

NTSE-2018 (International Conference on
Nuclear Theory in the Supercomputing Era)
IBS, Daejeon, Korea

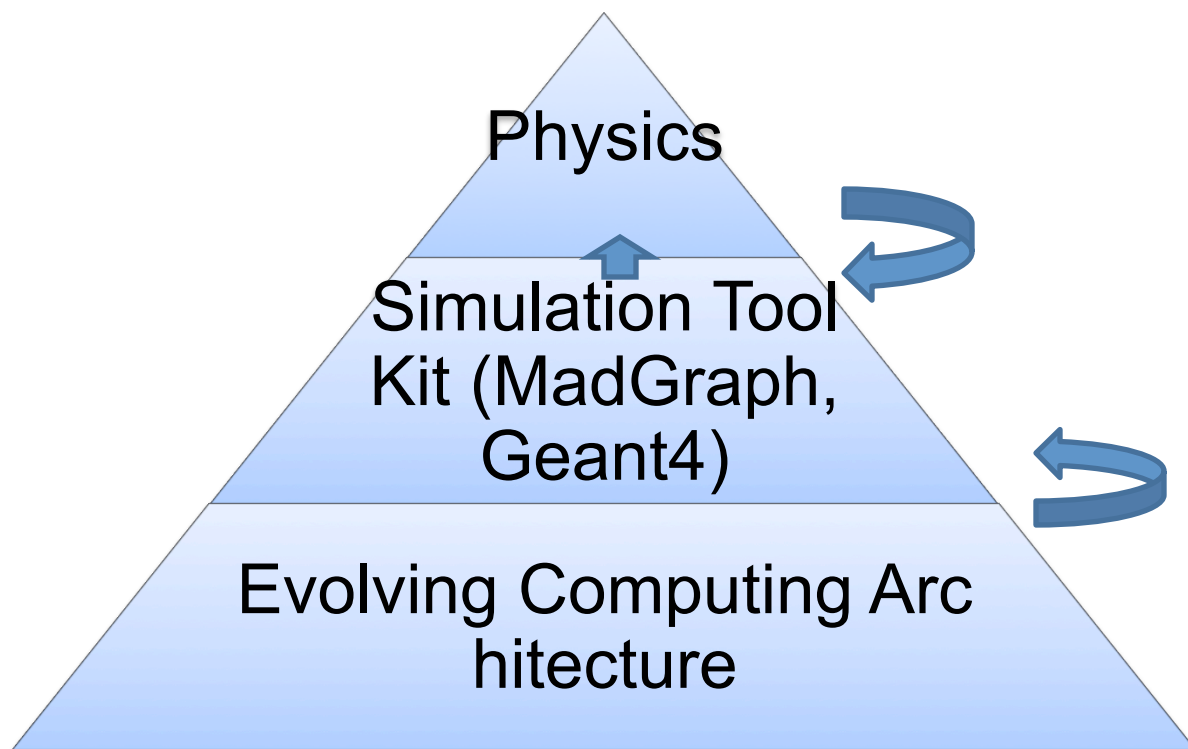
October 29 ~ November 2, 2018

Nuclear Theory in the 5th Supercomputing Era

Kihyeon CHO
(KISTI)

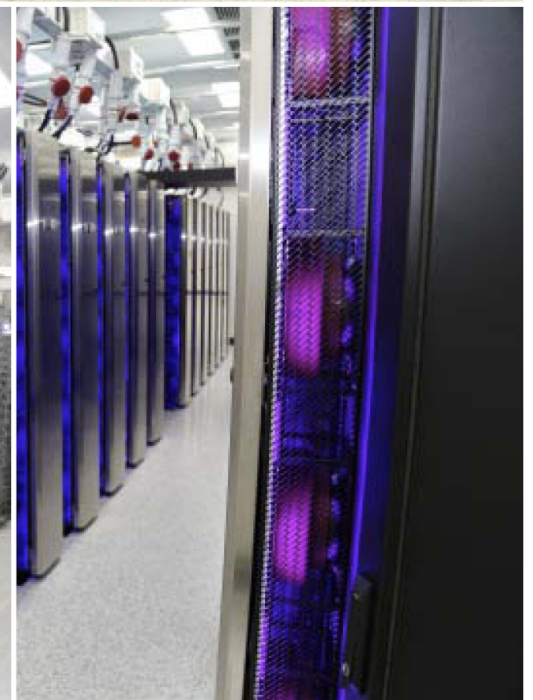
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- KISTI
- Evolving Computing Architecture
- Simulation
- Physics
- Summary



KISTI

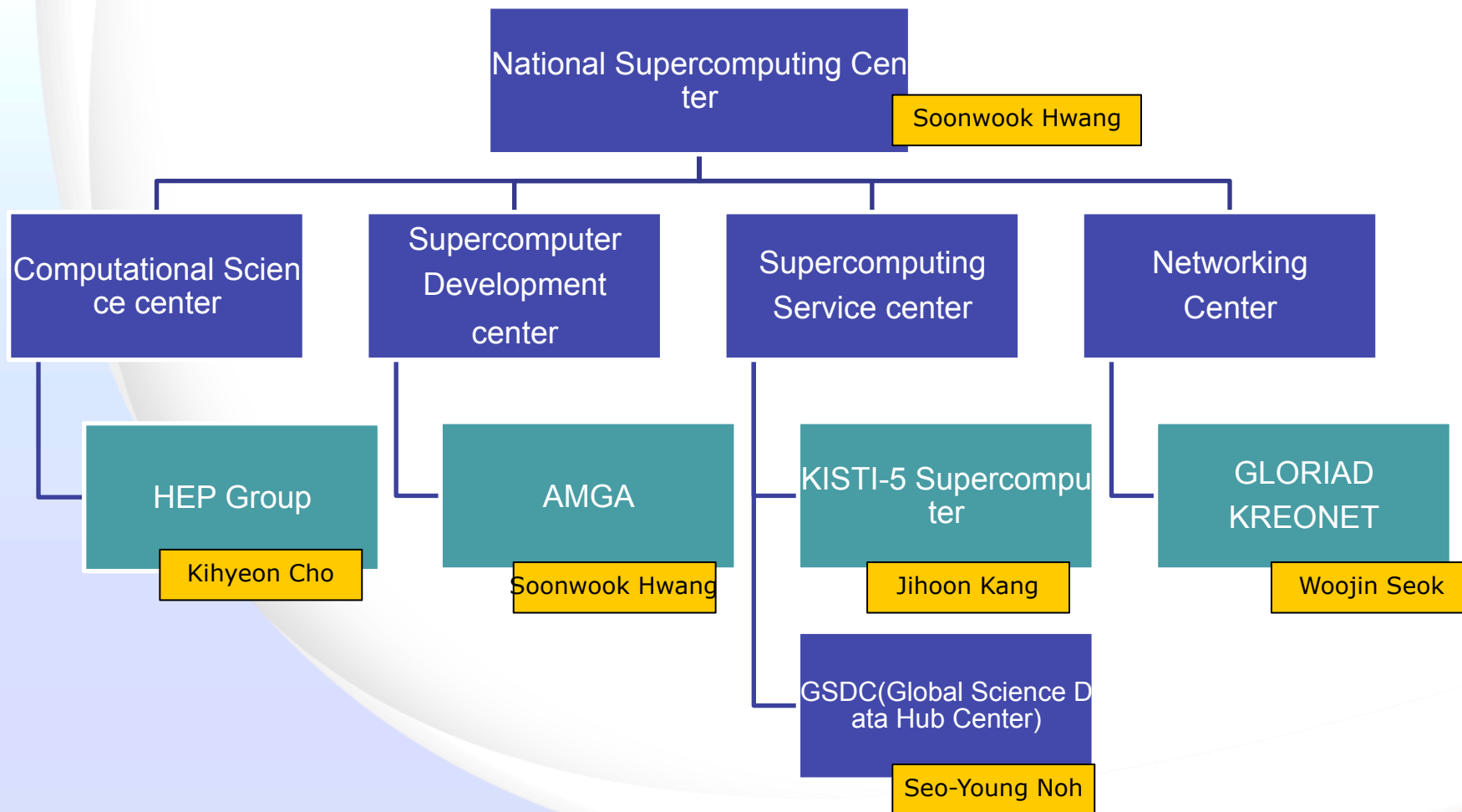




KISTI Organization



* KISTI has the only national supercomputing center in Korea.



* Describe HEP related departments only♪

Community
(Dark Matter Research Cluster)

KISTI

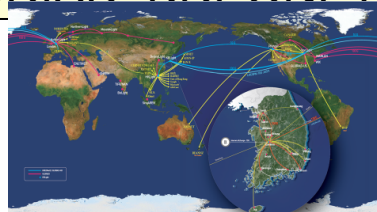
Supercomputing Center

Contact person (Kihyeon Cho)

Physics
- HEP Group (Kihyeon Cho)

Software/Middleware
-AMGA, Grid CA(KISTI CA)

Evolving Computing Architecture
-5th Supercomputer (KISTI-5),
-GSDC(ALICE T1, CMS T2, Belle2, LIGO Farm) -
GLORIAD KRFONET

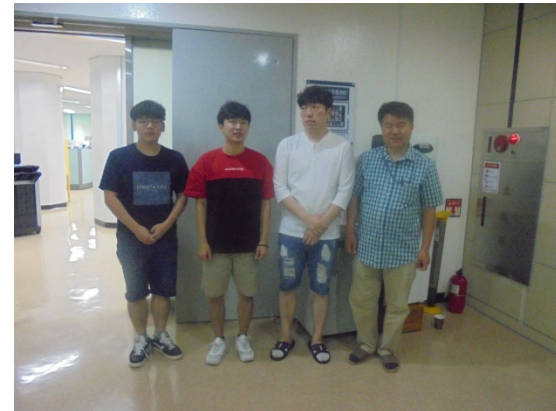


HEP Group @ KISTI

- Who are we?

Name	Ph.D.	Experiences	
Prof. Kihyeon Cho	Charm/B @ CLEO ('96, U. of Colorado)	Charm @ FOCUS ('96-06, U. of Tennessee & KNU), B @ CDF ('01- , KNU & KISTI)	
Dr. Inseong Yeo	RENO ('17, JNU)	Belle('17- , KISTI)	
Dr. Myeong Hwan Mun	Nuclear Theory ('15, KNU)	KAERI('15-18), UNIST('18)	

- Looking for M.S. and Ph.D students
- Intern for undergraduate student



Vision @ HEP Group

Technical Paper

J. Astron. Space Sci. 33(1), 63-67 (2016)
<http://dx.doi.org/10.5140/JASS.2016.33.1.63>



e-Science Paradigm for Astroparticle Physics at KISTI

Kihyeon Cho[†]

Korea Institute of Science and Technology Information, Daejeon 34141, Korea

The Korea Institute of Science and Technology Information (KISTI) has been studying the e-Science paradigm. With its successful application to particle physics, we consider the application of the paradigm to astroparticle physics. The Standard Model of particle physics is still not considered perfect even though the Higgs boson has recently been discovered. Astrophysical evidence shows that dark matter exists in the universe, hinting at new physics beyond the Standard Model. Therefore, there are efforts to search for dark matter candidates using direct detection, indirect detection, and collider detection. There are also efforts to build theoretical models for dark matter. Current astroparticle physics involves big investments in theories and computing along with experiments. The complexity of such an area of research is explained within the framework of the e-Science paradigm. The idea of the e-Science paradigm is to unify experiment, theory, and computing. The purpose is to study astroparticle physics anytime and anywhere. In this paper, an example of the application of the paradigm to astrophysics is presented.

Keywords: e-Science, astroparticle physics, dark matter

1. INTRODUCTION

Current research can be analyzed by big data in the framework of the e-Science paradigm. The e-Science paradigm unifies experiments, theories, and computing simulations that are related to big data (Lin & Yen 2009). Hey explained that a few thousands of years ago, science was described by experiments (Hey 2006). In the last few hundred years, science was described by theories and in the last few decades, science was described by computing simulations (Hey 2006). Today, science is described by big data through the unification of experiments, theories, and computing simulations (Cho et al. 2011).

We introduce the e-Science paradigm in the search for new physics beyond the Standard Model, as shown in Fig. 1. It is not a mere set of experiments, theories, and computing, but an efficient method of unifying researches. In this paper, we show an application of the e-Science paradigm to astroparticle physics.

Dark matter is one of three major principal constituents of the universe. The precision measurements in flavor physics

have confirmed the Cabibbo-Kobayashi-Maskawa (CKM) theory (Kobayashi & Maskawa 1973). However, the Standard Model leaves many unanswered questions in particle physics such as the origin of generations and masses, and the mixing and abundance of antimatter. Astrophysical evidence

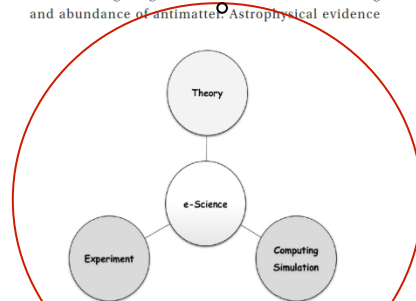


Fig. 1. Paradigm of e-Science in astroparticle physics represented as a unification of experiment, theory, and computing.

