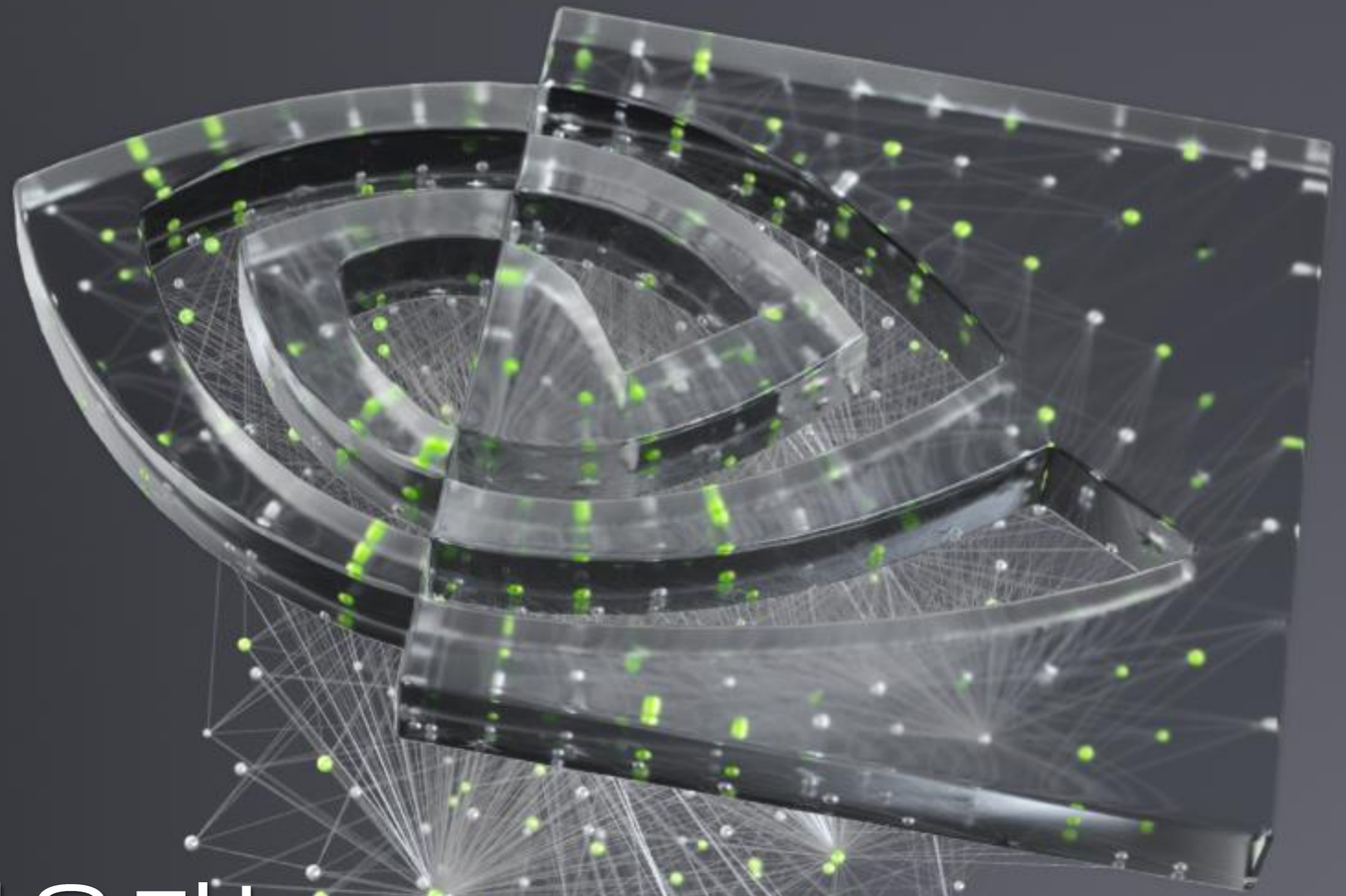


신약/신소재 개발에 사용되는
NVIDIA DGX SUPERPOD

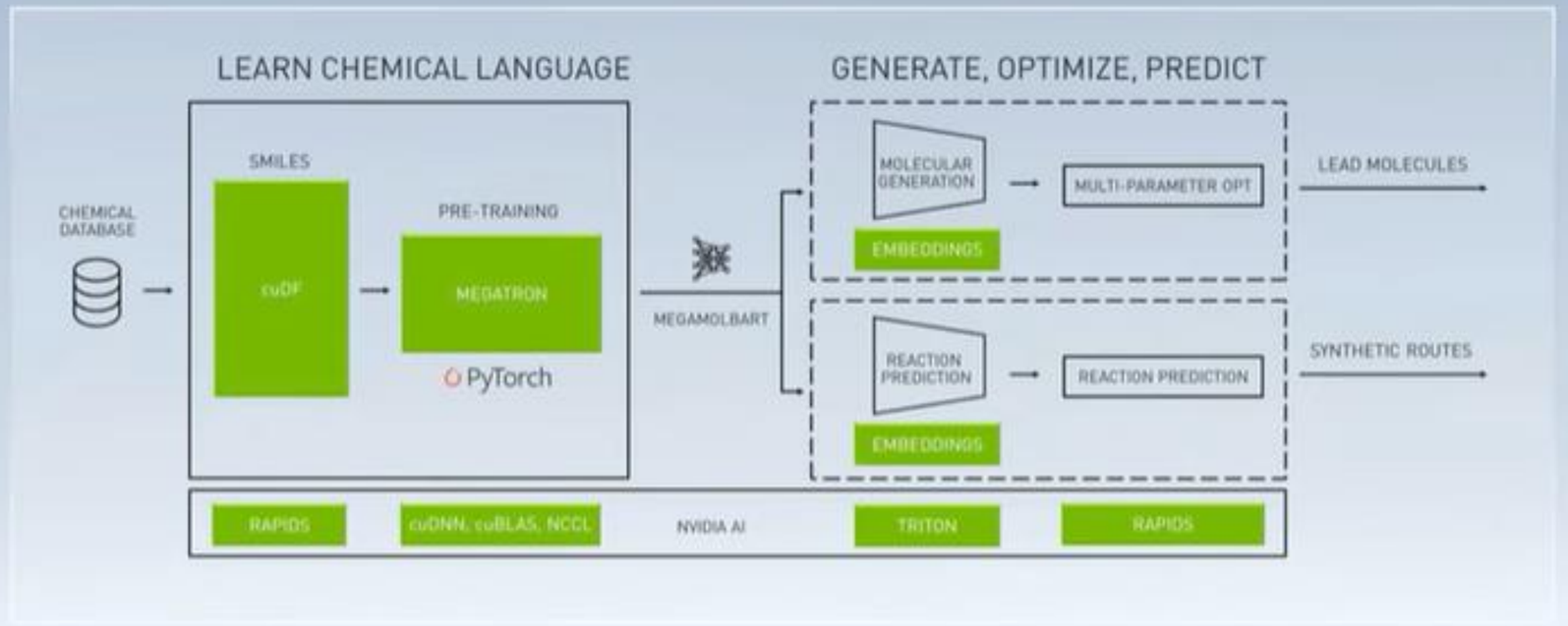
정구형 부장, Solutions Architect, NVIDIA Korea, 2021년 9월 7일

“GPT-3와 같은 초거대 AI 모델을 위한 NVIDIA DGX SuperPOD”

지난 6월 세션에 이어 이번 발표에서는...

ANNOUNCING MEGAMOLBART

Understanding the Language of Chemistry



AstraZeneca

Pre-Training with 1B Molecules in Zinc Database

Megatron Multi-GPU, Multi-Node Training
Across 32 DGX A100

Triton Inference 250M Molecules/Day on Cambridge-1

Molecule Generation |Molecular Optimization
Synthesis Prediction

Cambridge-1
DGX SuperPOD

NVIDIA

NVIDIA SELENE

running molecular dynamics applications

NVIDIA DGX SuperPOD for internal use

4,480 A100 GPUs

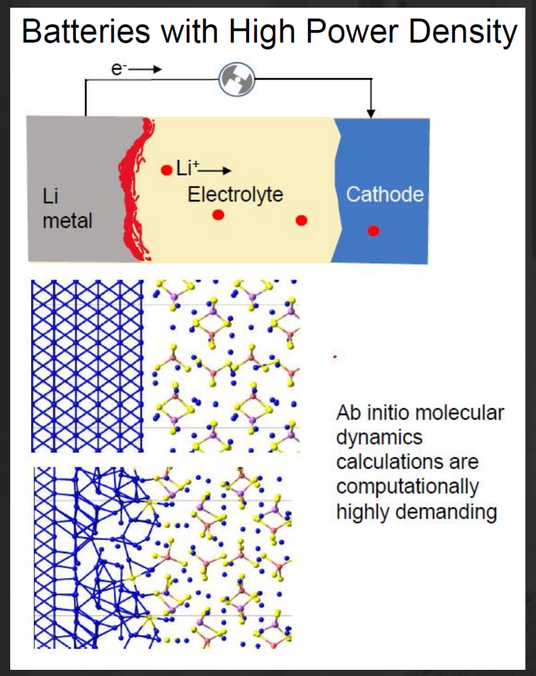
560 DGX A100 systems

850 Mellanox 200G HDR switches

14 PB of high-performance storage

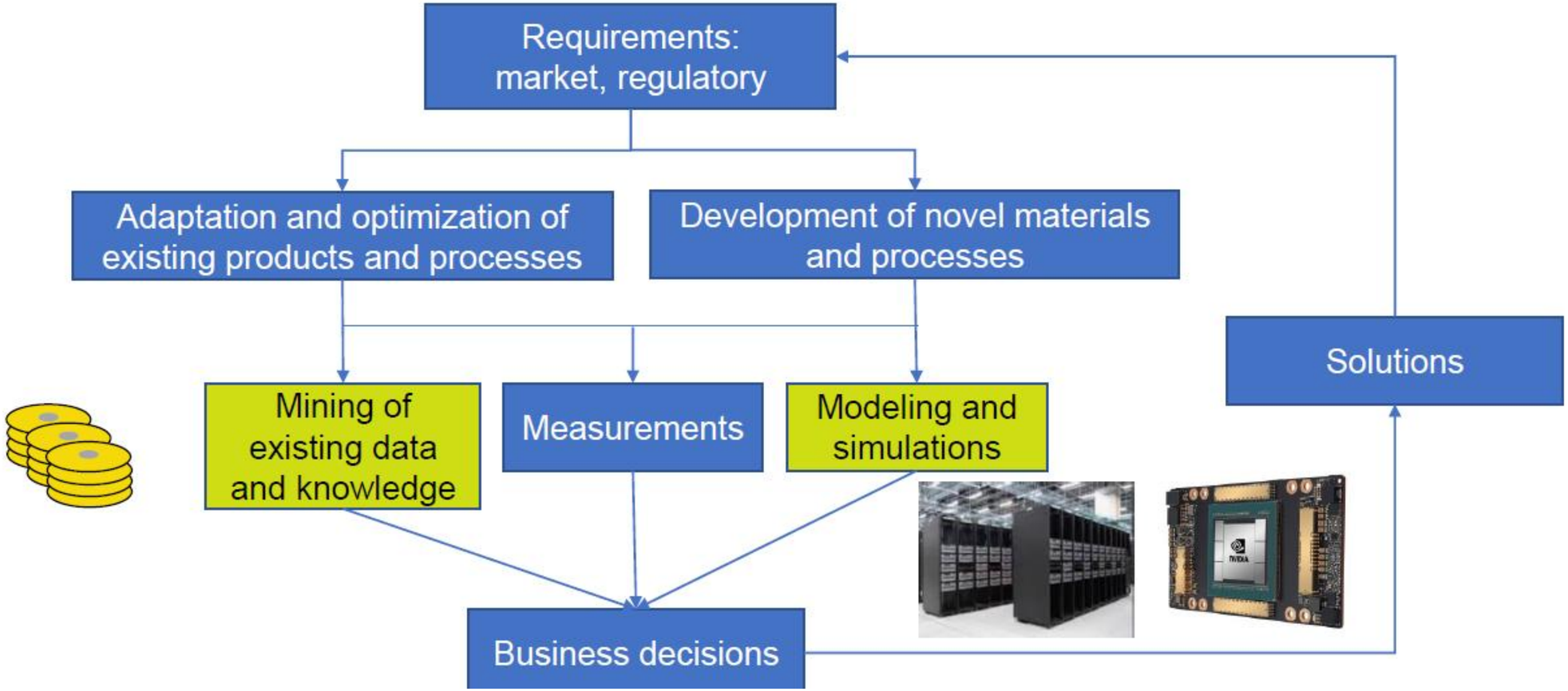
2.8 EFLOPS of AI peak performance

63 PFLOPS HPL @ 24GF/W



R&D WORKFLOW

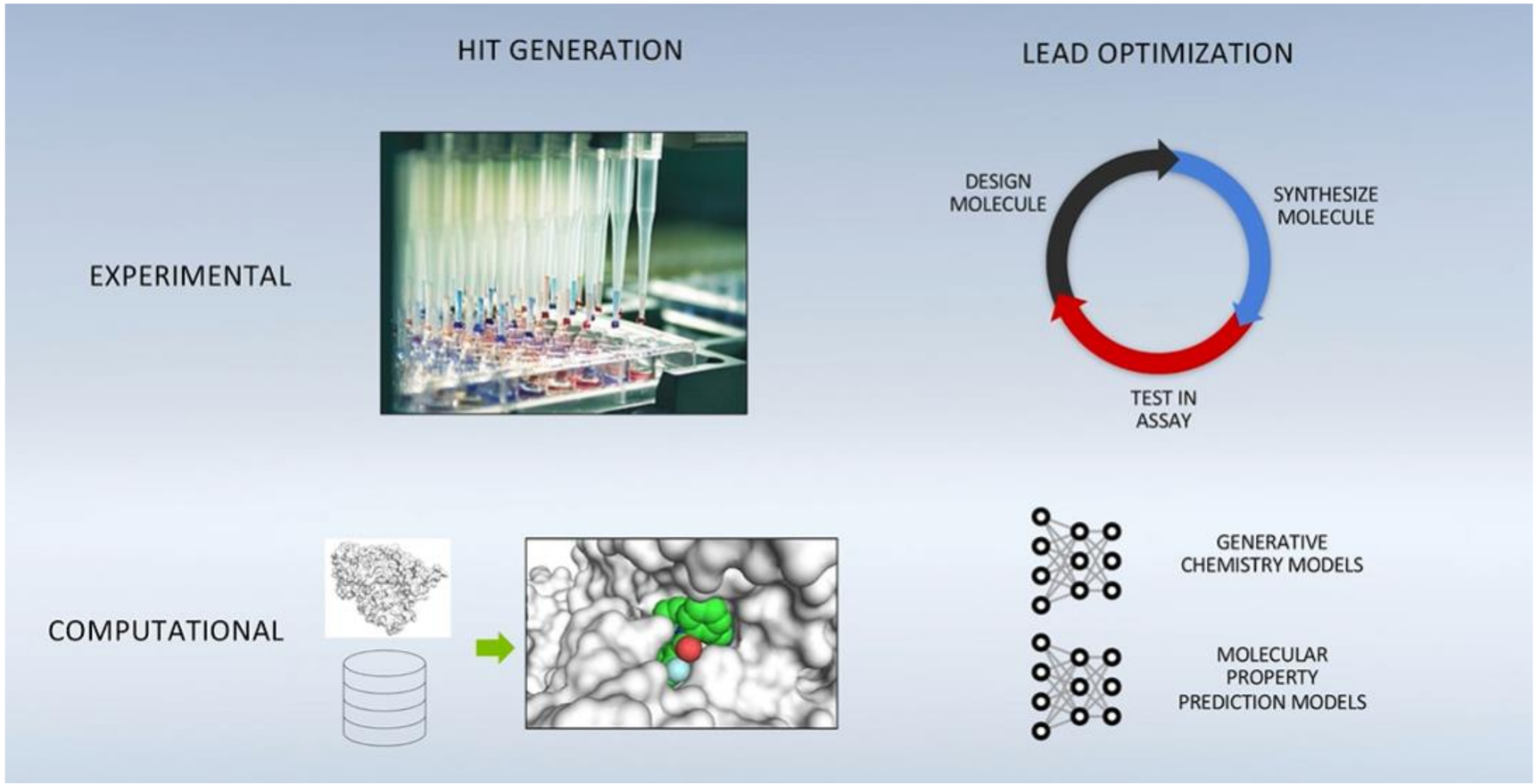
직접 실험 vs. Computational simulation



Source: THE INNOVATIVE FORCE OFHIGH PERFORMANCE COMPUTING IN MATERIALS SCIENCE, NVIDIA, Webinar (2021년 7월)

예. 신규 물질 개발

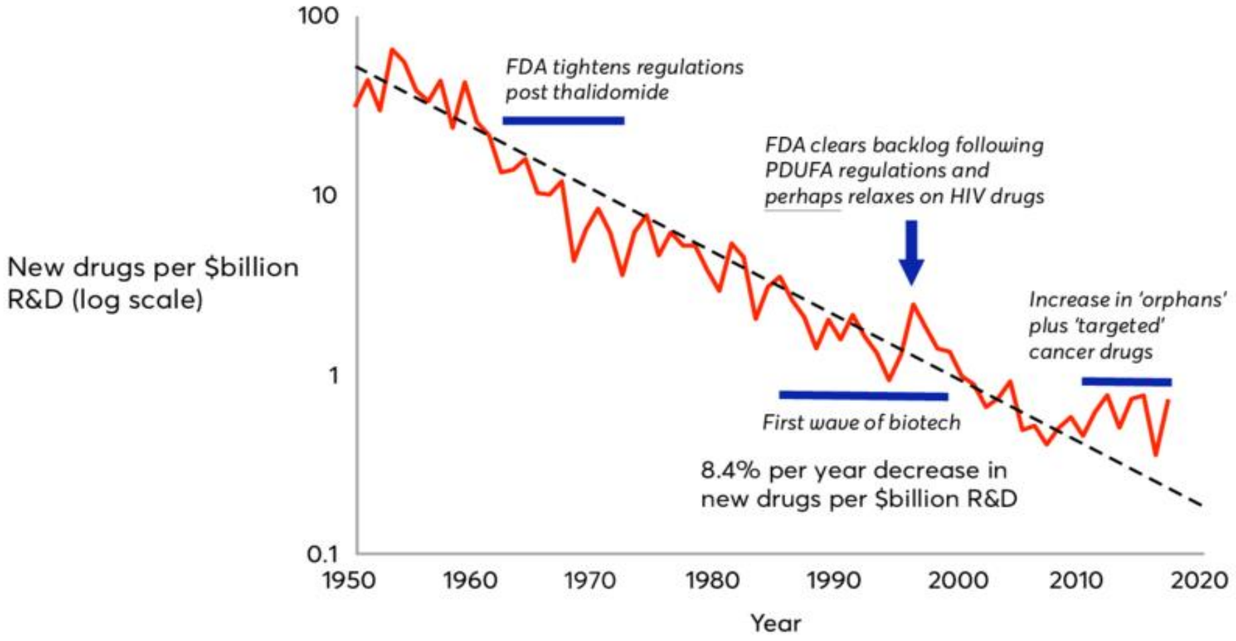
직접 실험 vs. Computational simulation



Source: Accelerating Drug Discovery with Clara Discovery's MegaMolBart, NVIDIA, YouTube (2021년 4월)

EROOM’S LAW – 신약 개발 성공률 저하

평균 10년이 넘는 시간 | 신약 1개 개발시 평균 $2B 비용 | 신약 개발 실패율 90%



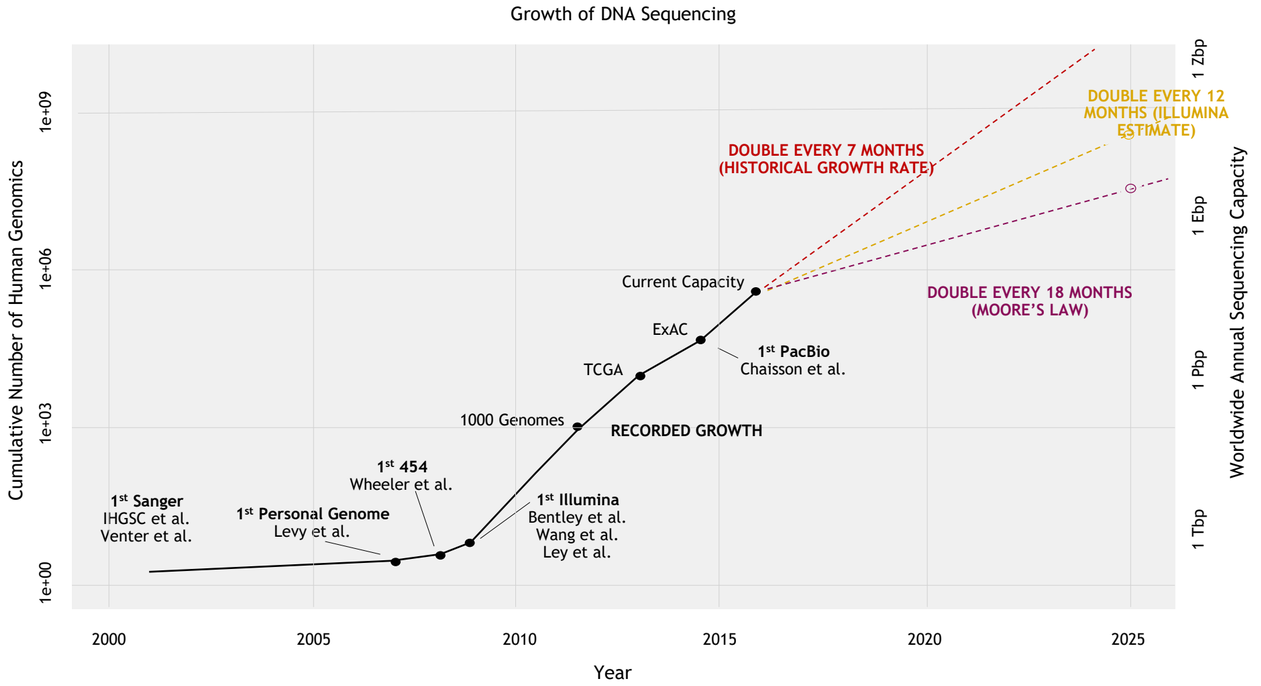
Eroom’s Law

Exponential Decline in Drug Discovery R&D Productivity

Source: Jones, R. & Wilsdon, James. (2018). The Biomedical Bubble: Why UK research and innovation needs a greater diversity of priorities, politics, places and people.

