3D Parallel FEM (III)
Parallel Visualization and ppOpen-HPC

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ppOpen-HPC: Overview

- Application framework with automatic tuning (AT)
  - ✓ “pp” : post-peta-scale
- Five-year project (FY.2011-2015) (since April 2011)
  - ✓ P.I.: Kengo Nakajima (ITC, The University of Tokyo)
  - ✓ Part of “Development of System Software Technologies for Post-Peta Scale High Performance Computing” funded by JST/CREST (Supervisor: Prof. M. Sato, RIKEN R-CCS)
  - ✓ Finally, it was extended to FY.2018 under collaborations with German Projects (SPPEXA/DFG)
- Team with 7 institutes, >50 people (5 PDs) from various fields: Co-Design
- Open Source Software
  - ✓ http://ppopenhpc.cc.u-tokyo.ac.jp/
  - ✓ https://github.com/Post-Peta-Crest/ppOpenHPC
  - ✓ English Documents, MIT License

独立行政法人 科学技術振興機構 Japan Science and Technology Agency

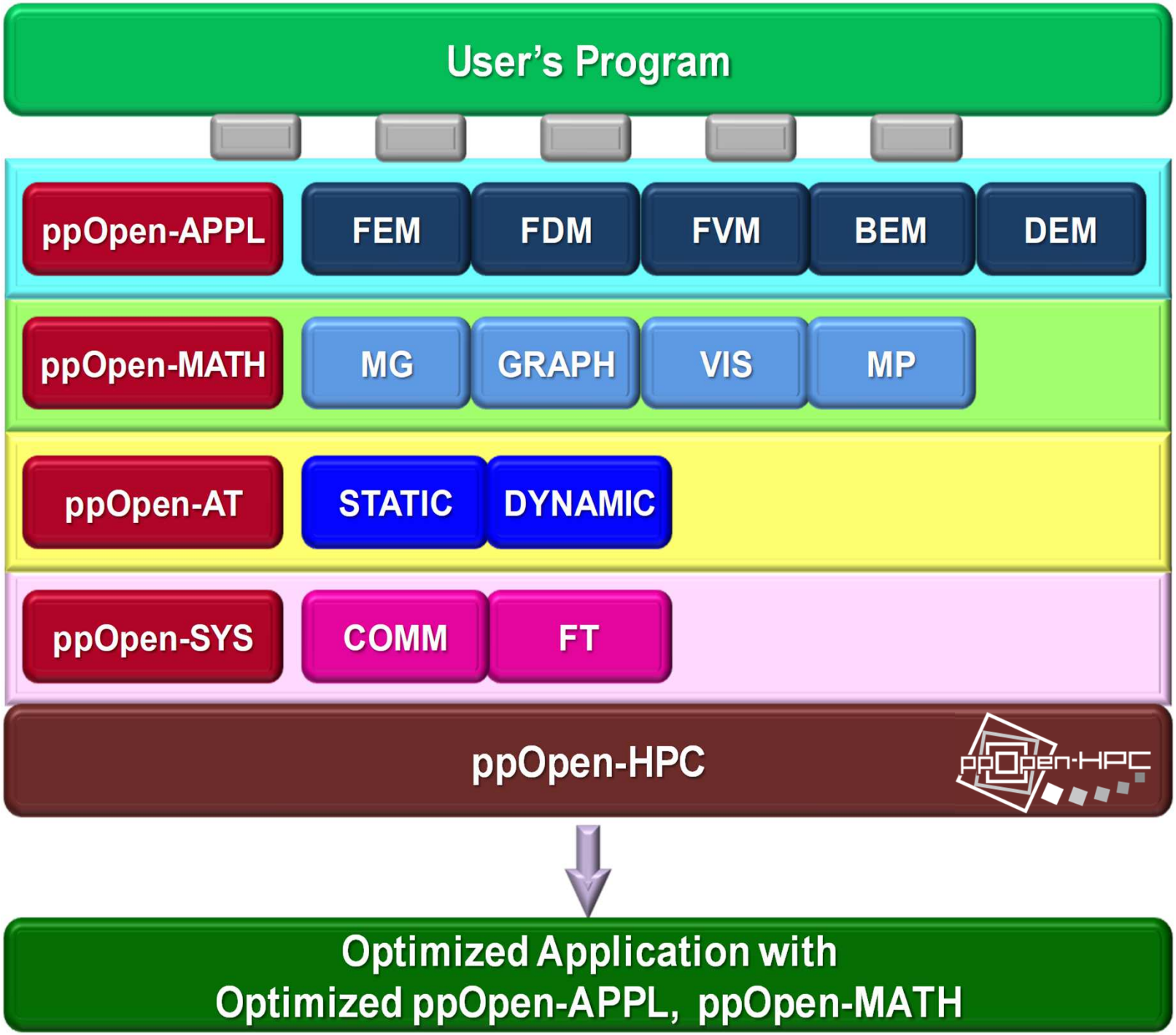
CREST 戦略的創造研究推進事業 Core Research for Evolutionary Science and Technology

Framework Appl. Dev.

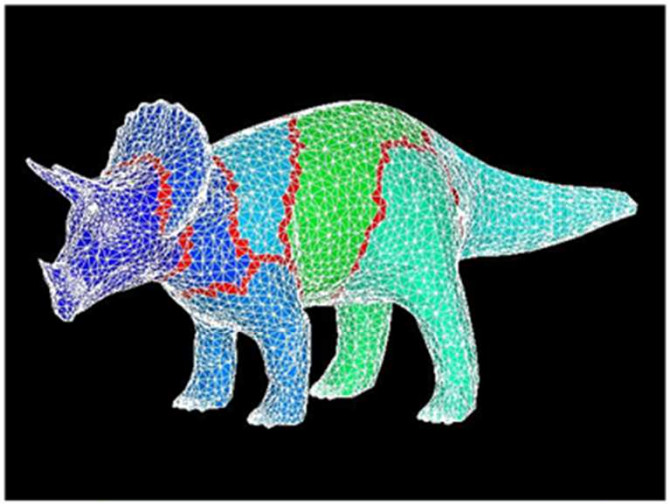
Math Libraries

Automatic Tuning (AT)

