

3D Parallel FEM (III)

Parallel Visualization and ppOpen-HPC

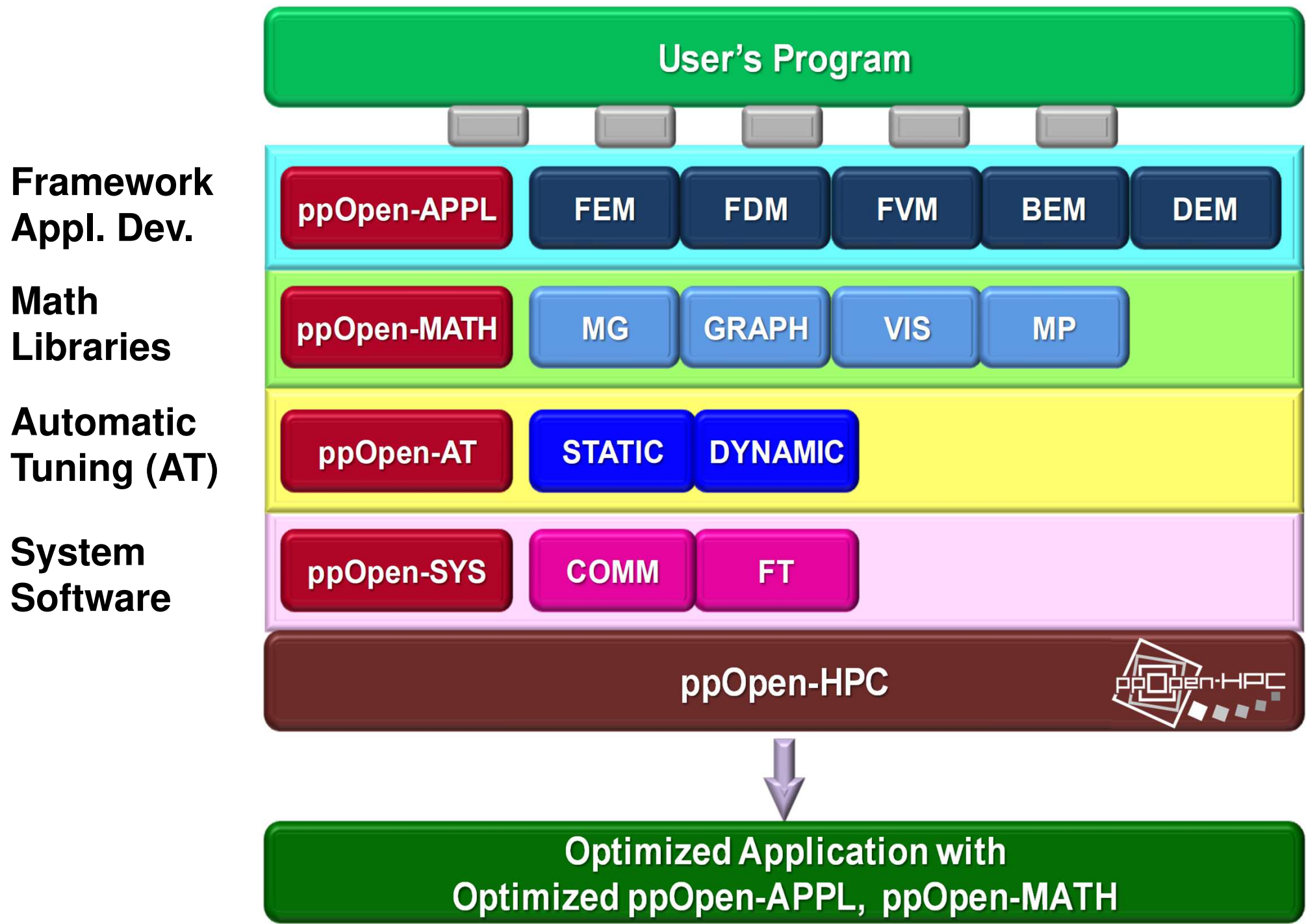
Kengo Nakajima
RIKEN R-CCS

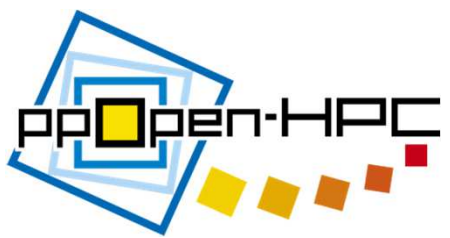


ppOpen-HPC: Overview

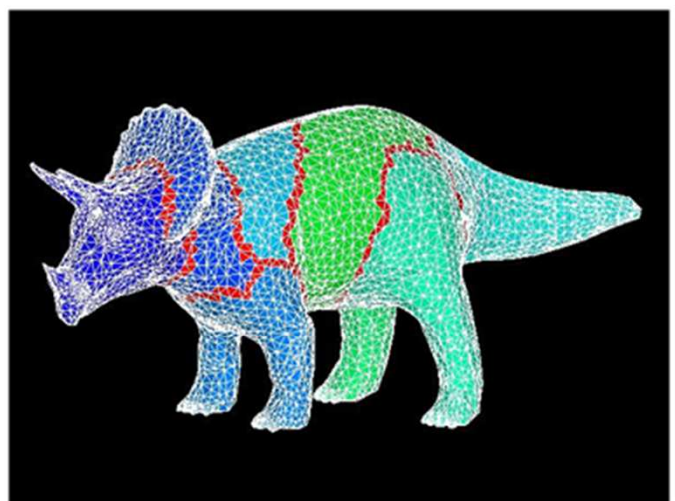
- Application framework with automatic tuning (AT)
 - ✓ “pp” : post-peta-scale
- Five-year project (FY.2011-2015) (since April 2011)
 - ✓ P.I.: Kengo Nakajima (ITC, The University of Tokyo)
 - ✓ Part of “Development of System Software Technologies for Post-Peta Scale High Performance Computing” funded 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