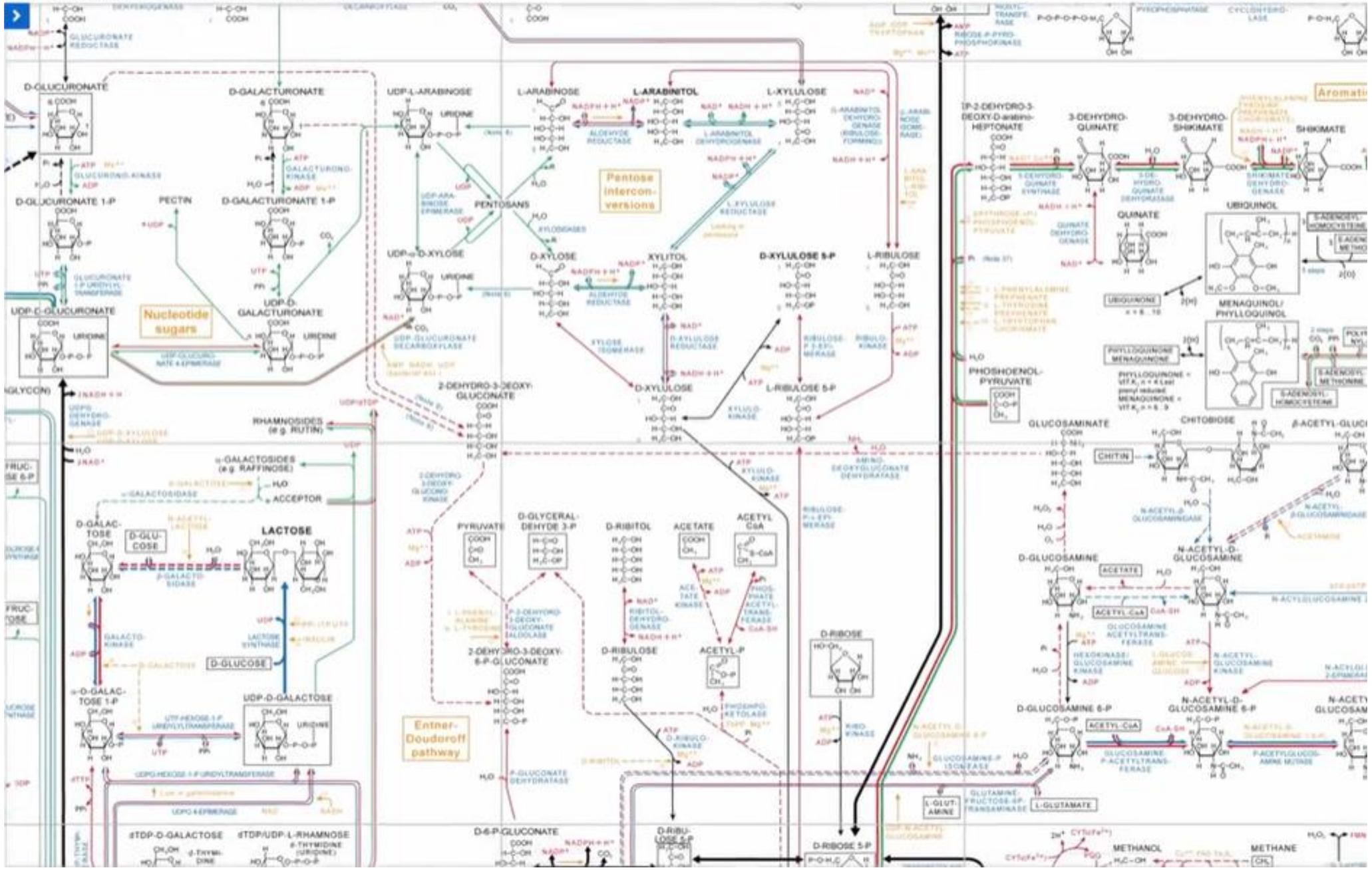
EROOM’S LAW – 신약 개발 성공률 저하

폭발적으로 늘어나는 biomedical 데이터

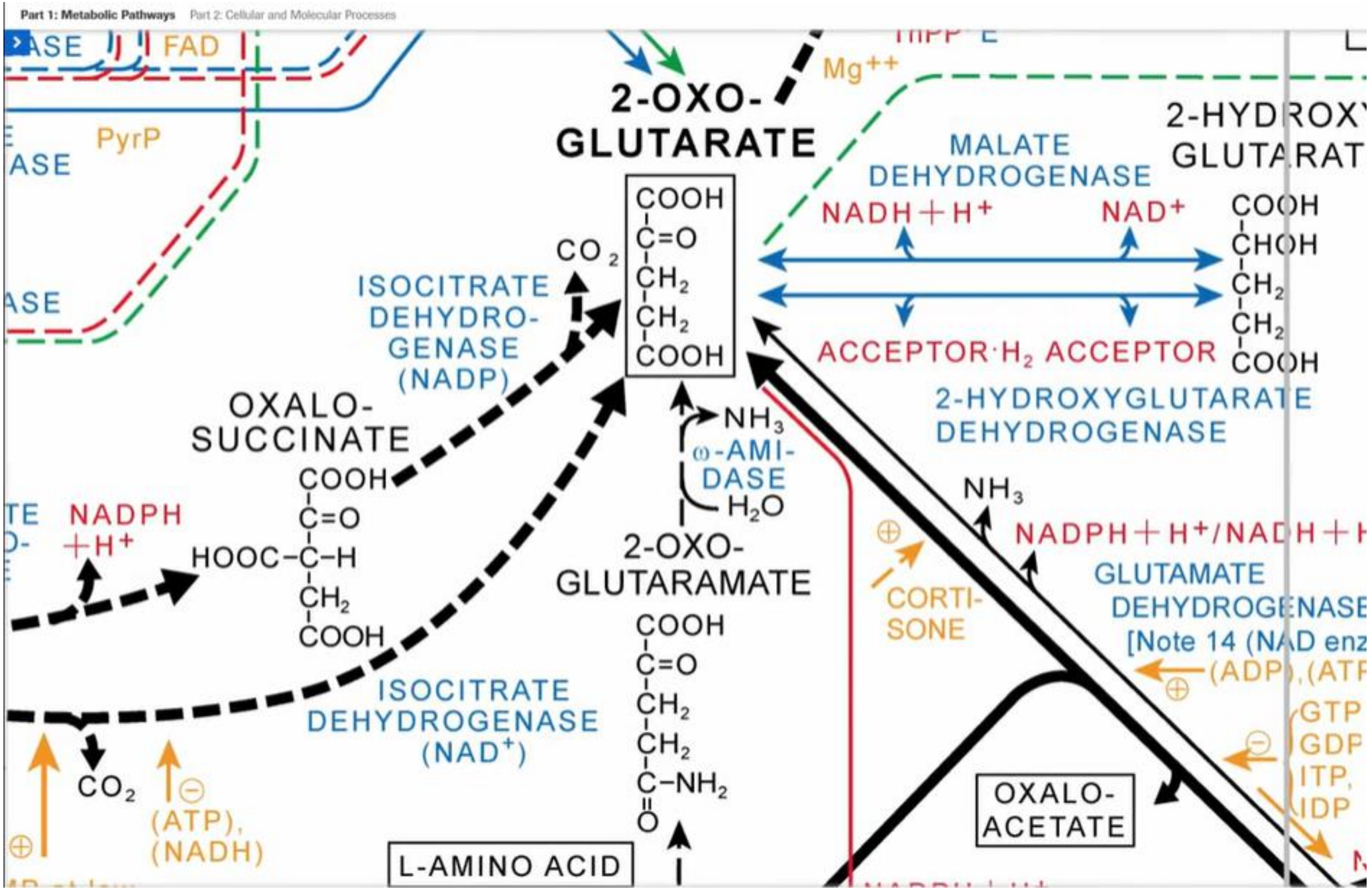


Biomedical Data Explosion

Sequencing, Protein, Imaging



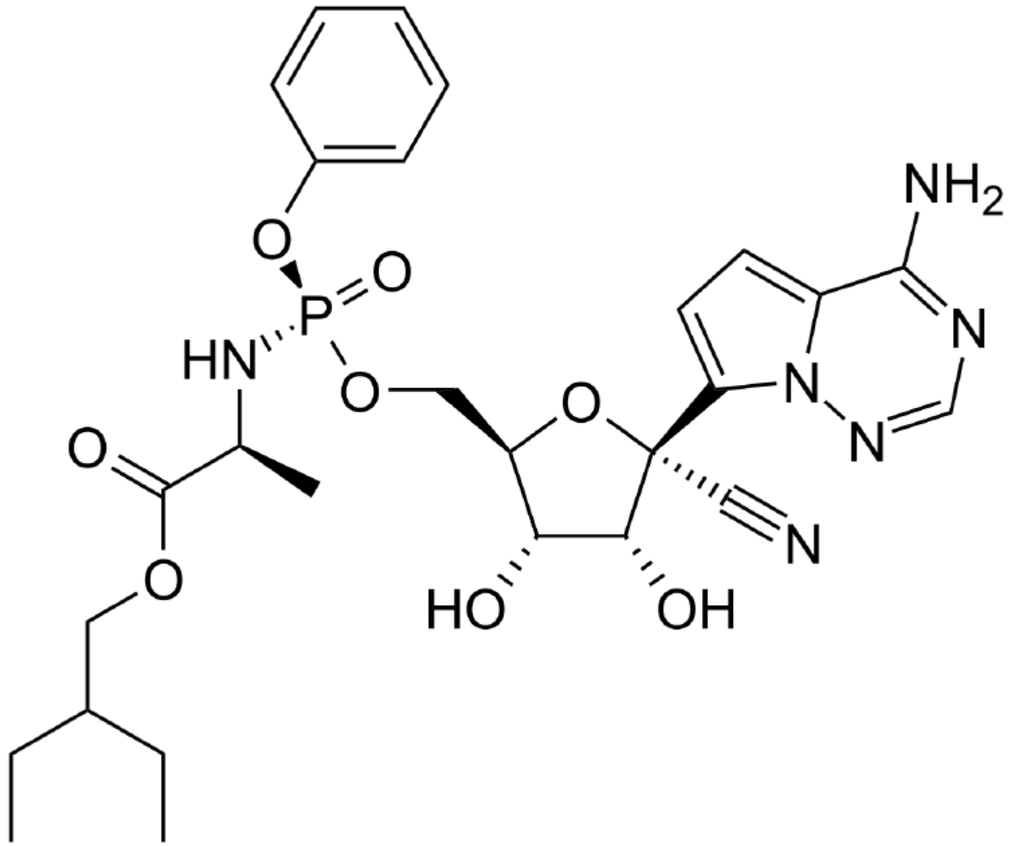
Source: [Introducing Clara Discovery: Modular Platform for Computational Drug Discovery](), NVIDIA, GTC (2021년 4월)



Source: [Introducing Clara Discovery: Modular Platform for Computational Drug Discovery](), NVIDIA, GTC (2021년 4월)

신약 개발은 얼마나 힘든 일일까요?

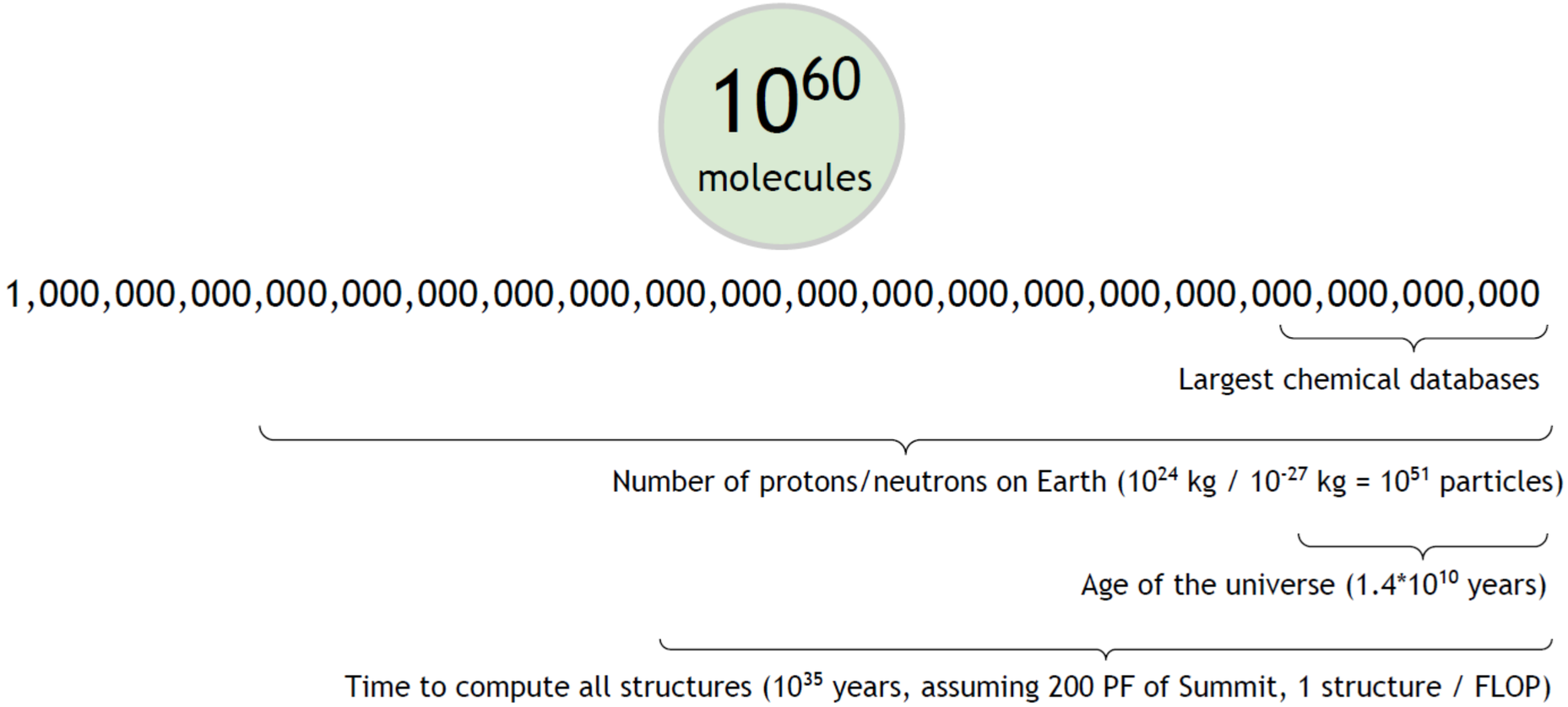
지금 여러분은 하나의 화학 구조물을 보고 계십니다.



Source: Introducing Clara Discovery: Modular Platform for Computational Drug Discovery, NVIDIA, GTC (2021년 4월)

화학 물질의 세계는 광대합니다.

30개의 원자로 구성할 수 있는 분자 구조 경우의 수

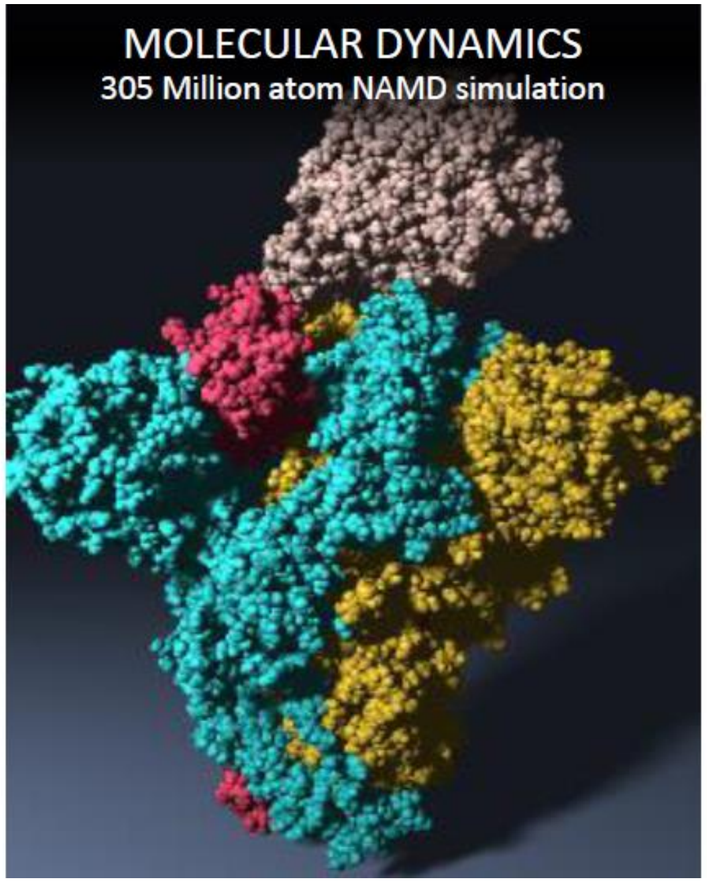


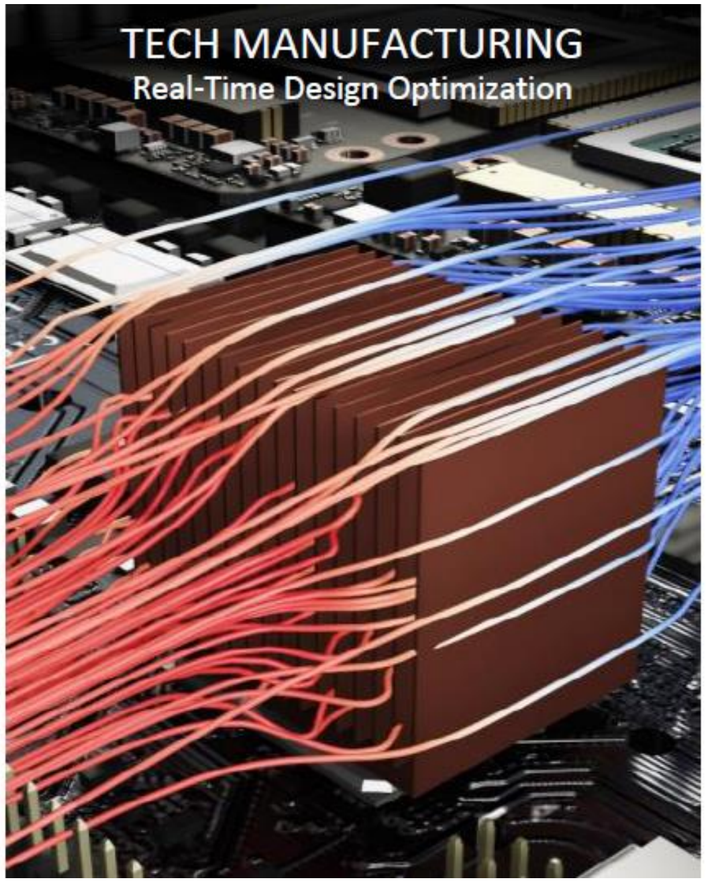
Source: Introducing Clara Discovery: Modular Platform for Computational Drug Discovery, NVIDIA, GTC (2021년 4월)

