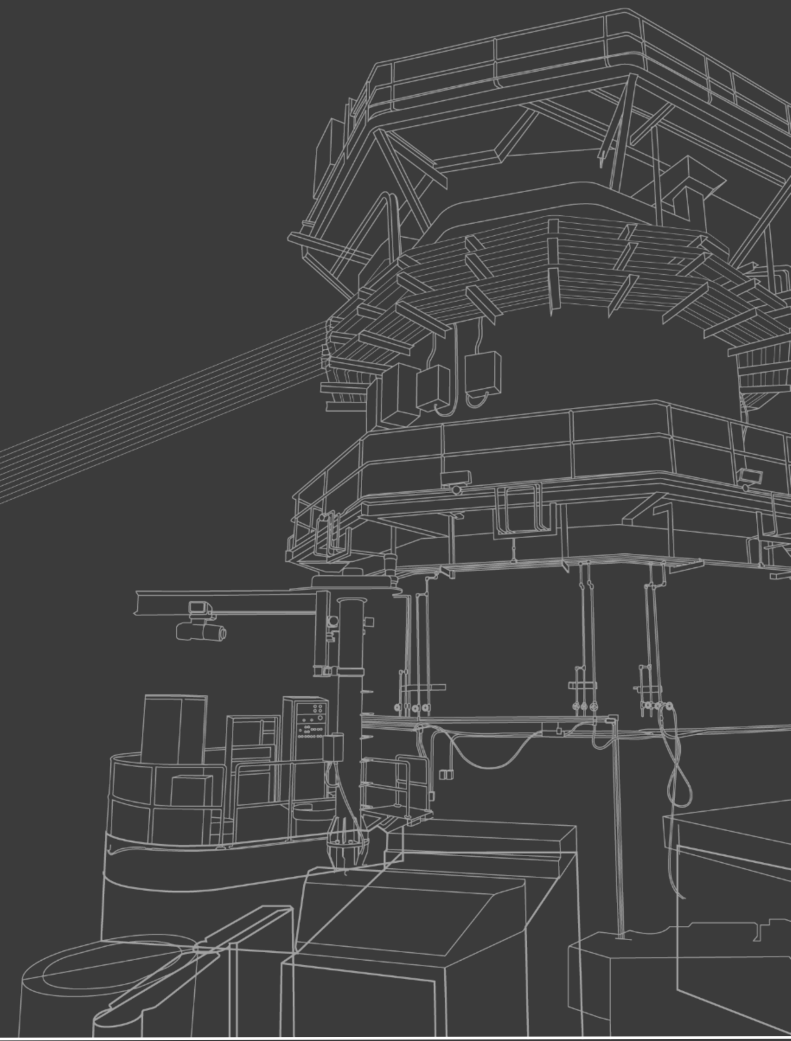
KAERI

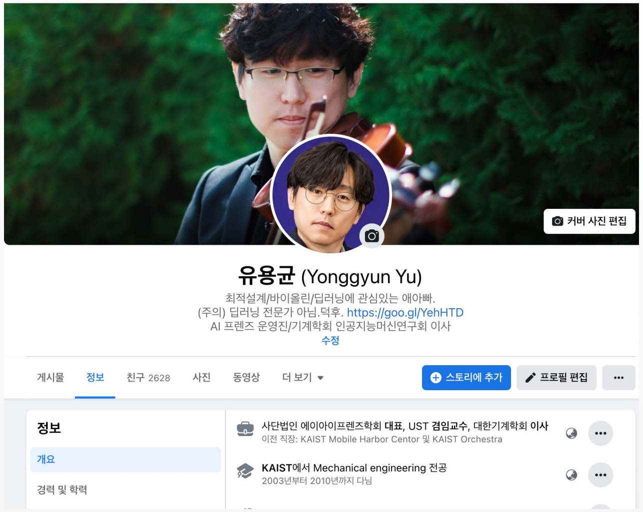
원자력(재료)에서의 인공지능 응용사례



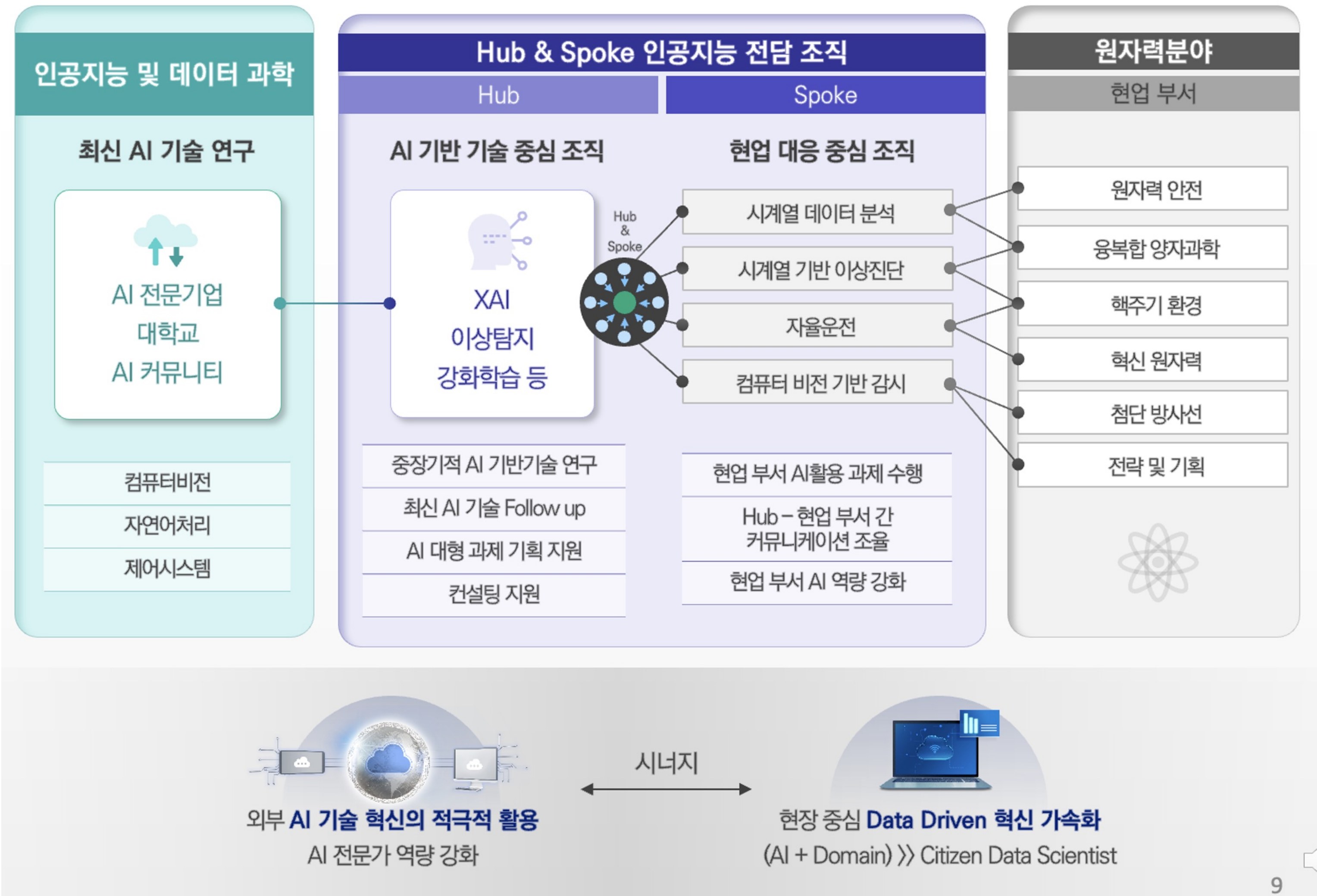
한국원자력연구원 유 용 균
(ygyu@kaeri.re.kr, yoyogo@gmail.com)

Korea Atomic Energy Research Institute

- 한국원자력연구원 인공지능응용전략실
- 사단법인/커뮤니티 AI프렌즈 대표
- Nvidia 앰배서더 / DLI Instructor
- UST 원자력 및 방사선 안전 겸임교수
- 대한기계학회 인공지능머신연구회 이사



Hub(인공지능응용전략실) & Spoke (현업부서 DS)



AI그랜드 챌린지…원자력연-젠티연합팀 1위로 3단계 진출

길애경 기자 | kilpaper@hellodd.com | 입력 2021.11.04 17:30 | 수정 2021.11.04 18:52 | 댓글 0

과기부, 5차대회 2단계 3팀 통과
연구비 팀별 4억7500만원 지원
3, 4차 대회 3단계 대회 내달 펼쳐져

인공지능 개발자들의 치열한 경연이 펼쳐지는가운데 한국원자력연구원과 기업 젠티 연합팀, 매스프레소 기업팀, 성균관대 인공지능대학원 연구팀이 5차대회 3단계에 올랐다.

과학기술정보통신부(장관 임혜숙)는 '인공지능 그랜드 챌린지' 5차 대회 2단계를 통과한 팀을 5일 대회 홈페이지에 발표하고 내달 10일부터 12일까지 3, 4차대회 3단계를 진행한다고 4일 밝혔다.

인공지능 그랜드 챌린지 대회는 제시된 문제를 해결하기 위해 참가자들이 자발적으로 진행한 사전 연구를 바탕으로 실력을 겨루는 도전·경쟁형 연구개발(R&D) 경진대회다. 5차 대회는 자연어의 이해와 수리적 사고 추론에 기반한 복합지능 기술 확보를 목표로 '인공지능 기술을 활용해 주어진 수학 문제를 해결'하는 것이다. 오는 22년까지 2년간 총3단계로 진행된다.

인공지능의 정의from state of AI 2022

인공 지능(AI): 인간과 동물이 보여주는 자연 지능과 달리 지능형 기계를 만드는 것을 목표로 하는 광범위한 분야입니다.

인공 일반 지능(AGI): 경제적으로 가치 있는 모든 작업에서 인간의 인지 능력의 전체 범위와 일치하고 초과할 수 있는 미래의 기계를 설명하는 데 사용되는 용어입니다.

AI 안전: 미래의 AI가 인류에게 가할 수 있는 치명적인 위험을 연구하고 완화하려는 분야입니다.

머신 러닝(ML): 통계 기술을 사용하여 머신이 명시적으로 수행 방법에 대한 지침을 받지 않고도 데이터에서 "학습"할 수 있는 기능을 제공하는 AI의 하위 집합입니다. 이 프로세스는 특정 작업에 대한 모델 성능을 점진적으로 향상시키는 학습 "알고리즘"을 사용하여 "모델"을 "훈련"하는 것으로 알려져 있습니다 .

딥 러닝(DL): 데이터의 복잡한 패턴을 인식하는 방법을 배우기 위해 뇌의 뉴런 층에서 활동을 모방하려고 시도하는 ML 영역입니다. "깊은"은 더 나은 성능 향상을 달성하기 위해 데이터의 풍부한 표현을 학습하는 데 도움이 되는 현대 모델의 많은 수의 뉴런 레이어를 나타냅니다.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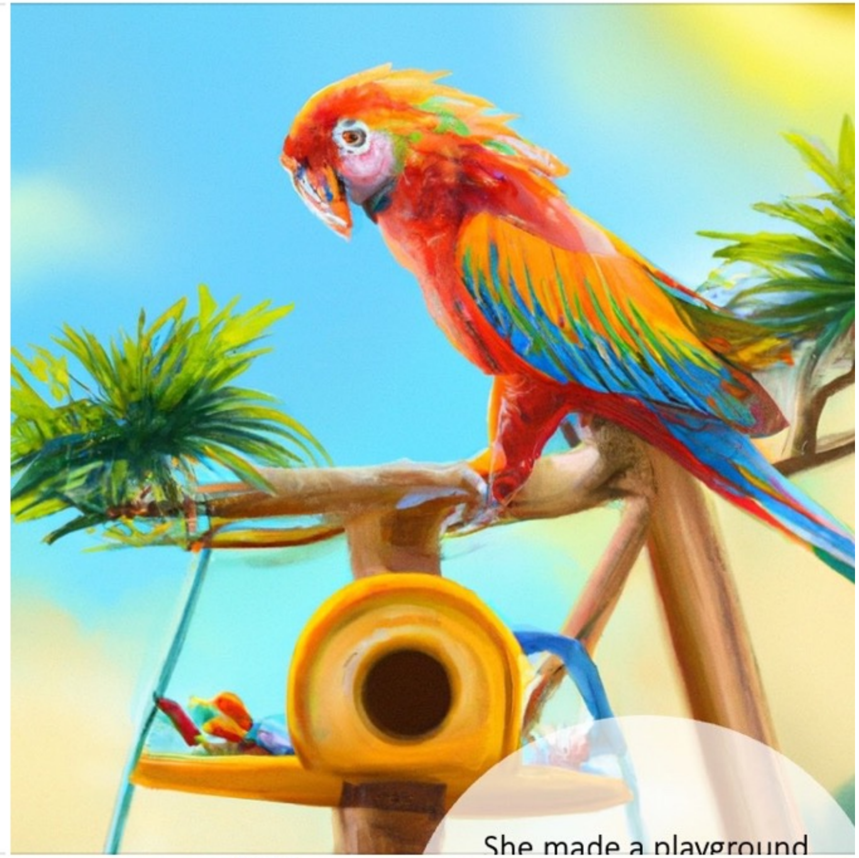
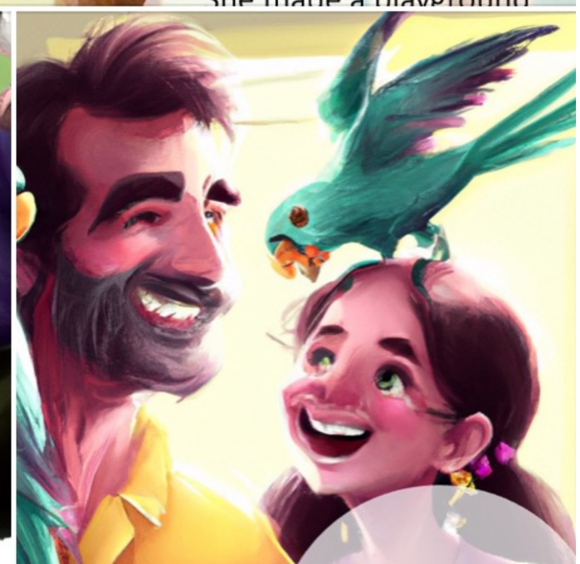
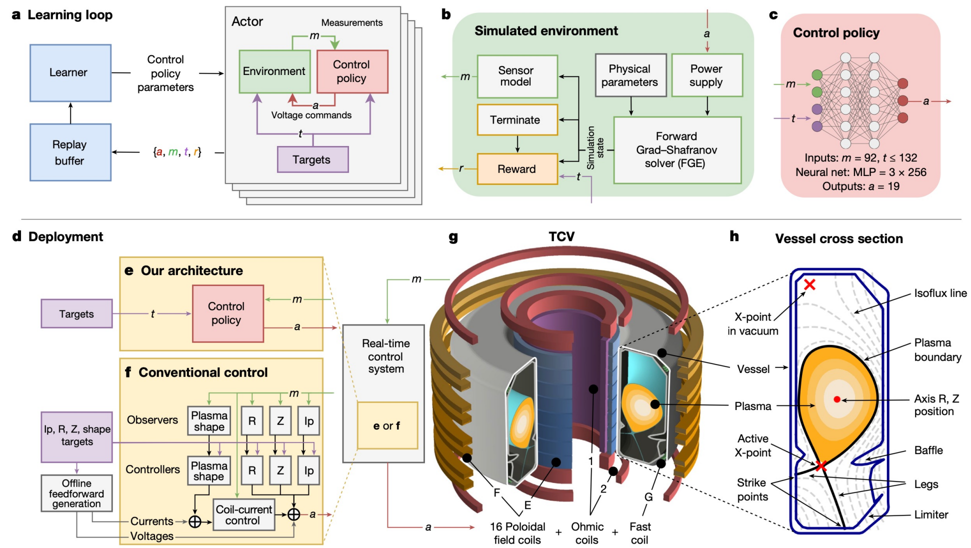
Once upon a time there lived a girl who





2022.2.16 핵융합(플라즈마) 제어하는 인공지능 (Deepmind)



ZDNet Korea

알파고 만든 딥마인드, 핵융합 제어 AI 개발

남혁우 기자 입력 2022. 02. 17. 08:52 댓글 3개

토카막 내부 플라즈마 자기장 안정화 제어

(지디넷코리아=남혁우 기자)바둑 인공지능(AI) 알파고를 만든 딥마인드가 핵융합로 내부 플라즈마를 제어하는 AI를 개발했다.

알파고를 만든 알파벳의 자회사 딥마인드는 스위스 로잔연방공과대학교(EPFL)의 플라즈마센터와 공동 연구 프로젝트로 핵융합 반응 제어용 AI를 개발 중이라고 과학저널 네이처에 16일(현지시간) 발표했다.

딥마인드는 이번 프로젝트에서 가변 구성 토카막(TCV) 핵융합로 내 자기장을 제어할 수 있는 신경망 AI를 개발했다고 밝혔다.

2022.2 수학문제 증명하는 인공지능 (OpenAI)

Solving (Some) Formal Math Olympiad Problems

We built a neural theorem prover for Lean that learned to solve a variety of challenging high-school olympiad problems, including problems from the AMC12 and AIME competitions, as well as two problems adapted from the IMO.[1] The prover uses a language model to find proofs of formal statements. Each time we find a new proof, we use it as new training data, which improves the neural network and enables it to iteratively find solutions to harder and harder statements.

These problems are not standard math exercises, they are used to let the best high-school students from the US (AMC12, AIME) or the world (IMO) compete against each other.

PROBLEM 3

Adapted from the MATH dataset[3]

Let $f(x) = Ax + B$ and $g(x) = Bx + A$, where $A \neq B$. If $f(g(x)) - g(f(x)) = B - A$, prove that $A + B = 0$.

FORMAL | **INFORMAL**

First we find that:

$$f(g(x)) = A(Bx + A) + B = ABx + A^2 + B$$

$$g(f(x)) = B(Ax + B) + A = ABx + B^2 + A$$

Now we plug this back in $f(g(x)) - g(f(x)) = B - A$ and get:

$$(ABx + A^2 + B) - (ABx + B^2 + A) = B - A$$

That is:

$$A^2 - B^2 + B - A = B - A$$

Hence:

$$A^2 - B^2 = (A - B)(A + B) = 0$$

Since we are given that $A \neq B$, necessarily, $A + B = 0$.

OBLEM 5

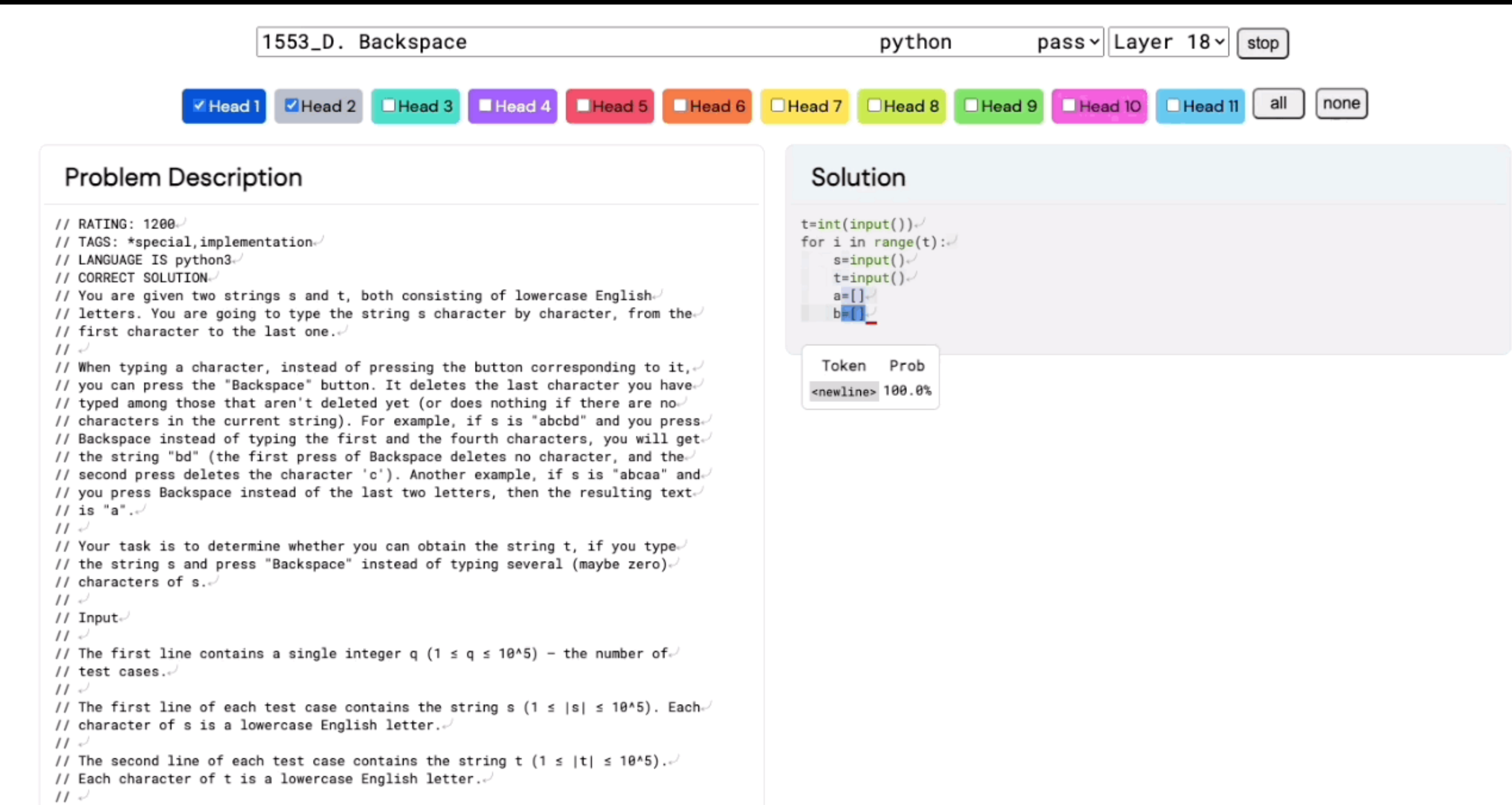
lapted from AIME 1984 Problem 1

ove that $a2 + a4 + a6 + a8 + ... + a98 = 93$ if $a1, a2, a3...$ is an arithmetic ogression with common difference 1, and $a1 + a2 + a3 + ... + a98 = 137$.

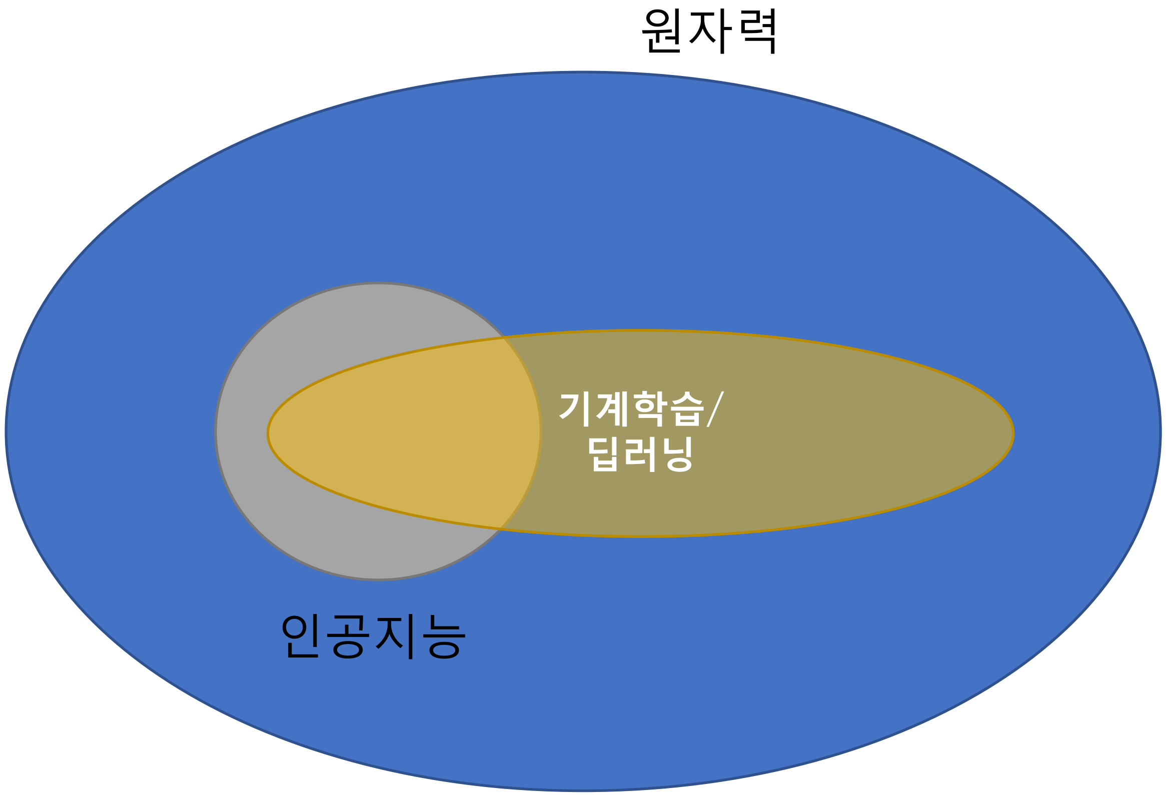
FORMAL | INFORMAL

```
theorem aime_1984_p1
  (u : ℕ → ℚ)
  (h₀ : ∀ n, u (n + 1) = u n + 1)
  (h₁ : ∑ k in finset.range 98, u k.succ = 137) :
  ∑ k in finset.range 49, u (2 * k.succ) = 93 :=
begin
  rw finset.sum_eq_multiset_sum,
  dsimp [finset.range] at h₁,
  simp [h₀],
  ring,
  norm_num at h₁,
  norm_num,
  apply eq_of_sub_eq_zero,
  { simp only [*, abs_of_pos, add_zero] at *, linarith },
end
```

2022.2 알파코드 (DeepMind)



원자력(재료)에서의 인공지능은?