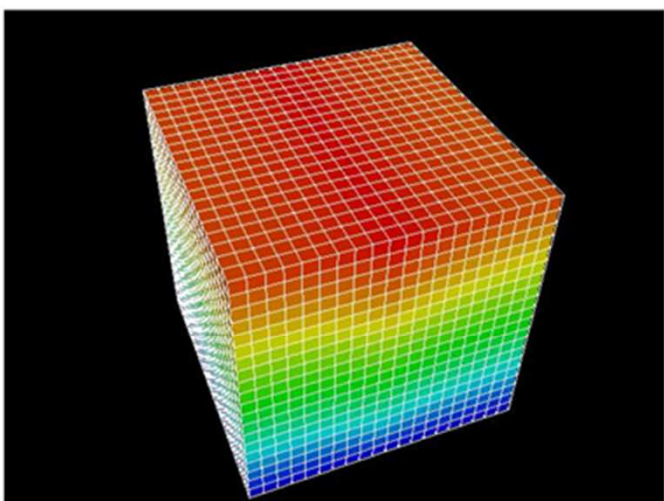




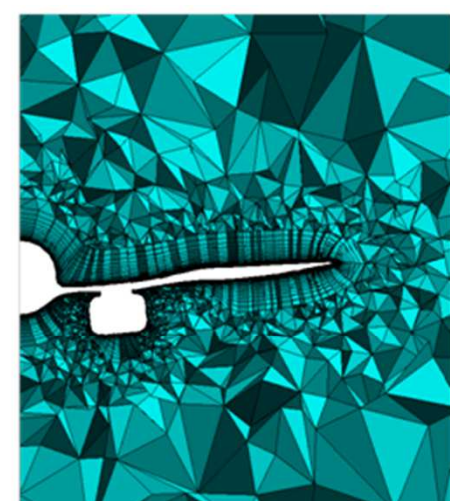
ppOpen-HPC covers ...



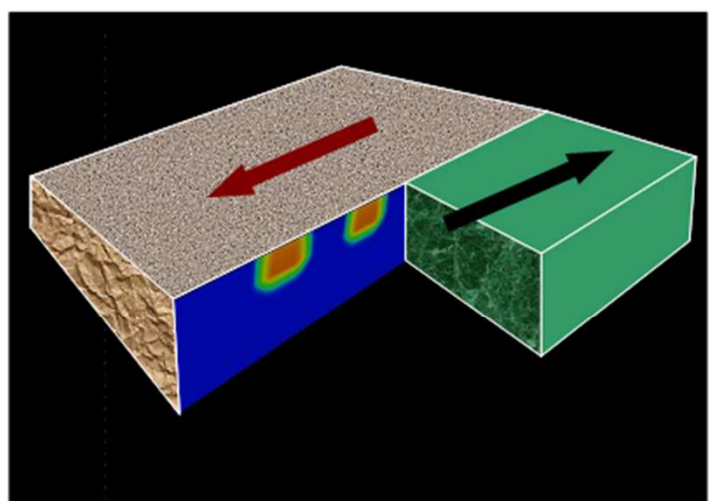
FEM
Finite Element Method



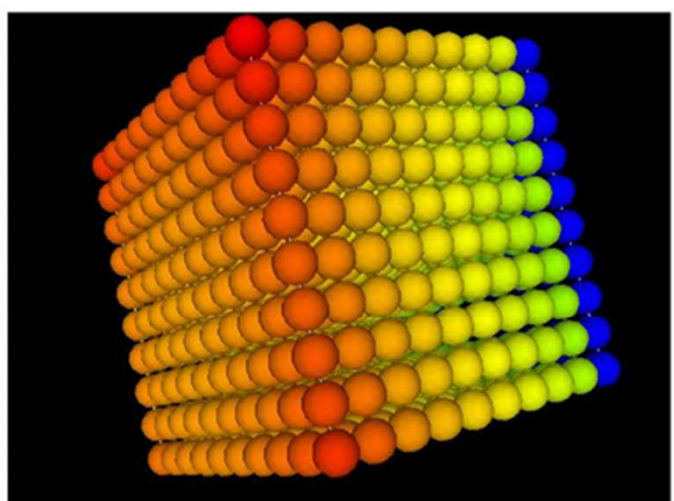
FDM
Finite Difference Method



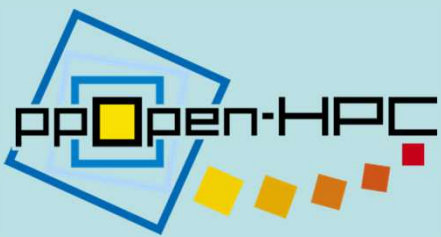
FVM
Finite Volume Method



BEM
Boundary Element Method

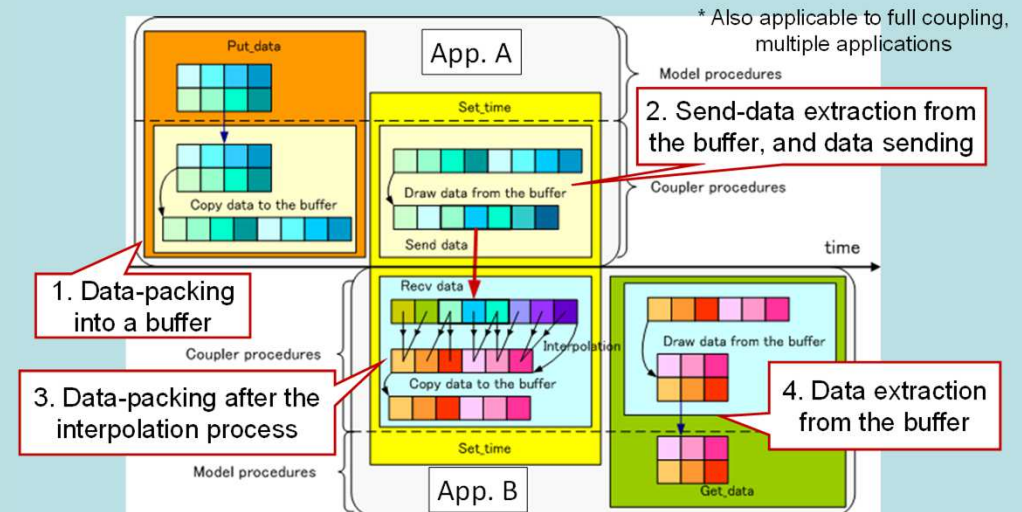
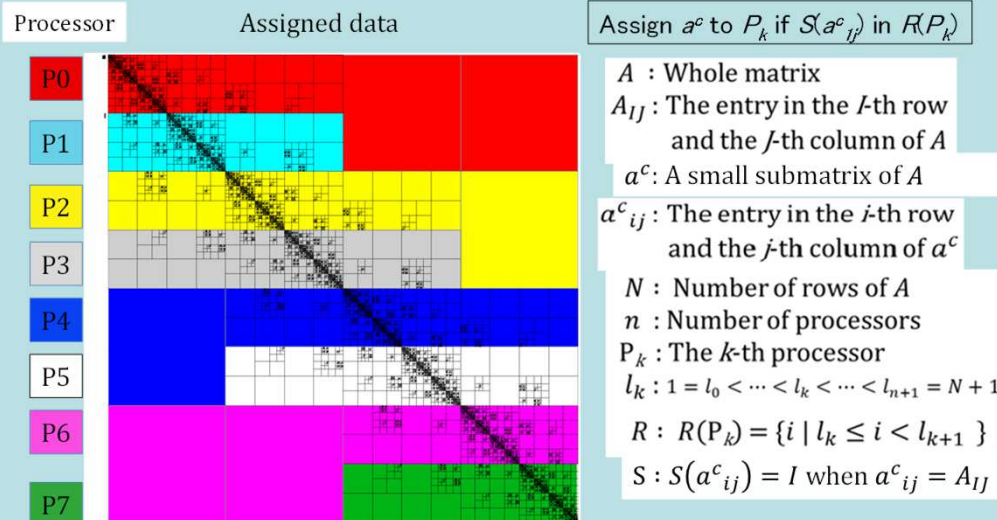