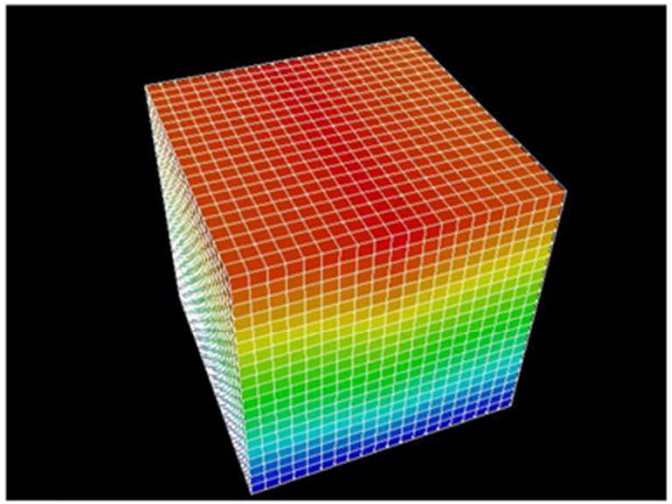
System Software



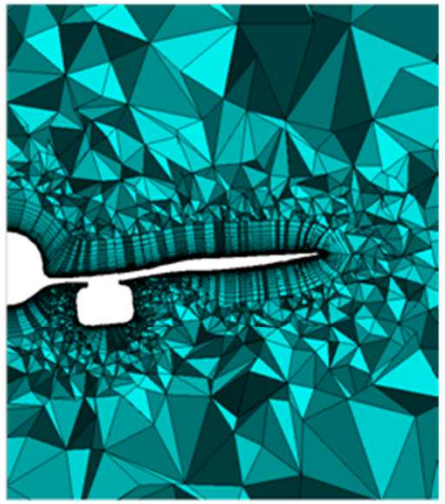
ppOpen-HPC covers …



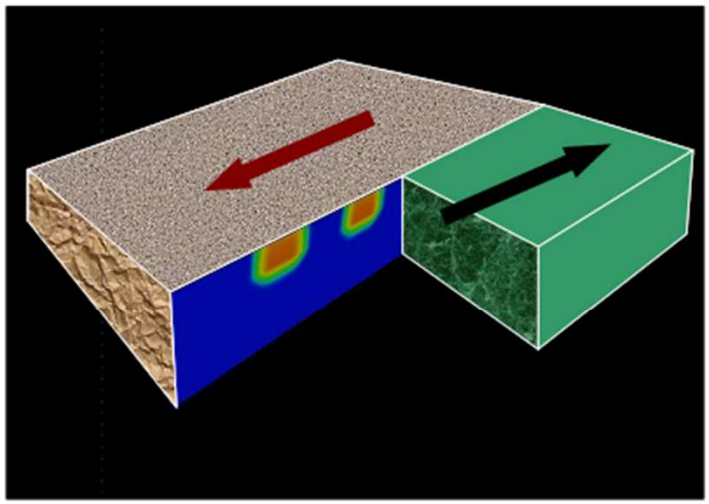
FEM
Finite Element Method



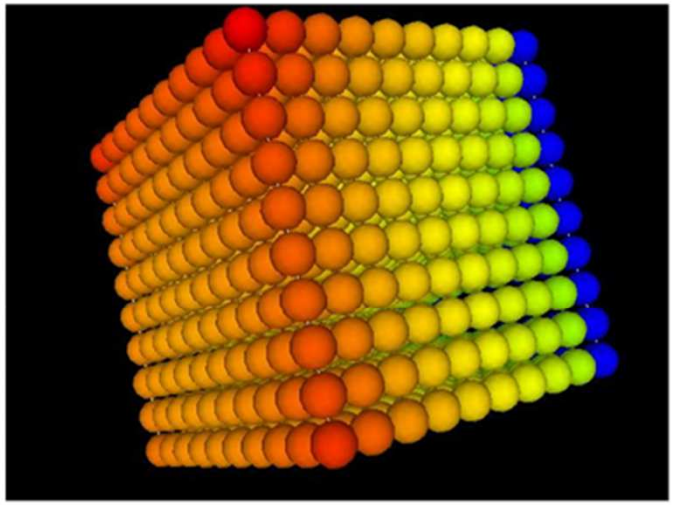
FDM
Finite Difference Method



FVM
Finite Volume Method



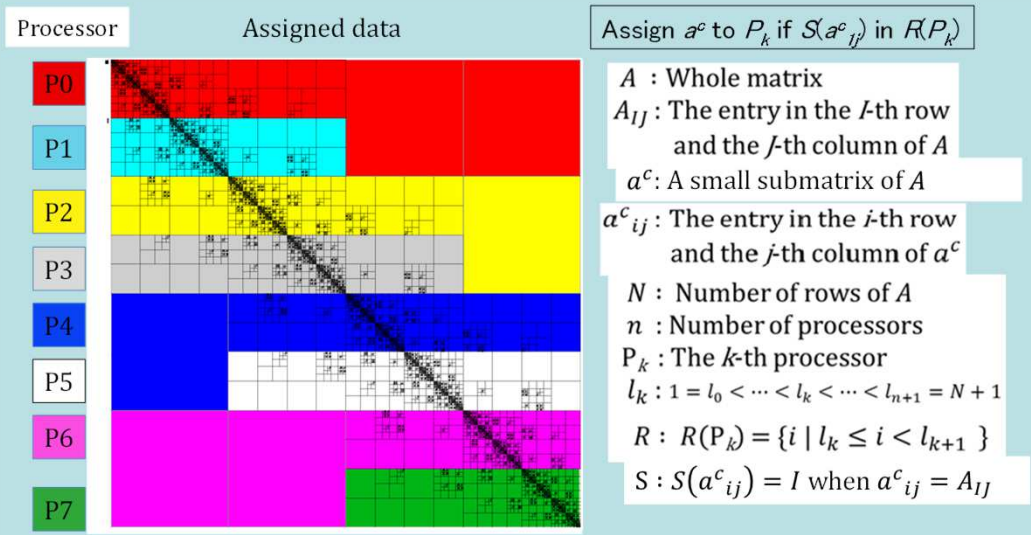
BEM
Boundary Element Method

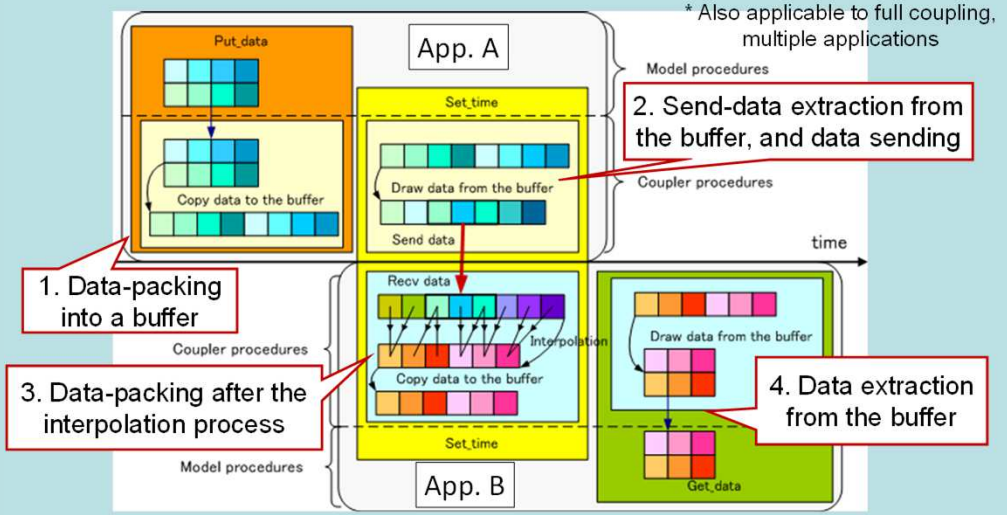