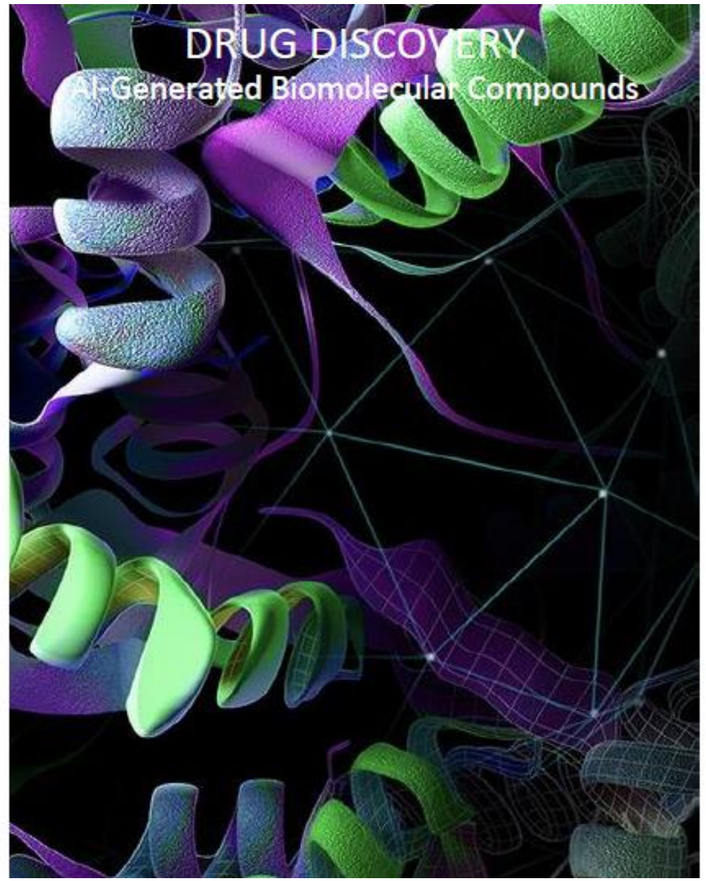
NVIDIA

R&D에서 *SIMULATION* 중요성 대두

Simulation이 활발히 적용될 수 있는 산업 분야

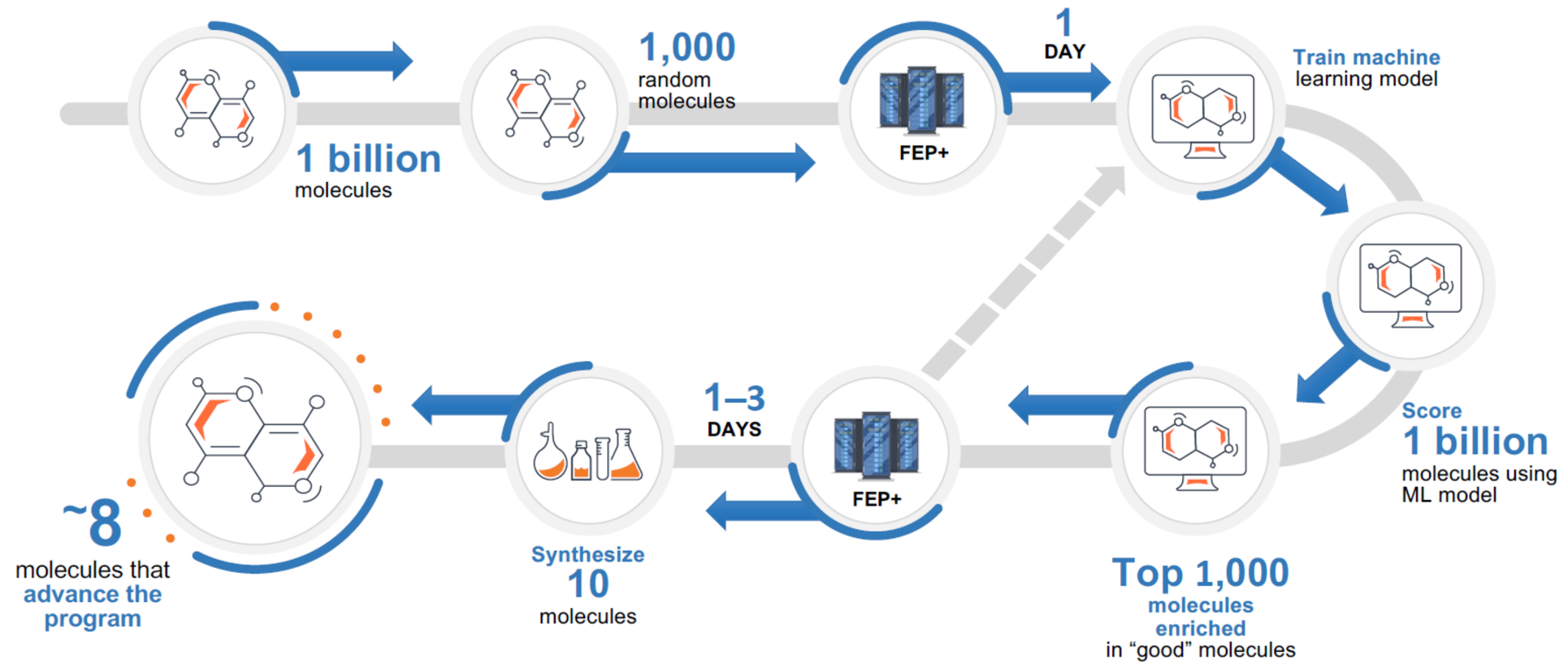






신규 물질 개발시 SIMULATION 역할

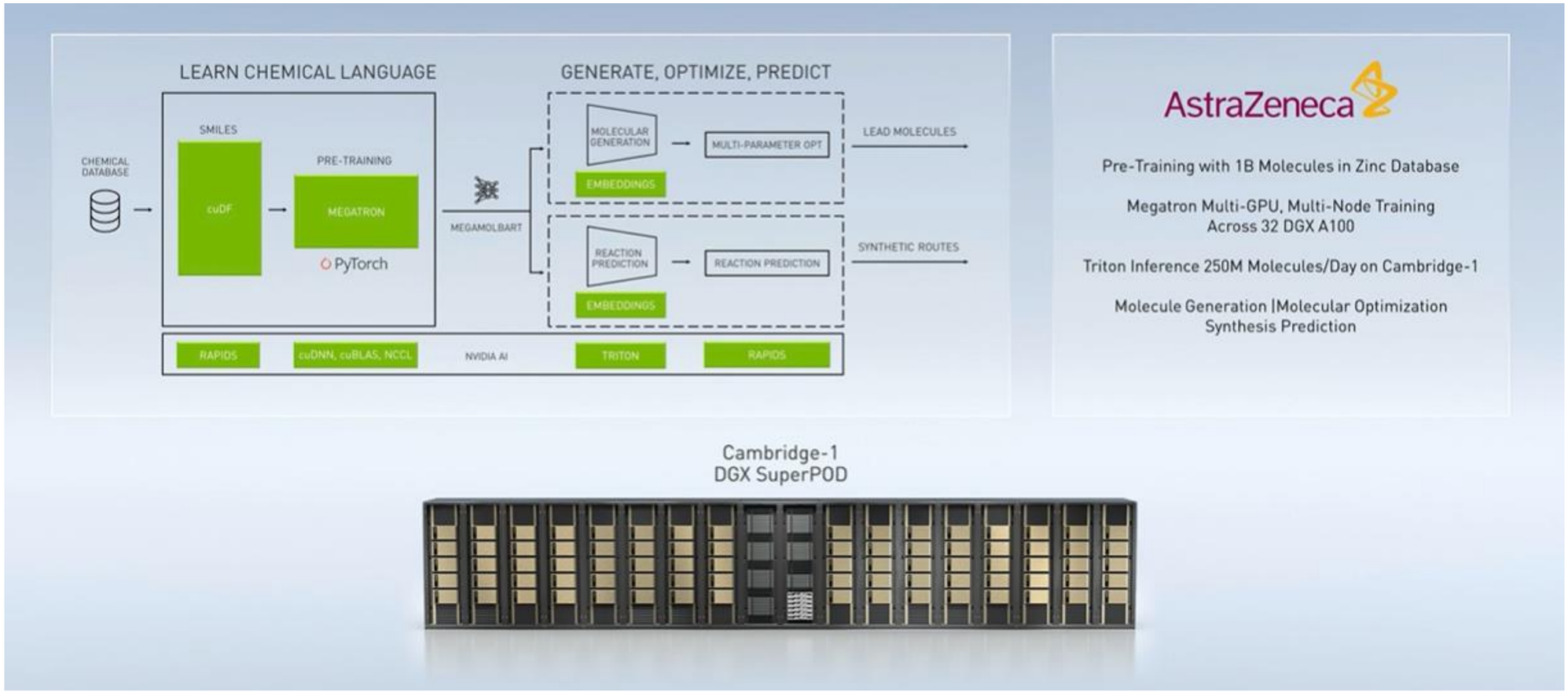
(1) 얼마나 적합한 후보 물질(HIT)을 찾느냐, (2) 찾은 후보 물질을 얼마나 빨리 시뮬레이션하느냐



Source: Accelerating Drug Discovery with Advanced Computational Modeling, Schrödinger, NVIDIA GTC (2021년 4월)

ASTRAZENECA 신약 개발에 활용된 NVIDIA DGX SUPERPOD

ZINC 데이터베이스에 저장된 10억 여 개 분자 구조 학습 → 타겟 화학 물질에 반응할 후보 hit 생성



Source: [Accelerating Drug Discovery with Clara Discovery's MegaMolBart](), NVIDIA, YouTube (2021년 4월)

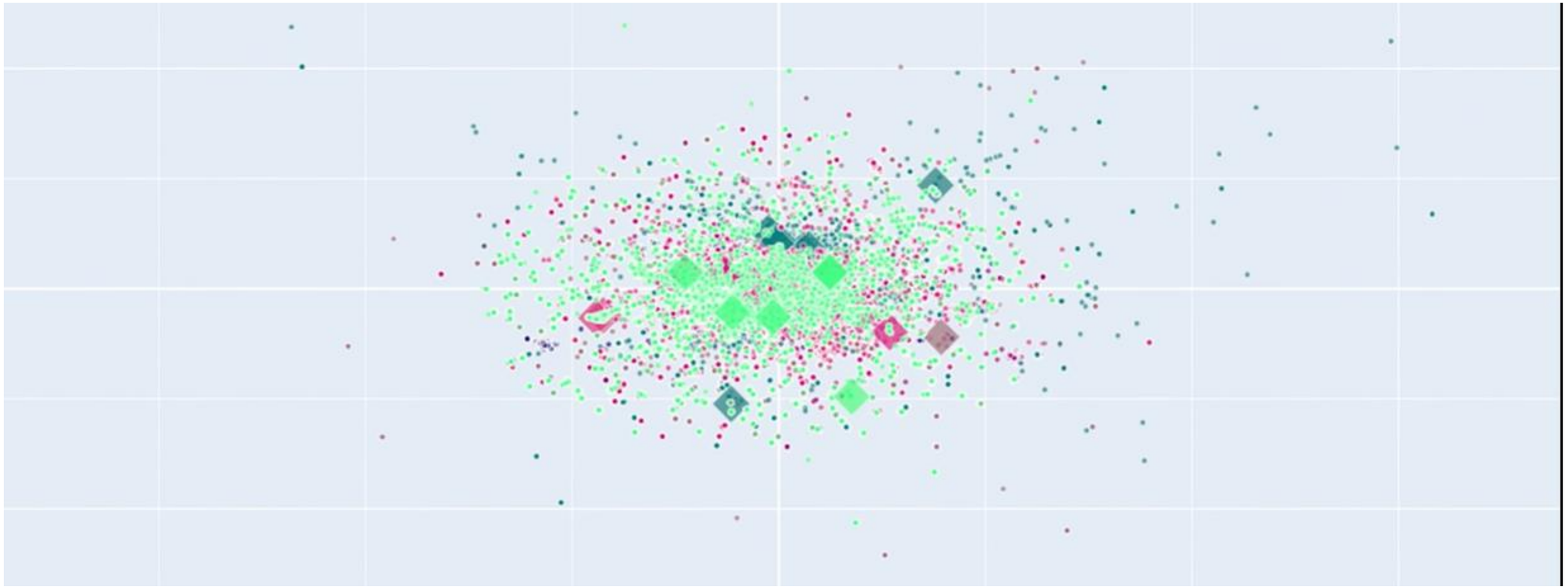
SARS-COV-2에 반응하는 화학 물질 찾기 (VIRTUAL SCREENING)

수 억 개의 분자를 이해하고 있는 AI가 1초에 약 4개 hit 생성 (CPU는 7초에 1개 hit 생성)

Source: Accelerating Drug Discovery with Clara Discovery's MegaMolBart, NVIDIA, YouTube (2021년 4월)

타겟 바이러스에 적합한 후보 물질 클러스터링

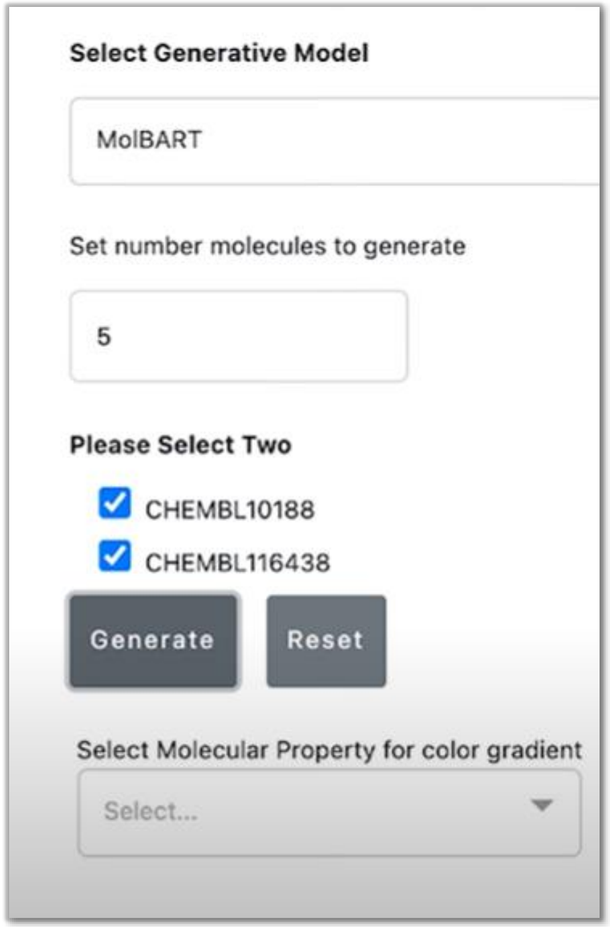
색깔은 클러스터 구분, 다이아몬드 모양은 클러스터 안에서 후보 hit 분자를 뜻함



Source: Accelerating Drug Discovery with Clara Discovery's MegaMolBart, NVIDIA, YouTube (2021년 4월)

이렇게 생성된 후보 HIT 분자 2개를 사용자가 지정하면

AI가 자동으로 그 범위 내 추가 후보 hit 분자 생성

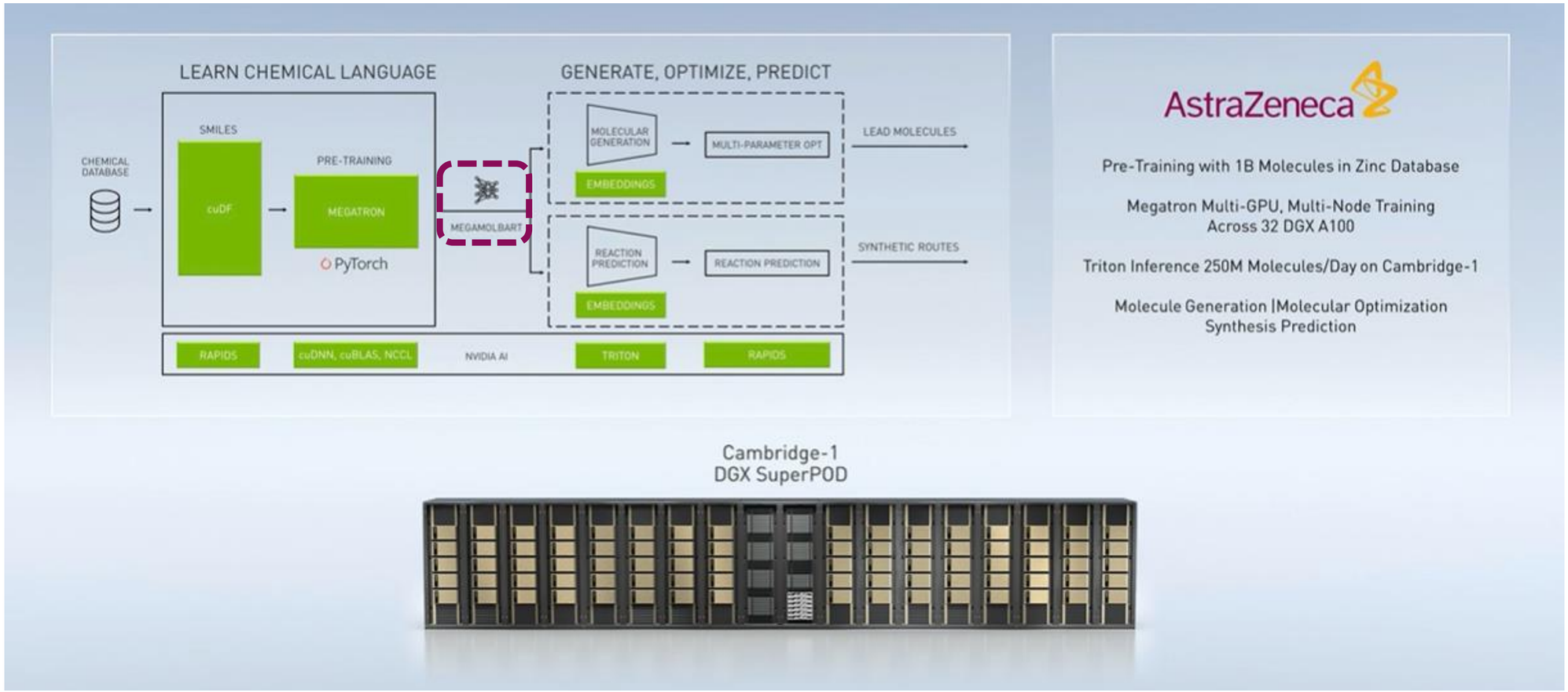


Source: [Accelerating Drug Discovery with Clara Discovery's MegaMolBart](), NVIDIA, YouTube (2021년 4월)

NVIDIA

ASTRAZENECA의 후보 HIT 생성에 사용된 기술들

MegaMolBART, transformer 기반 generative AI 모델 (NVIDIA와 AstraZeneca 협업)



Source: Accelerating Drug Discovery with Clara Discovery's MegaMolBart, NVIDIA, YouTube (2021년 4월)

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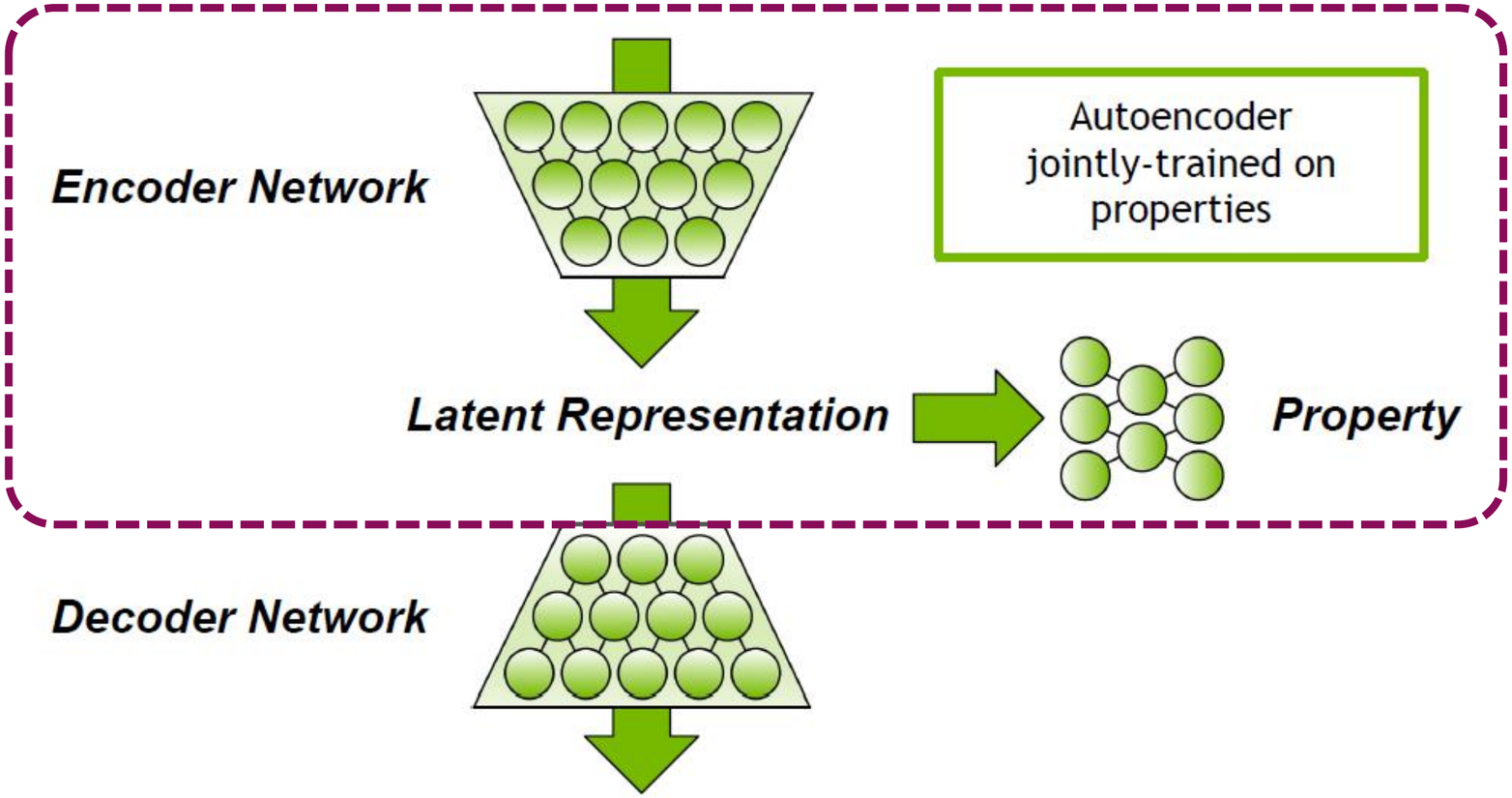

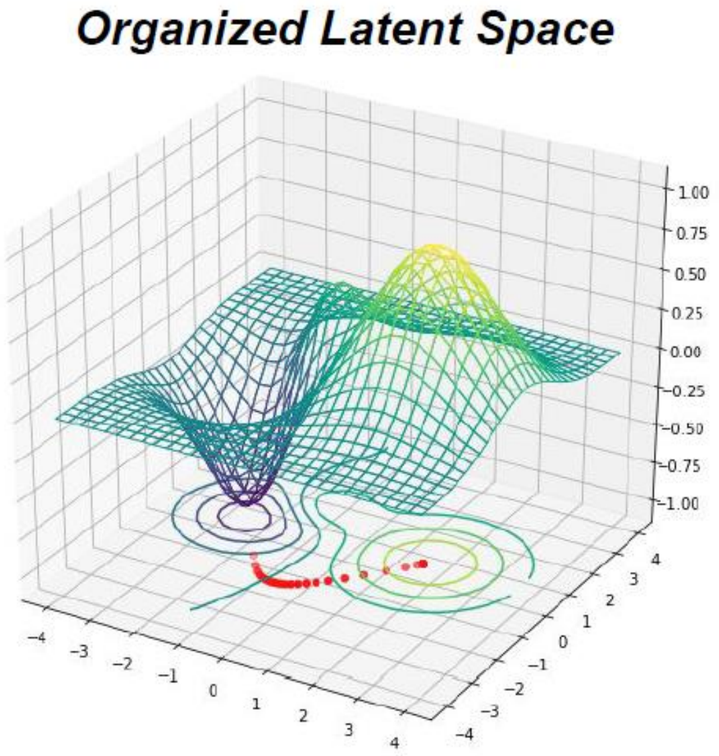

Source: Introducing Clara Discovery: Modular Platform for Computational Drug Discovery, NVIDIA, GTC (2021년 4월)

NVIDIA

ASTRAZENECA의 후보 HIT 생성에 사용된 기술들

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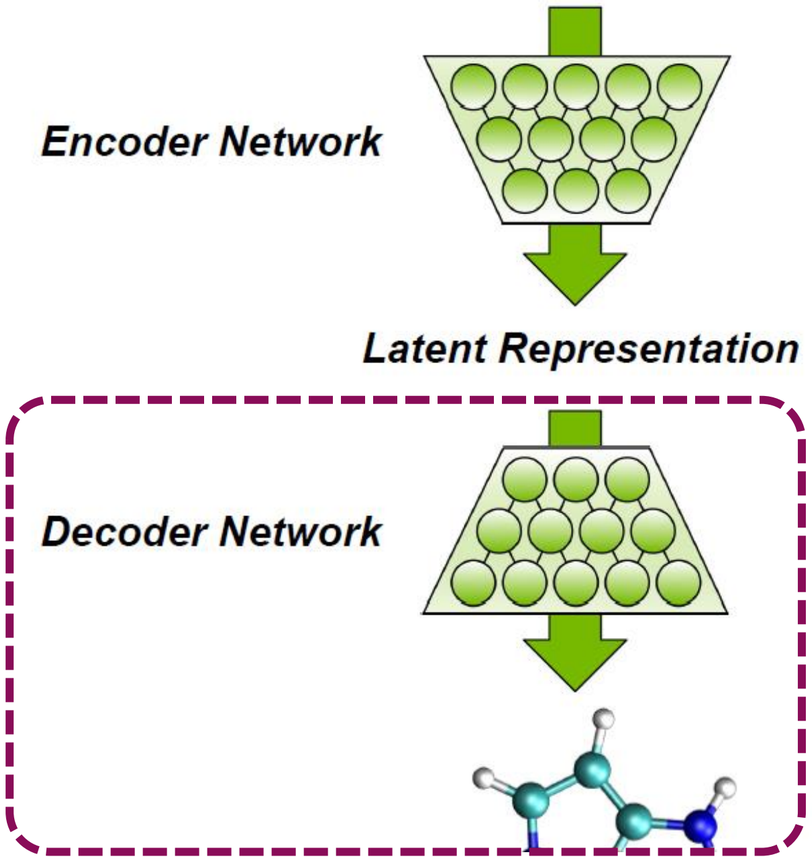
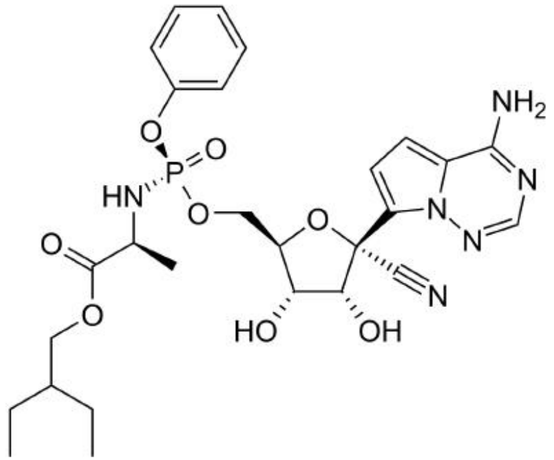


How Do We Make This?