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Tel: +82-42-869-0722, Fax: +82-42-869-0799

• Theory-Experiment
-Simulation
⇒ Computational
Science

KISTI HEP Group activities

DUNE@FNAL, USA

IN2P3@France

FKPPL

FKPPL

DMRC@KISTI, Daejeon Korea

Belle*/Belle II*
@ KEK, Japan

Geant4 Collaboration

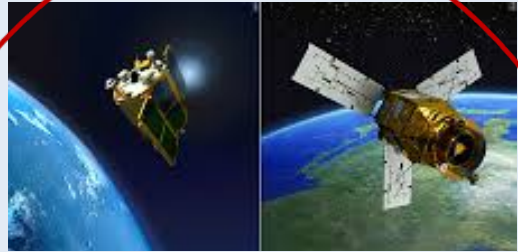


*** Official Collaborations**

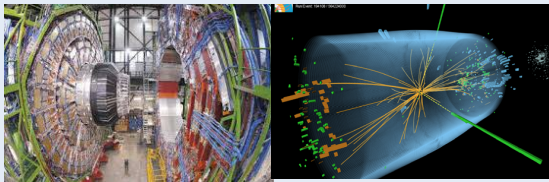
Collaborations

1. DUNE @ Fermilab
2. Belle/Belle II @ KEK
3. Geant4 Collaboration
4. FKPPL(France Korea Particle Physics Laboratory) Beam Simulation
5. Dark Matter Research Cluster @ KISTI

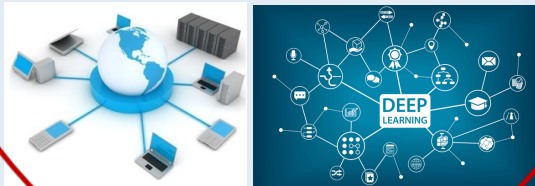
Dark Matter Research Cluster



KASI (Astronomical Data)



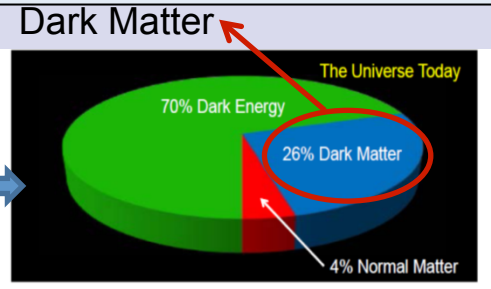
KISTI (Accelerator Data)



ICT

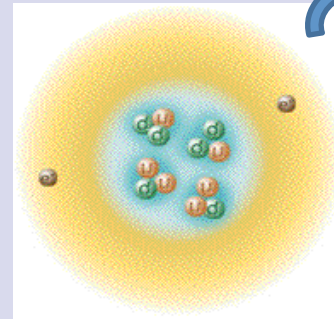


Evolution of Universe

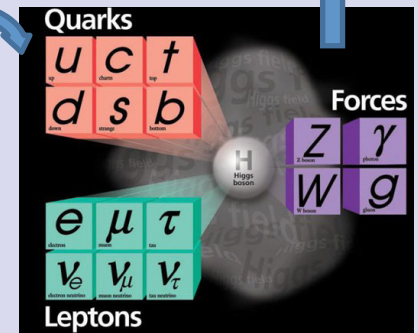


Component

SM



Origin of Matter

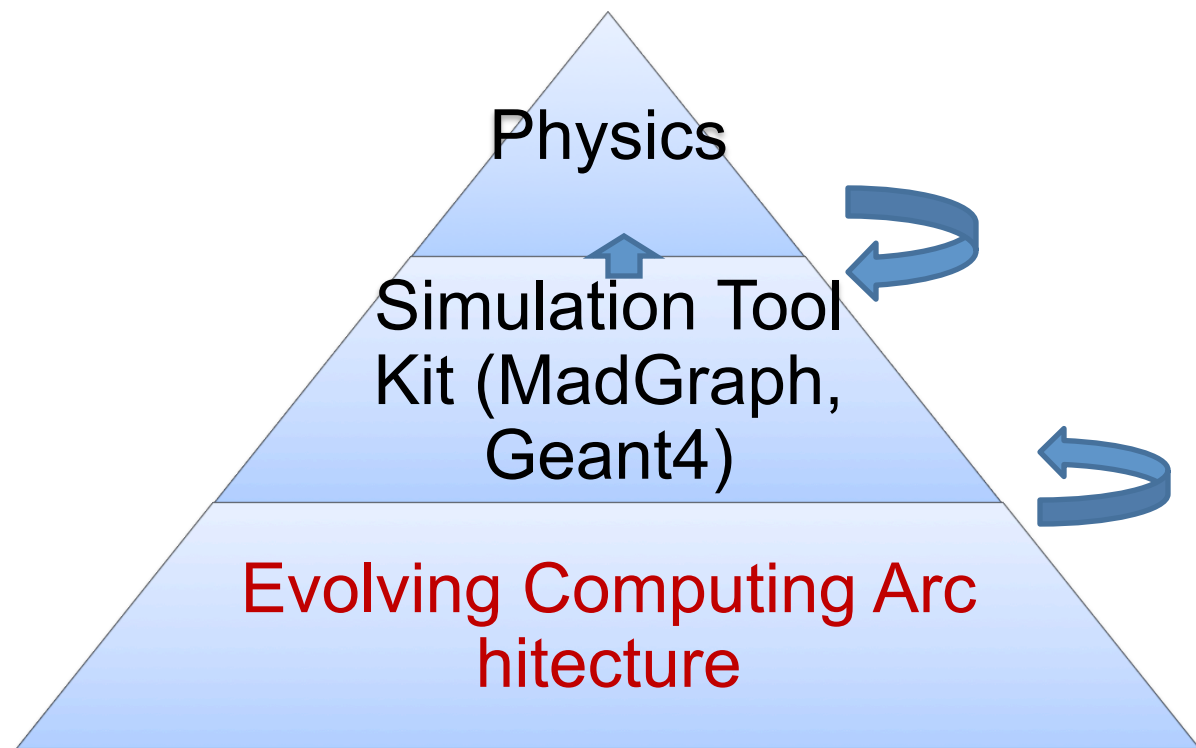


Standard Model



Big Data / Deep Learning

Evolving Computing Architecture

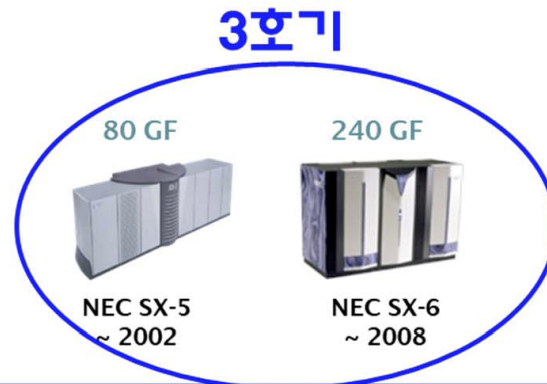


From KISTI-1 to KISTI-4 supercomputer

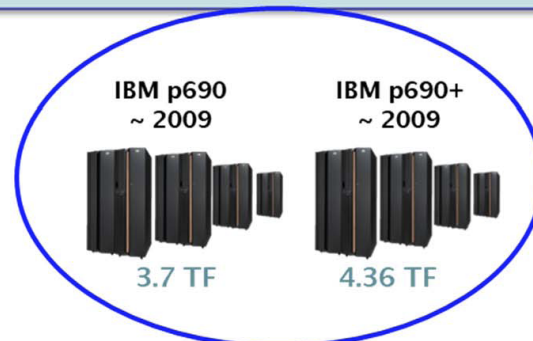
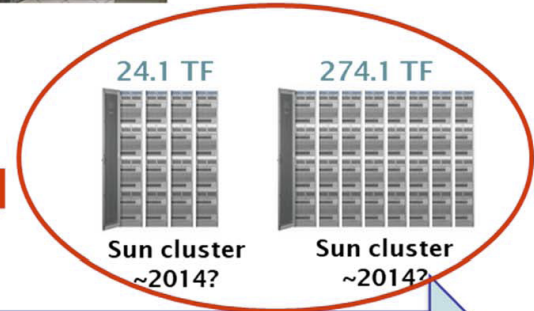
✓ 1988년 12월 6일 공식 서비스



[타키온]



4호기



[노벨]



[가이아]



KISTI-5 supercomputer (5th supercomputer)



KISTI-5 supercomputer building



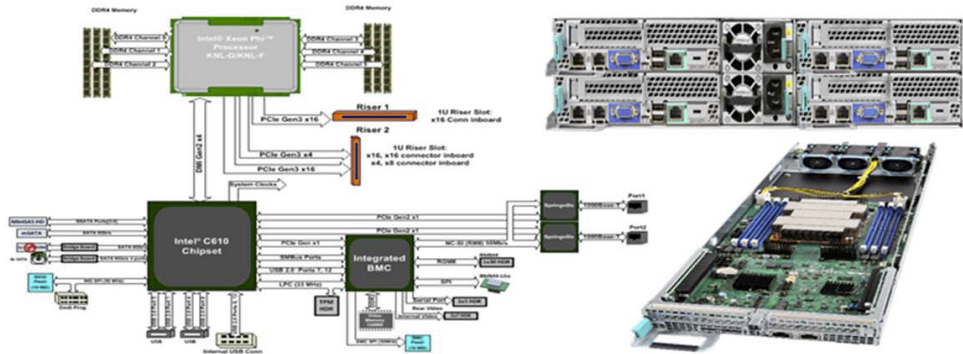
KISTI-5 supercomputer

Compute node

계산노드 Cray 3112-AA000T(2U enclosure), KNL 기반 계산 노드 (8,305개)

25.3PF

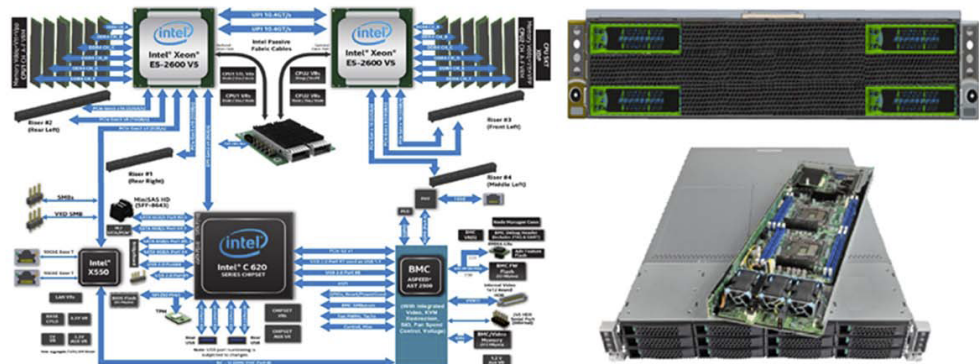
- 1x Intel Xeon Phi KNL 7250 processor
- 68 Cores per Processor
- 96GB (6x 16GB) DDR4-2400 RAM
- 1x Single-port 100Gbps OPA HFI card
- 1x On-board GigE (RJ45) port



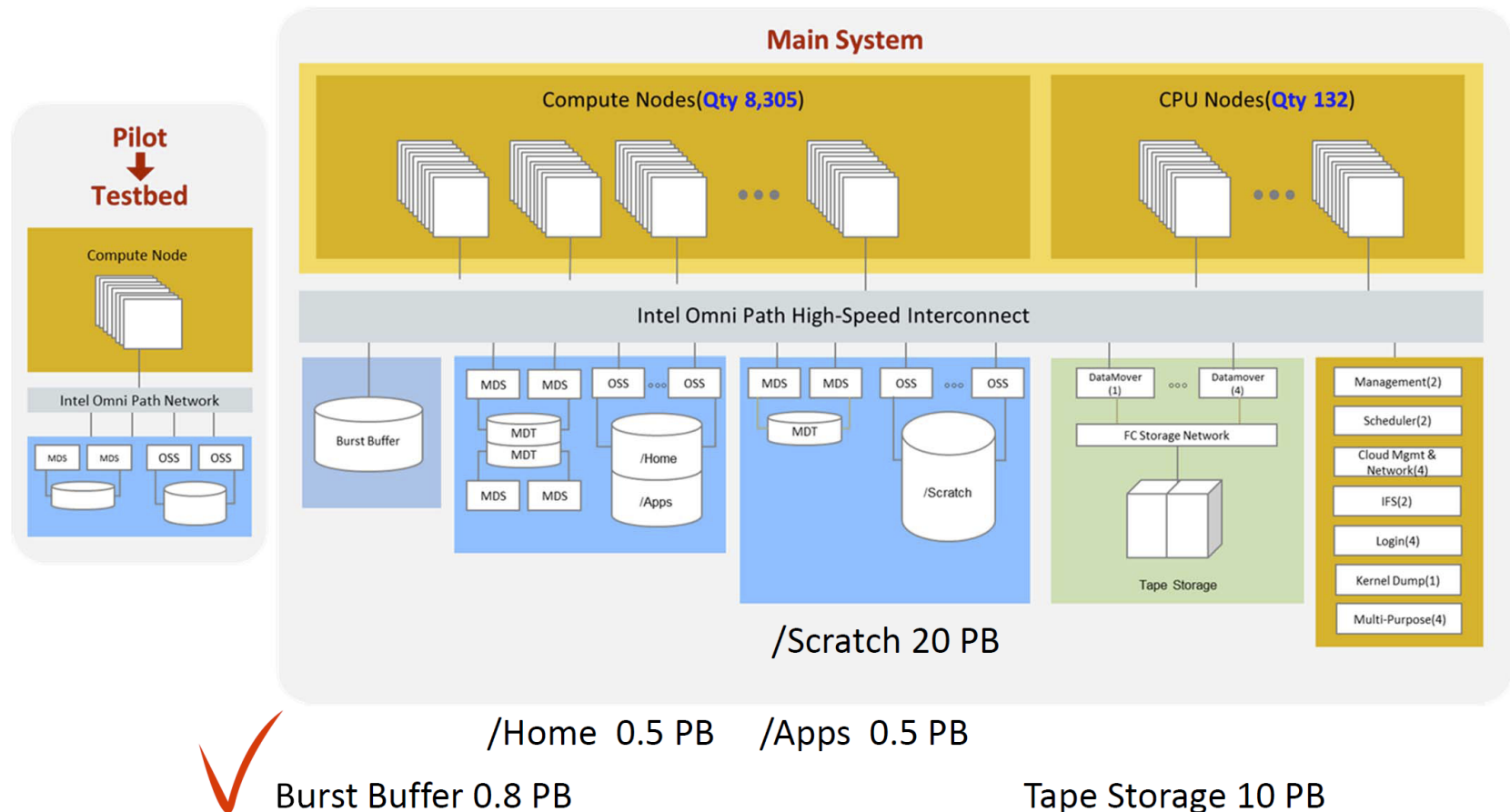
CPU-only Cray 3111-BA000T(2U enclosure), Skylake 기반 계산 노드 (132개)

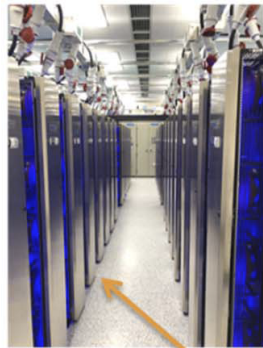
0.4PF

- 2x Intel Xeon SKL 6148 (2.4 GHz) processors
- 20 Cores per processor (total 40 Cores)
- 192GB (12x 16GB) DDR4-2666 RAM-6CH
- 1x Single-port 100Gbps OPA HFI card
- 1x On-board GigE (RJ45) port



