

Kenji ONO and Jorji Nonaka

High-performance Computing Team
Integrated Simulation of Living Matter Group
Computational Science Research Program
RIKEN





#### TOC

- Supercomputer development project
  - Computer Hardware development
  - Grand Challenge in Life Science
- Post-process system
  - Current status of system design

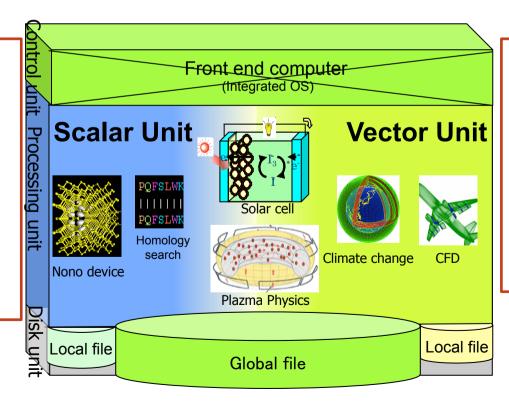
#### NEXT-GENERATION SUPERCOMPUTER



- Development
  - Under initiative of MEXT
  - Riken is responsible for dev. in collaboration with vendors
- Hybrid System composed of Scalar and Vector Units
  - LINPACK 10PFLOPS

Scalar Unit
Data base,
homology search
Similarity with PC

- high speed low power CPU
- New strong network for enormous parallelism



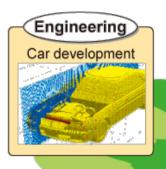
Vector Unit
Vector processor
based on the Earth
Simulator

 New generation low-power vector processor with optical network

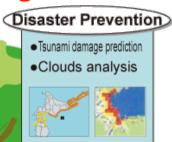
#### EXPECTED MAJOR APPLICATIONS





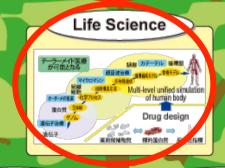




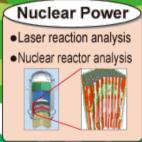


- Applications
- Benchmark
- Grand challenge
- •Focusing on life science









#### Astrophysics

- Milky Way formation process
- Aurora outbreak process
- Planet formation process





#### Issues to be considered

- Large-scale nature of data
  - computational space, time-varying, multivariate
  - Expected data size is order of 1PB (Peak)
- Data Tsunami
  - How to do vis., data processing, analysis?
  - Depend on each researcher
  - Various scenarios
- Complex hardware
  - Various configurations



#### **CURRENT STATUS AND GOAL**

- System design
  - To develop user-friendly post-processing system
  - Derive useful information from Large-scale dataset
  - Easy to use
  - Enhance productivity



 To assist scientific knowledge and understanding physical phenomena



 Operating this post-process system to assist research

# ISSUES ON POST-PROCESS OF LARGE-SCALE DATASET



- Size of dataset
  - Space, Temporal data, multivariate
- Distribution of dataset
  - Distributed parallel, GRID
- Complexity of HW system
  - Heterogeneous environment, File system, Network
- High cost of data copy, movement
  - MMU/HDD capacity
- o can not move any large-scale data
  - need appropriate tools to access large-scale data
- Many cumbersome procedures
  - File handling, preparation of process
  - need an environment to focus on "THINKING"



#### ORIENTATION OF POST-PROCESS

- o do note move data
  - beyond that…
    - Sharing data, collaboration
    - Remote, virtual organization

#### Data intensive service

- Data access, visualization, analysis, processing
- Sharing data, results, knowledge, resource
  - Data repository for group
  - o Data browse, search, break down