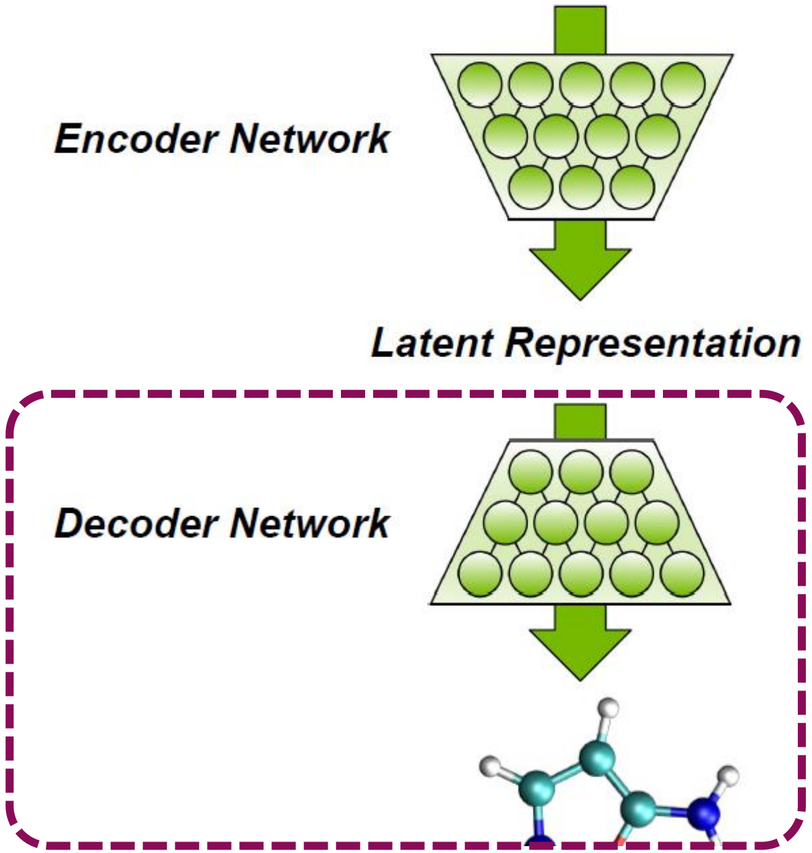
Esben Bjerrum, Ola Engkvist, Ross Irvin, Jiazhen He

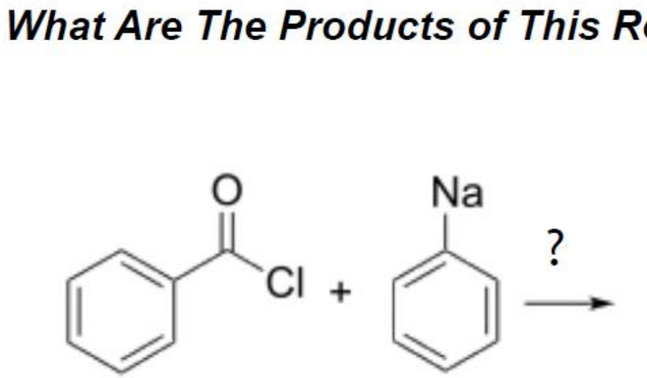
Source: Introducing Clara Discovery: Modular Platform for Computational Drug Discovery, NVIDIA, GTC (2021년 4월)

NVIDIA

ASTRAZENECA의 후보 HIT 생성에 사용된 기술들

MegaMolBART, transformer 기반 generative AI 모델 (NVIDIA와 AstraZeneca 협업)



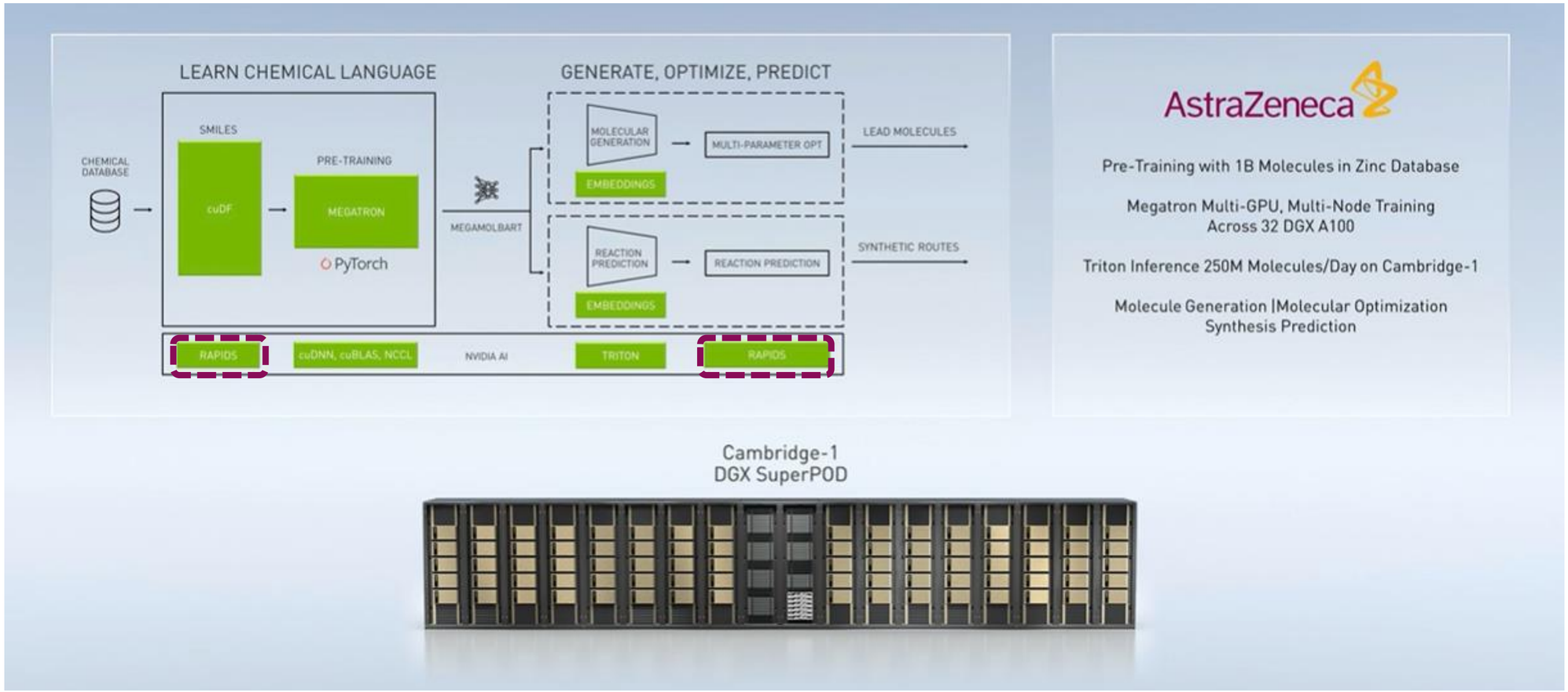


Esben Bjerrum, Ola Engkvist, Ross Irvin, Jiazhen He

Source: Introducing Clara Discovery: Modular Platform for Computational Drug Discovery, NVIDIA, GTC (2021년 4월)

ASTRAZENECA의 후보 HIT 생성에 사용된 기술들

RAPIDS 활용한 거대 데이터베이스 ELT 처리



Source: Accelerating Drug Discovery with Clara Discovery's MegaMolBart, NVIDIA, YouTube (2021년 4월)

ASTRAZENECA의 후보 HIT 생성에 사용된 기술들

RAPIDS 활용한 거대 데이터베이스 ELT 처리

Imports

Here we import cuDF and CuPy for GPU-accelerated dataframes and math operations, plus the CPU libraries Pandas and NumPy on which they are based and which we will use for performance comparisons:

In [1]:
```
import cudf
import cupy as cp
import pandas as pd
import numpy as np
```

ASTRAZENECA의 후보 HIT 생성에 사용된 기술들

RAPIDS 활용한 거대 데이터베이스 ELT 처리

- Reading 60 million records, entire population of England and Wales from official UK census data

from a local csv file directly into GPU memory:

In [2]:
```
%time gdf = cudf.read_csv('./data/pop_1-03.csv')
gdf.shape
```

```
CPU times: user 1.4 s, sys: 996 ms, total: 2.4 s
Wall time: 3.2 s
```

Here for comparison we read the same data into a Pandas dataframe:

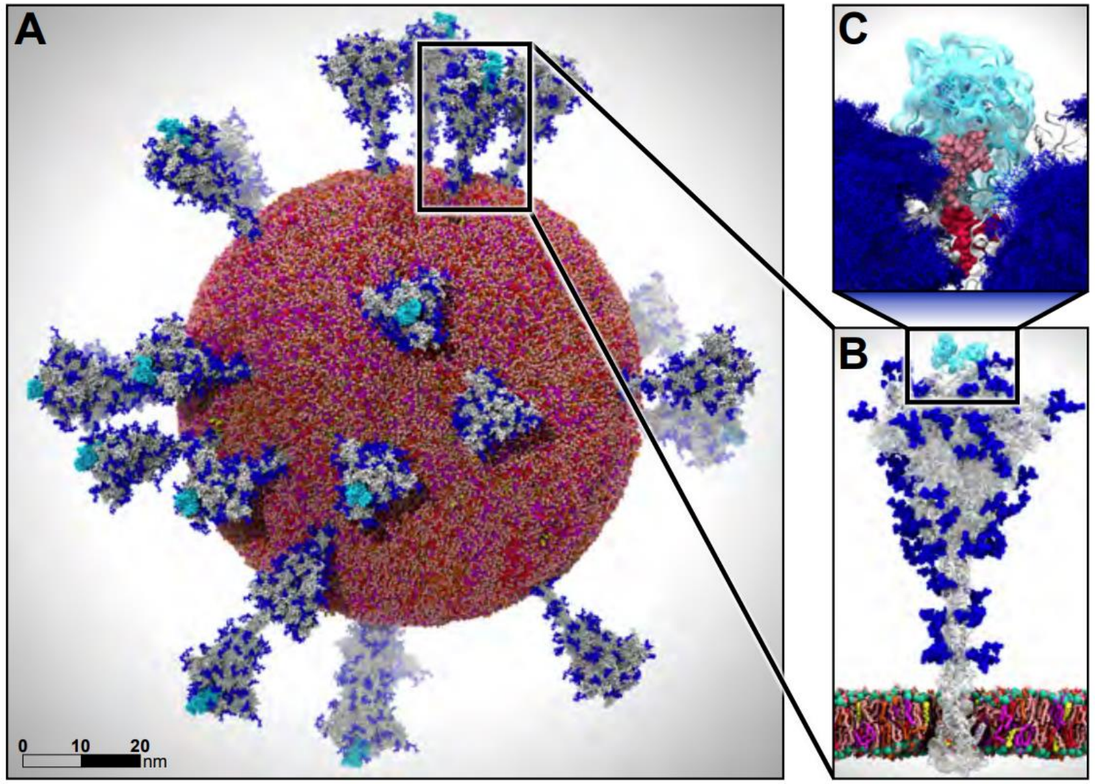
In [4]:
```
%time df = pd.read_csv('./data/pop_1-03.csv')
gdf.shape == df.shape
```

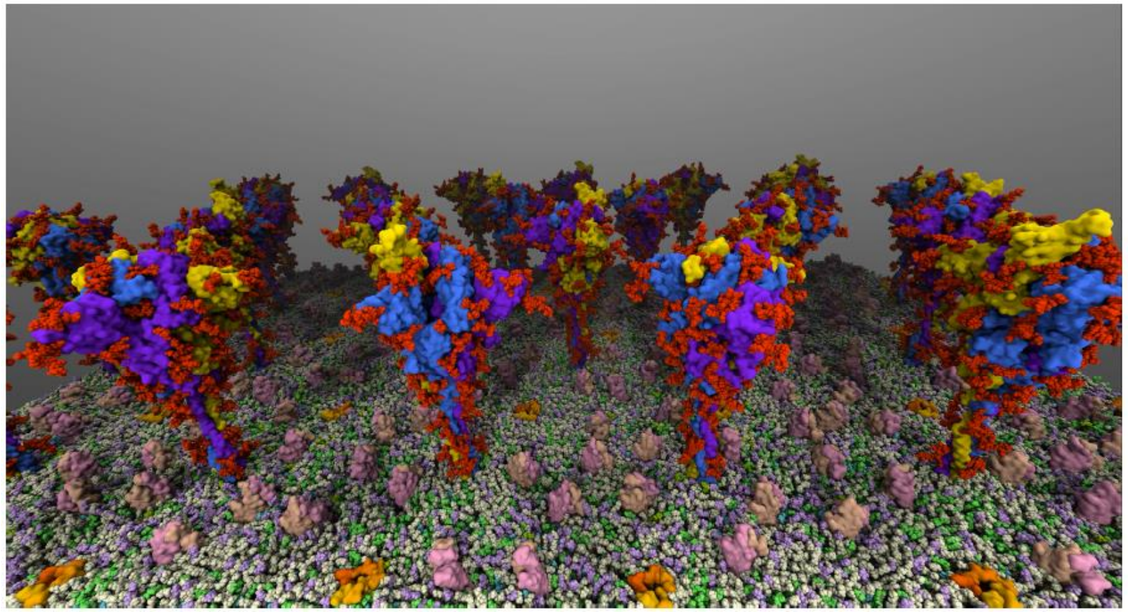
```
CPU times: user 32.1 s, sys: 4.55 s, total: 36.7 s
Wall time: 36.7 s
```

이제 후보 화학 물질을 얼마나 신속하게 SIMULATION하느냐

NAMD 소프트웨어 활용한 SARS-Cov-2 simulation (CUDA, NVIDIA GPU, NVIDIA DGX 시스템 활용)

- SC20 컨퍼런스에서 Gordon Bell Special Prize 차지





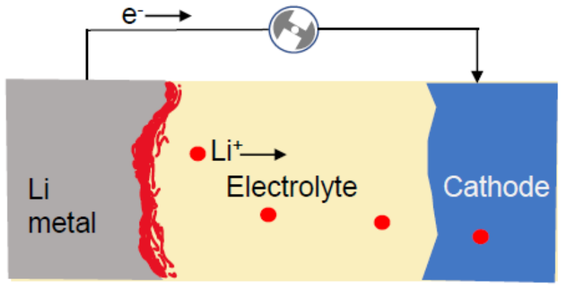
Source: Molecular Dynamics Simulations on GPU-Dense Architectures with NAMD, University of Illinois at Urbana-Champaign, GTC (2021년 4월)

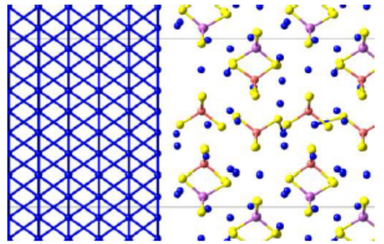
NVIDIA

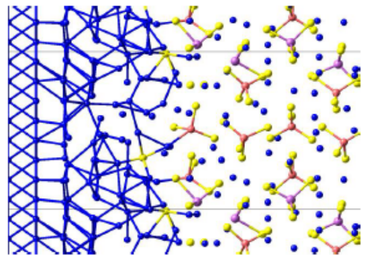
SIMULATION이 필요한 또 다른 예 - VASP (분자 역학 S/W)

리튬 이온 배터리에 사용할 가장 효율적인 전해질 물질 찾기

- The Challenge: increase the capacity of batteries while maintaining rigorous safety requirements
- Approach
  - Use Li metal rather than Li in graphite
  - Replace liquid electrolytes by solid state electrolytes
- The bottlenecks
  - Find solid state electrolytes with high ionic conductivity
  - Control the reaction of Li metal with the electrolyte
  - Find cathode materials with good mechanical match with solid state electrolytes
- The solution
  - Use large-scale accurate atomistic simulations to find optimal materials
  - Use quantum chemical calculations to understand and control the chemical reactions at interfaces







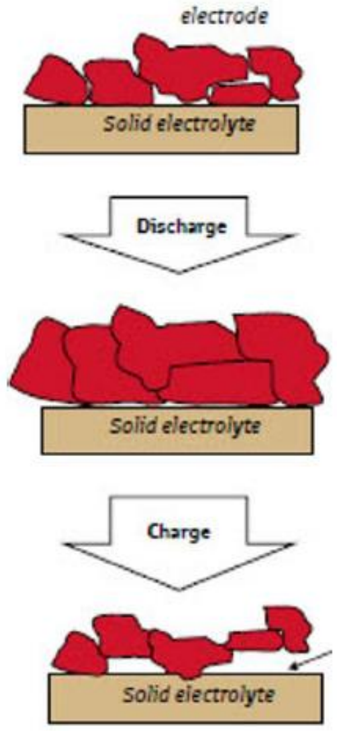
Ab initio molecular dynamics calculations are computationally highly demanding

Source: THE INNOVATIVE FORCE OFHIGH PERFORMANCE COMPUTING IN MATERIALS SCIENCE, NVIDIA, Webinar (2021년 7월)

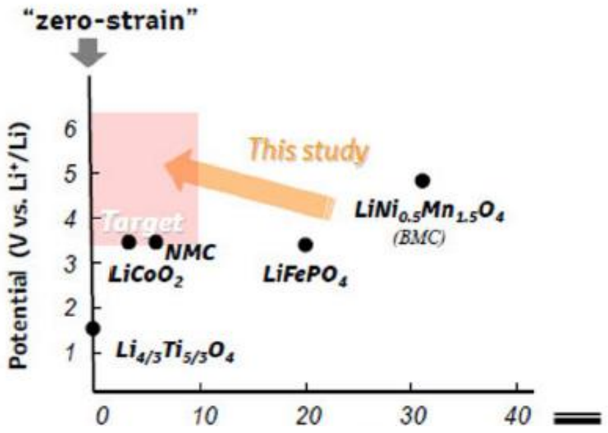
NVIDIA

VASP 활용한 고효율 리튬 이온 배터리 전해질 찾기

충전과 방전 반복시 변형이 최소로 발생하는 전해질 찾기



- Computational screening of candidates with *MedeA VASP*



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International Bureau

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4 December 2014 (04.12.2014)

WIPO | PCT

(10) International Publication Number
WO 2014/191018 A1

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C01G 45/12 (2006.01) *H01M 10/052* (2010.01)
H01M 4/505 (2010.01) *H01M 10/0562* (2010.01)

(21) International Application Number:
PCT/EP2013/060881

(22) International Filing Date:
27 May 2013 (27.05.2013)

(25) Filing Language: English

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(71) Applicant: **TOYOTA MOTOR EUROPE NV/SA** [BE/BE]; Avenue du Bourget 60, B-1140 Brussels (BE).

(72) Inventors: **ROSCIANO, Fabio**; Milcampslaan 127, B-1030 Schaarbeek (BE). **CHRISTENSEN, Mikael**; Branningevagen 1, S-120 54 Arsta (SE). **EYERT, Volker**; Baumschulenweg 6A, 14469 Potsdam (DE). **MAVRO-MARAS, Alexander**; Bergandsgatan 43, S-133 41 Saltsjobaden (SE). **WIMMER, Erich**; 3 avenue du Commerce, F-78000 Versailles (FR).