KISTI-5 supercomputer



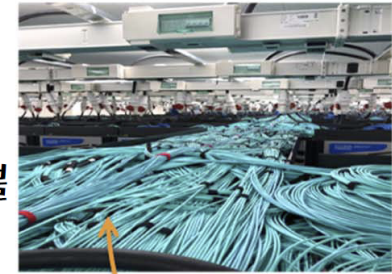


후면
냉각
도어

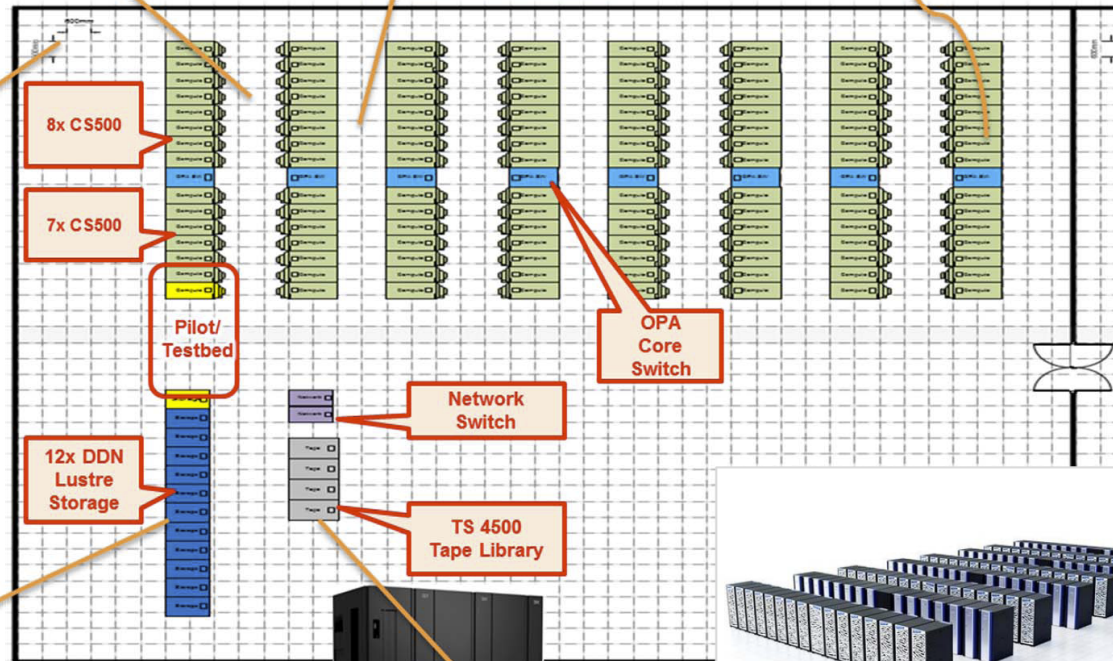
정면



상부
OPA
케이블



8열, 126랙



디스크
스토리지
(21PB)



테이프
스토리지
(10PB)



KISTI-5 Opening Ceremony



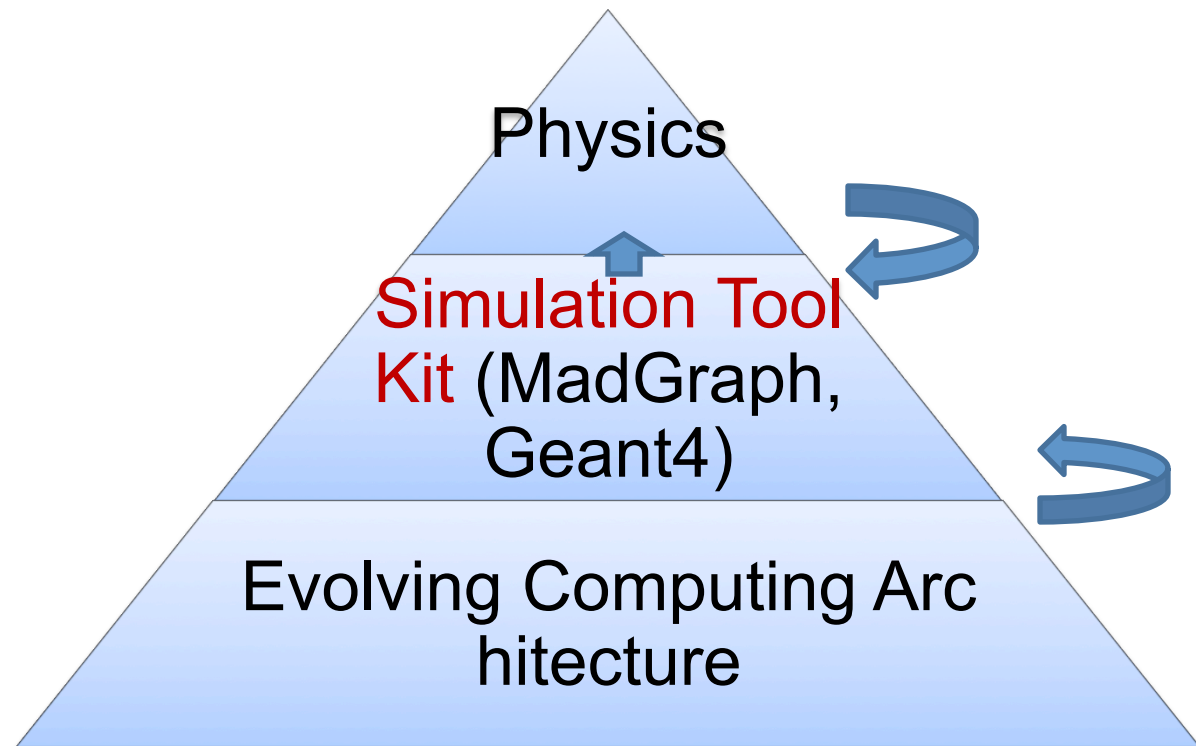
국제 워크숍

International workshop
Date: 2018. 11.7 13:50-17:30
Place: KISTI, Daejeon

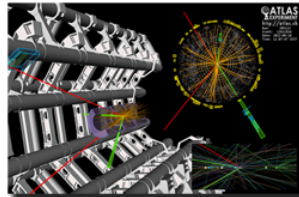
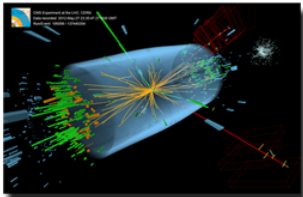
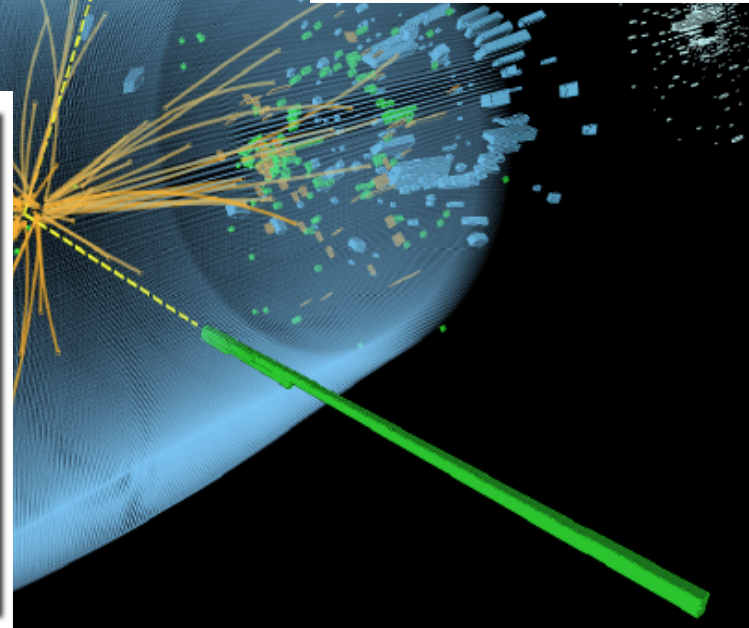
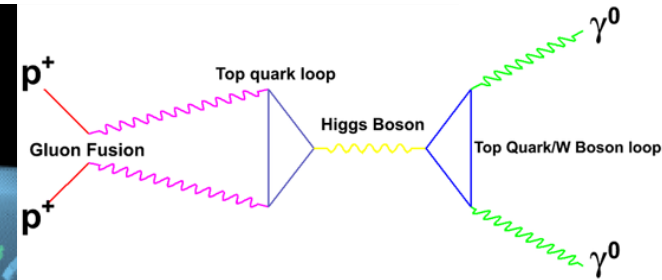
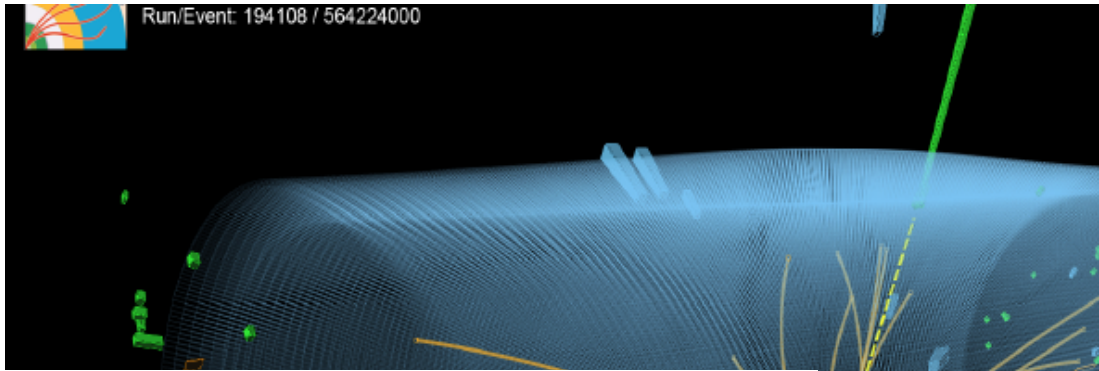
시간		제목/발표자
10:30 ~ 14:00	(10')	Welcome Speech Dr. Hee-yoon Choi (President of KISTI)
Keynote Speech Session		
14:00 ~ 14:30	(30')	The Direction and Policies of Exascale Computing, AI, Big Data in the US Prof. Daniel Reed (Chairs of Department of Energy's Advanced Computing Advisory Committee, SVP of University of Utah)
14:30 ~ 15:00	(30')	The ABCI Project and its AI Usage in Japan Dr. Satoshi Sekiguchi (Vice Director of AIST)
15:00 ~ 15:30	(30')	Coffee Break
The World Top KNL Supercomputers Session		
15:30 ~ 15:50	(20')	The successful experiences in OakForest-PACS system in Japan speaker : Prof. Taisuke Boku (University of Tsukuba)
15:50 ~ 16:10	(20')	The successful experiences in Cori System in USA speaker : Dr. Richard Gerber (HPC Department Head, NERSC)
16:10 ~ 16:30	(20')	The successful experiences in Stampede-2 system in USA speaker : Dr. Todd Evans (TACC)
16:30 ~ 16:50	(20')	The usage of KISTI-5 system in Korea speaker : Dr. Min Sun Yeom(KISTI)
16:50 ~ 17:30	(40')	Discussion Dr. Soonwook Hwang (General Director of KISTI)

You are welcome to join.

Simulation



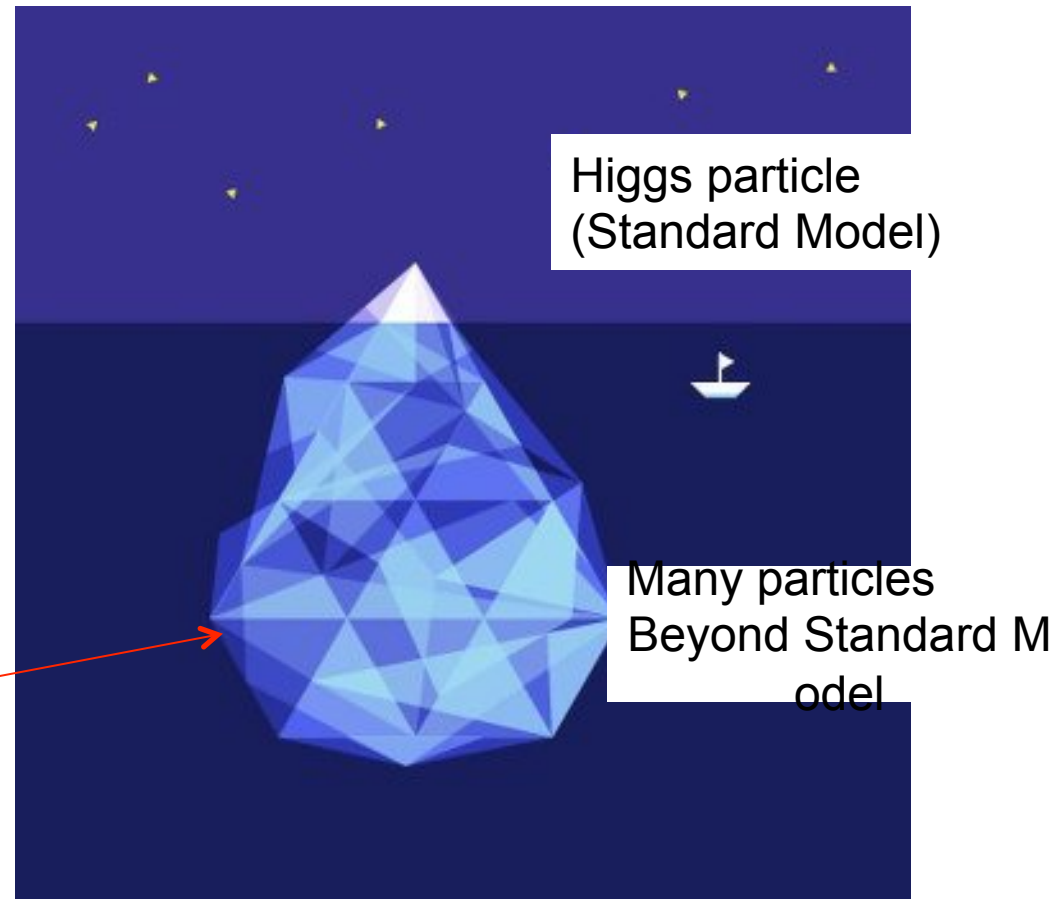
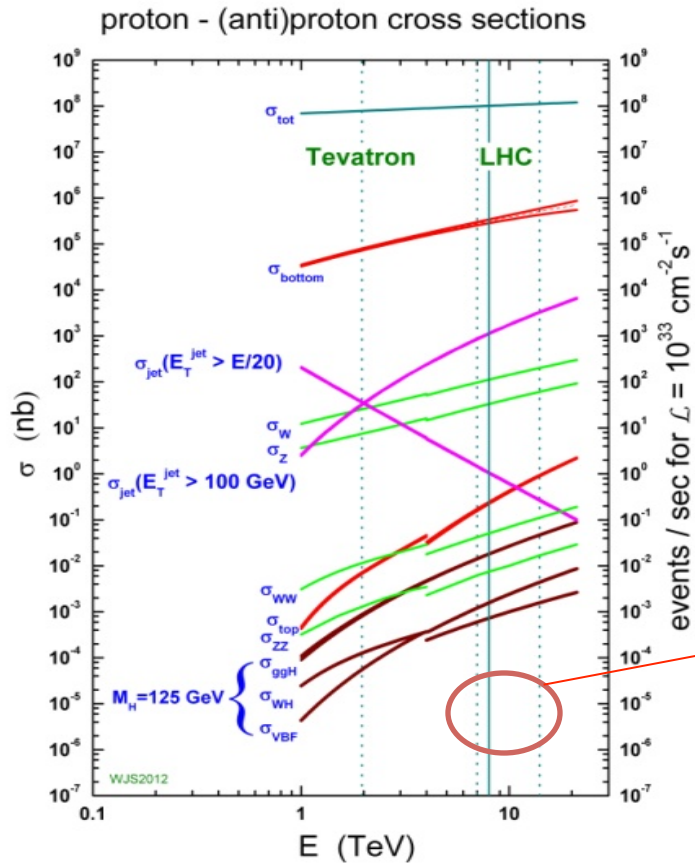
Higgs Discovery (July 4, 2012)



The SM is now complete?