케플러의 행성운동법칙

文A 79개 언어

위키백과, 우리 모두의 백과사전.

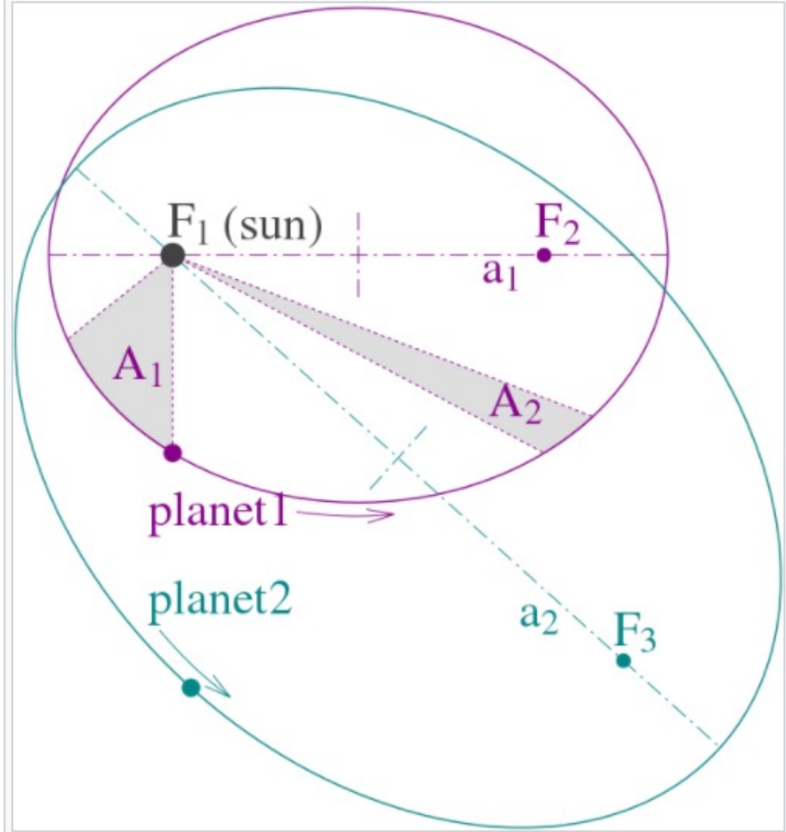
케플러의 행성운동법칙(行星運動法則, 영어: Kepler's laws of planetary motion)은 독일의 천문학자 요하네스 케플러가 발표한 행성의 운동에 대한 세 개의 물리학 법칙이다.

아이작 뉴턴이 만유인력의 법칙을 발견하기 약 반세기 전, 케플러는 티코 브라헤가 평생 동안 천체를 관측하면서 축적한 자료들을 분석하여 다음과 같은 케플러의 행성운동법칙을 발표하였다.

1. 행성은 모항성을 한 초점으로 하는 타원궤도를 그리면서 공전한다. (타원궤도 법칙)
2. 행성과 태양을 연결하는 가상적인 선분이 같은 시간 동안 쓸고 지나가는 면적은 항상 같다.
3. 행성의 공전주기의 제곱은 궤도의 긴반지름의 세제곱에 비례한다.[1]

아이작 뉴턴은 자신이 발견한 운동 법칙과 케플러 법칙 등을 기반으로 만유인력의 법칙을 유도해냈다. 즉, 케플러가 기술한 태양계의 행성의 운동은 뉴턴의 법칙에 따르는 두개의 질점간의 상호작용에 해당한다는 것을 밝혀낸 것이다.

따라서 케플러의 행성 운동 법칙은 태양과 행성 사이에만 성립하는 것이 아니라, 행성과 그 위성(인공위성을 포함하여), 위성과 위성이 갖는 손자위성 사이에도 성립한다.



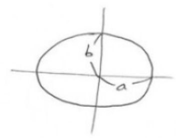
두 행성의 공전궤도를 통한 케플러의 세가지 법칙들에 대한 설명. (1) 첫 번째 행성의 공전궤도는 *f1*과 *f2*를 초점으로 갖는 타원궤도이고, 두 번째 행성의 공전궤도는 *f1*과 *f3*을 초점으로 갖는 타원궤도이다. 태양은 여기서 초점 *f1*에 있다. (2) 행성이 같은 시간 동안 휩쓸고 지나가는 음영으로 표시된 두 영역 *A1*과 *A2*는 같은 면적을 가지고 있다. (3) 두 행성의 공전주기의 비는 $a_1^{\frac{3}{2}} : a_2^{\frac{3}{2}}$이다.

목차 [숨기기]

수학적 설명 [편집]

⊙ 케플러 3법칙 (조화의 법칙) 의 증명.

케플러 2법칙에서, $\frac{dA}{dt} = \frac{L}{2m} = \frac{h}{2}$



$$\int_{\text{타원}} dA = \int_0^T \frac{h}{2}\,dt$$

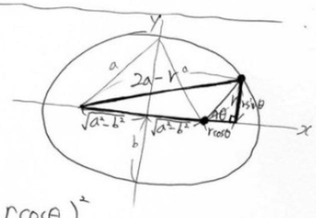
$$\pi ab = \frac{h}{2}T$$

$$T = \frac{2\pi ab}{h}$$

$T^2 = 4\pi^2 \frac{a^2b^2}{h^2}$ 인데 $\underbrace{h^2 = \frac{b^2}{a}GM}_{\text{증명은 (*)에...}}$ 이므로,

$$\boxed{T^2 = \frac{4\pi^2}{GM}a^3}$$ Q.E.D.//

(*) $h^2 = \frac{b^2}{a}GM$ 의 증명.



타원의 $\underbrace{\text{방정식을}}_{a,b\text{로}}$ 극좌표 형태로 나타내보자.

피타고라스 정리로부터,

$$(2a-r)^2 = r^2\sin^2\theta + \left(2\sqrt{a^2-b^2} + r\cos\theta\right)^2$$

위식을 정리하면,

$$r = \frac{\frac{b^2}{a}}{1 + \frac{\sqrt{a^2-b^2}}{a}\cos\theta}$$

이다. 그런데 케플러 1법칙 증명할때 ② 식과 비교하면, 분자의 $\frac{b^2}{a} = \frac{h^2}{GM}$ 임을 알수있다!! Q.E.D.//

참고로 여기서 a가 반장축 입니다

https://m.blog.naver.com/winzone/70138313312

요하네스 케플러

독일 수학자

요하네스 케플러는 독일의 수학자, 천문학자, 점성술사이자 17 세기 천문학 혁명의 핵심 인물이었다. 위키백과

출생: 1571년 12월 27일, 독일 바일데어슈타트

사망 정보: 1630년 11월 15일, 독일 레겐스부르크

자녀: 루드윅 케플러, 마르가레타 레지나 케플러, 시볼드 케플러, 더보기

학력: 튀빙겐 에버하르트 카를 대학교 (1589년-1591년), 더보기

배우자: Susanna Reuttinger (1613년-), 바바라 뮐러 (1597년-1611년)

부모: 카타리나 케플러, 하인리히 케플러

아이작 뉴턴

전 영국의 조폐국 장관

아이작 뉴턴 경은 잉글랜드의 수학자, 물리학자, 천문학자이다. 1687년 발간된 자연철학의 수학적 원리는 고전역학과 만유인력의 기본 바탕을 제시하며, 과학사에서 영향력 있는 저서 중의 하나로 꼽힌다. 위키백과

출생: 1643년 1월 4일, 영국 Woolsthorpe Manor House

사망 정보: 1727년 3월 31일, 영국 런던 켄싱턴

묘지: 영국 런던 웨스터 민스터 사원

영향을 준 인물: 갈릴레오 갈릴레이, 요하네스 케플러, 더보기

학력: 트리니티 대학 (1667년-1668년), 트리니티 대학 (1661년-1665년), The King's School (1655년-1659년)

국적: 그레이트브리튼 왕국, 영국, 잉글랜드, 잉글랜드 왕국

Kepler was a Data Scientist

Nikhil Verma Dec 9, 2020 · 4 min read ★

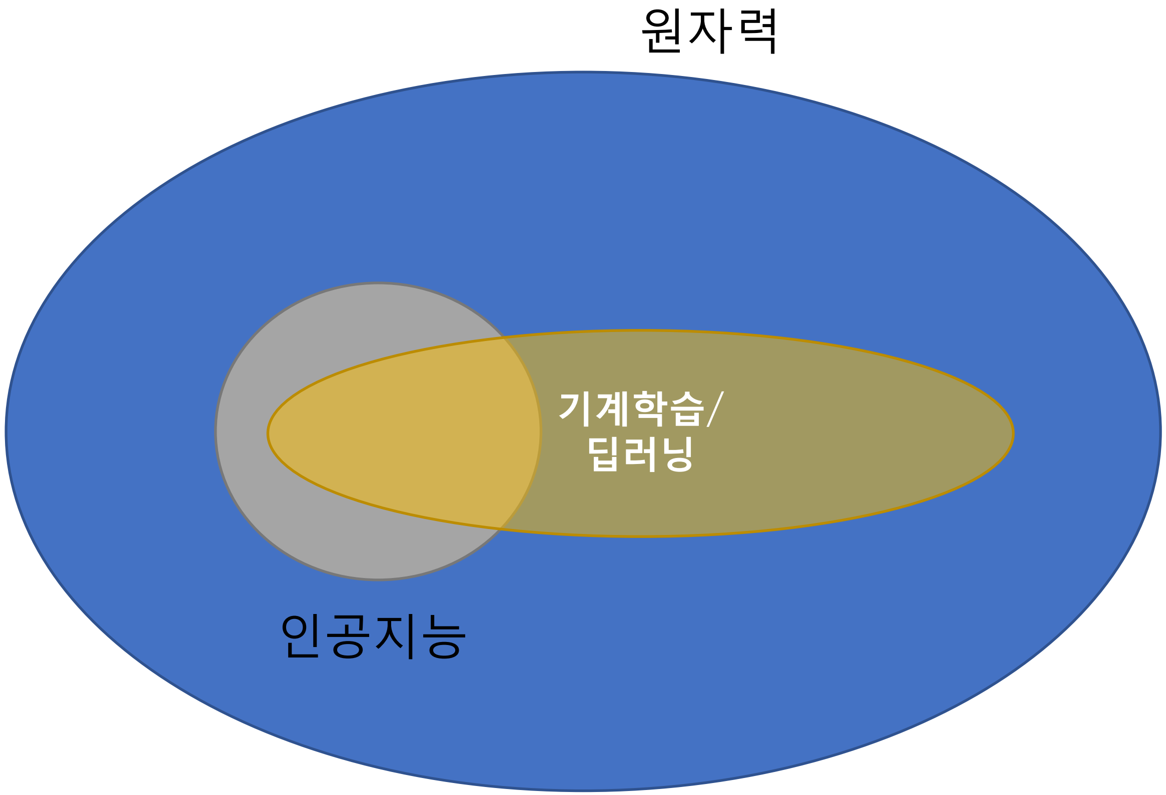
https://lih-verma.medium.com/kepler-was-a-data-scientist-b90b21315c85

Math Rule Based ML

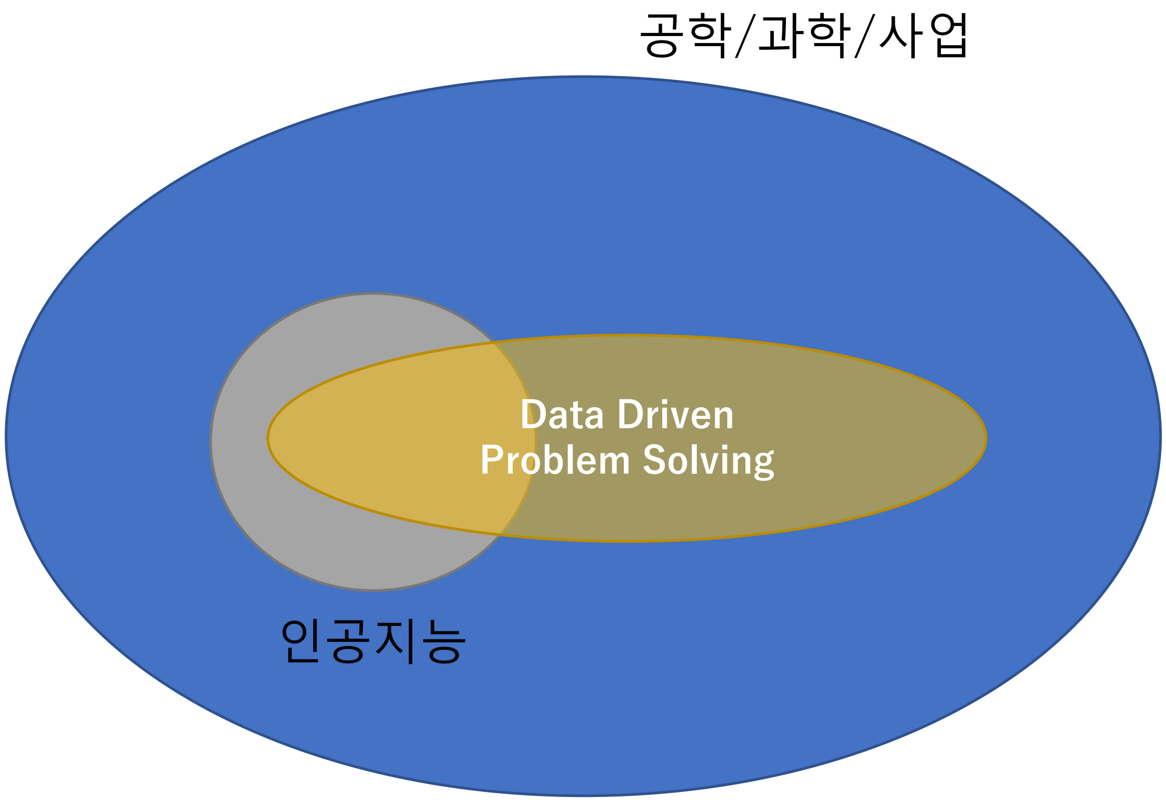
ML은 문제해결을 위한 방법론들 중 하나

한국원자력연구원

원자력(재료)에서의 인공지능은?



인공지능기술은 문제해결 방법



저의 관점…

인공지능(기계학습)은 뭔가 정의하거나
설명하기 애매모호한 것을
데이터를 이용해서 모델링 하기 좋은 기술…

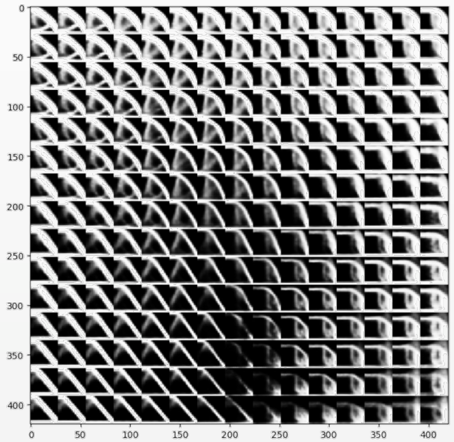
조건 $f(x)$

$$\underset{\rho}{\text{minimize}} \quad F = F(\mathbf{u}(\rho), \rho) = \int_{\Omega} f(\mathbf{u}(\rho), \rho)\mathrm{d}V$$

$$\text{subject to} \quad G_0(\rho) = \int_{\Omega} \rho \mathrm{d}V - V_0 \leq 0$$

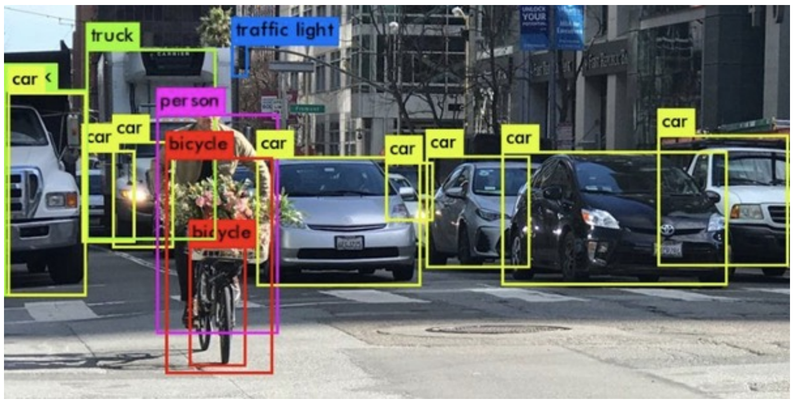
$$G_j(\mathbf{u}(\rho), \rho) \leq 0 \text{ with } j = 1, \ldots, m$$

조건 $f(x)$

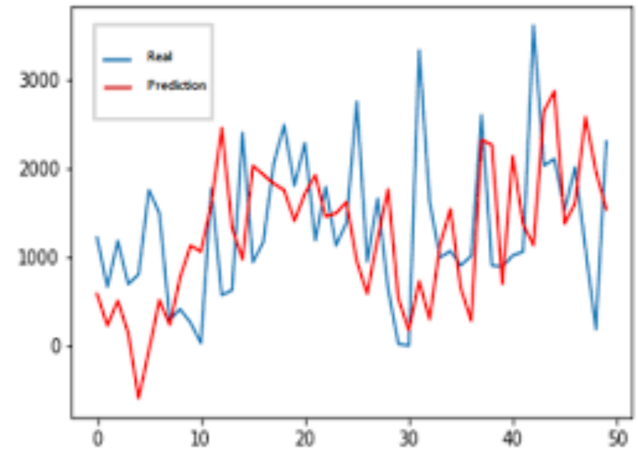


원자력분야의 인공지능

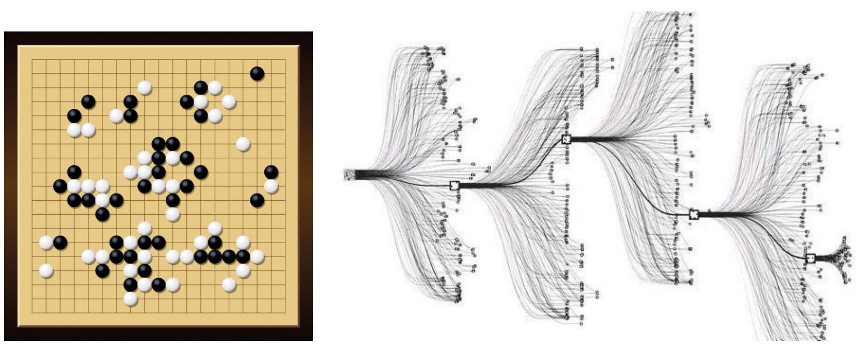
한국원자력연구원



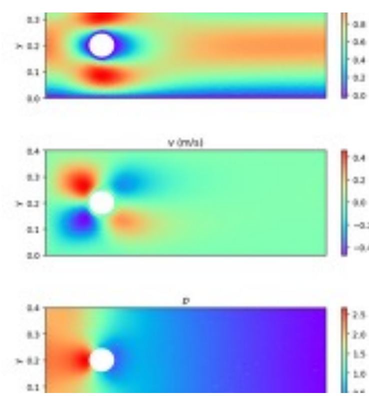
인지능력대체



데이터 분석

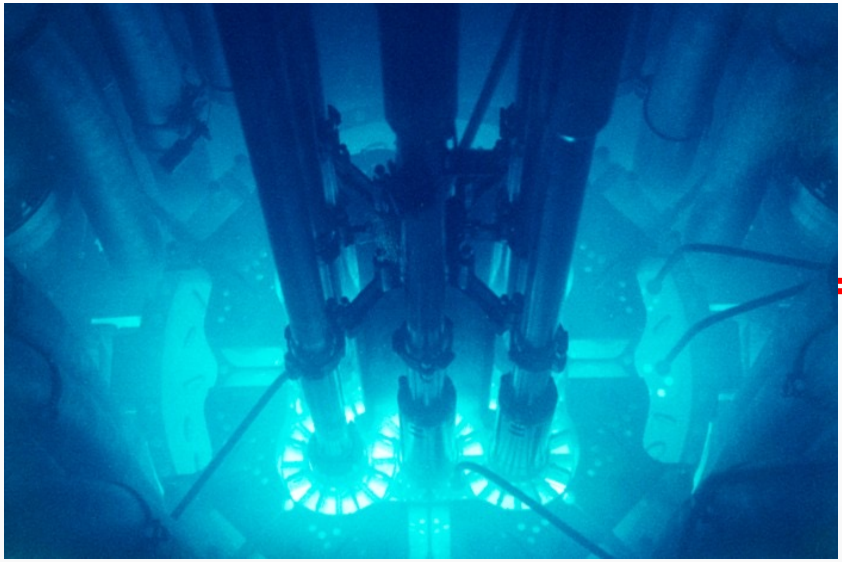


의사결정



Data driven Simulation

1. 인간의 인지/판단 능력을 대신하는 것



노심 감시
(기포 발생 등)

체렌코프 효과를 이용한 출력 모니터링

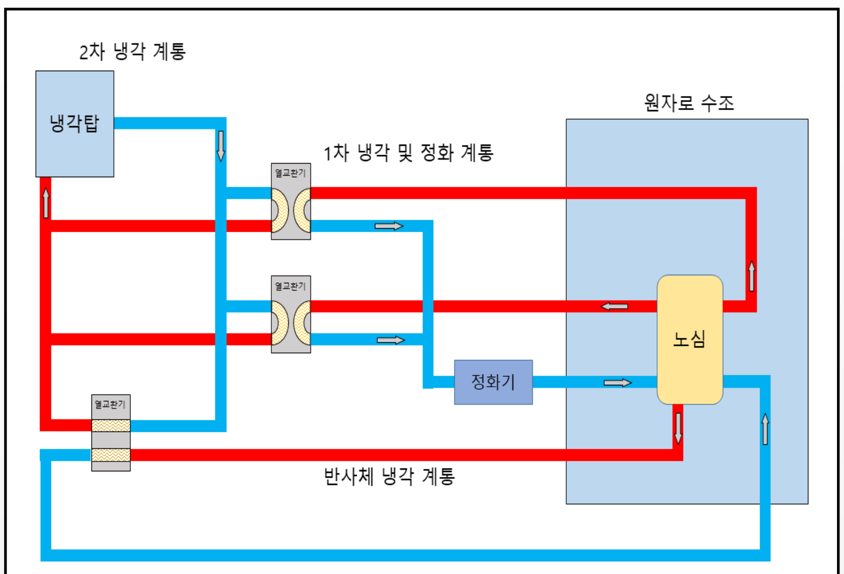
X-ray (+중성자) 영상분석

인공지능을 활용한 X-Ray 이미지 유해 물품 식별 모델 자문 및 기술이전 추진 중

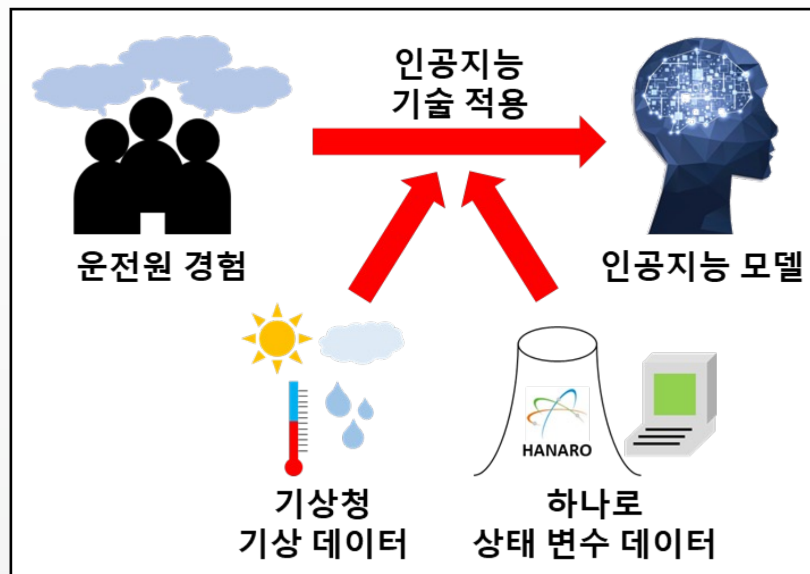
* ai hub 위해물품 엑스레이 이미지

1-2. 하나로 2차 계통 냉각팬 운전 모드 예측 모델 개발

- **하나로 2차 냉각 계통 시스템은 외부에 노출되어있는 냉각탑과 냉각팬을 포함.**
  → 2차 냉각 계통의 거동이 기상 상황에 영향을 받음.
- **이러한 특성이 고려된 절차가 정립되어있지 않아 운전원들의 경험에 따라 냉각팬 운전.**
  → 최적의 운전 방식이 아닐 뿐더러, 운전원들에게 부가적인 업무 부하 야기.
- **이러한 특성이 고려된 절차가 정립되어있지 않아 운전원들의 경험에 따라 냉각팬 운전.**
  → 하나로 상태 변수 데이터(냉각팬 운전 기록 포함)와 기상청 기상 데이터를 이용.
  → 지도학습을 통해 분류 모델을 학습시켜, 특정 상황에서의 냉각팬 운전 상태를 예측.



