

GridRPC and its Application

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GridRPC-WG history

- 1994 Ninf Project started
- 1995 NetSolve Project started
- 2003 GGF GridRPC WG established at GGF8 in Seattle, July
 - ▶ Defining two documents
 - @End-User Doc.
 - @Middleware Doc.
- 2005 GridRPC End-User Document became a Draft Recommendation
- 2006 ...

Outline

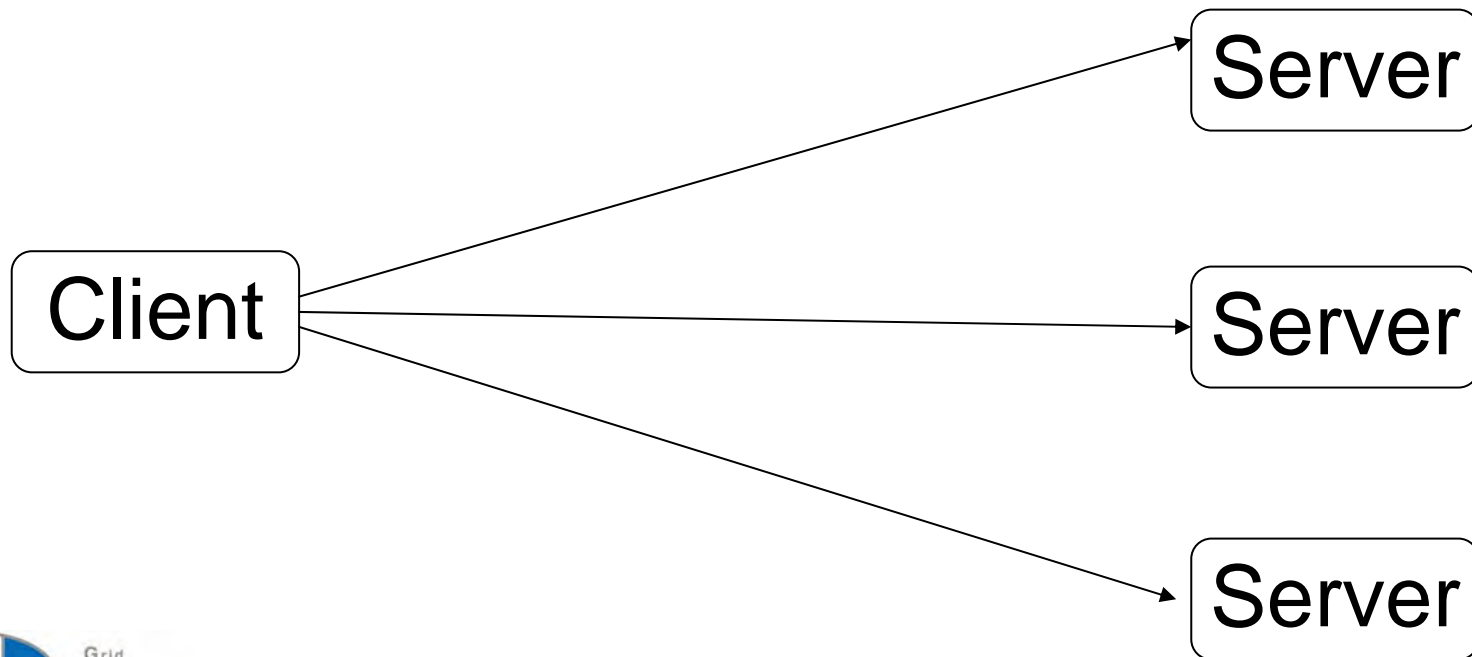
- GridRPC API

- GridRPC Implementation: Ninf-G

- GridRPC Applications

What is GridRPC

- RPC mechanism for Grid Environment
- Client can call server side functions with ease
- Parallel invocation is supported



Example

Client program with GridRPC API

```
/* initialize function handle */  
for (i = 0; i < NUM_HOSTS; i++)  
    grpc_function_handle_init(&handles[i], hosts[i],  
        port, "pi/pi_trial");  
for (i = 0; i < NUM_HOSTS; i++)  
/* parallel invocation */  
    grpc_call_async(&handles[i], i, times,  
        &count[i]);  
/* wait for all the calls */  
grpc_wait_all();
```