⇒ What is next?

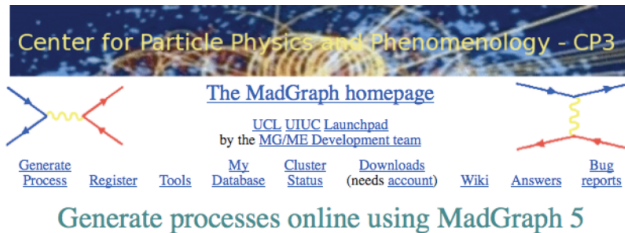
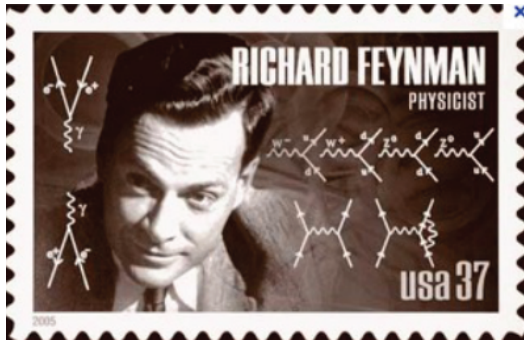
Beyond the Standard Model



Adam Martin

⇒ BSM needs 1000 more Higgs events.

HEP Simulation



New Physics Model



⇒ Feynman rules calculation

FeynRules



⇒ Model implementation

MadGraph/CalcHEP



⇒ Process creation

PYTHIA



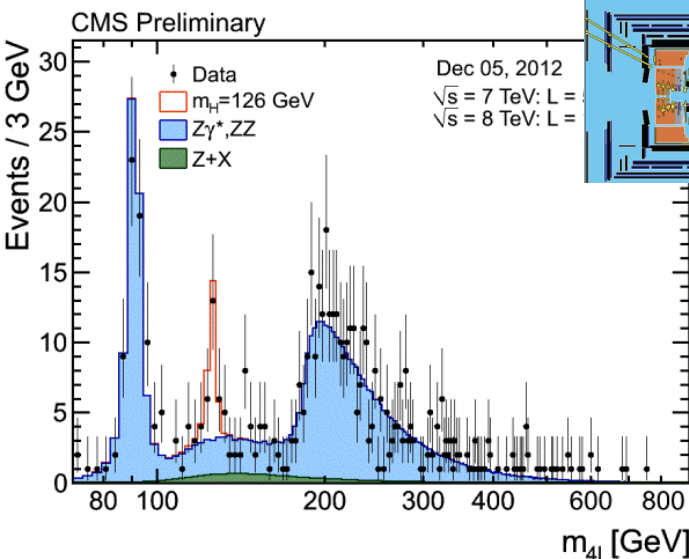
⇒ Event generation (physics)

PGS/Delphes/Geant4



⇒ Detector simulation

MadAnalysis/ROOT/Mathematica



We focus on MadGraph & Geant4



Geant4 Collaboration



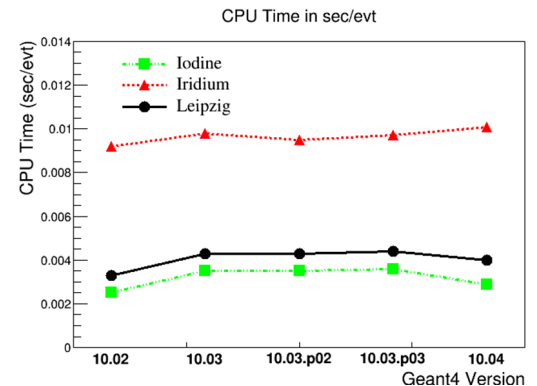
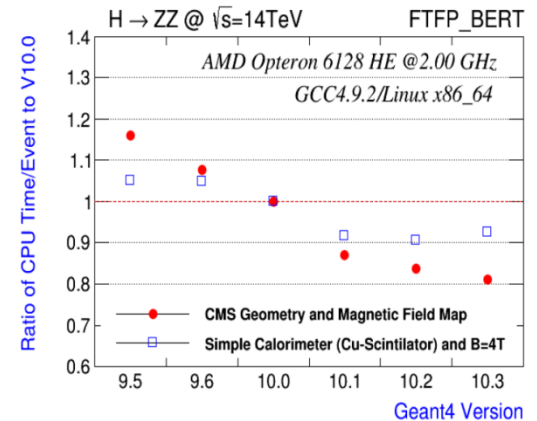
- Geant4 is the most successful model in HEP.
- HEP user community – BaBar(2001), LHC(2003), Belle II
- Prof. Kihyeon Cho is the contact person in Korea.

HEP Simulation

- Why profiling?
 - Diversity of physics applications
 - Evolving Computing
 - ⇒ S/W development
 - ⇒ Profiling tools
- ⇒ To draw community interests for collateral effort

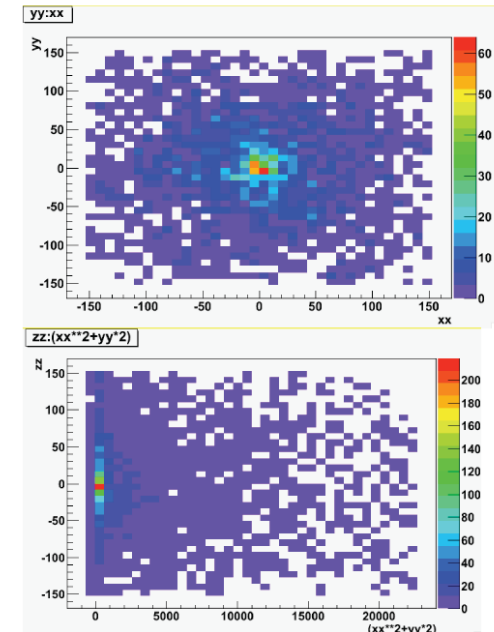
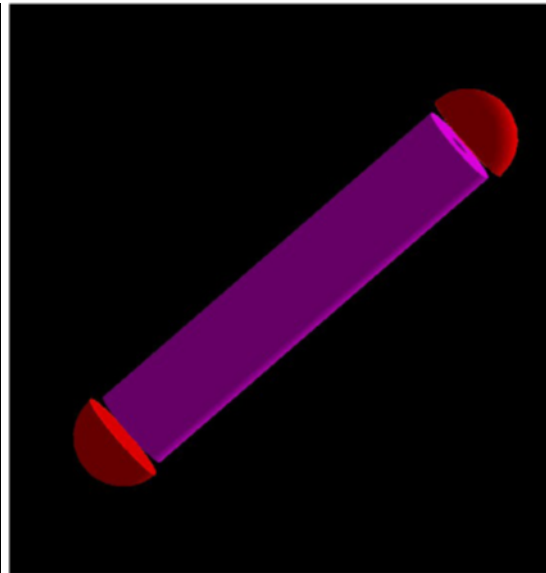
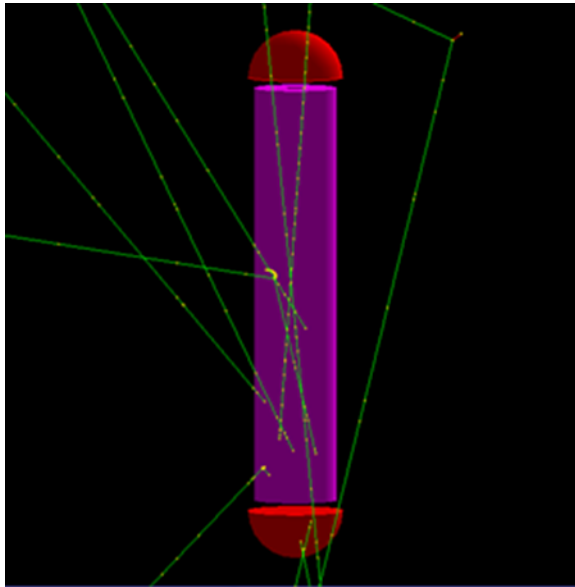
Profiling system

- Current status
 - High energy physics profiling (Fermilab)
 - SimpliCarlo (Sequential)
 - CMSExp (Multi-Thread)
 - Low energy physics profiling (KISTI)
 - Using Brachytherapy code



1. Profiling for low energy physics

- Profiling system using brachytherapy simulation (Low energy physics)
- - cf. Brachytherapy(MeV) vs. SimplifiedCarlo(TeV)



- Results (Brachytherapy v.10.02 & Geant4 v.10.04)
 - 1) CPU
 - 2) Memory size
 - 3) Version dependency
 - 4) Event number dependency
 - 5) KISTI-4 machine dependency

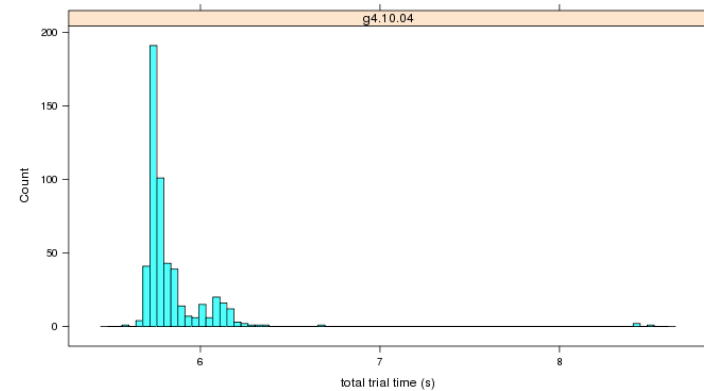
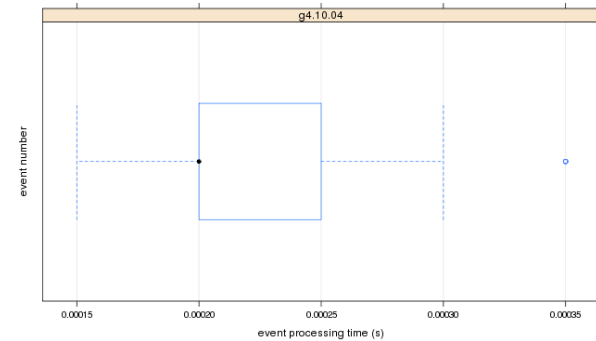
1) CPU time

CPU Time in seconds/event

Geant4.10.04 Brachy 01

Sample	Physics List	Energy	Process
Iodine	QGSP_BIC_EMY	35 KeV	0.0029
	QGSP_BIC_EMZ	35 KeV	0.0029
Iridium	QGSP_BIC_EMY	356 KeV	0.0102
	QGSP_BIC_EMZ	356 KeV	0.0101
Leipzig	QGSP_BIC_EMY	356 KeV	0.0040
	QGSP_BIC_EMZ	356 KeV	0.0040

QGSP_BIC_EMY



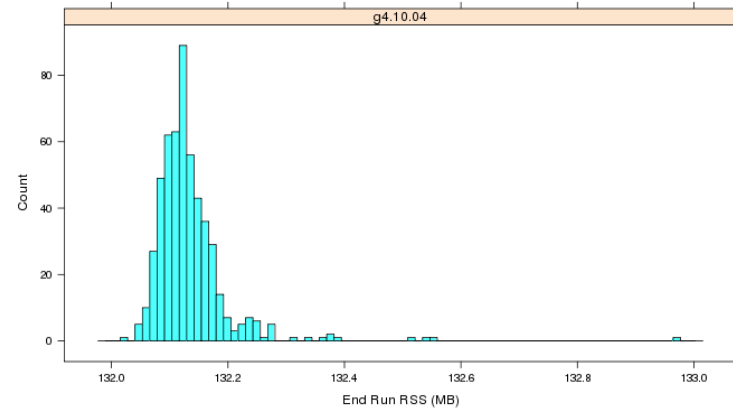
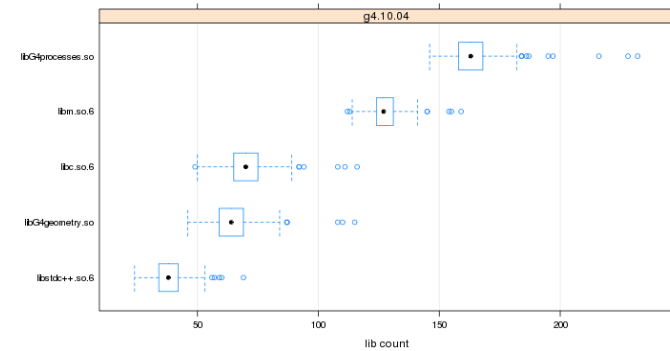
2) Memory size

Total Memory in Counts/10,000

Geant4.10.04 Brachy 01

Sample	Physics List	Energy	Process	
			First Event	Last Event
Iodine	QGSP_BIC_EMY	35 KeV	143.372	205.959
	QGSP_BIC_EMZ	35 KeV	143.372	205.968
Iridium	QGSP_BIC_EMY	356 KeV	174.434	233.229
	QGSP_BIC_EMZ	356 KeV	174.434	233.229
Leipzig	QGSP_BIC_EMY	356 KeV	184.667	256.539
	QGSP_BIC_EMZ	356 KeV	184.667	256.529

