Recent Activities in CCS

Masayuki Umemura

Director

Oakforest-PACS

JCAHPC

JCAHPC: Joint Center for Advanced High Performance Computing

U. Tsukuba

計算科学研究センター
Center for Computational Sciences

U. Tokyo

東京大学情報基盤センター
INFORMATION TECHNOLOGY CENTER, THE UNIVERSITY OF TOKYO

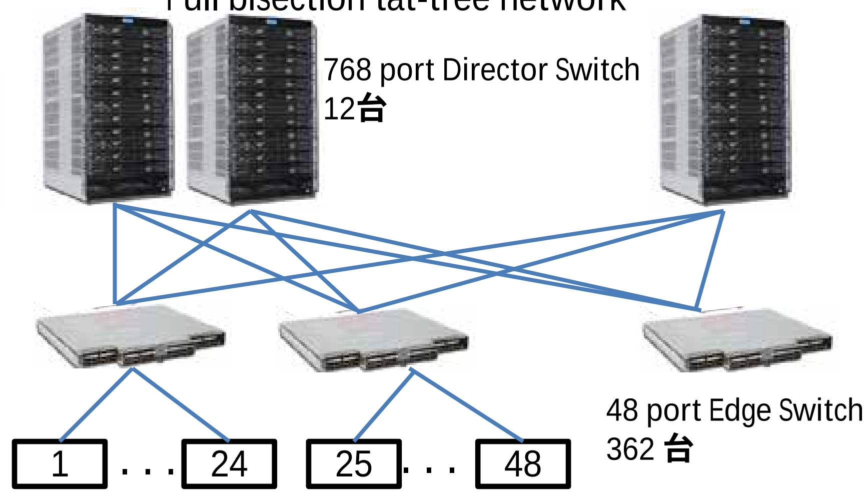
- Ø **Peak Performance 25 PFLOPS**
- Ø **LINPACK 13.55PFLOPS**

FUJITSU

Node (Fujitsu PRIMERGY CX1640 M1)
CPU Intel Xeon Phi 7250 (Knights Landing)

intel

Intel® Omni-Path Architecture
Full bisection tat-tree network



DataDirect NETWORKS

26 PB Parallel file system，940 TB High-performance file cash system

Oakforest-PACS ranks #1 in IO 500 list

Oakforest-PACS Storage System

Parallel file system (DataDirect Networks ES14KX)
File cache system (Infinite Memory Engine IME14KX): Improving the storage performance.

IO-500 benchmark in 2017

The file cache system achieved 742 GiB/s[1] for file-per-process write access that parallel processes access their own file.
and 600 GiB/s for single-shared-file write access that parallel processes access a single shared file but a different position.

OFP file cache system IME14KX

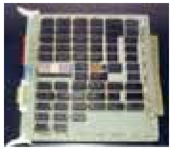
Development of Massively Parallel Computer Systems in CCS

- 1977 research begins (by Hoshino, Kawai)
- 1978 1st machine
- 1996 CP-PACS (top of Top500)
- 2006 7th machine PACS-CS
- 2012 8th machine HA-PACS

CP-PACS

- First large-scale general-purpose MPP system in Japan
    - Development supported by “Research of Field Physics with Dedicated Parallel Computers” funded by the Ministry of Education of the Japanese Government.
    - ranked as No. 1 system in the November 1996 Top 500 List.
- Collaboration by physicists and computer scientists
- Collaboration with industry, and released as Hitachi SR2201

1978
1st PACS-9



1980
2nd PAXS-32

1989
5th QCDPAX

1996
6th CP-PACS
(top of Top500 list in 1996)

2006
7th PACS-CS

2012
8th HA-PACS

2014
9th COMA

Year	System	Performance
1978	PACS-9 (PACS I)	7 KFLOPS
1980	PACS-32 (PACS II)	500 KFLOPS
1983	PAX-128 (PACS III)	4 MFLOPS
1984	PAX-32J (PACS IV)	3 MFLOPS
1989	QCDPAX (PACS V)	14 GFLOPS
1996	CP-PACS (PACS VI)	614 GFLOPS
2006	PACS-CS (PACS VII)	14.3 TFLOPS
2012	HA-PACS (PACS VIII)	1.166 PFLOPS
2014	COMA (PACS IX)	1.001 PFLOPS

2007
FIRST
(Hybrid Simulator)

36 TFLOPS

Timeline of Computing Systems in CCS

Fiscal Year | 2013 | 2014 | 2015 | 2016 | 2017 | 2018 | 2019 | 2020 | 2021 | 2022