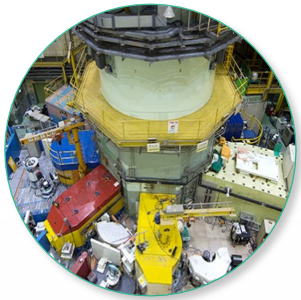
하나로 냉각 계통 구성도



인공지능 기술 적용을 통한 운전원 경험 모델링

2. 데이터 패턴 분석

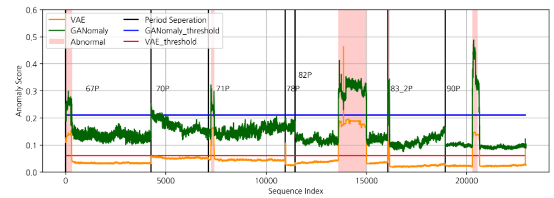
하나로원자로 이상탐지 기술개발



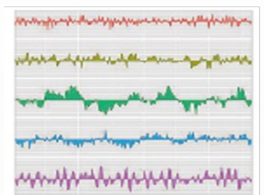
연구용 원자로 [하나로]

이상탐지 기술 동작 개요

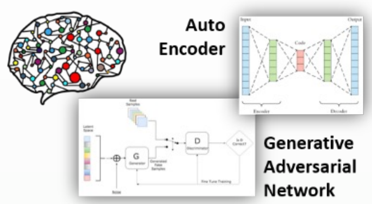
시계열 이상 탐지 및 예측



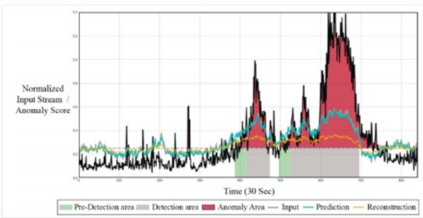
하나로 데이터 활용 이상탐지 결과



시계열 운전 데이터

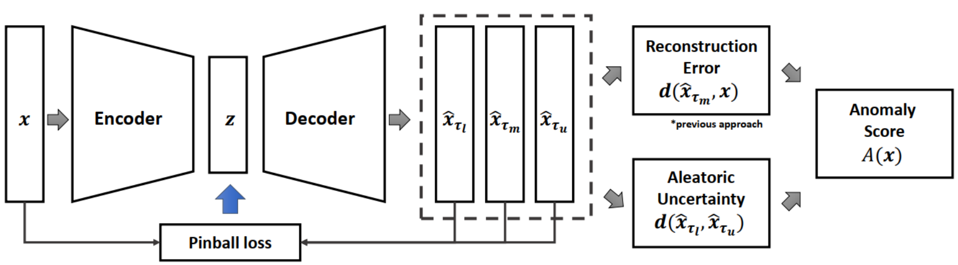


최적의 딥러닝 모델 탐색



이상 탐지 및 예측

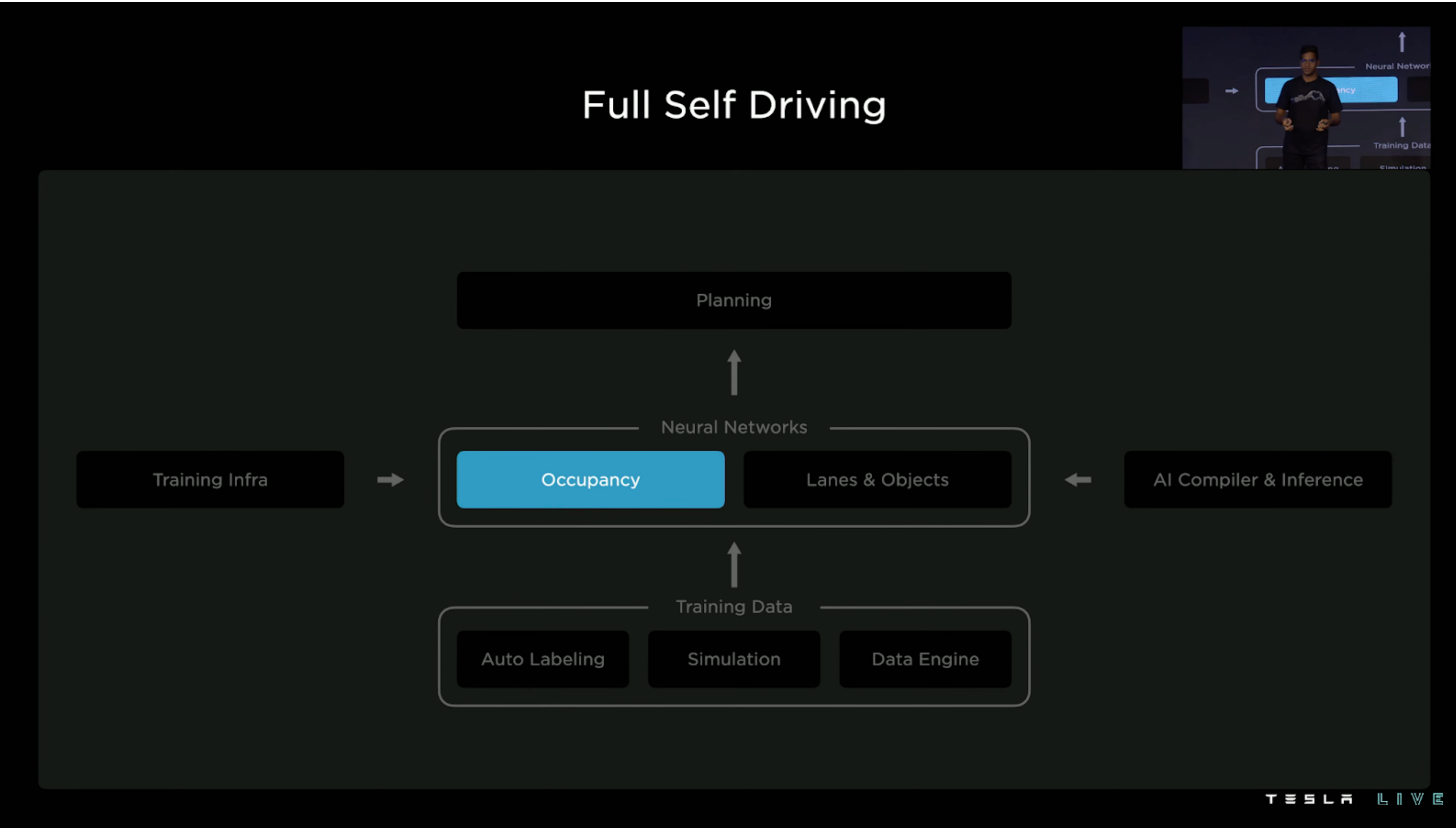
기술 개발 과정

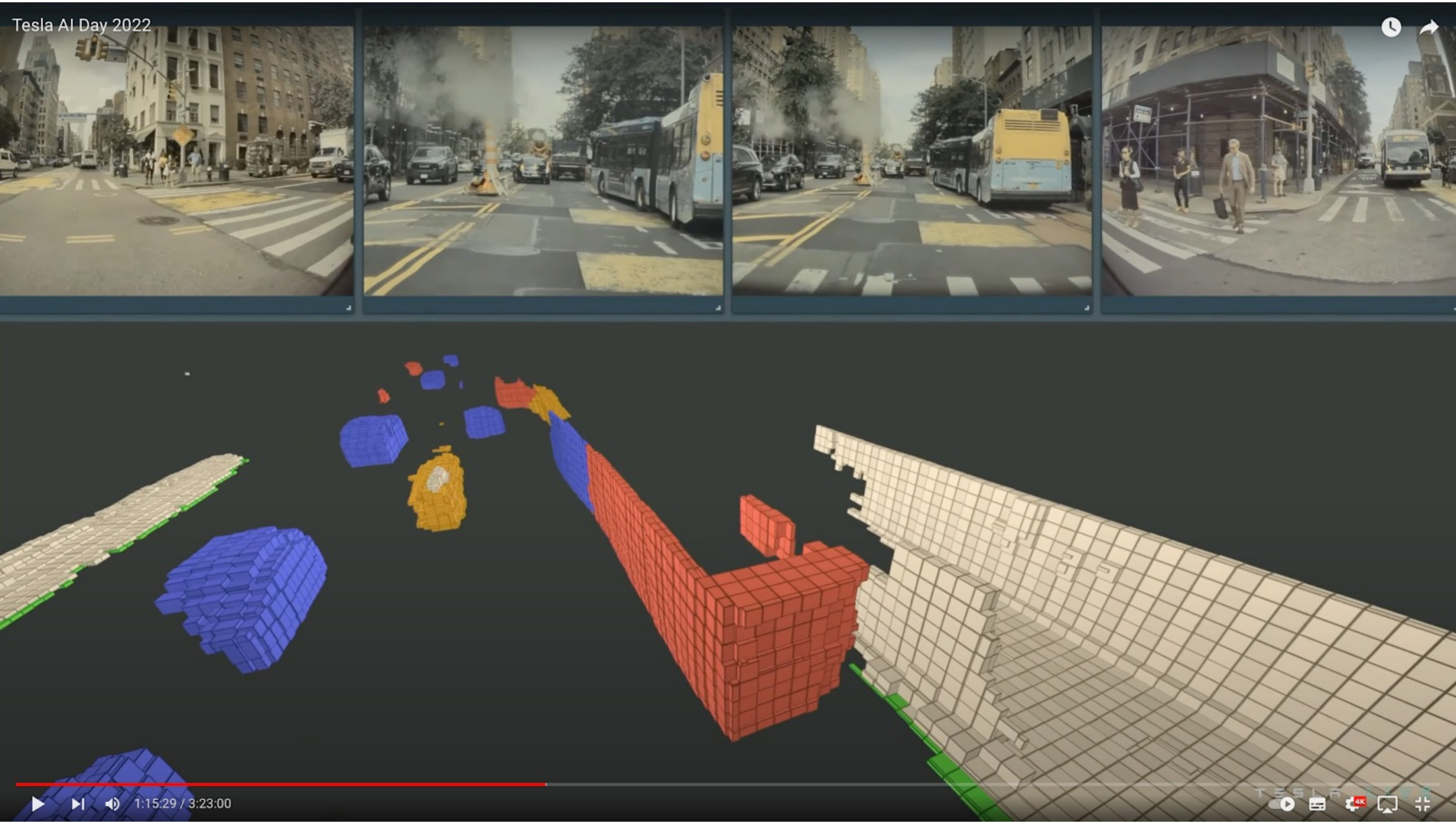


오토인코더 및 불확실성을 고려한 딥러닝 이상탐지 모델 구조

3. Digital Twin과 AI를 이용한 의사결정

Self-Driving
100m
48
mph


Full Self Driving
Planning
Neural Networks
Training Infra
Occupancy
Lanes & Objects
AI Compiler & Inference
Training Data
Auto Labeling
Simulation
Data Engine

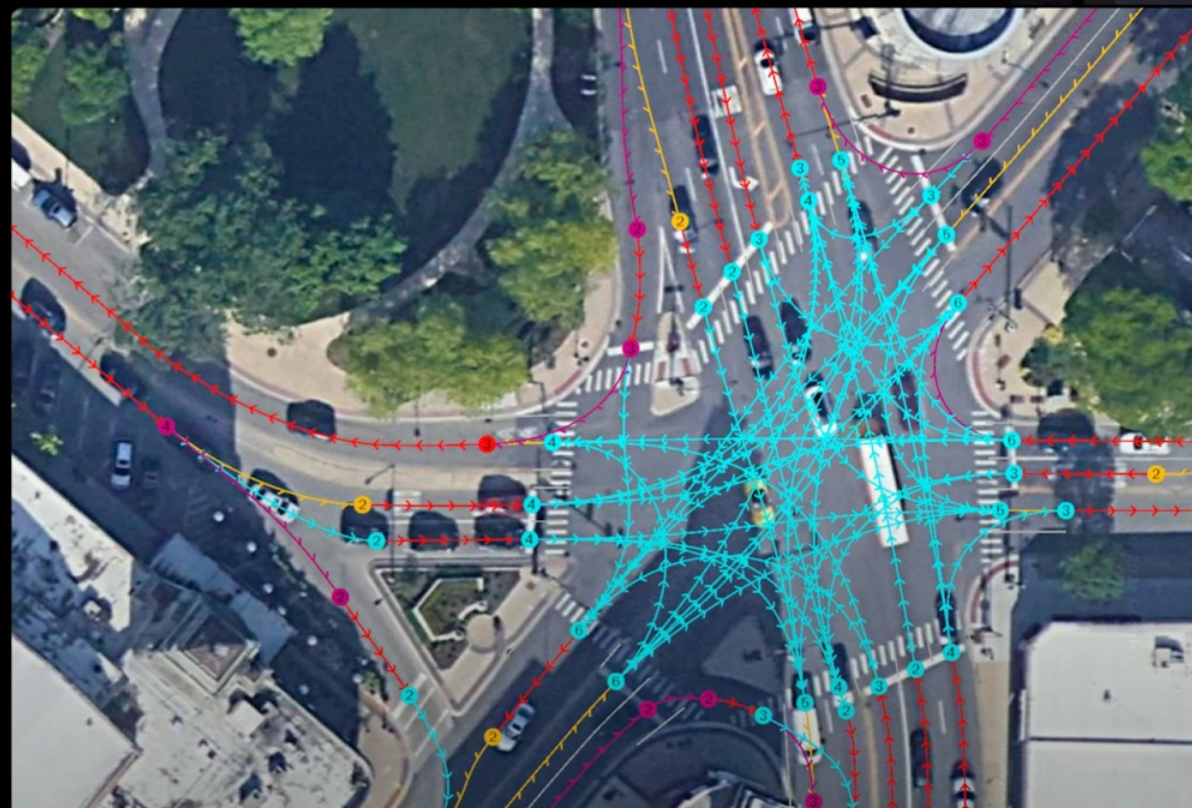

Tesla AI Day 2022
1:15:29 / 3:23:00

Tesla AI Day 2022

FSD Lanes

OBJECTIVE

Produce the full set lanes instances and their connectivity to each other.



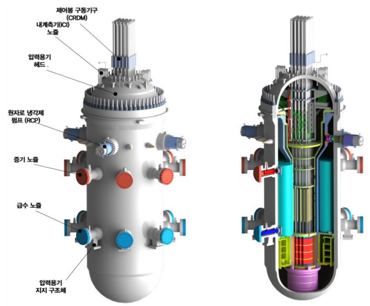
1:27:02 / 3:23:00


Tesla AI Day 2022
Find a Gap Between Pedestrian and Cr
Lanes
Occupancy
Moving Objects
$\hat{g}_0^0$ $\hat{g}_0^1$ $\hat{g}_0^2$ $\hat{g}_0^3$
$\hat{\tau}_1^0$ $\hat{\tau}_1^1$ $\hat{\tau}_1^2$ $\hat{\tau}_1^3$
$\hat{s}_2^0$ $\hat{s}_2^1$
$\hat{s}_3^0$ $\hat{s}_3^1$ $\hat{s}_3^2$ $\hat{s}_3^2$
$\hat{g}_4^0$
1:05:47 / 3:23:00

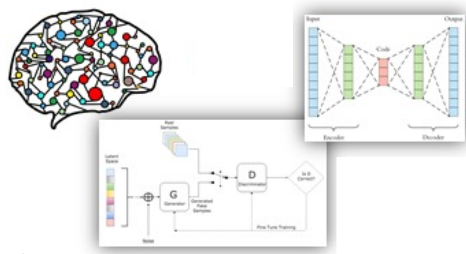
원자로 시뮬레이션 가속화 기술 연구 with 리스크·신뢰도평가연구실

한국원자력연구원

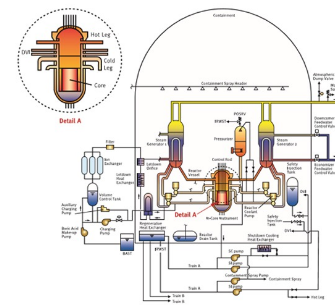
가상 모델



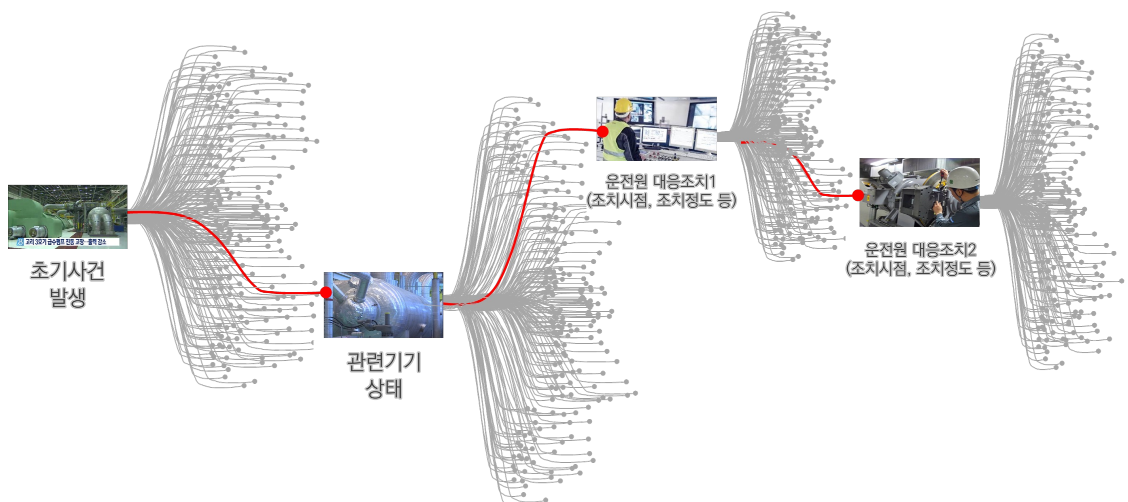
인공지능 기술



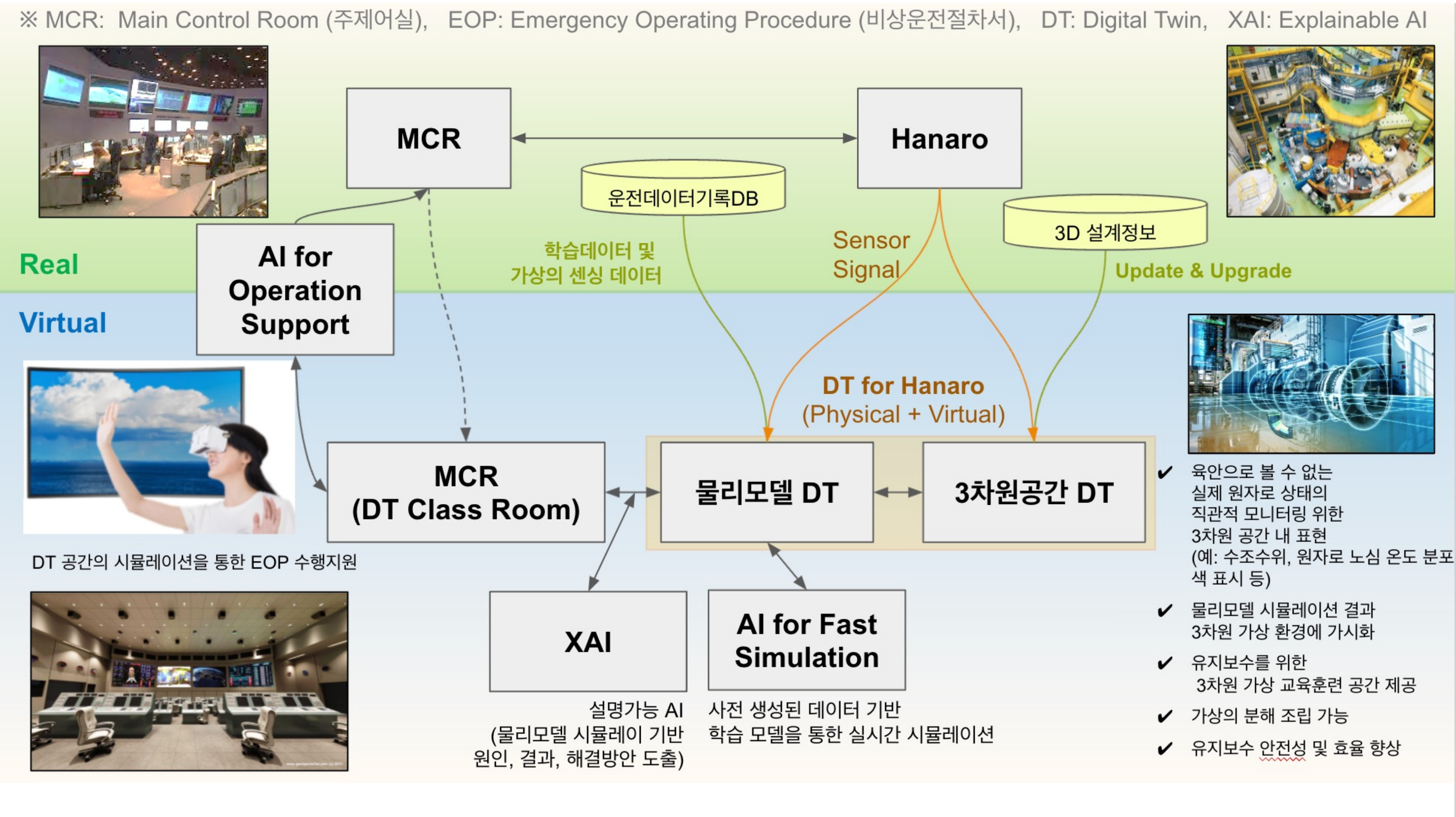
실제 원자로



- 고복잡도
- 다물리 시스템
- 실험의 어려움



고속 시뮬레이션



※ MCR: Main Control Room (주제어실), EOP: Emergency Operating Procedure (비상운전절차서), DT: Digital Twin, XAI: Explainable AI
MCR
Hanaro
운전데이터기록DB
3D 설계정보
Real
Virtual
AI for Operation Support
학습데이터 및 가상의 센싱 데이터
Sensor Signal
Update & Upgrade
DT for Hanaro (Physical + Virtual)
MCR (DT Class Room)
물리모델 DT
3차원공간 DT
DT 공간의 시뮬레이션을 통한 EOP 수행지원
XAI
AI for Fast Simulation
설명가능 AI (물리모델 시뮬레이 기반 원인, 결과, 해결방안 도출)
사전 생성된 데이터 기반 학습 모델을 통한 실시간 시뮬레이션
✔ 육안으로 볼 수 없는 실제 원자로 상태의 직관적 모니터링 위한 3차원 공간 내 표현 (예: 수조수위, 원자로 노심 온도 분포 색 표시 등)
✔ 물리모델 시뮬레이션 결과 3차원 가상 환경에 가시화
✔ 유지보수를 위한 3차원 가상 교육훈련 공간 제공
✔ 가상의 분해 조립 가능
✔ 유지보수 안전성 및 효율 향상

사고대응 시나리오 (훈련, 운전지원)

상황 1. 원자로 냉각재 상실 사고: 수조수 수위 저하 □ 최악의 경우 핵연료 노출

상황 2. 반응도 삽입사고: 제어봉구동장치 오동작

사전 징후 발생 → **상황 발생** → **현재상황 파악** → **DT 기반 미래상황 시뮬레이션** → **AI 기반 최적 대응 방안 제시**

AI 기반 이상징후 감시
(Anomaly Detection)

현재상황 Display

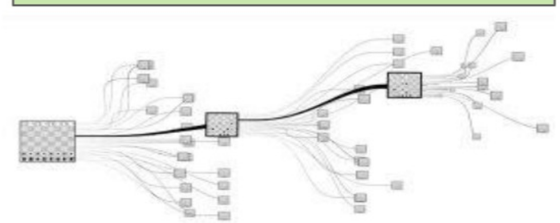
무대응 시,
상황 Display

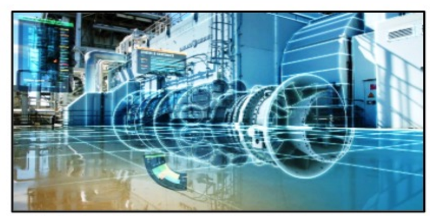
반복해석

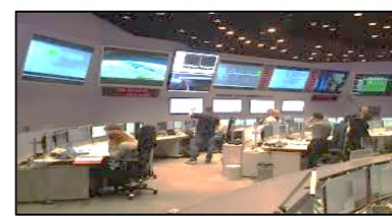
제시된 최적 혹은 다수의
방안에 대한 원자로 상태 변화 표기

XAI 기법을 이용한 원인 추정

XAI 기반 미래상황표시 → **대응 / 대응 훈련**

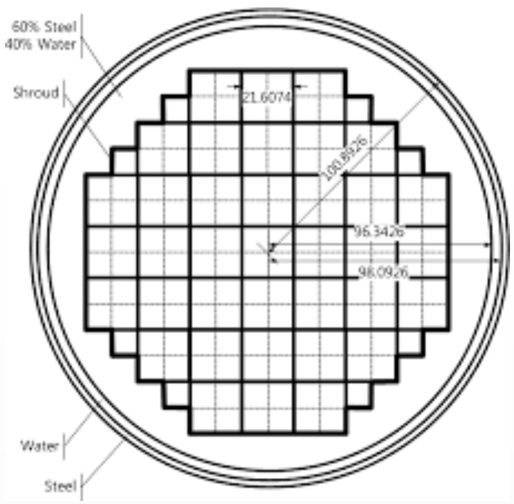


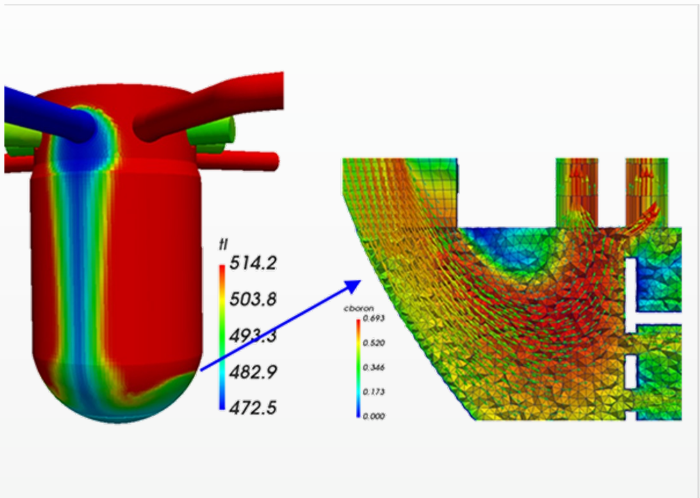




4. Physics Informed Machine Learning + Optimization

모든(많은) 원자력공학은 함수를 만드는 작업이다.