QGSP_BIC_EMY



3) Version dependency

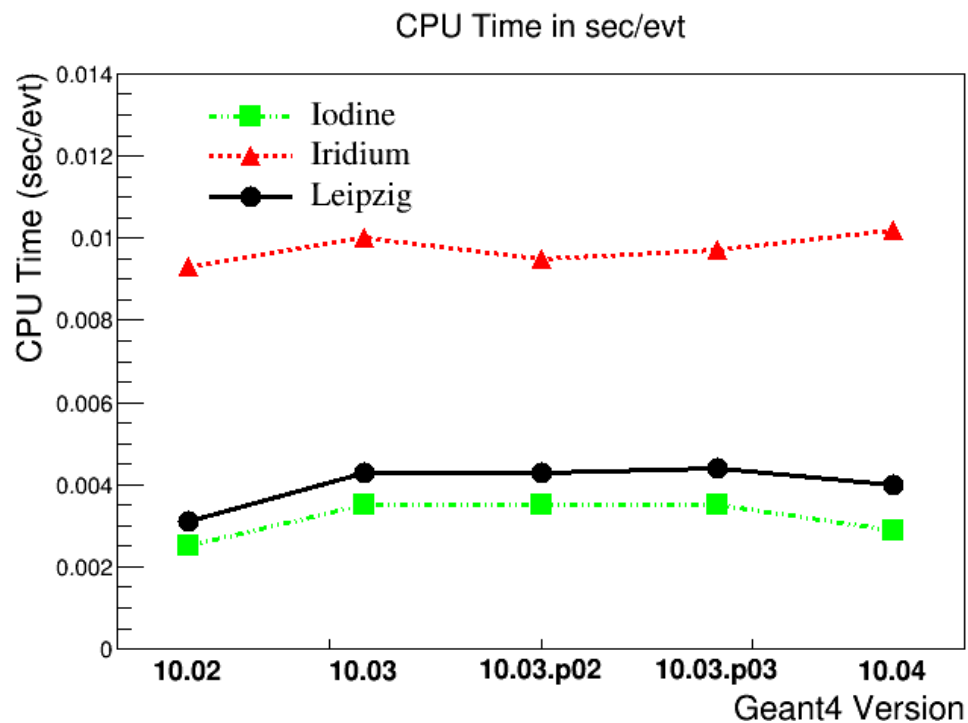
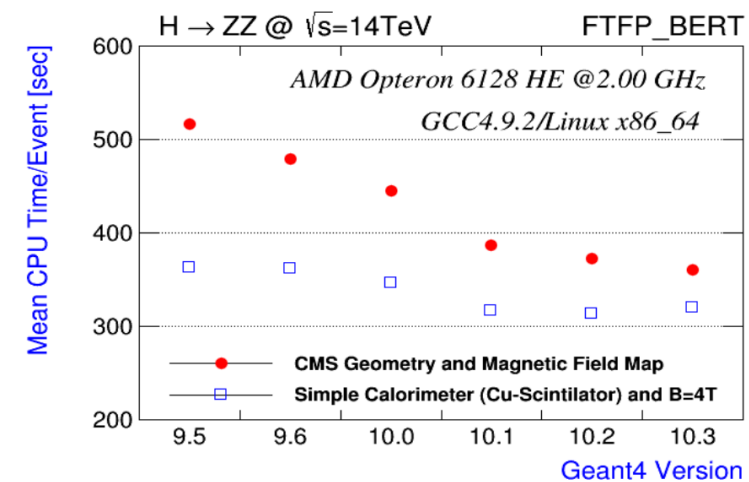
Content	Profiling				
Geant4 Version	10.02	10.03	10.03p02	10.03p03	10.04
Brachy version	10.02				

- Trial time: 528
- Macro file
 - IodineSourceMacro.mac (endocavitary brachytherapy)
 - IridiumSourceMacro.mac (interstitial brachytherapy)
 - LeipzigSourceMacro.mac (superficial brachytherapy)
- Physics list
 - QGSP_BIC_LIV
 - QGSP_BIC_EMZ
 - QGSP_BIC_EMY

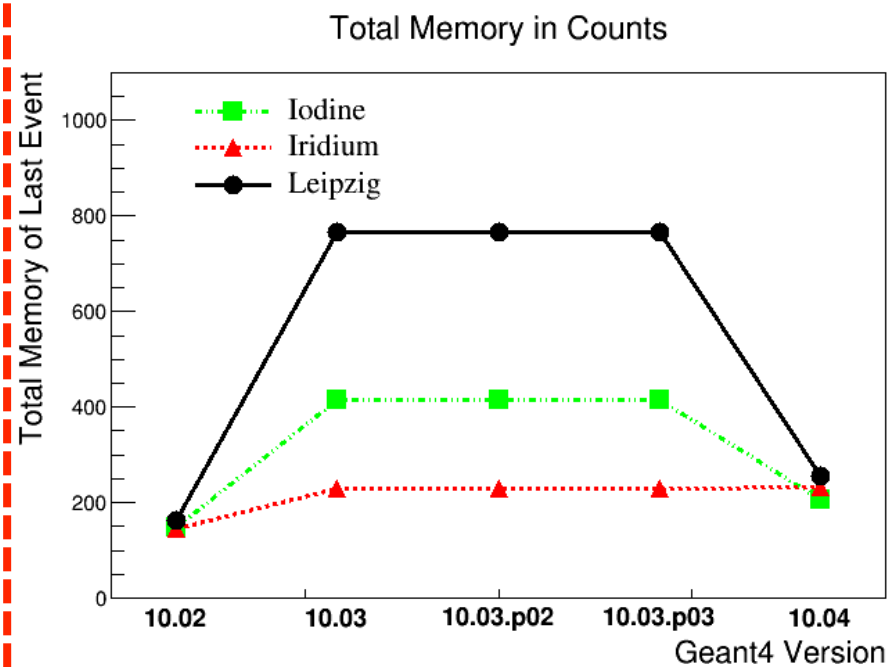
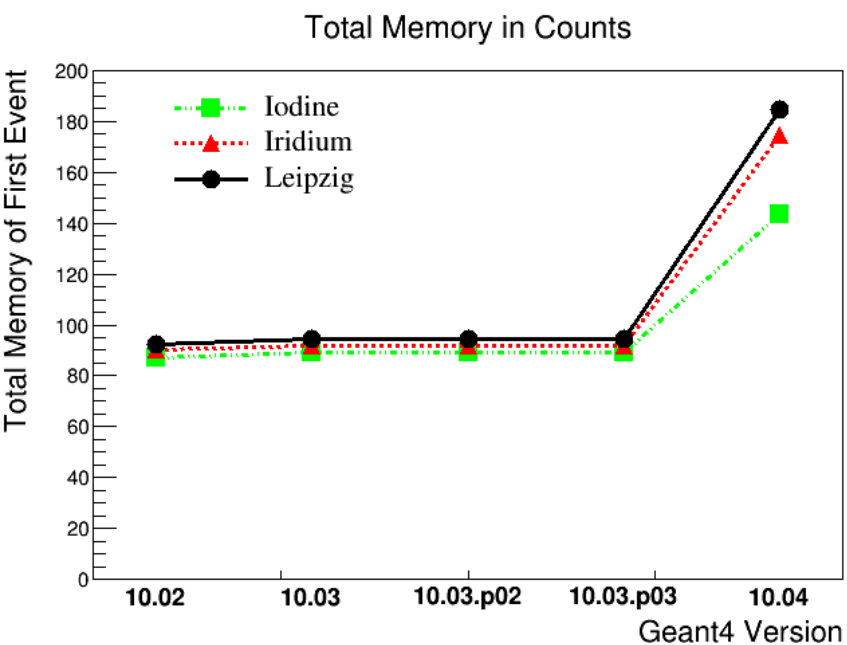
QGSP BIC EMY

Higgs -> ZZ Physics List = FTFP_BERT , Magnetic Field = 4 Tesla

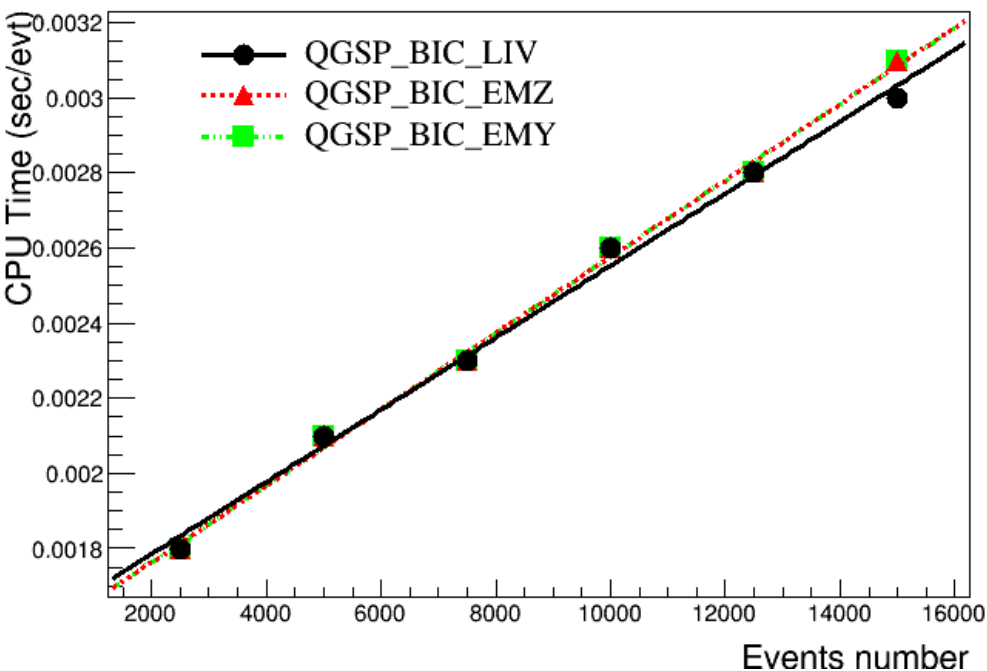
Beam Energy = 1400 GeV



Iodine QGSP BIC EMY



4) Event number dependency



QGSP BIC EMY

Chi2 = 3.42857e-09
 NDf = 4
 p0 = 0.00156 +/- 2.72554e-05
 p1 = 1.01714e-07 +/- 2.79942e-09

QGSP BIC EMZ

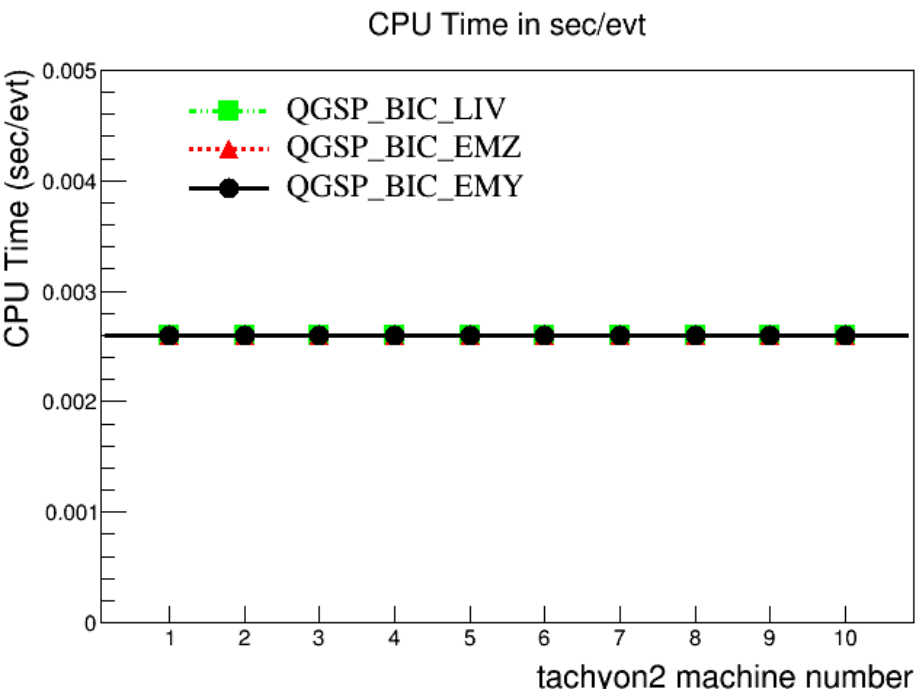
Chi2 = 3.42857e-09
 NDf = 4
 p0 = 0.00156 +/- 2.72554e-05
 p1 = 1.01714e-07 +/- 2.79942e-09

QGSP BIC LIV

Chi2 = 5.33333e-09
 NDf = 4
 p0 = 0.00159333 +/- 3.39935e-05
 p1 = 9.6e-08 +/- 3.49149e-09

- There is linearity on event number.

5) KISTI-4 machine dependency



QGSP BIC EMY

Chi2 = 1.88079e-36
 NDf = 9
 p0 = 0.0026 +/- 1.4456e-19

QGSP BIC EMZ

Chi2 = 1.88079e-36
 NDf = 9
 p0 = 0.0026 +/- 1.4456e-19

QGSP BIC LIV

Chi2 = 1.88079e-36
 NDf = 9
 p0 = 0.0026 +/- 1.4456e-19

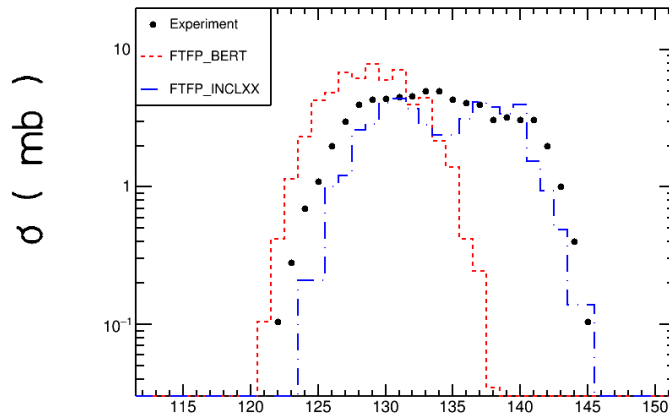
- There no machine dependency on KISTI-4 supercomputer.
- To check KISTI-5 supercomputer machine dependency

2. Beam Simulations (1/2)

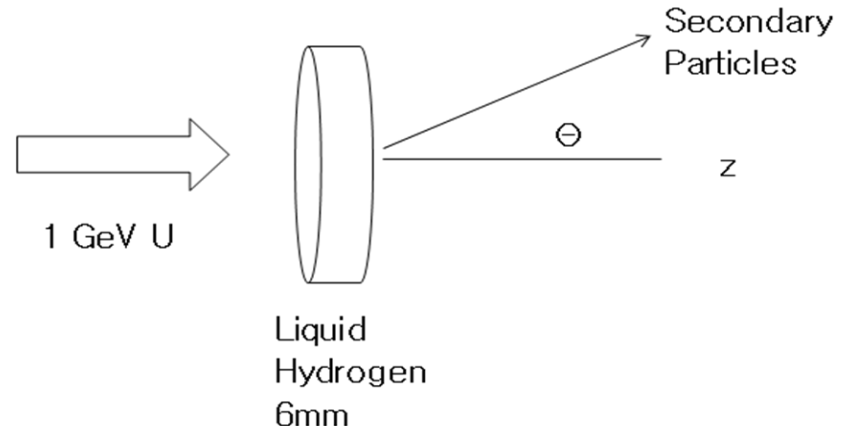
➤ Reliability of Geant4 models in producing spallation fragmentation species