DEM
Discrete Element Method

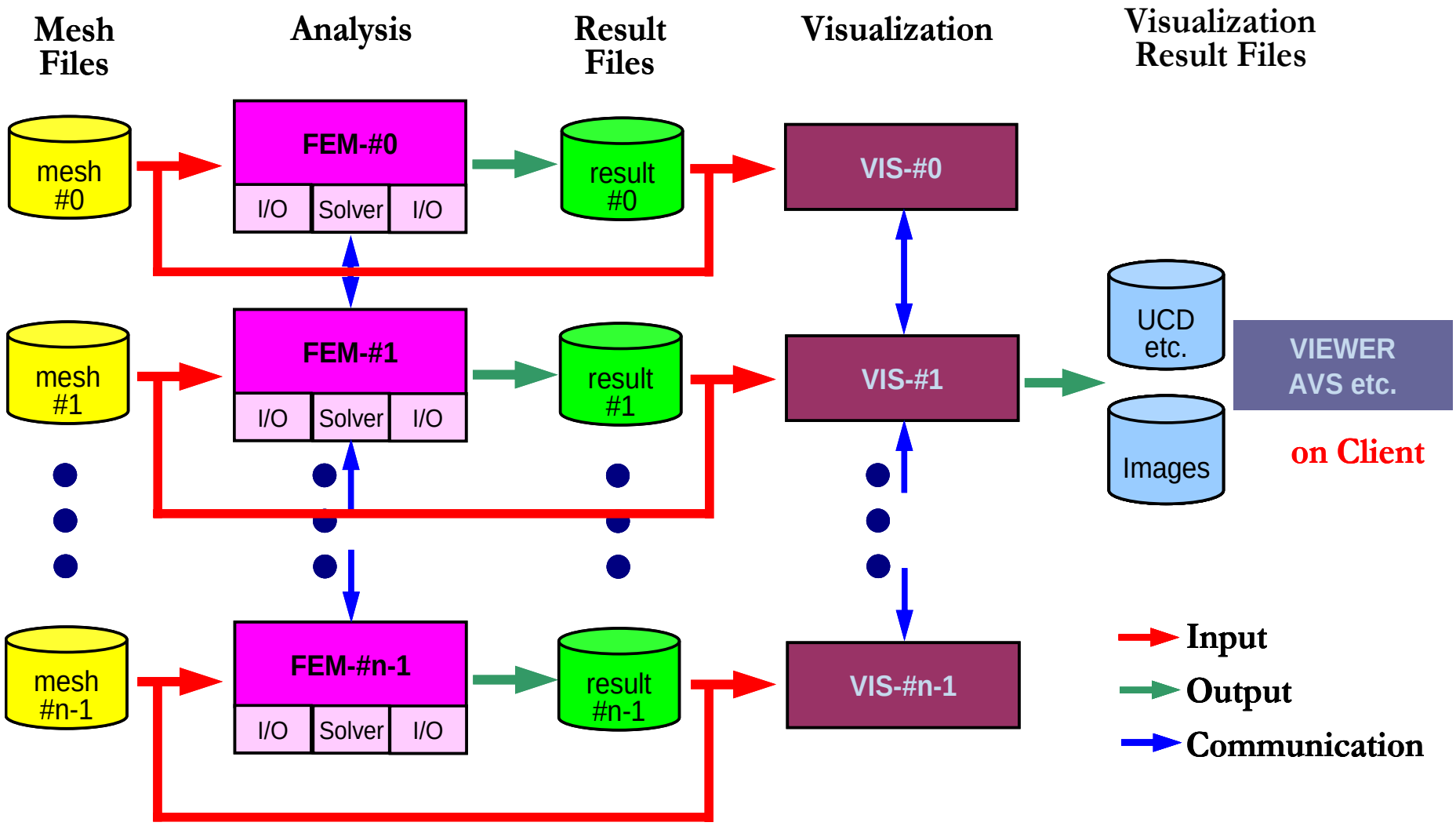
Featured Developments

- ppOpen-AT: AT Language for Loop Optimization
- HACApK library for H-matrix comp. in ppOpen-APPL/BEM (OpenMP/MPI Hybrid Version)
  - First Open Source Library by OpenMP/MPI Hybrid
- **ppOpen-MATH/MP (Coupler for Multiphysics Simulations, Loose Coupling of FEM & FDM)**
- **Sparse Linear Solvers**