Comparison with MPI

● MPI is more powerful

- ▶ RPC communication is limited to between client and server

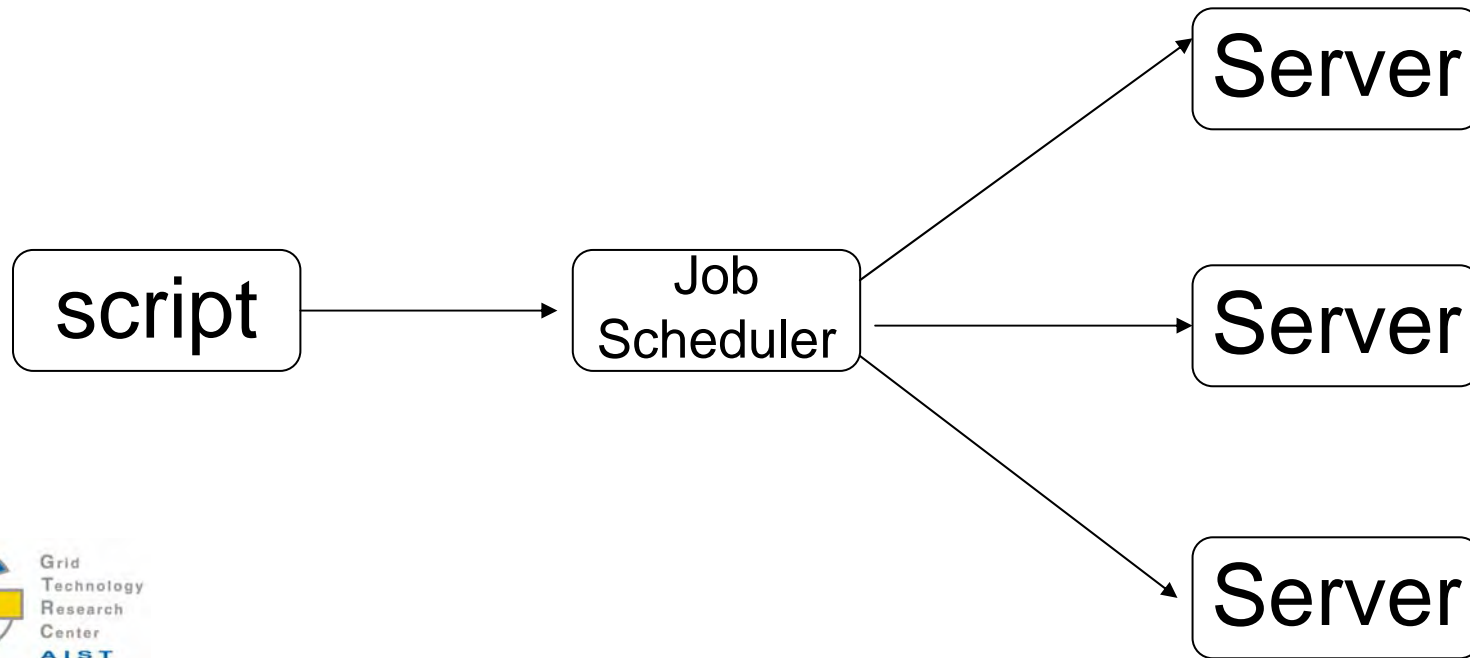
● RPC is more simple

- ▶ No explicit data packing

- ▶ No explicit data send/recv

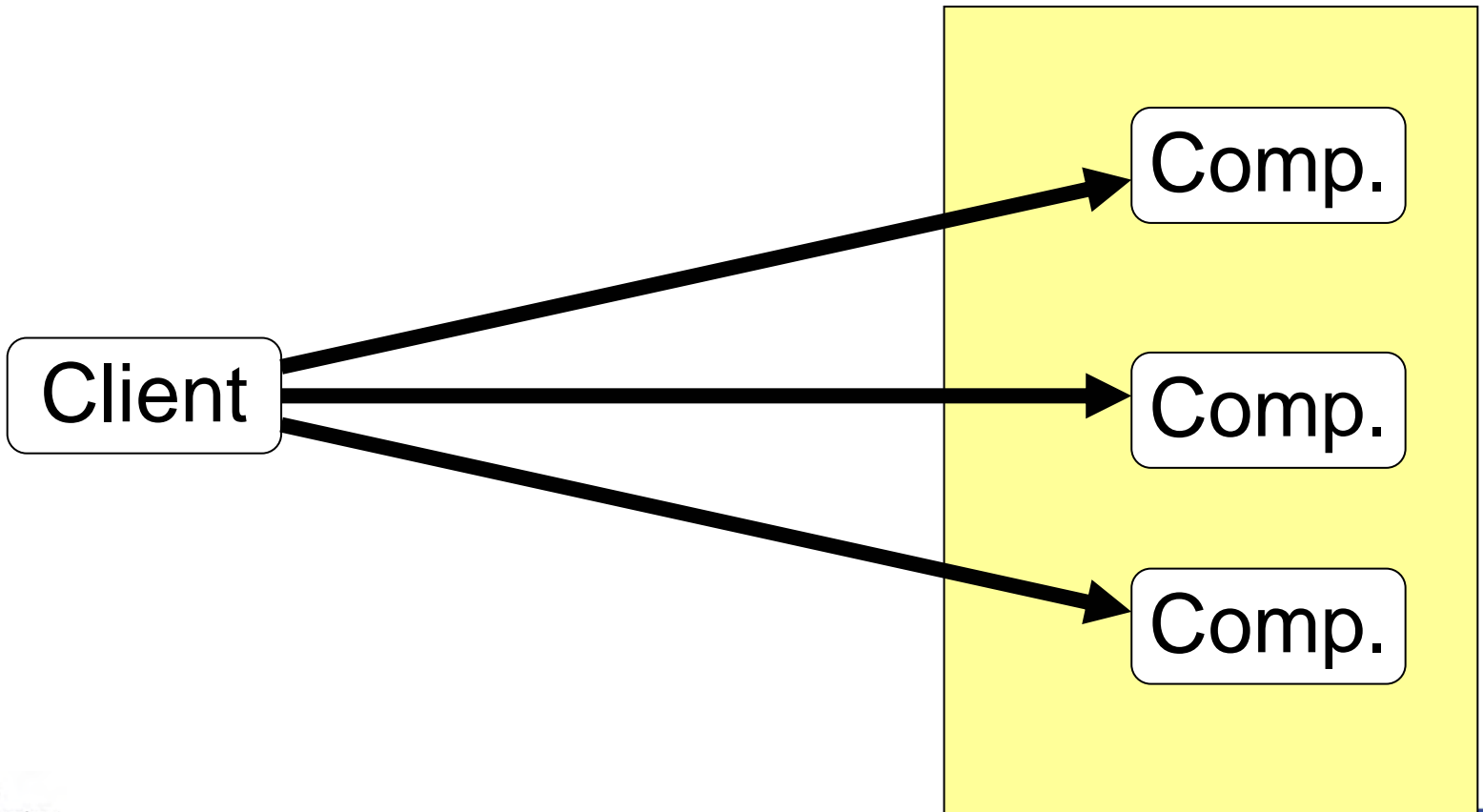
Comparison with script with some job scheduler

- With a script and a job scheduler (such as Condor), you can do the almost same thing, but
- RPC is suitable for more fine grained jobs
- Programming will be much easier