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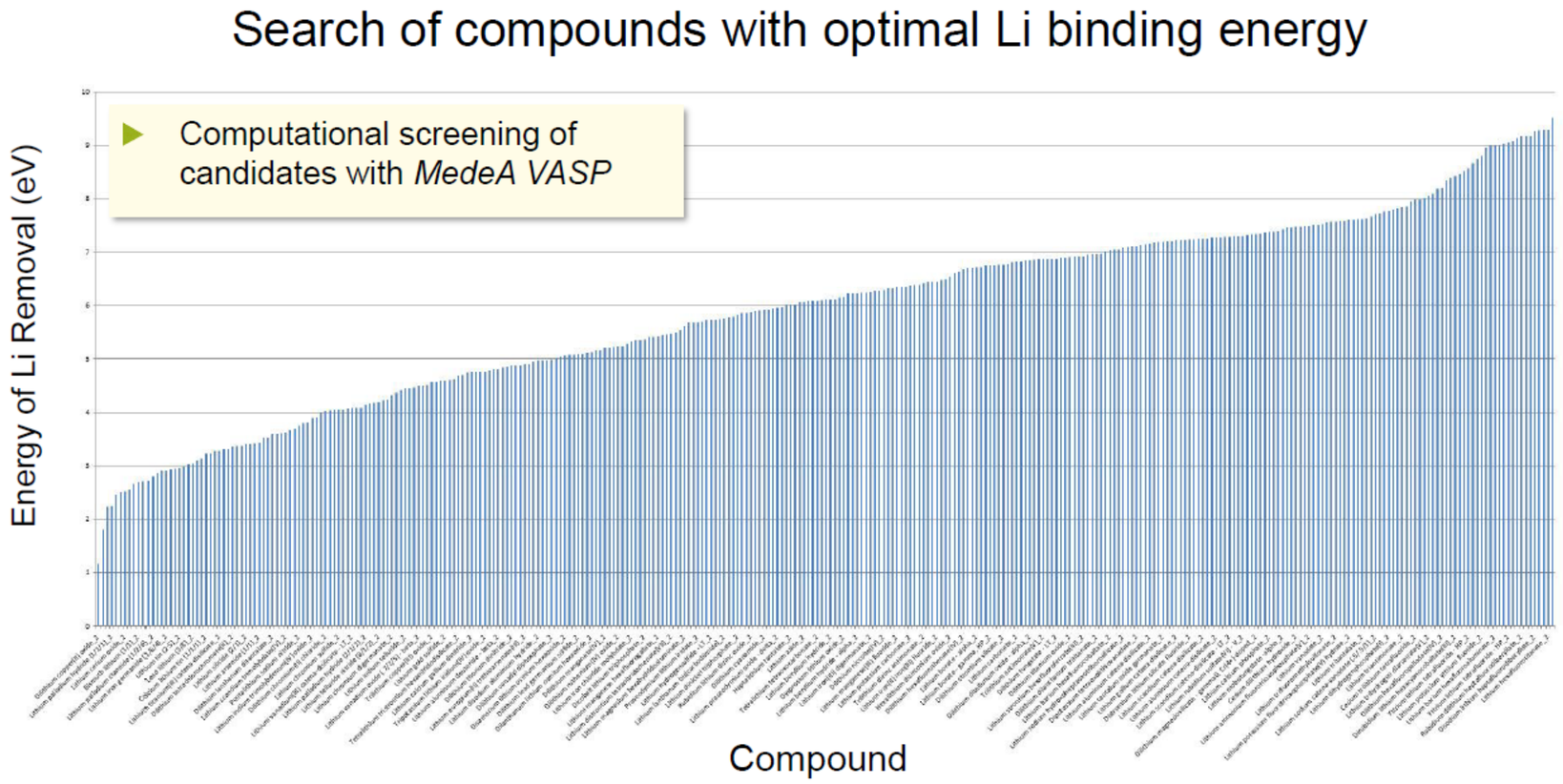
Published:

Source: THE INNOVATIVE FORCE OFHIGH PERFORMANCE COMPUTING IN MATERIALS SCIENCE, NVIDIA, Webinar (2021년 7월)

NVIDIA

VASP 활용한 고효율 리튬 이온 배터리 전해질 찾기

직접 실험을 한다면 현실적으로 불가능한 후보 물질 수, VASP 활용한 computational screening 활용



Source: THE INNOVATIVE FORCE OFHIGH PERFORMANCE COMPUTING IN MATERIALS SCIENCE, NVIDIA, Webinar (2021년 7월)

VASP 활용한 핵발전 SIMULATION

Zr(지르코늄)과 H_2O와의 반응 simulation (반복되는 핵융합에도 원료가 최대한 오래 지속되록)

- The Challenge: increase the life-time of materials in the reactor while maintaining their safe operation
- Approach
  - Use materials modeling to identify the key degradation mechanisms under irradiation
  - Develop a predictive computational approach
  - Predict the performance of improved and new materials prior to experimental testing which is expensive and time consuming
- The bottleneck
  - Highly accurate multi-scale models
  - 3D simulations require large-scale simulations
- The solution
  - HPC enables simulations of high complexity and accuracy with predictive power, thus accelerating the development and certification of advanced materials.

Source: THE INNOVATIVE FORCE OFHIGH PERFORMANCE COMPUTING IN MATERIALS SCIENCE, NVIDIA, Webinar (2021년 7월)

VASP 활용한 핵발전 SIMULATION

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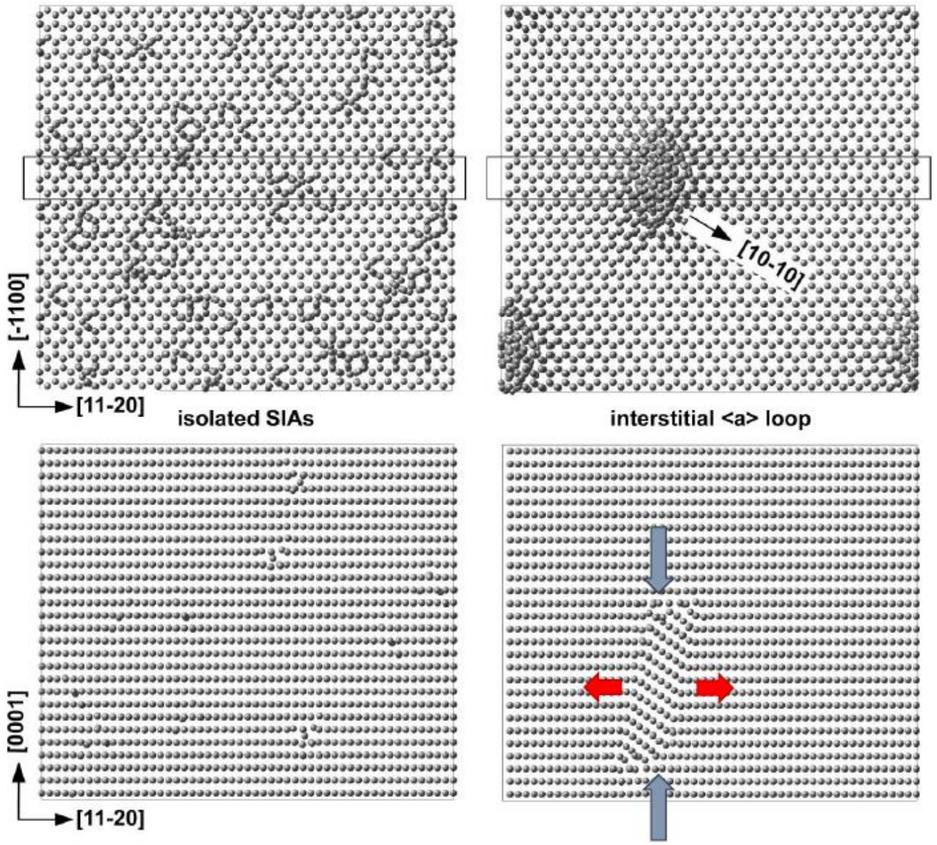
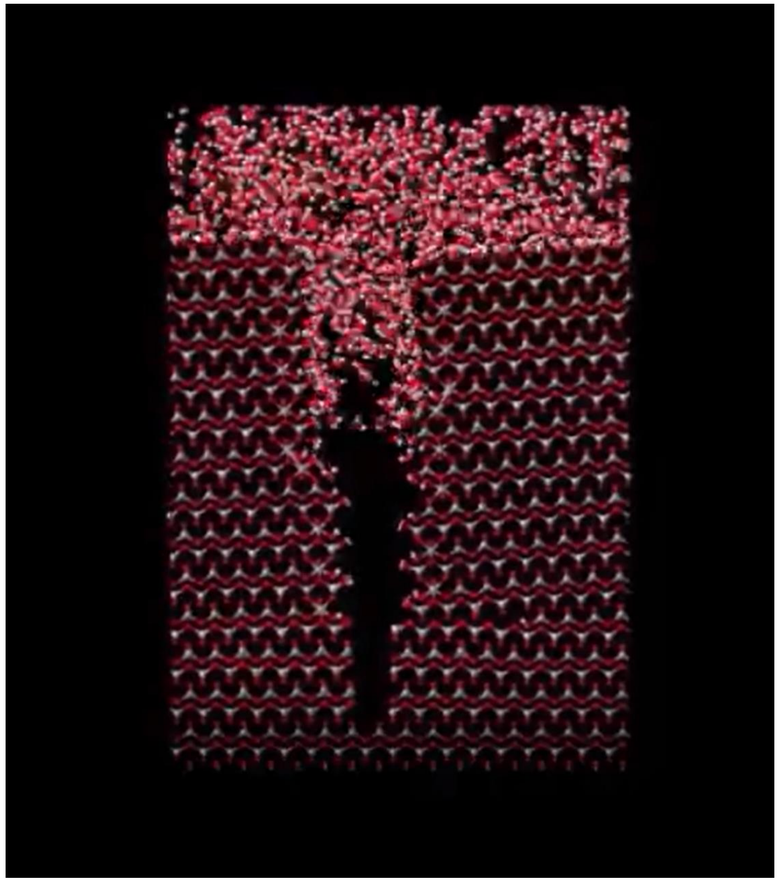
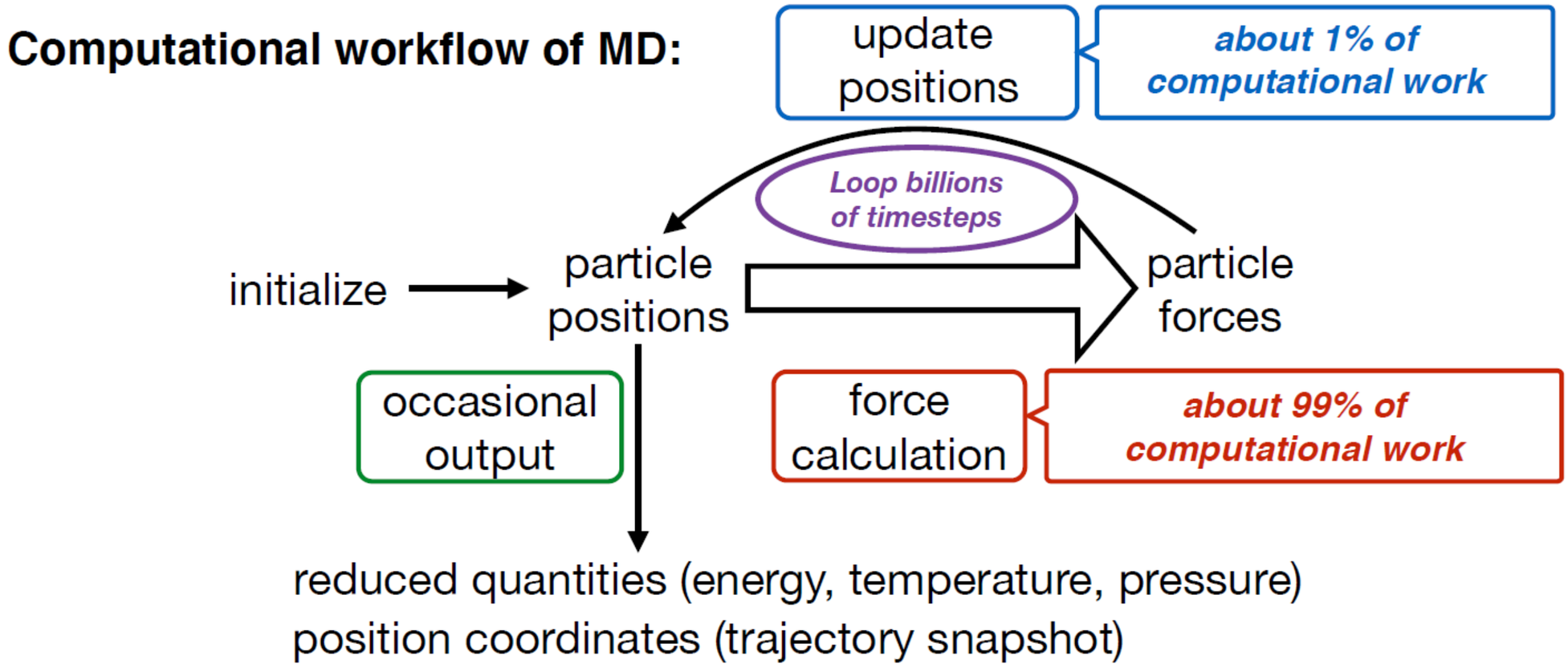




Source: *THE INNOVATIVE FORCE OFHIGH PERFORMANCE COMPUTING IN MATERIALS SCIENCE, NVIDIA, Webinar (2021년 7월)*

SIMULATION에서 요구되는 COMPUTATIONAL WORK

원자간 force calculation



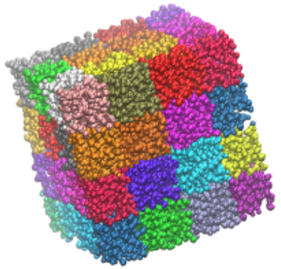
Source: Molecular Dynamics Simulations on GPU-Dense Architectures with NAMD, University of Illinois at Urbana-Champaign, GTC (2021년 4월)

분자 역학 SIMULATION에서 분산(병렬) 컴퓨팅의 중요성

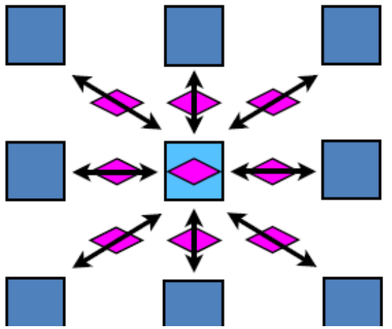
(준비) Patch라 불리는 공간에 원자들 배치 → (Simulation) 원자간 힘 적용 → 변화된 원자들 위치 적용

- Atoms are decomposed into fixed volume *patches* within the system
- Forces that move atoms are calculated in parallel at each step between adjacent patches
- Migrate atoms to adjacent patches, updating domain decomposition after every *cycle* (e.g. 20 steps)
- Performance is measured in **ns/day** — number of nanoseconds of simulated time achieved per day of running. (More is better!)

Spatial decomposition of atoms into patches



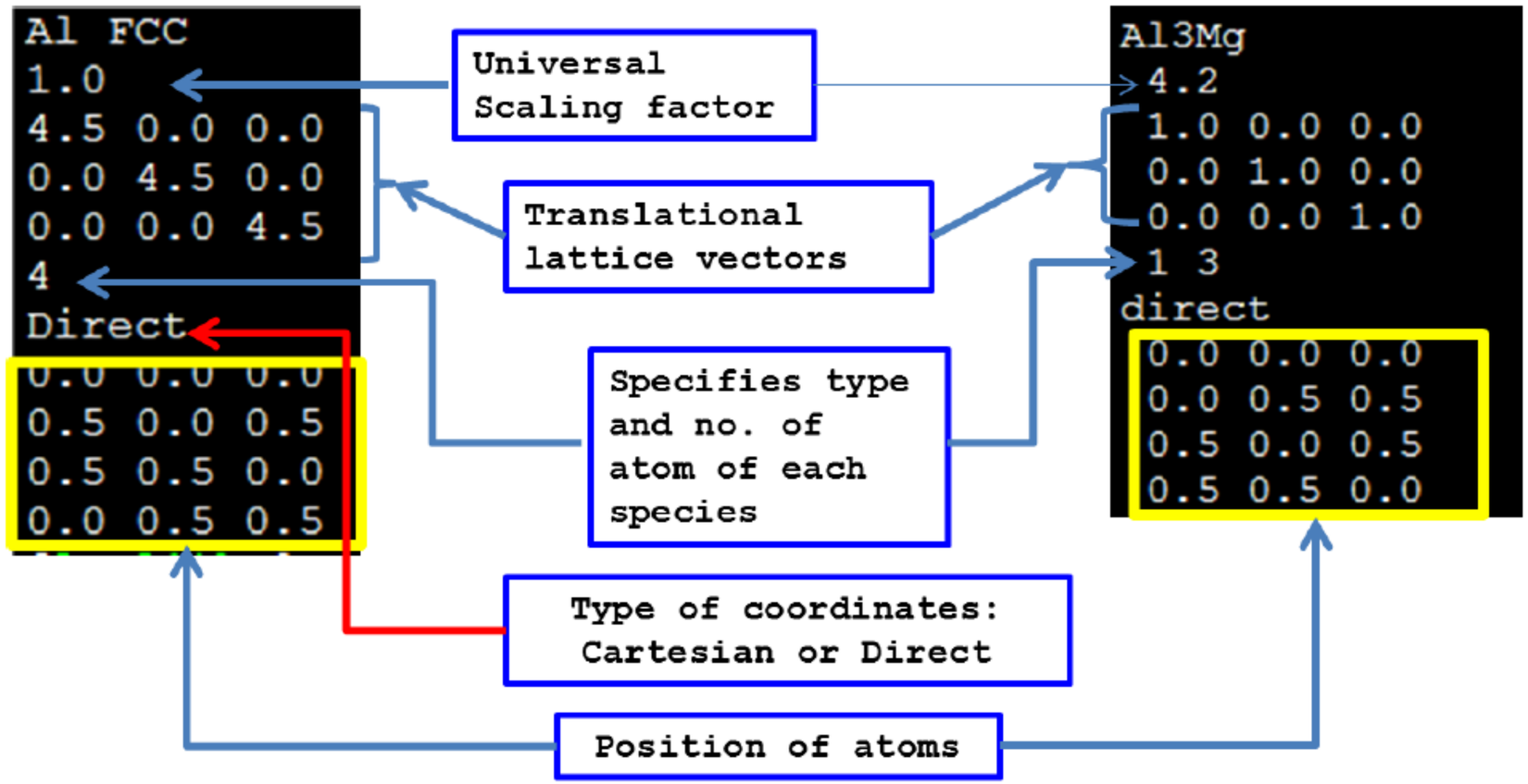
Work decomposition of patch interactions



Source: Molecular Dynamics Simulations on GPU-Dense Architectures with NAMD, University of Illinois at Urbana-Champaign, GTC (2021년 4월)

VASP SIMULATION에 필요한 INPUT FILES

중 *POSCAR* 파일에 명시되는 원자들 위치 (원자 개수 예. 200개, 2000개, LAMMPS 경우 80M도)

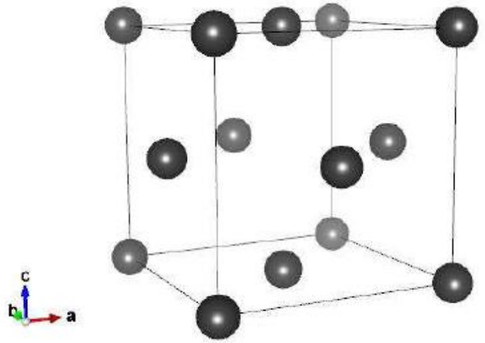


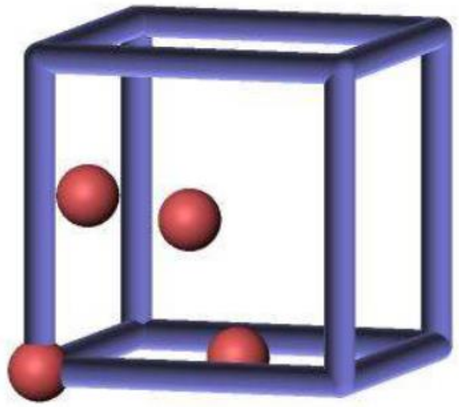
Source: Running a DFT calculation in VASP, Laalitha Liyanage, ICME (2012년)

VASP SIMULATION에 필요한 INPUT FILES

중 *POSCAR* 파일에 명시되는 원자들 위치 (원자 개수 예. 200개, 2000개, LAMMPS 경우 80M도)

- 4 atoms, fcc structure
  - Translational lattice vectors
    - a1 = (4.0; 0.0; 0.0)
    - a2 = (0.0; 4.0; 0.0)
    - a3 = (0.0; 0.0; 4.0)
  - Basis vectors
    - 0.0; 0.0; 0.0
    - 0.5; 0.0; 0.5
    - 0.5; 0.5; 0.0
    - 0.0; 0.5; 0.5