Cesium Isotopes

M. Bernas et al. / Nuclear Physics A 725 (2003) 213–253

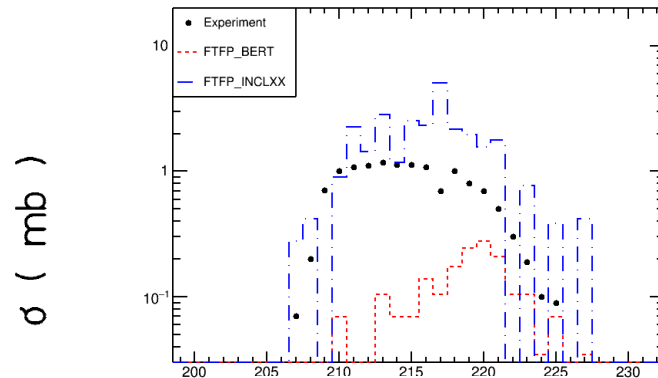


Number of mass



Francium Isotopes

J. Taïeb et al. / Nuclear Physics A 724 (2003) 413–430



Number of mass

FTFP_BERT

FTFP_BERT_HP

QGSP_BERT

QGSP_BERT_HP

QGSP_BIC

QGSP_BIC_HP

FTFP_INCLXX

FTFP_INCLXX_HP

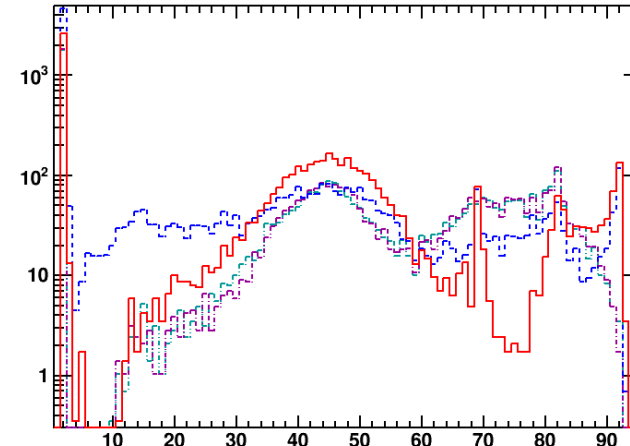
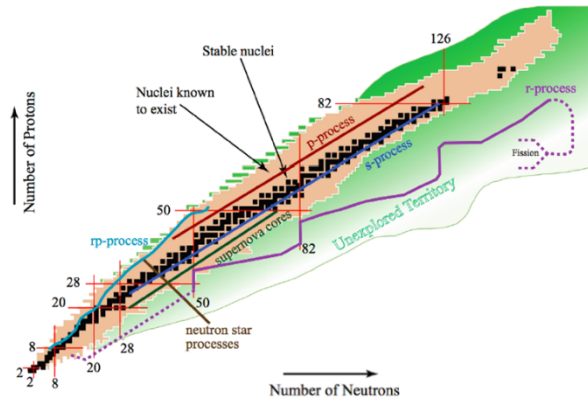
QGSP_INCLXX

QGSP_INCLXX_HP

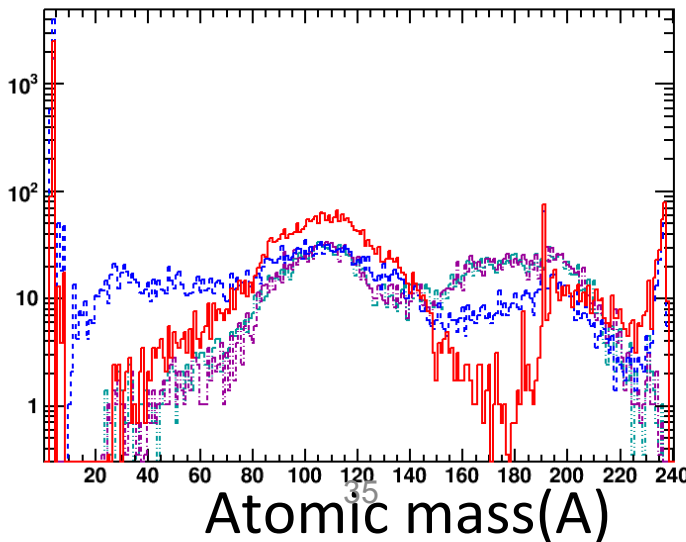
=> Selected FTFP_INCLXX

Beam Simulations (2/2)

- Application in astrophysics, nuclear imaging, ...

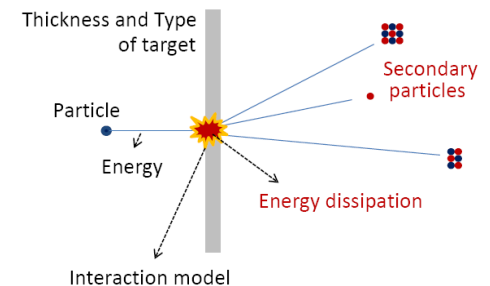


Atomic number(Z)

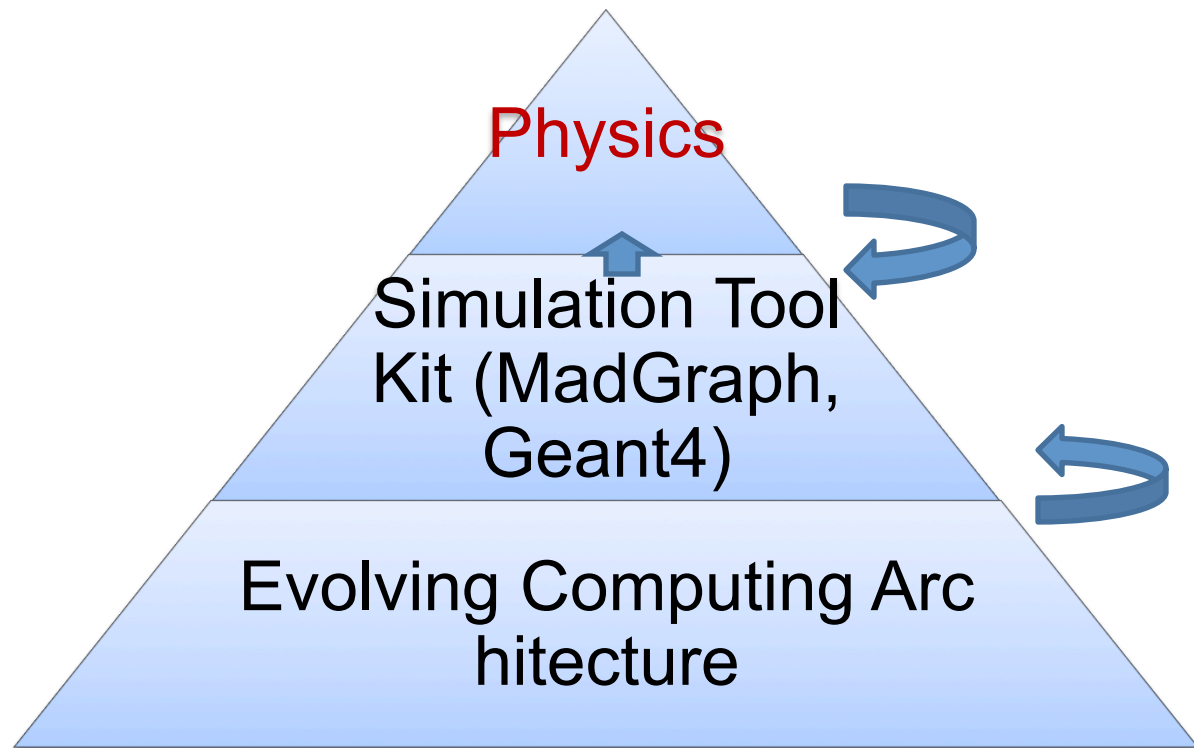


Proton beam with U Target

- 1000 GeV
- 100 GeV
- 10 GeV
- 1 GeV



Physics

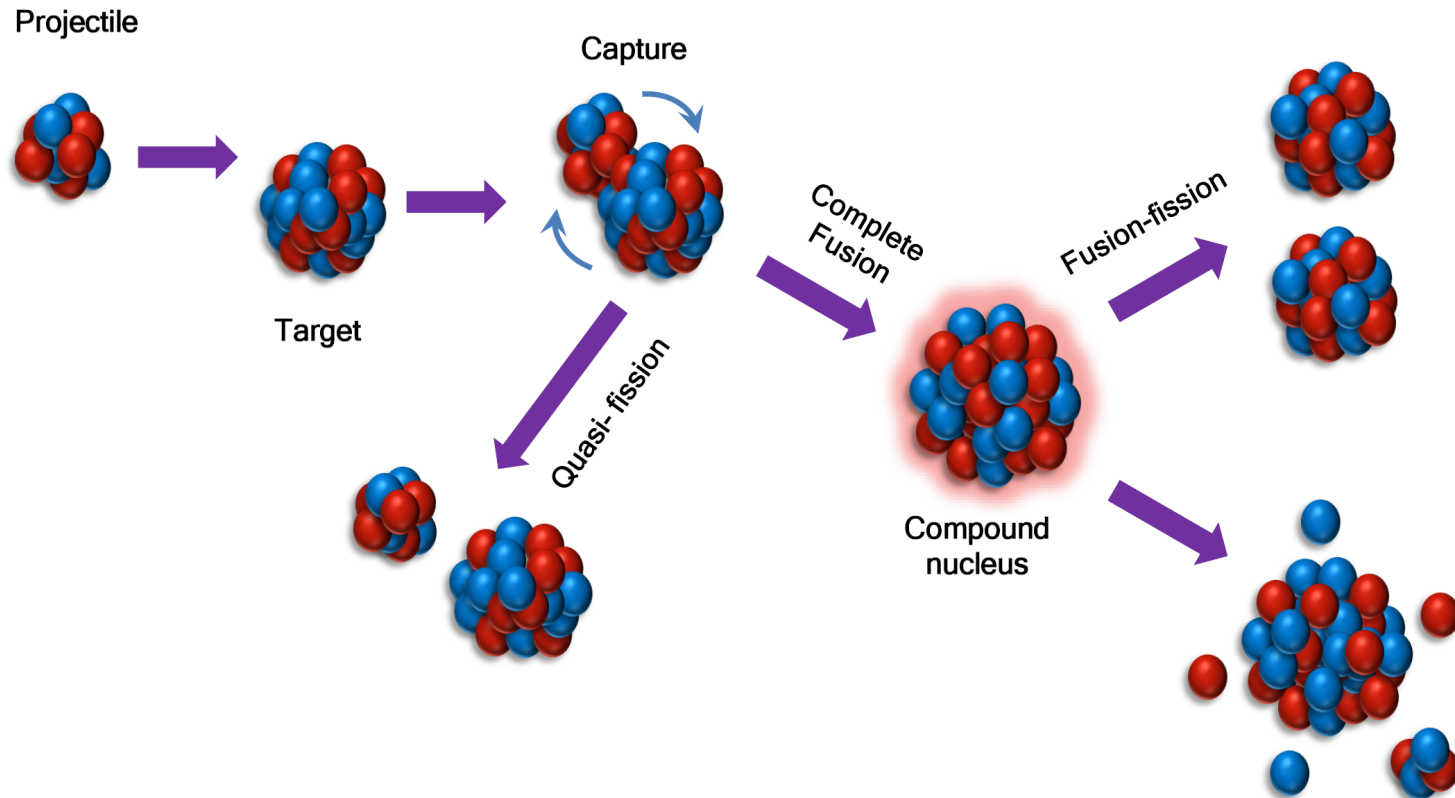


Physics

1. Production of exotic nuclei and heavy elements
2. Nuclear Structure and reactions from first principles

1. Production of exotic nuclei and heavy elements

Nuclear reactions at low energies
($< 10 \text{ MeV/n}$)



Production cross section

$$\sigma_{Z_i, N} = \sigma_{cap} \cdot Y_{Z_i, N}$$

Capture cross-section

$$\sigma_{cap} = \frac{\pi \hbar^2}{2\mu E_{cm}} J_{cap}(J_{cap} + 1)$$

J_{cap} : the value of angular momentum

$J_{cap} = 90$: $E_{c.m.}$ is 20 % larger than the Coulomb barrier energy

$J_{cap} = 30 \sim 40$: $E_{c.m.}$ is similar the Coulomb barrier energy

Formation-decay probability

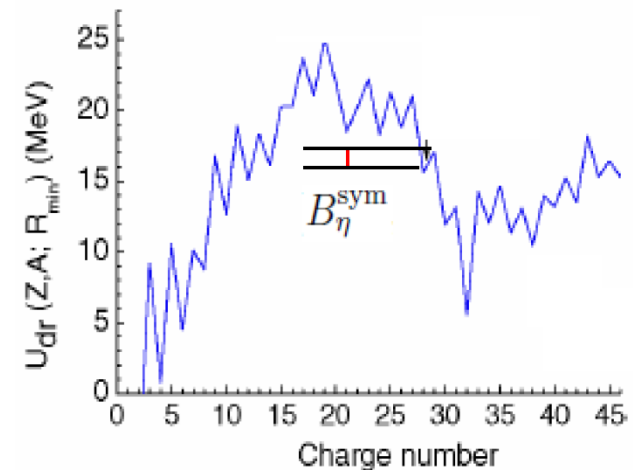
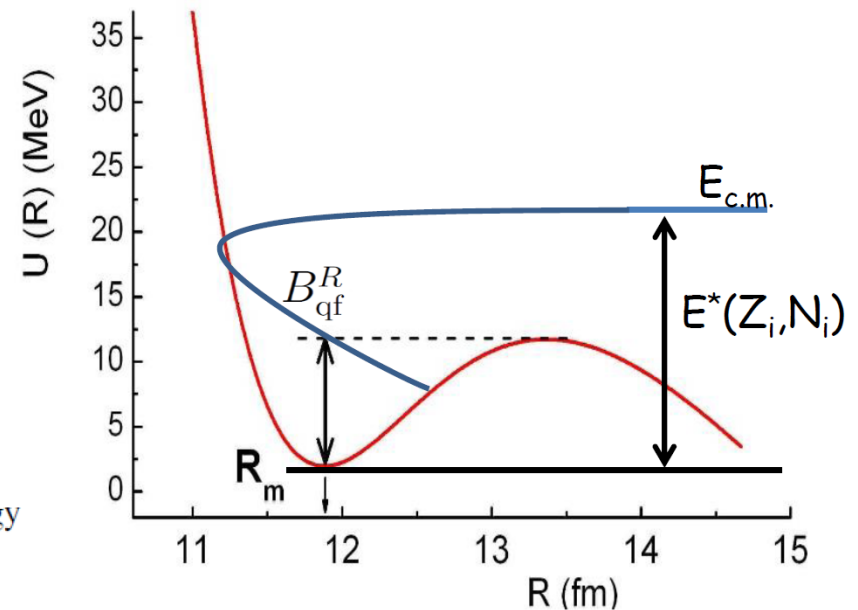
$$Y_{Z_i, N} \approx 0.5 \exp \left[-\frac{B_R(Z_i, N) - B_{qf}(Z_i, N_i)}{\Theta(Z_i, N_i)} \right]$$

$$B_R(Z, N) = U(R_b(Z, N), Z, N, J) - U(R_m(Z, N_e), Z, N_e, J)$$

$$B_{qf} = \min(B_{\eta}^{sym}, B_{qf}^R) \quad \Theta = \sqrt{E^*(Z_i, N_i)/a}. \quad a = A_{tot}/12 \text{ MeV}^{-1}$$

