Programming on the Grid using GridRPC

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Outline

- **What is GridRPC?**
  - Overview
  - v.s. MPI
  - Typical scenarios
- **Overview of Ninf-G and GridRPC API**
  - Ninf-G: Overview and architecture
  - GridRPC API
  - Ninf-G API
- **How to develop Grid applications using Ninf-G**
  - Build remote libraries
  - Develop a client program
  - Run
- **Practicals**
- **Recent activities/achievements in Ninf project**

What is GridRPC?

Programming model on Grid based on Grid Remote Procedure Call (GridRPC)

Layered Programming Model/Method

Portal / PSE
GridPort, HotPage,
GPDK, Grid PSE Builder,
etc...

Easy but inflexible

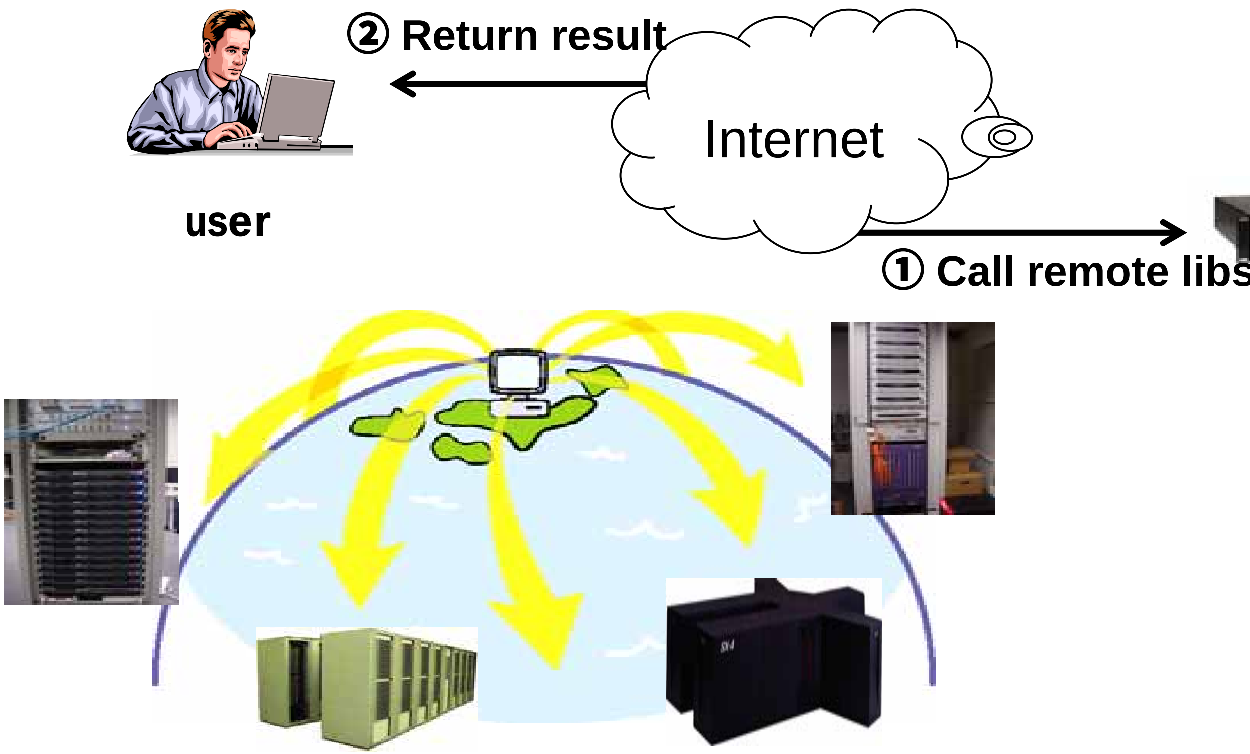
High-level Grid Middleware
MPI (MPICH-G2, PACX-MPI, ...)
GridRPC (Ninf-G, NetSolve, ...)

Low-level Grid Middleware
Globus Toolkit

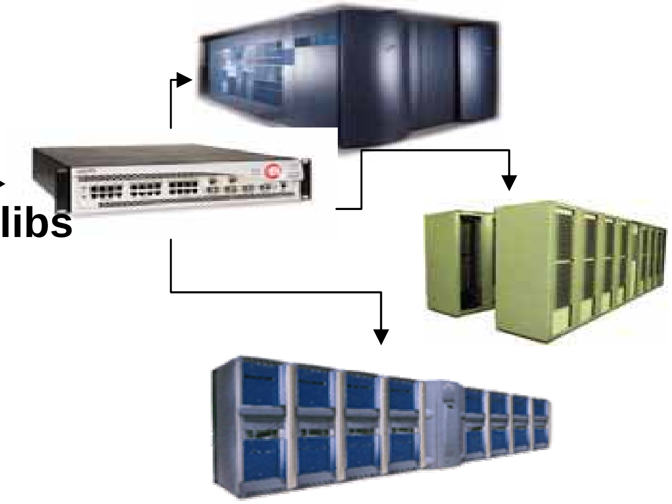
Primitives
Socket, system calls, ...

Difficult but flexible

GridRPC



Utilization of remote Supercomputers



Call remote (special) libraries

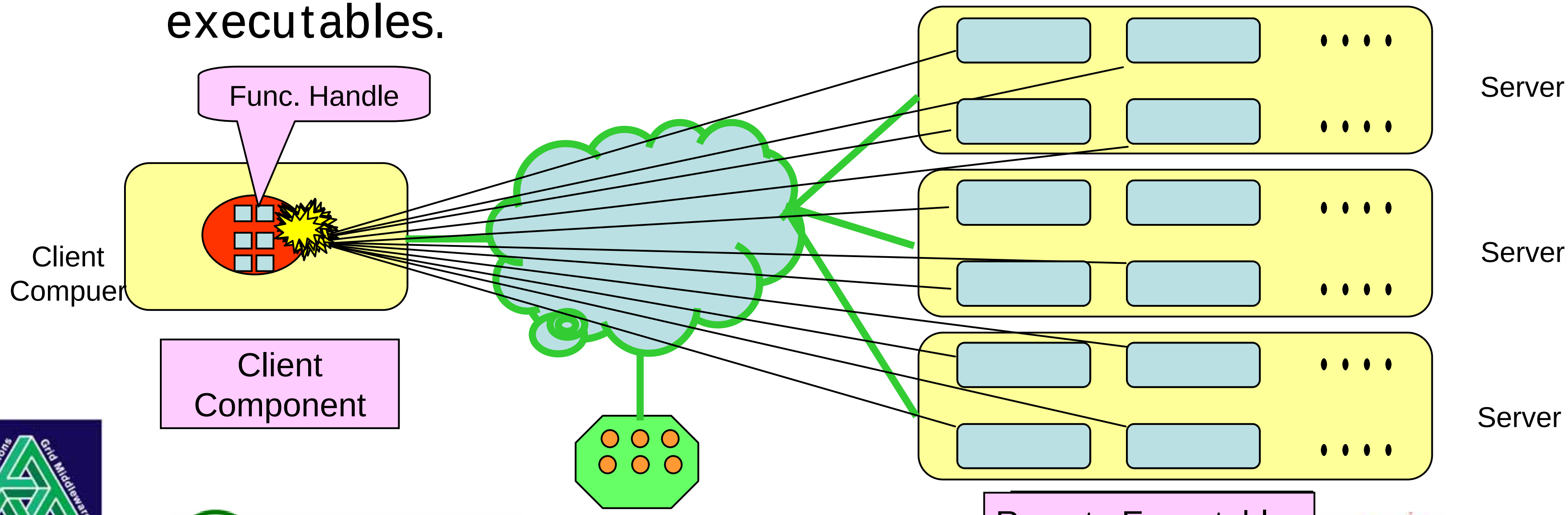
Large-scale distributed computing using multiple computing resources on Grids

Use as backend of portals / ASPs

Suitable for implementing task-parallel applications (compute independent tasks on distributed resources)

GridRPC Model

- **Client Component**
  - Caller of GridRPC.
  - Manages remote executables via function handles
- **Remote Executables**
  - Callee of GridRPC.
  - Dynamically generated on remote servers.
- **Information Manager**
  - Manages and provides interface information for remote executables.



GridRPC: RPC "tailored" for the Grid

- Medium to Coarse-grained calls
  - Call Duration < 1 sec to > week
- Task-Parallel Programming on the Grid
  - Asynchronous calls, 1000s of scalable parallel calls
- Large Matrix Data & File Transfer
  - Call-by-reference, shared-memory matrix arguments
- Grid-level Security (e.g., Ninf-G with GSI)
- Simple Client-side Programming & Management
  - No client-side stub programming or IDL management
- Other features…

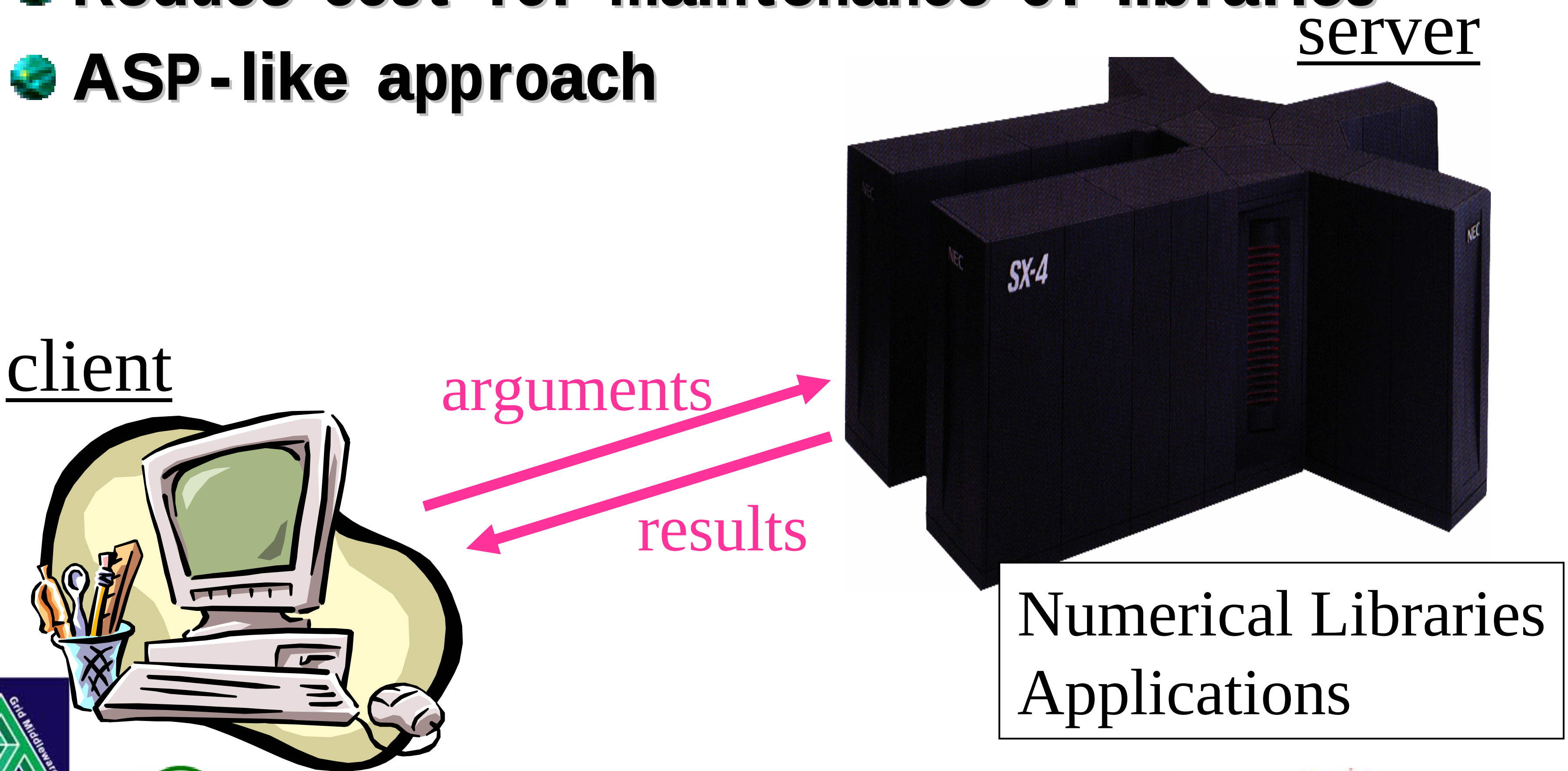
GridRPC v.s. MPI

	GridRPC	MPI
parallelism	task parallel	data parallel
model	client/server	SPMD
API	GridRPC API	MPI
co-allocation	dispensable	indispensable
fault tolerance	good	poor (fatal)
private IP nodes	available	unavailable
resources	can be dynamic	static*
others	easy to gridify existing apps.	well known seamlessly move to Grid

