In-Situ PBVR (v1.1) User Guide

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1 Introduction

This document is a user guide for In-Situ PBVR, which is an in-situ remote visualization system developed at the Center for Computational Science & e-Systems in Japan Atomic Energy Agency. In today's supercomputers, the computation speed greatly exceeds the I/O speed, making it difficult to output computation results. As a result, it has become difficult to apply the conventional visualization method, in which calculation results on a remote storage are transferred to a PC at hand for visualization. In-Situ visualization avoids large-scale data I/O by having the visualization program coupled to the simulation and processed simultaneously in the same environment as the simulation to reliably generate visualization images. In-Situ PBVR is a framework that enables interactive visualization through particle-based visualization and interactive in-situ control technology, whereas interactive in-situ visualization is difficult to achieve with conventional polygon-based methods. In-Situ PBVR is a C++ library built using the Particle Based Volume Rendering (PBVR) method, a particle-based volume rendering method developed by Koyamada Laboratory, Kyoto University, and the visualization library KVS. The framework consists of three components: a particle sampler, a daemon, and a PBVR client (Figure 1-1).

(1) Particle Sampler

The particle sampler is a visualization library that is coupled to a simulation code to generate particles in the same environment as the calculation. To build a simulation + in-situ visualization code, an array of calculation results is passed to the visualization functions provided by the particle sampler and inserted into the simulation code. The particle sampler refers to the visualization parameter file on the storage, converts the calculation results of each time step into compressed particles for visualization, and outputs them on the storage. The particle files are output from each process in a distributed manner.

(2) Daemon

The daemon runs on the login node or the interactive job and mediates between the particle files on the storage and the visualization parameters sent from the PBVR client. The daemon monitors the files on the storage, aggregates the distributed output particle files, and transfers them to the user PC via the network. The daemon also receives the visualization parameters sent from the PBVR client and outputs them as a visualization parameter file to be referenced by the particle sampler. Since this operation is executed asynchronously with the simulation, interactive control is possible without interfering with the simulation.

(3) PBVR Client

The PBVR Client runs on the user's PC and provides a viewer to display the visualization results and a GUI to edit the visualization parameters. PBVR Client communicates with the daemon using port forwarding. The PBVR client receives the particle data from the daemon, displays the volume rendered image on the viewer, and sends the visualization parameters edited by the user on the GUI to the daemon. In-Situ PBVR implements a multivariate visualization function that can be used universally for various simulations. In 3D data visualization, colors and opacity are assigned to the physical values of the simulation results, and the function that describes the relationship between them is called the transfer function. In conventional visualization, 1D transfer functions that assign color and opacity to a single physical value are used. However, it is difficult to design a multidimensional transfer function for multivariate data using conventional visualization methods. The In-Situ PBVR provides a transfer function editor that allows users to design multidimensional transfer functions using algebraic expressions. The transfer function editor allows users to edit the 1D transfer function of each physical variable, and to write a multidimensional transfer function using arbitrary algebraic expressions with these 1D transfer functions as variables. In this algebraic expression, basic operators, elementary functions, and differential operators can be used.

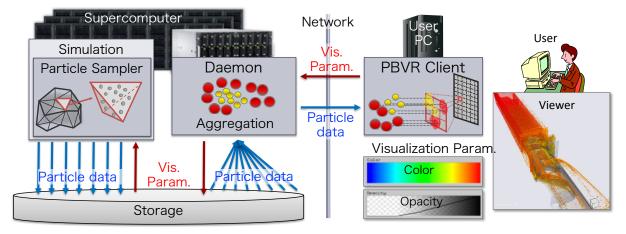


Figure 1-1 The configuration of In-Situ PBVR framework

1.1. Overview of Particle Sampler

The particle sampler is parallelized by hybrid of MPI/OMP programming model, and further accelerates the generation of particle data by using SIMD operation. The particle sampler is MPI parallelized without changing the domain decomposition of simulation, and generates particles in element parallel by OpenMP in each decomposed domain. The synthesis of physical values, the synthesis of transfer func tions, and the interpolation of physical values, which are required in multivariate visualization, are vectorized using SIMD operations.

Three types of particle samplers are available according to the simulation grid types, one for structured grids, one for unstructured grids, and one for hierarchical grids. The particle sampler supports simulation code written in C/C++ and FORTRAN. For in-situ visualization, the particle sampler is inserted into the time step loop of the simulation. At this time, multivariate data of simulation results, lattice data, and global coordinates of the region are input as arguments of the particle sampler. Also, the memory layout of multivariate data assumes an array structure (SOA).