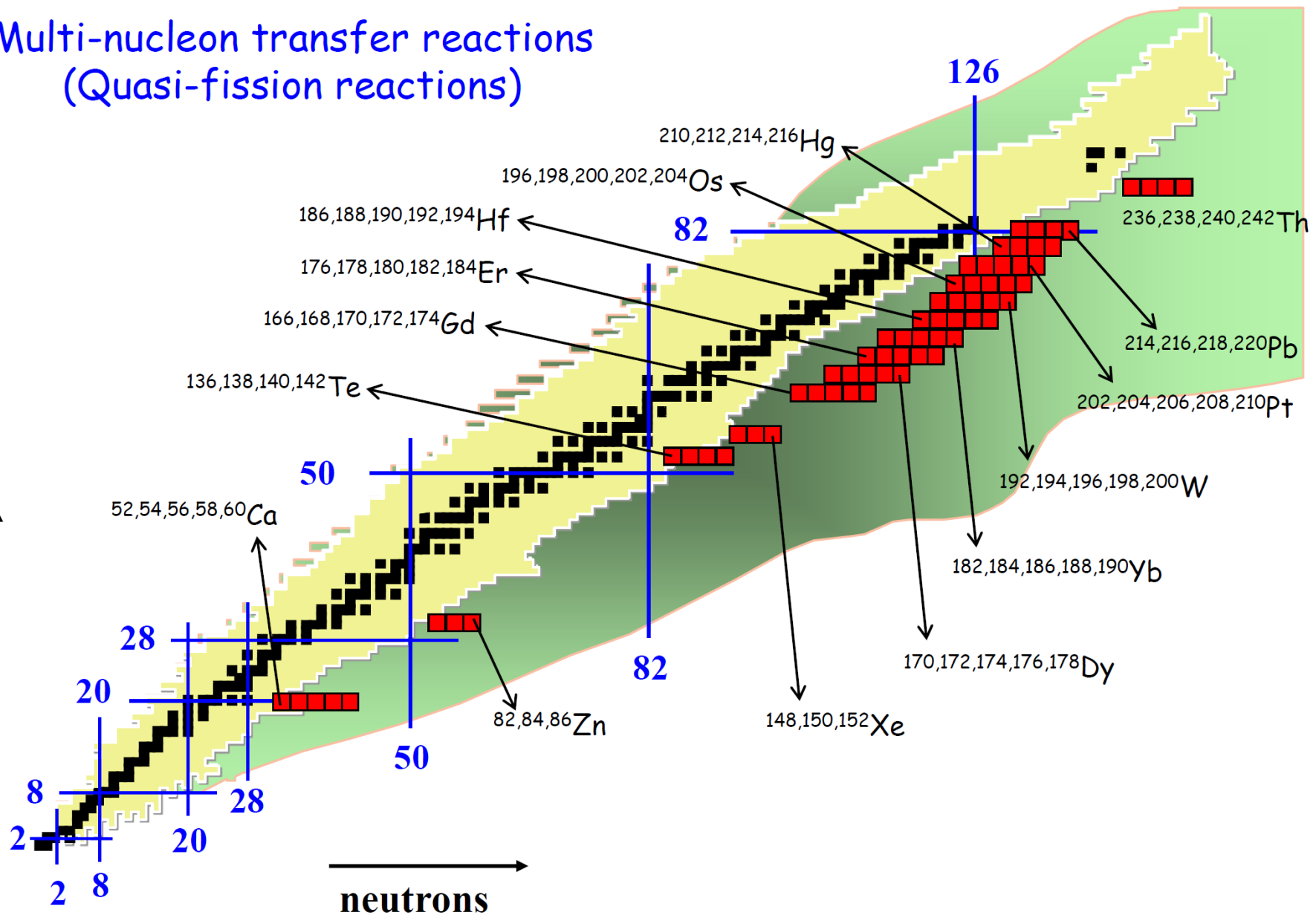
Yu.E. Penionzhkevich et al., *Phys. Lett. B* **621** 119 (2005).

M.H. Mun et al., *Phys. Rev. C* **89**, 034622 (2014).



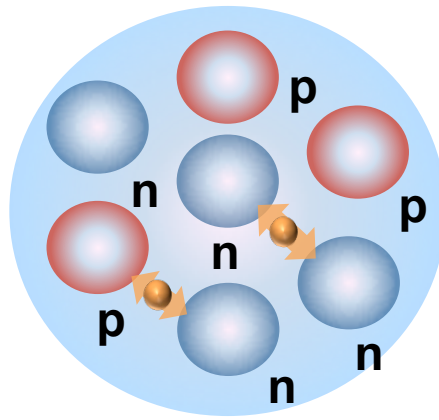
Multi-nucleon transfer reactions (Quasi-fission reactions)

protons



2. Nuclear Structure and reactions from first principles

- Ab initio: nuclei from first principles using fundamental interactions without uncontrolled approximations.
- No core: all nucleons are active, no inert core.
- Shell model: harmonic oscillator basis
- Point nucleons



- A -nucleon Schrödinger equation

$$\hat{H} \Psi(r_1, \dots, r_A) = E \Psi(r_1, \dots, r_A)$$

- Hamiltonian with $NN(+NNN)$ interactions

$$\hat{H} = \frac{1}{A} \sum_{i < j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i < j} V_{ij} + \sum_{i < j < k} V_{ijk} + \dots$$

- Wave functions are expanded in basis states

$$\Psi(r_1, \dots, r_A) = \sum a_i \Phi_i(r_1, \dots, r_A)$$

basis states Φ_i : Slater determinants of single particle states

Requested resources @KISTI-5 supercomputer	Total core time	1,500,000 node time - node/job: 4,000 node - Core time/job: 1 hours - Number of Total job: more than 20 /nuclide
	Memory	500 TB
	Hard disk	10 GB

Summary

- Computing needs solutions for the evolving architecture (KISTI-5).
- To fulfill the gap between physics and computing, we also need to focus on simulation R&D.

⇒ Physics goes beyond discovery.

Acknowledgement

- Insung Yeo
- Myeong Hwan Mun
- Soon Yung Jun
- Youngman Kim

Thank you.

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Backup

Expanding to other Scientific Domains

Experience on WLCG Tier-1 operation and service has given **many benefits** to expand its service availability to **other scientific domains in Korea**

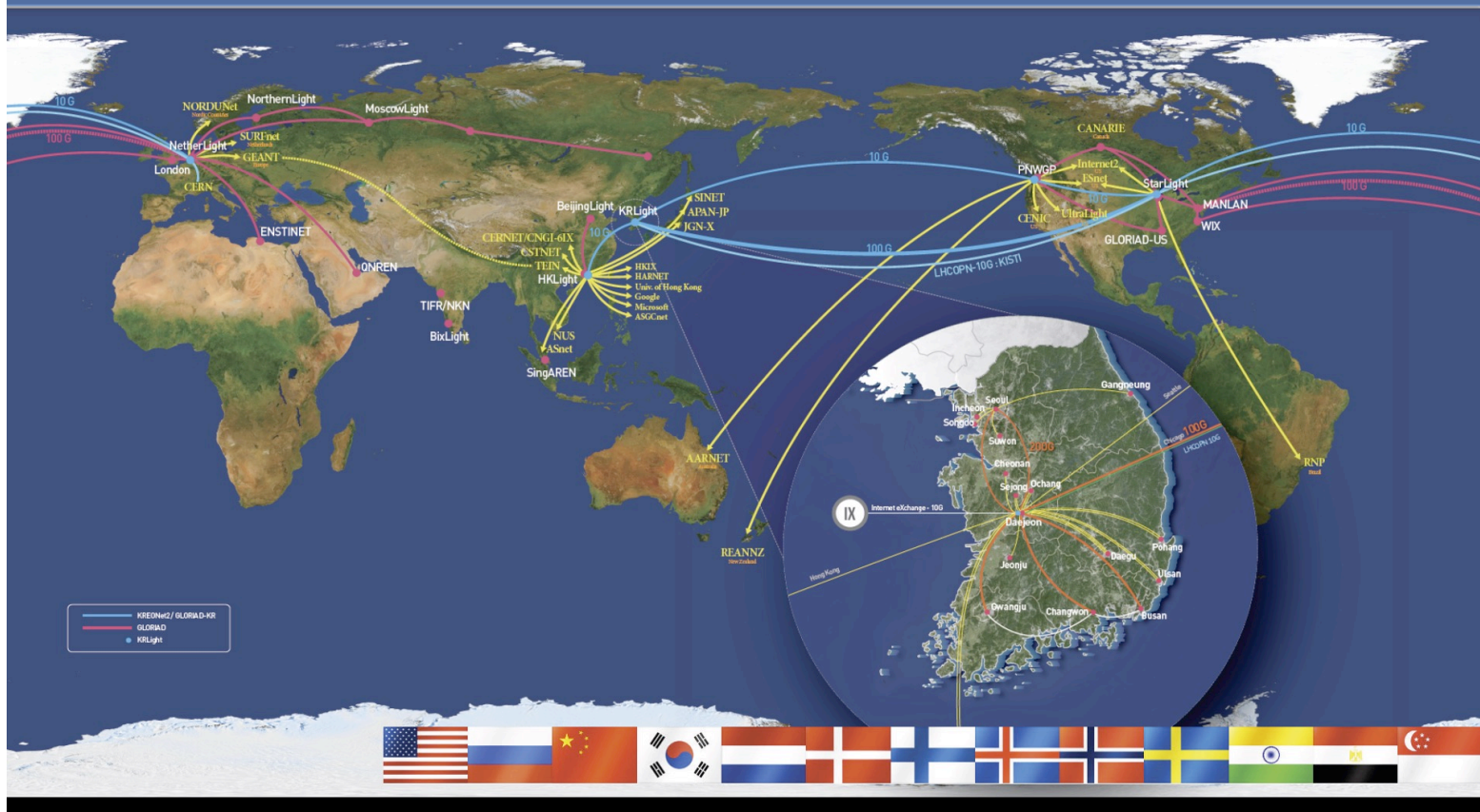


and it is still expanding to many other research areas.

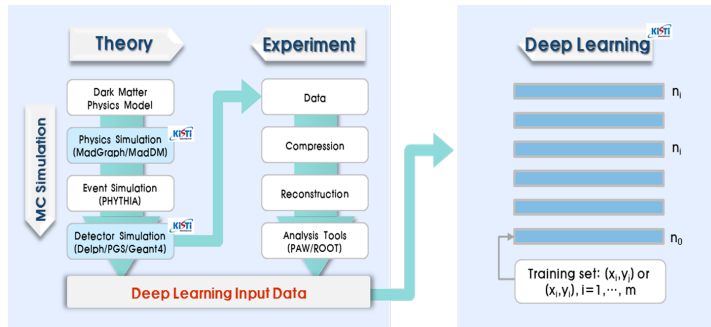
Service for additional domestic experiments is under preparation.

Network

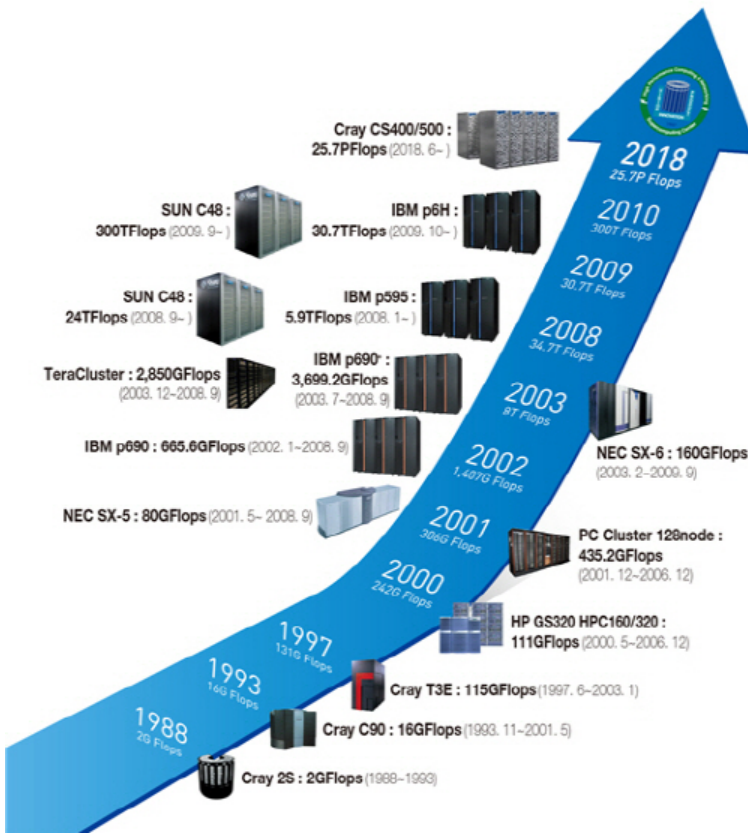
GLORIAD (GLObal RIng network for Advanced Application Development) : KREONet2, International Network of KREONET



KISTI Supercomputing



- 5th Supercomputer (KISTI-5)
 - Processing: 25.7PF
 - Heterogenous: 25.3PF CS400 w/KNL
 - CPU: 0.4PF CS500 w/SKL
 - Storage
 - 20PB SPS
 - 10PB Archive
 - Schedule
 - Installing now
 - Service (2Q, 2018)

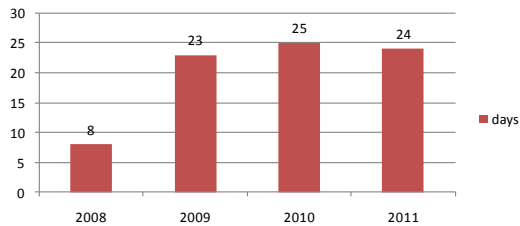


Cyber HEP environment

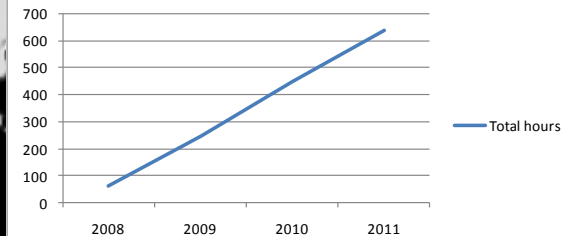
CDF Remote Control Room



CDF Remote Control Room
(2011.10.1)



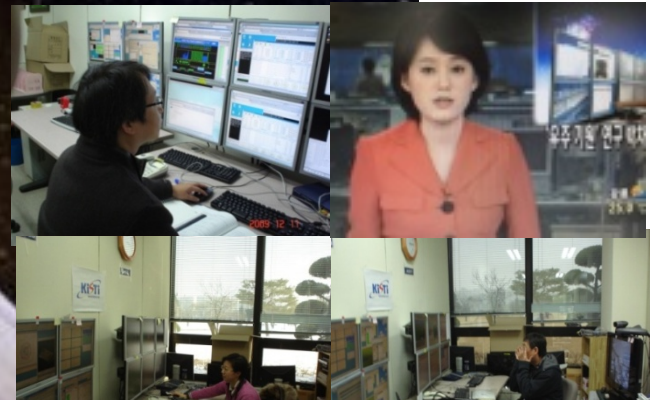
CDF Remote Control Room
Total used hours (2011.10.1)



CDF Operation Center



KISTI Remote Control Room



We take shifts at KISTI even if we are not at Fermilab.