CUPID 원자로 유동 해석

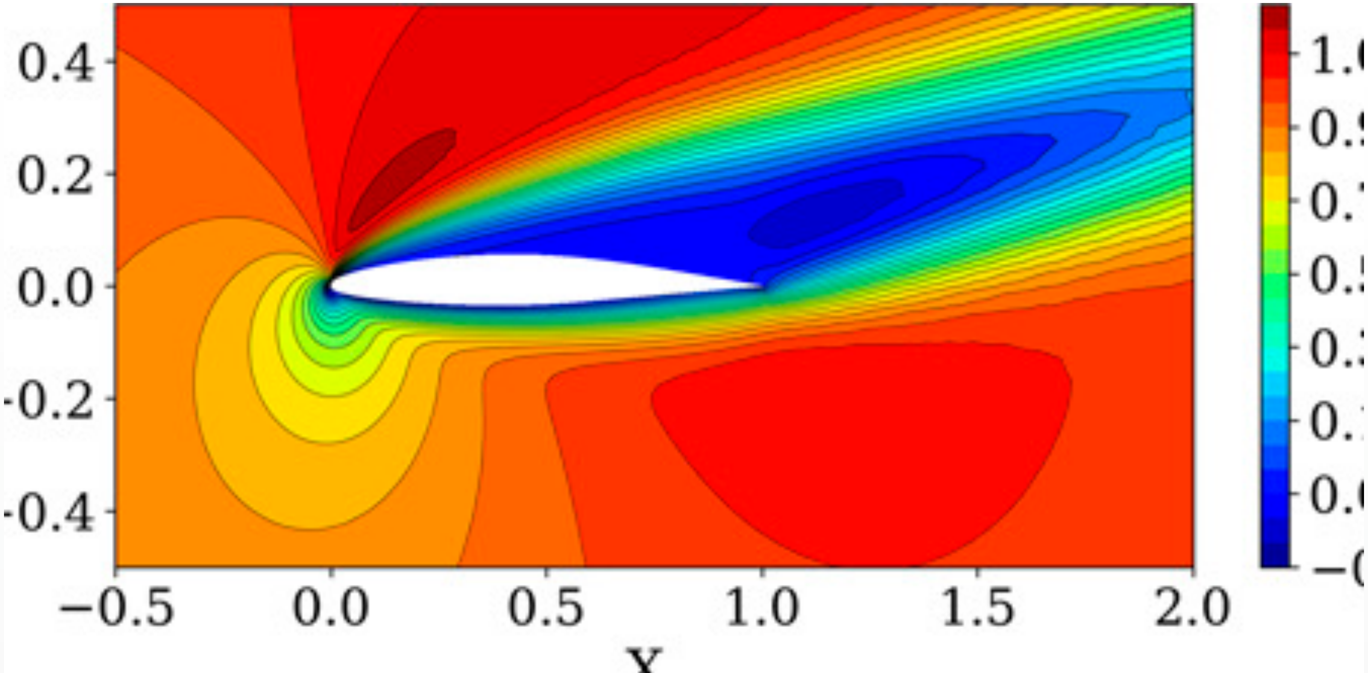
$$f(x)$$

성능

안전

https://www.kns.org/webzine/2018/w_5_6/sub_03.php

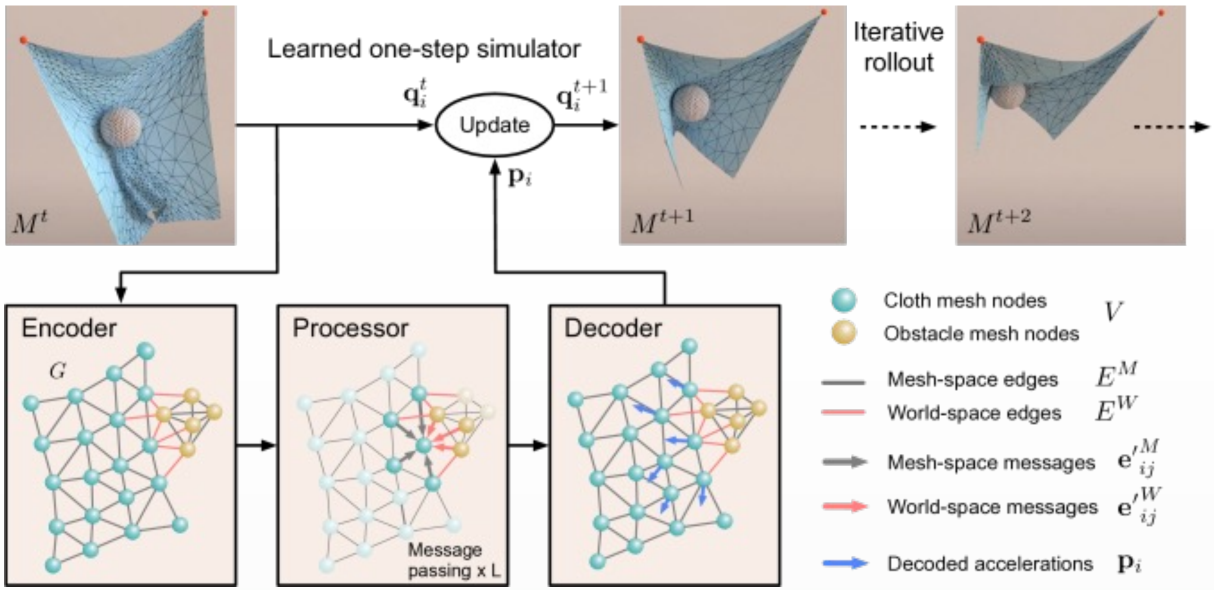
Fast flow field prediction over airfoils using deep learning

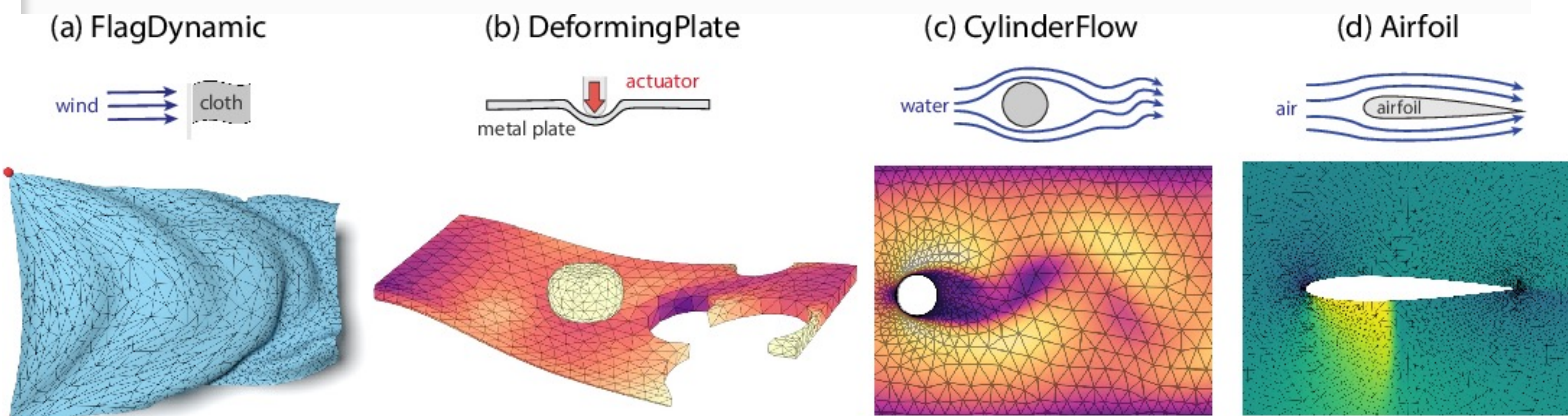


(c)

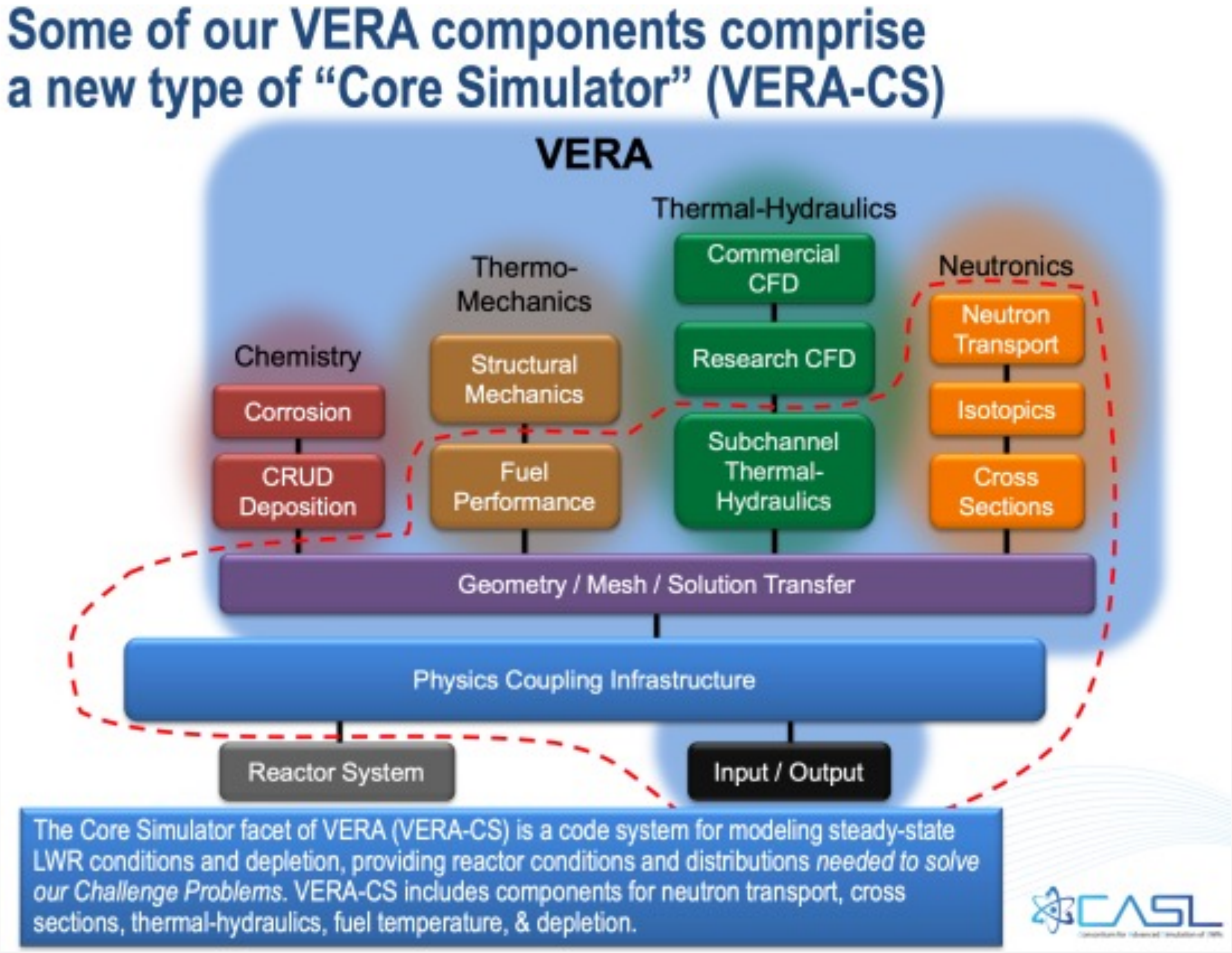
https://aip.scitation.org/doi/10.1063/1.5094943

Mesh based Simulation (Deepmind)





Argonne National Laboratory *is using AI to create* ***fast-running models*** *of various nuclear thermal-hydraulic processes.*



https://www.greencarcongress.com/2020/03/20200325-vera.html

"화학 연구에도 AI가?"···딥 마인드, 나노 계산 돕는 AI 공개

뉴스1 입력 2021.12.10 06:57 수정 2021.12.10 06:57

화학 반응을 비롯한 다양한 자연 현상을 원자와 분자 수준에서 이해하기 위해서는 물질·분자 내부에 전자의 분포와 에너지를 양자역학적으로 계산할 필요가 있다. 단순한 원자의 경우에는 양자역학적 계산이 가능하지만, 원자의 수가 늘어나고 관계가 복잡해질수록 필요한 계산량과 난이도는 급속히 늘어난다.

이후 밀도 범함수 이론(Density Functional Theory, DFT)이 나와 상대적으로 계산량이 줄었다. 이 이론을 발전시킨 월터 콘과 같은 학자는 이 공로로 노벨상을 수상하기도 했다.

딥마인드는 DFT 기반 계산을 개선하기 위한 인공신경망 기반의 인공지능을 개발했다. 전자 밀도와 상호 작용 에너지 사이의 정확한 매핑 특성(밀도 함수)는 계산의 핵심이지만, 알려지지 않았다. 딥마인드는 인공신경망을 사용해 이전에 달성할 수 있었던 것보다 더 정확한 밀도 및 전자 간의 상호 작용 관계 지도를 구축할 수 있음을 논문을 통해 밝혔다.

Web of Science 기준

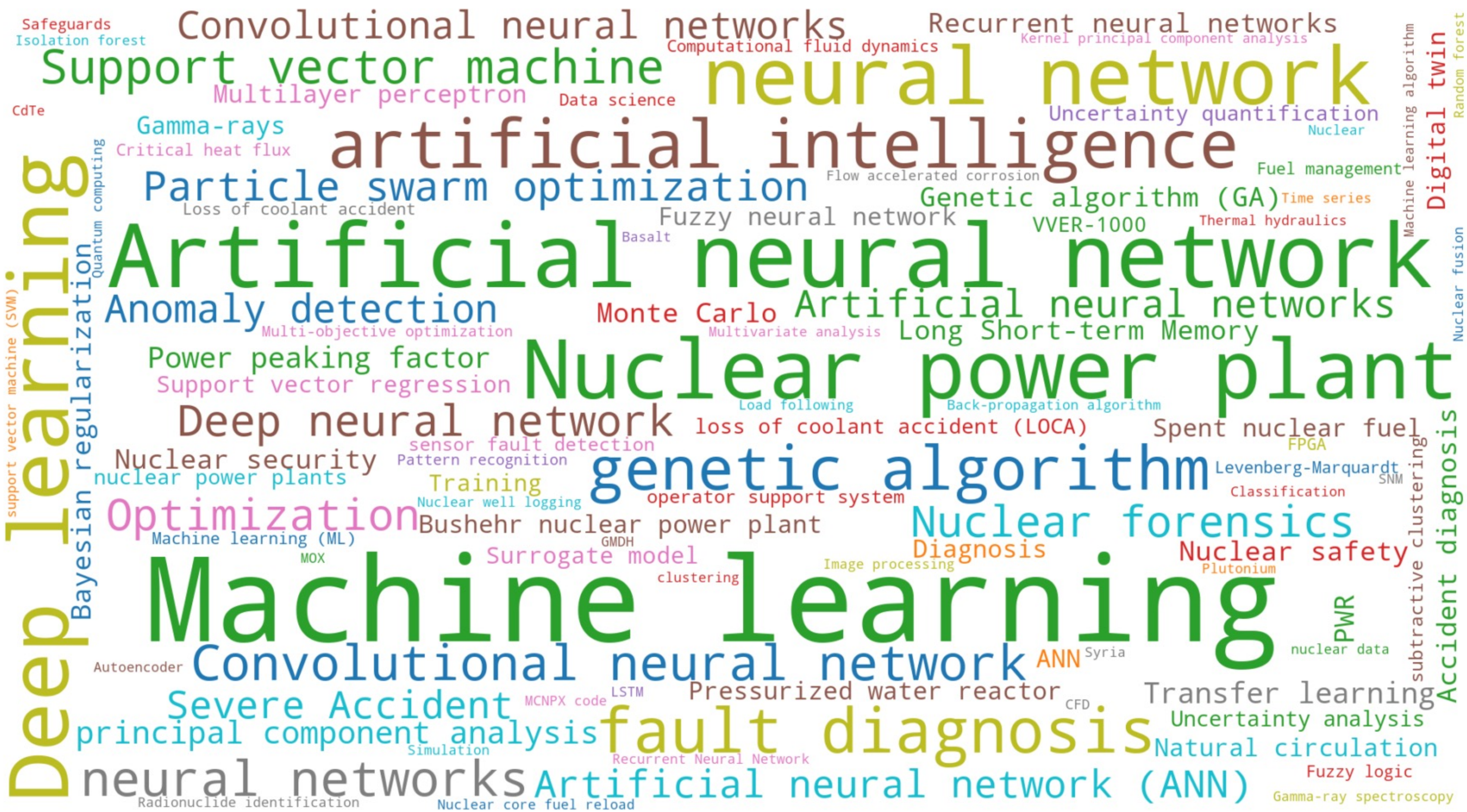
검색 키워드:
- Nuclear
- AI
    - Machine Learning
    - Artificial Intelligence
    - Deep Learning
    - Neural Network
    - Random forest, support vector machine….
    - Regression, classification

- Nuclear science and Technology 섹션

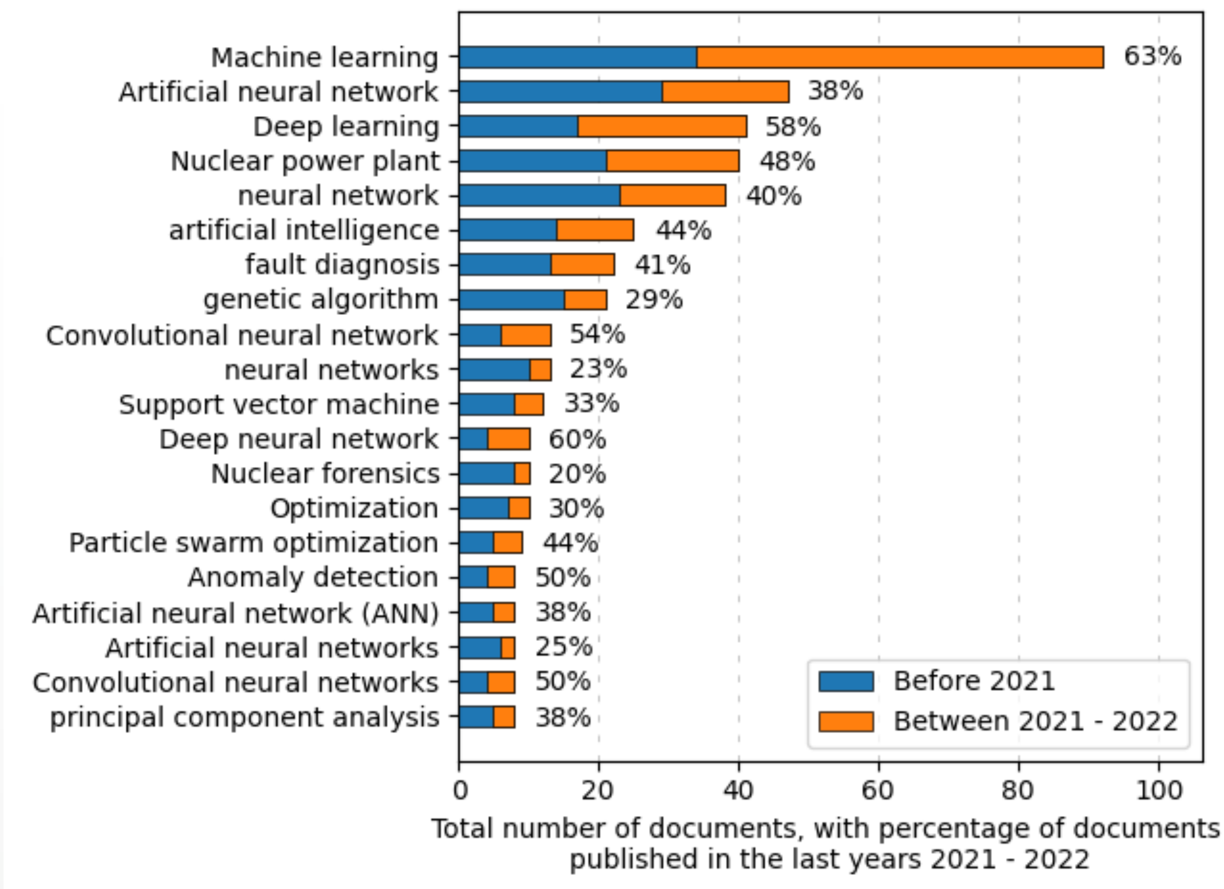
해당논문: 약 700개

분석 도구 : scientopy, vosviewer

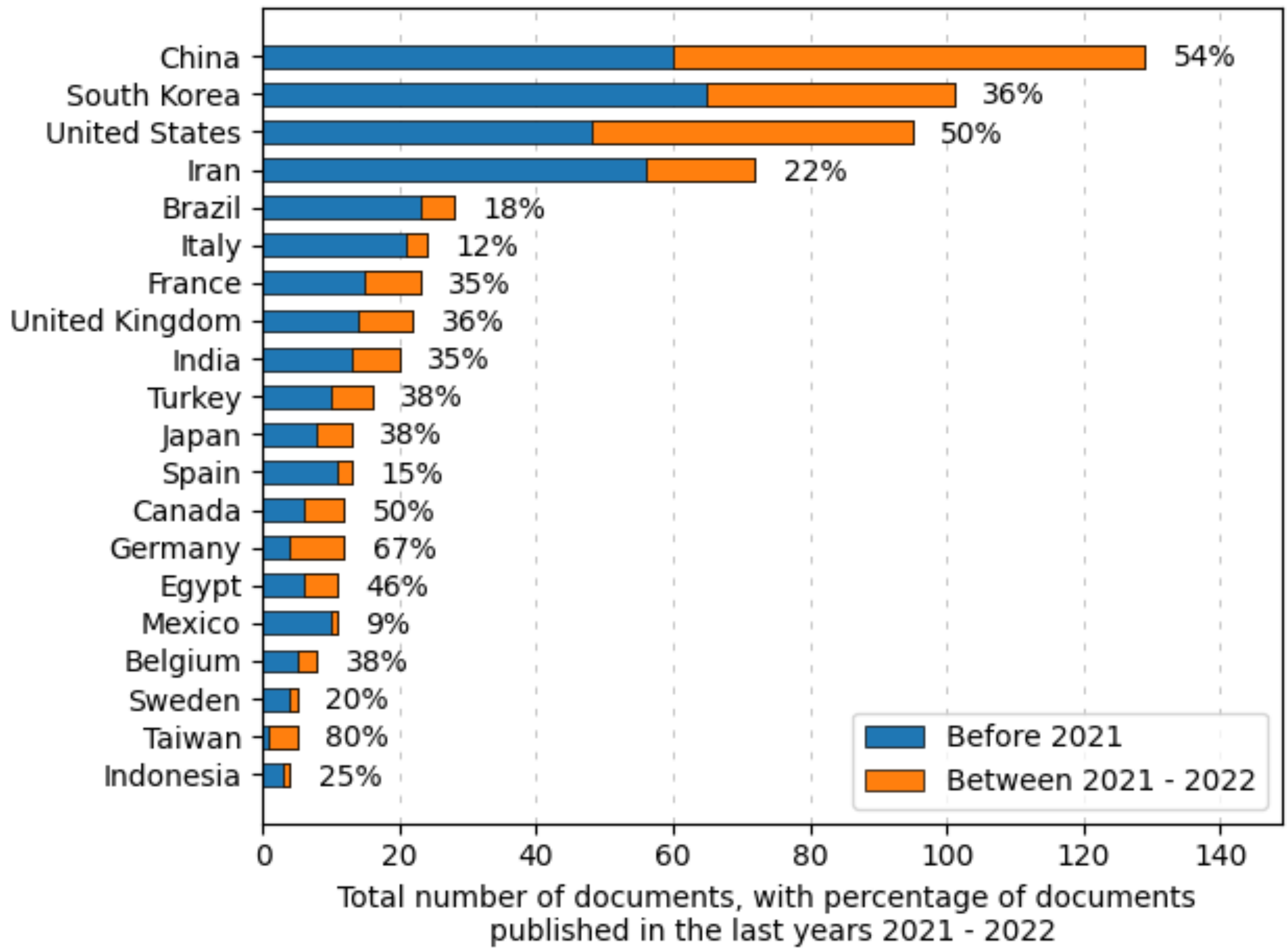
원자력 인공지능 문헌 분석(키워드)