1.2. Overview of Daemon

The daemon is executed on an interactive node or interactive job of the supercomputer, and is a key to realize interactive visualization during batch processing. The daemon constantly monitors files on

storage, and collects particle files output by the particle sampler. Because this collection is asynchronous with the particle sampler and the simulation, it does not impede the performance of the simulation. The collection of the particle files is parallelized by OpenMP, and the daemon aggregates the particle files into single particle data and sends it to the PBVR client. The daemon also receives the visualization parameters sent from the PBVR client and updates the visualization parameter file on the storage used by the particle sampler.

In the in-situ PBVR, since the daemon and the PBVR client send and receive data by socket communication via the Internet, the interactive node and the user PC need to be connected by port forwarding. Therefore, if the port forwarding is not permitted on a supercomputer, the daemon does not work and interactive visualization can not be used. In addition, interactive visualization can not be used even on a super computer that employs staging I/O where file output does not occur until the end of batch processing.

1.3. Overview of PBVR Client

The PBVR client is lunched on the user PC, and is comprised of a screen for displaying the visualization result, and a transfer function editor. In the transfer function editor, a "transfer function synthesizer" (TFS) is implemented in which is a function for realizing multivariate visualization. The TFS has a volume data synthesisis function which combines variables included in the result data to generate new volume data, and a transfer function synthesis function which combines multiple transfer functions. The user specifies the synthesis function by an algebraic expression on TFS. The algebraic expression is transferred to the PBVR sampler as a visualization parameter, and the volume data and transfer function synthesis are performed in real time by computer algebra system. Users can use initial mathematical functions and spatial derivatives of physical variables as algebraic expressions on TFS, and flexibly design the transfer function for the multivariate data by mathematical expressions.

1.4. Operating Environment

In-Situ PBVR is a cross-platform program and can be run on various supercomputers such as Fugaku, Oakforest PACS at the University of Tokyo/Tsukuba University, and SGI8600 owned by JAEA. The table below shows the operating environment.

Platform	OS	Compiler
Linux	Ubuntu18	g++
Мас	OSX10	clang
Windows	Windows10	MSVC

Table	1-1	PBVR Client
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Table 1-2 Daemon

Platform	OS	Compiler
Linux	RedHat	g++

Table 1-3 Particle Sampler

Platform	OS	Compiler
FUGAKU	A64FX (ARM)	Fujitsu compiler
OakforestPACS	Intel Xeon Phi (Knights Landing, KNL)	Intel compiler
SGI8600	Intel Xeon Gold	Intel compiler

2 Package Configuration

The source code and load module (binary) packages of the In-Situ PBVR are available from the <u>CCSE</u> <u>public page</u> (https://ccse.jaea.go.jp/software/); the PBVR client, daemon, and particle sampler are built independently and work together on the user PC, login node, and computation node, respectively.

2.1. Load Module Package

For the load module, we provide PBVR clients built for Windows, Linux, and Mac, and the daemon and the particle sampler built for a Linux server. The particle sampler and daemon are built on the supercomputer SGI8600 and Fugaku (clang-mode). The particle sampler consists of the following three libraries.

- 1. Particle generation library that provides particle generation functions
- 2. KVS library that provides visualization functions
- 3. Mathematical expression processing library that provides algebraic expression processing functions

In addition, the particle generation library supports three types of simulation lattice structures (structured and unstructured lattice, and hierarchical lattice). The table below shows the list of load modules.

Table 2	2-1	Load	modules	for	PBVR client
---------	-----	------	---------	-----	-------------

Machine type	Parallelization	Package name
Linux	OpenMP	pbvr_client_linux.tar.gz
Мас	OpenMP	pbvr_client_mac.tar.gz
Windows	OpenMP	pbvr_client_win.zip

Table 2-2 Daemon

Machine type	Parallelization	Package name
SGI8600	OpenMP	pbvr_daemon_s86.tar.gz
FUGAKU	OpenMP	pbvr_daemon_fugaku.tar.gz

Table 2-3 Load modules for particle sampler

Machine type	Parallelization	Package name
SGI8600	MPI+OpenMP	pbvr_sampler_s86.tar.gz
FUGAKU	MPI+OpenMP	pbvr_sampler_fugaku.tar.gz

2.2. Source Code Package

By compiling the source code package in user's environment, particle sampler, daemon, and PBVR client are generated. A source tree of In-Situ PBVR package are shown in Table 2-4. The source code package contains particle sampler coupled test simulation code.