DEM
Discrete Element Method



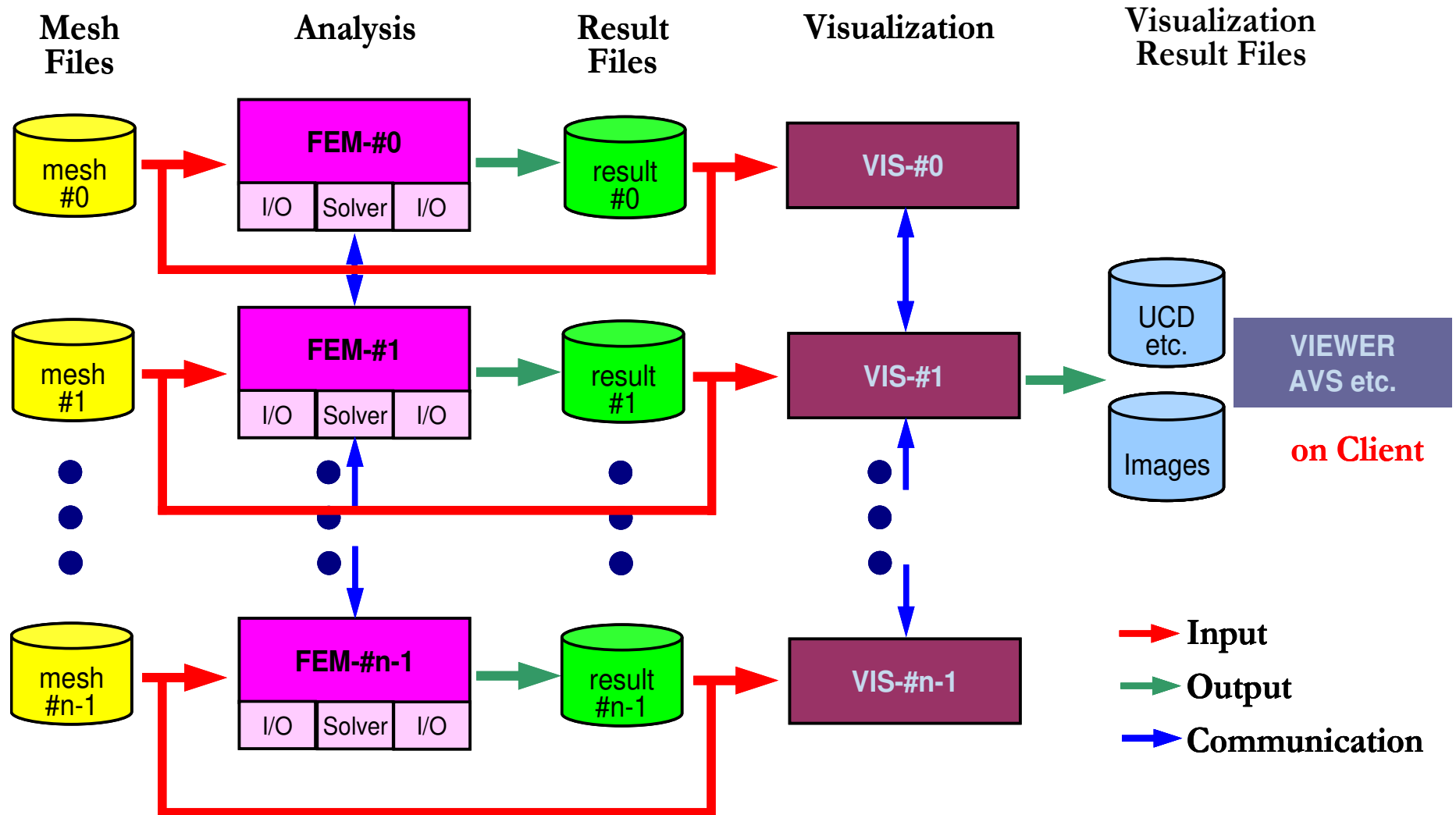
Featured Developments

- 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**

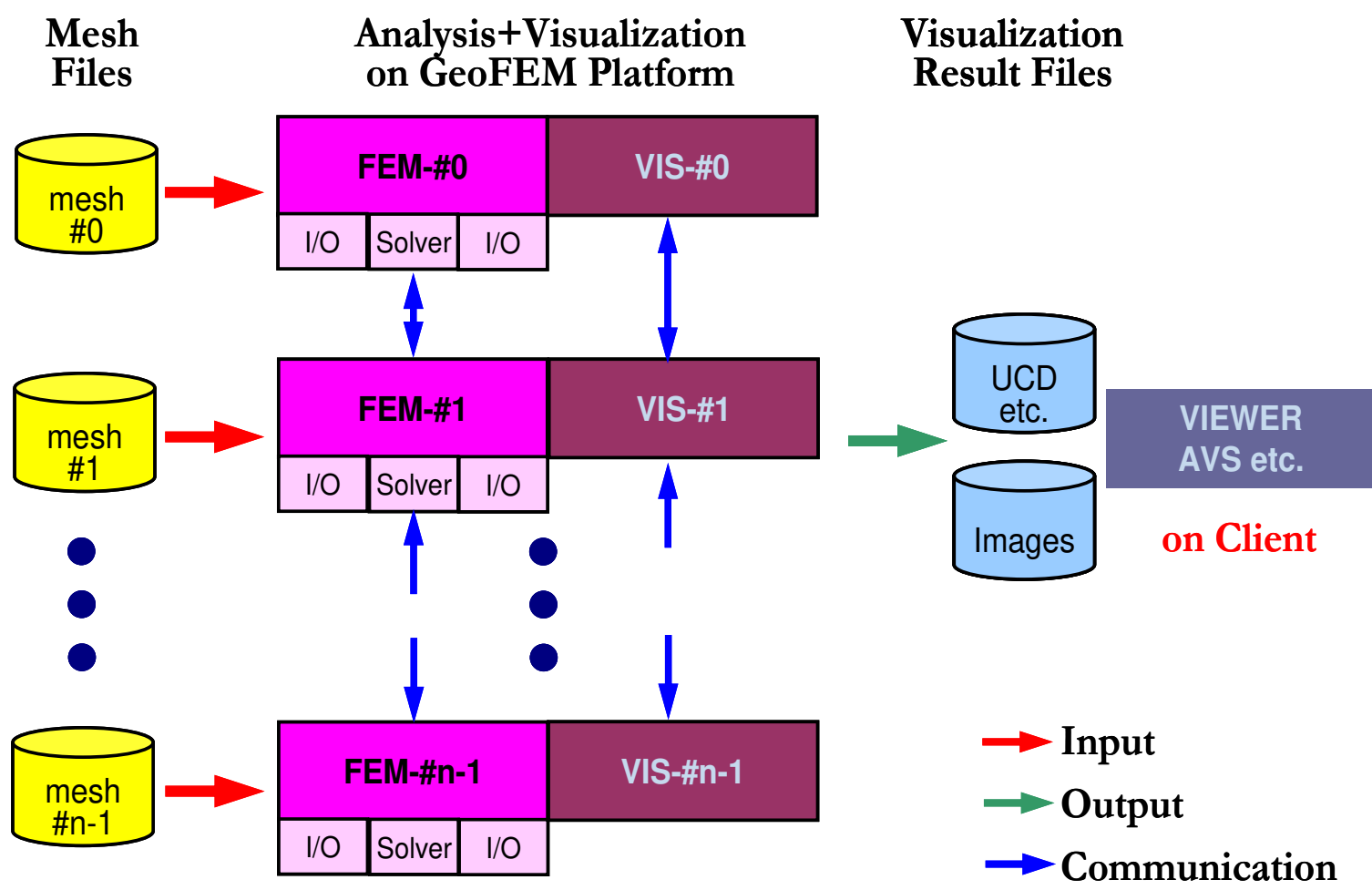