TPF

HA-PACS (PACS-VIII) 800TF → PPX 64TF → PPX2 64TF → PACS-X ～10PF

2MW

HA-PACS TCA +366TF

340kW

UCC+TPF

T2K-tsukuba

630kW

T2K-Todai

COMA (PACS-IX) 1PF

4.5MW

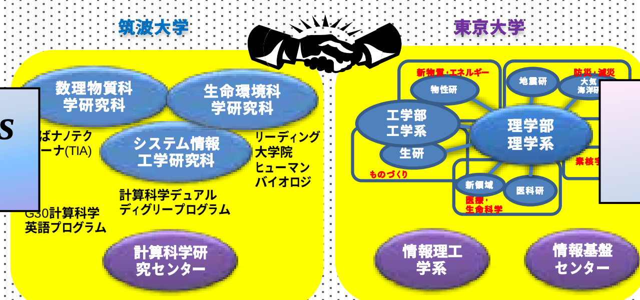
Oakforest-PACS 25PF

JCAHPC 4.2MW

TPF = Technology Path-Forward Machine
UCC = Upscale Commodity Cluster Machine

- **Joint Center for Advanced High Performance Computing (JCAHPC)**

Center for Computational Sciences
U. Tsukuba



Information Technology Center
U. Tokyo

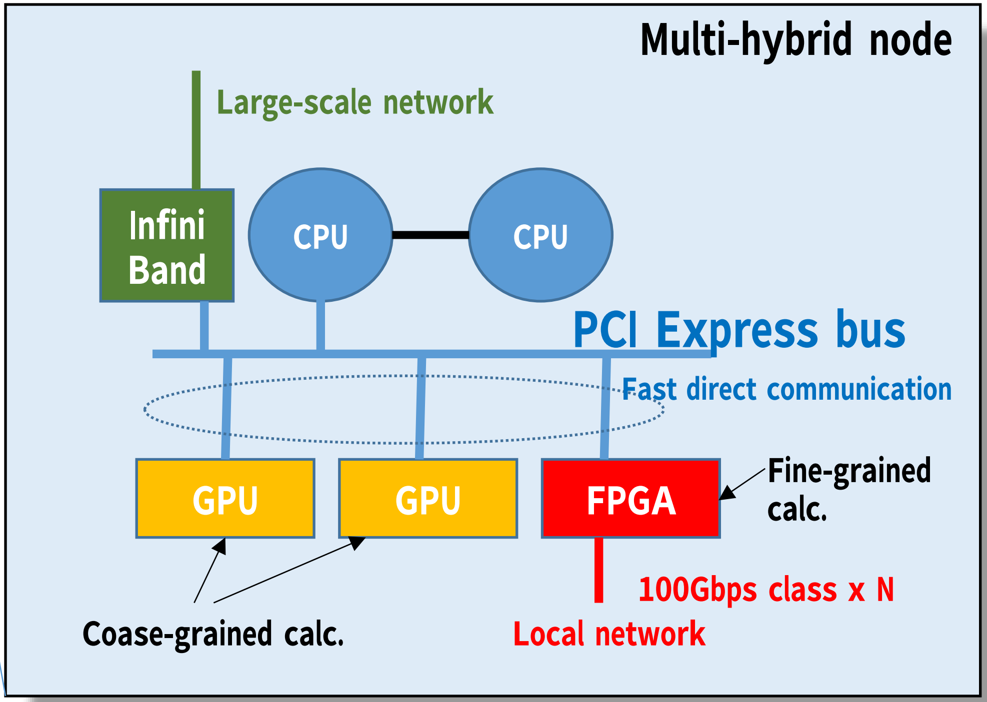
- **Feasibility Study toward Exa-scale Computing (National Project)**

PACS-X: Hybrid Accelerator System

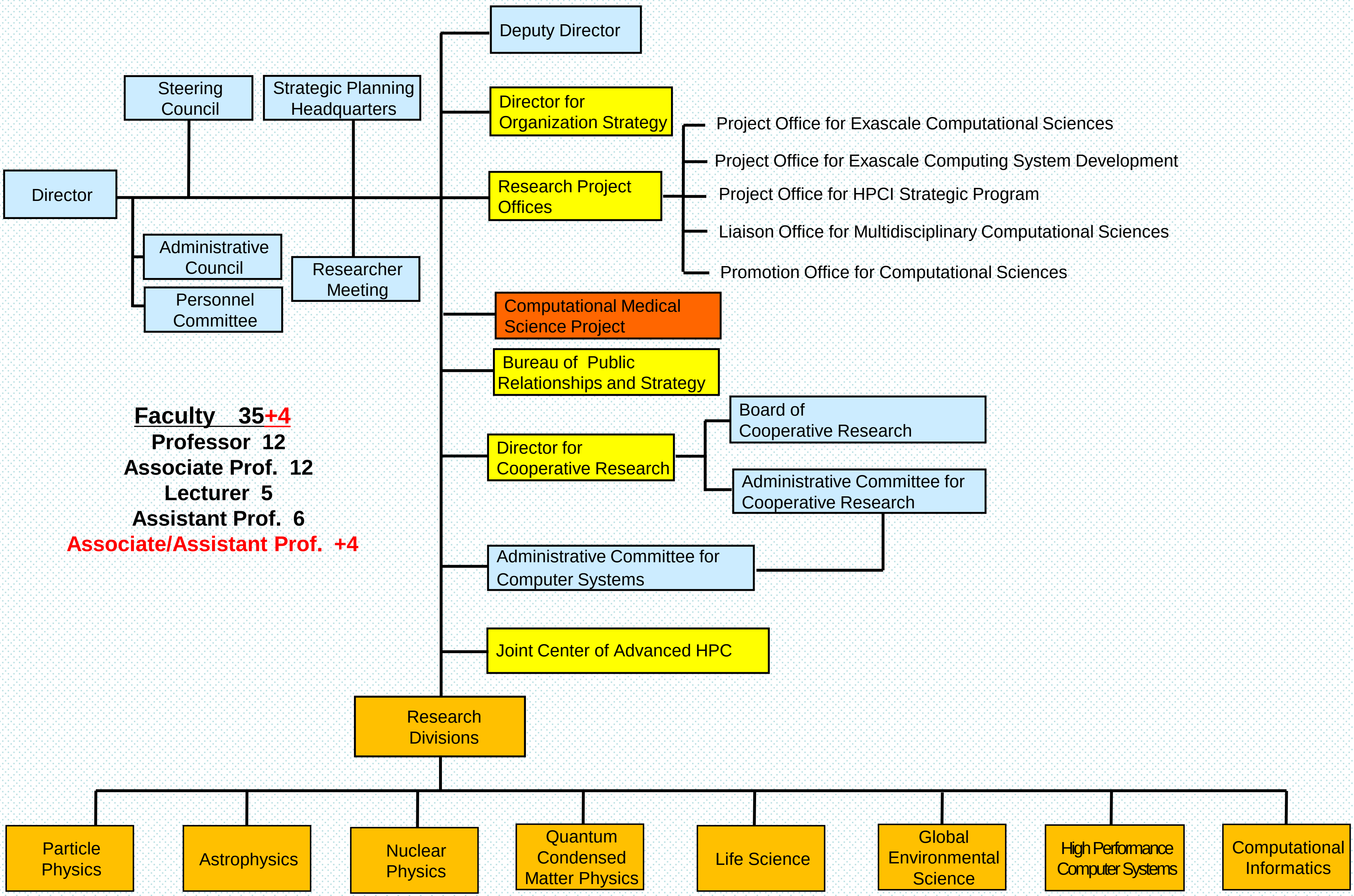
- GPU&FPGA are embedded with PCIe bas
- Local network system and off-loading with FPGA
- Acceleration of hot spots with GPU

Pre-PACS-X (PPX)

- PPX1(6nodes), PPX2(7nodes)
- Optimization of off-loading with FPGA



Organization of CCS



Faculty 35+4
Professor 12
Associate Prof. 12
Lecturer 5
Assistant Prof. 6
Associate/Assistant Prof. +4

Development of Novel Scientific Fields

Computational Medical Science Project

Development of medical technology by computational science in cooperation with medicine, physics, biology, mathematics, data science, and image processing technology.