Directory/File name	Explanation
is_pbvr/	Root directory for In-Situ PBVR
-pbvr.conf	Configuration file for the Makefile
-Makefile	Makefile for particle sampler, daemon, and PBVR client
-arch/	Setting files for various environments
-Client/	PBVR client program
-Common/	Protocol, communication and common library
-Daemon/	Daemon program
-Example/	Samples of test simulation code
C/	C version
-Hydrogen_struct/	for structured grid
-Hydrogen_AMR/	for AMR grid
-Hydrogen_unstruct/	for unstructured grid
-Fortran/	Fortran version
-Hydrogen_struct/	for structured grid
-Hydrogen_AMR/	for AMR grid
-Hydrogen_unstruct	for unstructured grid
-FunctionParser/	Computer algebra library
-InSituLib/	Particle generation library
-struct/	for structured grid
-AMR/	for AMR grid
-unstruct/	for unstructured grid
-KVS/	KVS library

Table 2-4 The source tree of In-Situ PBVR

3 Build from Source Codes

The PBVR client is generated on the user PC, while the daemon and particle sampler are generated by building the source code on the supercomputer.

3.1. Daemon and Particle Sampler

This section shows the procedure to build the daemon and particle sampler libraries from the source package. In the following procedure, we assume that the source package has already been downloaded on the supercomputer and the file download path is \$HOME.

1 Unzip pbvr_inSitu_1.10.tar.gz

\$ cd \$HOME
<pre>\$ tar xvfz pbvr_inSitu_1.10.tar.gz</pre>

2 Edit a config file.

The compiler used for the build is controlled by editing pbvr.conf to suit the environment. Table 3 1 gives an overview of a variable specified in pbvr.conf, and Table 3 2 lists the compilation configuration files that can be used as variable values.

Table 3-1 Variable in pbvr.conf	
---------------------------------	--

Variable	Input	Explanation	
PBVR_MACHINE	String	Specify a compile configuration file under arch	
P			

Table 3-2 Setting files for compilation

Filename	Explanation	
Makefile_machine_gcc	Setting of sequential version compilation with gcc	
Makefile_machine_gcc_omp	Setting of OpenMP version compilation with gcc	
Makefile_machine_gcc_mpi_omp	Setting of MPI+OpenMP version compilation with gcc	
Makefile_machine_intel	Setting of sequential version compilation with intel	
Makefile_machine_intel_omp	Setting of OpenMP version compilation with intel	
Makefile_machine_intel_mpi_omp	Setting of MPI+OpenMP version compilation with intel	
Makefile_machine_fugaku_clang	Setting of compilation on FUGAKU (clang-mode)	
Makefile_machine_fugaku_trad	Setting of compilation on FUGAKU (trad-mode)	
Makefile_machine_s86_mpi_omp	Setting of compilation on SGI8600	
Makefile_machine_ofp_mpi_omp	Setting of compilation on OakforestPACS	

```
$ cd $HOME/is_pbvr
$ cat pbvr.conf
PBVR_MACHINE=Makefile_machine_gcc_mpi_omp
PBVR_MAKE_CLIENT=0
```

③ The daemon and the particle sampler libralies are built by make.

```
$ cd $HOME/is_pbvr
$ make all_clean
```

\$ make

Table 3-3 Load modules of daemon and particle sampler

Directory	Load module	Explanation			
KVS	libkvsCore.a	KVS library providing particle format and			
		visualization functions			
Common	libpbvrCommon.a	Communication library providing protocol for socket			
		communication			
Daemon	pbvr_daemon	Daemon			
FuctionParser	libpbvrFunc.a	Computer algebra library			
InsituLib/struct	libInSituPBVR.a	Particle sampler			
InsituLib/unstruct	libInSituPBVR.a	Particle sampler			
InsituLib/AMR	libInSituPBVR.a	Particle sampler			

④ This completes the building of the daemon and particle sampler, and we will continue with the building of the test code under Example.

```
$ cd $HOME/is_pbvr/Example/C/Hydrogen_struct
```

\$ make

3.2. PBVR Client

The PBVR client is built with the same code as the <u>client-server PBVR</u> (https://ccse.jaea.go.jp/software/PBVR/). To build the PBVR client for In-Situ, edit qtpbvr.conf as follows to enable PBVR_MODE=IS.

```
#PBVR_MODE - Either CS (ClientServer), or IS (Insitu) - Needed on all
platforms
#PBVR_MODE = CS
PBVR_MODE = IS
```

For details on how to build a PBVR client, please refer to the manual for the client-server PBVR.

4 Setting up of In-SituVisualization

The collaboration of the particle sampler coupled to the simulation, the daemon operating on the interactive node, and the PBVR client on the user PC interactively visualizes the batch processed simulation. To accomplish this, some simple configuration and port forwarding connections are required.

4.1. Setting Environment Variables

The daemon and particle sampler use the environment variables shown in Table 41 below, and at runtime you need to set the environment variables with the export command.