Framework for Parallel Visualization 1

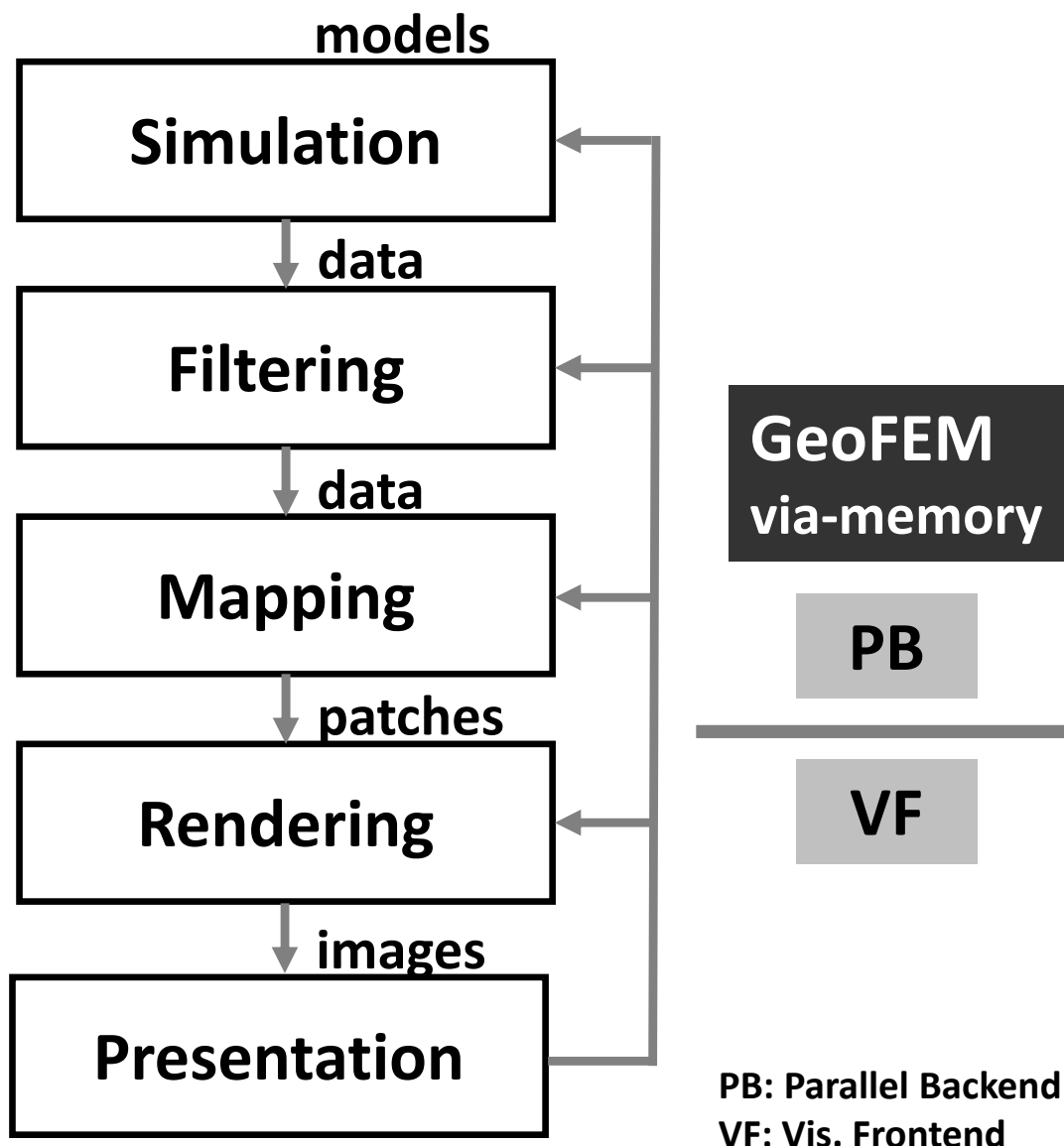
Via-File



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

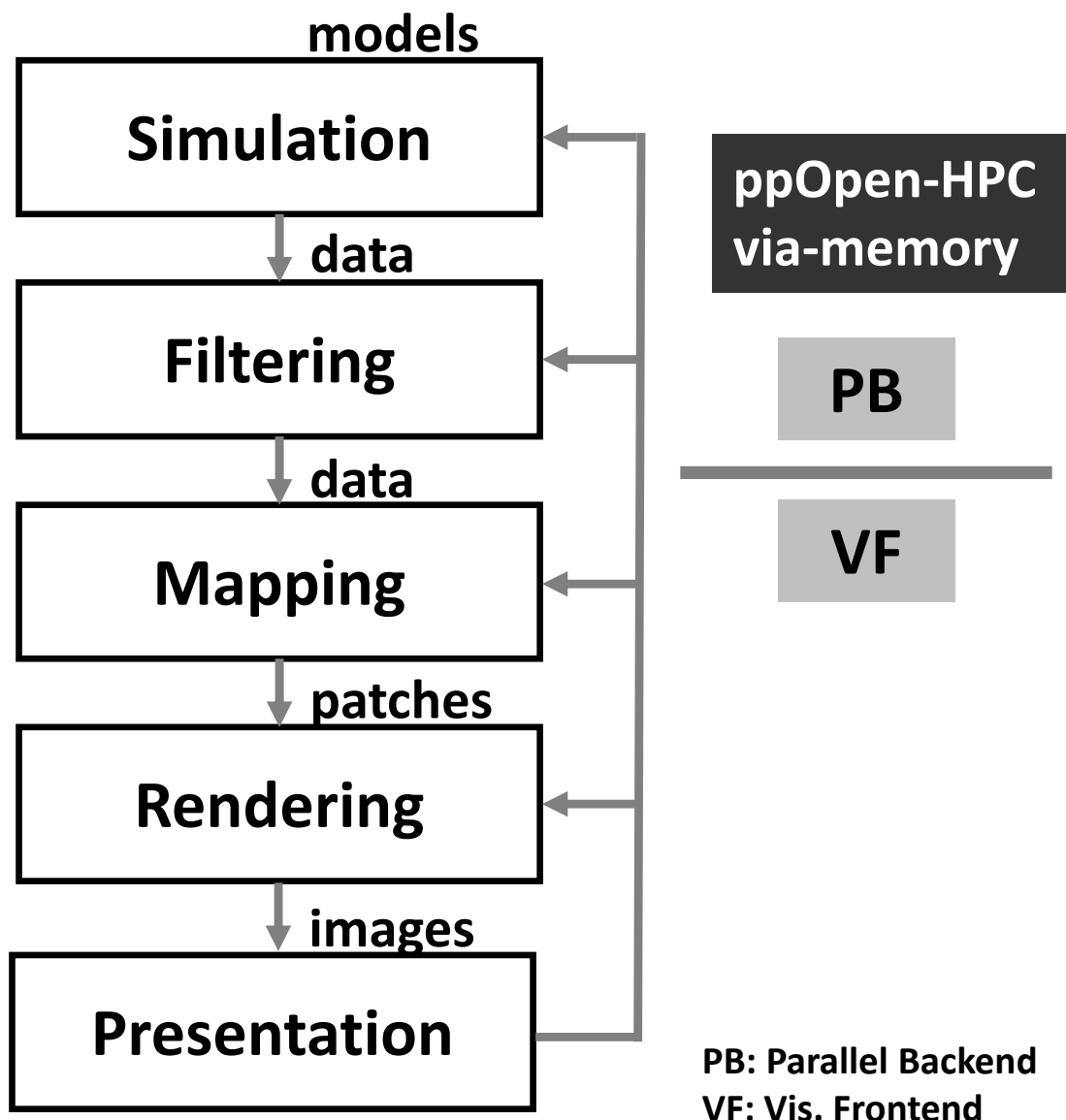


Visualization in GeoFEM (1997-2003)