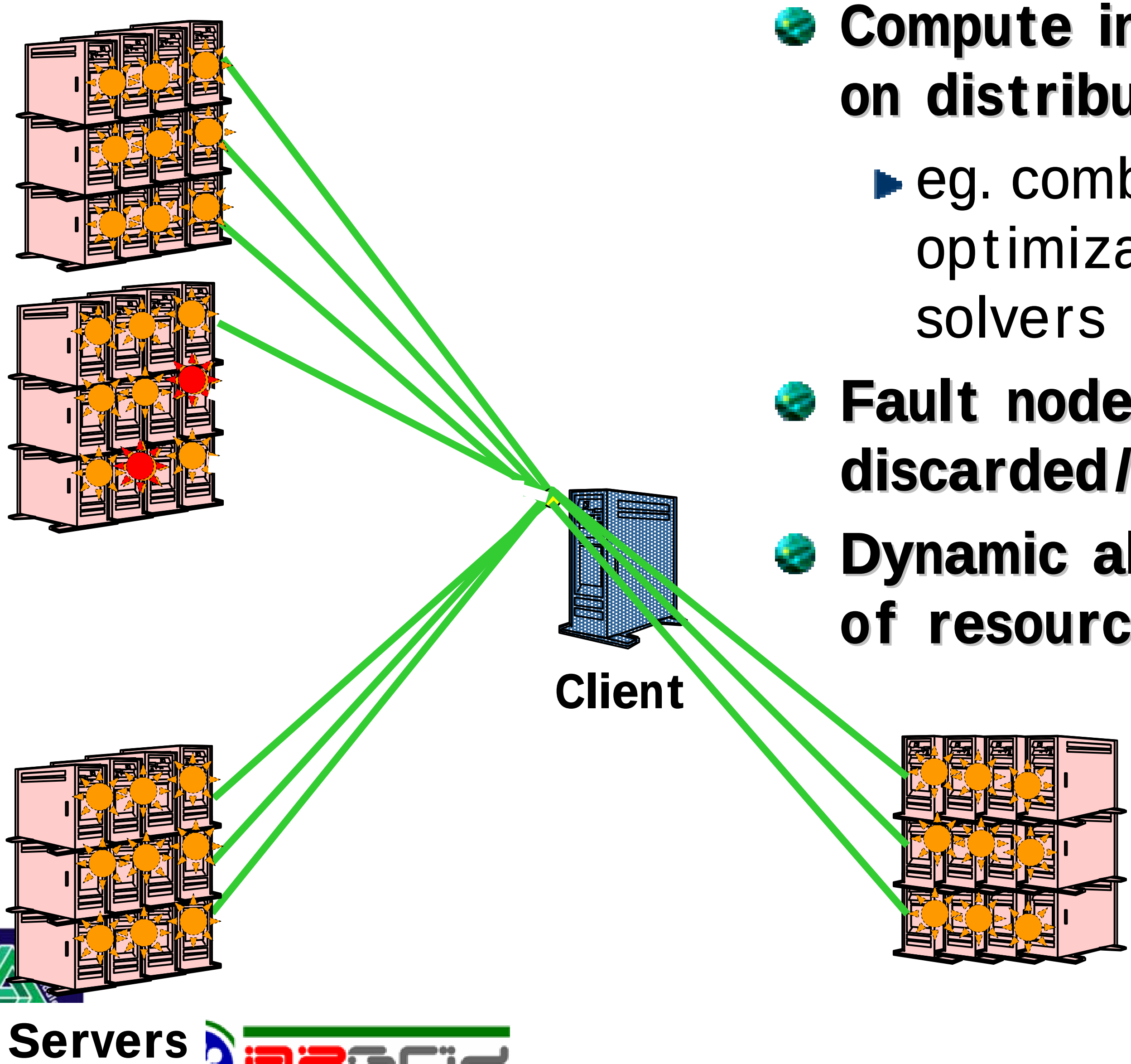
* May be dynamic using process spawning

Typical scenario 1: desktop supercomputing

- **Utilize remote supercomputers from your desktop computer**
- **Reduce cost for maintenance of libraries**
- **ASP-like approach**

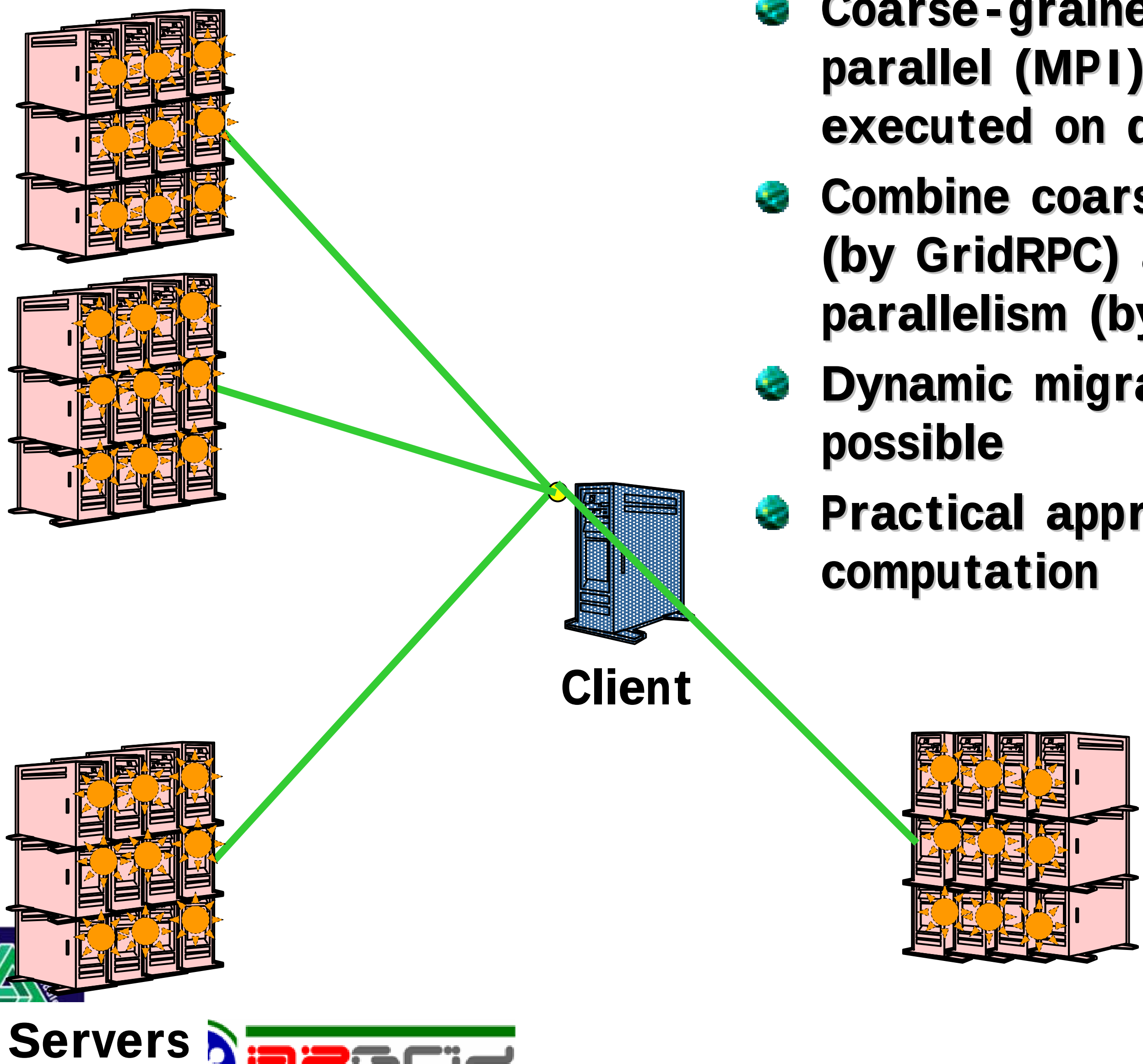


Typical scenario 2: parameter surevey



- **Compute independent tasks on distributed resources**
  - eg. combinatorial optimization problem solvers
- **Fault nodes can be discarded/retried**
- **Dynamic allocation / release of resources is possible**

Typical scenario 3: GridRPC + MPI



- Coarse-grained independent parallel (MPI) programs are executed on distributed clusters
- Combine coarse-grained parallelism (by GridRPC) and fine-grained parallelism (by MPI)
- Dynamic migration of MPI jobs is possible
- Practical approach for large-scale computation