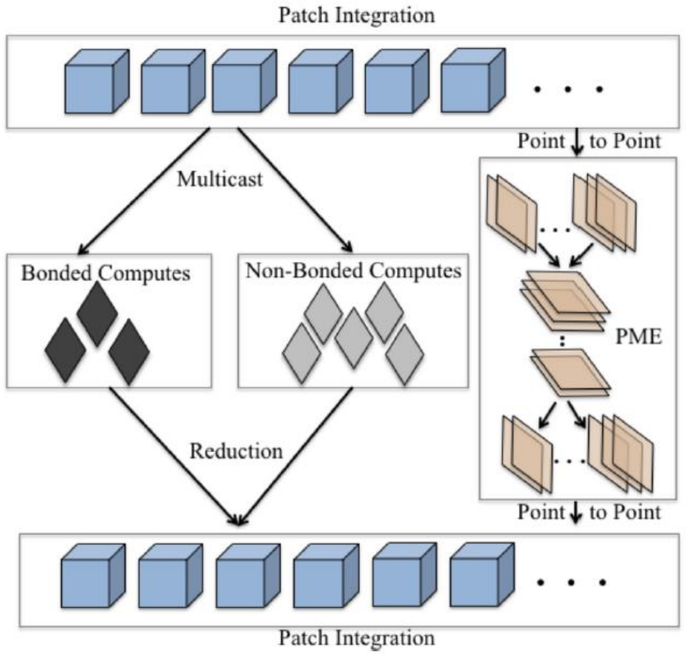


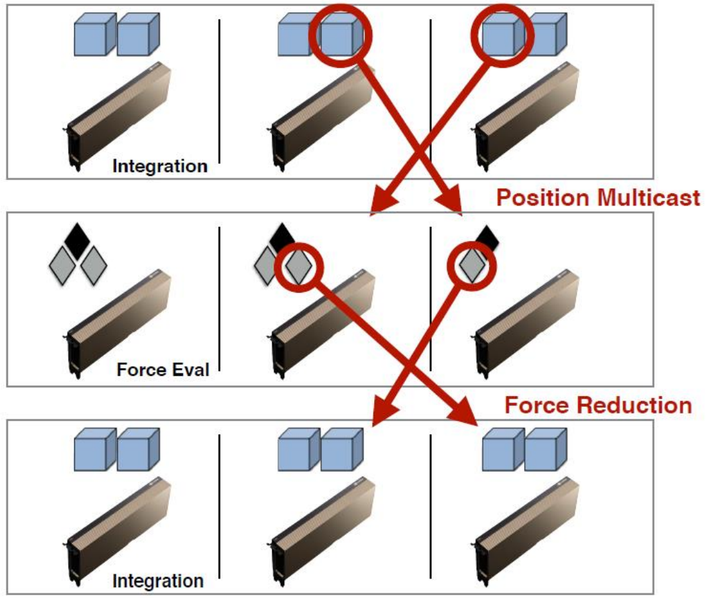


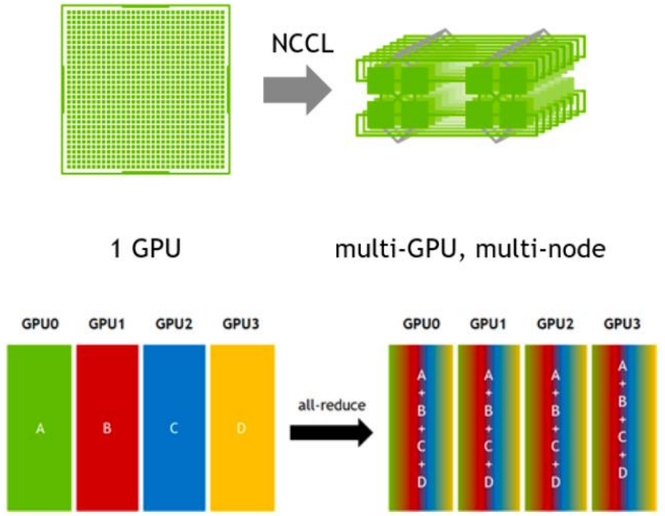
Source: Running a DFT calculation in VASP, Laalitha Liyanage, ICME (2012년)

분자 역학 SIMULATION에서 MULTI GPU 및 GPU간 통신 중요성

수많은 patch를 GPU당 하나씩 할당, iteration 끝날 때마다 변경된 원자 위치 모든 GPU에 업데이트







Source: [Molecular Dynamics Simulations on GPU-Dense Architectures with NAMD](), University of Illinois at Urbana-Champaign, GTC (2021년 4월)

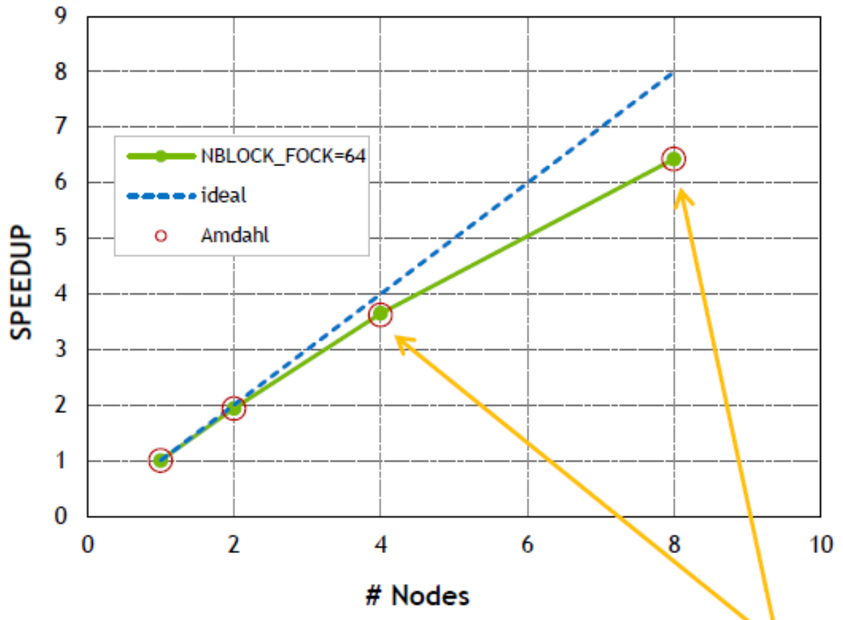
VASP COMPUTATION ENVIRONMENT

특별히 GPU간 통신 기술 주목

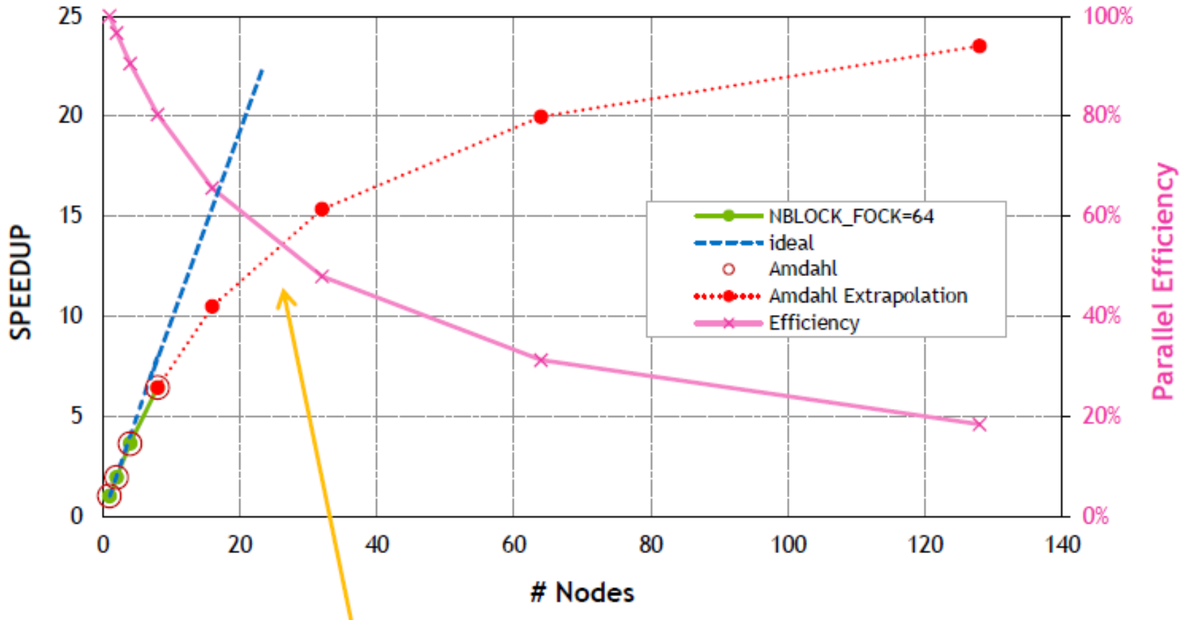
- H/W : NVIDIA Selene
- S/W
  - VASP 6.2.0 & 6.2.1
  - NVIDIA HPC SDK
  - CUDA 11.0: FFT libs – cuFFT, cuBLAS, cuSolver 11.0
  - Communication - openMPI 4.0.6rc1 using UCX 1.10.x branch; NCCL 2.9.9

VASP SIMULATION에서 MULTI GPU 노드의 위력

NVIDIA DGX SuperPOD



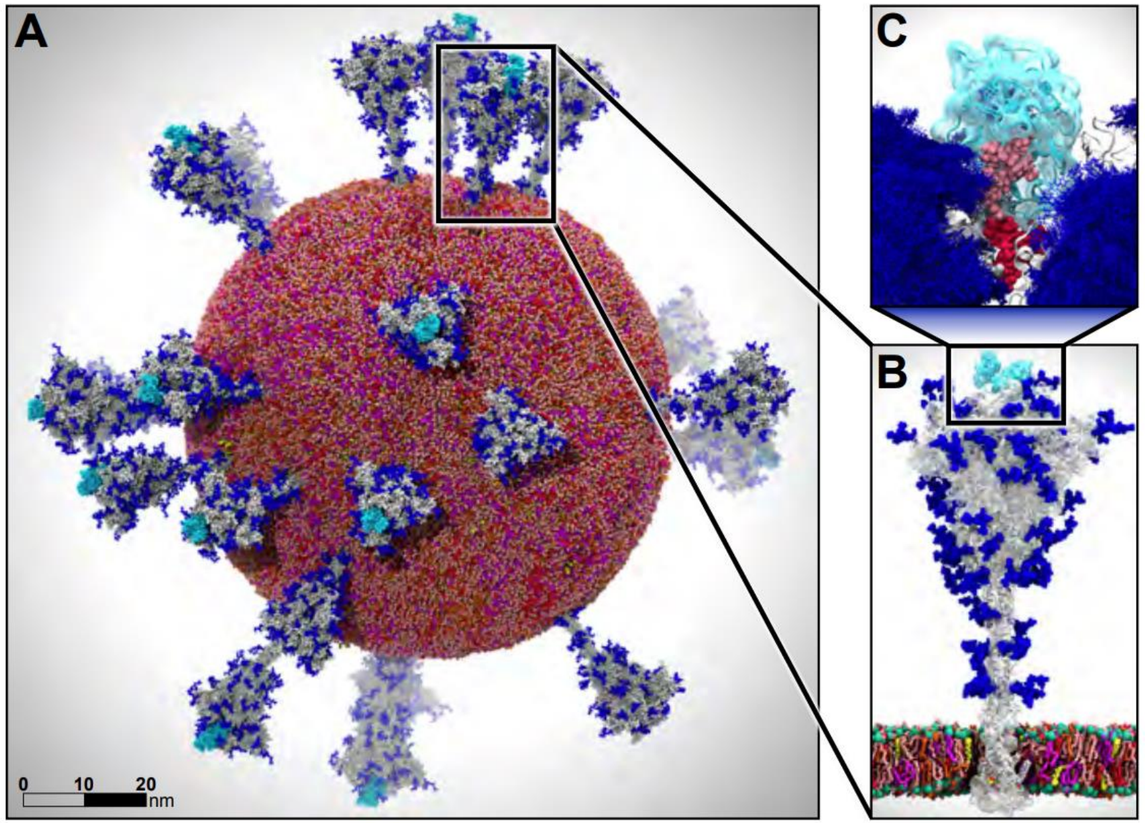
With an Amdahl's law numerical fit the approximation is quite good

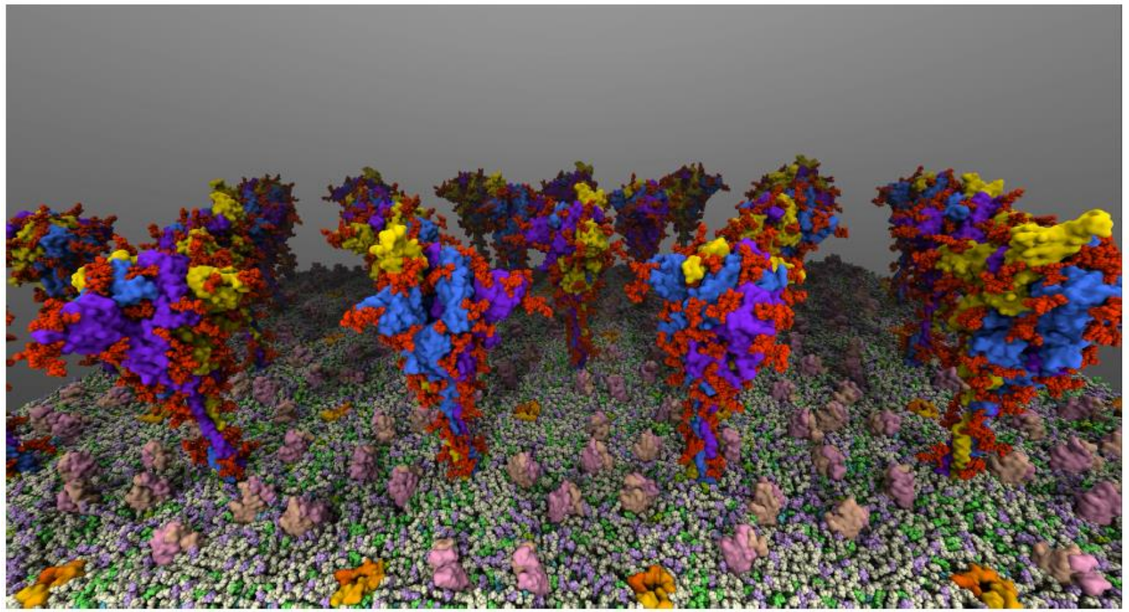


50% Scaling efficiency occurs at 30 nodes in this example

SIMULATION에서 이뤄지는 추가 움직임

NAMD 소프트웨어, GPU-Offload 에서 GPU-Resident 아키텍처로



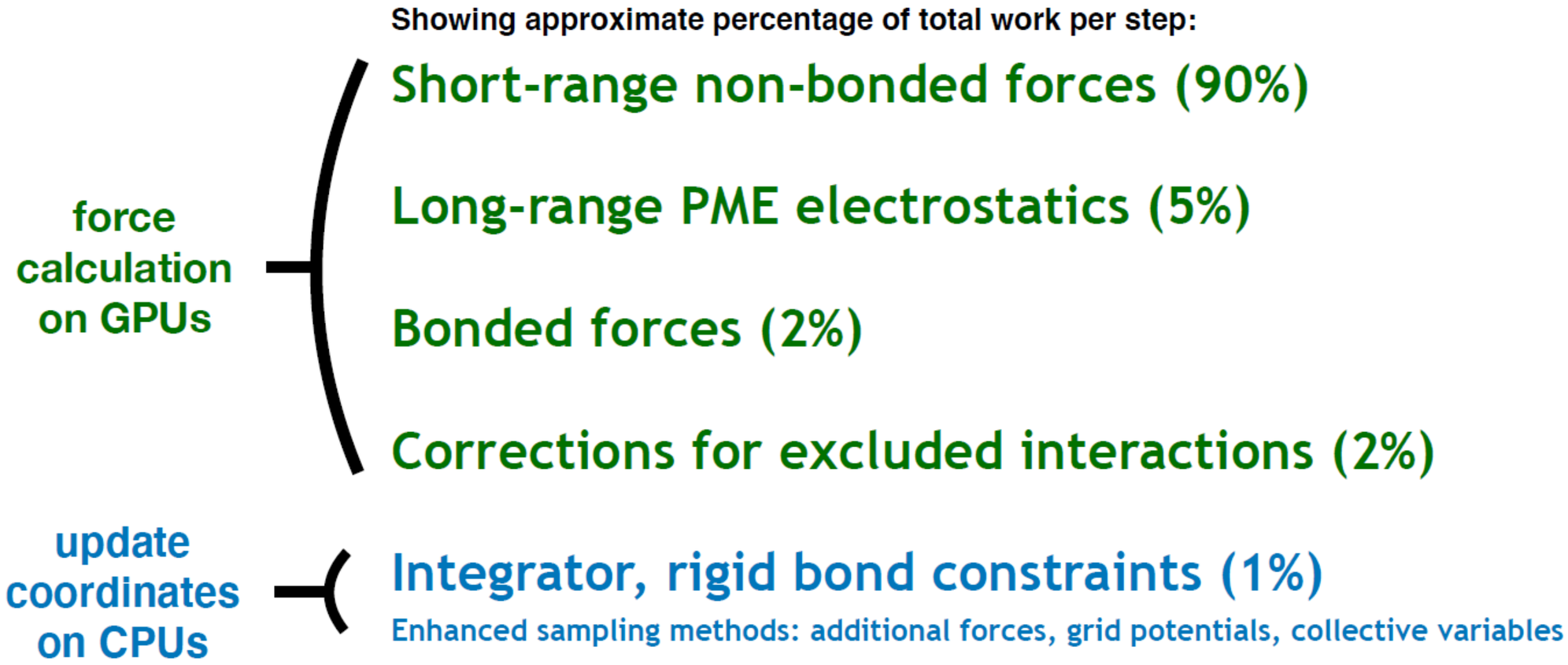


Source: Molecular Dynamics Simulations on GPU-Dense Architectures with NAMD, University of Illinois at Urbana-Champaign, GTC (2021년 4월)

NVIDIA.

기존 GPU-OFFLOAD 아키텍처

GPU는 force calculation, CPU는 원자 위치 업데이트

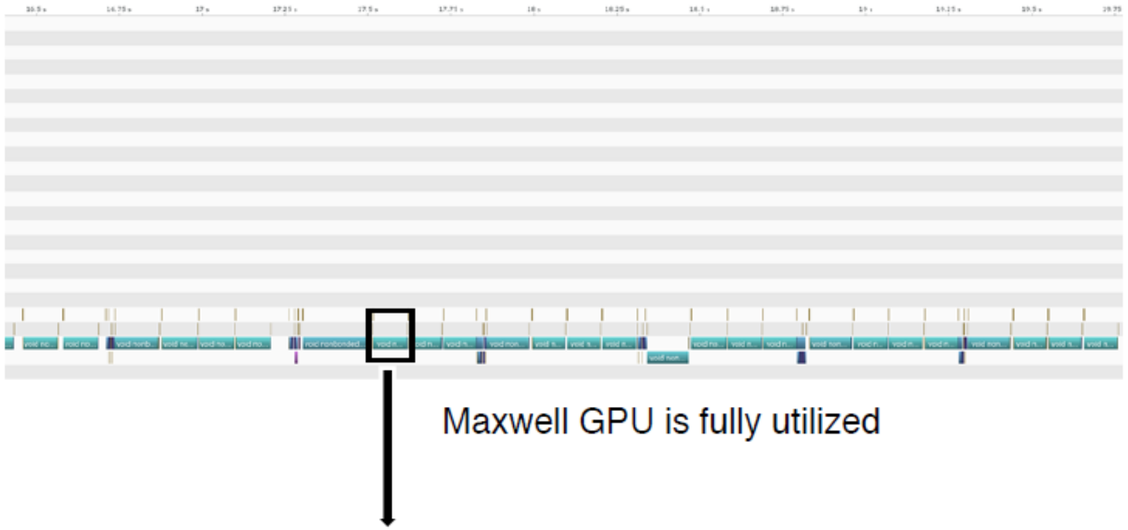


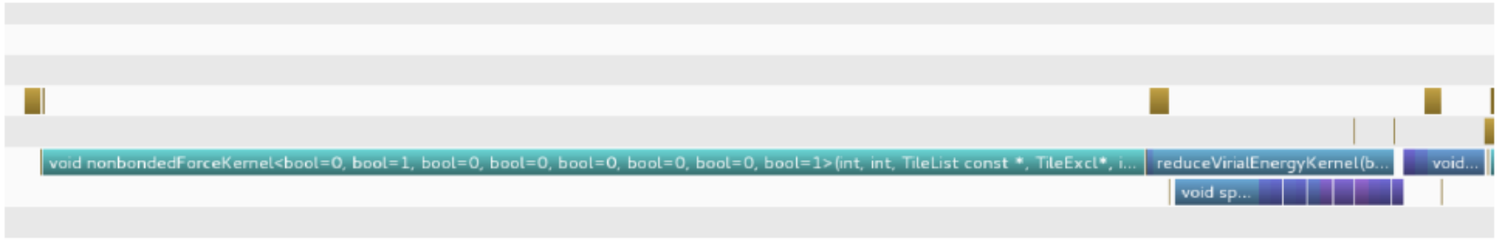
Source: Molecular Dynamics Simulations on GPU-Dense Architectures with NAMD, University of Illinois at Urbana-Champaign, GTC (2021년 4월)

기존 GPU-OFFLOAD 아키텍처

NVIDIA Pascal GPU까지는 force calculation도 어느 정도 시간 소요되어 CPU 연산과 overlap 됨

- GPUs weren't **that** fast back then
- Profiling shows GPUs are fully occupied by forces - no idle time
- Streaming forces allows overlap of CPU and GPU computation





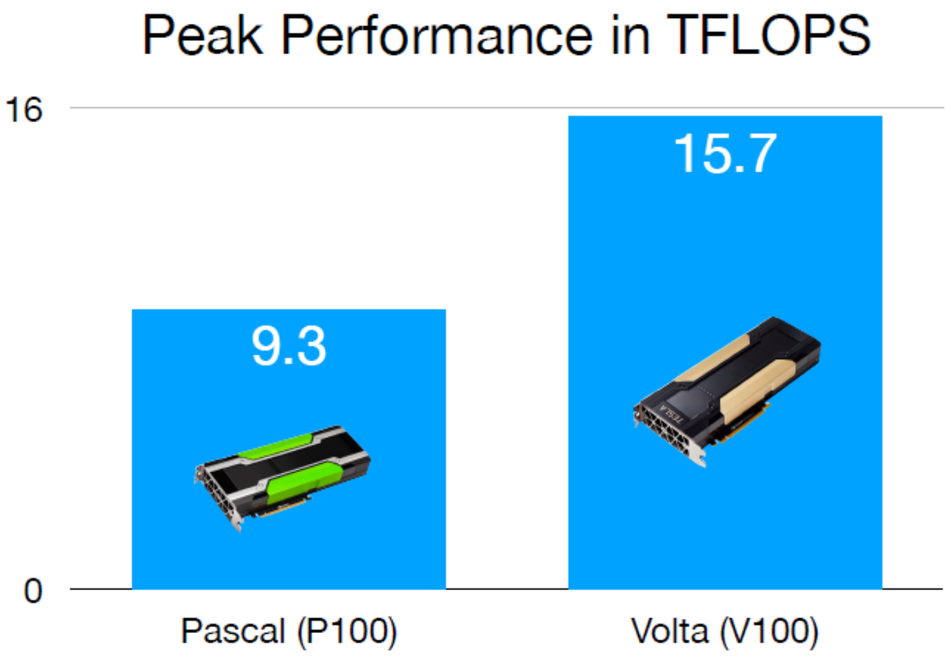
Source: Molecular Dynamics Simulations on GPU-Dense Architectures with NAMD, University of Illinois at Urbana-Champaign, GTC (2021년 4월)

NVIDIA

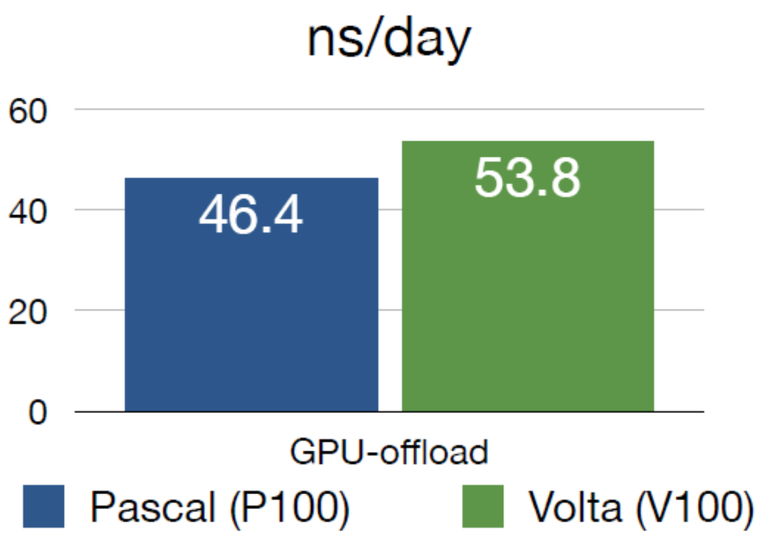
기존 GPU-OFFLOAD 아키텍처

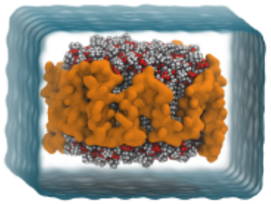
신규 GPU 성능 월등히 향상되었지만 NAMD 성능은 그만큼 향상되지 않았음. 왜?