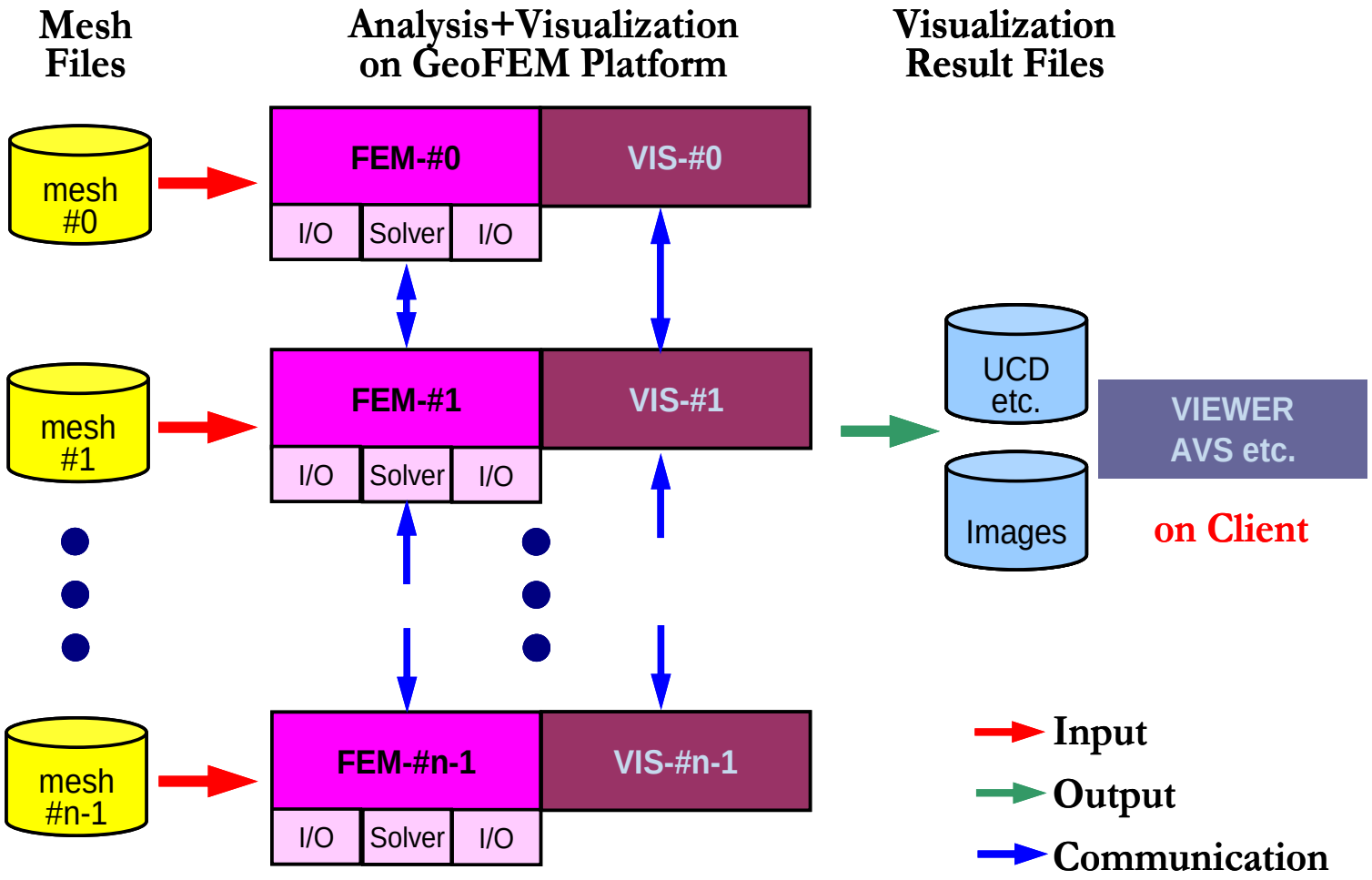




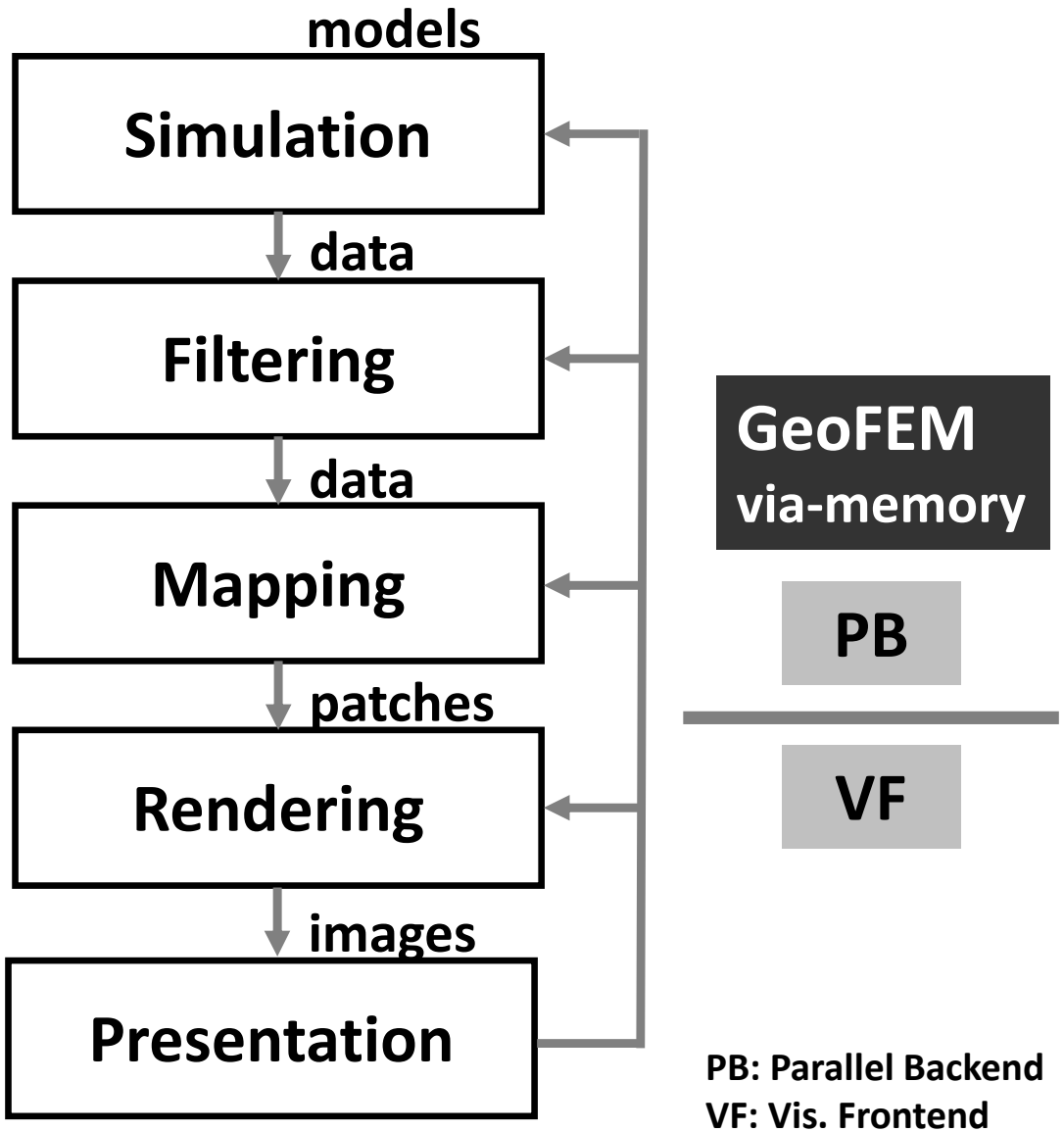
Framework for Parallel Visualization 1 Via-File



Framework for Parallel Visualization 2 Via-Memory (GeoFEM Project)

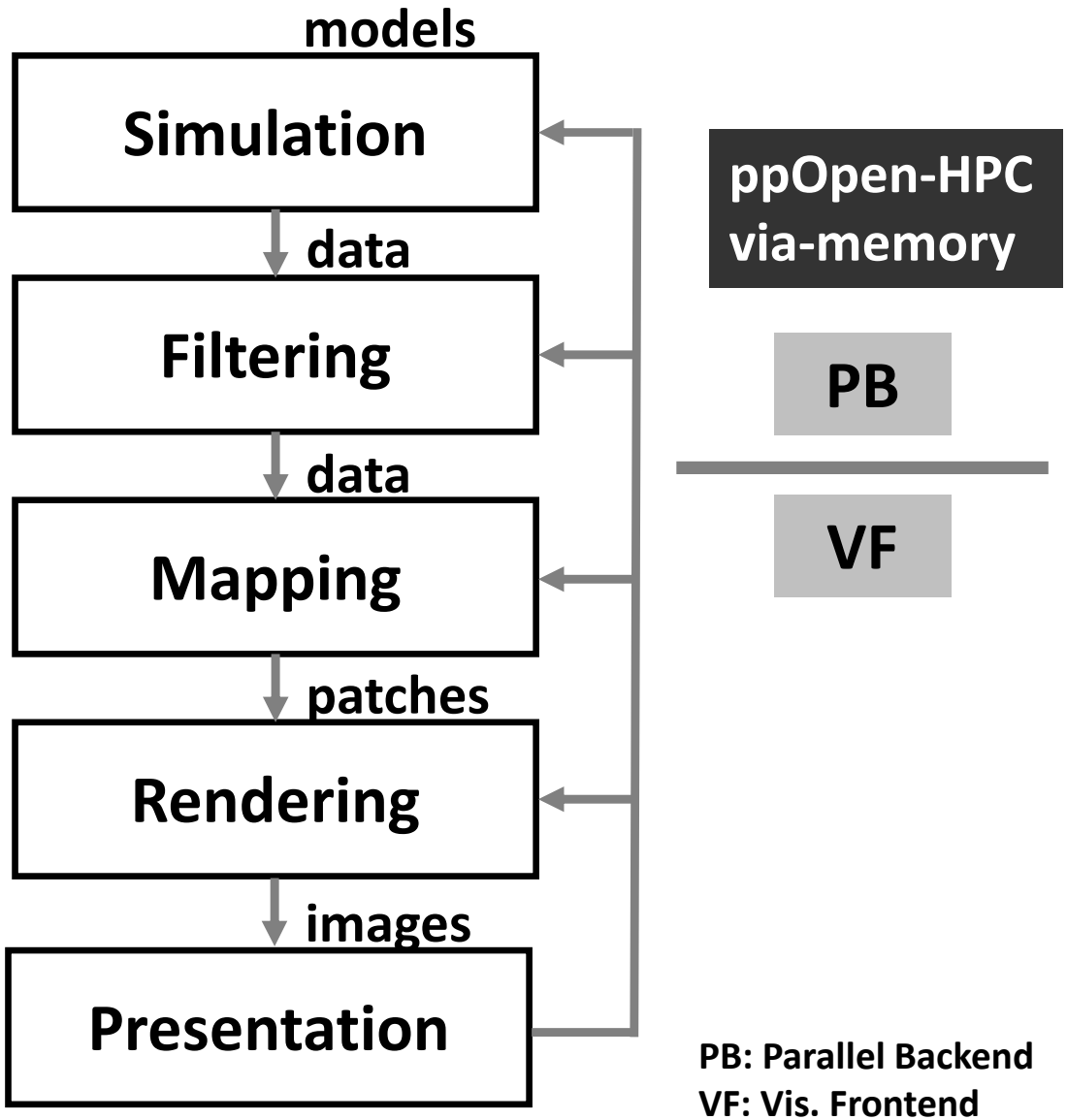


Visualization in GeoFEM (1997-2003)



- Concurrent Visualization-Computation (Via Memory)
- In GeoFEM (previous project), only patch files were obtained.