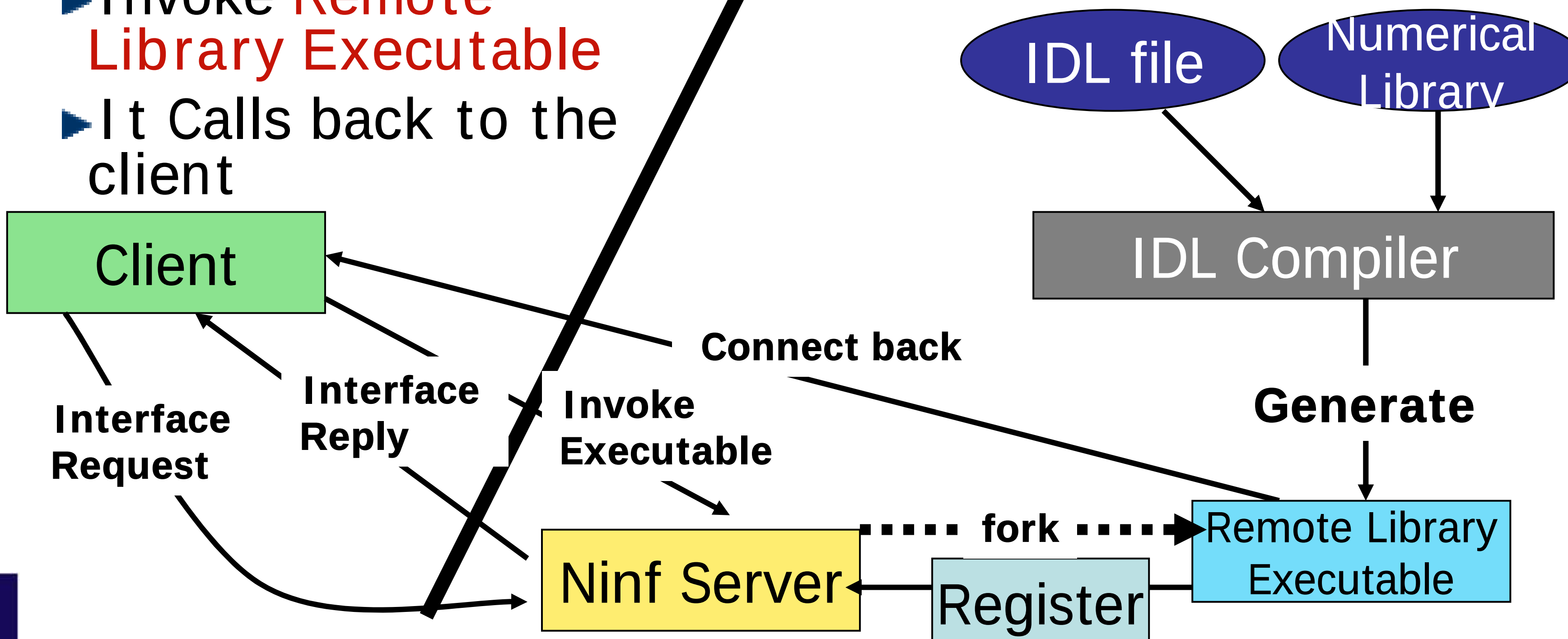
Sample Architecture and Protocol of GridRPC System – Ninf -

Client side

- **Call remote library**
  - Retrieve interface information
  - Invoke Remote Library Executable
  - It Calls back to the client

Server side

- **Server side setup**
  - **Build Remote Library Executable**
  - **Register it to the Ninf Server**



GridRPC: based on Client/Server model

- **Server-side setup**
  - Remote libraries must be installed in advance
    - Write IDL files to describe interface to the library
    - Build remote libraries
  - Syntax of IDL depends on GridRPC systems
    - e.g. Ninf-G and NetSolve have different IDL
- **Client-side setup**
  - Write a client program using GridRPC API
  - Write a client configuration file
  - Run the program

Ninf-G

Overview and Architecture

What is Ninf-G?

- **A software package which supports programming and execution of Grid applications using GridRPC.**
- **Three major versions**
  - Version 2 (Ninf-G2)
    - Works with pre-WS GRAM
    - The latest version is 2.3.0
    - 2.4.0 will come soon
  - Version 3 (Ninf-G3)
    - Works with GT3 WS GRAM
    - Obsolete version
    - Need to apply 3000lines patch to GT3.2.1
  - Version 4 (Ninf-G4)
    - Works with GT4 WS GRAM
    - Has an interface for working with other Grid middleware
    - 4.0.0 beta will come soon
    - 4.0.0 will be available on SC2005
- **Today's talk is based on Ninf-G2, but no differences in API between three versions**

What is Ninf-G? (cont'd)

- **Ninf-G is developed using Globus C and Java APIs**
  - Uses GSI, GRAM, MDS, GASS, and Globus-IO
- **Ninf-G includes**
  - C/C++, Java APIs, libraries for software development
  - IDL compiler for stub generation
  - Shell scripts to
    - compile client program
    - build and publish remote libraries
  - sample programs and manual documents

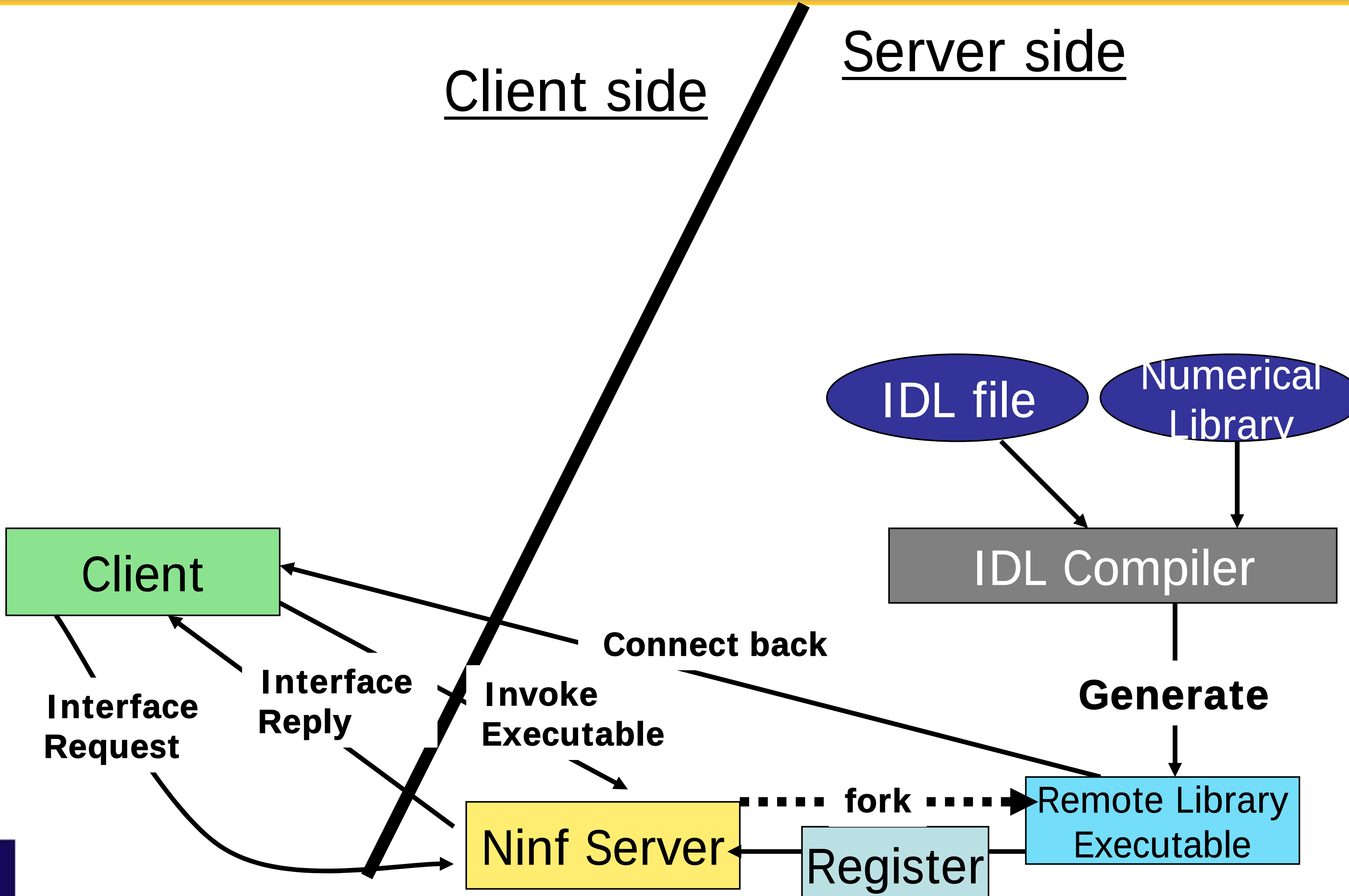
Terminology

- **Ninf-G Client**
  - This is a program written by a user for the purpose of controlling the execution of computation.
- **Ninf-G IDL**
  - Ninf-G IDL (Interface Description Language) is a language for describing interfaces for functions and objects those are expected to be called by Ninf-G client.
- **Ninf-G Stub**
  - Ninf-G stub is a wrapper function of a remote function/object. It is generated by the stub generator according to the interface description for user-defined functions and methods.

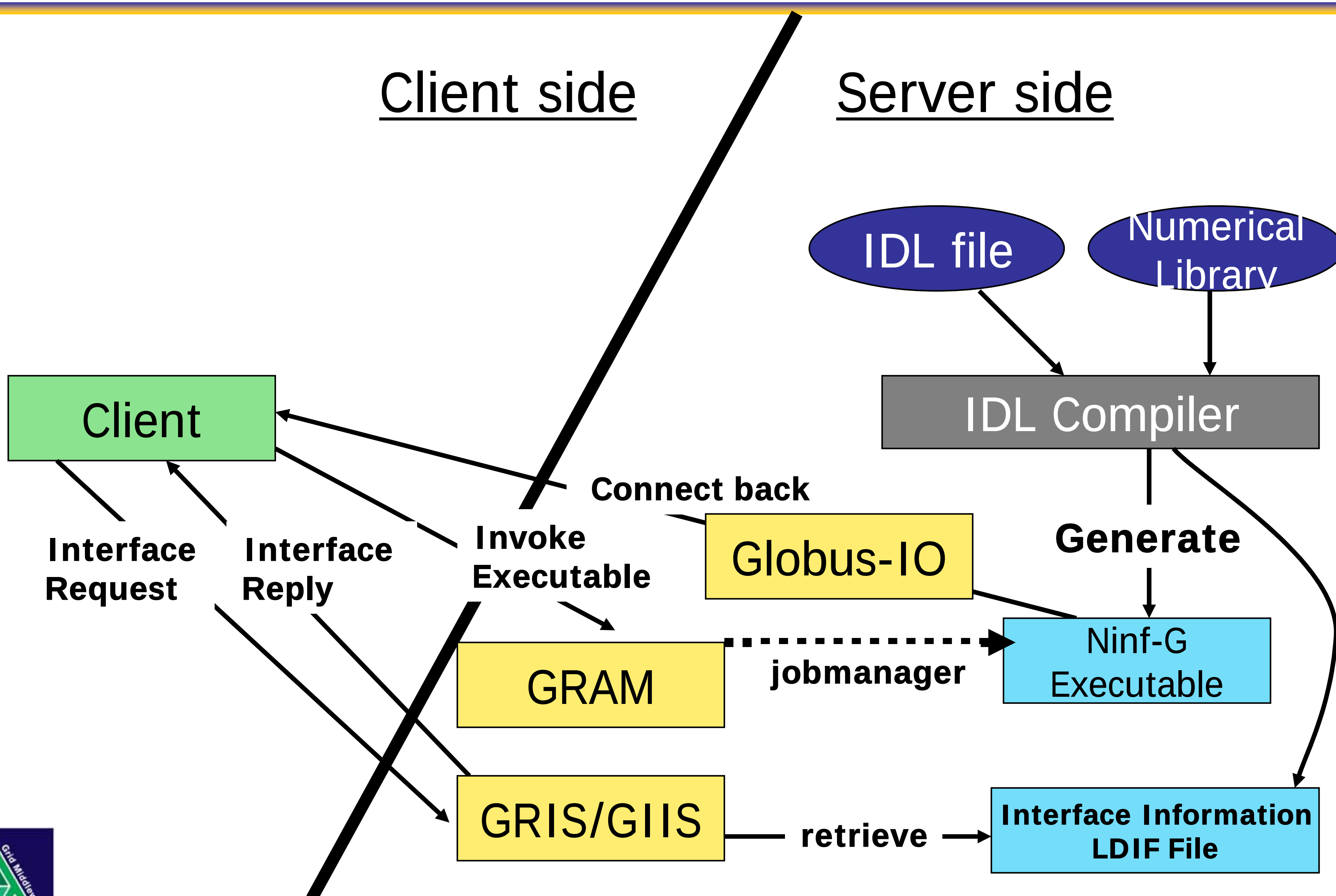
Terminloogy (cont'd)

- **Ninf-G Executable**
  - Ninf-G executable is an executable file that will be invoked by Ninf-G systems. It is obtained by linking a user-written function with the stub code, Ninf-G and the Globus Toolkit libraries.
- **Session**
  - A session corresponds to an individual RPC and it is identified by a non-negative integer called Session ID.
- **GridRPC API**
  - Application Programming Interface for GridRPC. The GridRPC API is going to be standardized at the GGF GridRPC WG.