Hardware has ~70% perf improvement!



NAMD (in 2018) less than 20% perf improvement!





ApoA1
92k atoms

Simulation details:
NVE, CHARMM force field, cutoff distance 12Å,
MTS with 2fs time step and 4fs PME, rigid bond constraints.
https://www.ks.uiuc.edu/Research/namd/benchmarks/

Source: Molecular Dynamics Simulations on GPU-Dense Architectures with NAMD, University of Illinois at Urbana-Champaign, GTC (2021년 4월)

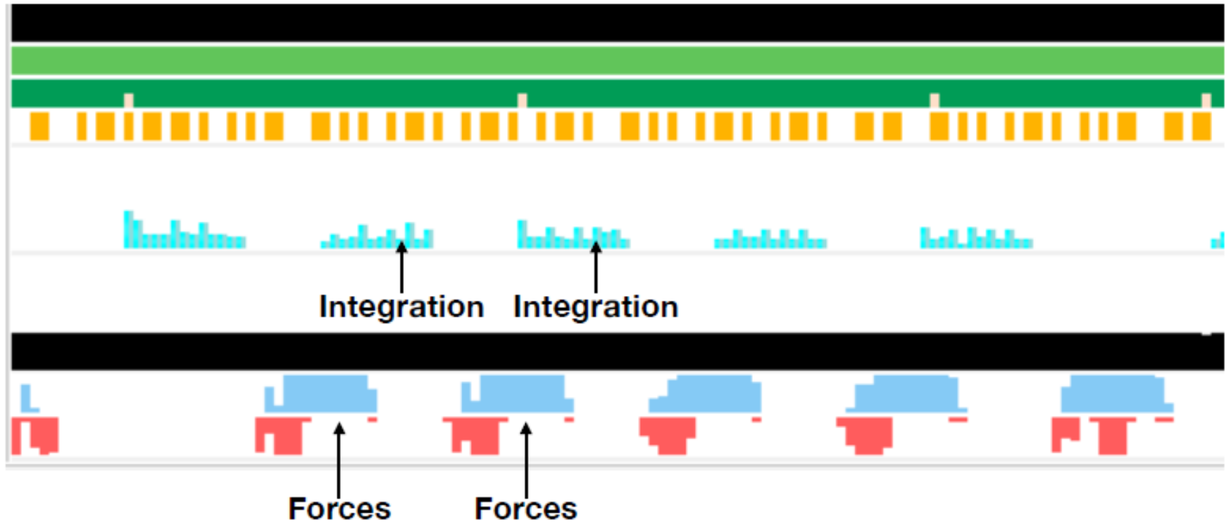
NVIDIA

기존 GPU-OFFLOAD 아키텍처

성능 대폭 향상된 GPU, 이제 force calculation 워낙 빨리 끝나 CPU 연산 마칠 때까지 idle time 발생

- GPUs became **much** faster!
- Attempt to overlap CPU and GPU causes performance bottleneck
- Unable to fully utilize GPU

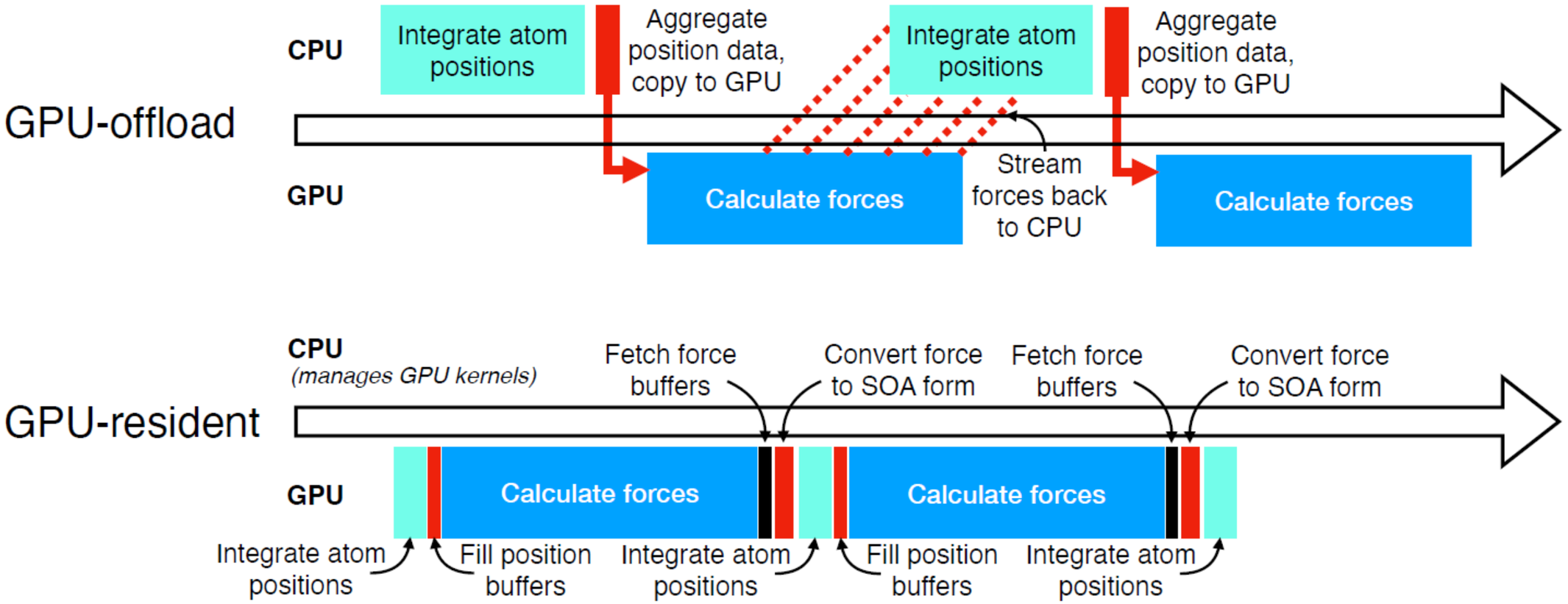
Profile using **Nsight Systems** with NVTX tags to trace execution of CPU kernels:



Source: Molecular Dynamics Simulations on GPU-Dense Architectures with NAMD, University of Illinois at Urbana-Champaign, GTC (2021년 4월)

신규 *GPU-RESIDENT* 아키텍처

기존 CPU가 하던 원자 위치 업데이트 연산도 이제 GPU로! (모든 연산을 GPU에서, “GPU-Resident”)

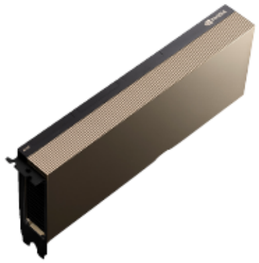


Source: Molecular Dynamics Simulations on GPU-Dense Architectures with NAMD, University of Illinois at Urbana-Champaign, GTC (2021년 4월)

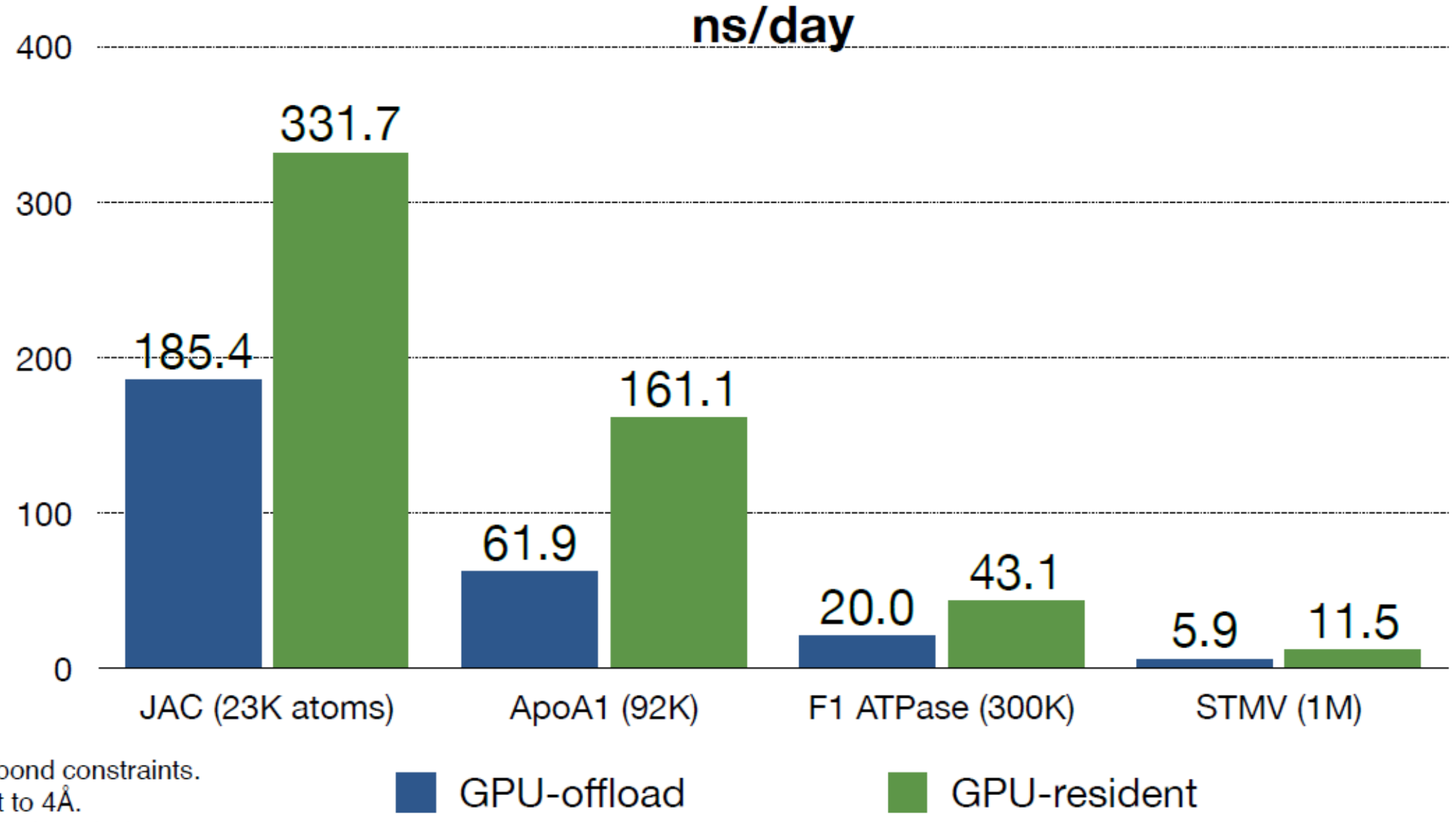
신규 *GPU-RESIDENT* 아키텍처에서 성능 향상

GPU-Offload 아키텍처 대비

Intel Xeon Gold 6134 @ 3.2 GHz



NVIDIA A100-PCIe



Simulation details:
CHARMM force field, cutoff distance 12Å,
MTS with 2fs time step and 4fs PME, rigid bond constraints.
Performance tuning parameter "margin" set to 4Å.
https://www.ks.uiuc.edu/Research/namd/benchmarks/

Source: Molecular Dynamics Simulations on GPU-Dense Architectures with NAMD, University of Illinois at Urbana-Champaign, GTC (2021년 4월)

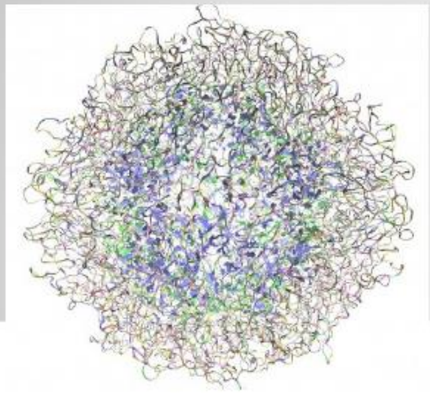
이런 기술들을 통해 얻어낸 SIMULATION 성과

AMOEBA 벤치마크 결과 내역 (Sorbonne Université & Institut Universitaire de France)

2016: TINKER (8 CORES-OPENMP/HASSWELL)
0.0007 NS/DAY

2018: CINES (Brodwell)
10000 cores: 0.25 ns/day

2019: IRENE JOLIOT-CURIE (SKYLAKE-AVX
10000 CORES MPI : 0.9 NS/DAY



2020: SELENE (NVIDIA DGX A100)
1 NODE, 8 GPUS: 4.51 NS/DAY

2016-2021: X 6000 ACCELERATION

Source: Accelerating Next-Generation Molecular Dynamics Simulations Using the Multi-GPU Tinker-HP Infras, Sorbonne Université, GTC (2021년 4월)

S/W 측면 특장점

GPU 어플리케이션 개발 방법 3가지

OpenACC DIRECTIVES EXAMPLE

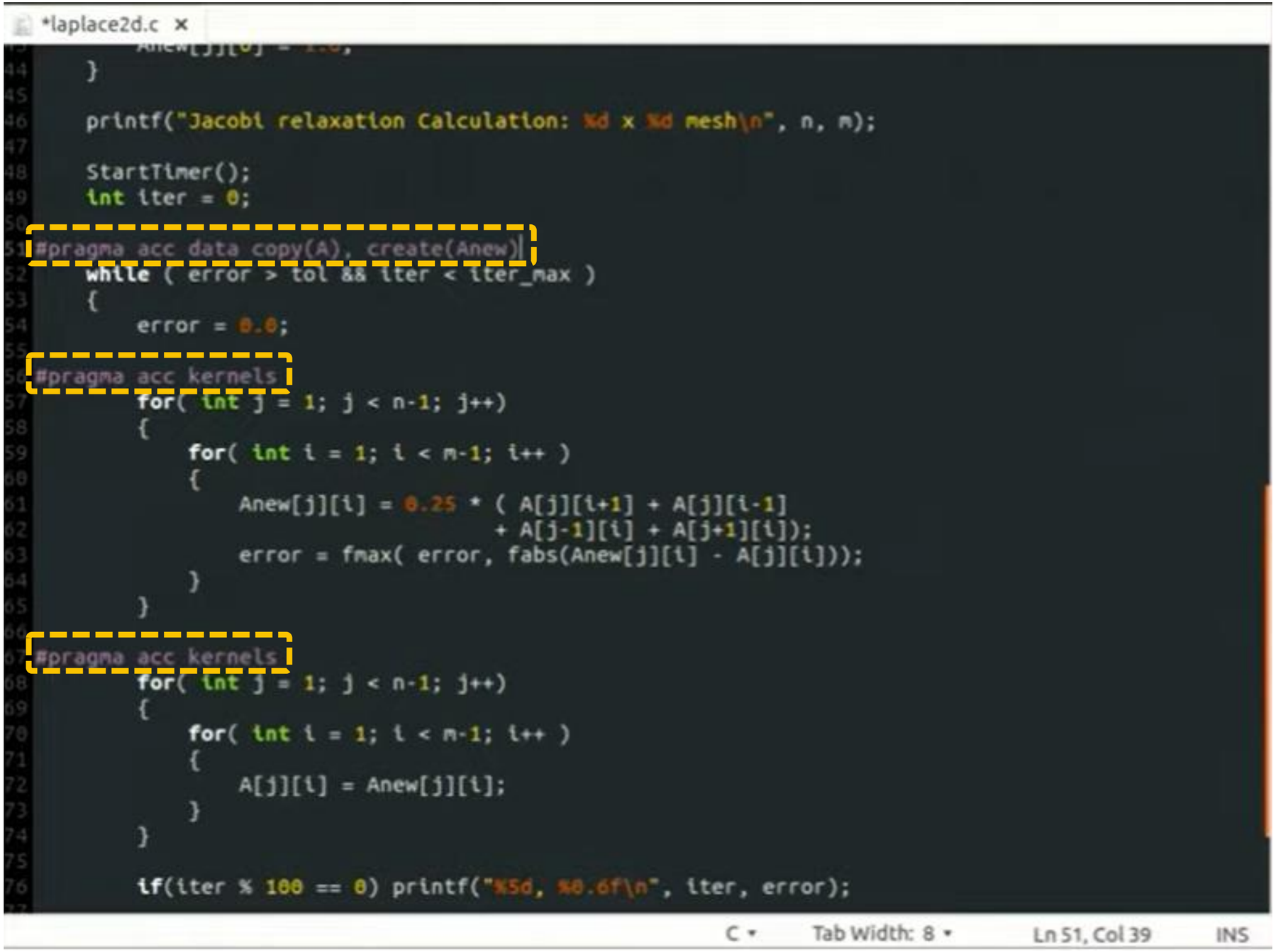
```
!$acc data copy(A,Anew)
 iter=0
 do while ( err > tol .and. iter < iter_max )

  iter = iter +1
  err=0._fp_kind

!$acc kernels
   do j=1,m
    do i=1,n
     Anew(i,j) = .25_fp_kind *( A(i+1,j  ) + A(i-1,j  ) &
                               +A(i  ,j-1) + A(i  ,j+1))
     err = max( err, Anew(i,j)-A(i,j))
    end do
   end do
!$acc end kernels
   IF(mod(iter,100)==0 .or. iter == 1)    print *, iter, err
   A= Anew

 end do
!$acc end data
```

Copy arrays into GPU memory within data region

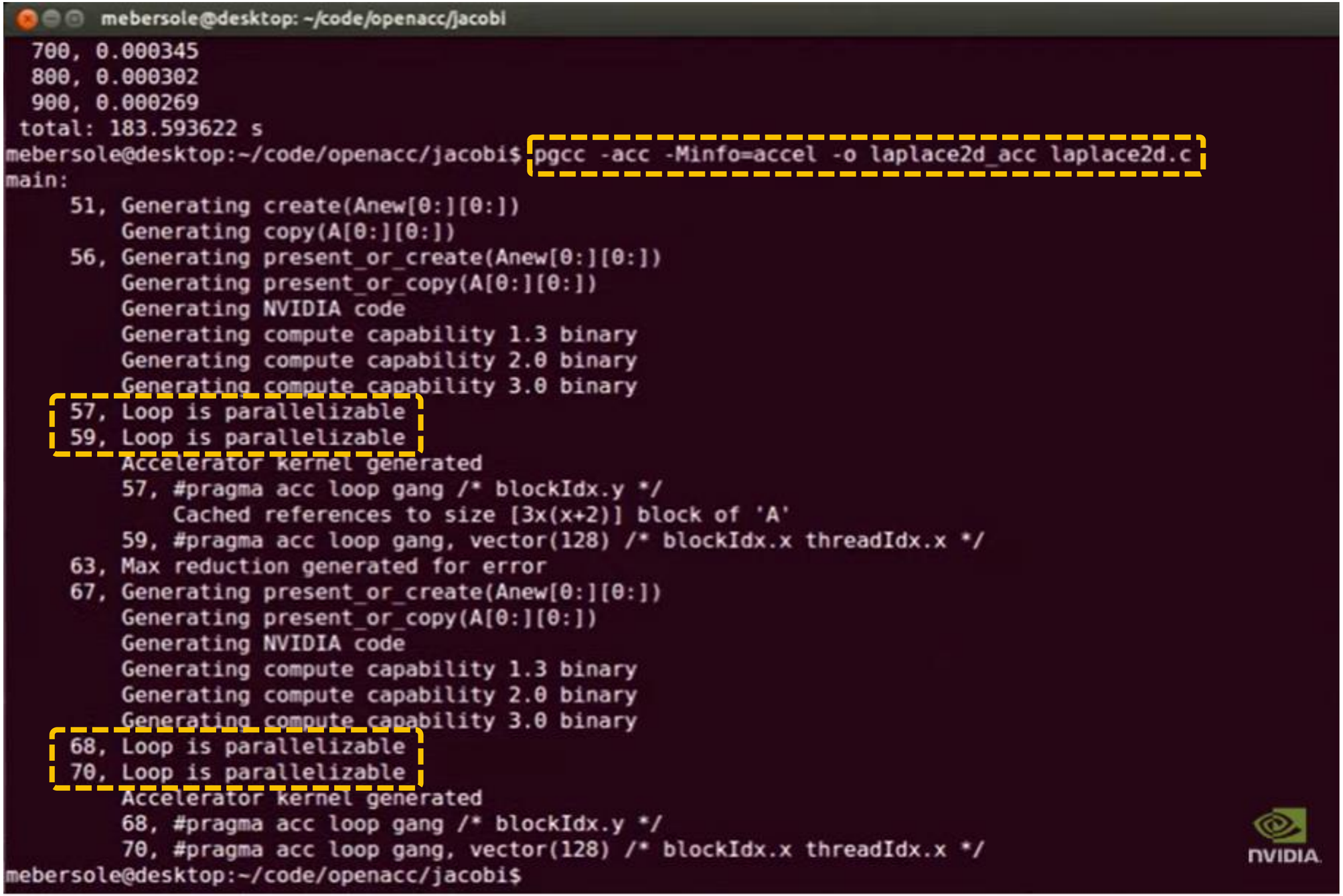
Parallelize code inside region

Close off parallel region

Close off data region, copy data back



Source: [CUDACast #3 - Your First OpenACC Program](), NVIDIA, YouTube (2013년 7월)