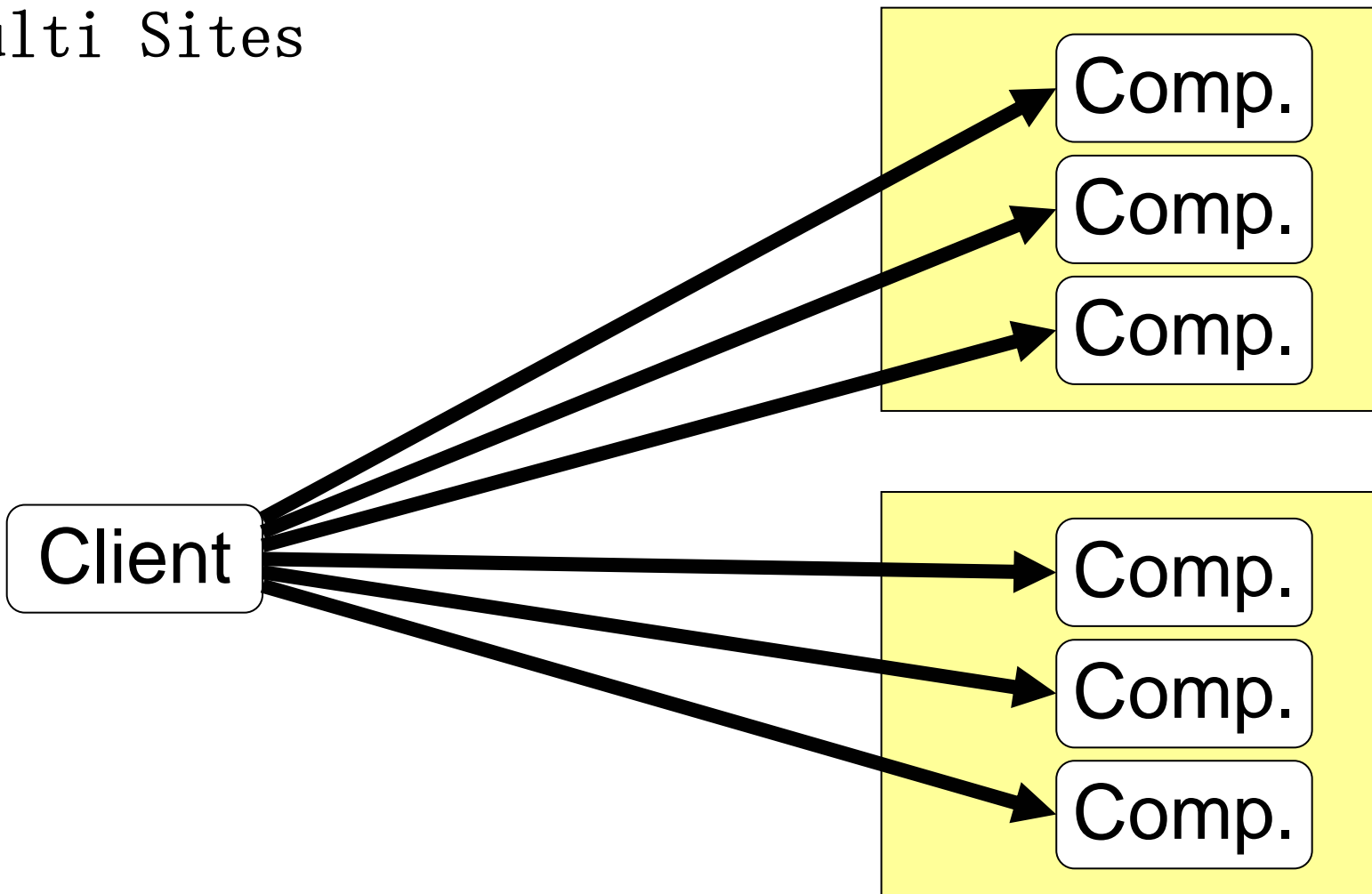
Application Configurations

Single Site



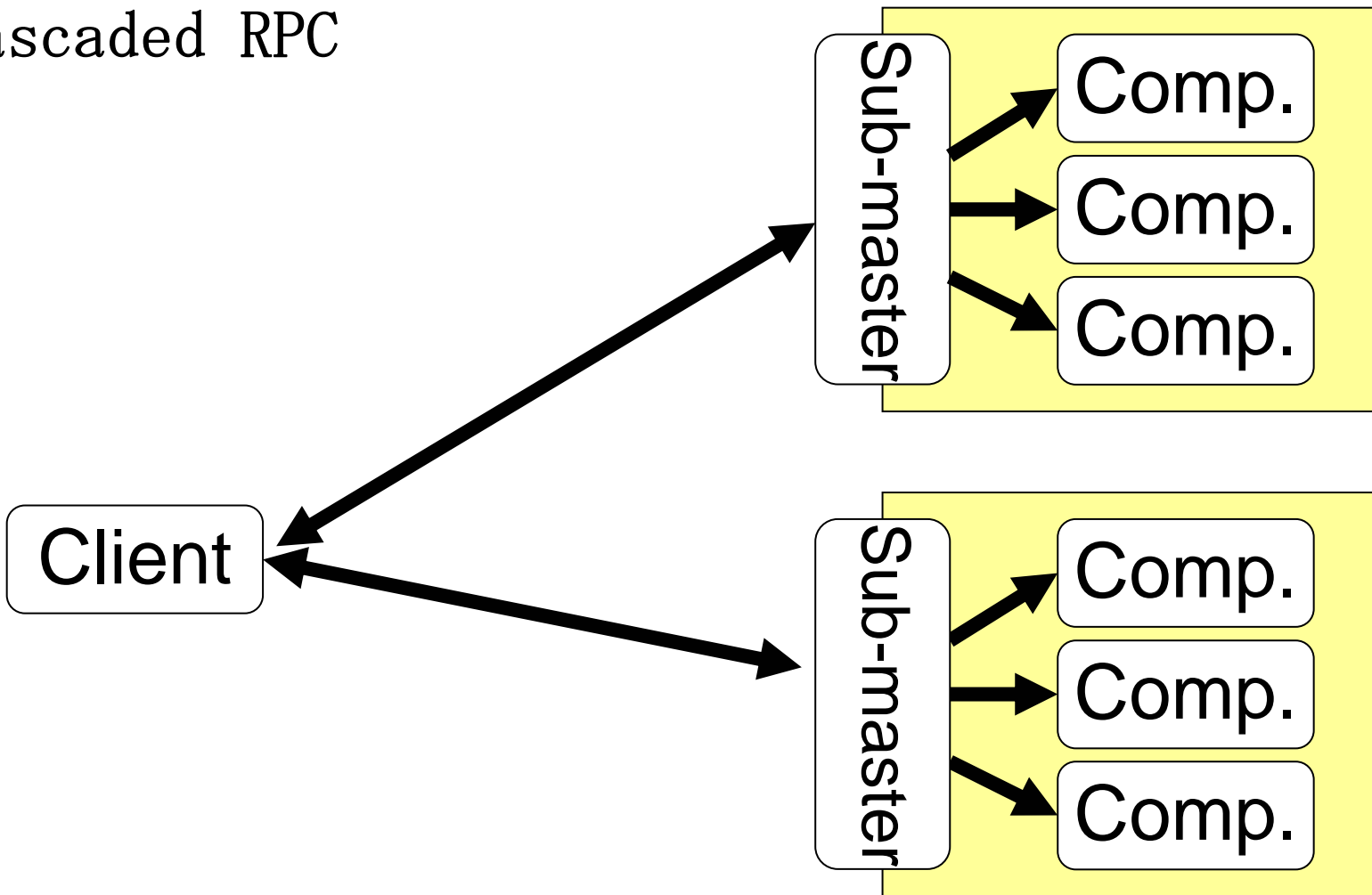
Application Configurations

Multi Sites



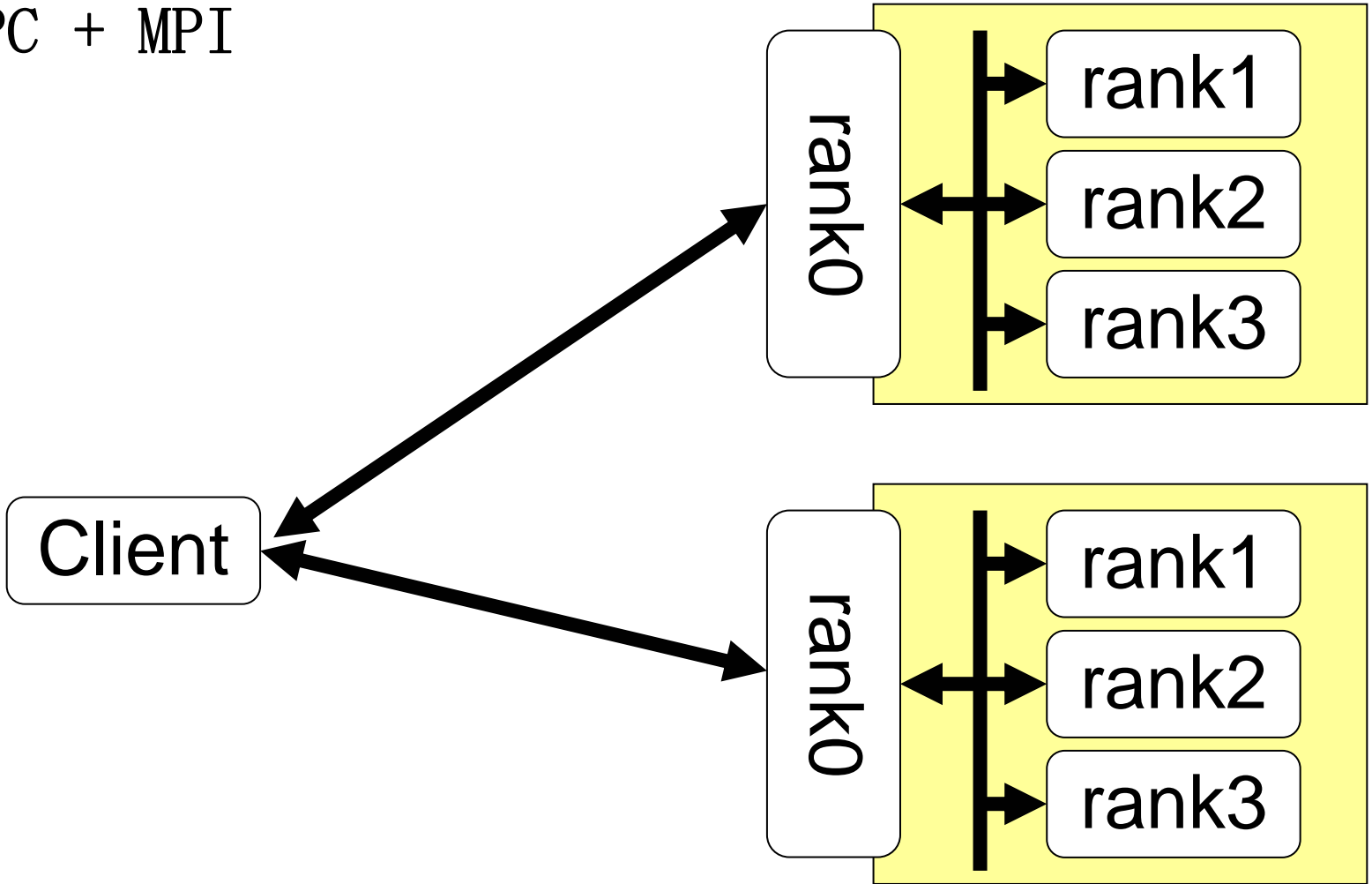
Application Configurations

🌐 Cascaded RPC



Application Configurations

RPC + MPI



Implementations

Ninf-G (AIST)

- ▶ Uses Globus 2/4 as the underlying layer

GridSolve (Univ. Tennessee)

- ▶ Based on NetSolve
- ▶ Automatic server selection with Agent

DIET (INRIA)