Computational Biomolecular Medical Science

Collaborations： Medicine, Biology, and Physics

Drug discovery, detection of SNP, and physical mechanism analysis by bioinformatics and simulations

Sleep Big Data Analytics & Automatic Sleep Diagnosis

Collaborations：IIIS, C-AIR, CCR

System for automatic analysis of EEG (electroencephalogram) in sleep with machine learning and deep learning

Computational Medical Science

Life Science

Data Science

Computational Media

Computational Physics

3DCG Virtual Surgery

Collaborations：Medicine, Engineering, Design

Development of surgical operation support system using computational surgery in cooperation with Medical, System Information Engineering, Information Media researches

Computational Optical Bioimaging

Collaborations：Biomedical optics, Mathematics

Development of non-invasive near-infrared computed tomography in cooperation with biomedical optics, radiation transfer physics, and mathematical inverse problem.

Industry

Computational Biomolecular Medical Science

Main Target
- Medium size drugs
- Covalent bond-type drugs
- Single Nucleotide Polymorphism

Current Problems
- Diversity in Structures (Vast Conformations)
- Reaction Control (First-principles Calculations)
- Fast Gene Analysis

Drug discovery needs long time (10～15 year) and a lot of fund ($1billion). But the success ratio is less than 1/20000
We needs a breakthrough for in silico drug discovery, i.e. detection of target, design of drug and proteins & etc.

→ Fusion of Biology, Medicine, and Physics to solve these problems

Evolution

Prof. Y. Inagaki
Department of Biology

Computational Biology

Next-generation sequencer

Fast Single Nucleotide Polymorphism detection

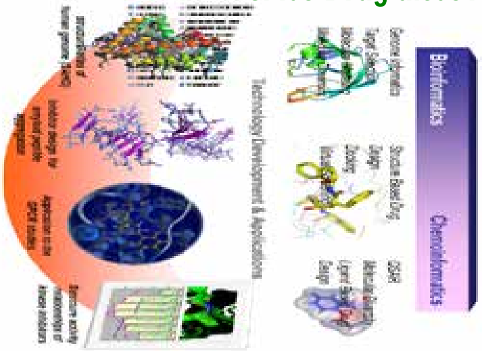
Phylogenetic tree analysis by GPU
Mitocondrial protein detection by supercomputer

Gene analysis
SNP analysis

Drug Simulation

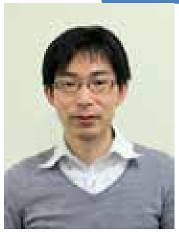
Prof. T. Hirokawa
Department of Medicine
& AIST

Bioinformatics,
In Silico Drug discovery



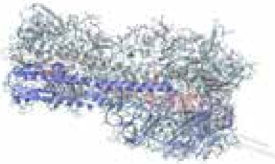
In Silico drug discovery project by AMED since 2017.

First-principle

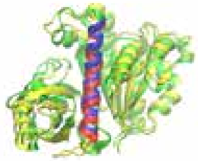


Prof. Y. Shigeta
Department of Physics

Biophysics, First-principles calculations



Influenza HA3
First-principles Calculation



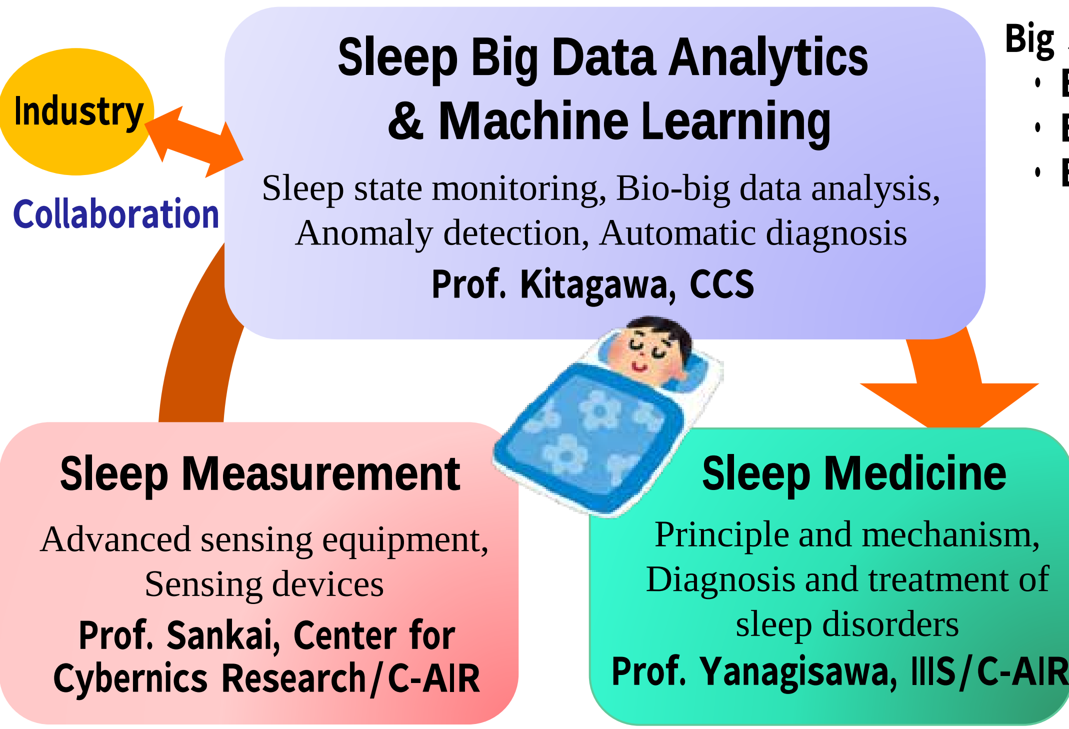
Molecular dynamics of FtsZ In cell fission