원자력 인공지능 문헌 분석(키워드)

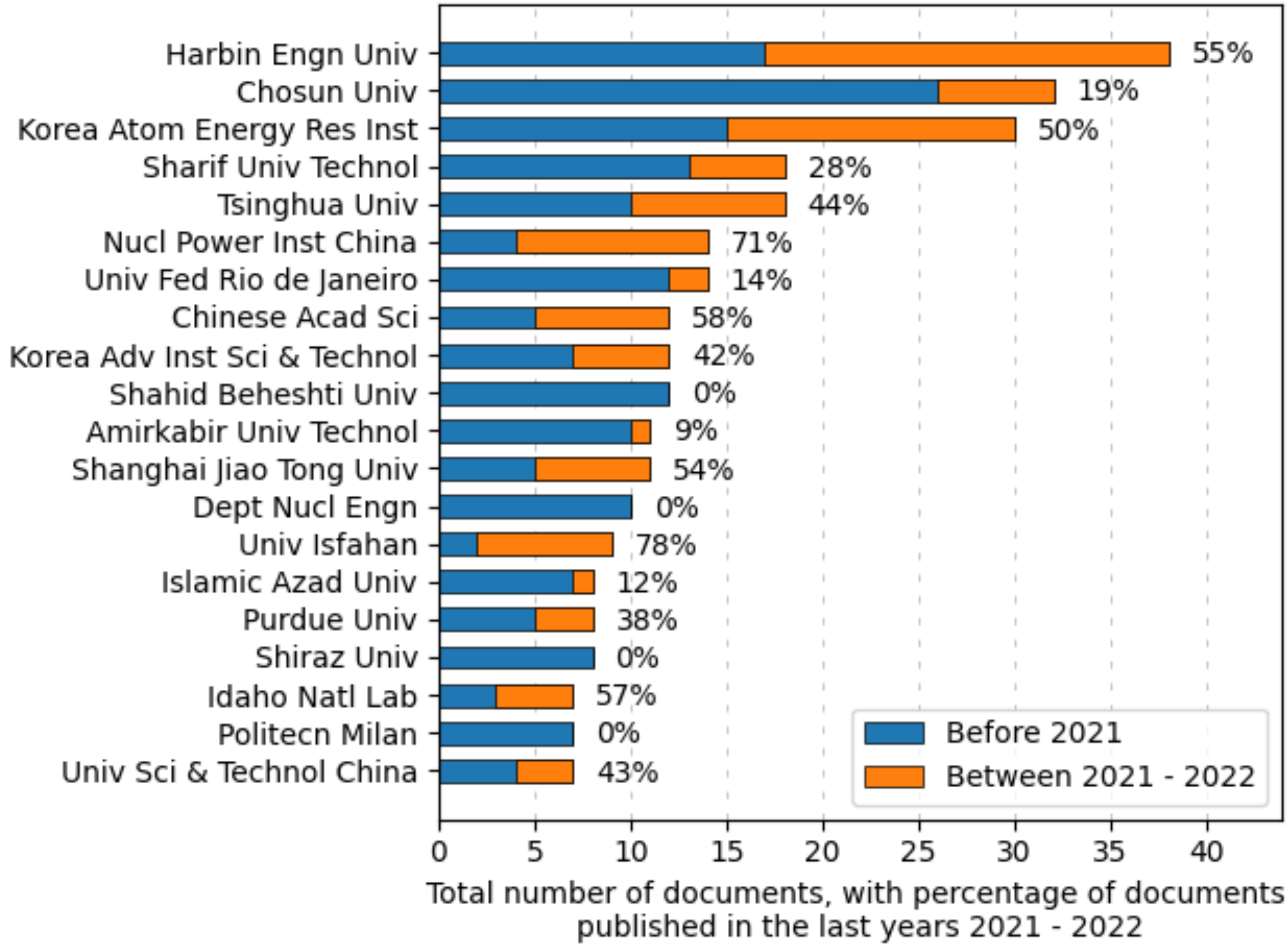


원자력 인공지능 문헌 분석(국가별)

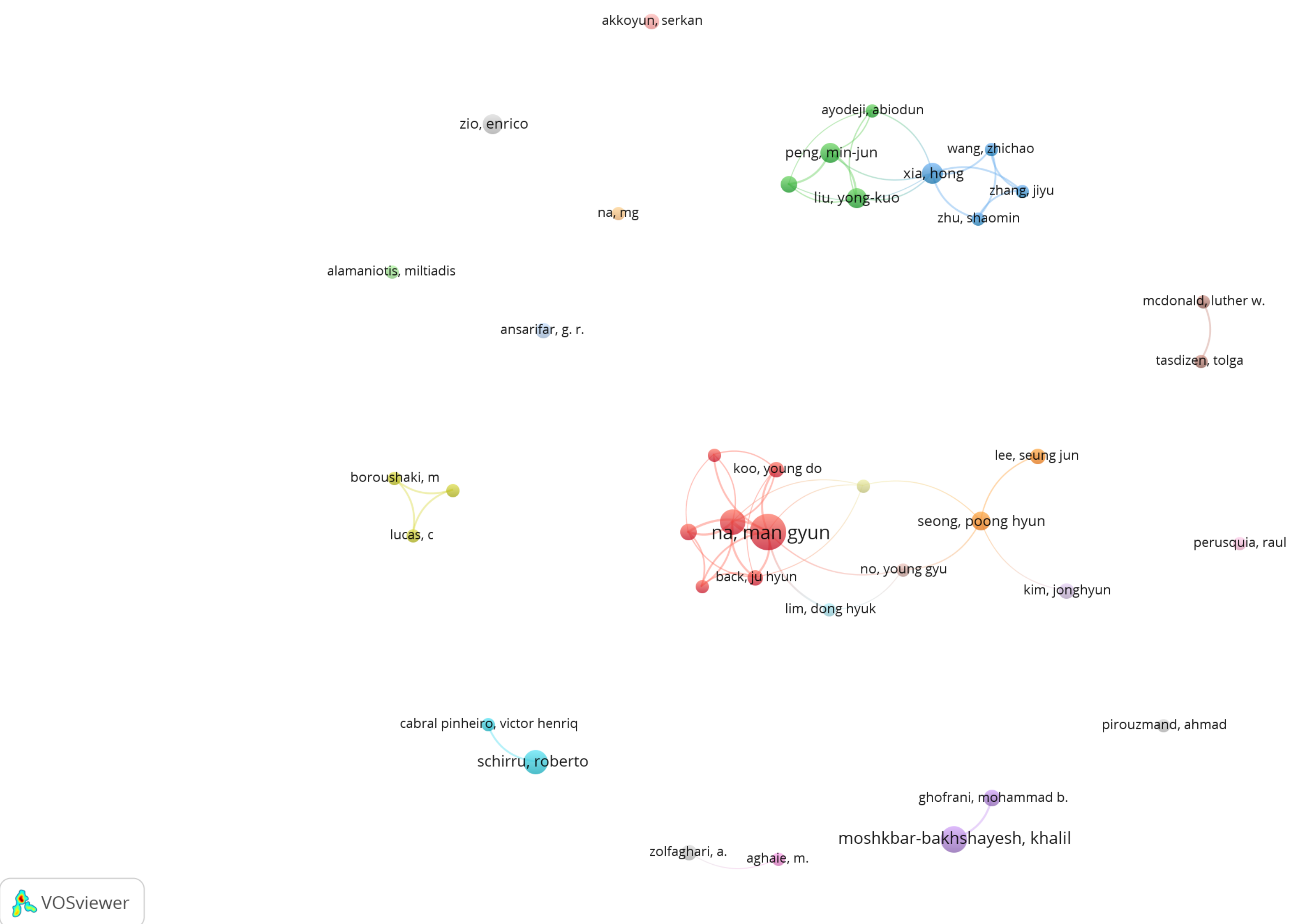


원자력 인공지능 문헌 분석(기관별)

한국원자력연구원



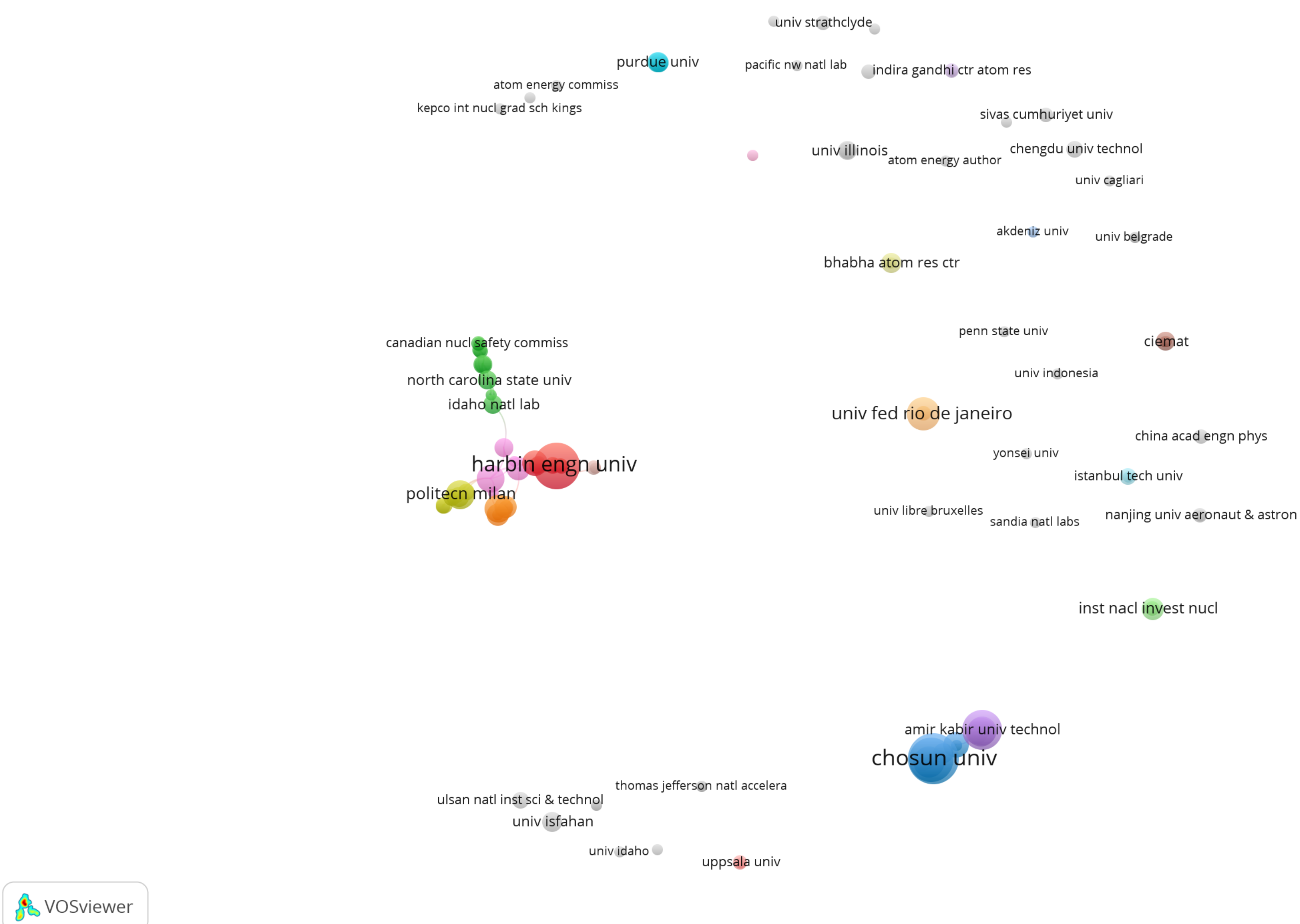
원자력 인공지능 문헌 분석(저자-네트워크)



원자력 인공지능 문헌 분석(저자-네트워크)

한국원자력연구원

원자력 인공지능 문헌 분석(기관-네트워크)



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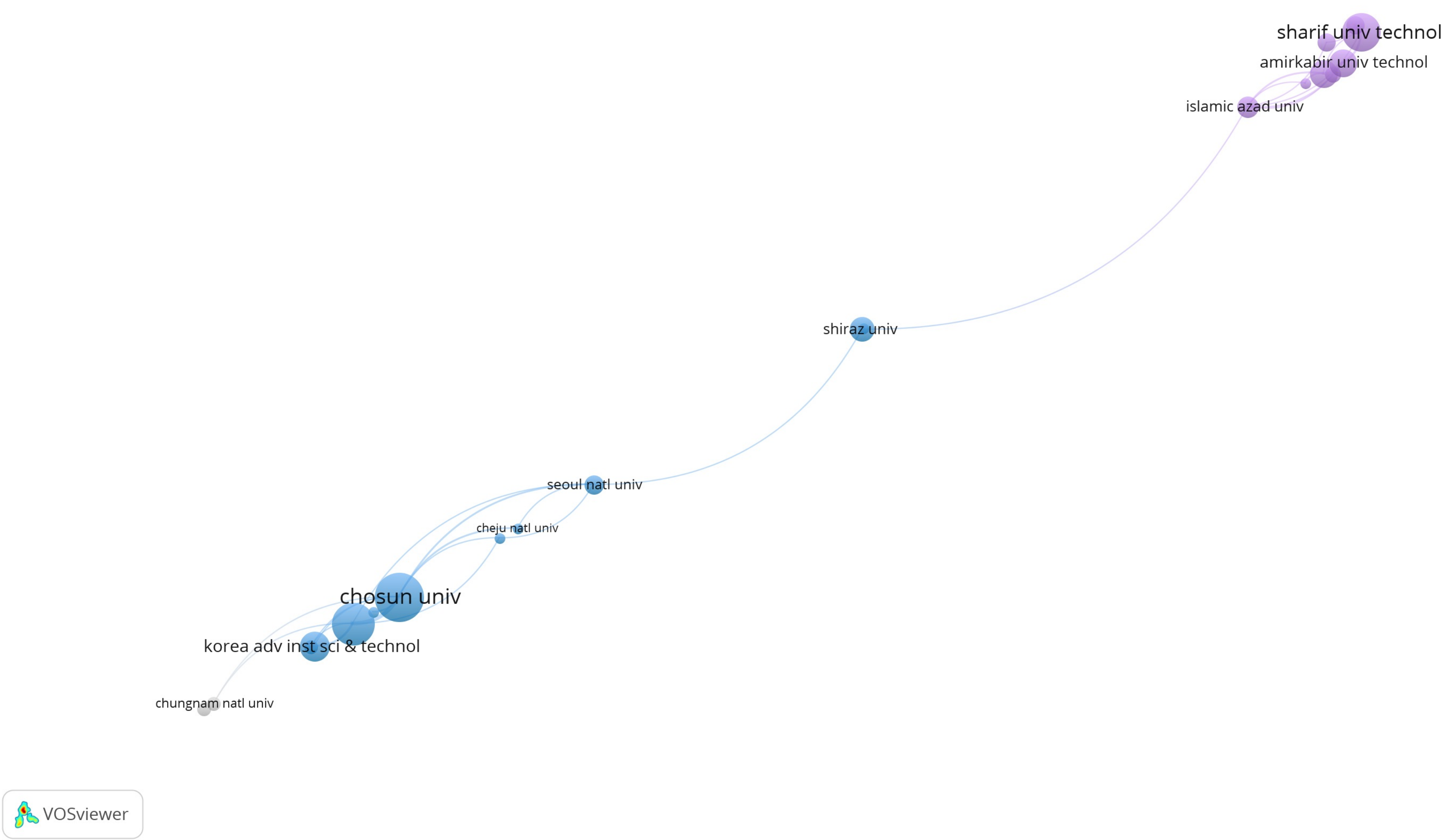

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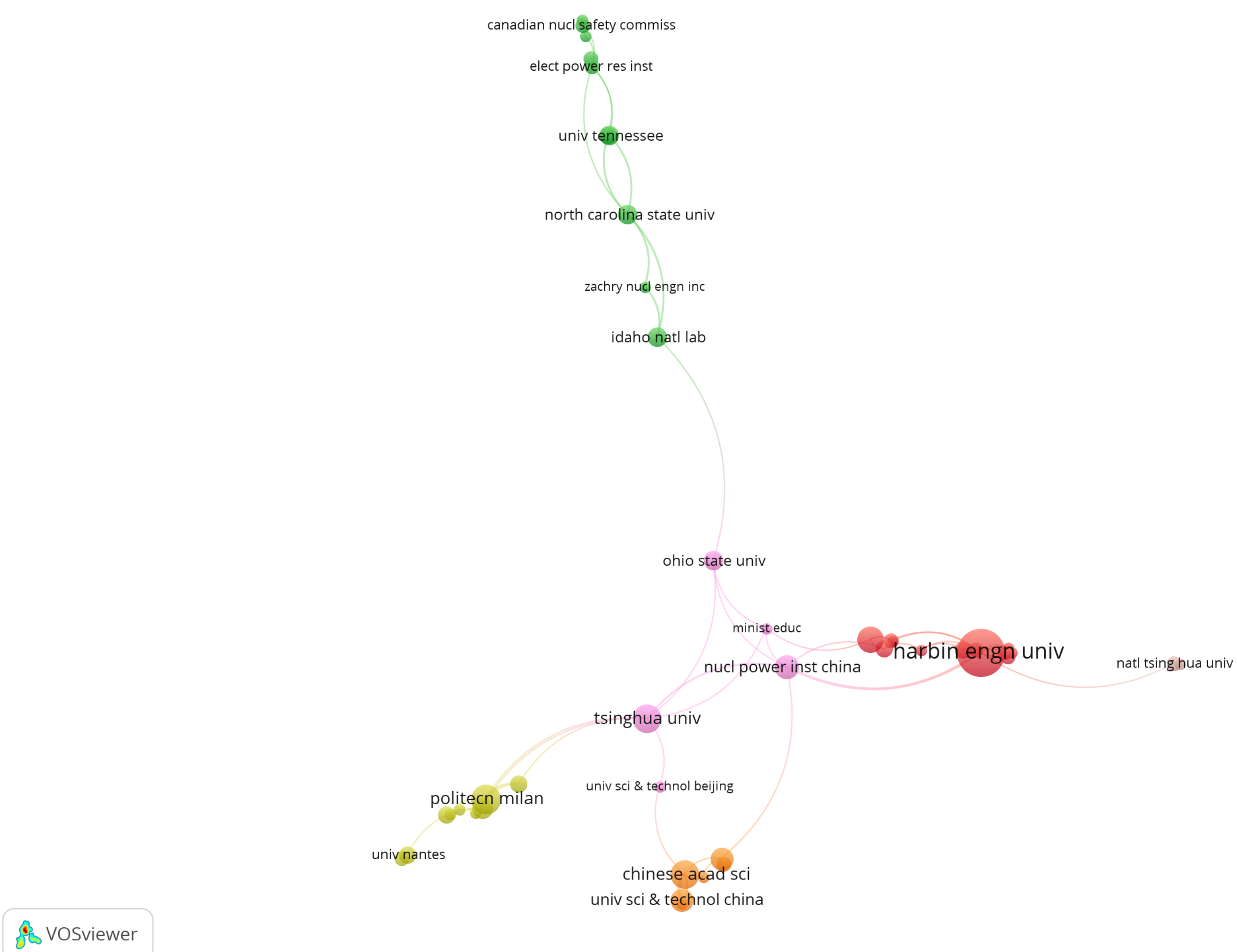

Web of Science 기준

키워드:

- Nuclear material OR Nuclear fuel
- AI
    - Machine Learning
    - Artificial Intelligence
    - Deep Learning
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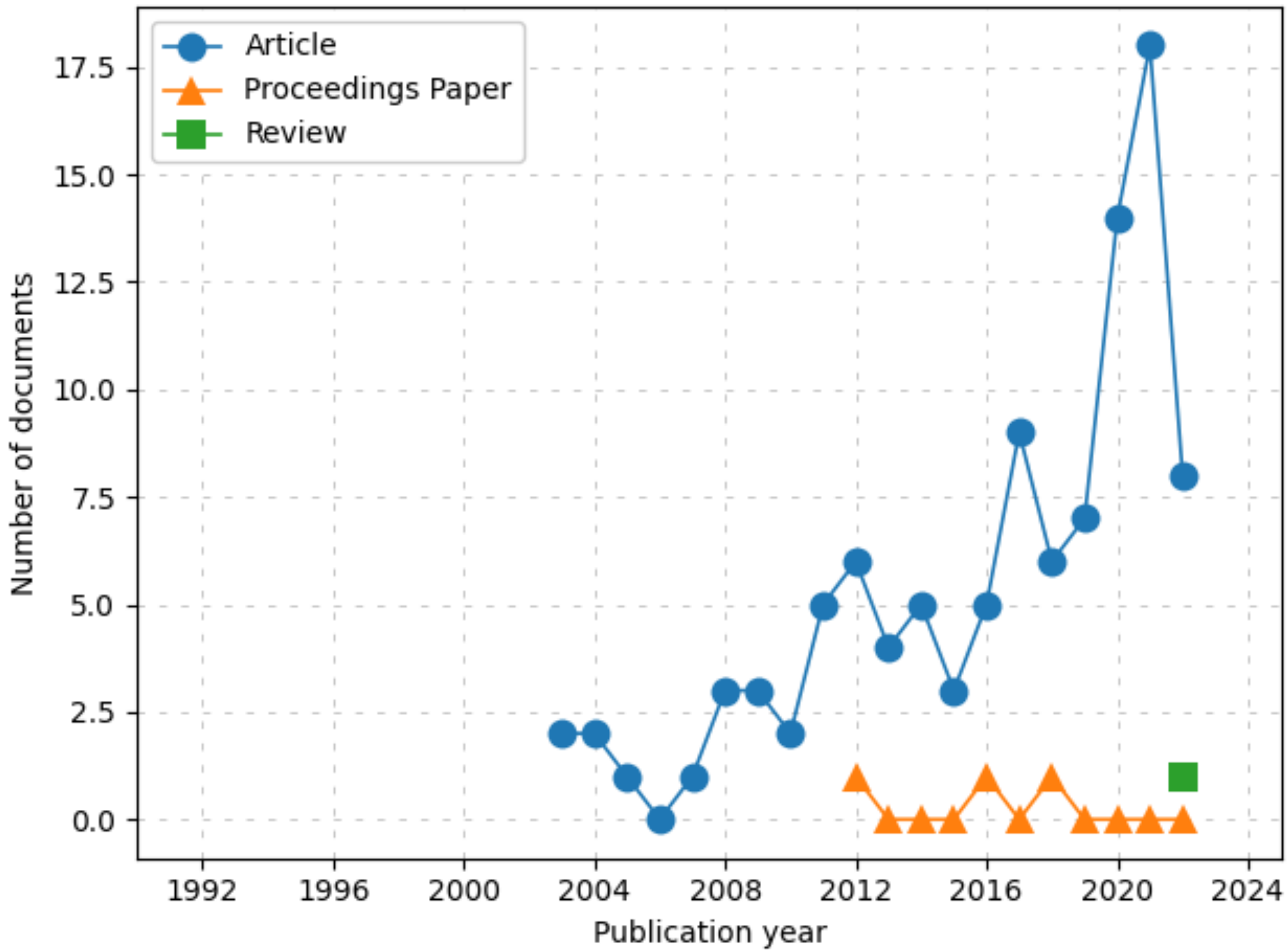
    - Random forest, support vector machine….
    - Regression, classification