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

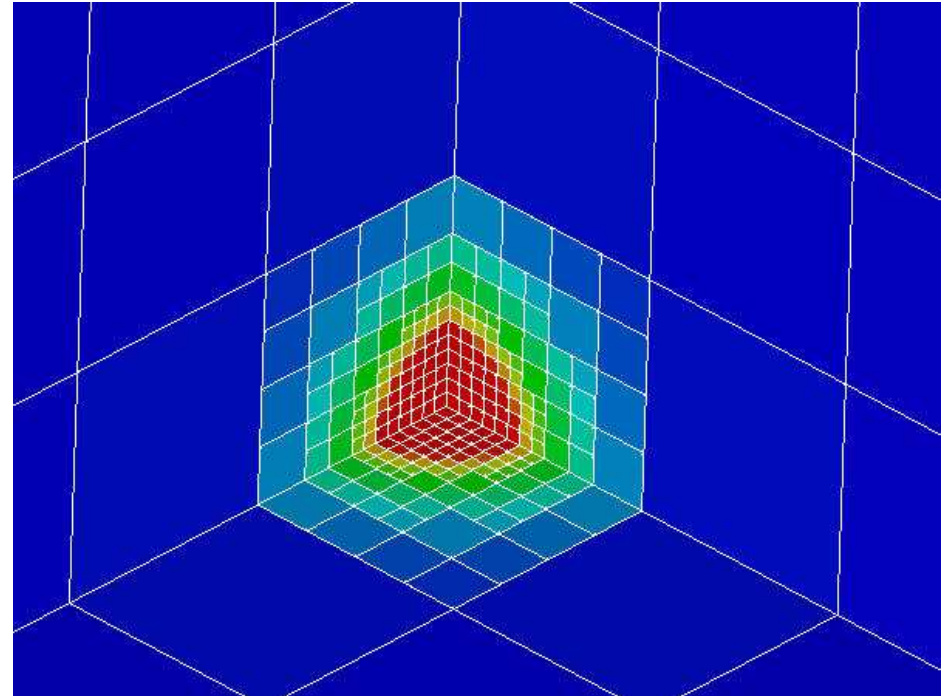
Visualization in ppOpen-HPC



- 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

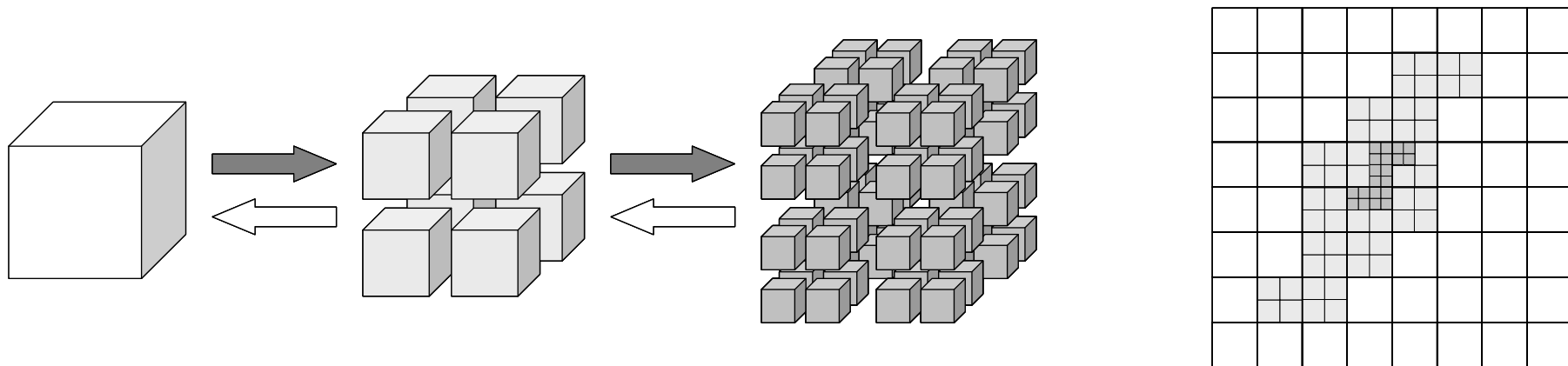


[Refine]

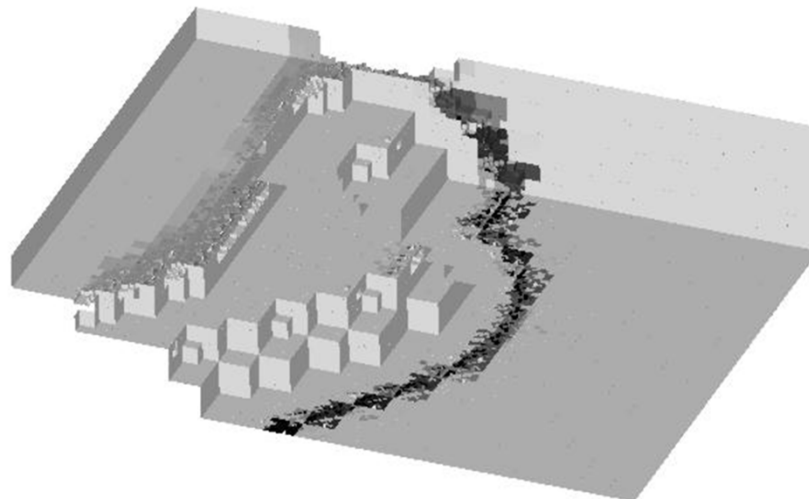