Sample Architecture and Protocol of GridRPC System – Ninf -



Architecture of Ninf-G



How to use Ninf-G

- **Build remote libraries on server machines**
  - Write IDL files
  - Compile the IDL files
  - Build and install remote executables
- **Develop a client program**
  - Programming using GridRPC API
  - Compile
- **Run**
  - Create a client configuration file
  - Generate a proxy certificate
  - Run

Sample Program

- **Parameter Survey**
  - No. of surveys: n
  - Survey function: survey(in1, in2, result)
  - Input Parameters: double in1, int in2
  - Output Value: double result[]

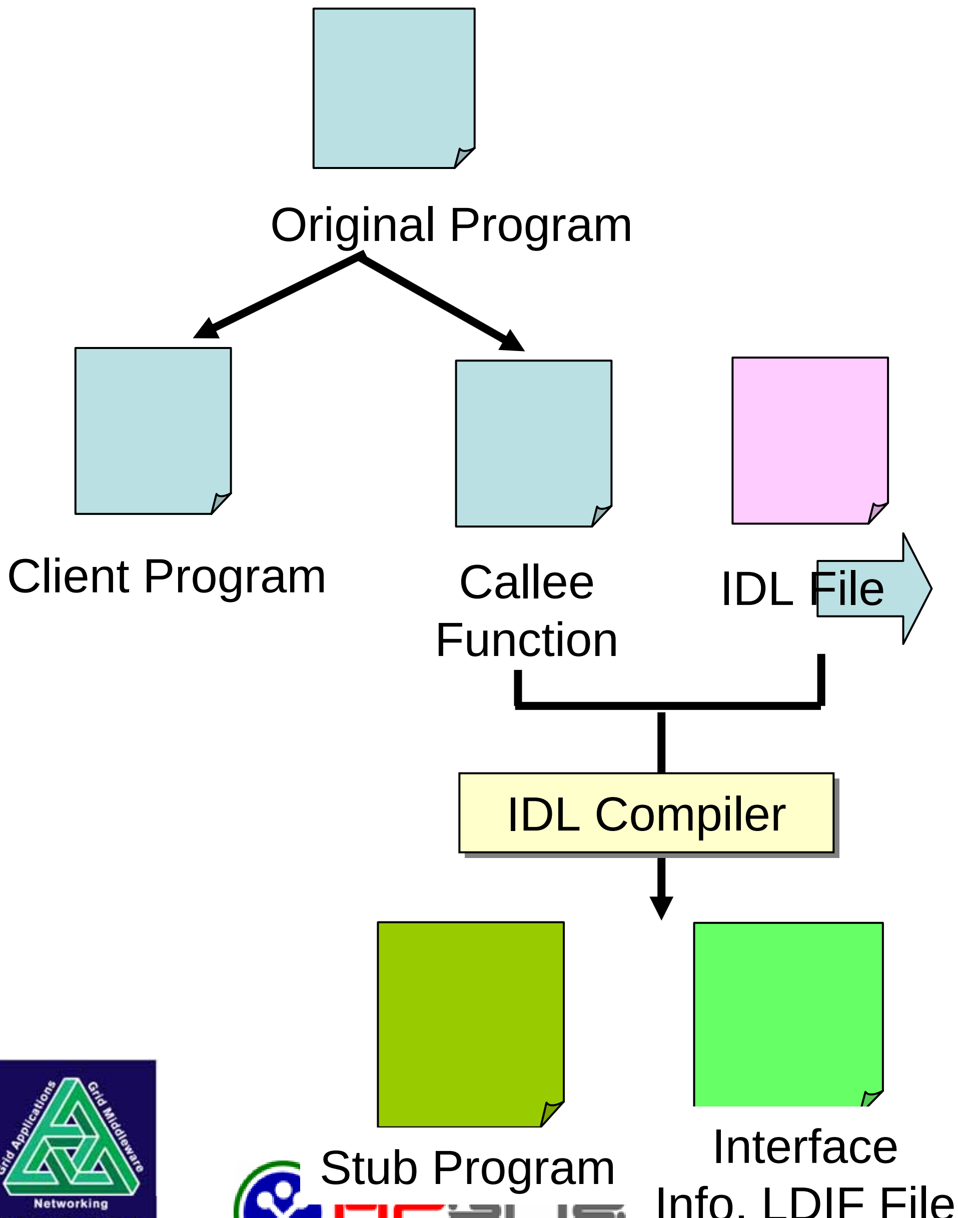
Main Program

```
Int main(int argc, char** argv)
{
int i, n, in2;
double in1, result[100][100];

Pre_processing();

For(I = 0; I < n, i++){
    survey(in1, in2, resul+100*n)
}

Post_processing();
```

Survey Function

```
survey(double in1, int in2, double* result)
{
・・・
  Do Survey
・・・

}
```

Build remote library (server-side operation)



Callee Function

```
survey
  (double in1, int in2, int size, double* result)

...
  Do Survey
...

}
```

Specify size of argument

IDL File

```
Module Survey_prog;

Define survey
  (IN double in1, IN int in2, IN int size,
                    OUT double* result);

Required "survey.o"
Calls "C" survey(in1, in2, size, result);
```

Ninfy the original code (client-side)

```
Int main(int argc, char** argv)
{
int i, n, in2;
double in1, result[100][100];

Pre_processing();

For(I = 0; I < n, i++){
    survey(in1, in2, resul+100*n)
}

Post_processing();
```

```
Int main(int argc, char** argv) {
int i, n, in2;
double in1, result[100][100];
grpc_function_handle_t handle [100];

Pre_processing();

grpc_initialize();
for(I = 0; I < n; i++) {
   handle[i] = grpc_function_handle_init();
}

For(I = 0; I < n, i++){
     grpc_call_async
          (handles, in1,in2,100, result+100*n)
}
grpc_wait_all();

for(I = 0; i<n; i++){
  grpc_function_handle_destruct();
}
grpc_finalize();

Post_processing();
```

Declare func. handles

Init func. handles

Async. RPC

Retrieve results

Destruct handles

NAREGI

ApGrid Asia-Pacific Grid

Ninf-G

How to build remote libraries

Ninf-G remote libraries

- **Ninf-G remote libraries are implemented as executable programs (Ninf-G executables) which**
  - contains stub routine and the main routine
  - will be spawned off by GRAM
- **The stub routine handles**
  - communication with clients and Ninf-G system itself
  - argument marshalling
- **Underlying executable (main routine) can be written in C, C++, Fortran, etc.**

Ninf-G remote libraries (cont'd)

- **Ninf-G provides two kinds of Ninf-G remote executables:**
  - Function
    - Stateless
    - Defined in standard GridRPC API
  - Ninf-G object
    - stateful
    - enables to avoid redundant data transfers
    - multiple methods can be defined
      - initialization
      - computation

How to build Ninf-G remote libraries (1/3)

- **Write an interface information using Ninf-G Interface Description Language (Ninf-G IDL).**
  Example:

```
Module mmul;
Define dmmul (IN int n,
              IN double A[n][n],
              IN double B[n][n],
              OUT double C[n][n])
Require "libmmul.o"
Calls "C" dmmul(n, A, B, C);
```

- **Compile the Ninf-G IDL with Ninf-G IDL compiler**

  % ng_gen <IDL_FILE>

  ns_gen generates stub source files and a makefile (<module_name>.mak)

How to build Ninf-G remote libraries (2/3)

- **Compile stub source files and generate Ninf-G executables and LDIF files (used to register Ninf-G remote libs information to GRIS).**

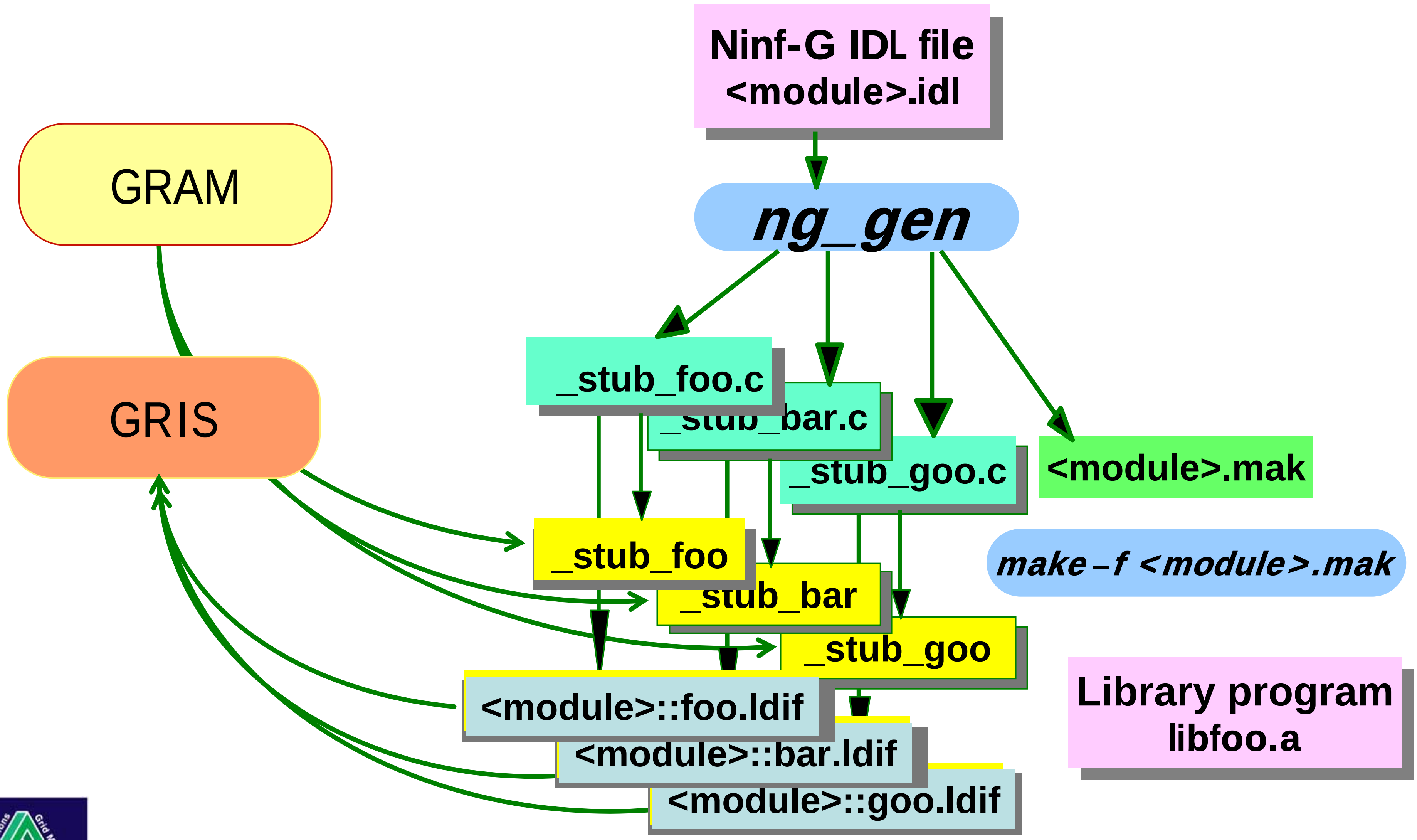
  % make –f <module_name>.mak

- **Publish the Ninf-G remote libraries**

  % make –f <module_name>.mak install

  This copies the LDIF files to ${GLOBUS_LOCATION}/var/gridrpc

How to build Ninf-G remote libraries (3/3)