- Nuclear science and Technology 섹션

해당논문: 약 200개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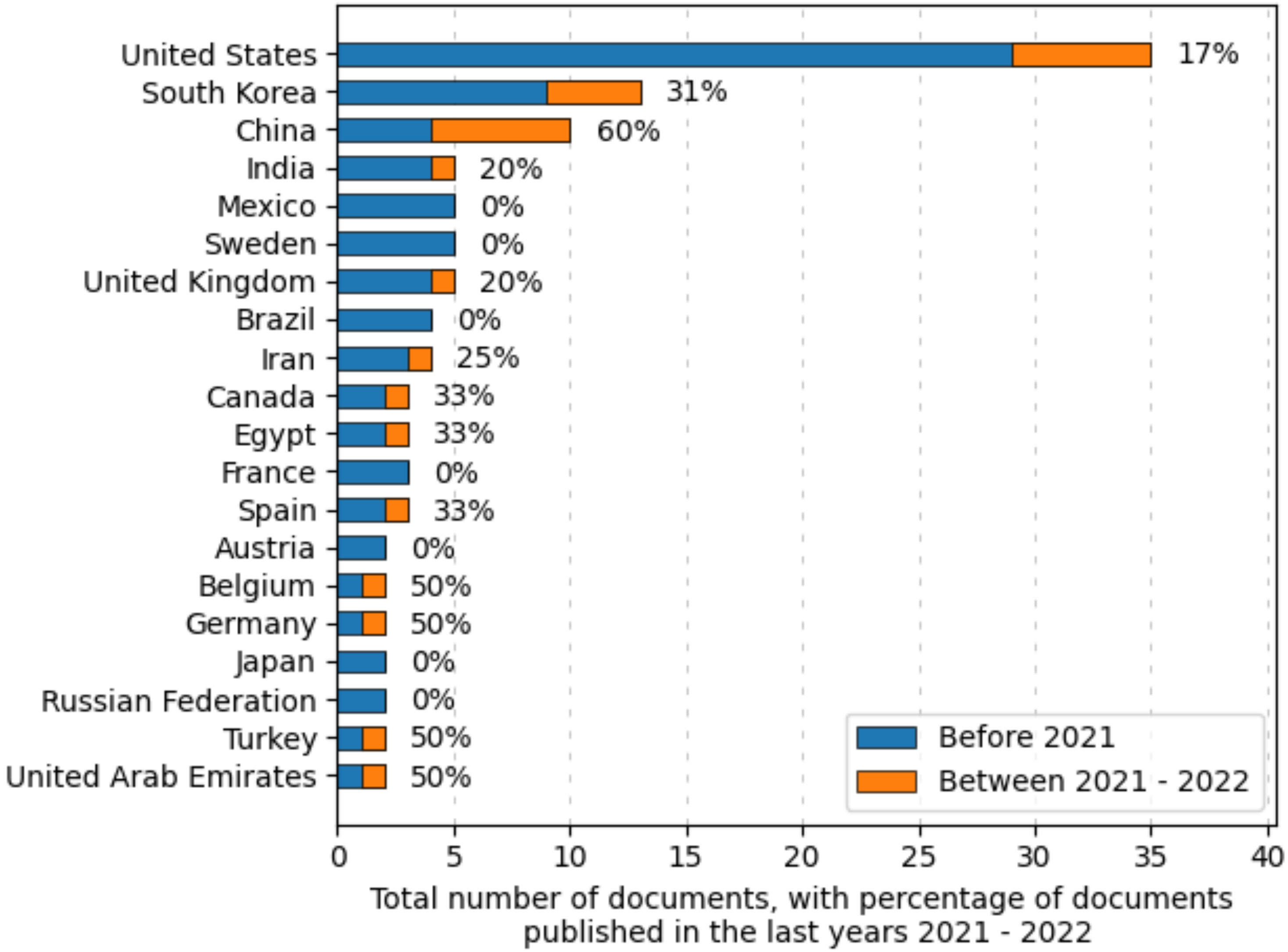

원자력 재료 & 핵연료 인공지능 문헌 분석 (기관별)

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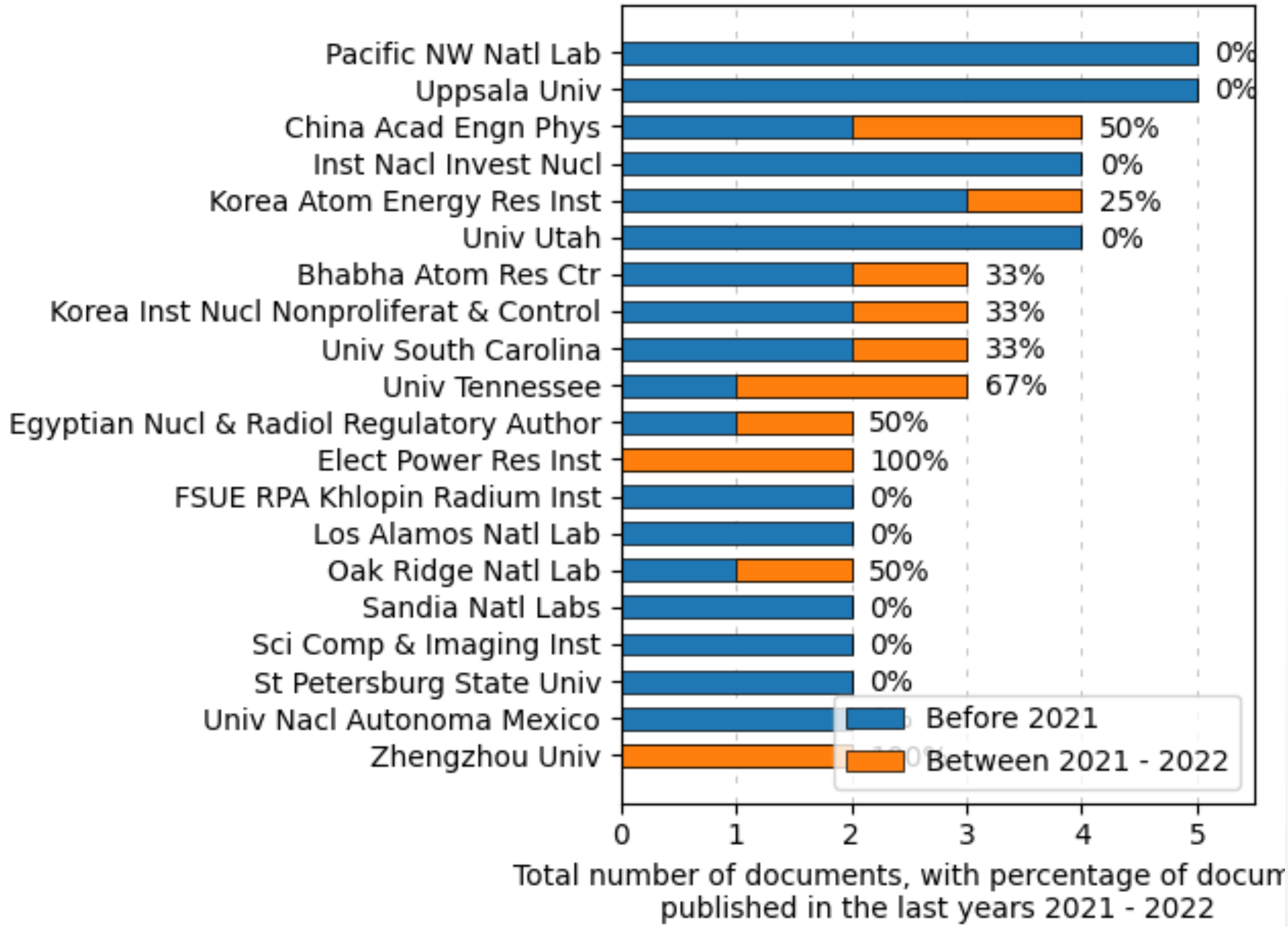
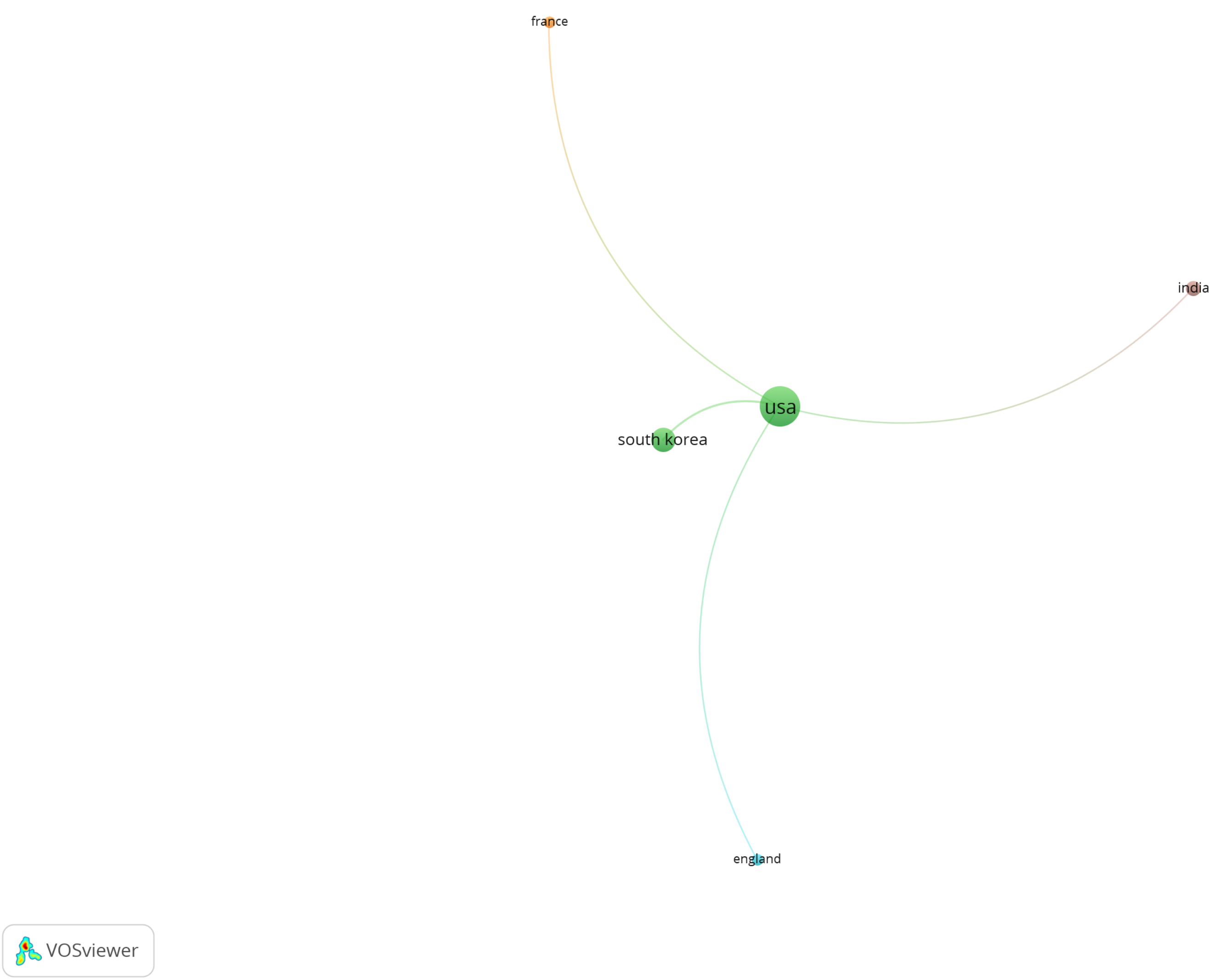


원자력 재료 & 핵연료 인공지능 문헌 분석 (국가별 네트워크)



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Machine learning molecular dynamics simulations toward exploration of high-temperature properties of nuclear fuel materials: case study of thorium dioxide

Keita Kobayashi[1✉], Masahiko Okumura[1,3], Hiroki Nakamura[1,3], Mitsuhiro Itakura[1,3], Masahiko Machida[1,3] & Michael W. D. Cooper[2,3]

Predicting materials properties of nuclear fuel compounds is a challenging task in materials science. Their thermodynamical behaviors around and above the operational temperature are essential for the design of nuclear reactors. However, they are not easy to measure, because the target temperature range is too high to perform various standard experiments safely and accurately. Moreover, theoretical methods such as first-principles calculations also suffer from the computational limitations in calculating thermodynamical properties due to their high calculation-costs and complicated electronic structures stemming from f-orbital occupations of valence electrons in actinide elements. Here, we demonstrate, for the first time, machine-learning molecular-dynamics to theoretically explore high-temperature thermodynamical properties of a nuclear fuel material, thorium dioxide. The target compound satisfies first-principles calculation accuracy because f-electron occupation coincidentally diminishes and the scheme meets sampling sufficiency because it works at the computational cost of classical molecular-dynamics levels. We prepare a set of training data using first-principles molecular dynamics with small number of atoms, which cannot directly evaluate thermodynamical properties but captures essential atomistic dynamics at the high temperature range. Then, we construct a machine-learning molecular-dynamics potential and carry out large-scale molecular-dynamics calculations. Consequently, we successfully access two kinds of thermodynamic phase transitions, namely the melting and the anomalous λ transition induced by large diffusions of oxygen atoms. Furthermore, we quantitatively reproduce various experimental data in the best agreement manner by selecting a density functional scheme known as SCAN. Our results suggest that the present scale-up simulation-scheme using machine-learning techniques opens up a new pathway on theoretical studies of not only nuclear fuel compounds, but also a variety of similar materials that contain both heavy and light elements, like thorium dioxide.

Images

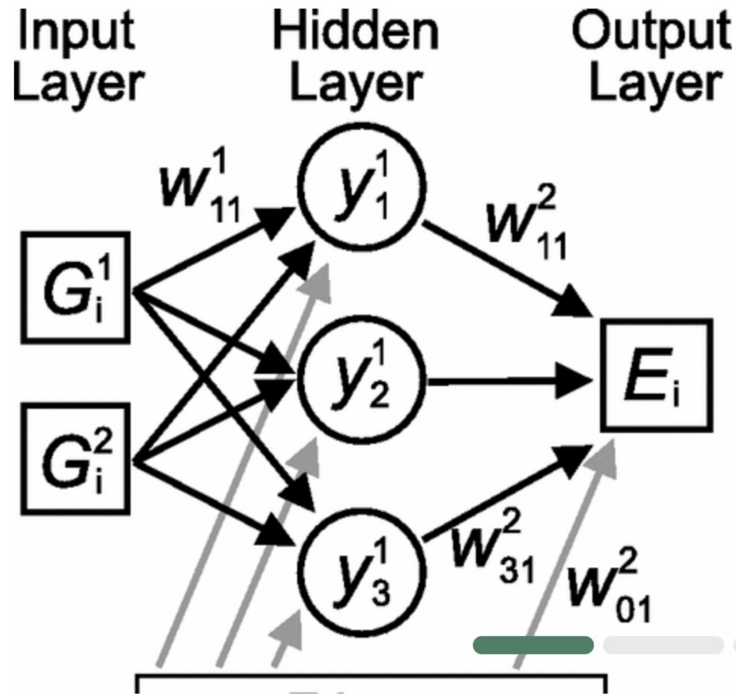

Figure 1

Example of a standard neural network employed for fitting potential-energy surfaces [5, 6]. The node in the output layer yields the energy E_i, which in this case depends on the values of the two input nodes, G_i^1 and G_i^2. In between the input and the output layer there is a hidden layer with three nodes represented by the circles. The arrows correspond to the 13 weight parameters w_{ij}^k, which connect node j in layer k with node i in layer $k-1$. The bias node is used to adapt the nonlinearity region of the activation functions. The functional form of this small network is given in Eq. (1).

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DEGREE PROJECT IN NUCLEAR ENERGY ENGINEERING,
SECOND CYCLE, 30 CREDITS

STOCKHOLM, SWEDEN 2020

A Machine Learning Approach to the Nuclear Fuel Fabrication Process

ELINA CHARATSIDOU

KTH Royal Institute of Technology
School of Engineering Sciences
Department of Physics
MSc in Nuclear Energy Engineering

The nuclear fuel fabrication is a complex process which requires precise control of many process parameters to obtain a final product conforming to stringent specifications. Hence, the yield improvement is one of the most important topics in nuclear fuel fabrication. The yield is driven down by demands on the final quality of the pellet: density, impurities, surface defects, etc., forcing to recycle some of the pellets, with the associated cost.

Over time, the process was able to reach a significant yield thanks to the use of traditional statistical methods on the various sub-processes. However, traditional approaches have limits in extracting the full benefits of the data, since trends can be hard to find. Therefore, the manufacturing data is currently poorly explored even in the most sophisticated process.

In this work, data from the nuclear fuel factory of Westinghouse Electric AB in Västerås, Sweden, were manually collected, organized, and structured in a way useful for data analysis and machine learning implementations. Afterwards, machine learning algorithms, namely neural network and gradient boosting, were applied to build models, feature weights of the parameter process, and understand correlations: the trained models were later used to predict output label values based on new datasets, and an evaluation of these predictions was performed, alongside with the comparison of the performance of both neural networks and gradient boosting for such problems. Through this method, it will be possible to model the fabrication process and use this tool to pursue improvements based on data.

Hence, the aim of this work is to facilitate the preprocessing of the fabrication data, creating an automated, high performance, accurate algorithm which will minimize human error as well as improve fabrication time and lower the cost of the fabrication process.

Abstract

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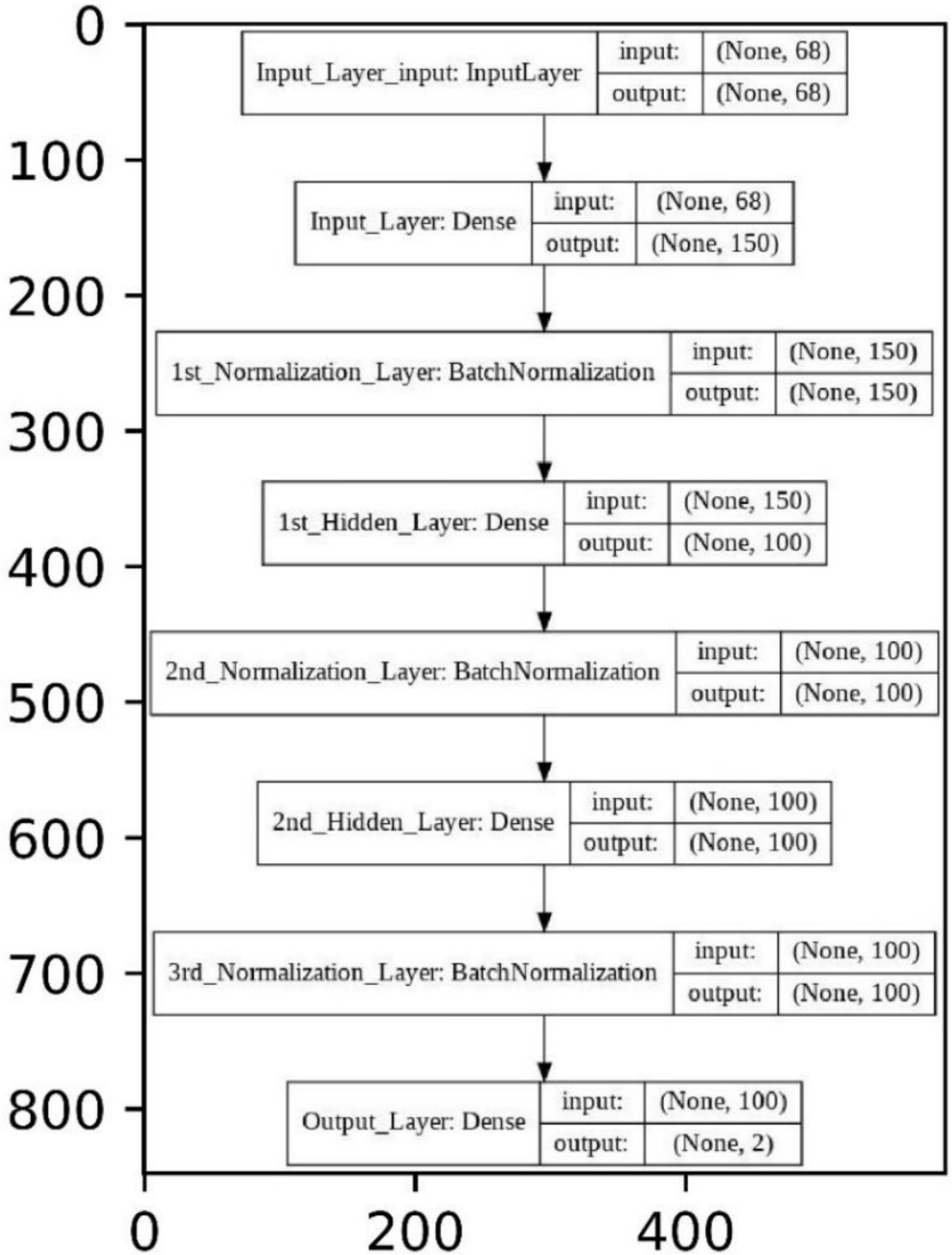

Figure 7. Neural Network Model Schematic

Using Machine Learning to Predict the Fuel Peak Cladding Temperature for a Large Break Loss of Coolant Accident

Wazif Sallehhudin[1] *and Aya Diab*[1,2]*

[1]*Nuclear Power Plant Engineering Department, KEPCO International Nuclear Graduate School (KINGS), Ulsan, South Korea,*
[2]*Mechanical Power Engineering Department, Faculty of Engineering, Ain Shams University, Cairo, Egypt*

In this paper the use of machine learning (ML) is explored as an efficient tool for uncertainty quantification. A machine learning algorithm is developed to predict the peak cladding temperature (PCT) under the conditions of a large break loss of coolant accident given the various underlying uncertainties. The best estimate approach is used to simulate the thermal-hydraulic system of APR1400 large break loss of coolant accident (LBLOCA) scenario using the multidimensional reactor safety analysis code (MARS-KS) lumped parameter system code developed by Korea Atomic Energy Research Institute (KAERI). To generate the database necessary to train the ML model, a set of uncertainty parameters derived from the phenomena identification and ranking table (PIRT) is propagated through the thermal hydraulic model using the Dakota-MARS uncertainty quantification framework. The developed ML model uses the database created by the uncertainty quantification framework along with Keras library and Talos optimization to construct the artificial neural network (ANN). After learning and validation, the ML model can predict the peak cladding temperature (PCT) reasonably well with a mean squared error (MSE) of ~0.002 and R^2 of ~0.9 with 9 to 11 key uncertain parameters. As a bounding accident scenario analysis of the LBLOCA case paves the way to using machine learning as a decision making tool for design extension conditions as well as severe accidents.

Keywords: nuclear safety, large break LOCA, artificial neural network, machine learning, uncertainty quantification, peak cladding temperature

Uncertainty Quantification Framework Development

The statistical tool, Dakota (Adams et al., 2020), is used in this work to propagate the uncertainty parameters into the thermal hydraulic model. Dakota is an open source statistical software tool developed by Sandia National Laboratory. It can be used for optimization, sensitivity analysis and uncertainty quantification. The uncertainty propagation process is achieved by developing the uncertainty quantification framework by loosely coupling the best estimate system code, MARS-KS, and the statistical tool, Dakota, via a python script to manage the data exchange process. Several important files such as, the Dakota input file, the python interface script, the MARS steady state file and the MARS transient file are necessary for the uncertainty quantification framework to run smoothly and propagate the uncertainty parameters.

TABLE 3 | Normalized uncertain parameters.