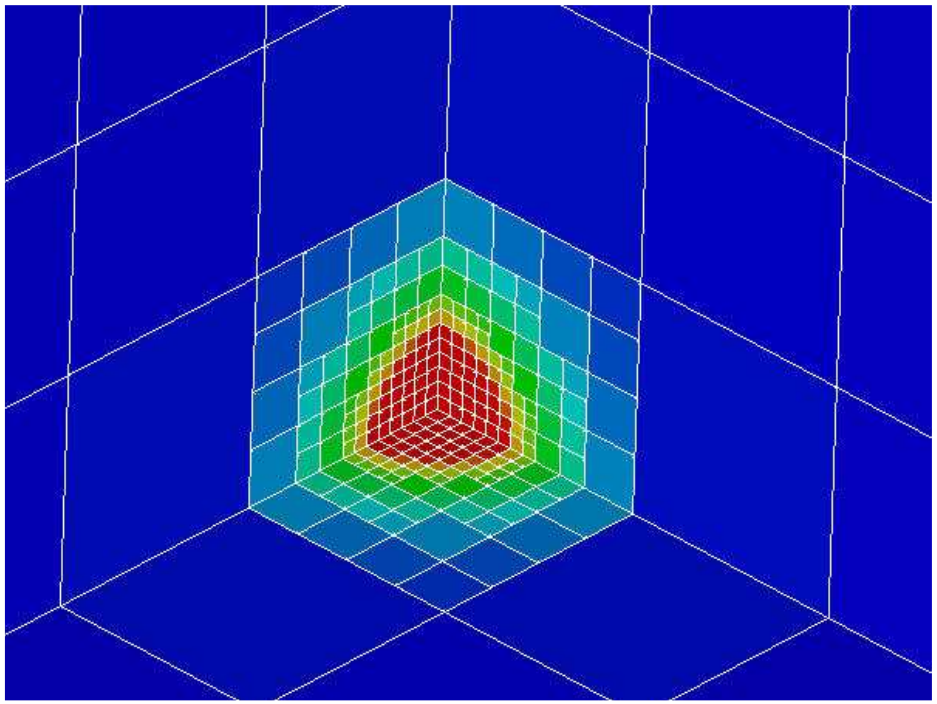
Visualization in ppOpen-HPC



- Concurrent Visualization-Computation (Via Memory)
- Output files (single “self-contained（自己完結）” file) are browsed by MicroAVS & Paraview on a PC
  - ✓ Different from GeoFEM (previous project), where only patch files were obtained.
- Not detailed visualization.
- Just for understanding MIN-MAX, and peaks
- Detailed geometry is preferable

ppOpen-MATH/VIS

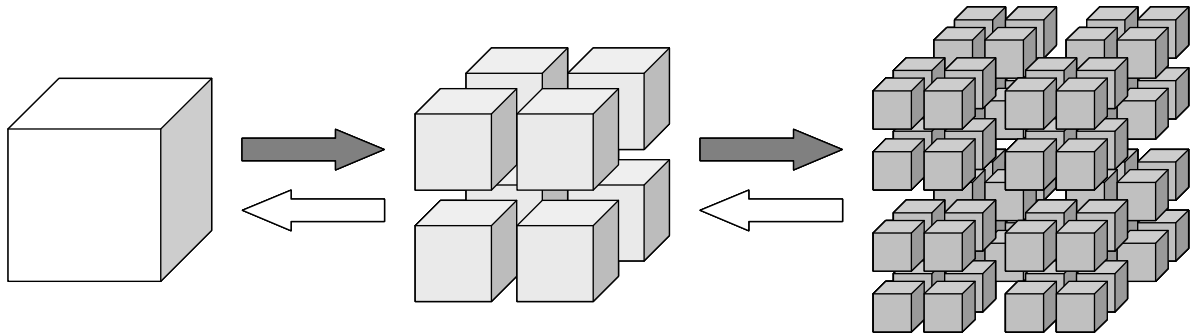
- Parallel Visualization using Information of Background Voxels [Nakajima & Chen 2006]
  - FDM version is released: ppOpen-MATH/VIS-FDM3D
- UCD single file

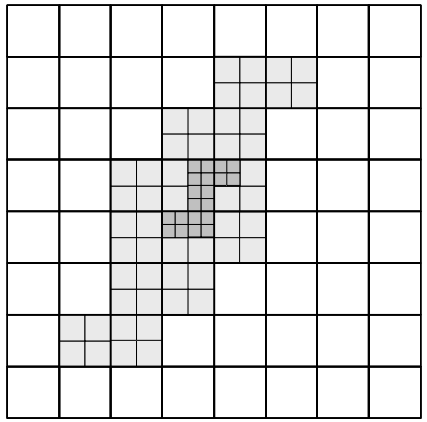


```
[Refine]
AvailableMemory = 2.0    Available memory size (GB), not available in this version.
MaxVoxelCount   = 500    Maximum number of voxels
MaxRefineLevel  = 20     Maximum number of refinement levels
```

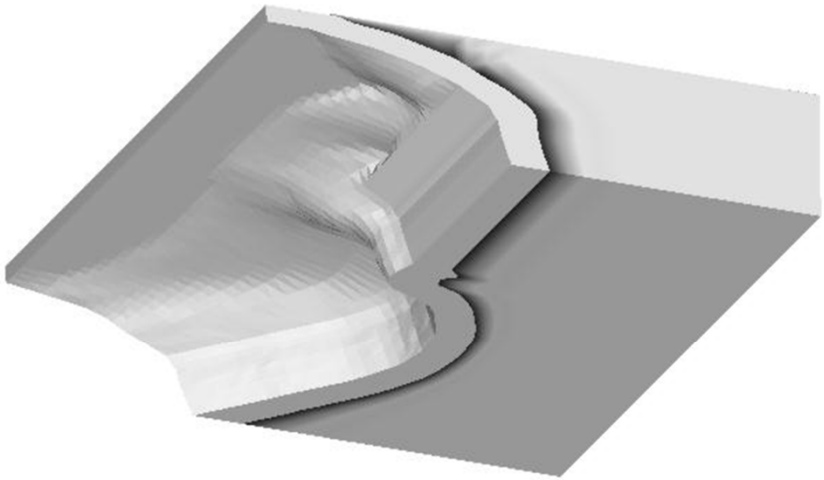
Simplified Parallel Visualization using Background Voxels

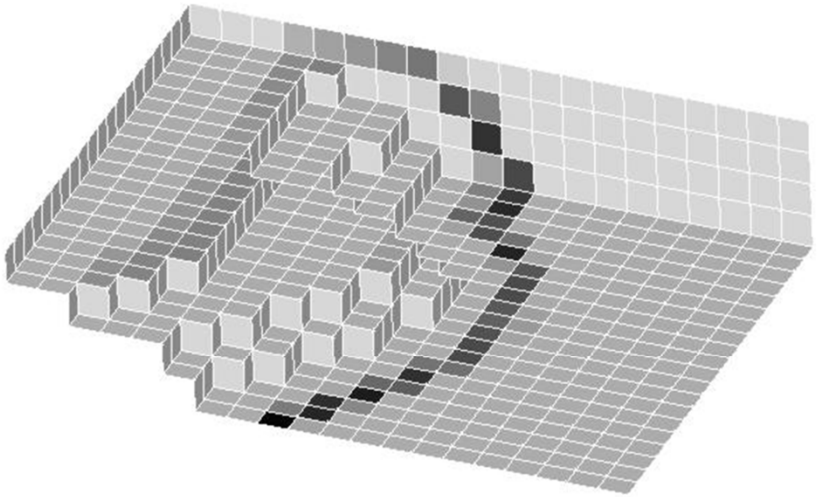
- Octree-based AMR
- AMR applied to the region where gradient of field values are large
  - stress concentration, shock wave, separation etc.
- If the number of voxels are controlled, a single file with 10^5 meshes is possible, even though entire problem size is 10^9 with distributed data sets.

