time permitted, we will also talk about an alternative free energy calculation method that is free of the charging process and far more efficient than the thermodynamic integration or free energy perturbation methods.

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Toward Multimodal AI for Drug Discovery: From ADMET Prediction and Molecular Generation to Foundation Models

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Artificial intelligence has been increasingly applied across various stages of drug discovery, from molecular property prediction to de novo molecular generation. Among these applications, accurate prediction of ADMET properties directly from molecular structures has remained a major challenge in drug discovery. To address this challenge, we developed a AutoML-based predictive models for 11 ADMET endpoints using SMILES-derived molecular descriptors and fingerprints [1]. Automated optimization of algorithms and hyperparameters achieved AUC values above 0.80 across all endpoints, with model generalizability further evaluated through cross-validation and external validation. Beyond property prediction, we explored molecular generation with an improved molecular representation [2]. Although SMILES is a widely used and general representation of chemical structures, its atom-level representation has limitations in distinguishing identical atoms in different chemical environments. To address this limitation, a hybrid SMILES and atom-in-SMILES (AIS) representation was introduced to incorporate local atomic environment information. This representation improves token diversity and reduces token imbalance, providing a more informative representation for molecular generation. Extending these efforts, we introduce a new multimodal foundation model that aligns three complementary molecular views—SMILES, property, and distance features—through contrastive learning, enabling its application to diverse downstream tasks.

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

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Q-CAR: A Noise and Congestion-Aware Deployment Scheme for Quantum Job Scheduling on Slurm Clusters

Jiwon Ha[†1], Sookyoung Park[†2], Hyeonsang Eom[1], and Yoonhee Kim[2*]

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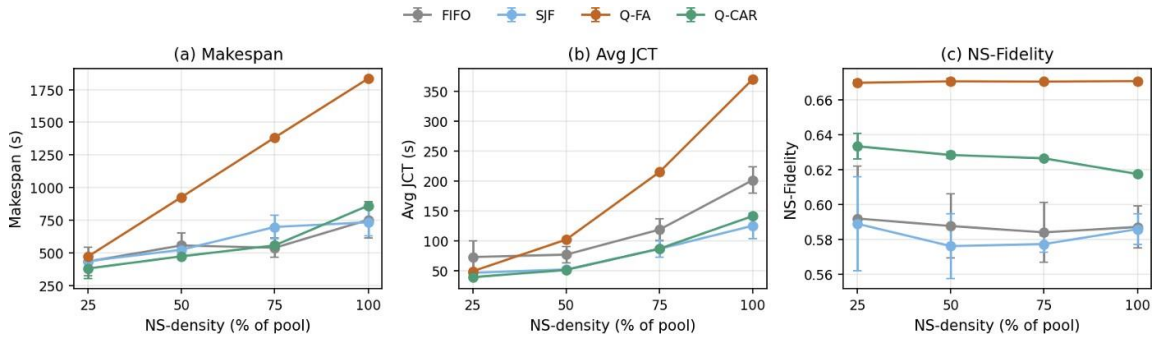
NISQ-era quantum computing increasingly requires resource managers to schedule jobs across heterogeneous backends with different noise levels and queue conditions. Although noise-aware placement can improve execution fidelity by assigning sensitive circuits to low-noise devices, concentrating many such jobs on a premium backend can create severe queueing and increase overall makespan. This work presents Q-CAR (Congestion-Aware Quantum Resource Allocation), a lightweight adaptive scheduling policy for Slurm-managed heterogeneous quantum clusters. Q-CAR follows a three-stage approach: it first restricts each job to a candidate set according to per-instance noise sensitivity, then selects a node by minimizing a composite cost that combines expected waiting time, service time, and fidelity loss, and finally allows a one-tier escape when congestion on the premium node exceeds a threshold. We evaluate Q-CAR on a real Slurm resource-management layer with per-node Qiskit Aer GPU simulators configured with three controlled noise tiers. The workload consists of five MQT Bench circuit families over 2-16 qubits, and congestion is varied by changing the density of noise-sensitive jobs. Compared with a fidelity-aware baseline that sends all high- and medium-sensitivity jobs to the lowest-noise node, Q-CAR reduces makespan by 49% and 60% at 50% and 75% noise-sensitive job density, respectively, while limiting the loss in noise-sensitive fidelity to approximately 0.04-0.05. The throughput advantage remains consistent under different arrival patterns. These results show that separating fidelity-oriented candidate gating from congestion-aware allocation is an effective way to balance fidelity and throughput in the evaluated heterogeneous quantum-cluster environment.