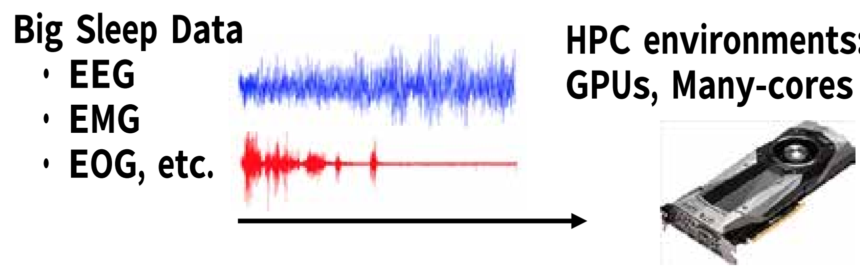
Fragment molecular orbital by GPU architecture
Efficient sampling method by Molecular Dynamics

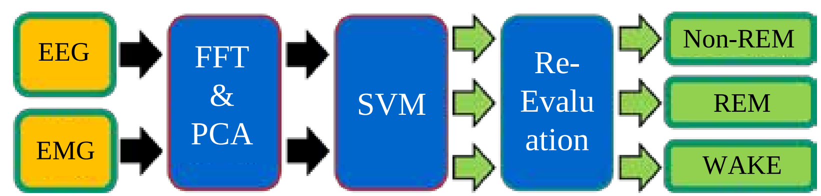
Post K Computer Project by MEXT since 2015

Sleep Big Data Analytics & Automatic Sleep Diagnosis

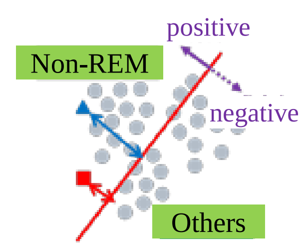
- Sleep plays an important role in daily life of people. Sleeping problems could trigger various diseases.
- There has not been any means for conveniently measuring the sleep state as accurately as medical doctors and technicians.
- Integrate bio-big data analysis, machine learning, and new sensing technology to realize automatic analysis and diagnosis of sleep.



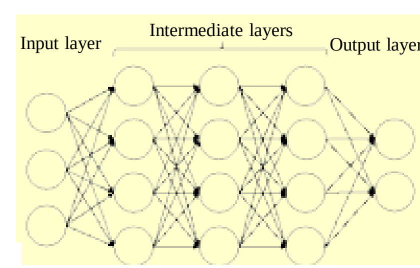




Big data analytics: Machine Learning, Deep Learning



Classifier for Non-REM



Collaboration within campus

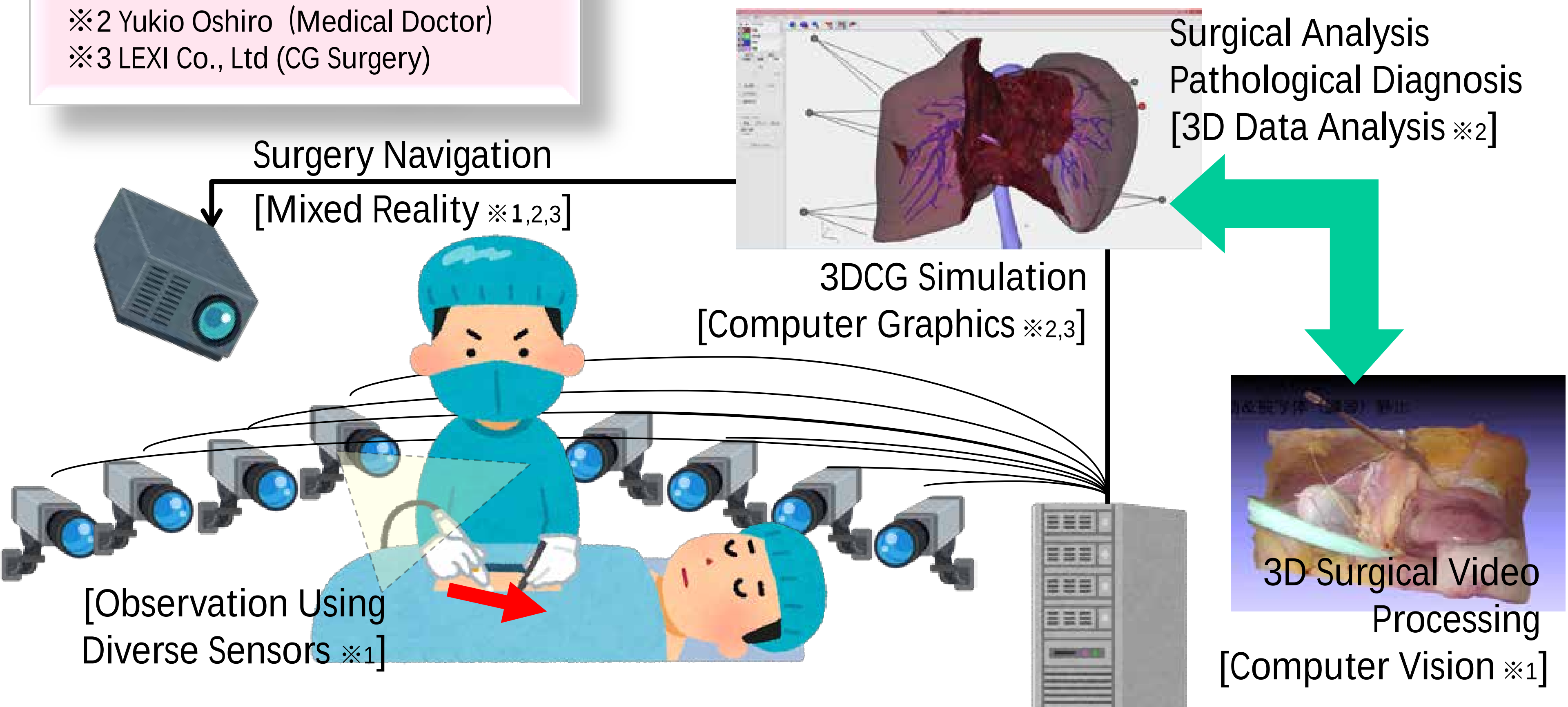
MEXT: Regional Innovation Eco-system Development