Belle II Data Handling system

KISTI-5 supercomputer

누리온
NURION

온 국민이
다 함께 누리는
슈퍼컴퓨터



KISTI-5 supercomputer



구분	소구분	계산노드	CPU-only 노드
모델명	시스템 모델명	Cray CS400	Cray CS500
	노드수	8,304 +1	132
	랙수	116	2
성능	이론성능	25.297306 PFLOPS	0.405504 PFLOPS
CPU (또는 가속기)	모델명	Intel Xeon Phi 7250 (KNL)	Intel Xeon 6148 (Skylake)
	CPU 이론 성능	3.0464 TFLOPS	1.536 TFLOPS
	CPU당 코어수	68	20
	노드당 CPU수	1	2
	on-package 메모리	16 GB, 490 GB/s	-
HCA	모델명	Intel 100HFA016LS	Intel 100HFA016LS
메인 메모리 (off-package)	메모리 모델	16 GB DDR4-2400	8 GB DDR4-2666
	메모리 구성	16GB x6, 6ch per CPU	8GB x12, 6ch per CPU
	노드 당 메모리 크기(GB)	96 GB	96 GB
	CPU와 메모리 간 대역폭	115.2 GB/s	128 GB/s
	전체 메모리 용량	778.50 TB	12.38 TB
로컬디스크	모델 및 노드당 용량	N/A	N/A
고성능 인터커넥트	토폴로지	FatTree	
	Blocking Ratio	50% Blocking	
	네트워크스위치	274x 48-port OPA edge switches 8x 768-port OPA core switches	
	포트당 단방향 대역폭	12.3 GB/sec	
	Bisectional Bandwidth	27,060 GB/sec	
Burst Buffer (BB)	서버수	DDN IME240서버 40대	
	노드 구성안(NVDRAM, SSD)	NVMe SSD	
	전체 용량	0.8PB usable	
	서버당 대역폭	서버당 20 GB/sec, 전체는 0.8TB/s	
	Scratch MDS	DDN SFA7700X 1대, MDS 2대	
	Home/Apps MDS	DDN SFA7700X 1대, MDS 4대	
	Scratch OSS	DDN ES14KX 9대(각360 x 8TB장착)	
	Home/Apps OSS	DDN ES14KX 1대(각400 x 4TB 장착)	
	전체용량	20PB usable, RAID6 (8D+2P)	
	전체대역폭	0.3TB/s	

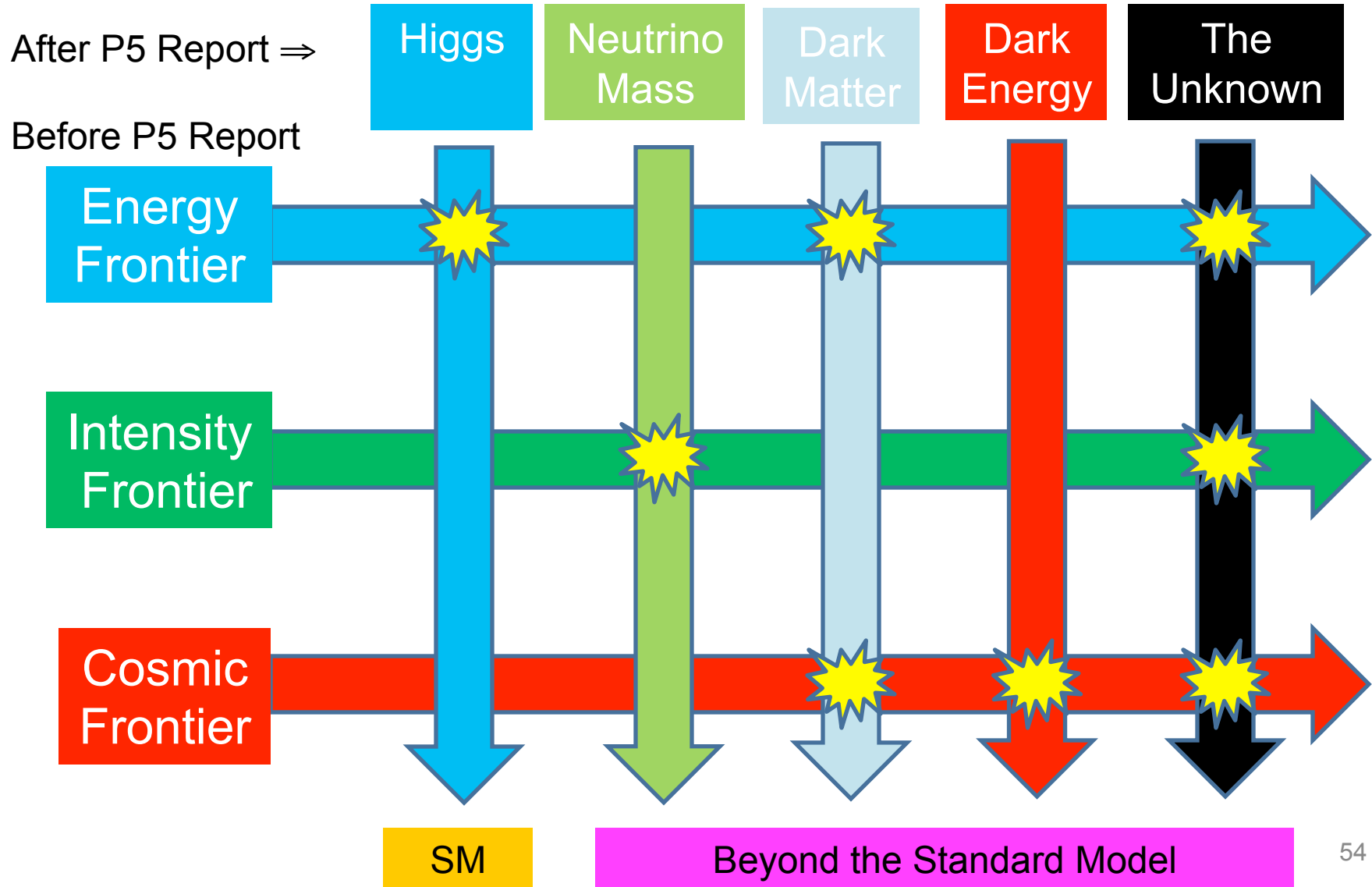


✓ 멀티코어 프로세서인
인텔 제온(Xeon)
스카이레이크(Skylake)
프로세서를 장착한
CPU 노드

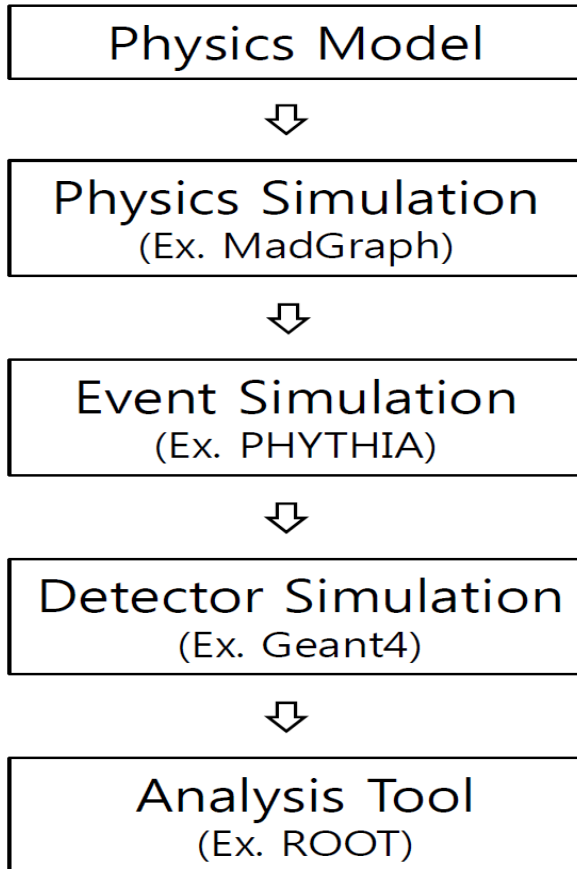
✓ 미니 코어 프로세서인
인텔 제온 파이(Xeon Phi)
나이트랜딩(Knights Landing)
프로세서를 장착한 가속기 노드

0.4 PF 대용량
25.3 PF 스토리지

P5 Report (May 22, 2015)



HEP Simulation



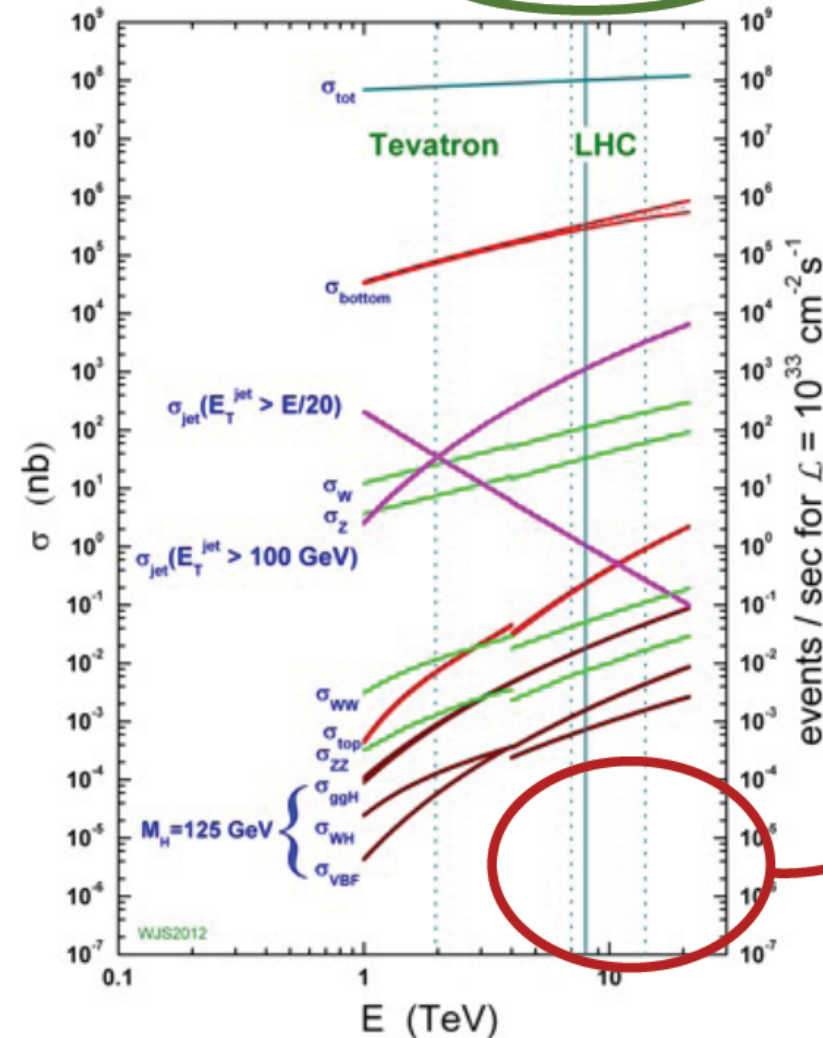
Geant4 Collaboration



Beyond the Standard Model

proton - (anti)proton cross sections

= production rate: to be calculated



◆ This is where any new phenomenon would hide

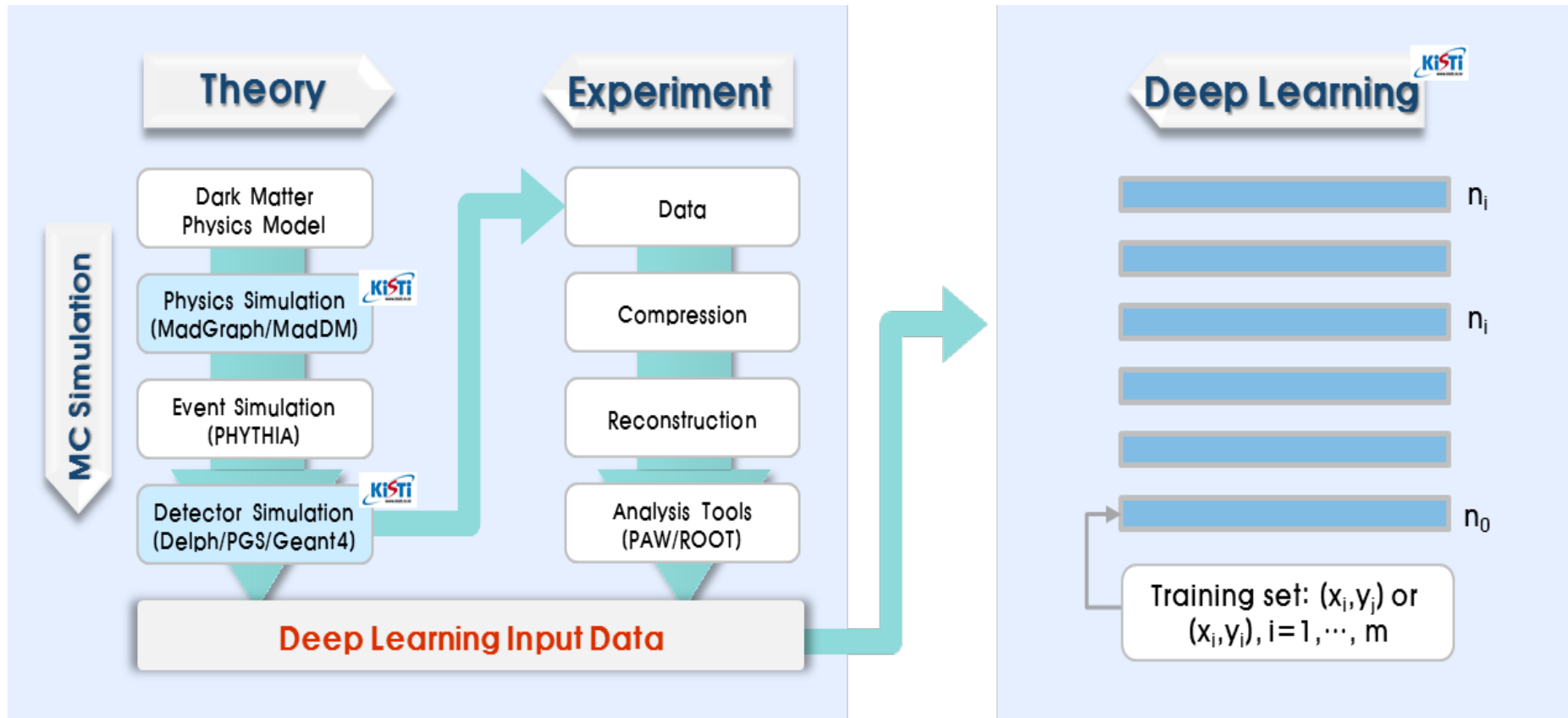
- ❖ Supersymmetry
- ❖ Extra-dimensions
- ❖ Grand-Unified Theories
- ❖ etc.

◆ Cross sections = production rate

- ❖ 1 possible new physics event (if any)
- ❖ 1.000 Higgs events
- ❖ 1.000.000.000.000 Standard Model events



Deep Learning



Thank you.

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