Table 4-1 Environment variables referenced by daemon and particle sampler

Env. var.	Explanation			
VIS_PARAM_DIR	R Directory placed the transfer function file (visualization param.) %1			
PARTICLE_DIR Destination directory for the particle files generated by particle sampler				
TF_NAME	File name of the transfer function (without extension)%2			

※1 If not specified this, the daemon and particle sampler will search the current directory in which each is running.

*2 If not specified this, daemon and particle sampler adopt default.tf as the transfer function name.

4.2. Setting of Visualization Parameters

When the particle sampler converts volume data into visualization particle data, visualization parameters such as a transfer function, a range of physical values to be visualized, and a screen resolution are required. Each item of the visualization parameters are described on a tag basis in the transfer function file. The user can use default.tf stored in the example of the source package as the transfer function file at first startup.

In order to execute In-Situ PBVR, the user needs to place the transfer function file in the directory specified by VIS_PARAM_DIR in Table 4-1 with the file name specified by TF_NAME.

The user can edit the contents of the transfer function file by the GUI by activating the daemon and the PBVR client. The transfer function file specified by the environment variable is read by the daemon, displayed on the PBVR client, and overwritten after editing.

4.3. Port Forwarding Connection

The particle data and visualization parameters are sent and received by socket communication between the daemon and the PBVR client. In order to perform socket communication between the interactive node on the remote supercomputer and the local PC, the user needs to connect both ports by ssh port forwarding.

4.3.1. Remote Connection between Tow Machines

The following example shows how to connect local machineA to remote machine using port forwarding.

machineA> ssh -L portnumA:hostnameB:portnumB username@machineB

In the above command, portnumA is the port number of machineA, hostnameB is the host name of machineB, and portnumB is the port number of machineB. hostnameB is often displayed on the terminal of machine B, and can also be confirmed by the hostname command. Also, if port forwarding is permitted on the login node of machine B, there is no need to enter a special host name for hostname B, but localhost can be used.

4.3.2. Remote Connection with Sseveral Machines

This section provides an example of connecting PBVR Server and PBVR Client on two remote machines 'machineA' and 'machineB' via 'machineC' for some reason, e.g. security. Once the SSH port forwading is established, the launching method is basically the same as the stand-alone mode, as with the two point remote concection mentioned before.

Step 1 [SSH port forwarding $A \rightarrow C$]

machineA> ssh -L 60000:localhost:60000 username@machineC

(Forwarding the 60000 port of machineA to the 60000 port of machineC)

Step 2[SSH port forwarding $C \rightarrow B$]

machineC> ssh -L 60000:localhost:60000 username@machineB (Forwarding the 60000 port of machineC to the 60000 port of machineB)

4.4. Launching Daemon and Port Forwarding

The daemon is started at an interactive node or job, and performs socket communication with the PBVR client. The user performs ssh port forwarding from the terminal on your PC to the interactive node, moves to the directory where the daemon load module is located, and starts the daemon as follows.

\$./pbvr_daemon first reading time[ms]:0 Server initialize done Server bind done Server listen done Waiting for connection ...

As described above, when waiting for the socket communication connection with the client, start the PBVR client from another terminal. The default port number at daemon startup is 60000. The port number can be changed with the command line option -p at startup as shown below.

\$./pbvr_daemon -p 71000

The daemon aggregates particle files and updates transfer function files with reference to the environment variables. Then, daemon sends and receives data with the PBVR client through the port specified at startup.

5 Particle Sampler

By inserting the generate_particles function into the simulation code, the particle sampler can generate particles for in-situ visualization. This function is defined in kvs_wrapper.h and can be used by referencing and linking particle generation libraries.

The particle sampler is executed with batch processing of the simulation, and converts the calculated volume data to the particle data referring to the environment variables (section 4.1) and the transfer function file (section 4.2). In the directory specified by PARTICLE_DIR, the particle sampler outputs a particle data file and a t_pfi_coords_minmax.txt file which has the maximum and minimum coordinates of the area. The particle data file consists of a header file (kvsml), a coordinate file (coord.dat), a color file (color.dat), and a normal file (normal.dat), output one set per node at each time step. At the same time, the particle sampler outputs \$TF_NAME_timestep.tf file recording history of transfer function change, history_timestep.txt file recording histogram and the range of physical values, state.txt recording time step interval in VIS_PARAM_DIR.

5.1. Particle Generation Function for Structured Grid

#include "kvs_wrapper.h"

void generate_particles(

int time_step, domain_patameters dom, Typs** volume_data, int num_volume_data);

This function takes as arguments the time step of simulation, information on calculation area, and volume data of simulation result.