MEXT: Grant-in-Aid for Scientific Research on Innovative Areas

3DCG Virtual Surgery

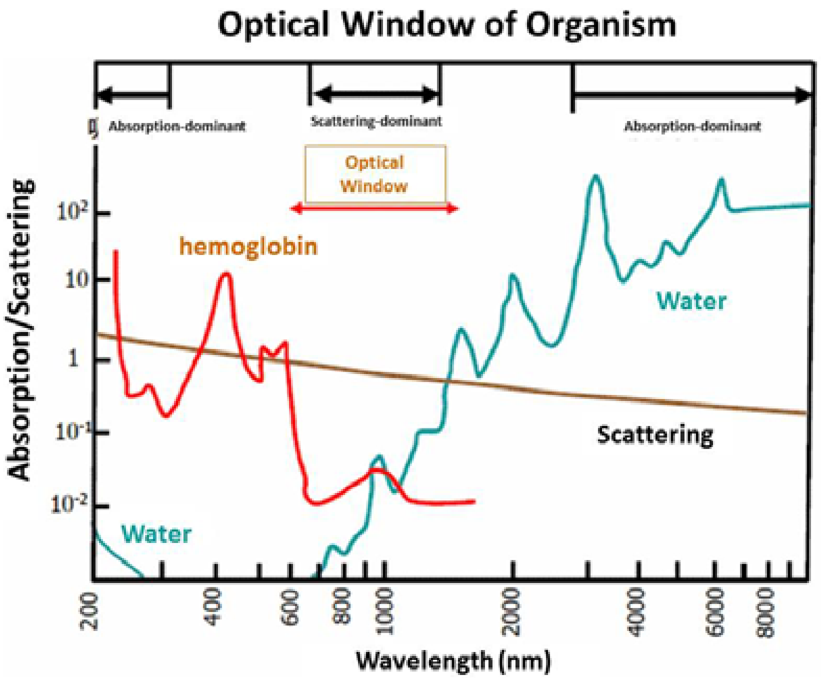
- **Improving instruction level**: Integration of 3D CG simulation and onsite navigation.
- **Solving surgeon shortage**: VR remote operation, advanced skill passing.
- **Boosting medical education**: Evaluation of surgical procedures and proficiency.

Collaboration Team
※1 Itaru Kitahara (CCS)
※2 Yukio Oshiro (Medical Doctor)
※3 LEXI Co., Ltd (CG Surgery)

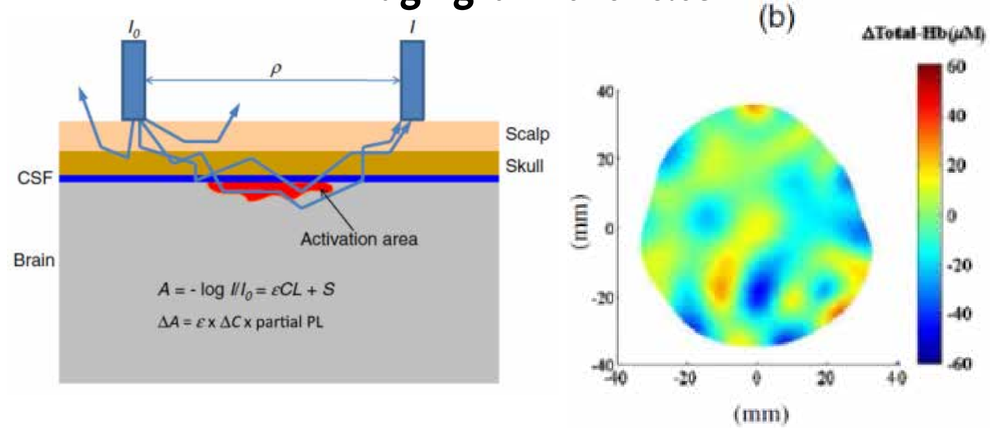


Computational Optical Bioimaging

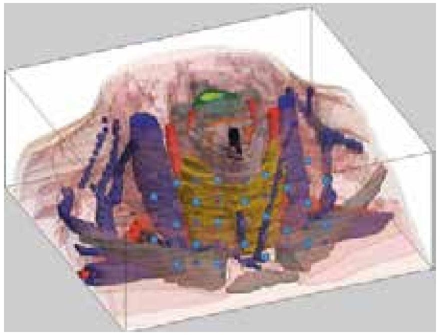
- No explosure, non-invasive, no side effects like CT or MRI, applicable to new-born babies and infants
- Bed side inspection, low cost, low restraint, high time resolution, automatic and remote diagnosis, monitoring, screening
- Diagnosis of cancers in thyroid, mammary gland, surface tissue, blood flow, ventricles, subarachnoid, etc.