Ninf-G System

● An implementation of GridRPC Interface

- ▶ Realizing remote procedure call (RPC) on the Grid
- ▶ GridRPC WG standardizes the interface
- ▶ Supports C and Java Client API

● Usage scenarios

- ▶ Remote library call
 - Ⓢ Executing compute-intensive tasks on a remote high performance computing resource
- ▶ Task parallel processing
 - Ⓢ Executing large numbers of independent tasks on distributed computing resources



Ninf-G Programming

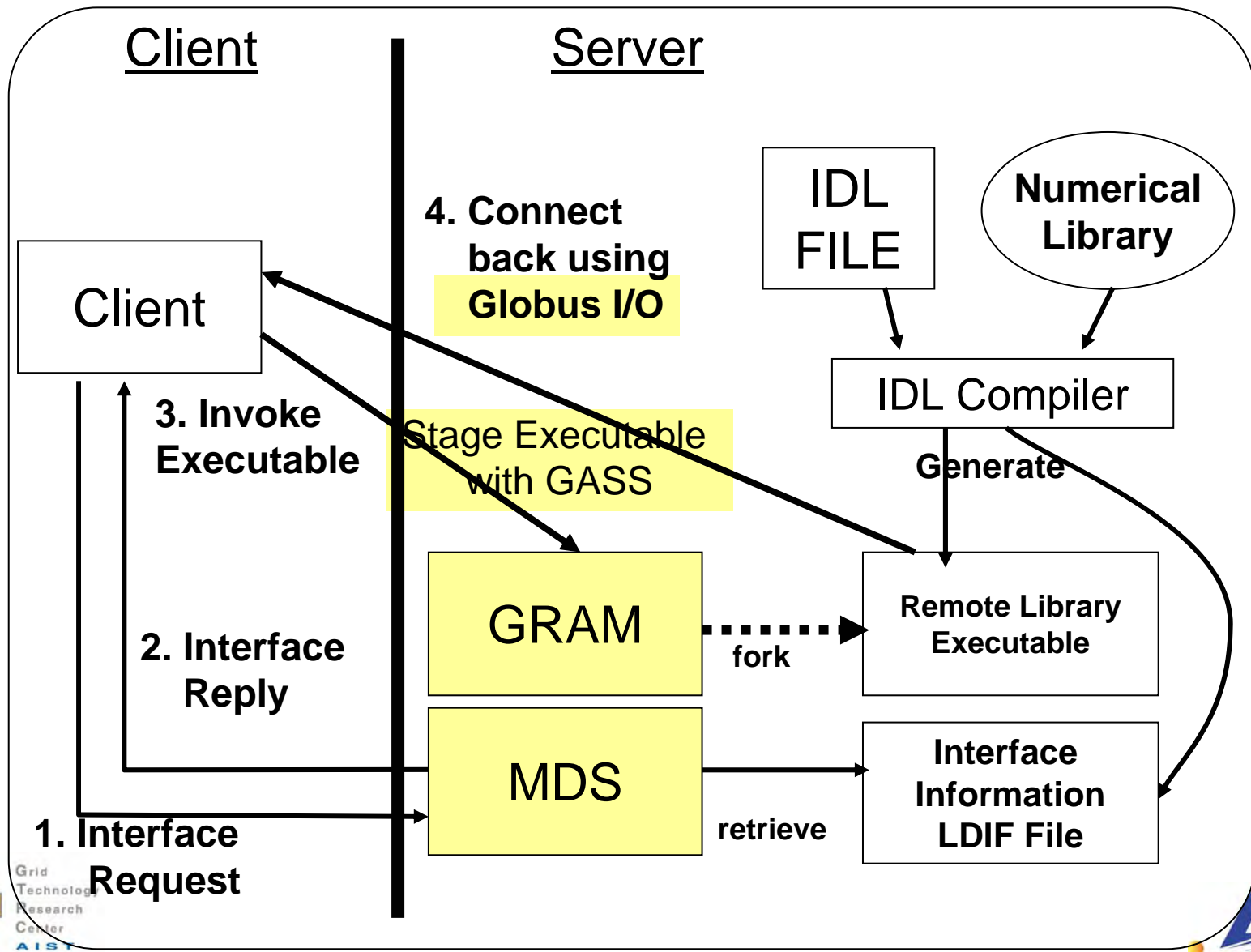
Client program with GridRPC API

```
/* initialize function handle */
for (i = 0; i < NUM_HOSTS; i++)
    grpc_function_handle_init(&handles[i], hosts[i], port, "pi/pi_trial");
for (i = 0; i < NUM_HOSTS; i++)
    /* parallel invocation */
    grpc_call_async(&handles[i], i, times, &count[i]);
/* wait for all the calls */
grpc_wait_all();
```

Server interface description with

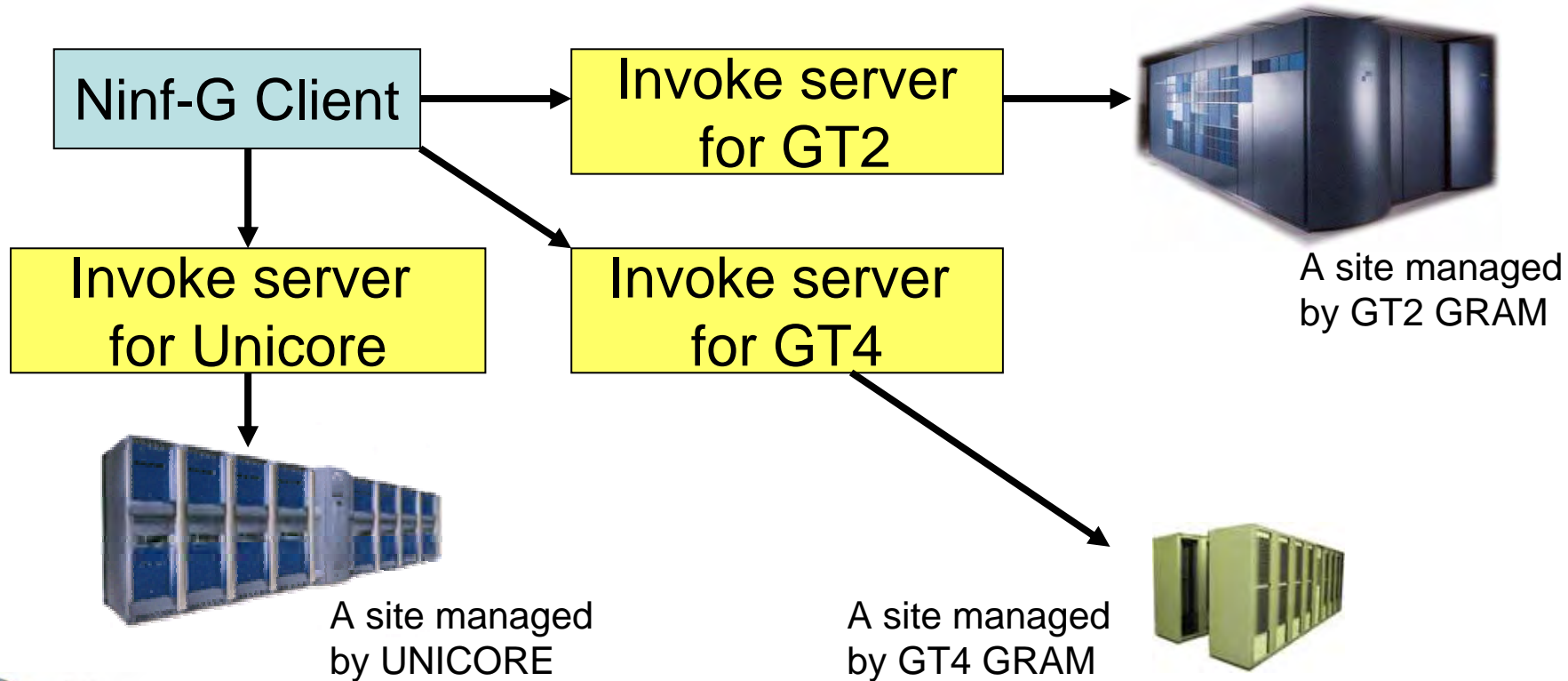
```
Define dmmul(
    mode_in int n, mode_in double A[n][n],
    mode_in double B[n][n], mode_out double C[n][n])
Required "mmul.o"
Calls "C" mmul(n,A,B,C);
```