- int time_step : simulation time step
- domain_patameters dom : data structure defines following calculation domain

typedef struct	
{	
float x_global_min;	// Minimum of x coordinates in whole domain
float y_global_min;	// Minimum of y coordinates in whole domain
float z_global_min;	// Minimum of z coordinates in whole domain
float x_global_max;	// Maximum of x coordinates in whole domain
float y_global_max;	// Maximum of ycoordinates in whole domain
float z_global_max;	// Maximum of z coordinates in whole domain
float x_min;	// Minimum of x coordinates in subdomain
float y_min;	// Minimum of y coordinates in subdomain
float z_min;	// Minimum of z coordinates in subdomain
int* resolution;	// Pointer to int resolution[3]
float cell_length;	//Length of a cell
} domain_parameters;	

Typs ** volume_data: A pointer to an array of volume data of simulation results. "Type" is a type of user-specified physical value, and multi-variable volume data is defined as a two-dimensional array.

In volume data of lattice resolution (X, Y, Z), the value of the position (i, j, k) of the n-th variable is referred to as volume_data [n] [i + j * X + k * X * Y].

int num_volume_data : number of volume data

5.2. Particle Generation Function for Unstructured Grid

#include "kvs_wrapper.h"

void generate_particles(

int time_step, domain_parameters dom, Type** values, int nvariables, float* coordinates,

int ncoords, unsigned int* connections, int ncells);

This function takes as arguments the time step of the simulation and information on the calculation area, volume data of the simulation result, and lattice information of the unstructured lattice.

- · int time_step ∶ simulation time step
- domain_patameters dom : data structure defines following calculation domain

type	edef struct	
{		
	float x_global_min;	// Minimum of x coordinates in whole domain
	float y_global_min;	// Minimum of y coordinates in whole domain
	float z_global_min;	// Minimum of z coordinates in whole domain
	float x_global_max;	// Maximum of x coordinates in whole domain
	float y_global_max;	// Maximum of ycoordinates in whole domain
	float z_global_max;	// Maximum of z coordinates in whole domain
} do	main_parameters;	

- Typs ** volume_data: A pointer to an array of volume data of simulation results. "Type" is a type of user-specified physical value, and multi-variable volume data is defined as a two-dimensional array. The value on the cell vertex of the nth variable is referred to by volume_data [n] [cell].
- float* coordinates: Pointer to an array of vertex coordinates. The i-th vertex coordinates (x, y, z) are referenced by (coordinates [3 * i], coordinates [3 * i + 1], coordinates [3 * i + 2]).
- int ncoords : number of coordinates
- unsigned int * connections: A pointer to the connection list of vertex IDs that make up a hexahedral element. The configuration of the hexahedral element is shown in Figure 5-1. The n-th vertex of the i-th hexahedral element is referred to by connections [6 * i + n].
- int ncells : number of elements

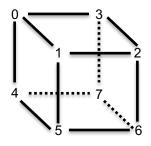


Figure 5-1 Connection of vetices of a hexahedral element

5.3. Particle Generation Function for AMR Grid

In-Situ PBVR supports Block Structured AMR, which is optimized for the memory layout of many-core computers. In this type of grid, an orthogonal grid of N³ is defined as a unit of the minimum processing area called "leaf", and leaves of different sizes are connected in each layer. Therefore, Block Structured AMR is defined as a four-dimensional grid of NxNxNxL (L is the number of leaves). Figure 5-2 shows a two-dimensional example.

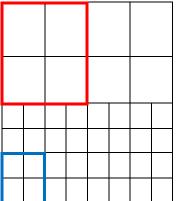
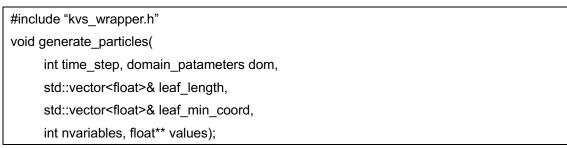


Figure 5-2 Example of a two-dimensional hierarchical grid. The upper part is the lattice of the hierarchy Lv. 1 and the lower part is the hierarchy Lv. 2. The leaf is defined by a 2×2 orthogonal grid, red is a leaf of Lv.1, blue is a leaf of Lv.2.



This function takes as arguments the time step of simulation, information of calculation area, configuration information of hierarchical lattice, and volume data of simulation result.