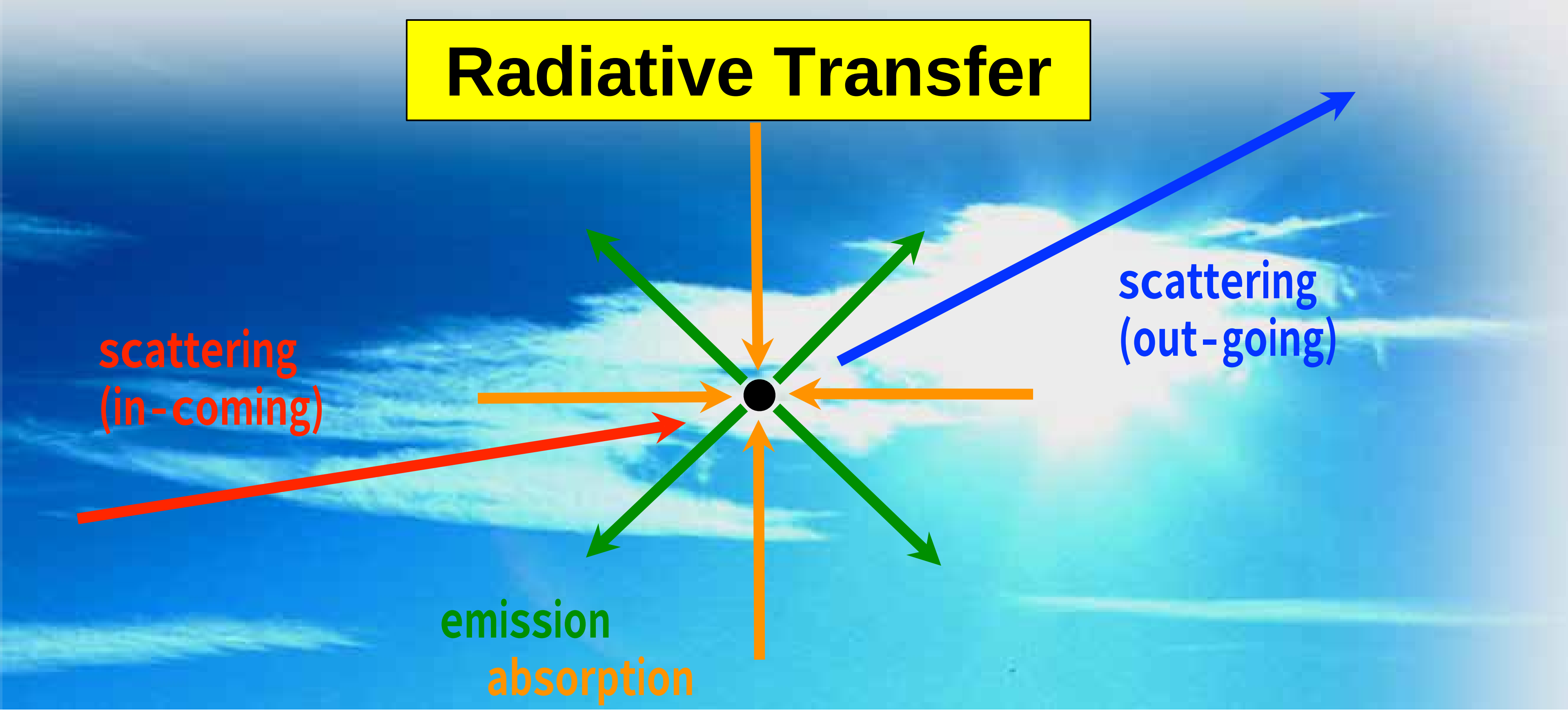
Imaging of ventricles



Imaging of thyroid gland



Radiative Transfer



Time-dependent Radiative Transfer Equation

(Photon Boltzmann equation in phase space of 3D space, 2D direction, and 1D frequency.)

$$\frac{1}{c}\frac{\partial I_\nu(\mathbf{n})}{\partial t} + \mathbf{n}\cdot\nabla I_\nu(\mathbf{n}) = \frac{\eta_\nu}{4\pi} - \kappa_\nu I_\nu(\mathbf{n}) - \sigma_\nu I_\nu(\mathbf{n}) + \sigma_\nu \int \phi(\mathbf{n};\mathbf{n}') I_\nu(\mathbf{n}') d\Omega'$$

emission

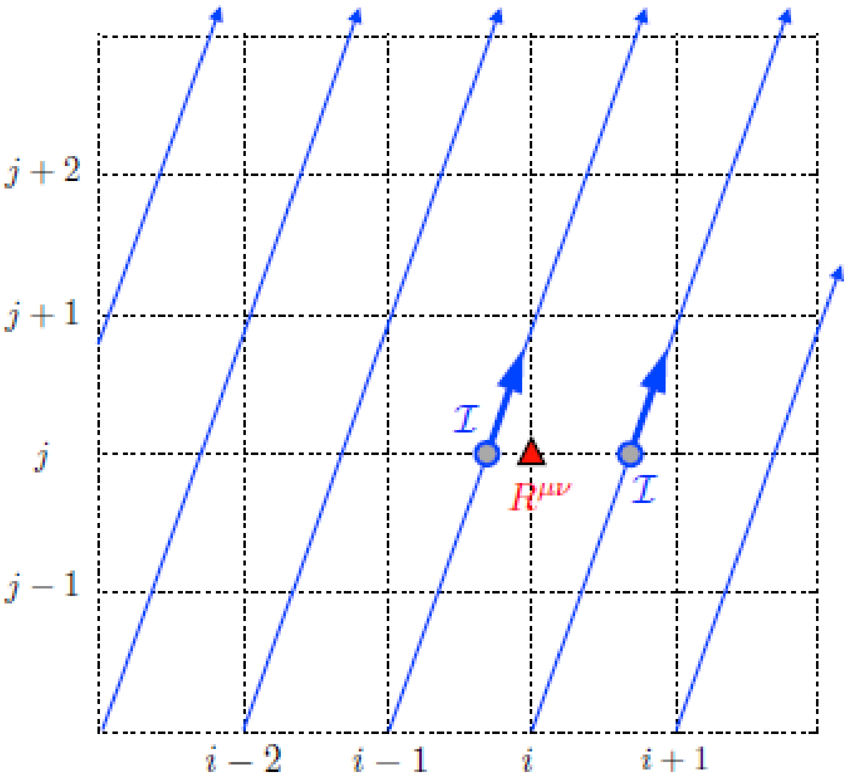
absorption

scattering (out-going)

scattering (in-coming)