Ninf-G Over view



Ninf-G4 architecture

- A single client can use several sites with different protocols simultaneously



Ninf-G4 Current Status

4.1 is released

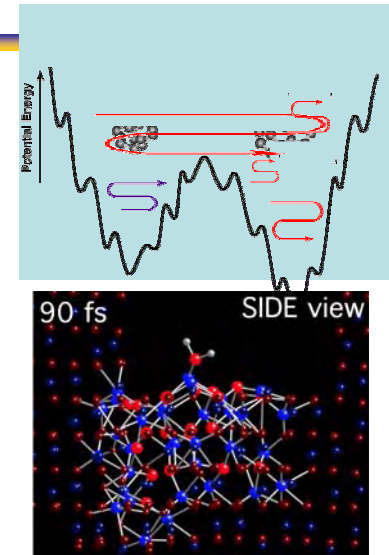
- ▶ C / Java Client
- ▶ MDS 2/4 are supported
- ▶ Works for Linux, Solaris, AIX, Mac OS X

<http://ninf.apgrid.org>

Examples of Ninf-G Applications

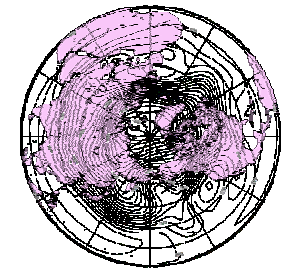
● Molecular Simulation

- ▶ Replica Exchange Monte-Carlo :
 - ⊗ Potential survey of a molecule
- ▶ Time Dependent DFT Simulation :
 - ⊗ Calculating electron status of a molecule
 - ⊗ Used for evaluating PRAGMA Testbed
- ▶ **QM/MD Coupled simulation**
 - ⊗ Efficient and accurate molecular simulation



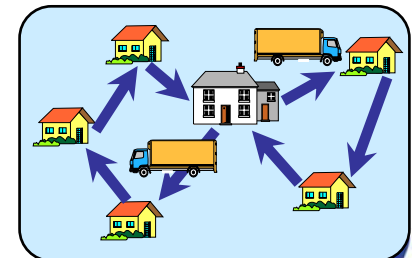
● Weather forecasting Simulation

- ▶ S-model :
 - ⊗ Global weather prediction using ensemble simulation
 - ⊗ Demonstrated in PRAGMA WS (Taiwan)



● Optimization Problem

- ▶ Traveling salesman problem :
 - ⊗ Searching shortest path



Hybrid QM/MD Simulation on the Grid

■ *Nano-structured Si system under stress*

- ◆ two slabs connected with a slanted pillar
- ◆ 0.11 million atoms

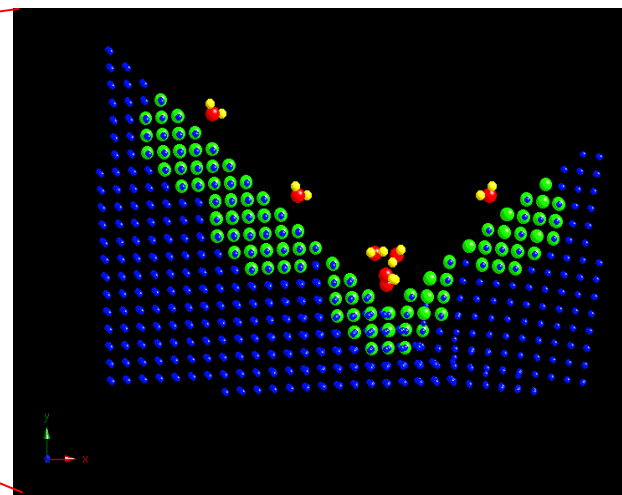
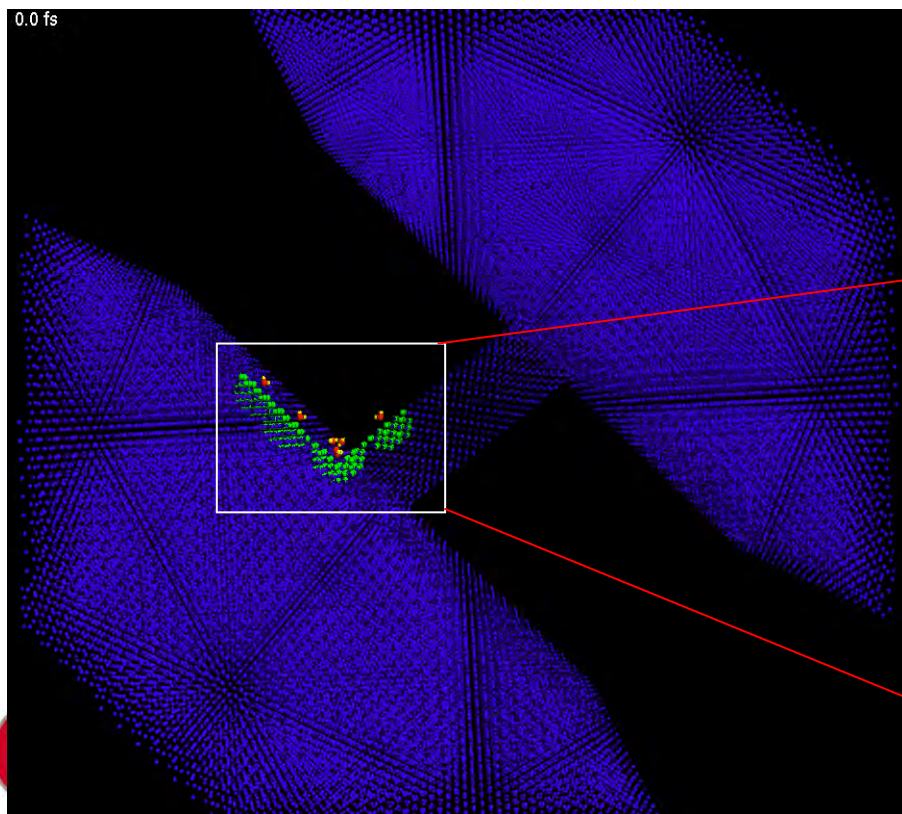
4 quantum regions:

#0: 69 atoms
including
 $2\text{H}_2\text{O}+2\text{OH}$

#2: 44 atoms
including H_2O

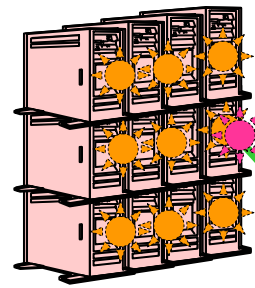
#1: 68 atoms
including H_2O

#3: 56 atoms
including H_2O

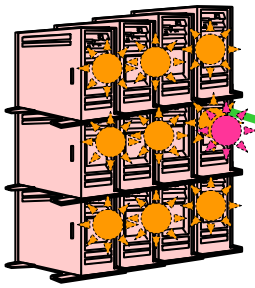


Close-up view

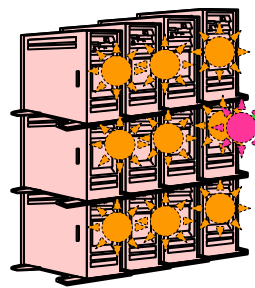
QM/MD simulation over the Pacific



P32 (512 CPU)



P32 (512 CPU)