Ninf-G IDL Statements (1/3)

- **Module** ***module_name***
  - specifies the module name.
- **CompileOptions** ***"options"***
  - specifies compile options which should be used in the resulting makefile
- **Library** ***"object files and libraries"***
  - specifies object files and libraries
- **FortranFormat** ***"format"***
  - provides translation format from C to Fortran.
  - Following two specifiers can be used:
    - %s: original function name
    - %l: capitalized original function name
  - Example:
    FortranFormat "_%l_";
    Calls "Fortran" fft(n, x, y);
    will generate function call
    FFT(n, x, y);
    in C.
- **Globals** ***{ ... C descriptions }***
  - declares global variables shared by all functions

How to define a remote function

- **Define** ***routine_name*** **(*parameters*...)**
  [“*description*”]
  [Required “*object files or libraries*”]
  [Backend “MPI”|”BLACS”]
  [Shrink “yes”|”no”]
  {*{C descriptions}* |
  Calls “C”|”Fortran” *calling sequence*}
  - declares function interface, required libraries and the main routine.
  - Syntax of parameter description:
    [mode-spec] [type-spec] formal_parameter
    [[dimension [:range]]+]+

How to define a remote object

- **DefClass class name**
  ["description"]
  [Required "*object files or libraries*"]
  [Backend "MPI" | "BLACS"]
  [Language "C" | "fortran"]
  [Shrink "yes" | "no"]
  { [DefState{ ... }]
  DefMethod method name (args…)
  {calling sequence}
  - Declares an interface for Ninf-G objects

Syntax of parameter description (detailed)

- **mode-spec: one of the following**
  - IN: parameter will be transferred from client to server
  - OUT: parameter will be transferred from server to client
  - INOUT: at the beginning of RPC, parameter will be transferred from client to server. at the end of RPC, parameter will be transferred from server to client
  - WORK: no transfers will be occurred. Specified memory will be allocated at the server side.
- **type-spec should be either *char, short, int, float, long, longlong, double, complex, or filename*.**
- **For arrays, you can specify the size of the array. The size can be specified using scalar IN parameters.**
  - Example: IN int n, IN double a[n]

Sample Ninf-G IDL (1/3)

Matrix Multiply

```
Module matrix;

Define dmmul (IN int n,
              IN double A[n][n],
              IN double B[n][n],
              OUT double C[n][n])
"Matrix multiply: C = A x B"
Required "libmmul.o"
Calls "C" dmmul(n, A, B, C);
```

Sample Ninf-G IDL (2/3)

```
Module sample_object;

DefClass sample_object
"This is test object"
Required "sample.o"
{
   DefMethod mmul(IN long n, IN double A[n][n],
      IN double B[n][n], OUT double C[n][n])
   Calls "C" mmul(n,A,B,C);

   DefMethod mmul2(IN long n, IN double A[n*n+1-1],
         IN double B[n*n+2-3+1], OUT double C[n*n])
   Calls "C" mmul(n,A,B,C);

   DefMethod FFT(IN int n,IN int m, OUT float x[n][m], float INOUT y[m][n]
)
   Calls "Fortran" FFT(n,x,y);
}
```

Sample Ninf-G IDL (3/3)

ScaLAPACK (pdgesv)

```
Module SCALAPACK;

CompileOptions "NS_COMPILER = cc";
CompileOptions "NS_LINKER = f77";
CompileOptions "CFLAGS = -DAdd_ -O2 –64 –mips4 –r10000";
CompileOptions "FFLAGS = -O2 -64 –mips4 –r10000";
Library "scalapack.a pblas.a redist.a tools.a libmpiblacs.a –lblas –lmpi –lm";

Define pdgesv (IN int n, IN int nrhs, INOUT double global_a[n][lda:n], IN int lda,
                    INOUT double global_b[nrhs][ldb:n], IN int ldb, OUT int info[1])
Backend "BLACS"
Shrink "yes"
Required "procmap.o pdgesv_ninf.o ninf_make_grid.of Cnumroc.o descinit.o"
Calls "C" ninf_pdgesv(n, nrhs, global_a, lda, global_b, ldb, info);
```

Ninf-G

How to call Remote Libraries

- client side APIs and operations -

(Client) User's Scenario

- **Write client programs in C/C++/Java using APIs provided by Ninf-G**
- **Compile and link with the supplied Ninf-G client compile driver (*ngcc*)**
- **Write a client configuration file in which runtime environments can be described**
- **Run *grid-proxy-init* command**
- **Run the program**

GridRPC API / Ninf-G API

APIs for programming client applications

The GridRPC API and Ninf-G API

GridRPC API

- Standard C API defined by the GGF GridRPC WG.
- Provides portable and simple programming interface.
- Enable interoperability between implementations suchas Ninf-G and NetSolve.

Ninf-G API

- Non-standard API (Ninf-G specific)
- complement to the GridRPC API
- provided for high performance, usability, etc.
- ended by _np
  - eg: grpc_function_handle_array_init_np(...)

Rough steps for RPC

- **Initialization**

```
grpc_initialize(config_file);
```

- **Create a function handle**
  - abstraction of a connection to a remote executable

```
grpc_function_handle_t  handle;

grpc_function_handle_init(
  &handle, host, port, “lib_name”);
```

- **Call a remote library**

```
grpc_call(&handle, args…);
          or
grpc_call_async(&handle, args…);
grpc_wait( );
```

Data types

- **Function handle – *grpc_function_handle_t***
  - A structure that contains a mapping between a client and an instance of a remote function
- **Object handle – *grpc_object_handle_t_np***
  - A structure that contains a mapping between a client and an instance of a remote object
- **Session ID – *grpc_sessionid_t***
  - Non-nevative integer that identifies a session
  - Session ID can be used for status check, cancellation, etc. of outstanding RPCs.
- **Error and status code – *grpc_error_t***
  - Integer that describes error and status of GridRPC APIs.
  - All GridRPC APIs return error code or status code.

Initialization / Finalization

- **grpc_error_t grpc_initialize(char *config_file_name)**
  - reads the configuration file and initialize client.
  - Any calls of other GRPC APIs prior to grpc_initialize would fail
  - Returns GRPC_OK (success) or GRPC_ERROR (failure)
- **grpc_error_t grpc_finalize()**
  - Frees resources (memory, etc.)
  - Any calls of other GRPC APIs after grpc_finalize would fail
  - Returns GRPC_OK (success) or GRPC_ERROR (failure)

Function handles

- **grpc_error_t grpc_function_handle_default(**
  grpc_function_handle_t *handle,
  char *func_name)
  - Creates a function handle to the default server
- **grpc_error_t grpc_function_handle_init(**
  grpc_function_handle_t *handle,
  char *host_port_str,
  char *func_name)
  - Specifies the server explicitly by the second argument.
- **grpc_error_t grpc_function_handle_destruct(**
  grpc_function_handle_t *handle)
  - Frees memory allocated to the function handle

Function handles (cont'd)

- **grpc_error_t grpc_function_handle_array_default_np (**
  grpc_function_handle_t *handle,
  size_t nhandles,
  char *func_name)
  - Creates multiple function handles via a single GRAM call
- **grpc_error_t grpc_function_handle_array_init_np (**
  grpc_function_handle_t *handle,
  size_t nhandles,
  char *host_port_str,
  char *func_name)
  - Specifies the server explicitly by the second argument.
- **grpc_error_t grpc_function_handle_array_destruct_np (**
  grpc_function_handle_t *handle,
  size_t nhandles)
  - Specifies the server explicitly by the second argument.

Object handles

- **grpc_error_t grpc_object_handle_default_np (**
  grpc_object_handle_t_np *handle,
  char *class_name)
  - Creates an object handle to the default server
- **grpc_error_t grpc_object_handle_init_np (**
  grpc_function_object_t_np *handle,
  char *host_port_str,
  char *class_name)
  - Specifies the server explicitly by the second argument.
- **grpc_error_t grpc_function_object_destruct_np (**
  grpc_object_handle_t_np *handle)
  - Frees memory allocated to the function handle.

Object handles (cont'd)

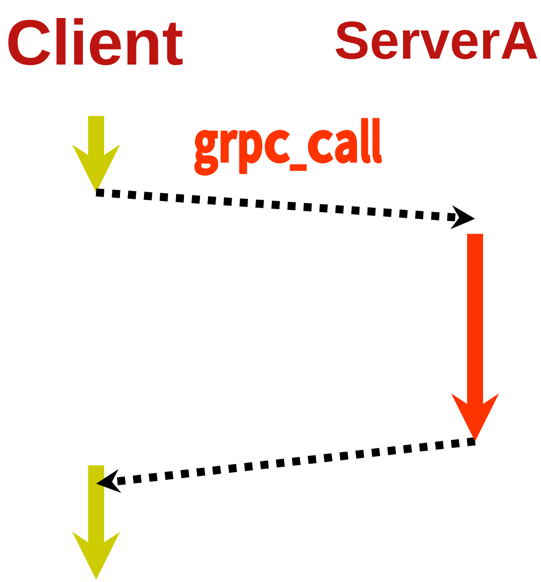
- **grpc_error_t grpc_object_handle_array_default (**
  grpc_objct_handle_t_np *handle,
  size_t nhandles,
  char *class_name)
  - Creates multiple object handles via a single GRAM call.
- **grpc_error_t grpc_object_handle_array_init_np (**
  grpc_object_handle_t_np *handle,
  size_t nhandles,
  char *host_port_str,
  char *class_name)
  - Specifies the server explicitly by the second argument.
- **grpc_error_t grpc_object_handle_array_destruct_np (**
  grpc_object_handle_t_np *handle,
  size_t nhandles)
  - Frees memory allocated to the function handles.

Synchronous RPC v.s. Asynchronous RPC

Synchronous RPC

- Blocking Call
- Same semantics with a local function call.