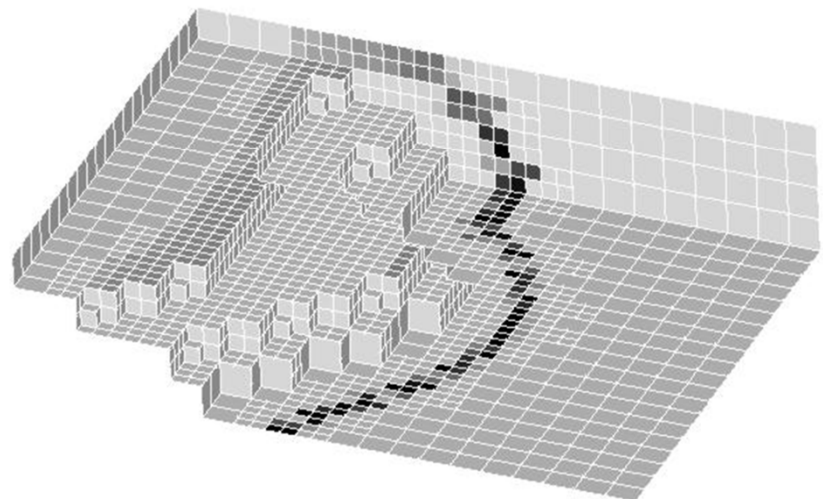
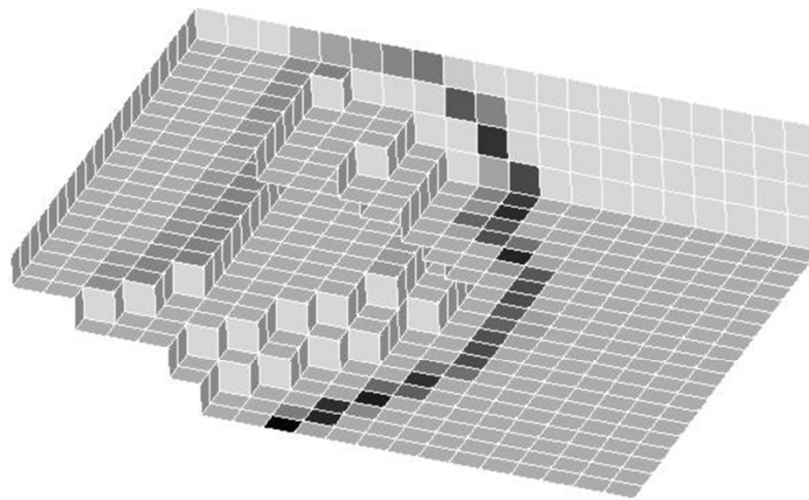
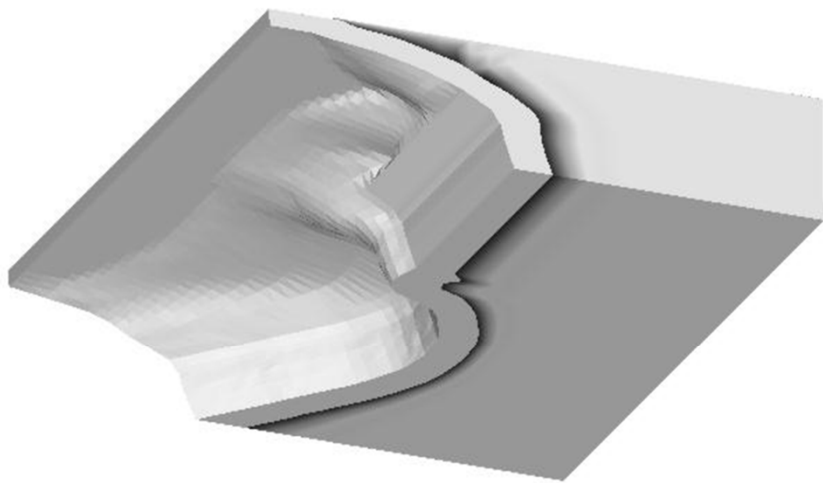
AvailableMemory = 2.0	Available memory size (GB), not available in this version.
MaxVoxelCount = 500	Maximum number of voxels
MaxRefineLevel = 20	Maximum number of refinement levels