- int time_step : simulation time step
- domain_patameters dom : data structure defines following calculation domain

typedef struct	
{	
float x_global_mi	n; // Minimum of x coordinates in whole domain
float y_global_mi	n; // Minimum of y coordinates in whole domain
float z_global_mi	n; // Minimum of z coordinates in whole domain
float x_global_ma	ax; // Maximum of x coordinates in whole domain
float y_global_ma	ax; // Maximum of ycoordinates in whole domain
float z_global_ma	ax; // Maximum of z coordinates in whole domain
int* resolution;	// Pointer to int resolution[4]
} domain_parameters;	

•

- std::vector<float>& leaf_length : A reference to an array of leaf lengths. The length of the l-th leaf is referred to by leaf_length [I].
- std::vector<float>& leaf_min_coord : A reference to an array of leaf minimum position coordinates. The coordinates of the l-th leaf are referenced by (leaf_min_coord [3 * I], leaf_min_coord [3 * I + 1], leaf_min_coord [3 * I + 2]).
- float** values : Pointer to the array of resulting volume data. Multivariate volume data is defined as a two-dimensional array. In the volume data of the grid resolution (X, Y, Z, L), the value of the position (i, j, k, l) of the nth variable is values [n] [i + j * X + k * X * Y Refer to + I * X * Y * Z].
- int nvariables : number of variables

5.4. Connection into Simulation Code

In-Situ visualization is possible by compiling the generate_particles function into the simulation code of the user. This chapter shows the procedure for connecting particle sampler to test simulation code as an example. The test simulation code calculates the value of charge density on the lattice vertex at each time step according to the charge density equation of hydrogen. Therefore, the class name to be calculated is Hydrogen. The code without particle sampler integration is as follows.

```
#include "Hydrogen.h"
#include <iostream>
#include <mpi.h>
int main( int argc, char** argv )
{
    MPl_Init(&argc, &argv);
    Hydrogen hydro;
    int time_step = 0;
    for(;;)
    {
        hydro.values;
        time_step++;
    }
    MPl_Finalize();
    return 0;
}
```

In the above source code, Hydrogen class outputs volume data of each time step in hydro.values in for loop.

5.4.1. Domain Information and Particle Generation Function

The generate_particles function obtains domain information through the structure domain_parameters. The user needs to copy the area information obtained from the simulation code to the structure.

int mpi_rank;
MPI_Comm_rank(MPI_COMM_WORLD, &(mpi_rank));
<pre>int resol[3] = { hydro.resolution.x(), hydro.resolution.y(), hydro.resolution.z() };</pre>
domain_parameters dom = {
hydro.global_min_coord.x(),
hydro.global_min_coord.y(),
hydro.global_min_coord.z(),
hydro.global_max_coord.x(),
hydro.global_max_coord.y(),
hydro.global_max_coord.z(),
hydro.global_region[mpi_rank].x(),
hydro.global_region[mpi_rank].y(),
0.0,
resol,
hydro.cell_length
};

In the above code, the rank number of MPI is used to calculate area of subdomain of Hydrogen. The domain information, resolution, MPI rank, and volume data becomes arguments of generate_particles function. The generate_particles function is called after simulation inside the time step loop. In the case of Hydrogen, it is inserted as follows.

int t	ime_step = 0;
for(;;) {
	generate_particles(time_step, dom, hydro.values, hydro.nvariables)
	time_step++;
l	

6 **PBVR Client**

In default mode, PBVR client draws particle data of the latest time step received from daemon. Viewer of PBVR client draws particle data using OpenGL. The PBVR client provides a GUI to edit visualization parameters, including transfer functions, and sends the visualization parameters to the daemon. Sending and receiving data between the daemon and the PBVR client is performed through an arbitrary port number by socket communication.

6.1. Launching PBVR Client

The following examples show how to launch PBVR client.

\$ pbvr_client [command line options]

option	value	default	explanation
-p	ポート番号	60000	port number
-viewer	100 \sim 9999 \times	620×620	resolution of PBVR client
	100~9999		
-shading	{L/P/B},ka,kd,ks,n	_	shading method %1

%1. This argument specifies the shading parameters.

L: Lambert Shading

This method ignores specular reflection in the shading process.

Parameters 'ka' and 'kd' are the coefficient for ambient and diffusion, respectively. They can have a value between 0-1.

P: Phong Shading

This method adds the specular reflection to Lambert shading. Phong shading imitates smooth metal and mirrors. (This is sometimes called highlight).

Parameter 'ka', 'kd','ks' (coefficients for specular reflection lying between 0-1) and 'n' (strength of highlight lying between 0-100) are used.

B : Blinn-Phong Shading

This is a shading model that simplifies Phong shading. Parameters 'ka', 'kd', 'ks', and 'n' exist.

6.2. Terminating of PBVR Client

PBVR client is terminated by pressing Ctrl + c on the console where you started the program. When you press Ctrl + c, the PBVR client synchronizes with the daemon at the time of the time update, and both ends. However, if communication is interrupted with the Stop button on the time step control panel, the Ctrl + c key input is ignored. Also note that if you terminate the daemon with Ctrl + c, you will not be able to terminate the PBVR client with Ctrl + c.

6.2.1. Forced Termination

If the PBVR client and daemon are not terminated by pressing the Ctrl + c key for some reason, forced termination is required using kill command with the process numbers of the client and daemon by ps command as shown below.