UP	Parameter description	Mean, μ	Standard deviation, σ	Range, L_{high}-L_{low}
1	Core power	1.0	0.01	0.98–1.02
2	Groeneveld-CHF	1.0	0.414	0.173–1.827
3	Chen nucleate boiling HTC	1.0	0.234	0.553–1.467
4	Transition boiling HTC	1.0	0.230	0.54–1.46
5	Dittus-Boelter liquid HTC	1.0	0.196	0.607–1.393
6	Dittus-Boelter vapor HTC	1.0	0.196	0.607–1.393
7	Film boiling HTC	1.0	0.287	0.426–1.574
8	Break discharge coefficient	1.0	0.115	0.77–1.23
9	Decay heat	1.0	0.033	0.934–1.066
10	Gap conductance	1.0	0.289	0.421–1.579
11	SIT actuation pressure (MPa)	1.0	0.025	0.949–1.051
12	SIT water inventory (m^3)	1.0	0.046	0.907–1.093
13	SIT loss coefficient	1.0	0.20	0.6–1.4
14	Pressurizer pressure (MPa)	1.0	0.113	0.77–1.23
15	Fuel thermal conductivity	-	-	0.847–1.153
16	Pump two phase head multiplier	-	-	0.0–1.0
17	Pump two phase head multiplier	-	-	0.0–1.0
18	SIT water temperature (K)	-	-	0.955–1.045
19	SIP (IRWST) water temperature (K)	-	-	0.936–1.064

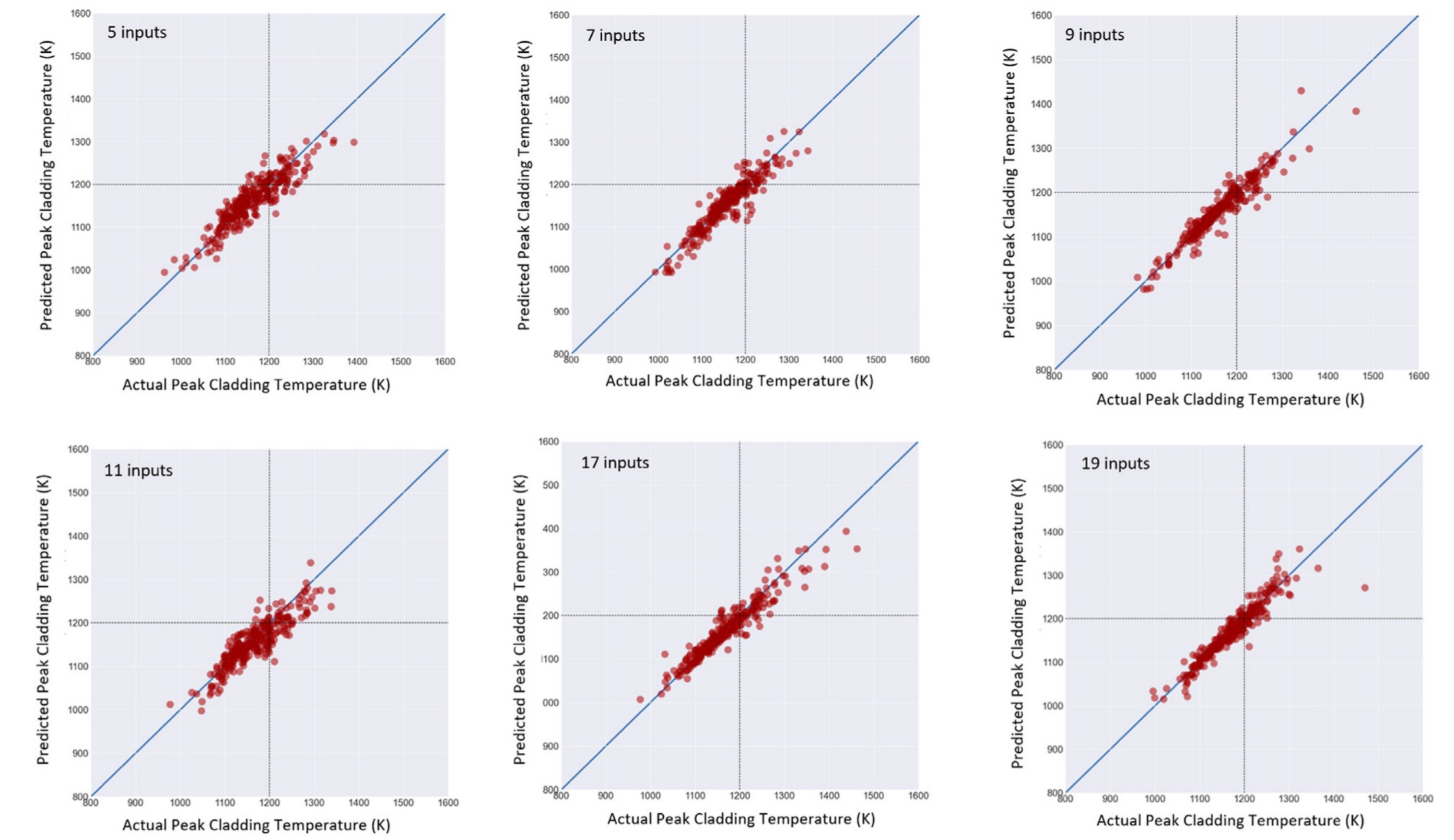

FIGURE 6 | Scatter plot for PCT using different number of uncertain parameters as inputs.

Deep learning approach to nuclear fuel transmutation in a fuel cycle simulator

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Keywords:
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A B S T R A C T

We trained a neural network model to predict Pressurized Water Reactor (PWR) Used Nuclear Fuel (UNF) composition given initial enrichment and burnup. This quick, flexible, medium-fidelity method to estimate depleted PWR fuel assembly compositions is used to model scenarios in which the PWR fuel burnup and enrichment vary over time. The Used Nuclear Fuel Storage, Transportation & Disposal Analysis Resource and Data System (UNF-ST&DARDS) Unified Database (UDB) provided a ground truth on which the model trained. We validated the model by comparing the U.S. UNF inventory profile predicted by the model with the UDB UNF inventory profile. The neural network yields less than 1% error for UNF inventory decay heat and activity and less than 2% error for major isotopic inventory. The neural network model takes 0.27 s for 100 predictions, compared to 118 s for 100 Oak Ridge Isotope GENeration (ORIGEN) calculations.

We also implemented this model into CYCLUS, an agent-based Nuclear Fuel Cycle (NFC) simulator, to perform rapid, medium-fidelity PWR depletion calculations. This model also allows discharge of batches with assemblies of varying burnup.

Since the original private data cannot be retrieved from the model, this trained model can provide open-source depletion capabilities to NFC simulators. We show that training an artificial neural network with a dataset from a complex fuel depletion model can provide rapid, medium-fidelity depletion capabilities to large-scale fuel cycle simulations.

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Machine learning of LWR spent nuclear fuel assembly decay heat measurements

Bamidele Ebiwonjumi, Alexey Cherezov, Siarhei Dzianisau, Deokjung Lee*

Department of Nuclear Engineering, Ulsan National Institute of Science and Technology, 50 UNIST-gil, Eonyang-eup, Ulju-gun, Ulsan, 44919, Republic of Korea

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A B S T R A C T

Measured decay heat data of light water reactor (LWR) spent nuclear fuel (SNF) assemblies are adopted to train machine learning (ML) models. The measured data is available for fuel assemblies irradiated in commercial reactors operated in the United States and Sweden. The data comes from calorimetric measurements of discharged pressurized water reactor (PWR) and boiling water reactor (BWR) fuel assemblies. 91 and 171 measurements of PWR and BWR assembly decay heat data are used, respectively. Due to the small size of the measurement dataset, we propose: (*i*) to use the method of multiple runs (*ii*) to generate and use synthetic data, as large dataset which has similar statistical characteristics as the original dataset. Three ML models are developed based on Gaussian process (GP), support vector machines (SVM) and neural networks (NN), with four inputs including the fuel assembly averaged enrichment, assembly averaged burnup, initial heavy metal mass, and cooling time after discharge. The outcomes of this work are (*i*) development of ML models which predict LWR fuel assembly decay heat from the four inputs (*ii*) generation and application of synthetic data which improves the performance of the ML models (*iii*) uncertainty analysis of the ML models and their predictions.

Table 4
Dataset input and output features.

Input features	Ranges	
	PWR dataset	BWR dataset
Decay time (days)	859–9734	857–9750
Discharge burnup (GWd/tU)	19.699–50.962	5.28–46.648
^{235}U enrichment (wt.%)	2.09–4.005	1.09–3.15
Heavy metal mass (kg)	361.72–463.898	126.68–195.48
Output feature		
Decay heat (W)	209.79–1550	19.5–395.40

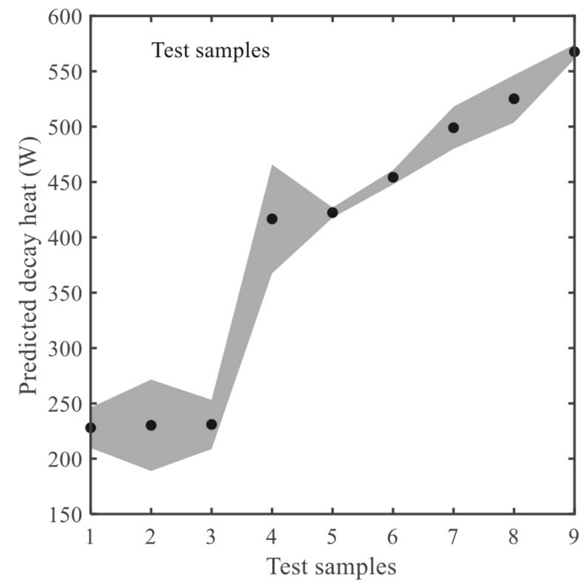


Fig. 6. GPR predictions and uncertainties at 95% confidence interval (original PWR dataset).

정리 및 제안

원자력 (재료) 분야 인공지능 연구는 증가하고 있으나 절대적인 양이 많지 않음

찾은 논문들을 AI (응용) 논문이라고 볼 수 있는가?

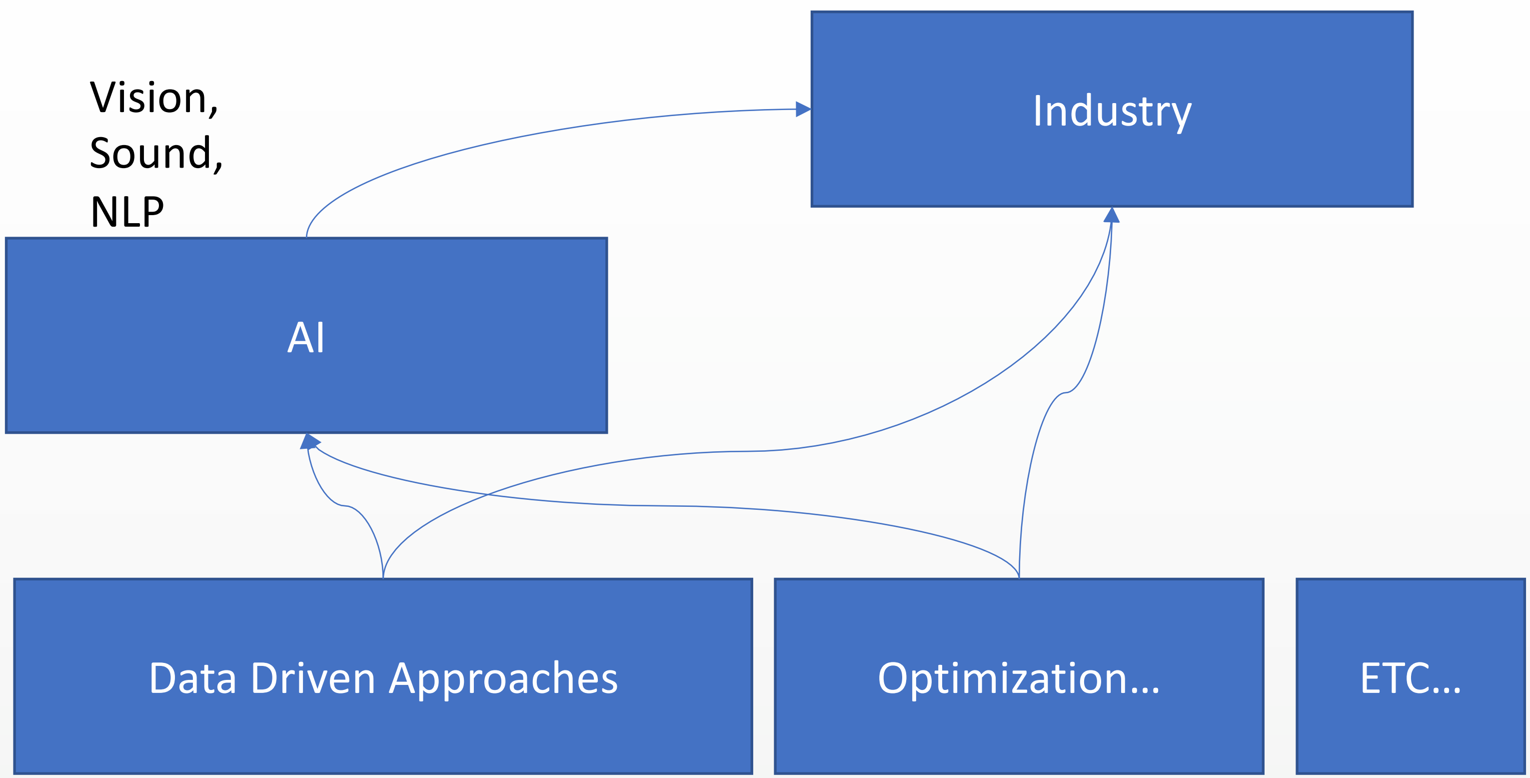
- Neural Network 를 사용하면 인공지능인가?
- 좀 복잡한 함수로 Curve fitting 했다는 것을 AI라고 불러야 하는가?
  (컴퓨터써서 연구하면 컴퓨터 사이언스인가?)
- AI 보다는 Data Mining /Data Science 이 더 어울리는 표현과 방향이 아닐지

Douglas Richard Hofstadter
AI is whatever hasn't been yet.

Neural Network가 최선인가?

- 대부분 Neural Network 등의 머신러닝 모델을 이용한 Data regression 사례
- neural network가 최선이 아닐 가능성이 큼

정말 필요해서 인공지능 기술을 사용한 건 맞나?
유행따라 인공지능 일단 적용하고 보자는 것은 아닌지?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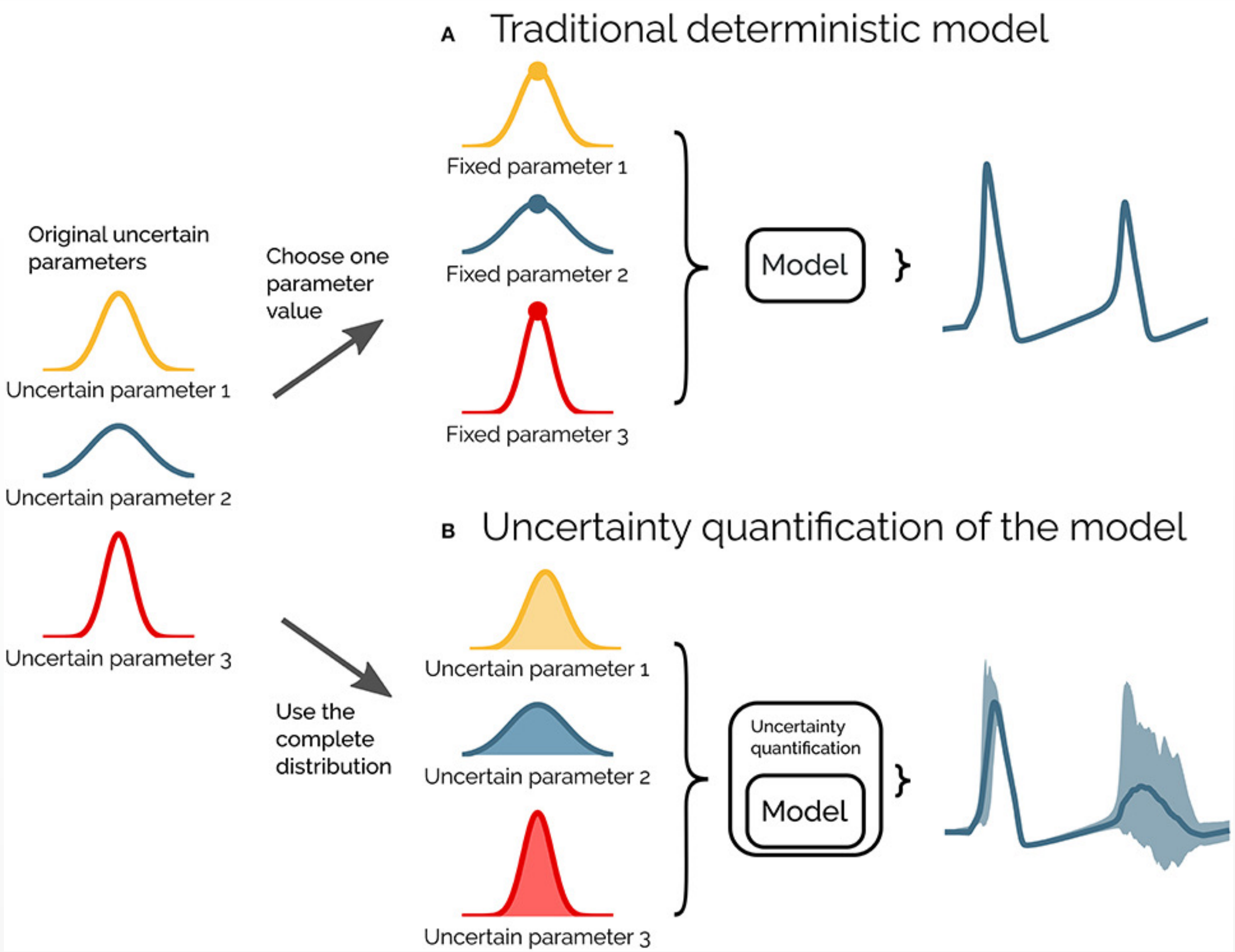
NLP
Industry
AI
Data Driven Approaches
Optimization...
ETC...



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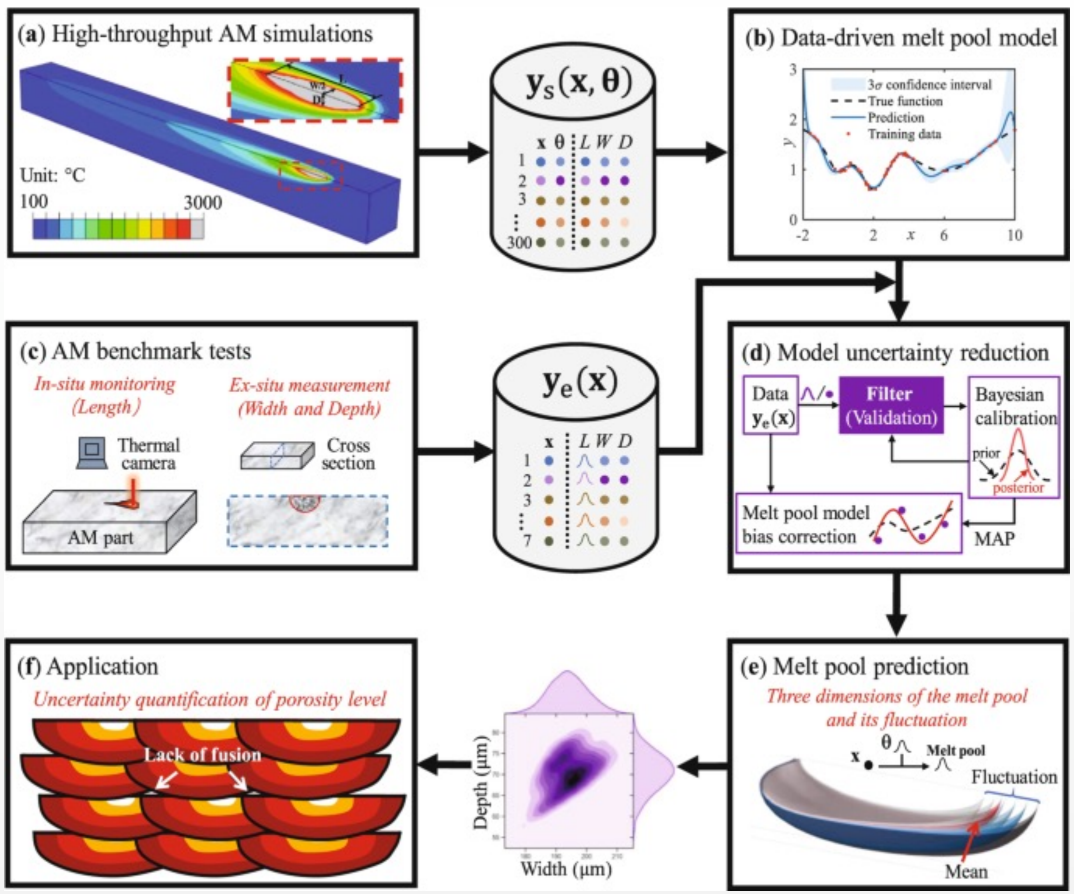
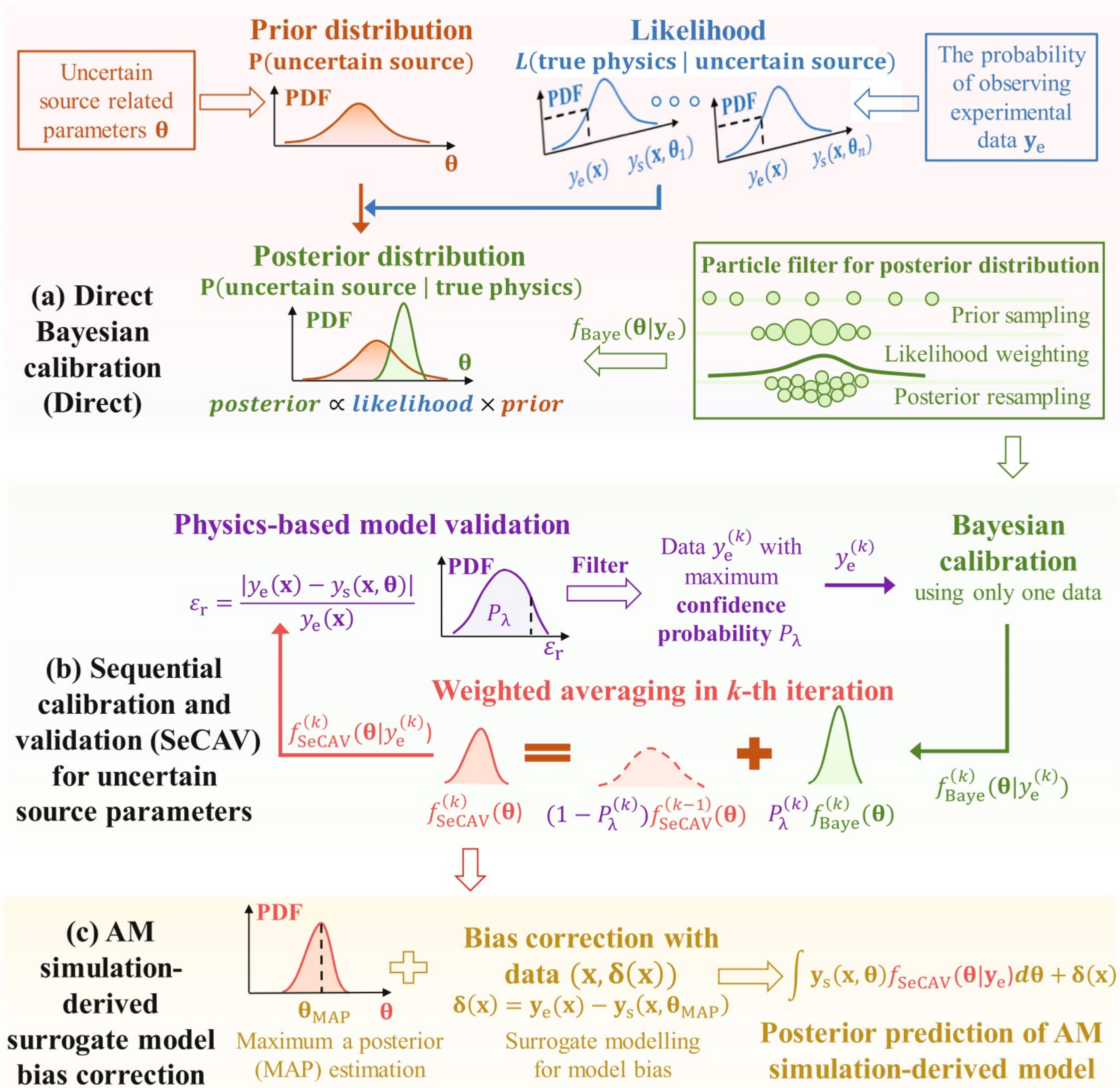
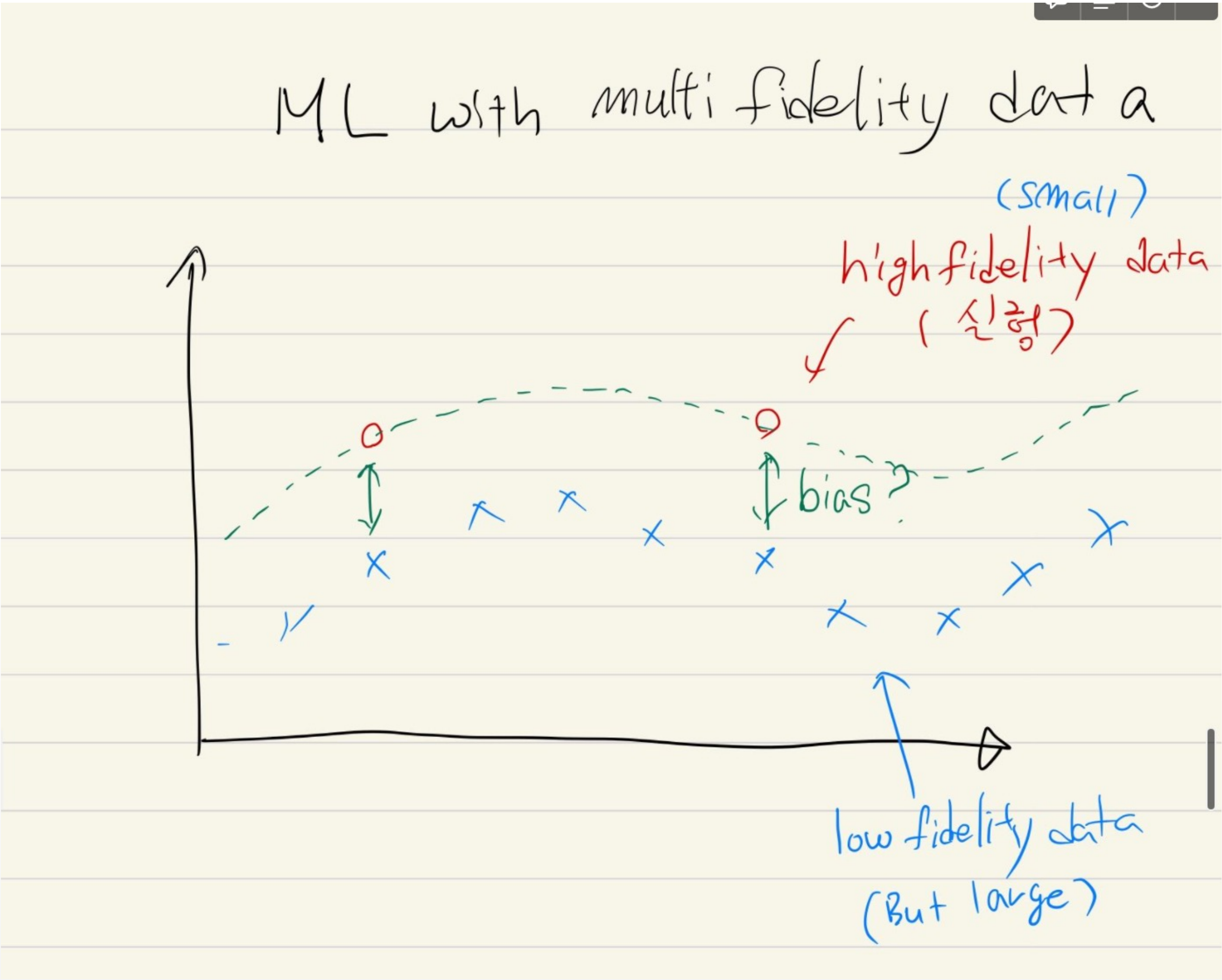
Uncertainty quantification and reduction in metal additive manufacturing