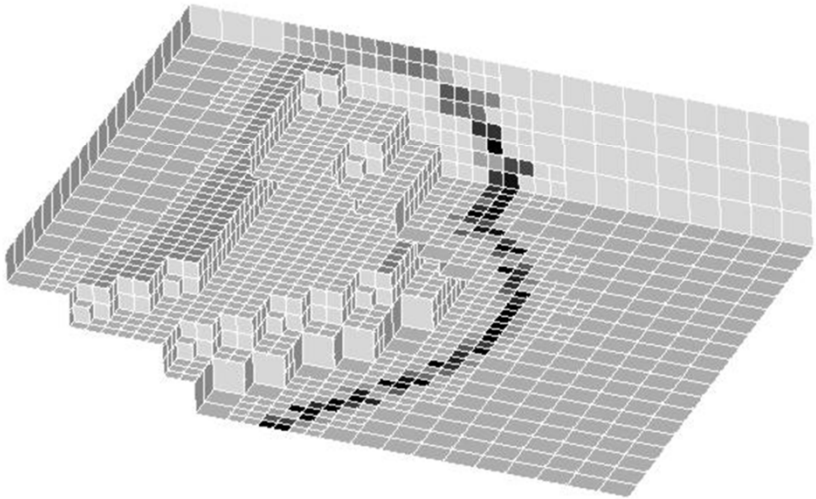


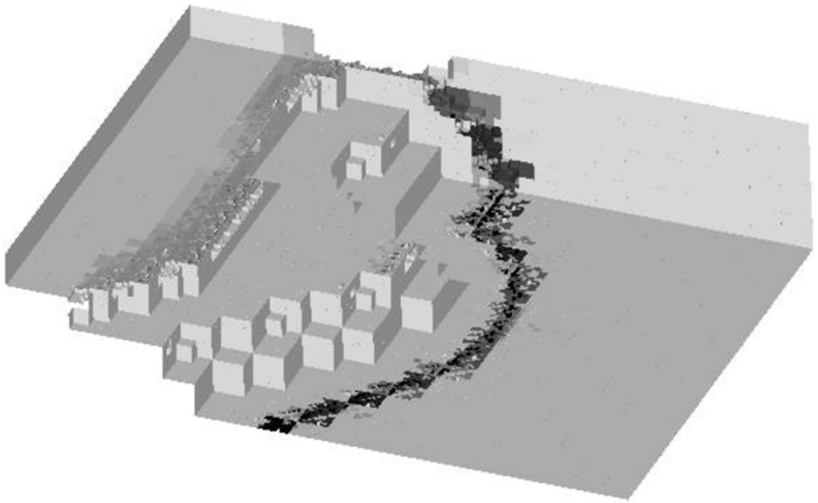


Voxel Mesh (adapted)

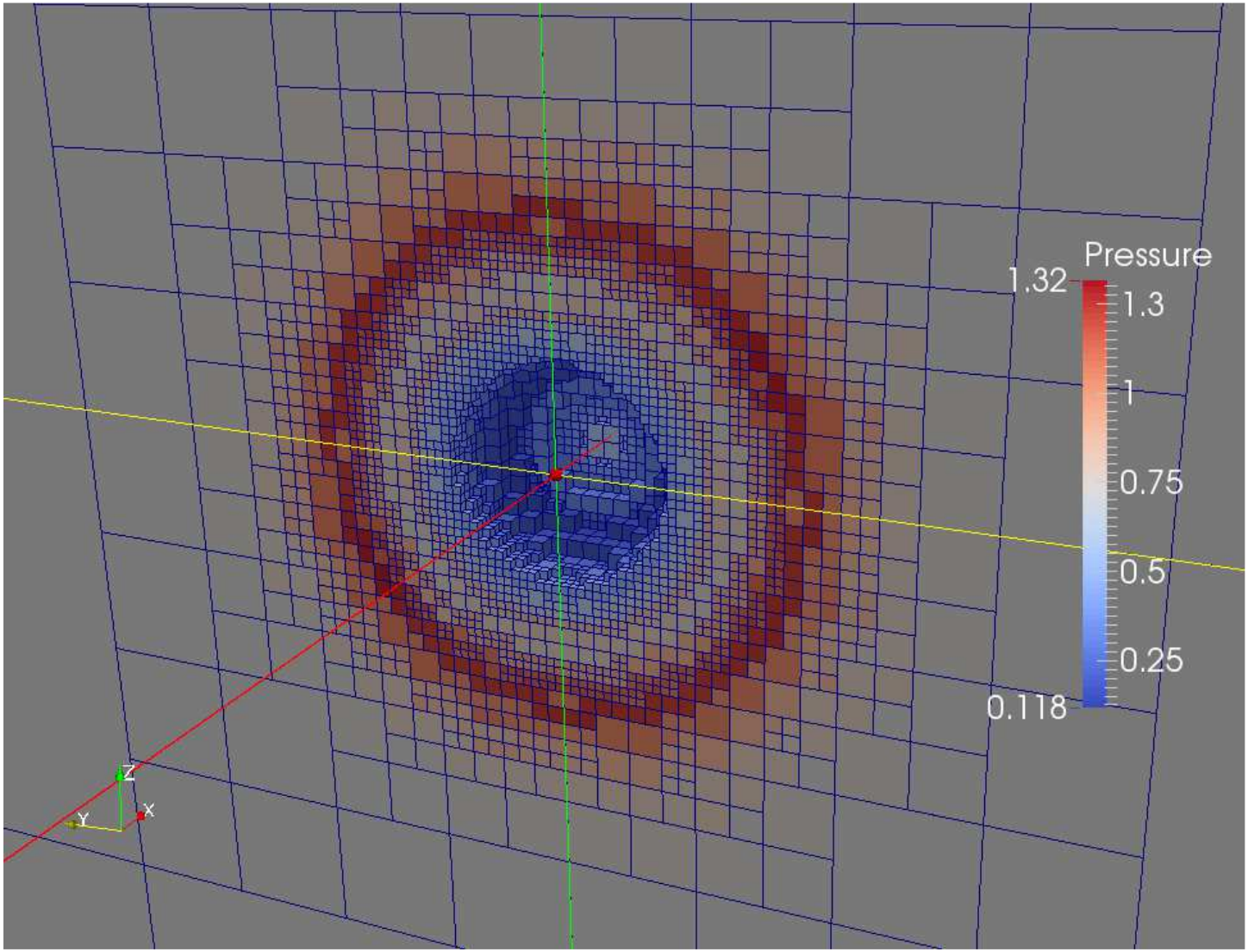








Flow around a sphere



pFEM3D + ppOpen-MATH/VIS

Fortran

```
>$ cd /work/gt36/t36XXX/pFEM
>$ cp /work/gt00/z30088/pFEM/F/pfem3dVIS.tar .
>$ tar xvf pfem3dVIS.tar
>$ cd pfem3d/srcV
>$ module load fj
>$ make
>$ cd ../runV
>$ ls solv
     solv
```

C

```
>$ cd /work/gt36/t36XXX/pFEM
>$ cp /work/gt00/z30088/pFEM/C/pfem3dVIS.tar .
>$ tar xvf pfem3dVIS.tar
>$ cd pfem3d/srcV
>$ module load fj
>$ make
>$ cd ../runV
>$ ls solv
     solv
```

pFEM/pfem3d/srcV/Makefile（F）

```
include Makefile.in

FFLAGSL   = -I/work/gt00/share/ppohVIS/include
FLDFLAGSL = -L/work/gt00/share/ppohVIS/lib
LIBSL     = -lfppohvispfem3d -lppohvispfem3d

.SUFFIXES:
.SUFFIXES: .o .f90 .f

.f.o:
        $(FC) -c $(FFLAGS) $(FFLAGSL) $< -o $@
.f90.o:
        $(F90) -c $(F90FLAGS) $(FFLAGSL) $< -o $@
TARGET = ../run/solv
OBJS = ¥
        pfem_util.o …

all: $(TARGET)

$(TARGET): $(OBJS)
        $(F90) -o $(TARGET) $(F90FLAGS) $(FFLAGSL) $(OBJS)
$(LDFLAGSL) $(LIBS) $(LIBSL) $(FLDFLAGSL)

clean:
        rm -f *.o *.mod $(TARGET)
distclean:
        rm -f *.o *.mod $(TARGET)
```

pFEM/pfem3d/srcV/Makefile（C）

```
include Makefile.in

CFLAGSL  = -I/work/gt00/share/ppohVIS/include
LDFLAGSL = -L/work/gt00/share/ppohVIS/lib
LIBSL    = -lppohvispfem3d

.SUFFIXES:
.SUFFIXES: .o .c

.c.o:
        $(CC) -c $(CFLAGS) $(CFLAGSL) $< -o $@

TARGET = ../run/solv

OBJS = test1.o …

all: $(TARGET)

$(TARGET): $(OBJS)
        $(CC) -o $(TARGET) $(CFLAGS) $(CFLAGSL) $(OBJS)
$(LDFLAGSL) $(LIBS) $(LIBSL)
clean:
        rm -f *.o *.mod $(TARGET)

distclean:
        rm -f *.o *.mod $(TARGET)
```