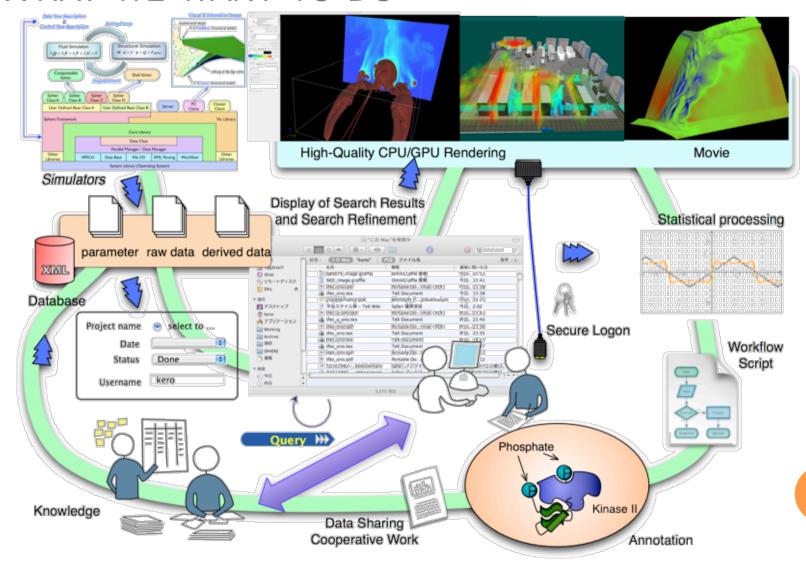


- Comprehension of phenomena
- Sharing information, knowledge



9

#### WHAT WE WANT TO DO



# SWEETS SCIENTIFIC KNOWLEDGE DISCOVERY TOOLS



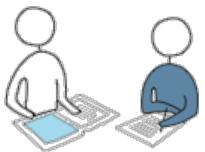
- Script based loosely coupling
  - script glues modules in sub-systems
  - scalability, flexibility and sustainability
- Sub-system
  - Visualization
  - Data / project management
  - Automation of a routine task using a workflow
  - Data sharing
  - •
  - module works independently, but provide full capability when working together
- Efficiently extract useful information from simulated results

10



#### REQUIRED TASKS FOR RESEARCH

# Thinking



Visualization
Data analysis

Task

Visualization
Data/project mgmt
Automation
Data sharing
Analysis

Service (sub-system)

#### Cumbersome

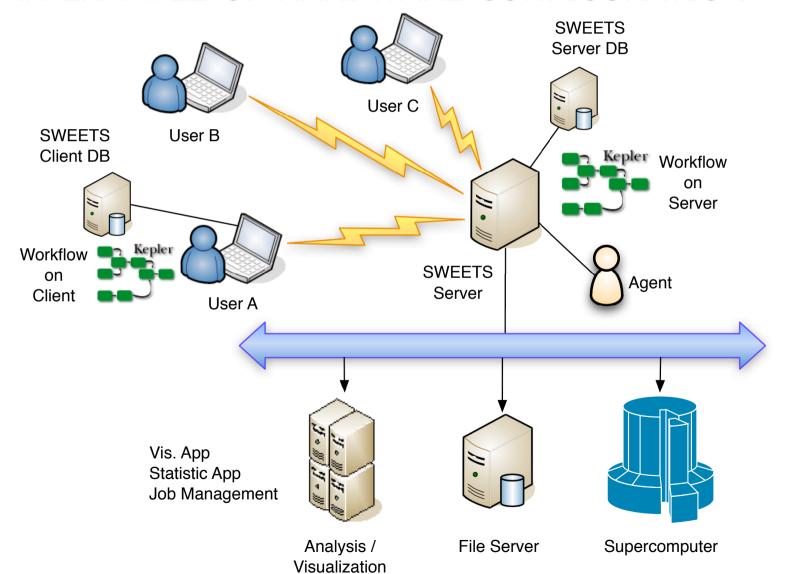
Parameter edit
Data copy/move
Submit a batch job
Program launch

Low level procedure

11

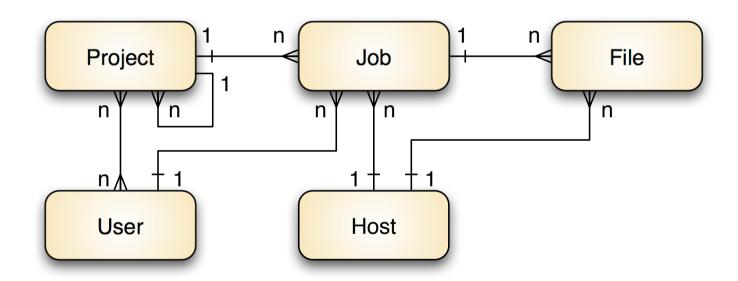


#### AN EXAMPLE OF HARDWARE CONFIGURATION



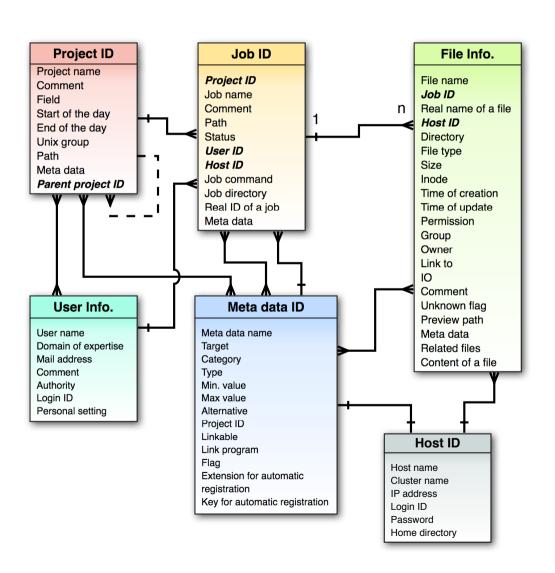


#### A CONCEPT MODEL OF DATA ENTITY





#### DATA ENTITY OF SWEETS SYSTEM





#### PREREQUISITE OF VIS. SUB-SYSTEM

#### Various scenarios for each researcher's approach

- Remote or local visualization
  - Provides unified environment by a common client
- Real-time or post visualization
  - Basically, file based visualization
- Interactive or batch visualization
- Software or hardware rendering
- Large-scale data handling
- Parallel rendering
- Platform
  - Linux, Windows, Max OSX, PC cluster, Supercomputer

