

Programming of Supercomputers

1st Assignment

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Outline

1. About this lab course
2. Fire benchmark
3. SuperMUC at LRZ
4. 1st assignment

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Programming of Supercomputers (PoS13) Lab

- Every other week on Friday
 - Time: 13:30 – 15:00
 - Dates: 18 Oct. 2013, **25 Oct. 2013**, 15 Nov. 2013, 29 Nov. 2013 & 13 Dec. 2013
 - Room: MI 01.06.020
 - Final Presentations (20 min.): 31 Jan. 2014, 10:00 o'clock
 - Office Hours: Tuesday, 10:30 – 12:00
- Registration in TUMonline
- News, source code and assignments
www.lrr.in.tum.de/~berariu/teaching/superprog1314.php



Programming of Supercomputers (PoS13) Lab

- **Last semester: Introduction to Parallel Programming**
 - Theoretical background about OpenMP and MPI
 - Tutorials using small exercises covering the basic usage
 - Team work allowed
 - Guided problem solving
- **This semester: Programming of Supercomputers**
 - Application of the gained knowledge on a single simulation code
 - Project-based format – more involved and autonomous work
 - Teams of 2 students: code together, tune and report individually
 - „Inter-teams“ submissions lead to course failure

PoS13: Assignments

- 1st assignment– Sequential optimization (30%)
 - Getting to know the application & the **coding guidelines**
 - Single-core compiler-based optimization
 - IO effects on performance
 - Visualization of results with ParaView
- 2nd assignment – MPI Parallelization (65%)
 - Milestone 1: Data Distribution
 - Milestone 2: Communication Model
 - Milestone 3: Parallelization using MPI
 - Milestone 4: Performance analysis and tuning
- Final report and presentation (5%)
 - Report on modeling, implementation and performance tuning results
 - 15 min. presentation + 10 min. Q&A session

PoS13: Submission

- Deadlines: 2nd Friday after each presentation @ 08:00 CET
- Plan for unscheduled maintenances & overbooked job queues
<http://www.lrz.de/services/compute/supermuc/>
- Commit all required files to the Git repository
 - separate repository for each team with restricted access for every student
 - about Git:
<http://git-scm.com/book/en/Git-Basics-Getting-a-Git-Repository>
 - address:
<http://periscope.in.tum.de/lectures/IN2190/teamXX>
 - username/pass – per email after registration
- Check-in as often as you need and use meaningful commit messages



PoS13: Grading

- Each team member receives an **individual grade**
- Maximum points for each assignment: 100
- Contribution of the separate assignments:
 - Assignment 1: 30%
 - Assignment 2: 65%
 - Milestone 1 - Data distribution: 15 points
 - Milestone 2 - Communication model: 15 points
 - Milestone 3 - MPI Implementation: 15 points
 - Milestone 4 - Performance measurements and tuning: 25 points
 - Final Report: 30 points
 - Final Presentation: 5%
- Minimum points to pass: 50
- Both assignment 1 and 2 are required to pass!

PoS13: Coding Guidelines

- Special guidelines for the coding style
 - One uniform format and look
 - Higher quality code & less misunderstandings
- Current version based on industry standards
 - Google C++ Style Guide
 - id Software Coding Style
- Not following these guidelines leads to negative points and could contribute to failing the lab course
- Full version of the Coding Guidelines:
http://www.lrr.in.tum.de/~berariu/teaching/res/pos1314/PoS1314_CodingStyle.pdf

PoS13: Coding Guidelines (1)

- Indentation
 - 4 spaces per level
 - never use tabs (configure your editor to emit 4 spaces on a Tab)
- Each code line should be at most 100 characters long
 - break up longer lines.
- Use whitespace liberally within expressions, but only one space at a time
 - 1 space before and after all operators and after every comma
- Non-ASCII characters should be rare and must use UTF-8 formatting

PoS13: Coding Guidelines (2)