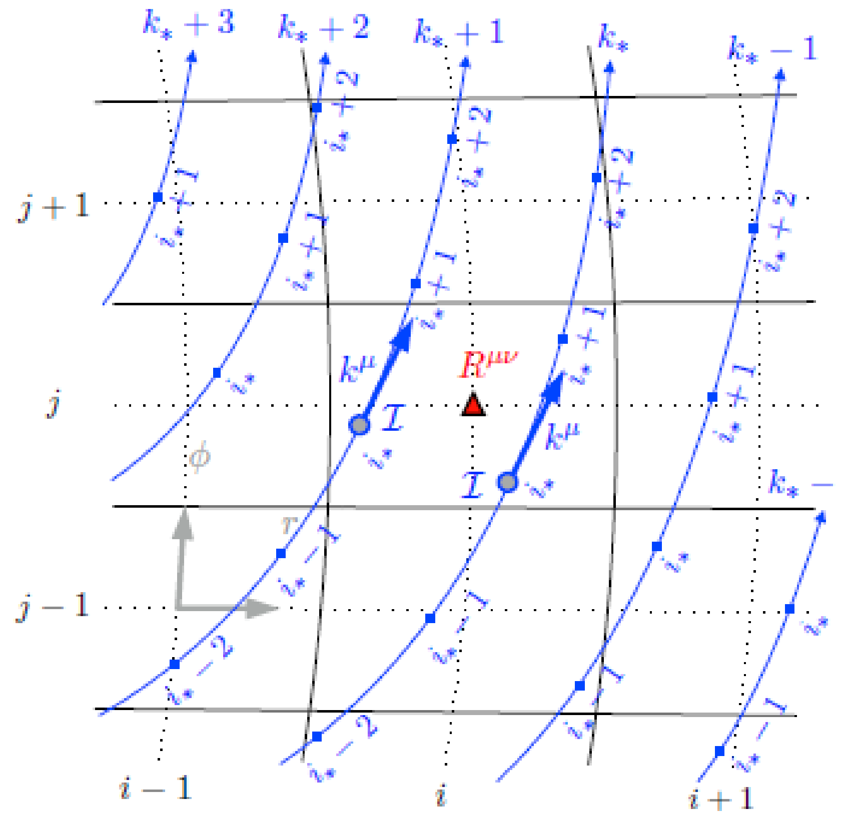
ART code
(Authentic Radiative Transfer)

Non-relativistic steady-state radiation transfer



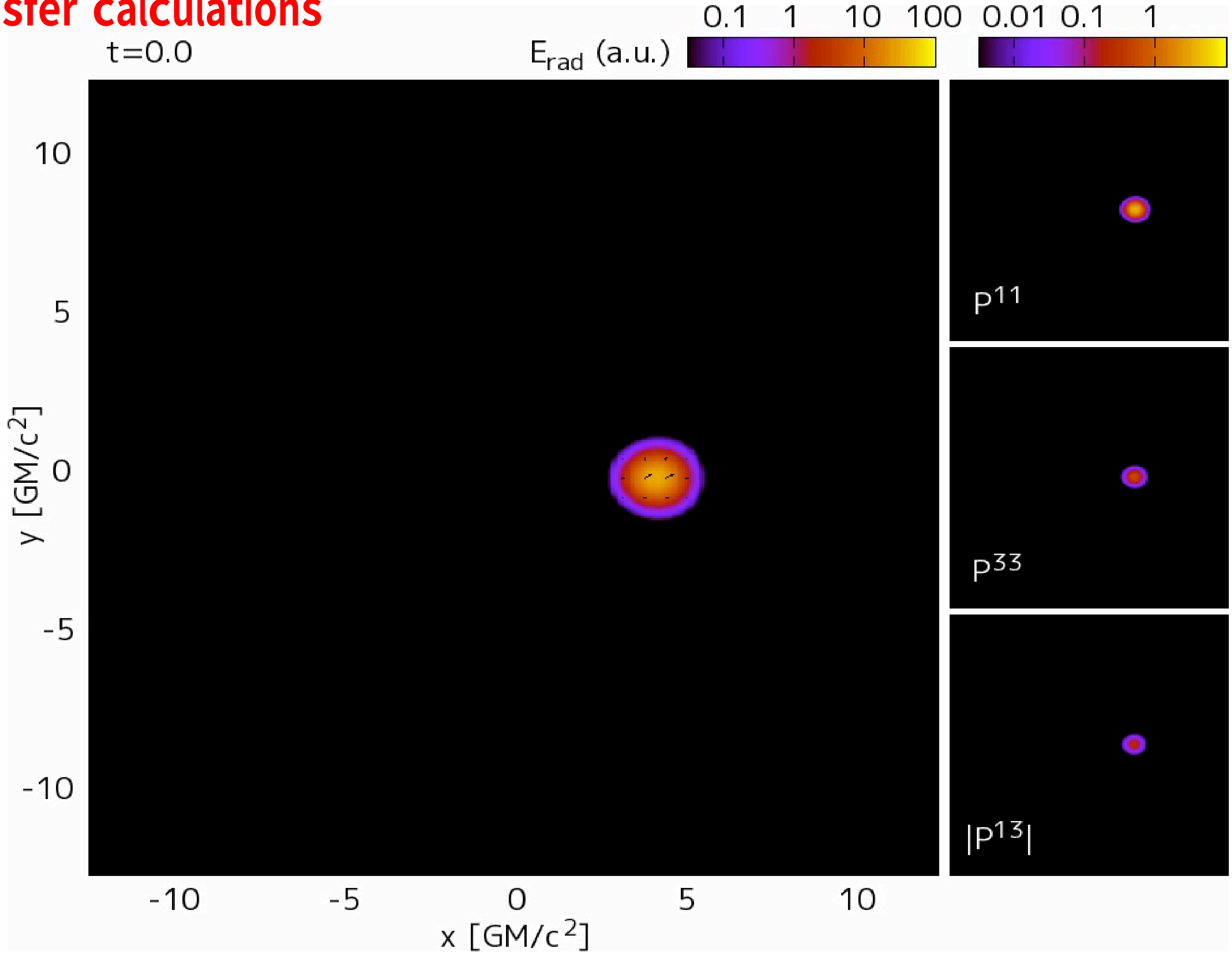
ARTIST code
(Authentic Radiative Transfer In Space-Time)