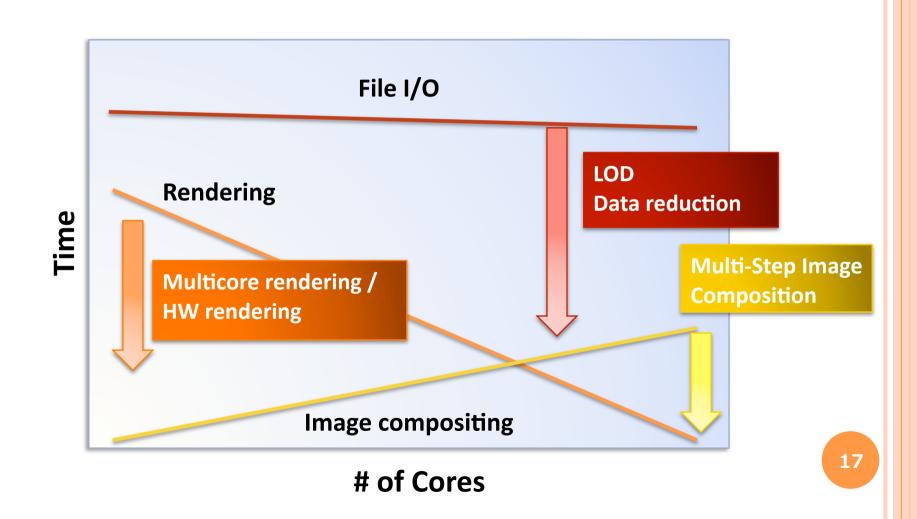


#### 2-WAY SCENARIO

- 1st step: Visualization on supercomputer
  - Sever client system
    - with basic visualization function
    - Data reduction, ROI
  - Operation is only batch job by its policy
- 2nd step: Visualization on CPU/GPU cluster
  - Capability of interactive visualization by GPU
  - Relatively small MMU (Data reduction is necessary)
  - Reduce risk of development
  - Reduce utility time of supercomputer
  - can use existing software, COTS



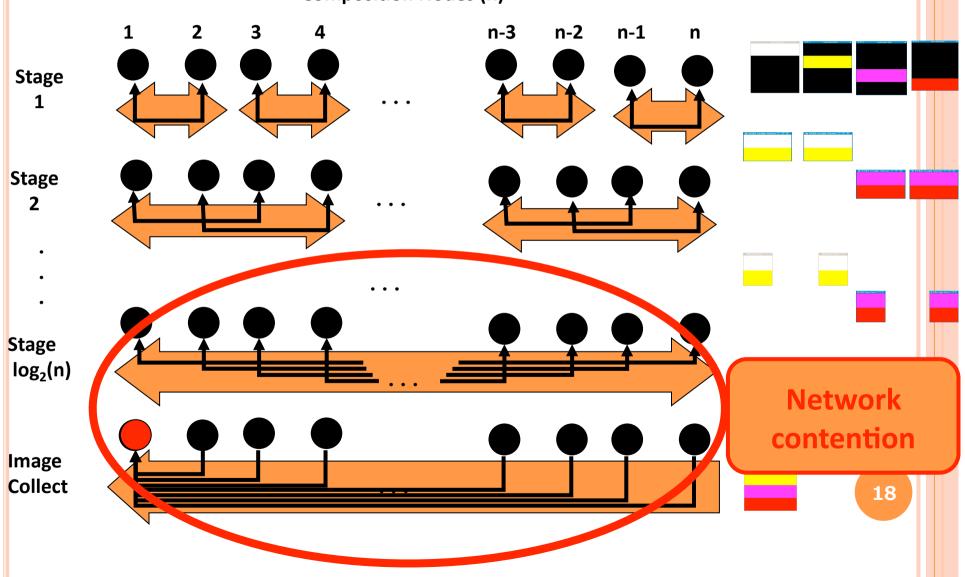
#### STRATEGY: INTERACTIVITY AND SCALABILITY