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DeepKinomeWeb: a Quantitative, Panel-Level Platform for Kinase Inhibitor Screening and Selectivity Profiling

Hyeonsu Na[1,2], Jisu Eun[1,3], Yeeun Lee[4], Seunghoon Yang[1,2], Donghwan Choi[1], Hyeyun Cho[1,2], Seungyoon Nam[4,5*], and Jinhyuk Lee[1,2*]

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Protein kinases constitute one of the largest enzyme families in the human genome and remain among the most important therapeutic target classes in oncology [1, 2]. In early-stage drug discovery, however, identifying potent and selective inhibitors is constrained by the cost of competition-based high-throughput screening and by the difficulty of reading selectivity across an entire kinase panel rather than kinase by kinase. Few available tools combine panel-level screening, quantitative affinity estimation, and off-target assessment in a single workflow.

To address this gap, we developed DeepKinomeWeb, an integrated web platform for quantitative kinase inhibitor screening and selectivity profiling [4]. It builds on DeepKinome, a 20-layer convolutional neural network regression model trained on LINCS KINOMEscan data that predicts binding affinity as a continuous percent inhibition value (RMSE = 1.157, PCC = 0.743, R^2 = 0.535) [3]. Compounds submitted as PubChem identifiers or SDF files [7] are screened against a 229-kinase panel, and results are returned on one interactive page: an affinity heatmap, two selectivity indices (SI_mean, SI_worst), promiscuity/specificity radar plots, optional AutoDock Vina docking with a 3D viewer [5], and ADMET profiling [6].

In a case study of three FDA-approved ATP-competitive inhibitors absent from the training data, the platform recovered their known profiles: brigatinib gave a sharp, spike-like specificity profile toward ALK (SI_mean = 4.6934), whereas ponatinib (1.7903) and sunitinib (0.9928) were broader, and the docking poses matched their reported Type I and Type II binding modes. Validation against DrugBank sets showed SI_mean shifted upward for approved on-target pairs (n = 422; Wilcoxon $P = 2.48 \times 10^{-9}$), and DeepKinome ranked approved targets above AutoDock Vina. The server is freely available at https://str.kribb.re.kr/deepkinome.

Keywords kinase inhibitor, deep learning, binding affinity prediction, selectivity profiling, drug discovery

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pH-dependent membrane insertion and folding of the Caveolin-3-derived peptide Cav3(7–26): an all-atom molecular dynamics study

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Caveolin-3 (Cav3) is a muscle-specific scaffolding protein of caveolae whose flexible N-terminal region is intrinsically disordered in solution yet undergoes a pH-dependent conformational switch at membrane-mimetic interfaces [1, 2]. Circular dichroism and NMR show that acidification promotes α-helix formation in the Cav3(7–26) peptide, most strongly at anionic membrane surfaces, but ensemble spectroscopy cannot resolve the time-ordered, residue-level pathway by which the peptide approaches, inserts into, and folds within the bilayer, nor which residues initiate the transition. To obtain this atomic-resolution mechanism, we performed all-atom molecular dynamics (MD) simulations.