General relativistic time-dependent radiation transfer

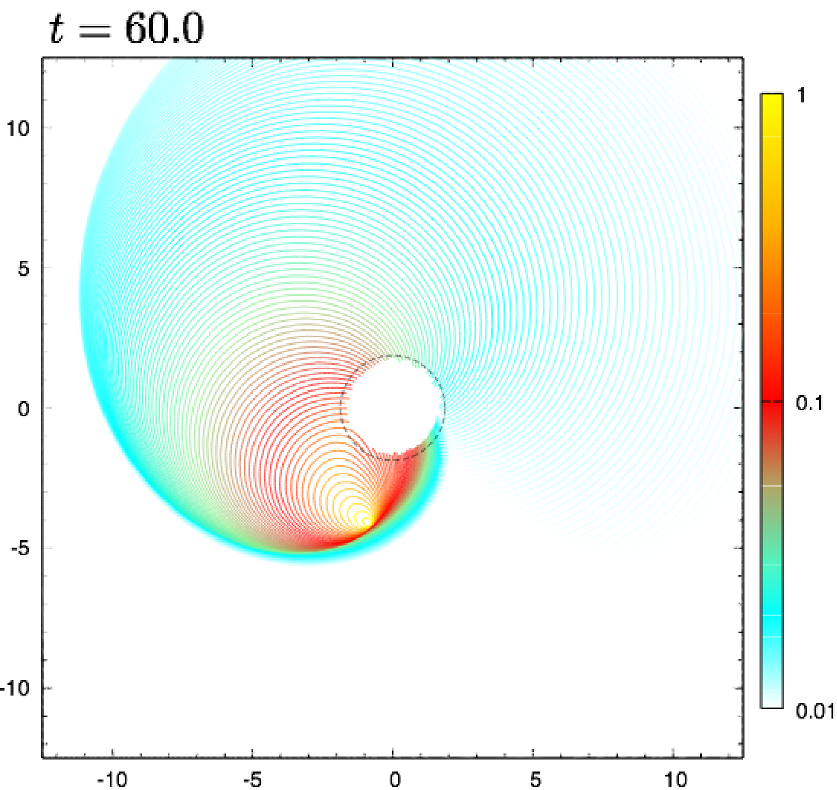


Dynamical Test 2 by *ARTIST* : Photon wave front from a rotating hot spot

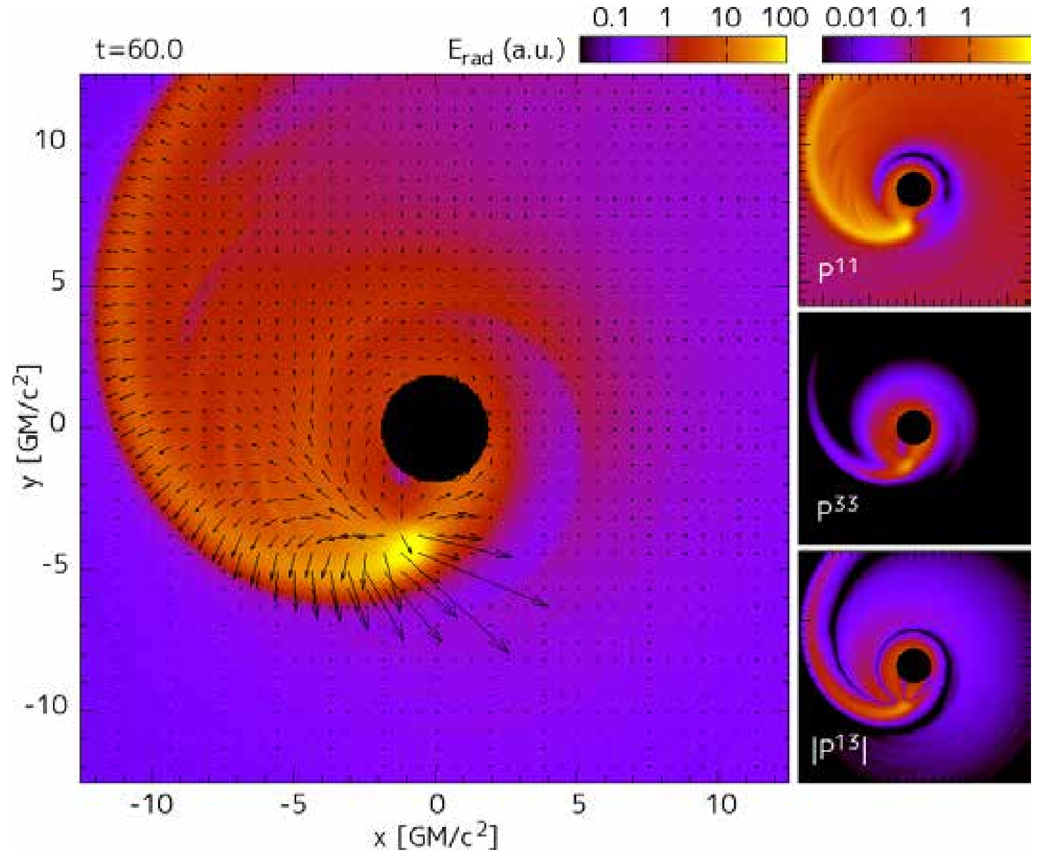
Transfer calculations



Ray-tracing calculations by *MASTER*



Transfer calculations by *ARTIST*



N_i (r)=90, N_j (f) =256

Geodesics=4608

Accurate Algorism of Image Reconstruction

Biomedical Optics

Diffuse Optical Tomography (DOT) , Photoacoustic Imaging (PAI), Fluorescence Tomography

Direct Problem Analysis

Numerical solution of radiative transfer with absorption, scattering, and reflection.

Inverse Problem Analysis

Mathematical Analysis of non-linear optimization problem.