# BINARY-SWAP IMAGE COMPOSITION

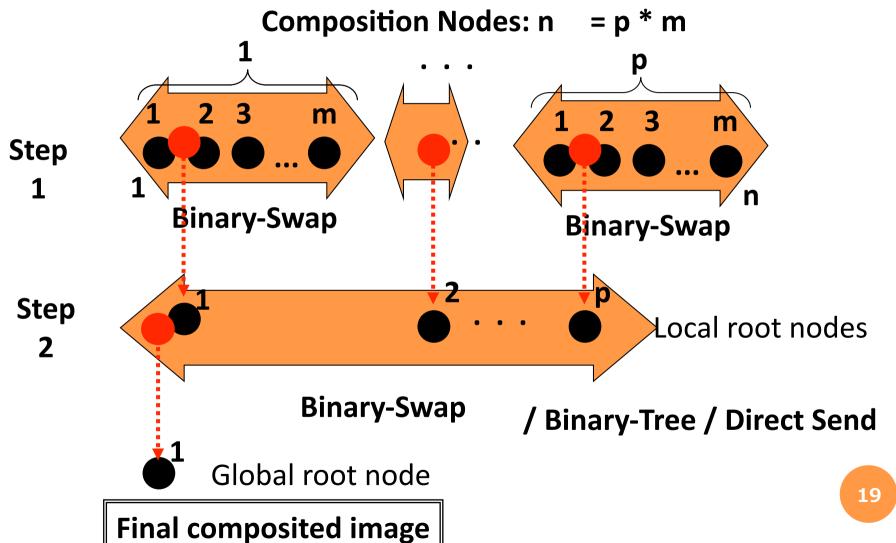






### MULTI-STEP IMAGE COMPOSITION

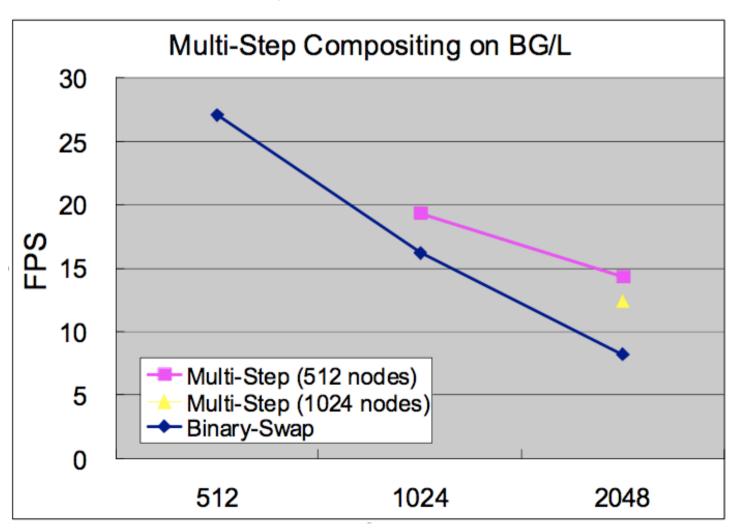






# MSIC BG/L (RIKEN)

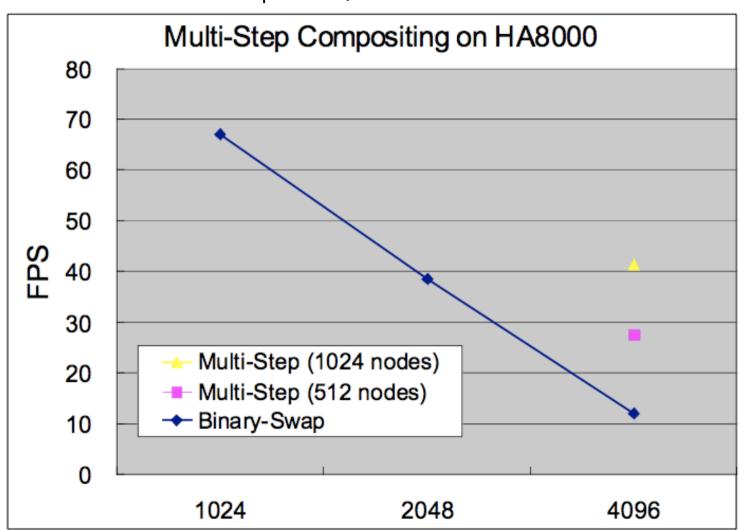
BlueGene / L Dual core x 1024 nodes





### MSIC - T2K (UNIV. OF TOKYO)

AMD Opteron Quad Core x 4 Sockets





#### OTHER SUB-SYSTEMS

- Workflow
  - Kepler
- Data base
  - RDB ? XML feature
- Scripting
  - python ... plays glue
- Analysis
  - R
  - user program
- Other useful existing tools...



#### CONCLUDING REMARKS

- Design and current development status
  - to assist discovery and understanding
  - Database centered structure
  - sub-systems take part in the system
    - Visualization
    - Workflow
    - Other programs
  - resource mgmt and access control provide data sharing
  - reuse of existing useful software
  - script base
- Supercomputer will be fully operational on 2011
- Combining existing software, enhancing capability