- **Function names**

- should be descriptive
- use a “command” verb, or a verb followed by noun
- avoid starting function names with nouns
- start with a lower case:

```
void function( int arg1, double r );
```
- for multi-word function names, all words should be lower case with underscores (`_`) between words

```
void do_something_function( void );
```

- **Variable names – follow the function name rules**

PoS13: Coding Guidelines (3)

- **Function calls**
 - on one line if it fits
 - otherwise, wrap arguments at the parenthesis
- **Function length and contents**
 - use single empty lines to add clarity where necessary
 - never have more than one consecutive blank line
 - each function should be a coherent unit of work
 - no longer than 50 lines / 1 page of code - factor out common code
 - avoid having more than 5 nesting levels

PoS13: Coding Guidelines (4)

- Use a Doxygen compliant header for all functions

```
/**
 * Calculate the distribution factor of a dataset.
 *
 * @param nintci start element
 * @param nintcf end element
 * @param cgup data array for which a factor is calculated
 *
 * @return distribution factor
 */
double calc_distribution_factor( int nintci,
                                int nintcf,
                                double* cgup );
```

Doxygen Manual: www.doxygen.org

PoS13: Coding Guidelines (5)

- Use trailing braces everywhere: if, else, functions, structures, typedefs, class definitions, etc.
- Else statement starts on the same line as the last closing brace
- Pad parenthesized expressions with spaces
- Always indent the following
 - Statements within function body
 - Statements within blocks
 - Statements within 'case' body of switch operators

```
if ( x ) {  
    // ...  
} else {  
    // ...  
}
```

```
x = ( y * z );
```

PoS13: Coding Guidelines (6)

- **Comments**
 - should be brief
 - should explain WHY instead of HOW
 - do not restate code in the comments
 - give reasons
 - why a particular algorithm was chosen
 - why a particular data structure is used
 - why a certain action must be taken

Bad Example

```
// set product to "base"
product = base;

// loop from 2 to "num"
for ( int i = 2; i <= num; i++ ) {
    // multiply "base" by "product"
    product = product * base;
}
```

Good Example

```
// compute the square root of num using
// Newton-Raphson approximation
r = num / 2;

while ( abs( r - (num/r) ) > EPSILON ) {
    r = 0.5 * ( r + (num/r) );
}
```