pFEM/pfem3d/srcV/Makefile.in (1/2)

```
# Install directory
PREFIX      = /work/gt00/share/ppohVISflat
BINDIR      = $(PREFIX)/bin
INCDIR      = $(PREFIX)/include
LIBDIR      = $(PREFIX)/lib

# TetGen directory
TETGENDIR   = $(HOME)/usr/local/tetgen1.4.3
TETINCDIR   = $(TETGENDIR)
TETLIBDIR   = $(TETGENDIR)

# C compiler settings
CC          = mpifccpx
CFLAGS      = $(CINCDIR) $(COPTFLAGS)
COPTFLAGS   = -Nclang -Kfast –Kopenmp
CINCDIR     = -I. -I$(TETINCDIR)

# C++ compiler settings
CXX         = mpiFCCpx
CXXFLAGS    = $(CXXINCDIR) $(CXXOPTFLAGS) -DTETGEN -DTETLIBRARY
CXXOPTFLAGS = -Nclang -Kfast –Kopenmp
CXXINCDIR   = -I. -I$(TETINCDIR)

# Fortran 77 compiler settings
FC          = mpifrtpx
FFLAGS      = $(FINCDIR) $(FOPTFLAGS)
FOPTFLAGS   = -Kfast -Kopenmp
FINCDIR     = -I.
```

pFEM/pfem3d/srcV/Makefile.in (2/2)

```
# Fortran 90 compiler settings
F90          = mpifrtpx
F90FLAGS     = $(F90INCDIR) $(F90OPTFLAGS)
F90OPTFLAGS = -Kfast -Kopenmp
F90INCDIR    = -I.

# Linker settings
LD           = $(CC)
LDFLAGS      = $(LIBS)
#LIBS         = -L$(TETLIBDIR) -ltet -lm
LIBS         = -L$(TETLIBDIR) -lm
LDLIBDIR     =

# Archiver settings
AR           = ar rv

# ETC
CP           = cp -f
RM           = rm -rf
MKDIR        = mkdir -p
```

Fortran/main (1/2)

```
      use solver11
      use pfem_util
      use ppohvis_pfem3d_util

      implicit REAL*8(A-H,O-Z)
      type(ppohVIS_BASE_stControl)               :: pControl
      type(ppohVIS_BASE_stResultCollection)      :: pNodeResult
      type(ppohVIS_BASE_stResultCollection)      :: pElemResult
      character(len=PPOHVIS_BASE_FILE_NAME_LEN) :: CtrlName
      character(len=PPOHVIS_BASE_FILE_NAME_LEN) :: VisName
      character(len=PPOHVIS_BASE_LABEL_LEN)      :: ValLabel
      integer(kind=4)                             :: iErr

      CtrlName = ""
      CtrlName = "vis.cnt"

      VisName = ""
      VisName = "vis"

      ValLabel = ""
      ValLabel = "temp"

      call PFEM_INIT

      call ppohVIS_PFEM3D_Init(MPI_COMM_WORLD, iErr)
      call ppohVIS_PFEM3D_GetControl(CtrlName, pControl, iErr);
      call INPUT_CNTL
      call INPUT_GRID

      call ppohVIS_PFEM3D_SETMESHEX(                                    &
     &       NP,       N,            NODE_ID, XYZ,                    &
     &       ICELTOT, ICELTOT_INT, ELEM_ID, ICELNOD,                    &
     &       NEIBPETOT, NEIBPE, IMPORT_INDEX, IMPORT_ITEM,              &
     &                          EXPORT_INDEX, EXPORT_ITEM, iErr)
```

Fortran/main (2/2)

```
      call MAT_ASS_MAIN
      call MAT_ASS_BC

      call SOLVE11

      pNodeResult%ListCount = 1
      pElemResult%ListCount = 0
      allocate(pNodeResult%Results(1))

      call ppohVIS_PFEM3D_ConvResultNodeItem1N(                          &
     &       NP, ValLabel, X, pNodeResult%Results(1), iErr)

      call ppohVIS_PFEM3D_Visualize(pNodeResult, pElemResult, pControl, &
     &                              VisName, 1, iErr)

      call PFEM_FINALIZE

      end program heat3Dp
```

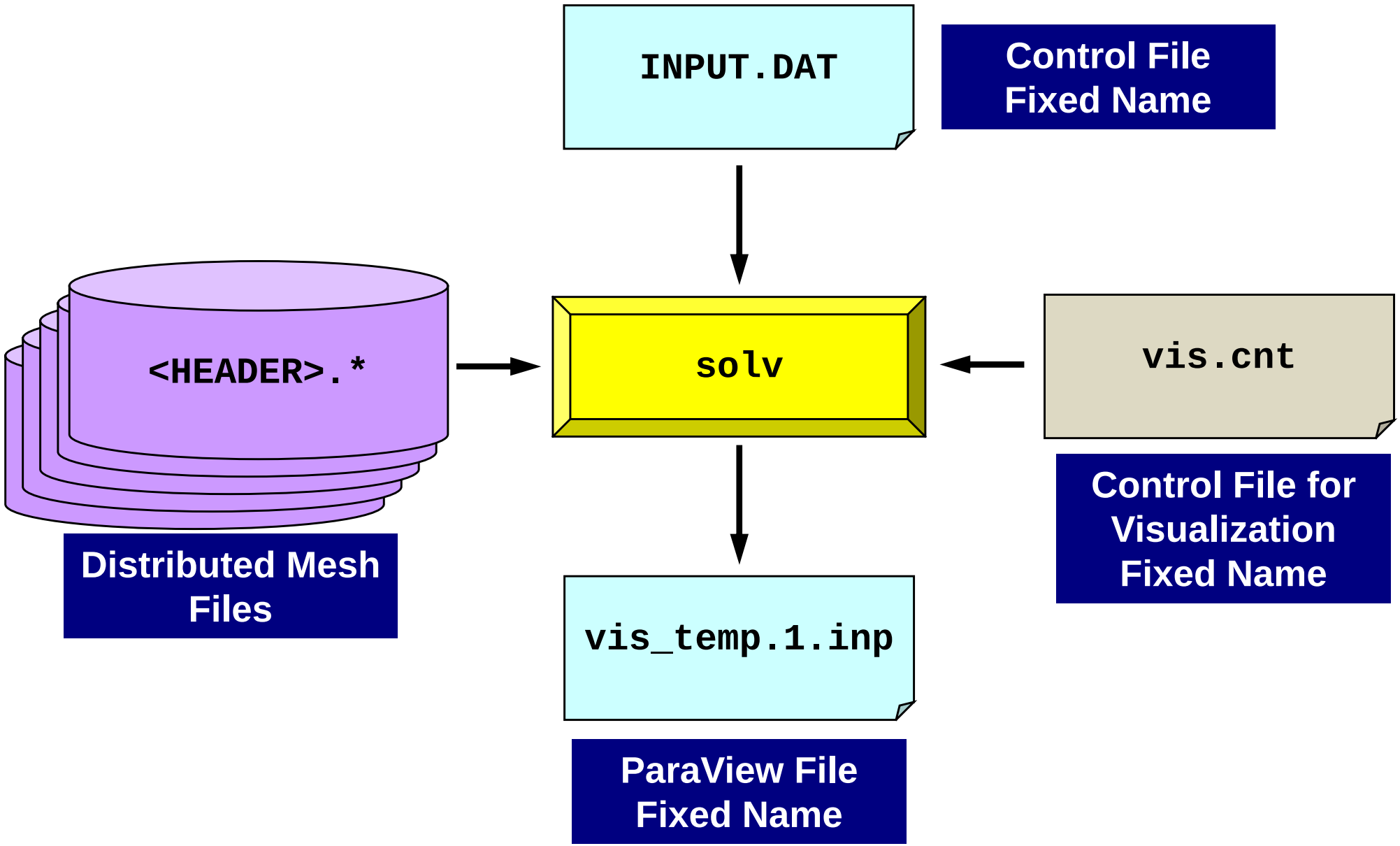
C/main (1/2)

```
#include <stdio.h>
#include <stdlib.h>
FILE* fp_log;
#define GLOBAL_VALUE_DEFINE
#include "pfem_util.h"
#include "ppohVIS_PFEM3D_Util.h"
extern void PFEM_INIT(int,char**);
extern void INPUT_CNTL();
extern void INPUT_GRID();
extern void MAT_CON0();
extern void MAT_CON1();
extern void MAT_ASS_MAIN();
extern void MAT_ASS_BC();
extern void SOLVE11();
extern void OUTPUT_UCD();
extern void PFEM_FINALIZE();
int main(int argc,char* argv[])
{
  double START_TIME,END_TIME;
  struct ppohVIS_FDM3D_stControl *pControl = NULL;
  struct ppohVIS_FDM3D_stResultCollection *pNodeResult = NULL;

  PFEM_INIT(argc,argv);
  ppohVIS_PFEM3D_Init(MPI_COMM_WORLD);
  pControl = ppohVIS_FDM3D_GetControl("vis.cnt");

  INPUT_CNTL();
  INPUT_GRID();

  if(ppohVIS_PFEM3D_SetMeshEx(
      NP,N,NODE_ID,XYZ,
      ICELTOT,ICELTOT_INT,ELEM_ID,ICELNOD,
      NEIBPETOT,NEIBPE,IMPORT_INDEX,IMPORT_ITEM,EXPORT_INDEX,EXPORT_ITEM)) {
              ppohVIS_BASE_PrintError(stderr);
              MPI_Abort(MPI_COMM_WORLD,errno);
  };
```