Simplified Parallel Visualization using Background Voxels

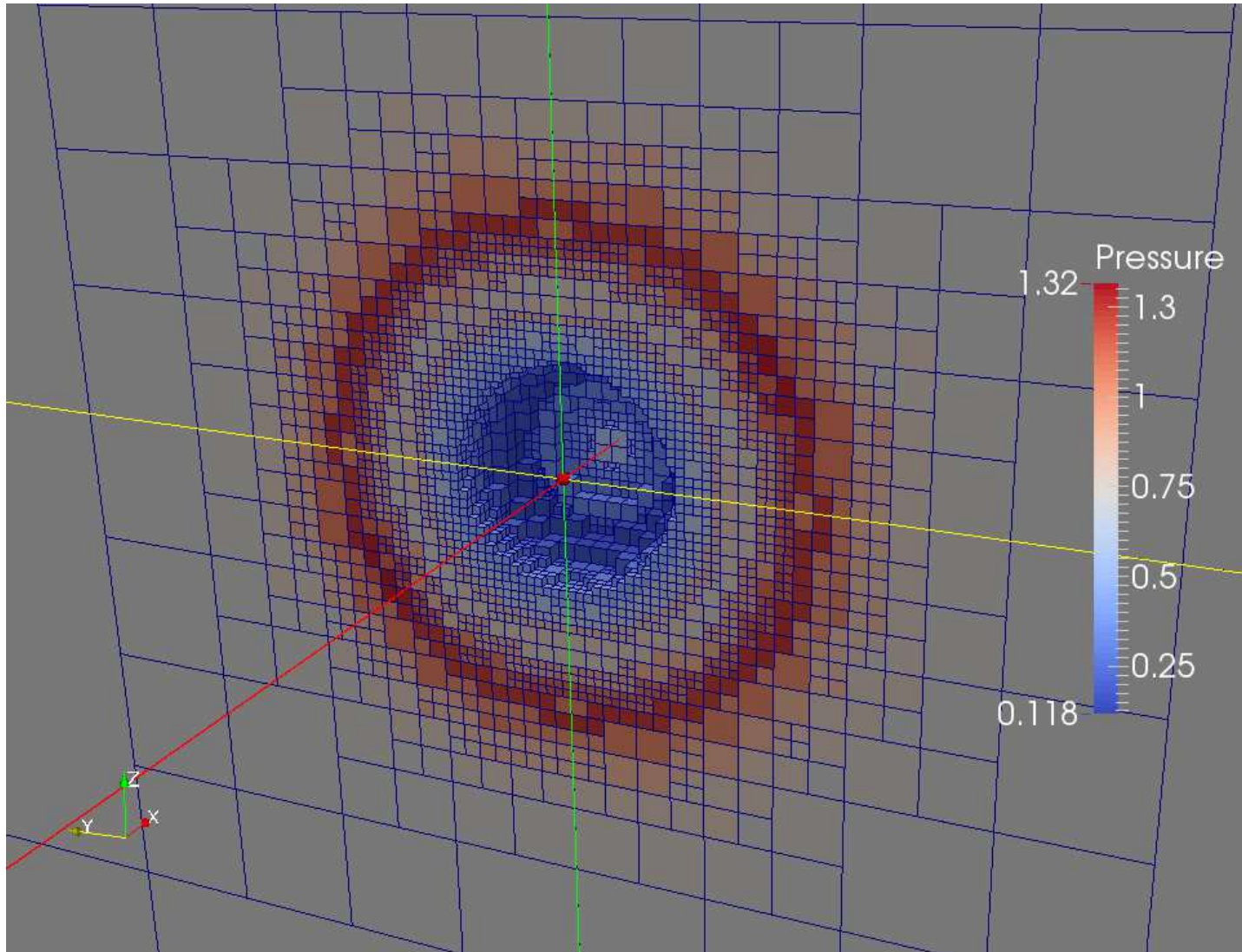
- Octree-based AMR
- AMR applied to the region where gradient of field values are large
 - stress concentration, shock wave, separation etc.
- If the number of voxels are controlled, a single file with 10^5 meshes is possible, even though entire problem size is 10^9 with distributed data sets.



Voxel Mesh (adapted)