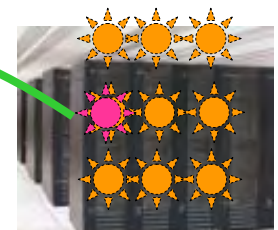
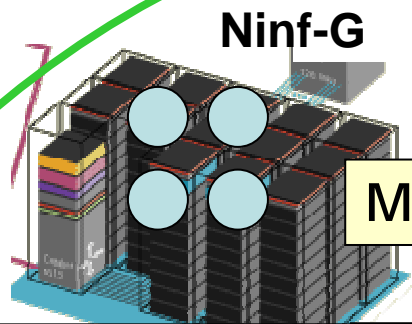


F32 (256 CPU)

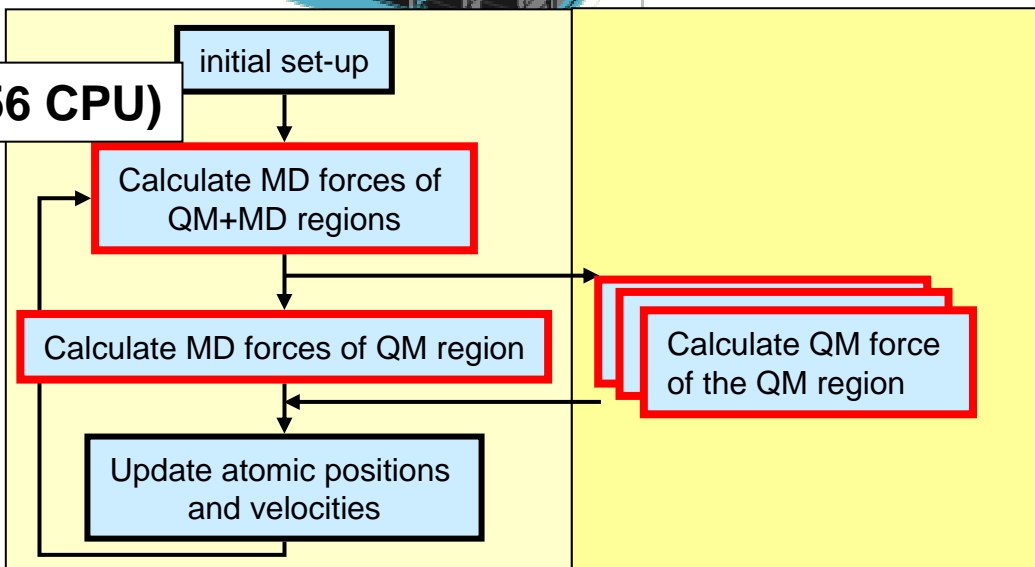
QM Server

Total number of CPUs: 1792

**TCS (512 CPU)
@ PSC**

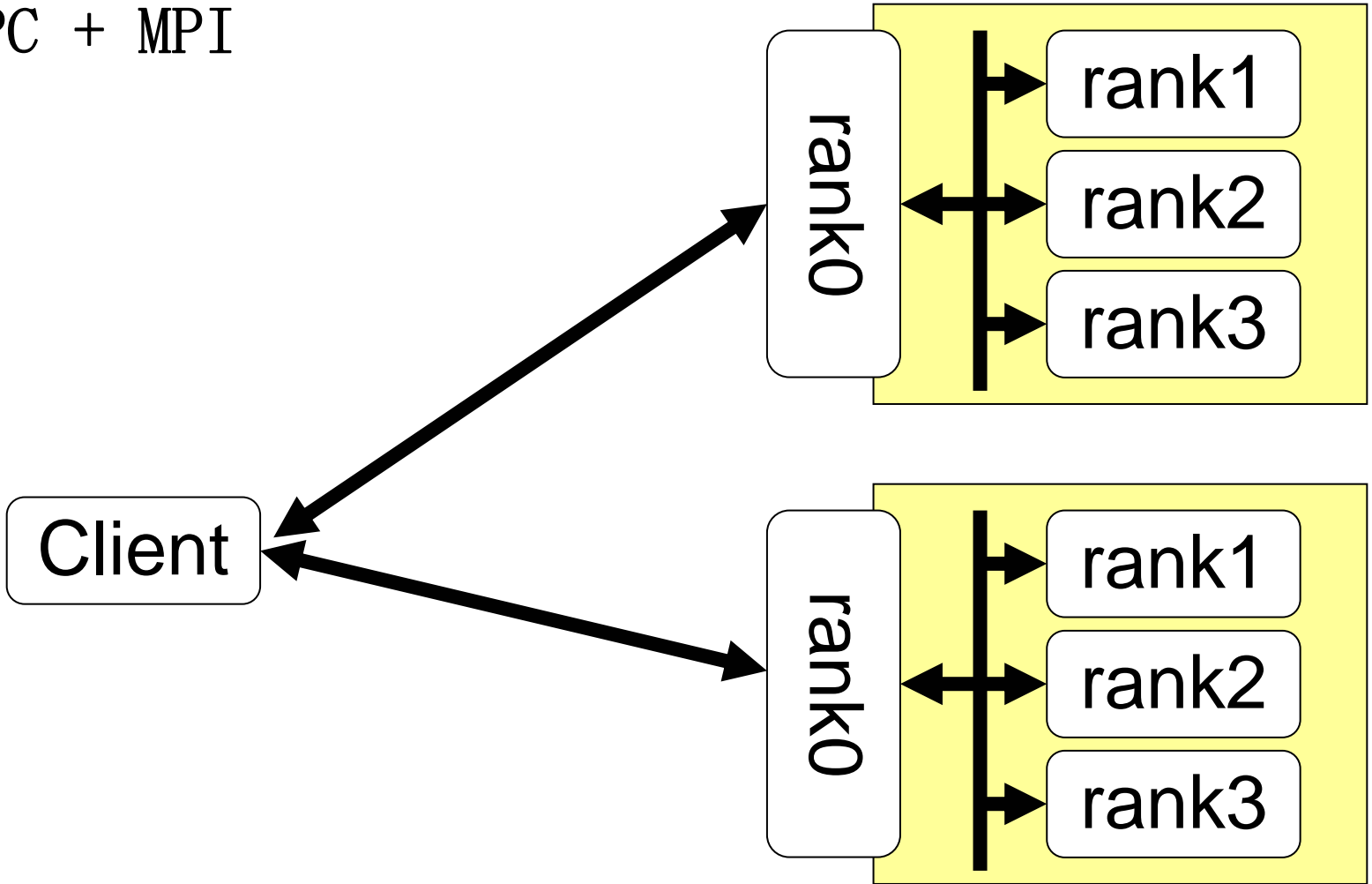


QM Server



Application Configurations

RPC + MPI



Another Application: TDDFT

Application: TDDFT Equation

- ▶ Original program is written in **Fortran 90**.
- ▶ A hotspot is divided into multiple tasks and processed in parallel.
- ▶ **Task-parallel** part is implemented with **Ninf-G** which is a reference implementation of **the GridRPC**.

Previous Experiment

- ▶ Schedule: June 1, 2004 ~ August 31, 2004 (For 3 months)
- ▶ Participants: 10 Sites (in 8 countries): AIST, SDSC, KU, KISTI, NCHC, USM, BII, NCSA, TITECH, UNAM
- ▶ Resource: 198 CPUs (on 106 nodes)

TDDFT program

```
main(){
```

```
:
```

```
Numerical integration part
```

```
:
```

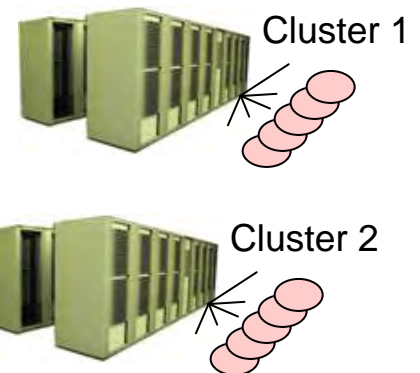
```
}
```

5000 iterations

Independent tasks



GridRPC server side



Details of Application (1)

TDDFT: Time-Dependent Density Functional Theory

© By Nobusada (IMS) and Yabana (Tsukuba Univ.)