C/main (2/2)

```
  MAT_CON0();
  MAT_CON1();

  MAT_ASS_MAIN();
  MAT_ASS_BC()  ;

  SOLVE11();

  OUTPUT_UCD();

  pNodeResult=ppohVIS_BASE_AllocateResultCollection();
        if(pNodeResult == NULL) {
                ppohVIS_BASE_PrintError(stderr);
                MPI_Abort(MPI_COMM_WORLD,errno);
        };
        if(ppohVIS_BASE_InitResultCollection(pNodeResult, 1)) {
                ppohVIS_BASE_PrintError(stderr);
                MPI_Abort(MPI_COMM_WORLD,errno);
        };

        pNodeResult->Results[0] =

  ppohVIS_PFEM3D_ConvResultNodeItemPart(NP,1,0,"temp",X);

  START_TIME= MPI_Wtime();
        if(ppohVIS_PFEM3D_Visualize(pNodeResult,NULL,pControl,"vis",1)) {
                ppohVIS_BASE_PrintError(stderr);
                MPI_Abort(MPI_COMM_WORLD,errno);
        };

  ppohVIS_PFEM3D_Finalize();

  PFEM_FINALIZE() ;
}
```

pFEM3D + ppOpen-MATH/VIS



Preparing Distributed Mesh Files

```
>$ cd /work/gt36/t36XYZ/pFEM/pfem3d/runV
(mesh.inp, mg.sh)
>$ pjsub mg.sh
```

mesh.inp

```
256 256 256
  8   8   4
pcube
```

256^3 nodes into $8 \times 8 \times 4 = 256$ partitions
16,777,216 nodes
16,581,375 elements
Each MPI process has 32x32x64 nodes

mg.sh

```
#!/bin/sh
#PJM -N "pmg"
#PJM -L rscgrp=lecture6-o
#PJM -L node=8
#PJM --mpi proc=256
#PJM -L elapse=00:10:00
#PJM -g gt36
#PJM -j
#PJM -e err
#PJM -o pmg.lst

module load fj
module load fjmpi
mpiexec ./pmesh
rm wk.*
```

Computation + Visualization

```
>$ cd /work/gt36/t36XYZ/pFEM/pfem3d/runV
(INPUT.DAT, go.sh)
>$ pjsub gg.sh
```

INPUT.DAT

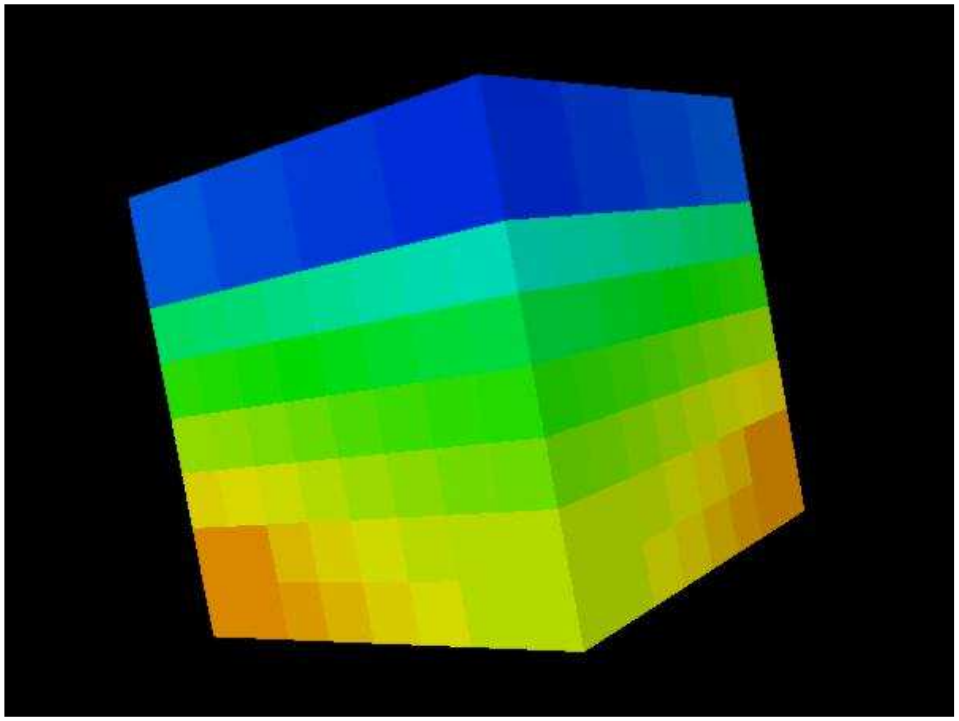
```
pcube
2000
1.0 1.0
1.0e-08
```

gg.sh

```
#!/bin/sh
#PJM -N "VIS"
#PJM -L rscgrp=lecture6-o
#PJM -L node=8
#PJM --mpi proc=256
#PJM -L elapse=00:15:00
#PJM -g gt36
#PJM -j
#PJM -e err
#PJM -o testV.lst

module load fj
module load fjmpi
mpiexec ./solv
```

vis.cnt

```
[Refine]                    Control Info. for Refinement
AvailableMemory = 2.0       Available Memory (GB) not in use
MaxVoxelCount = 1000        Max Voxel #
MaxRefineLevel = 20         Max Voxel Refinement Level
[Simple]                    Control Info. for Simplification
ReductionRate = 0.0         Reduction Rate of Surface Patches
[Output]                    Output Format
FileFormat    = 2           =1:MicroAVS, =2:ParaView
```



Values at Cell Ctr.

16,777,216 nodes
16,581,375 elem's, 256 MPI proc's

vis_temp.1.inp
1,436 nodes
1,002 elements

COPY the File to Your PC

Odyssey

```
>$ cd /work/gt36/t36XXX/pFEM/pfem3d/runV
>$ cp vis_temp.1.inp ~/.
```

PC

```
>$ scp t36XXX@wisteria.cc.u-tokyo.ac.jp:~/vis_temp.1.inp .
```