Cav3(7–26) was placed at a mixed DMPC/LPPG bilayer interface and simulated for ~10 μs each under fixed protonation states approximating pH 3 (folding) and pH 7 (control) using GROMACS with the CHARMM36m force field [3–5]. At pH 3 the peptide followed an ordered, partly overlapping insertion-and-folding pathway: N-terminal residues made first interfacial contact (~0.8 μs), a short helix was seeded (~1.8 μs), and the peptide settled into a stable 11–17 α-helix buried beneath the lipid phosphates (~6.5–10 μs; modal helix content ~35%). An amphipathic hydrophobic face (Leu9, Ile13, Val14, Ile17) led insertion, with N-terminal residues initiating contact and central residues providing the deepest, most persistent anchor (deepest ~6.5 Å from the bilayer center). At pH 7 the peptide remained disordered in solution (~0% helix), matching the neutral-pH random-coil signature.

To test the role of the flexible termini, the truncation Cav3(10–24), lacking N-terminal 7–9 and C-terminal 25–26, was simulated under the same pH 3 protocol. It formed no 11–17 helix (~0% helix content) and failed to insert (deepest ~19.3 Å, short of the ~17.3 Å bilayer half-thickness), with the deepest position shifting from the helix core to the truncated terminus. This confirms that the terminal residues are essential for the pH-dependent insertion-and-folding transition, consistent with the reduced helical CD of the truncated peptide. Together, the simulations provide a residue-level mechanistic model that unifies the spectroscopic observations and suggest that local acidification, such as lactic-acid accumulation during intense muscle activity or ischemia, could modulate the conformational ensemble of the Cav3 N terminus.

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[Key words] Caveolin-3, molecular dynamics, membrane insertion, pH-dependent folding, amphipathic helx

Virtual Screening of Covalent Inhibitors Targeting PNPLA3-I148M

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The PNPLA3 I148M variant is a major genetic risk factor for metabolic dysfunction-associated steatotic liver disease (MASLD) and accumulates on the lipid droplet surface due to reduced ubiquitination and proteasomal degradation [1]. PF-07853578 has been reported to covalently bind to the catalytic Ser47 residue, promoting the dissociation of PNPLA3 from lipid droplets and subsequent protein degradation [2]. In this study, we aimed to identify novel covalent inhibitor candidates by considering both Ser47 and the local environment surrounding the mutation-specific Met148 residue.

WT and I148M receptor models were constructed from the AlphaFold-predicted human PNPLA3 structure (UniProt Q9NST1). In 1,200 ns MD simulations, the global Cα RMSD was 0.48 Å, while the residue 148–Ser47 OG distance increased from 4.41 Å in WT to 5.27 Å in I148M, indicating a localized active-site difference. Stepwise virtual screening of 24,959 compounds from PF-07853578-based PubChem, amine-ring-expanded, and REINVENT4 de novo libraries yielded 551 candidates for AutoDock4 Flexible Side Chain covalent docking [3] and WT/I148M selectivity assessment. The top-ranked candidate showed an adduct interaction energy of −9.66 kcal/mol with complete pose and energy convergence but dissociated from the catalytic pocket during 100 ns non-covalent MD (ligand RMSD, 12.47 Å; COM displacement, 10.37 Å). In contrast, PF-07853578 remained stable (2.04 Å; 1.56 Å, respectively), while additional top-ranked candidates are currently undergoing MD validation.

This study established an integrated PNPLA3-I148M-targeted virtual screening workflow combining compound filtering, covalent docking, and MD-based validation. The results obtained to date suggest that a high docking score alone does not ensure dynamic binding stability and that MD evaluation incorporating both reactive geometry toward Ser47 and binding stability around Met148 is important for prioritizing candidate compounds.

Keywords PNPLA3-I148M, covalent docking, flexible side chain method, molecular dynamics, Ser47, virtual screening

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Computational modeling of the AAVX–AAVR complex from Cryo-EM density map

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Adeno-associated virus (AAV) is widely utilized in gene therapy due to its efficient transduction, favorable tissue tropism, and low immunogenicity. Despite its growing therapeutic relevance, the structural basis of its interaction with cellular receptors remains incompletely understood.