[Forced termination of PBVR client] \$ ps -C PBVRViewer PID TTY TIME CMD 19582 pts/6 00:00:00 PBVRViewer \$ kill -9 19582 [Forced termination of daemon] \$ ps -C CPUServer PID TTY TIME CMD 19539 pts/5 00:00:00 CPUServer \$ kill -9 19539

6.3. Using PBVR Client GUI

The PBVR client is built on the same GUI as the <u>client-server type PBVR</u> (https://ccse.jaea.go.jp/software/PBVR/); for details on how to operate the PBVR client, please refer to the manual of the client-server type PBVR.

7 How to Execute Examples

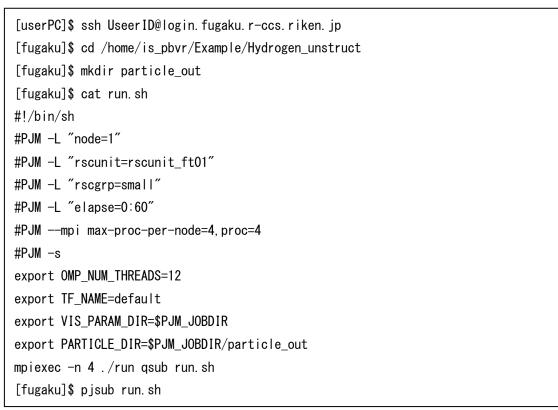
This section shows an example of port-forward connection from Linux/Mac to FUGAKU using Examples included in the source code package to execute In-Situ PBVR. In this section, we will show you how to use a login node that are allowed to execute programs and how to use interactive jobs. This section also shows an example of accessing a remote server from Windows and executing In-Situ PBVR.

7.1. Login node

The following is the procedure for running the test program for the unstructured lattice (is_pbvr/Example/Hydrogen_unstruct) on the FUGAKU by using the login node that are allowed to execute programs. In this example, we assume that the RSA public key and the ssh host name and user name have been configured, the source package has been placed in /home/ on FUGAKU, and the build is complete. In this procedure, the test program combined with In-Situ PBVR is submitted to job, and the daemon is launched on the login node and the PBVR client is launched on the user PC.

Start up the first terminal, log in to FUGAKU, and submit the test program to the job using a script "run.sh".

[Terminal 1]



In the second terminal, make a port-forward connection between FUGAKU and the user PC and start the daemon.

[Terminal 2]

```
[userPC]$ ssh -L 61000:localhost:61000 UserID@loginX.fugaku.r-ccs.riken.jp
[fugaku]$ source /opt/intel/bin/compilervars.sh intel64
[fugaku]$ cd /home/is_pbvr/Daemon
[fugaku]$ export VIS_PARAM_DIR=/home/is_pbvr/Example/Hydrogen_unstruct
[fugaku]$ export PARTICLE_DIR=$VIS_PARAM_DIR/particle_out
[fugaku]$ ./pbvr_daemon -p 61000
```

In the third terminal, launche the PBVR client on the user PC.

[Terminal 3]

[usrPC]\$./pbvr_client -p 61000

7.2. Interactive Job

Start up the first terminal, log in to Fugaku, and submit the test program to the job using a script "run.sh".

[Terminal 1]

```
[userPC]$ ssh FUGAKU
[fugaku]$ cd /home/is_pbvr/Example/Hydrogen_unstruct
[fugaku]$ mkdir particle_out
[fugaku]$ cat run.sh
#!/bin/sh
#PJM -L "node=1"
#PJM -L "rscunit=rscunit_ft01"
#PJM -L "rscgrp=small"
#PJM -L "elapse=0:60"
#PJM --mpi max-proc-per-node=4, proc=4
#PJM -s
export OMP_NUM_THREADS=12
export TF_NAME=default
export VIS_PARAM_DIR=$PJM_JOBDIR
export PARTICLE_DIR=$PJM_JOBDIR/particle_out
mpiexec -n 4 ./run qsub run.sh
```

Since Fugaku is not allowed to execute programs on the login node, the computation node and the user PC are connected port-forward and the daemon is executed in an interactive job.

Start the interactive job on terminal 2 and get the IP address of the computation node running the interactive job. "ip" command displays the network information, and a IP address after "inet" is the computation node's IP.

[Terminal2]

[userPC]\$ ssh FUGAKU
[fugaku]\$ cd /home/is_pbvr/Example/Hydrogen_unstruct
[fugaku]\$ In -s /home/is_pbvr/Daemon/pbvr_daemon
[fugaku]\$ pjsubinteract -L "node=1" -L "rscgrp=int" ¥
[fugaku]\$ -L "elapse=0:10:00"sparam "wait-time=600"
[intrct]\$ ip address show tofu1
inet **.**.**.**/12 brd 10.255.255.255 scope global noprefixroute tofu1

Using the IP address of the computation node, port forward connection is made between the user PC and the computation node at terminal 3.