Flow around a sphere



pFEM3D + ppOpen-MATH/VIS

Fortran

```
>$ cd /work/gt18/t18XXX/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/gt18/t18XXX/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] =

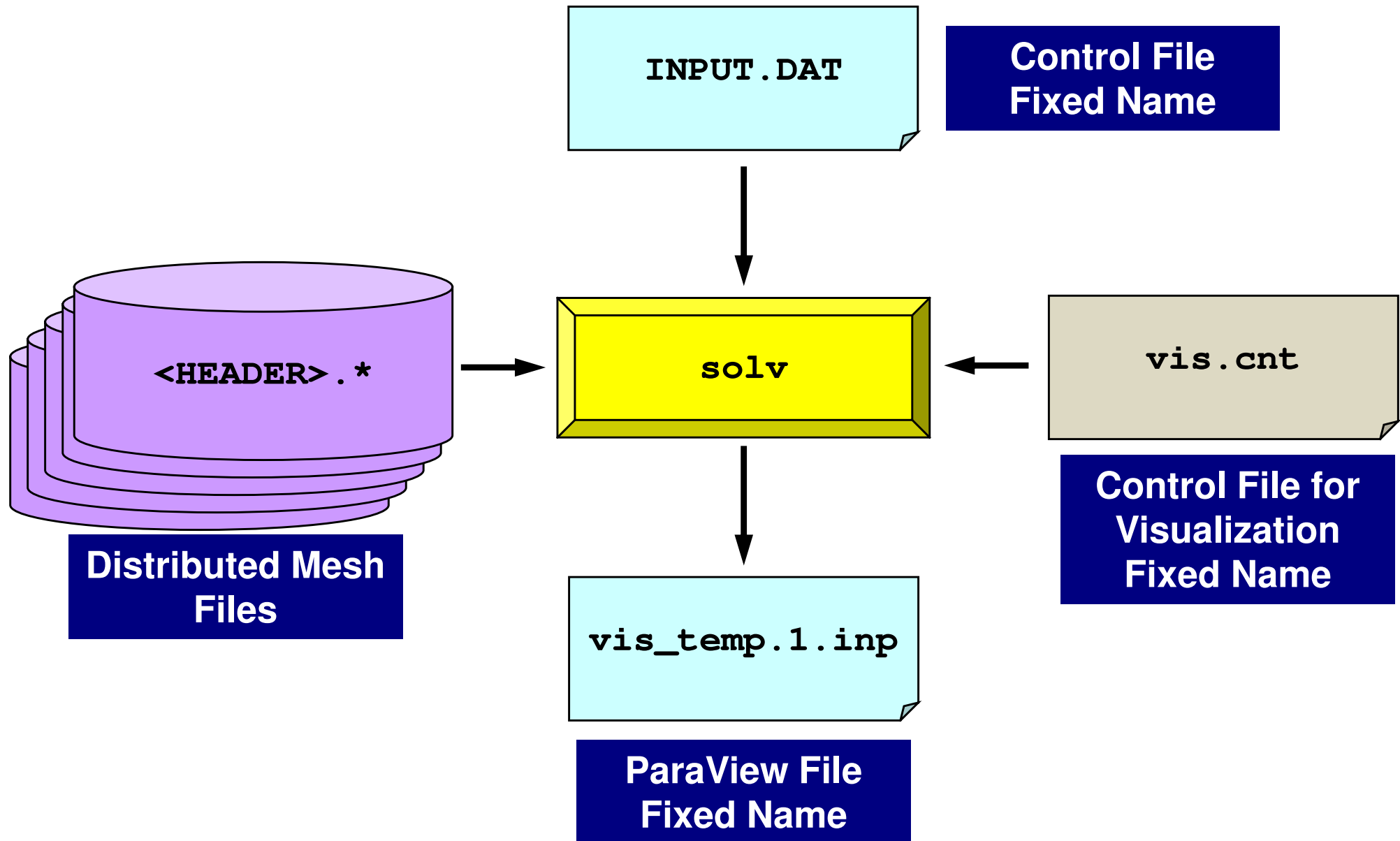
ppohVIS_PFEM3D_ConvResultNodeItemPart (NP, 1, 0, "temp", X);

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/gt18/t18XYZ/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 $32 \times 32 \times 64$ nodes

mg.sh

```
#!/bin/sh  
#PJM -N "pmg"  
#PJM -L rscgrp=lecture8-o  
#PJM -L node=8  
#PJM --mpi proc=256  
#PJM -L elapse=00:10:00  
#PJM -g gt18  
#PJM -j  
#PJM -e err  
#PJM -o pmg.lst
```

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


Computation + Visualization

```
>$ cd /work/gt18/t18XYZ/pFEM/pfem3d/runV  
(INPUT.DAT, go.sh)  
>$ pjsub go.sh
```

INPUT.DAT

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

go.sh

```
#!/bin/sh  
#PJM -N "VIS"  
#PJM -L rscgrp=lecture8-o  
#PJM -L node=8  
#PJM --mpi proc=256  
#PJM -L elapse=00:15:00  
#PJM -g gt18  
#PJM -j  
#PJM -e err  
#PJM -o testV.lst
```

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

vis.cnt

[Refine]

AvailableMemory = 2.0

MaxVoxelCount = 1000

MaxRefineLevel = 20

[Simple]

ReductionRate = 0.0

[Output]

FileFormat = 2

Control Info. for Refinement

Available Memory (GB) not in use

Max Voxel #

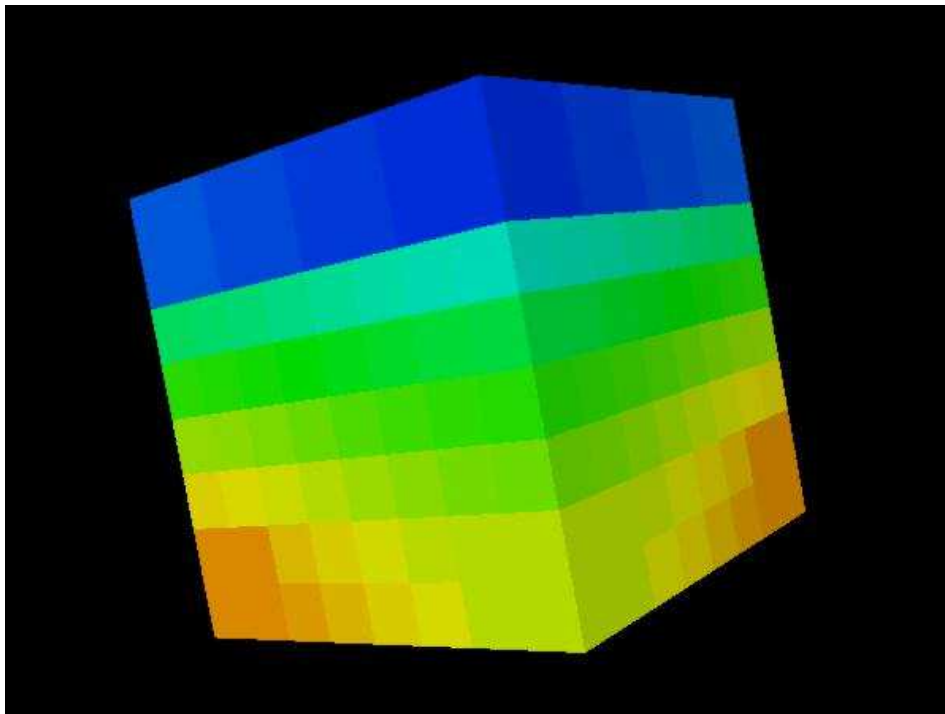
Max Voxel Refinement Level

Control Info. for Simplification

Reduction Rate of Surface Patches

Output Format

=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/gt18/t18XXX/pFEM/pfem3d/runV  
>$ cp vis_temp.1.inp ~/.
```

PC

```
>$ scp t18XXX@wisteria.cc.u-tokyo.ac.jp:~/vis_temp.1.inp .
```