- ▶ Application of the computational quantum chemistry
- ▶ Simulate how the electronic system evolves in time after excitation

Time dependent N-electron wave function is

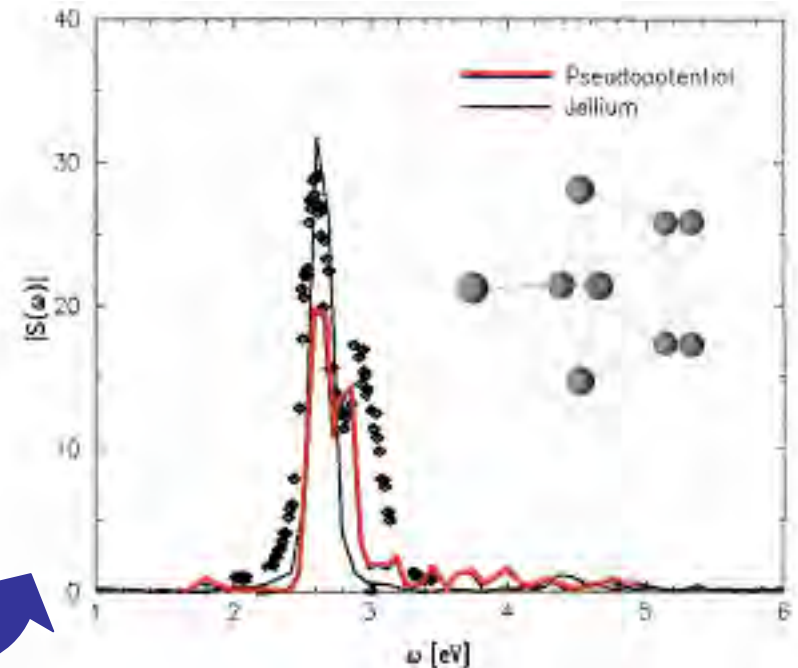
$$|\Psi\rangle = |\psi_1 \psi_2 \dots \psi_N\rangle$$

which is approximated and transformed to

$$i \frac{\partial}{\partial t} \psi_i = \left(-\frac{1}{2} \nabla^2 + V_{ion} + V_H + V_{ex} \right) \psi_i$$

then applied to numerical integration.

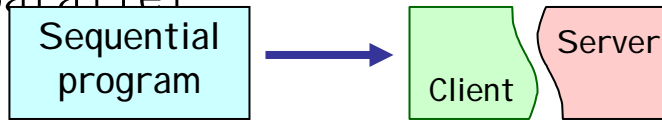
A spectrum graph by calculated real-time dipole moments



Details of Application (2)

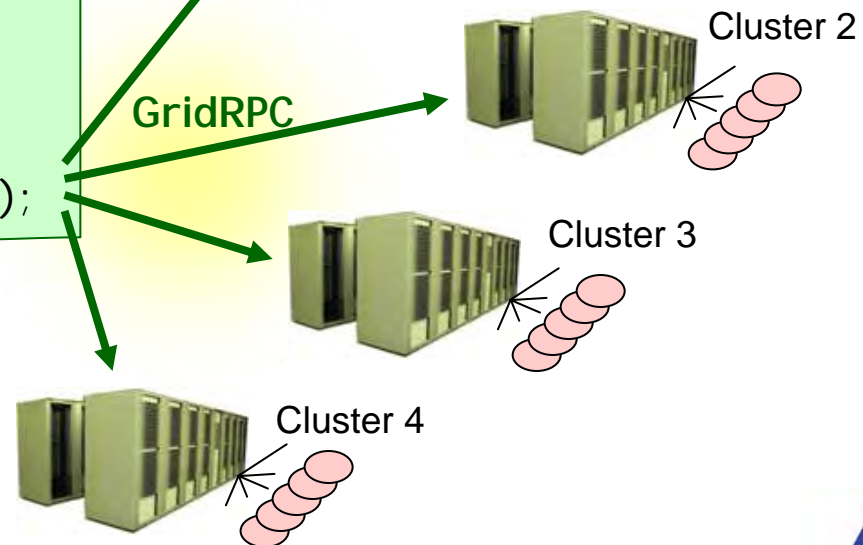
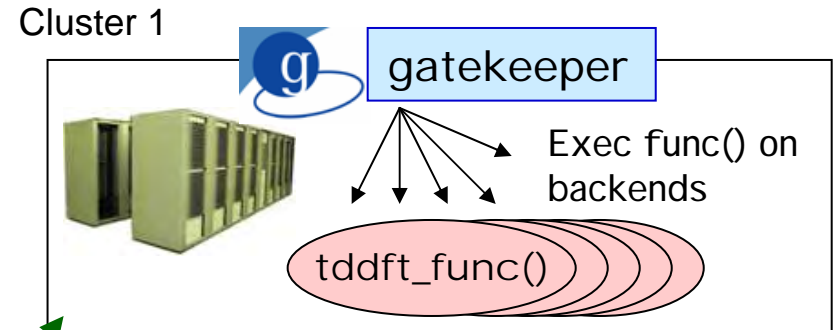
GridRPC model using Ninf-G

- ▶ Execute some partial calculations on multiple servers in parallel



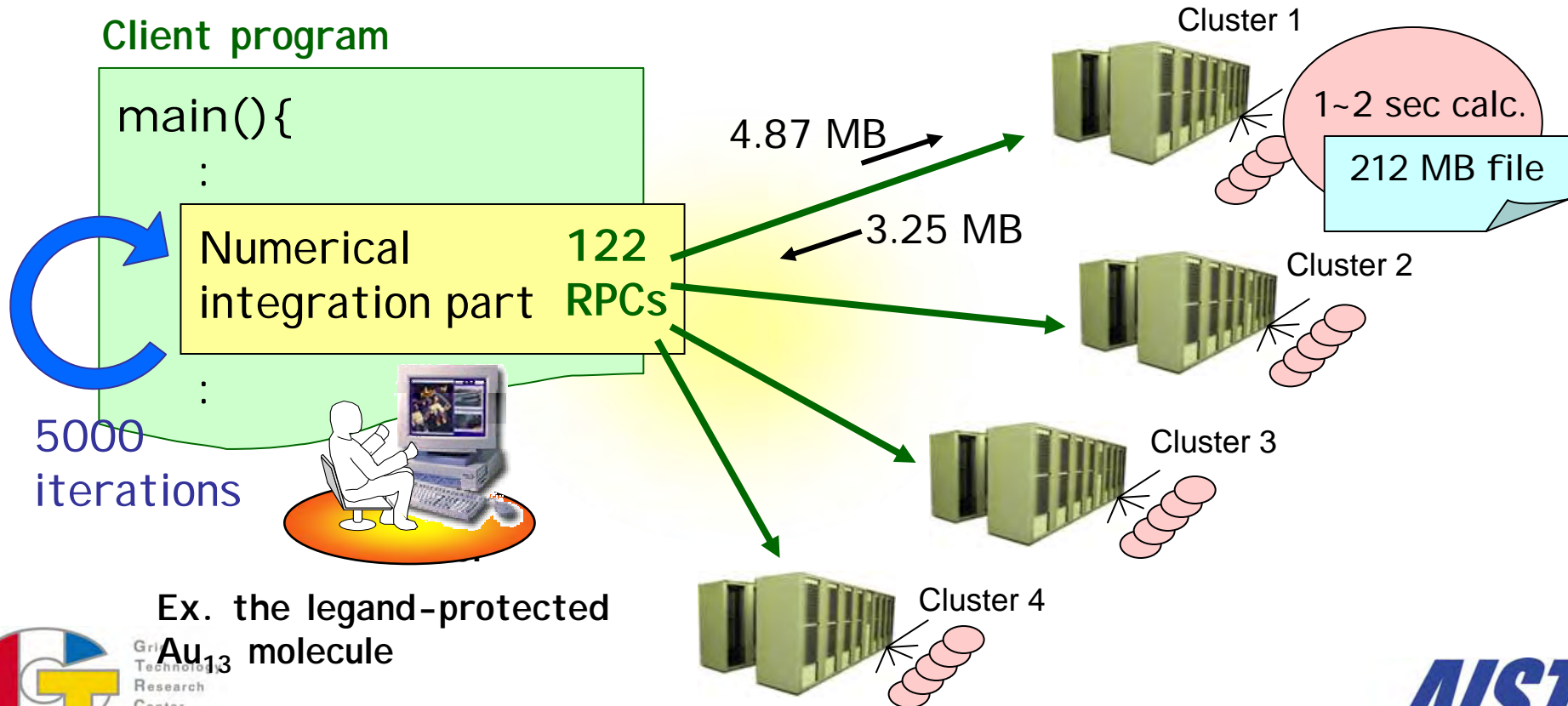
Client program of TDDFT

```
main(){  
:  
  grpc_function_handle_default(  
    &server, "tddft_func");  
:  
  grpc_call(&server, input, result);  
:  
}
```