To elucidate the mechanism of cellular entry and receptor recognition, we determined the cryo-electron microscopy (cryo-EM) structure of the AAV serotype X (AAVX) capsid in the complex with its cellular receptor, receptor A, at a resolution of 2.66 Å. CHARMM was used to derive an energetically optimized structure with maximal density map–to–model correlation., which provided energetically favorable conformations for the complex, guided initial model construction. Subsequent structural refinement was performed using Phenix real-space refinement and manual corrections in Coot. Interaction analysis provided to identify key contact residues involved in receptor engagement.

This high-resolution density map allowed accurate atomic modeling of the AAVX–receptor A complex, revealing detail interface characterization. These structural insights provide a foundation for understanding the unique receptor engagement of AAVX.

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EpiSearch: Identifying Disease-Specific Leading Search Indicators Using Wastewater Surveillance Data in Korea

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Early detection and rapid response to infectious diseases are crucial for effectively managing their spread. Currently, various methods such as clinical surveillance and wastewater-based epidemiology (WBE) are used for infectious disease surveillance[1]. However, these approaches have limitations, as time delays can occur during processes such as diagnosis, specimen collection, and analysis. To address these limitations, research has been conducted to utilize web search data which reflects people's disease related concerns and behaviors as a supplementary indicator for infectious disease surveillance[2,3]. G. Lippi et al. demonstrated that trends in internet search volume can serve as an indicator to predict local COVID-19 outbreaks three weeks in advance, and Z. Alessandro et al. demonstrated the predictive power of Google search volume using wastewater surveillance data. However, no systematic studies have yet been sufficiently established regarding the optimal combination of search keywords that most effectively reflects the characteristics of each disease.

Therefore, in this study, we designed various keyword composition strategies for SARS-CoV-2, Influenza, and Norovirus in Korea by categorizing search keywords into single keywords, groups of disease names and symptom keywords, and groups combining two or more keywords. We then analyzed the temporal correlation between the search trends for each strategy and pathogen concentrations in wastewater to identify the optimal search indicators for each infectious disease where search trends precede WBE signals.

The analysis revealed that for SARS-CoV-2, the highest correlation (r = 0.90) was observed when search volume for the keywords "코로나" and "코로나"+"제반증상" preceded WBE signals by one week. For influenza, the search volume for the keyword "오한" showed the highest correlation (r = 0.89) when it preceded WBE signals by one week, while for norovirus, the search volume for the keyword combinations "노로바이러스"+"구토"+"물설사" and "노로바이러스"+"구토" showed the highest correlation (r = 0.65) when it preceded WBE signals by two weeks. All correlations were statistically significant ($p < 0.001$). This study confirmed that the lead time between web search trends and WBE signals varies depending on the search keyword composition strategy for each infectious disease. Furthermore, by identifying keywords and combinations that show high correlations for each infectious disease, the study demonstrated the potential for using web search data as an early infectious disease surveillance indicator.

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The Intelligent Frontier: Synergizing HPC, AI and Quantum

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PROGRAM

DAY 1 | September 08, 2026

- 기조연설 1, 2
- KSC2026 개회식
- Track
  - HPC·AI 인프라 최신 기술 동향 및 국내 대형 시스템 소개 • 2026년 한국계산과학공학회 추계학술대회 • AI for Science: 과학적 발견과 혁신
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DAY 2 | September 09, 2026

- Track
  - HPC 활용을 위한 대규모 데이터 처리 기술 워크숍 · HPC 수치모의실험 전문학 워크숍 · Quantum Intelligence: 양자-AI 융합과 신약 바이오 혁신
  - 국가슈퍼컴퓨터 6호기 '한강' 및 시범·공식서비스(혁신지원사업) 설명회 · HPC 활용 산업 기술 워크숍 · 기상 기후 분야 초고성능컴퓨팅 활용고도화 워크숍
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