Zhuo Wang[1,8], Chen Jiang[2,8], Pengwei Liu[3], Wenhua Yang[4], Ying Zhao[2], Mark F. Horstemeyer[5], Long-Qing Chen[6], Zhen Hu[2,7]✉ and Lei Chen[1,7]✉




Prior distribution
P(uncertain source)
Likelihood
L(true physics | uncertain source)
Uncertain source related parameters $\boldsymbol{\theta}$
The probability of observing experimental data $\mathbf{y}_e$
PDF
$\boldsymbol{\theta}$
$y_e(\mathbf{x})$
$y_s(\mathbf{x}, \boldsymbol{\theta}_1)$
$y_s(\mathbf{x}, \boldsymbol{\theta}_n)$
Posterior distribution
P(uncertain source | true physics)
(a) Direct Bayesian calibration (Direct)
$posterior \propto likelihood \times prior$
$f_{Baye}(\boldsymbol{\theta}|\mathbf{y}_e)$
Particle filter for posterior distribution
Prior sampling
Likelihood weighting
Posterior resampling
Physics-based model validation
$\varepsilon_r = \frac{|y_e(\mathbf{x}) - y_s(\mathbf{x}, \boldsymbol{\theta})|}{y_e(\mathbf{x})}$
P_λ
ε_r
Filter
Data $y_e^{(k)}$ with maximum confidence probability P_λ
$y_e^{(k)}$
Bayesian calibration
using only one data
(b) Sequential calibration and validation (SeCAV) for uncertain source parameters
$f_{SeCAV}^{(k)}(\boldsymbol{\theta}|y_e^{(k)})$
Weighted averaging in k-th iteration
$f_{SeCAV}^{(k)}(\boldsymbol{\theta})$
$(1 - P_\lambda^{(k)}) f_{SeCAV}^{(k-1)}(\boldsymbol{\theta})$
$P_\lambda^{(k)} f_{Baye}^{(k)}(\boldsymbol{\theta})$
$f_{Baye}^{(k)}(\boldsymbol{\theta}|y_e^{(k)})$
(c) AM simulation-derived surrogate model bias correction
$\boldsymbol{\theta}_{MAP}$
Maximum a posterior (MAP) estimation
Bias correction with data $(\mathbf{x}, \boldsymbol{\delta}(\mathbf{x}))$
$\boldsymbol{\delta}(\mathbf{x}) = \mathbf{y}_e(\mathbf{x}) - \mathbf{y}_s(\mathbf{x}, \boldsymbol{\theta}_{MAP})$
Surrogate modelling for model bias
$\int \mathbf{y}_s(\mathbf{x}, \boldsymbol{\theta}) f_{SeCAV}(\boldsymbol{\theta}|\mathbf{y}_e) d\boldsymbol{\theta} + \boldsymbol{\delta}(\mathbf{x})$
Posterior prediction of AM simulation-derived model



ML with multi fidelity data
(small)
high fidelity data
(실험)
bias?
low fidelity data
(But large)

Nuclear Material Science

Strategic nuclear material production and processing

SCIENTIFIC DISCOVERY
SUSTAINABLE ENERGY
NATIONAL SECURITY
Chemical & Biothreat Signatures
Cybersecurity
Nuclear Material Science
Nuclear Nonproliferation
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Systems Integration & Deployment
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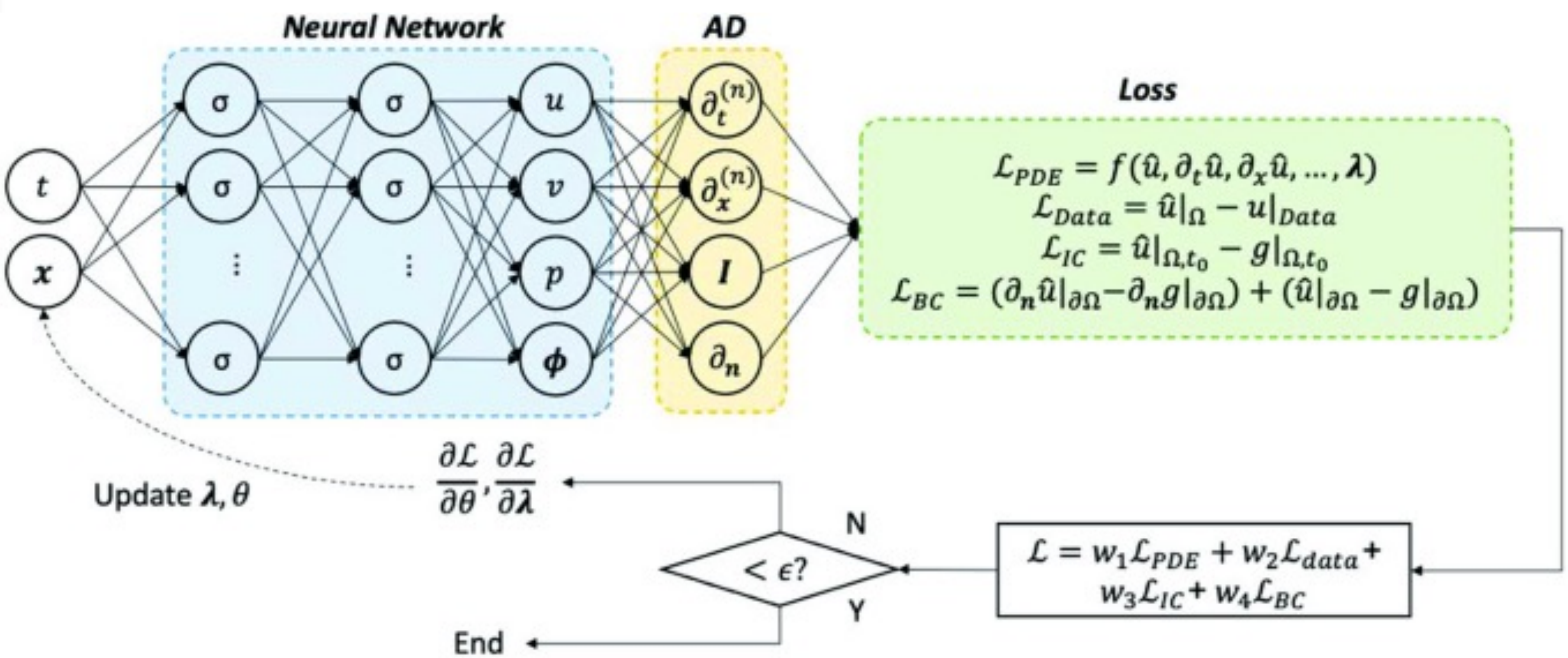
Pacific Northwest National Laboratory (PNNL) is a leader in the science and technology of strategic material production and processing, including tritium, uranium, and plutonium. Our cutting-edge nuclear material science capabilities are rooted in the support for Hanford's defense mission during the Manhattan Project and the Cold War. The resources, facilities, and collaborations across disciplines at PNNL, the national laboratory system, academia, and industry enable us to develop and use a deep understanding of nuclear materials to drive mission impact in stockpile stewardship, nonproliferation, and nuclear energy.

PNNL continues to invest in the expansion and enhancement of our capabilities in nuclear-material processing. For example, we are working to accelerate modeling-based prediction of material microstructure through targeted application of high-fidelity models for fundamental phenomena; lower-resolution models to characterize trends across broad ranges of the process parameter space; and science-informed machine learning to accelerate the discovery and interpretation of relationships across length and time scales. We are also developing and applying advanced noninvasive diagnostic methods that can provide real-time validation of product characteristics to reduce the need for sampling-based offline characterization and to inform data-driven process control. PNNL has numerous activities in the development and use of physics-informed data analytics methods tailored to material processing, including the interpretation of complex patterns in the process–structure–property relationships that govern material performance.

Nuclear material science is the foundation of reliable tritium production

PNNL is the design authority for the tritium-producing burnable absorber rods (TPBARs) used to produce tritium for the nuclear weapons stockpile. PNNL is the recognized leader in the science and engineering of



Note: $\hat{u} = [u, v, p, \phi]$, $x = [x, y]$, θ: weights/biases, λ: unknown PDE parameters, $w_i, i = 1, \ldots, 4$: weights

https://link.springer.com/article/10.1007/s10409-021-01148-1

"화학 연구에도 AI가?"···딥 마인드, 나노 계산 돕는 AI 공개

뉴스1 입력 2021.12.10 06:57 수정 2021.12.10 06:57

화학 반응을 비롯한 다양한 자연 현상을 원자와 분자 수준에서 이해하기 위해서는 물질·분자 내부에 전자의 분포와 에너지를 양자역학적으로 계산할 필요가 있다. 단순한 원자의 경우에는 양자역학적 계산이 가능하지만, 원자의 수가 늘어나고 관계가 복잡해질수록 필요한 계산량과 난이도는 급속히 늘어난다.

이후 밀도 범함수 이론(Density Functional Theory, DFT)이 나와 상대적으로 계산량이 줄었다. 이 이론을 발전시킨 월터 콘과 같은 학자는 이 공로로 노벨상을 수상하기도 했다.

딥마인드는 DFT 기반 계산을 개선하기 위한 인공신경망 기반의 인공지능을 개발했다. 전자 밀도와 상호 작용 에너지 사이의 정확한 매핑 특성(밀도 함수)는 계산의 핵심이지만, 알려지지 않았다. 딥마인드는 인공신경망을 사용해 이전에 달성할 수 있었던 것보다 더 정확한 밀도 및 전자 간의 상호 작용 관계 지도를 구축할 수 있음을 논문을 통해 밝혔다.

Pushing the frontiers of density functionals by solving the fractional electron problem

JAMES KIRKPATRICK, BRENDAN MCMORROW, DAVID H. P. TURBAN, ALEXANDER L. GAUNT, JAMES S. SPENCER, ALEXANDER G. D. G
ANNETTE OBIKA, LOUIS THIRY, MEIRE FORTUNATO, [...] ARON J. COHEN +8 authors Authors Info & Affiliations

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BY JOHN P. PERDEW

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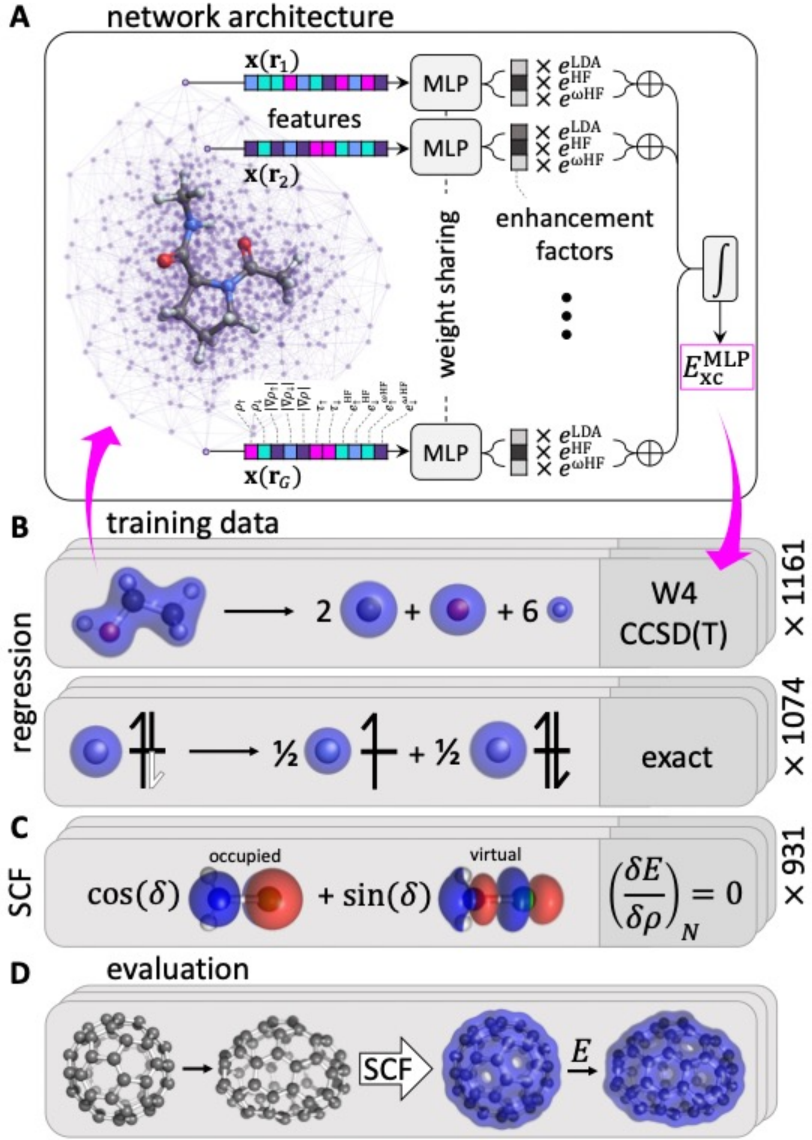
Response to Comment on "Pushing the frontiers of density functionals by solving the frac-tional electron problem"

BY JAMES KIRKPATRICK, BRENDAN MCMORROW, DAVID H. P. TURBAN, ET AL.

Improving DFT with deep learning

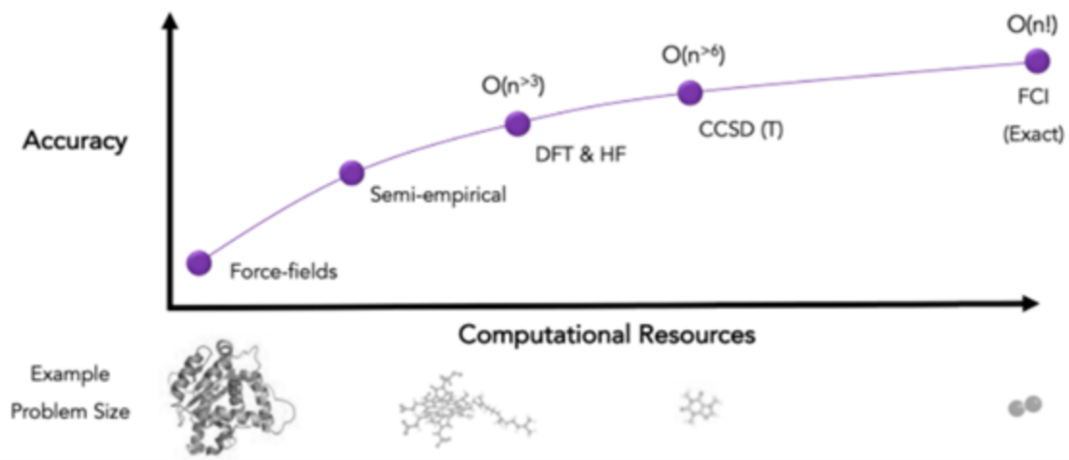
In the past 30 years, density functional theory (DFT) has emerged as the most widely used electronic structure method to predict the properties of various systems in chemistry, biology, and materials science. Despite a long history of successes, state-of-the-art DFT functionals have crucial limitations. In particular, significant systematic errors are observed for charge densities involving mobile charges and spins. Kirkpatrick *et al*. developed a framework to train a deep neural network on accurate chemical data and fractional electron constraints (see the Perspective by Perdew). The resulting functional outperforms traditional functionals on thorough benchmarks for main-group atoms and molecules. The present work offers a solution to a long-standing critical problem in DFT and demonstrates the success of combining DFT with the modern machine-learning methodology. —YS



The intersection of quantum computation and chemistry

Many problems in chemistry have to do with quantum nature of electrons. Many of the physiochemical properties of compounds can be derived from quantum mechanics descriptions of the electronic structure of a molecule. Complexity observed in biological systems has its origin in quantum mechanics. It is then inevitable to think that the underlying physical device to perform computation on nature must be quantum itself.

In the field of computational chemistry, classical computing has set the bar very high. Overtime physicists and chemists have come with clever simplifications to solve the Schrödinger equation of chemical systems, sacrificing accuracy while remaining efficient. Ab initio quantum chemical calculations must compete with a wide list of competitive alternatives with different levels of accuracy (FF, DFT, Hartree-Fock, coupled-cluster theory) and years of extensive development on CPU and GPU chips.



https://pharmacelera.com/blog/science/quantum-computing/

NEW LABORATORY TO EXPLORE THE QUANTUM MYSTERIES OF NUCLEAR MATERIALS

Replete with tunneling particles, electron wells, charmed quarks and zombie cats, quantum mechanics takes everything Sir Isaac Newton taught about physics and throws it out the window.

Every day, researchers discover new details about the laws that govern the tiniest building blocks of the universe. These details not only increase scientific understanding of quantum physics, but they also hold the potential to unlock a host of technologies, from quantum computers to lasers to next-generation solar cells.

But there's one area that remains a mystery even in this most mysterious of sciences: the quantum mechanics of nuclear fuels.

EXPLORING THE FRONTIERS OF QUANTUM MECHANICS

Until now, most fundamental scientific research of quantum mechanics has focused on elements such as silicon because these materials are relatively inexpensive, easy to obtain and easy to work with.

Now, Idaho National Laboratory researchers are planning to explore the frontiers of quantum mechanics with a new synthesis laboratory that can work with radioactive elements such as uranium and thorium.

An announcement about the new laboratory appears online in the journal Nature Communications.

Uranium and thorium, which are part of a larger group of elements called actinides, are used as fuels in nuclear power reactors because they can undergo nuclear fission under certain conditions.

Open-Source Quantum Development

Qiskit [kiss-kit] is an open-source SDK for working with quantum computers at the level of pulses, circuits, and application modules.

Get started

Run a quantum program

```
[python3] $ pip install qiskit
```

```
from qiskit import QuantumProgram
qp = QuantumProgram()
qr = qp.create_quantum_register('qr',2)
cr = qp.create_classical_register('cr',2)
qc = qp.create_circuit('Bell',[qr],[cr])
qc.h(qr[0])
qc.cx(qr[0], qr[1])
qc.measure(qr[0], cr[0])
qc.measure(qr[1], cr[1])
result = qp.execute('Bell')
print(result.get_counts('Bell'))
```

AI·로봇 연구원 24시간 실험도 'OK'… '무인연구실' 현실?

허나영 수습기자 | nyheo2022@HelloDD.com | 입력 2022.01.18 17:40 | 수정 2022.01.20 18:42 | 댓글 0

> 연구로봇 배양방법 배워 실험·연구자 창의적 작업 몰두
> 美카네기멜론대·日리켄 각각 무인실험실 마련

연구실 무인화가 본격화되고 있다. 인공지능과 로봇기술 접목으로 실험을 완전히 자동화하며 365일 가동되는 실험실이 현실로 다가왔다.

일본경제신문에 의하면 미국 카네기멜론대학은 올해 초 24시간, 365일 가동하는 대규모 자동화 실험실을 갖췄다. 일본에서도 이화학연구소(이하 리켄), 시마즈제작소 등이 의약품 재료 연구시설을 자동화 했다. 실험 데이터 품질도 사람과 차이가 없는 것으로 확인된다. 완전 자동화 실험실 구축으로 연구성과도 증가하며 혁신을 가속화 할 것으로 기대된다.

◆ 카네기멜론대, '무인 실험실'과 '클라우드 실험실'

카네기멜론대 스타트업 에메랄드 클라우드 랩. [영상=에메랄드 클라우드 랩 유튜브]

댓글 마당

- 3. 추가적으로 일정 수준이 넘어서면 대부분의 교수와...
- 1. 대학등록금 올린다고 학교 예산이 크게 증가하지는...
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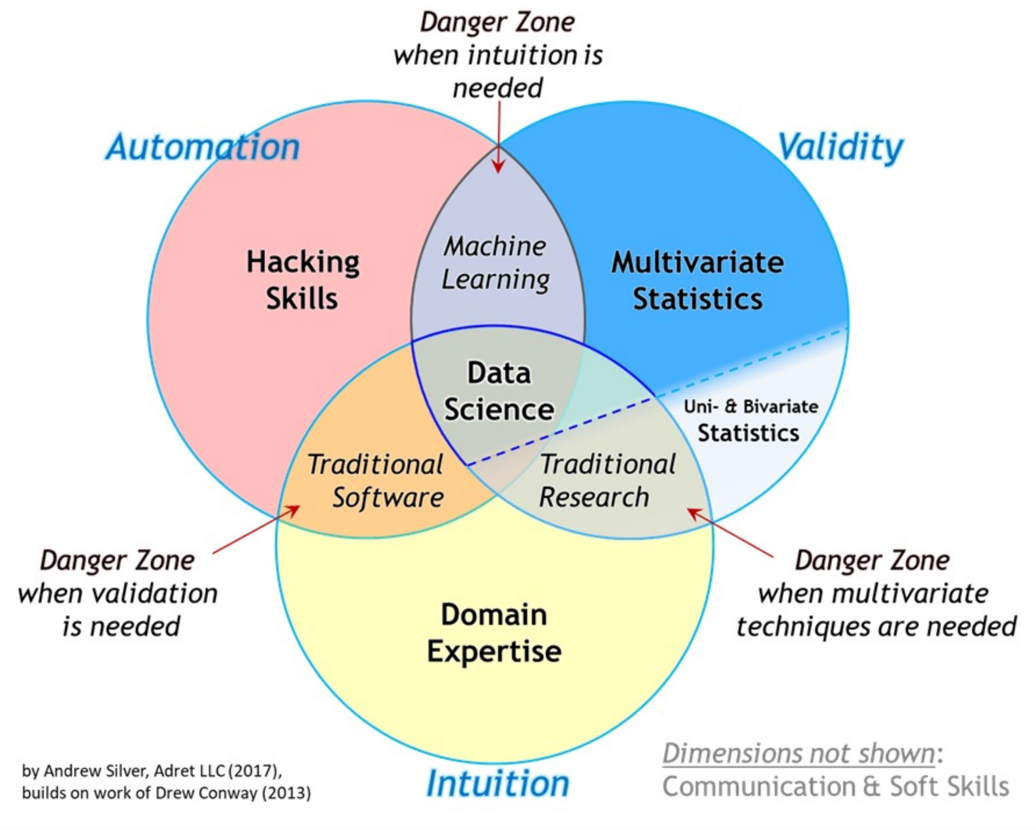

도메인 지식과 데이터과학의 이해가 필요
-> 인공지능응용전략실과 협업 환영합니다!