Details of Application (3)

- Parallelism: Suitable to GridRPC framework
- Real Science: Long-time run, Large data
 - ▶ Require 6.1 millions of RPCs (Take about 1 week)

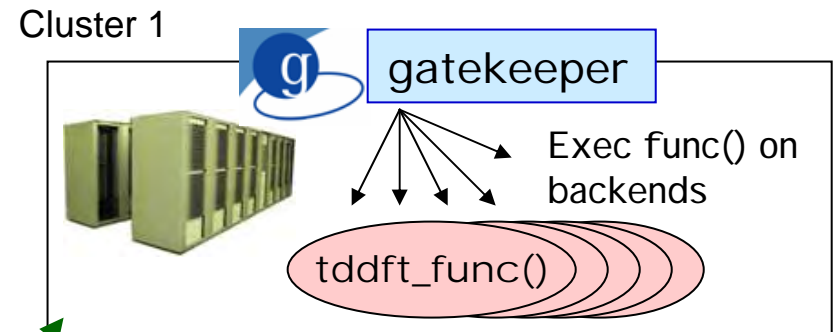
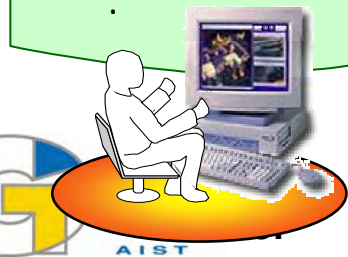


Experiment

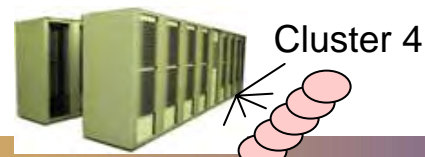
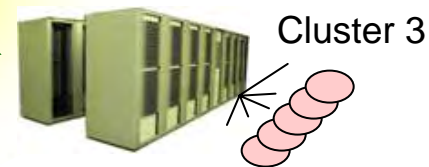
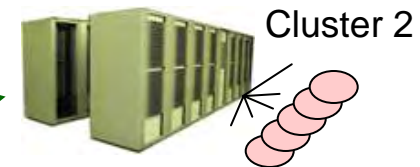
- We have testbed with both of pre-WS and WS GRAM
 - ▶ 5-6 sites on PRAGMA test bed with 60 nodes, for 3 months
 - ▶ Ninf-G4 hides the heterogeneity

Client program of TDDFT

```
main(){  
  :  
  grpc_function_handle_default(  
    &server, "tddft_func");  
  :  
  grpc_call(&server, input, result);  
  :  
}
```

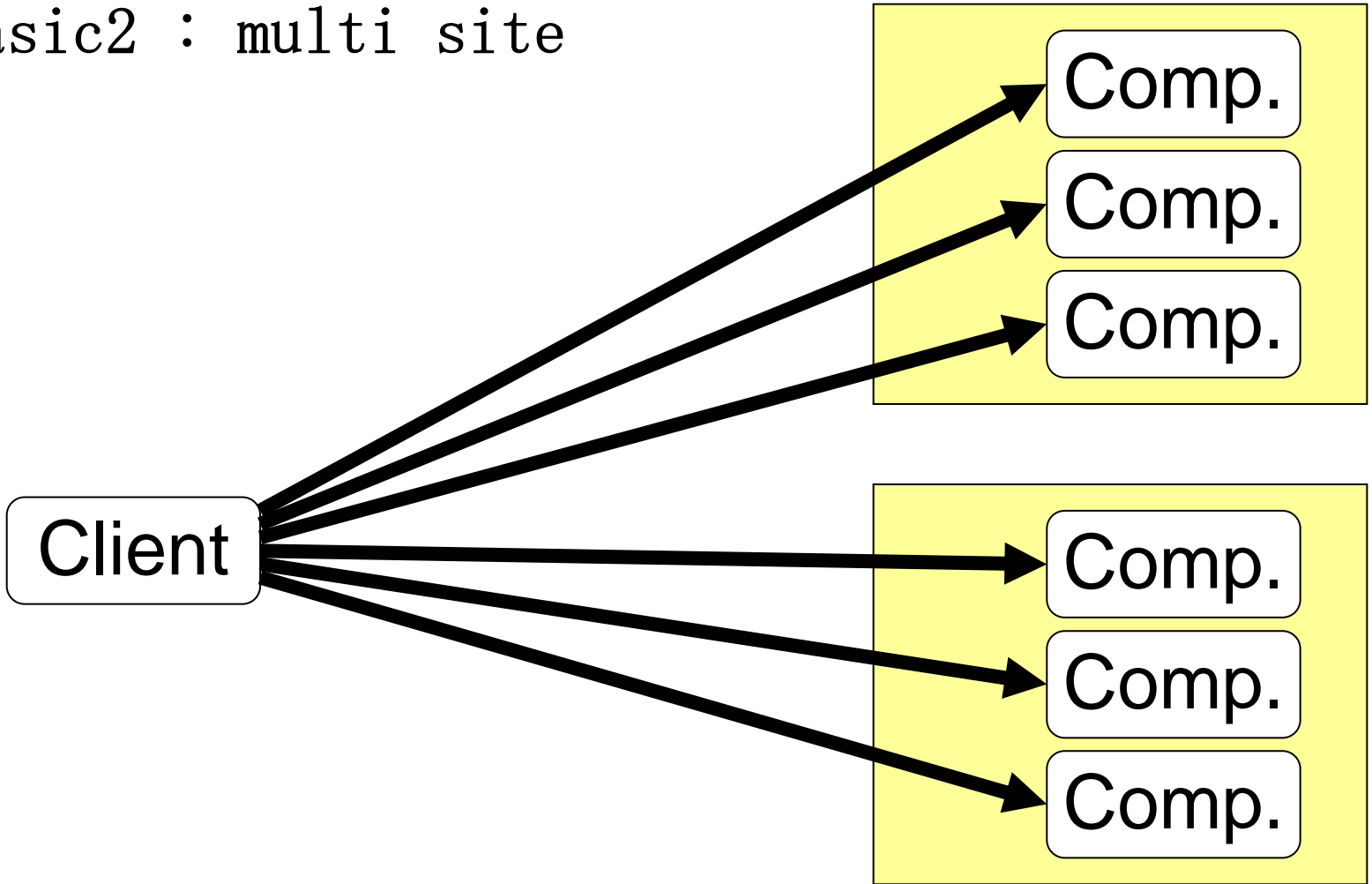


GridRPC



Application Configurations

Basic2 : multi site



Summary

🌐 GridRPC API is now a Draft Recommendation

- ▶ Drafted experience report.
- ▶ Hopefully, it will become formal Recommendation soon.

🌐 GridRPC Implementation: Ninf-G

- ▶ Implemented on Globus Toolkit

🌐 GridRPC Applications

- ▶ Several Scientific applications