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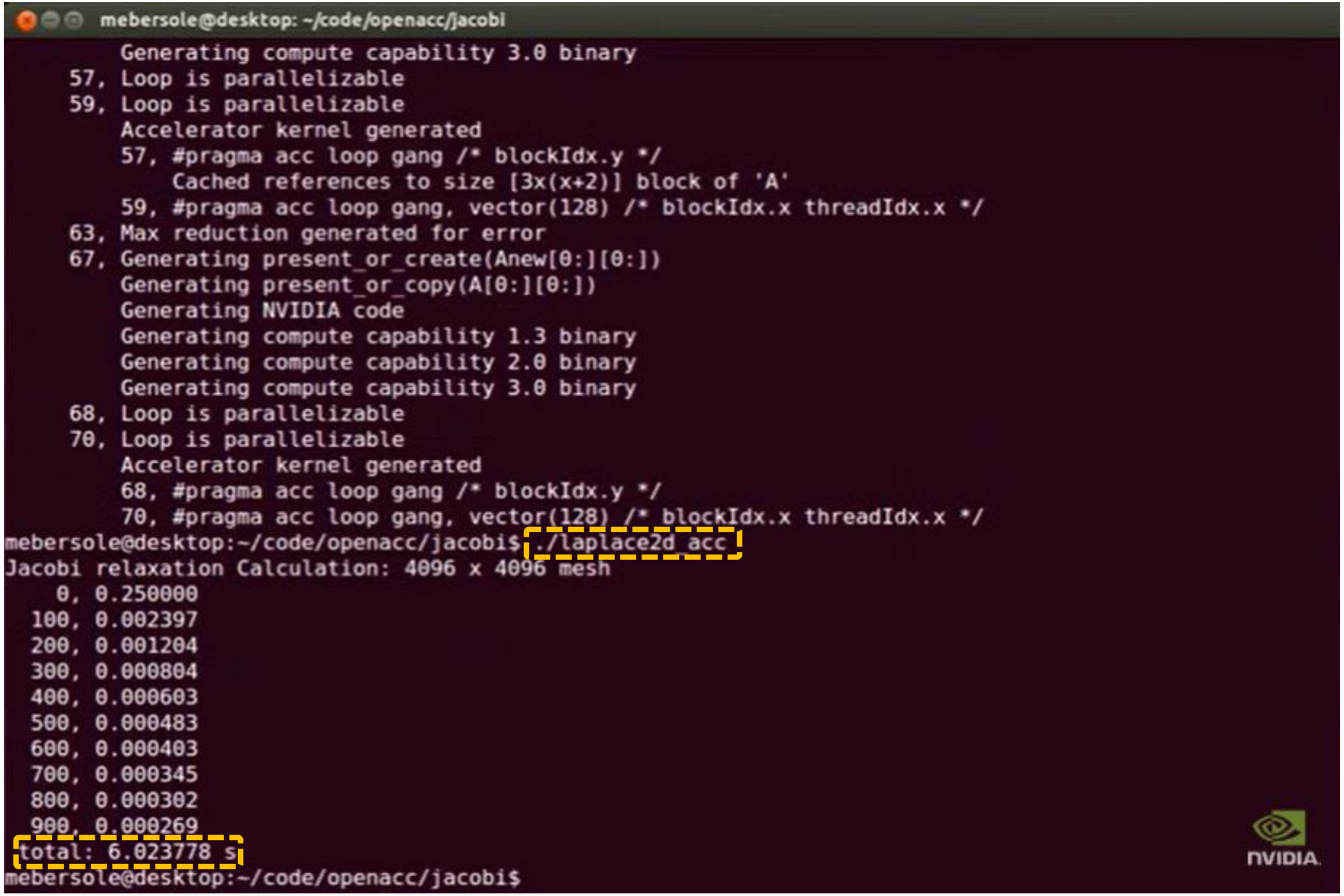
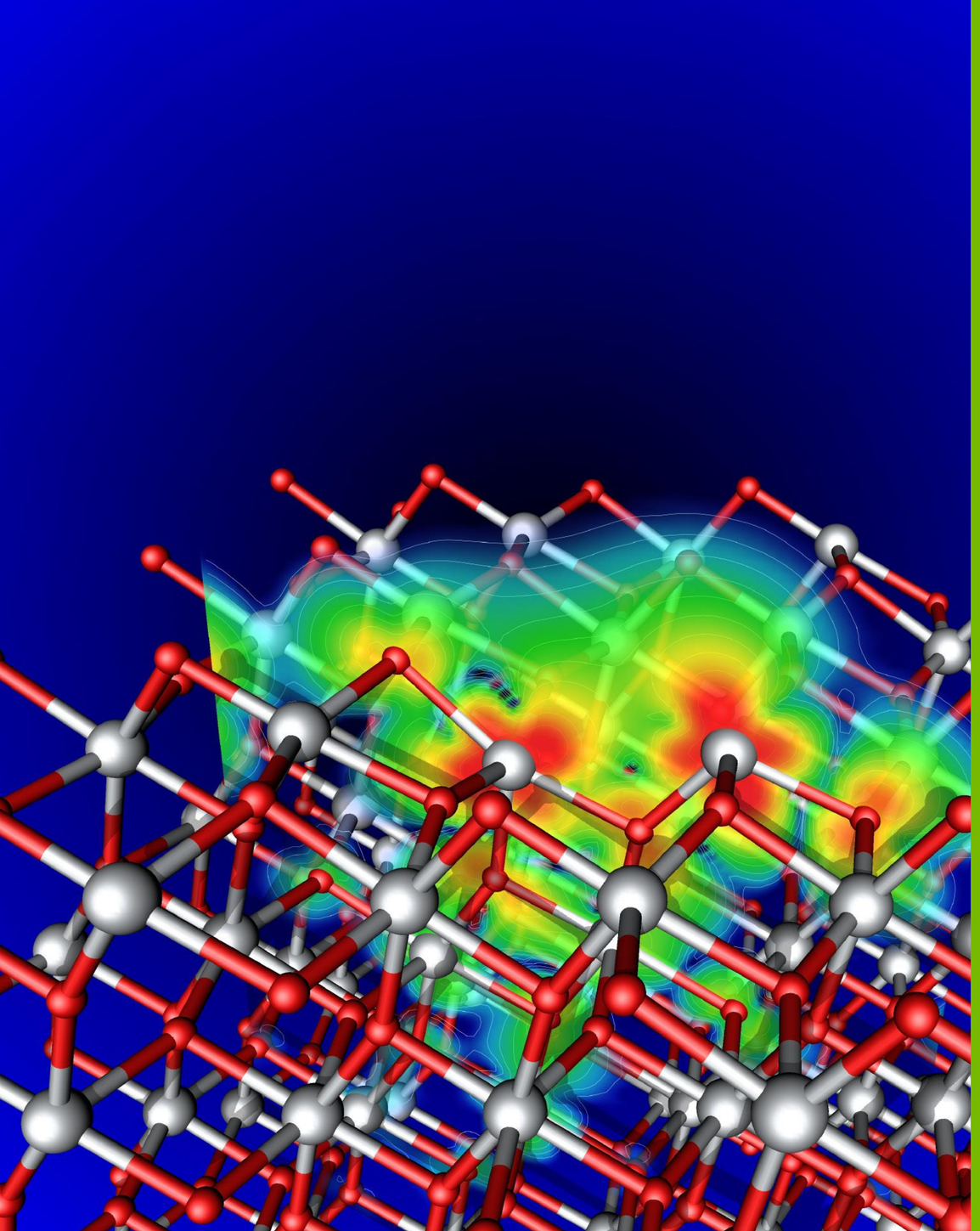


OpenACC 적용 전 약 78초 소요

Source: CUDACast #3 - Your First OpenACC Program, NVIDIA, YouTube (2013년 7월)

VASP ON GPU

- VASP has organically grown over more than 25 years (450k+ lines of Fortran code)
- Previous VASP5.4.4 release: some features were ported with CUDA C
- Current VASP6.1.X releases: re-ported to GPU using OpenACC
- The OpenACC port is more complete already than the CUDA port.

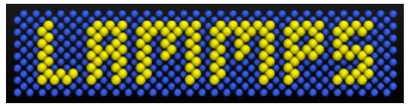


VASP

Prof. Georg Kresse
Computational Materials Physics
University of Vienna

“For VASP, OpenACC is ***the*** way forward for GPU acceleration. Performance is similar and in some cases better than CUDA C, and OpenACC dramatically decreases GPU development and maintenance efforts. We’re excited to collaborate with NVIDIA and PGI as an early adopter of CUDA Unified Memory.”

NVIDIA ACCELERATES COMPUTATIONAL CHEMISTRY



Parabricks™


이를 위해 탄생한
CAMBRIDGE-1

ANNOUNCING CAMBRIDGE-1 AI SUPERCOMPUTER

AstraZeneca

NHS
Guy's and St Thomas'
NHS Foundation Trust

gsk

King's College London

Oxford NANOPORE Technologies

80 NVIDIA DGX A100 | 400 PETAFLOPS AI COMPUTE | 20 TERABYTES/SEC INFINIBAND | 2PB NVME | 500KW

HEALTHCARE &
LIFE SCIENCE RESEARCH

LARGE-SCALE AI &
DATA SCIENCE RESEARCH

COLLABORATION WITH UK INDUSTRY,
UNIVERSITIES, STARTUPS

EDUCATE FUTURE
AI PRACTITIONERS

NVIDIA

CAMBRIDGE-1
POWERING THE FUTURE OF HEALTHCARE WITH AI

AstraZeneca

Lindsay Edwards
Head of AI, Respiratory & Immunology

gsk

Steve Crossan
VP, AI and Machine Learning

King's College London

Sebastien Ourselin
Professor of Healthcare Engineering

NHS

Nadine Hachach-Haram
Clinical Innovation Lead

Oxford Nanopore Technologies

Rosemary Sinclair Dokos
VP, Product & Programme Management

NVIDIA

David Hogan
VP, Enterprise EMEA

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COMPUTATIONAL DRUG DISCOVERY CALCULATOR

Sizing DGX A100 Infrastructure

Mix Traditional HPC + New AI Workloads

Specify Experiment Turn Around Time

Customize AI Models per Project

Plan for Future Compute Needs

Contact NVIDIA Account Executive

Summary End-to-End Needs for Drug Development					
Domain (row titles, right)	Genomics	CryoEM	AI / ML / QSAR	CADD	TOTALS
Phase (column, below)	DGX A100	DGX A100	DGX A100	DGX A100	DGX A100
Phase 1: Target Identification	TBD	TBD	1	-	1
Phase 2: Structure Determination	-	3	1	TBD	4
Phase 3: Computer-Aided Drug Design	-	-	14	26	40
Phase 4: HTScreening / Bioimaging	-	-	2	-	2
TOTALS	0	3	18	26	47

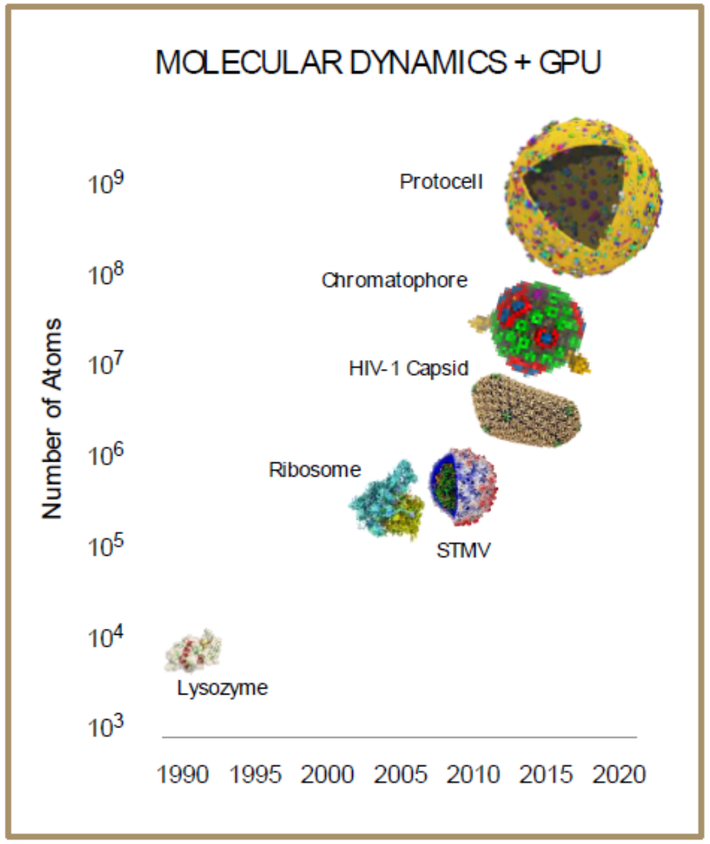
Target Identification		
	Turn-Around-Time	Num. of DGX A100
Sequencing	2	TBD
Genomics Analyses	2	TBD

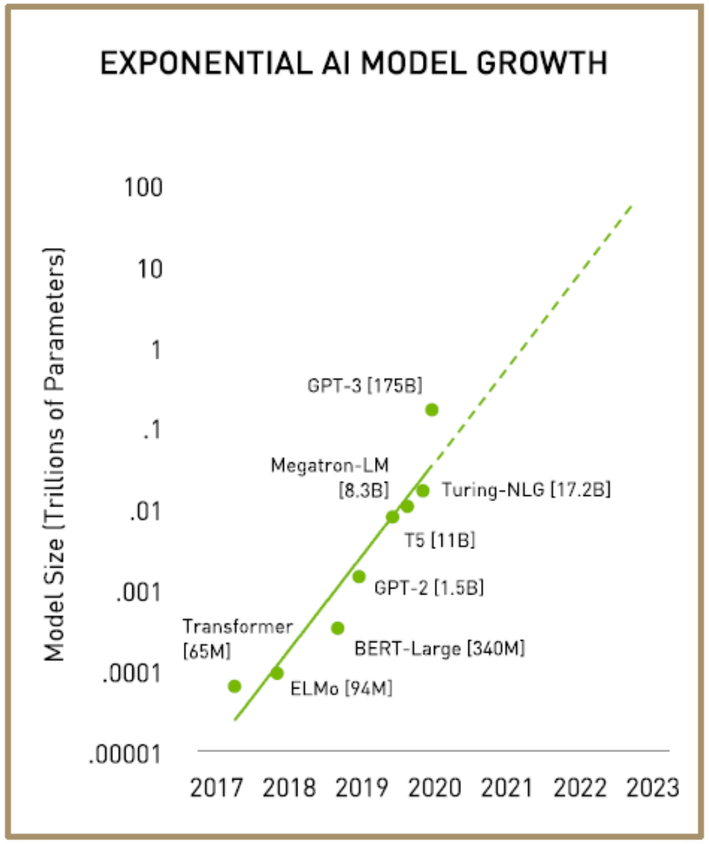
Structure Determination		
	Turn-Around-Time	Num. of DGX A100
Cryogenic EM	2	3
Physics-Based Structure Prediction	1	TBD
Homology Modeling	1	TBD

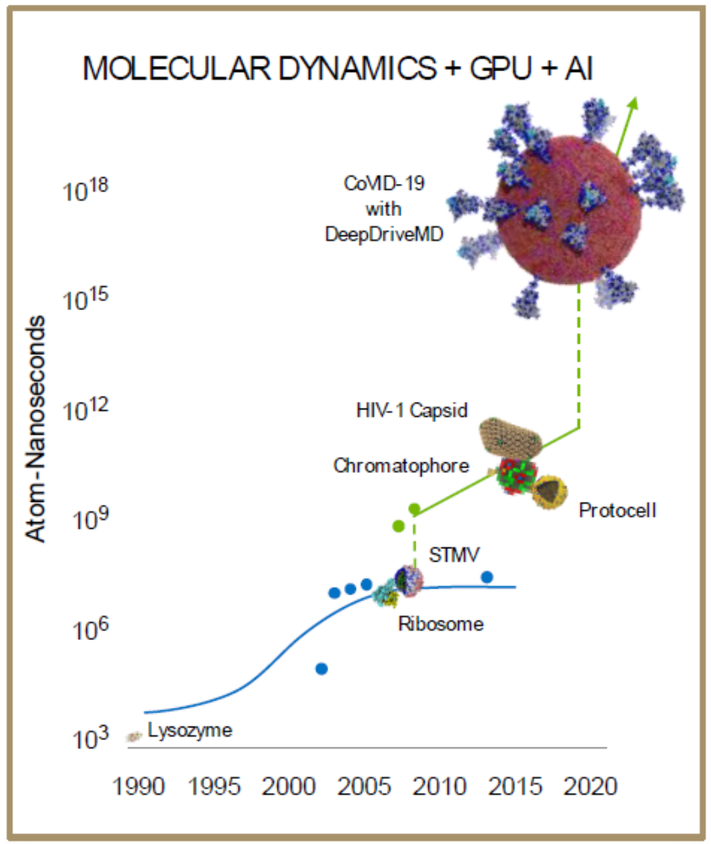
Computer-Aided Drug Design		
	Turn-Around-Time	Num. of DGX A100
Docking	1	15
Free Energy Methods	5	9
Molecular Dynamics	5	2
Quantum	3	

AI model training			
	Number of Models (per project)	Turn-Around-Time	Num. of DGX A100
Phase 1: Target Identification models	1	5	1
Phase 2: Protein structure prediction models	1	5	1
Phase 3: AI-accelerated MD models	2	3	4
Phase 3: Generative models for lead discovery	2	3	4
Phase 3: Ligand binding score models	2	3	4
Phase 3: ADMET models	2	5	2
Phase 4: Bioimaging models	1	3	2

INDUSTRIAL HPC AT THE TIPPING POINT







Source: THE INNOVATIVE FORCE OFHIGH PERFORMANCE COMPUTING IN MATERIALS SCIENCE, NVIDIA, Webinar (2021년 7월)

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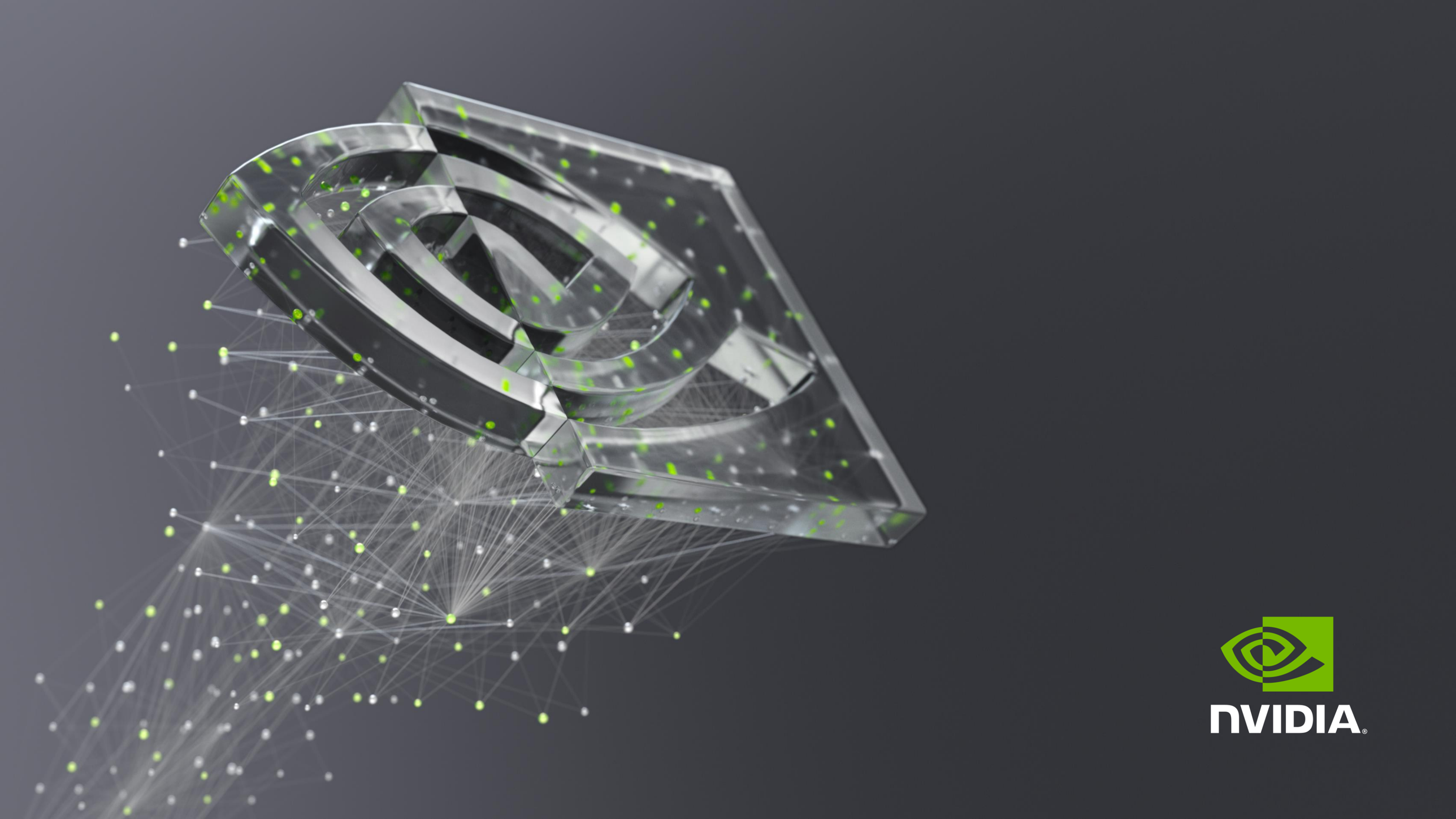
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