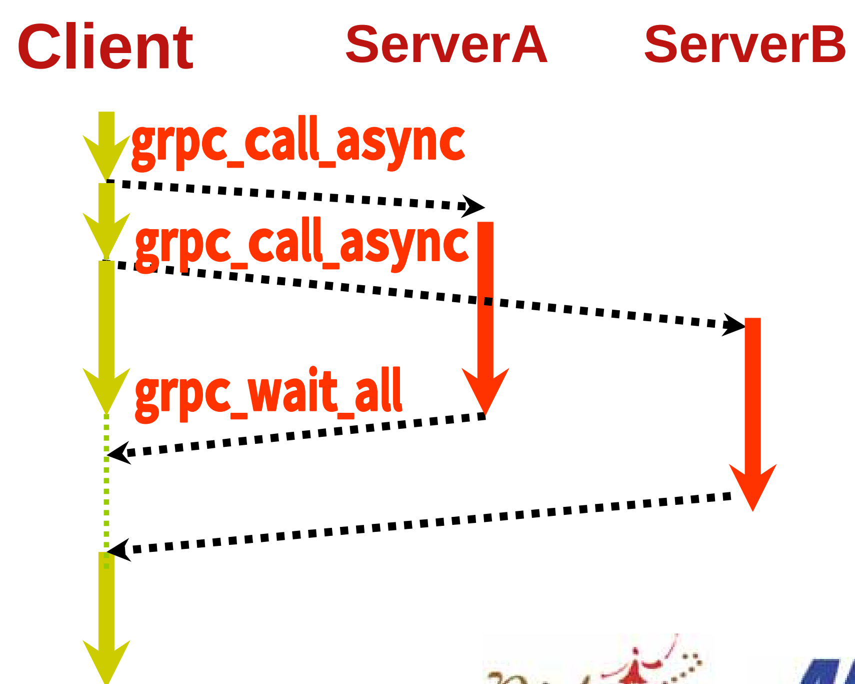
```
grpc_call(...);
```



Asynchronous RPC

- Non-blocking Call
- Useful for task-parallel applications

```
grpc_call_async(...);
grpc_wait_*(...);
```



RPC functions

- **grpc_error_t grpc_call (**
  grpc_function_handle_t *handle, ...)
  - Synchronous (blocking) call
- **grpc_error_t grpc_call_async (**
  grpc_function_handle_t *handle,
  grpc_sessionid_t *sessionID,
  ...)
  - Asynchronous (non-blocking) call
  - Session ID is stored in the second argument.

Ninf-G method invocation

- **grpc_error_t grpc_invoke_np (**
  grpc_object_handle_t_np *handle,
  char *method_name,
  ...
)
  - Synchronous (blocking) method invocation
- **grpc_error_t grpc_invoke_async_np (**
  grpc_object_handle_t_np *handle,
  char *method_name,
  grpc_sessionid_t *sessionID,
  ...)
  - Asynchronous (non-blocking) method invocation
  - session ID is stored in the third argument.

Session control functions

- **grpc_error_t grpc_probe (grpc_sessionid_t sessionID)**
  - probes the job specified by SessionID whether the job has been completed.
- **grpc_error_t grpc_probe_or (grpc_sessionid_t *idArray, size_t length, grpc_sessionid_t *idPtr)**
  - probes whether at least one of jobs in the array has been
- **grpc_error_t grpc_cancel (grpc_sessionid_t sessionID)**
  - Cancels a session
- **grpc_error_t grpc_cancel_all ()**
  - Cancels all outstanding sessions

Wait functions

- **grpc_error_t grpc_wait (grpc_sessionid_t sessionID)**
  - Waits outstanding RPC specified by sessionID
- **grpc_error_t grpc_wait_and (grpc_sessionid_t *idArray, size_t length)**
  - Waits all outstanding RPCs specified by an array of sessionIDs

Wait functions (cont'd)

- **grpc_error_t grpc_wait_or (
  grpc_sessionid_t *idArray,
  size_t length,
  grpc_sessionid_t *idPtr)**
  - Waits any one of RPCs specified by an array of sessionIDs.
- **grpc_error_t grpc_wait_all ()**
  - Waits until all outstanding RPCs are completed.
- **grpc_error_t grpc_wait_any (
  grpc_sessionid_t *idPtr)**
  - Waits any one of outstanding RPCs.

Ninf-G

Compile and run

Prerequisite

- **Environment variables**
  - GPT_LOCATION
  - GLOBUS_LOCATION
  - NG_DIR
- **PATH**
  - ${GLOBUS_LOCATION}/etc/globus-user-env.{csh,sh}
  - ${NG_DIR}/etc/ninfg-user-env.{csh,sh}
- **Globus-level settings**
  - User certificate, CA certificate, grid-mapfile
  - test

    % grid-proxy-init

    % globus-job-run server.foo.org /bin/hostname
- **Notes for dynamic linkage of the Globus shared libraries:**
  - Globus dynamic libraries (shared libraries) must be linked with the Ninf-G stub executables. For example on Linux, this is enabled by adding ${GLOBUS_LOCATION}/lib in /etc/ld.so.conf and run ldconfig command.

Compile and run

- **Compile the client application using *ngcc* command**
  % ng_cc –o myapp app.c

- **Create a proxy certificate**
  % grid-proxy-init

- **Prepare a client configuration file**

- **Run**
  % ./myapp config.cl [args…]

NAREGI

Asia-Pacific Grid

AIST

Client configuration file

- **Specifies runtime environments**
- **Available attributes are categorized to sections:**
  - INCLUDE section
  - CLIENT section
  - LOCAL_LDIF section
  - FUNCTION_INFO section
  - MDS_SERVER section
  - SERVER section
  - SERVER_DEFAULT section

Frequently used attributes

- **<CLIENT> </CLIENT> section**
  - loglevel
  - refresh_credential
- **<SERVER> </SERVER> section**
  - hostname
  - mpi_runNoOfCPUs
  - jobmanager
  - job_startTimeout
  - job_queue
  - heatbeat / heatbeat_timeoutCount
  - redirect_outerr
- **<FUNCTION_INFO> </FUNCTION_INFO> section**
  - session_timeout
- **<LOCAL_LDIF> </LOCAL_LDIF> section**
  - filename

Ninf-G

Summary

How to use Ninf-G (again)

- **Build remote libraries on server machines**
  - Write IDL files
  - Compile the IDL files
  - Build and install remote executables
- **Develop a client program**
  - Programming using GridRPC API
  - Compile
- **Run**
  - Create a client configuration file
  - Generate a proxy certificate
  - Run

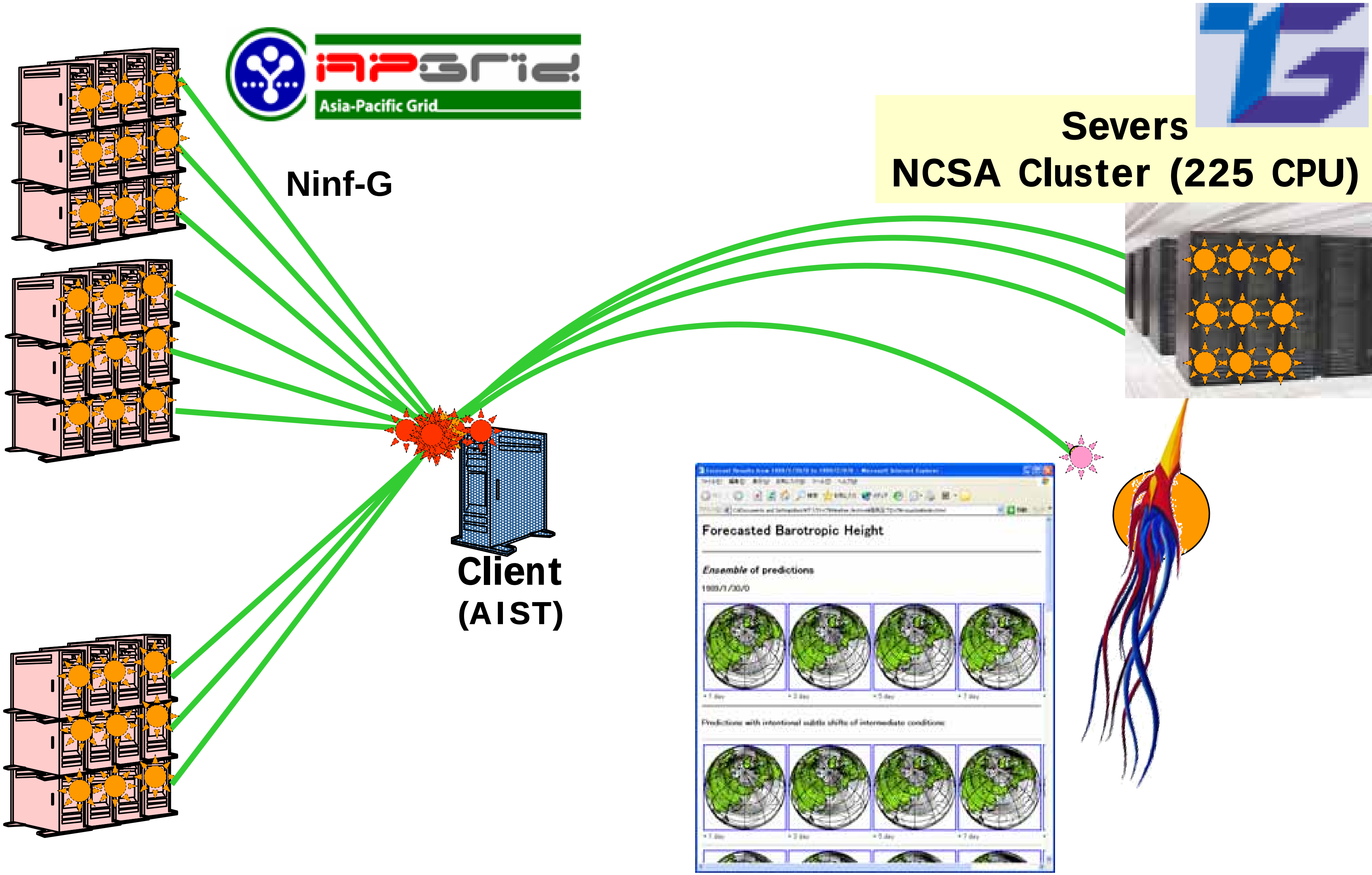
Ninf-G tips

- **How the server can be specified?**
  - Server is determined when the function handle is initialized.
    - *grpc_function_handle_init();*
      - hostname is given as the second argument
    - *grpc_function_handle_default();*
      - hostname is specified in the client configuration file which must be passed as the first argument of the client program.
  - Ninf-G does not provide broker/scheduler/meta-server.
- **Should use LOCAL LDIF rather than MDS.**
  - easy, efficient and stable
- **How should I deploy Ninf-G executables?**
  - Deploy Ninf-G executables manually
  - Ninf-G provides automatic staging of executables
- **Other functionalities?**
  - heatbeating
  - timeout
  - client callbacks
  - attaching to debugger
  - ...