[Terminal3]

```
[userPC]$ ssh -L 60000: **. **. **: **: 60000 FUGAKU
```

Run the daemon at terminal 2.

[Terminal2]

```
[intrct]$ export TF_NAME=default
[intrct]$ export VIS_PARAM_DIR=$PJM_JOBDIR
[intrct]$ export PARTICLE_DIR=$PJM_JOBDIR/particle_out
[intrct]$ ./pbvr_daemon
```

Launch PBVR client on the user PC in terminal 4.

[userPC]\$./pbvr_client -p 60000

7.3. Windows

The procedure for connecting remotely from a Windows client to a remote server is shown below. The following procedure assumes transfer from the port 60000 of the client to the port 60000 of the server. To connect PBVR Client in a Windows machine to PBVR Server in a remote machine, setup port forwarding with the help of an SSH client software such as TeraTerm or Putty. The following shows an example for TeraTerm.

Tera Term: New	connection		
● TCP/IP	Service: (<mark>z820.edo.ja</mark> ☑ History ◎ Telnet ◎ SSH ◎ Other	TCP <u>p</u> ort#: 22 SSH <u>v</u> ersion: SSH2 → Proto <u>c</u> ol: UNSPEC →
🗢 Serial	Po <u>r</u> t: (OK	Cance	· · · · · · · · · · · · · · · · · · ·

1) Launch TeraTerm and hit cancel in the "New connection" dialog.

Figure 7-1 Tera Term dialog 1)

 Select Setup > SSH Transfer from the menu bar. Click Add... in the Forwarding Setup dialog.

TTSSH: Forwarding Setup	x	
Port Forwarding		
Add Edit Remove X Forwarding ✓ Display remote X applications on local X server		
OK Cancel		

Figure 7-2 Tera Term dialog 2)

3) In the **Select Direction for Forwarded Port** dialog, select **Forward Local Port** and enter the port number to be used for PBVR Client. In the **to remote machine** text field, enter the domain name or the IP address of the server. In the **port** field, enter the port number to be used on PBVR Server. Click on **OK** to complete the setup of port forwarding.

SSH Port Forwarding		X		
Select direction for forwarde	d port:			
Forward local port	61000 🔻	l <u>i</u> sten		
to remote <u>m</u> achine	z820.edo.jaea.go.jp	port 61000 -		
Forward remote server port Iisten to local machine port				
OK Cancel				

Figure 7-3 Tera Term dialog 3)

4) Connect to the server. Select File > New Connection from the menu bar. In the New Connection panel, enter the host name of the serve and click on OK. In the SSH Authentication panel, enter the user name and passphrase, or specify the location of the private key file, and click on OK.

SSH Authentication				
Logging in to z820.ed	o.jaea.go.jp			
Authentication require	ed.			
User <u>n</u> ame:	******			
Passphrase:				
	Remember password in memory			
	Forward agent			
🔘 Use p <u>l</u> ain passw	ord to log in			
Use <u>R</u> SA/DSA/E	CDSA key to log in Private key file: dot_ssh¥id_rsa			
Use rhosts to log in (SSH1) Local user name:				
O Use challenge/response to log in(keyboard-interactive)				
O Use P <u>ag</u> eant				
	OK			

Figure 7-4 Tera Term dialog 4)

The following procedures show how to launch PBVR Server and Client after establishing port forwarding. This example uses the Visual Studio 2013 x64 Cross Tools command prompt in Visual Studio 2013 as the terminal for launching PBVR Client.

Step1 [Launch PBVR Server] Server> mpiexec -n 4 pbvr_server -p port_number Step2 [Set a client parameter for Windows] Windows> set TIMER_EVENT_INTERVAL=1000 Step3 [Launch PBVR Client] Windows> pbvr_client.exe -vin filename -p port_number

Note that PBVR Client on a Windows machine can be launched also by executing a batch file with the following lines.

set TIMER_EVENT_INTERVAL=1000 pbvr_client.exe -vin filename -p port_number ファイル名: IS-PBVRManualEng.docx

フォルダー:

/Users/kawamura/Documents/PBVROpenSourceProject/ISPBV

R/v.1.1/ReleaseCandidate/v.1.1/Manual/Japanese

テンプレート: /Users/kawamura/Library/Group

Containers/UBF8T346G9.Office/User

Content.localized/Templates.localized/Normal.dotm

表題:

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作成者:	y ido
キーワード:	
説明:	
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