Ninf-G

Recent achievements

Climate simulation on AIST-TeraGrid @SC2003



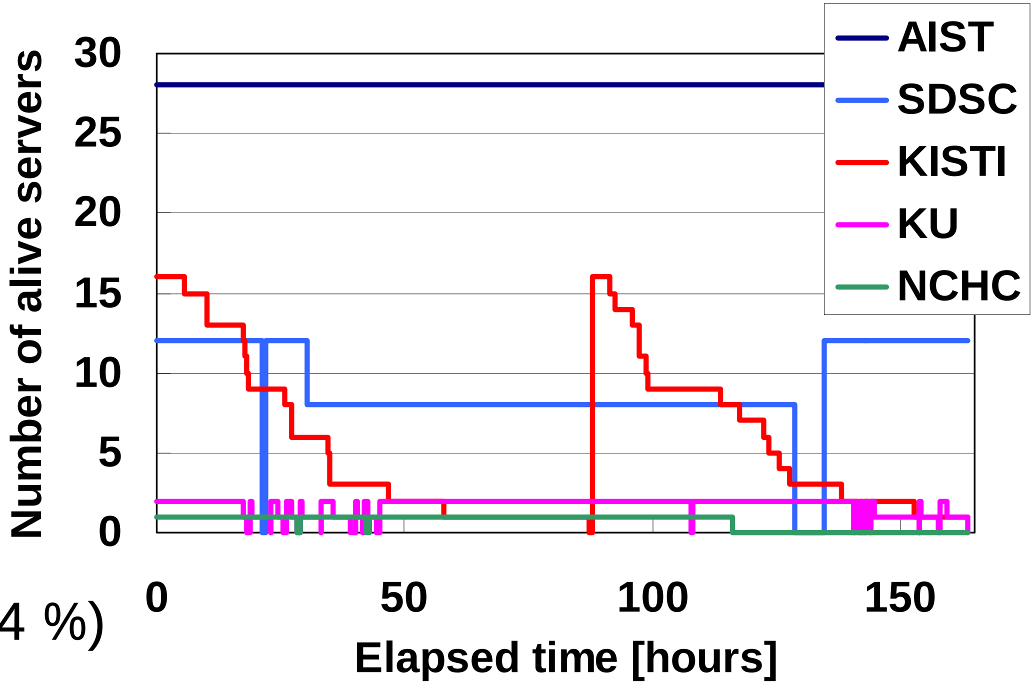
Experiments on long-run

Purpose

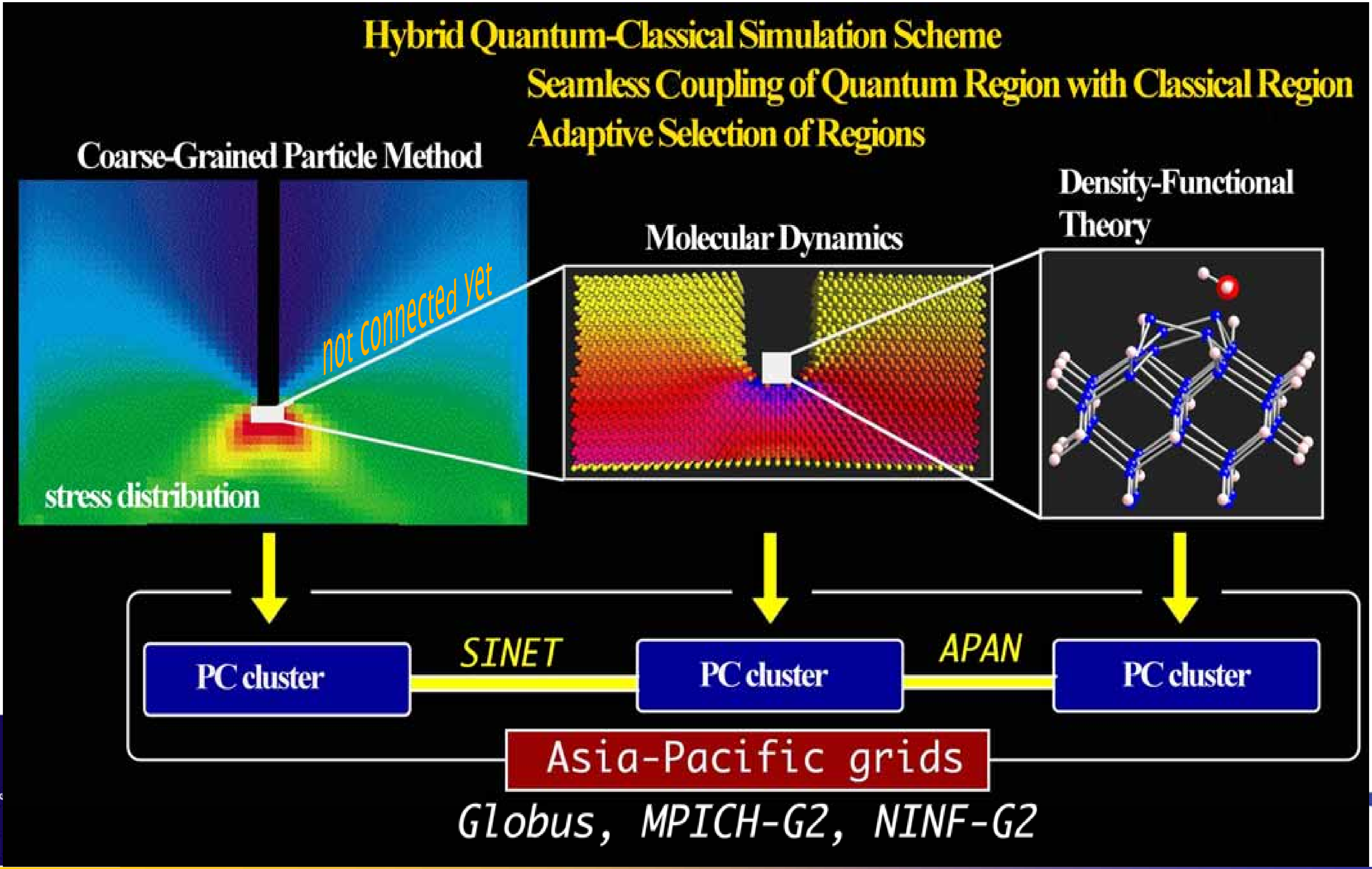
- Evaluate quality of Ninf-G2
- Have experiences on how GridRPC can adapt to faults

Ninf-G stability

- Number of executions : 43
- Execution time
  (Total) : 50.4 days
  (Max) : 6.8 days
  (Ave) : 1.2 days
- Number of RPCs:
  more than 2,500,000
- Number of RPC failures:
  more than 1,600
  (Error rate is about 0.064 %)

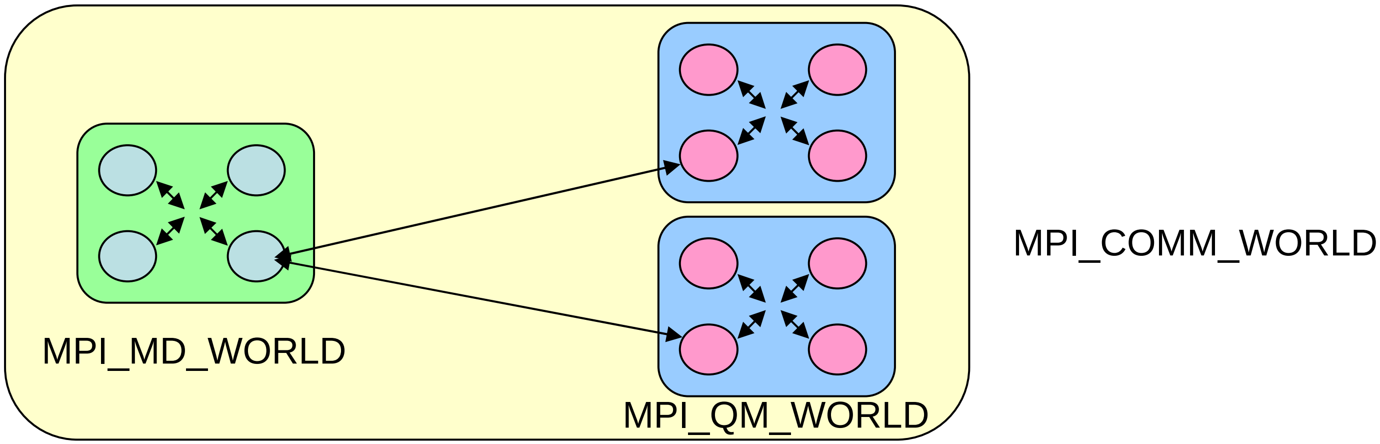


Hybrid Quantum-Classical Simulation Scheme on Grid

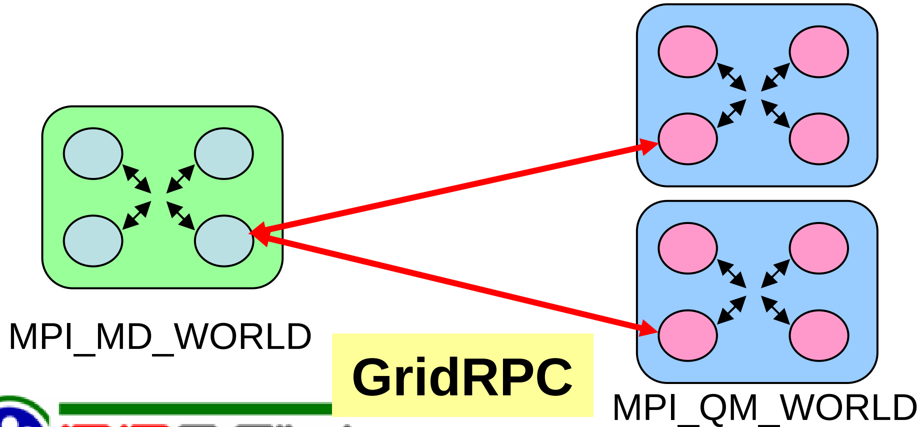


Re-implementation using GridRPC

Original implementation (MPI)



New implementation (GridRPC + MPI)



Hybrid QM-MD Simulation of Nano-structured Si in Corrosive Environment

Nano-structured Si system under stress

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

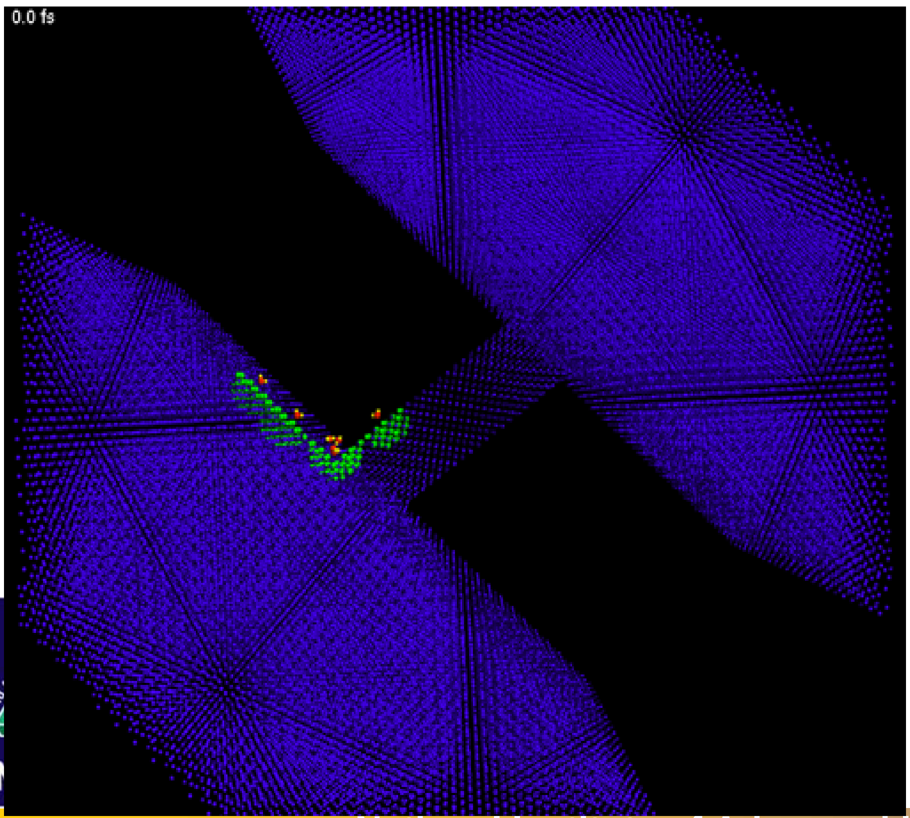
4 quantum regions:

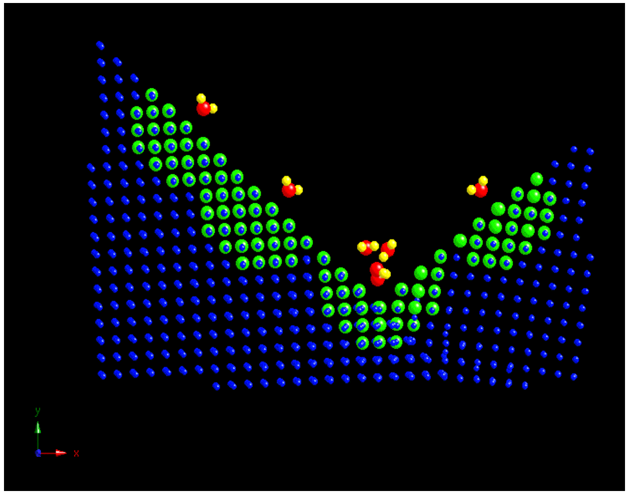
#0: 69 atoms including $2H_2O+2OH$

#1: 68 atoms including H_2O

#2: 44 atoms including H_2O

#3: 56 atoms including H_2O





Close-up view

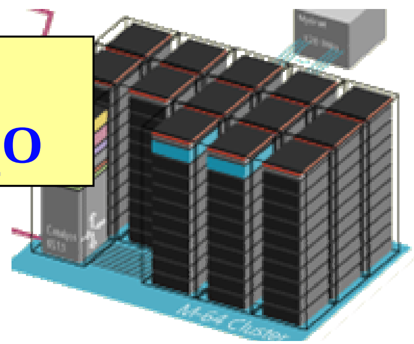
Testbed used in the experiment @ SC2004

P32 (512 CPU)

#0: 69 atoms including $2H_2O+2OH$

P32 (512 CPU)

#1: 68 atoms including H_2O



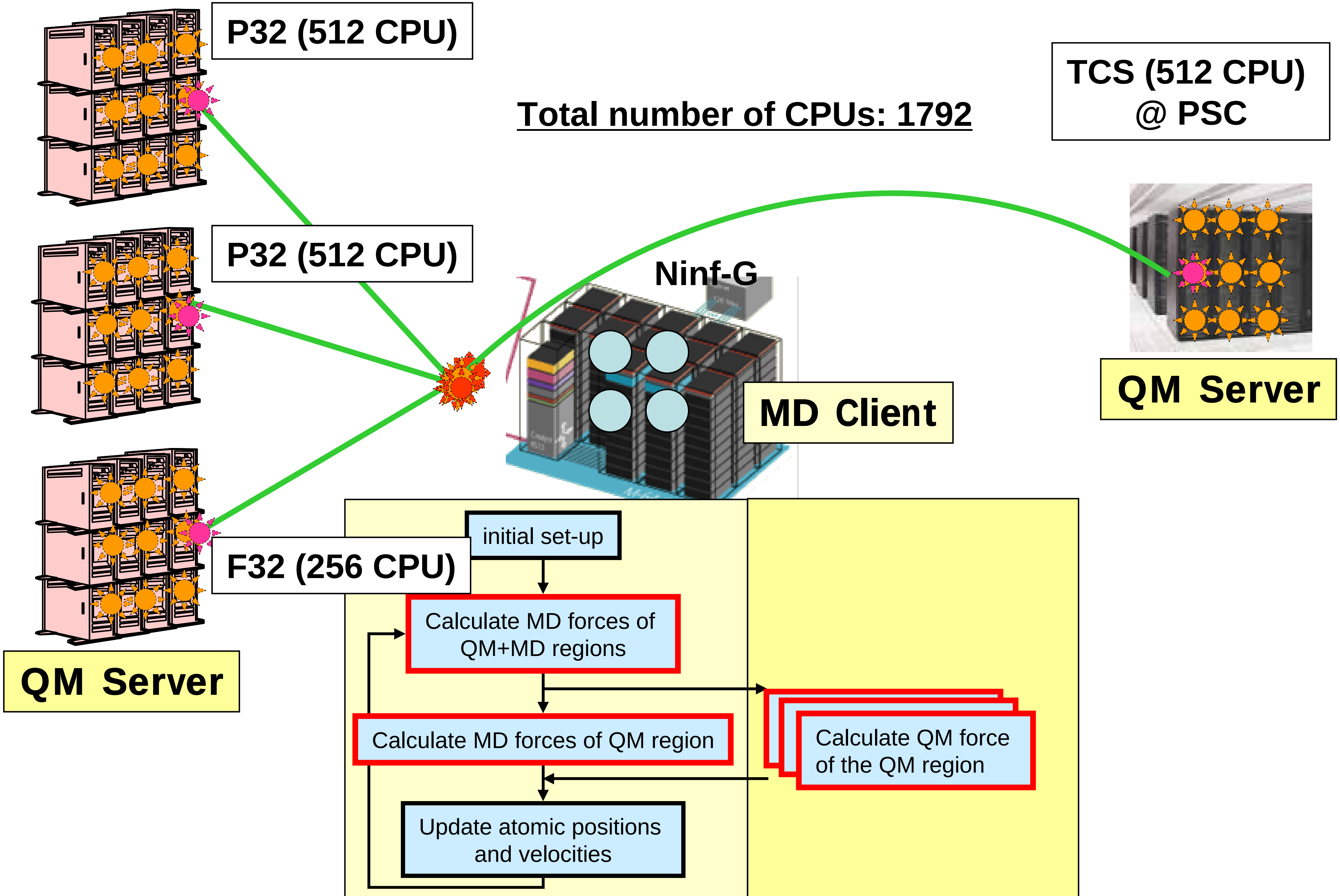
F32 (256 CPU)

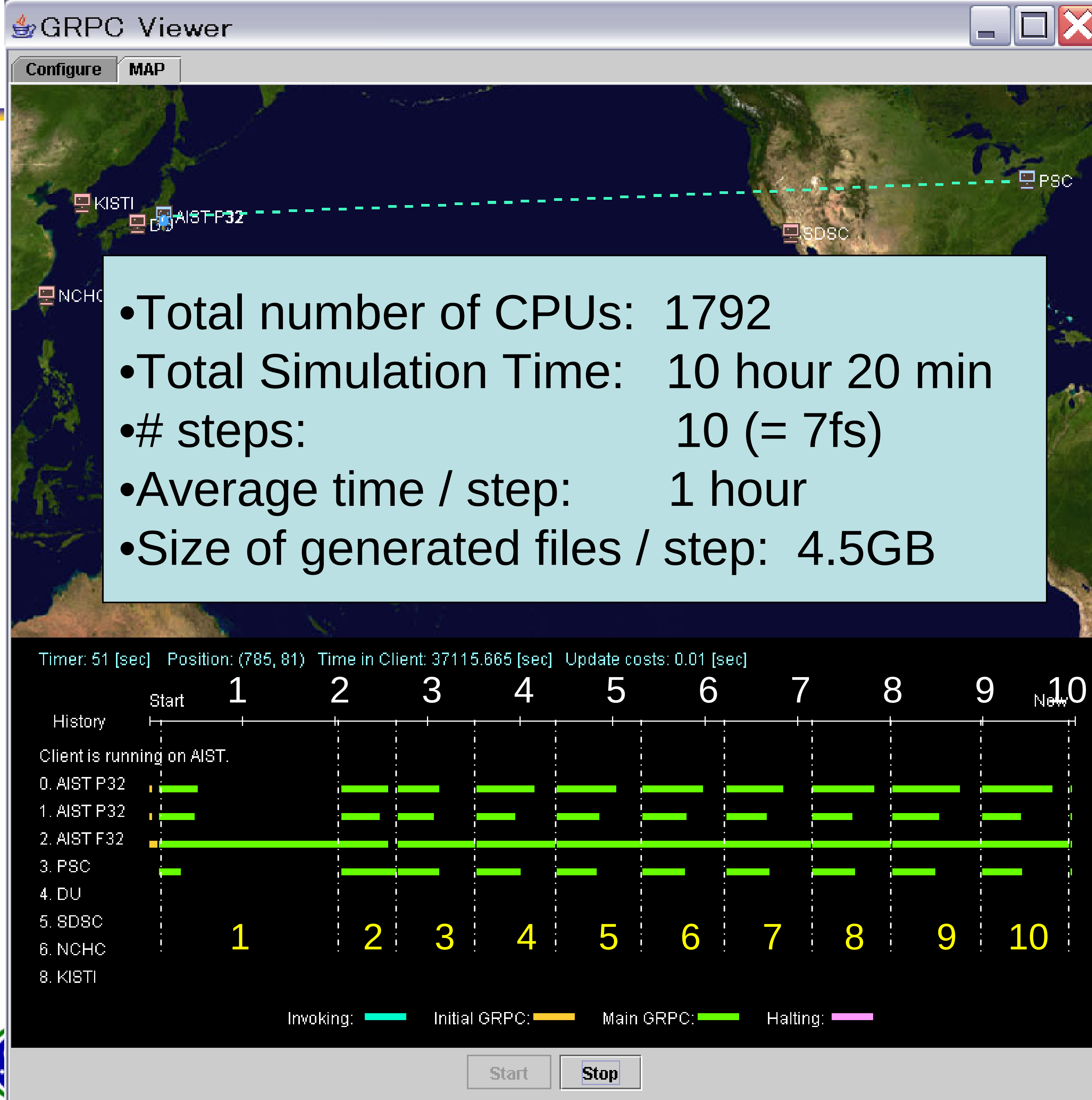
#2: 44 atoms including H_2O

TCS (512 CPU) @ PSC

#3: 56 atoms including H_2O

QM/MD simulation over the Pacific





- Total number of CPUs: 1792
- Total Simulation Time: 10 hour 20 min
- # steps: 10 (= 7fs)
- Average time / step: 1 hour
- Size of generated files / step: 4.5GB

For more info, related links

- **Ninf project ML**
  - ninf@apgrid.org
- **Ninf-G Users' ML**
  - ninf-users@apgrid.org
- **Ninf project home page**
  - http://ninf.apgrid.org
- **Global Grid Forum**
  - http://www.ggf.org/
- **GGF GridRPC WG**
  - http://forge.gridforum.org/projects/gridrpc-wg/
- **Globus Alliance**
  - http://www.globus.org/