Outline

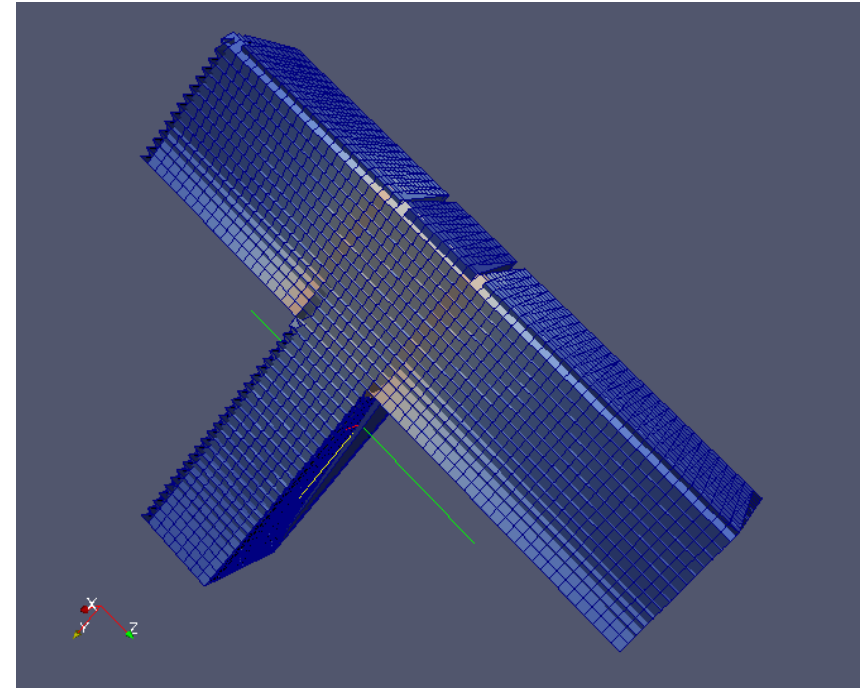
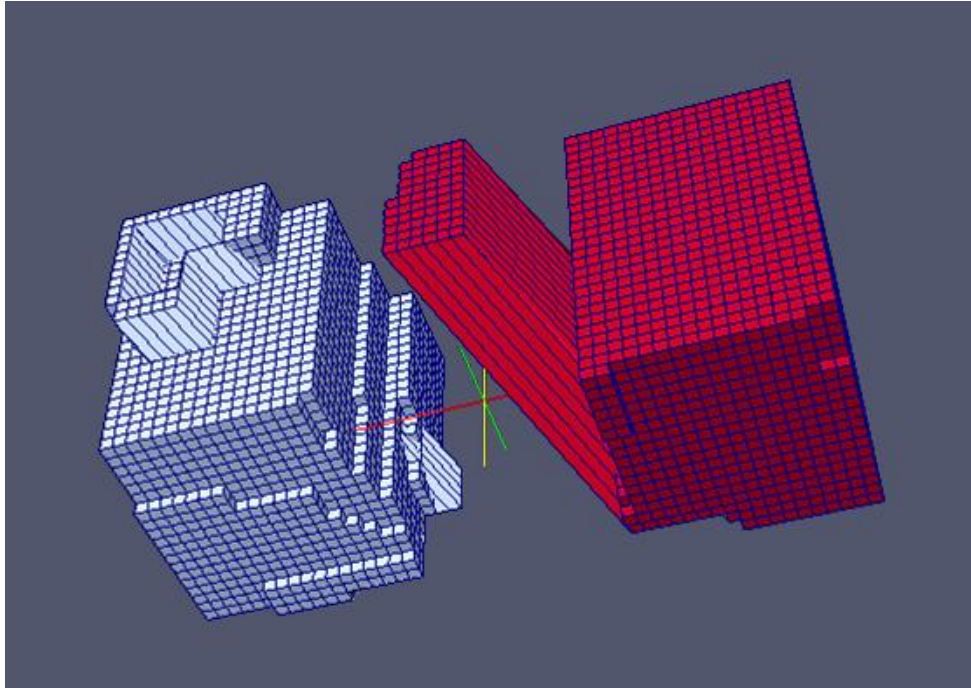
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Fire Benchmark

Two- or three-dimensional (un-)steady simulations of flow and heat transfer within arbitrarily complex geometries with moving or fixed boundaries

- Computational Fluid Dynamics (CFD) solver framework for arbitrary geometries
- Developed by AVL LIST GmbH, Graz, Austria
- Written in C
 - main computational function is only 350 lines
 - two extra files for data import and export
- Black-box approach
 - do not spend time on understanding the physics behind
 - concentrate on the performance and optimization and not the theory!!

Fire Benchmark - Geometries



Fire Benchmark - GCCG

- GCCG – generalized orthomin solver with diagonal scaling
- Linearized Continuity Equation

$$A_p \varphi_p = \sum_{c=E,S,N,\dots} A_c \varphi_c + S_\varphi$$

given

- source value $S_\varphi \rightarrow SU$
- boundary cell coefficients $A_c \rightarrow BE, BS, \dots$
- boundary pole coefficients $A_p \rightarrow BP$

wanted

- variation vector/flow to be transported $\varphi_p \rightarrow VAR$

Fire Benchmark - GCCG

- Domain discretisation in volume cells
- Unstructured grid with neighboring information (LCC) and indirect addressing
- Internal and external (ghost) cells
- Iterate until acceptable residual achieved
 - Phase 1: compute the new *directional* values from the old ones
 - Phase 2:
 - normalize and update values
 - compute new residual
- More details with the 2nd assignment

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SuperMUC @ Leibniz Supercomputer Centre

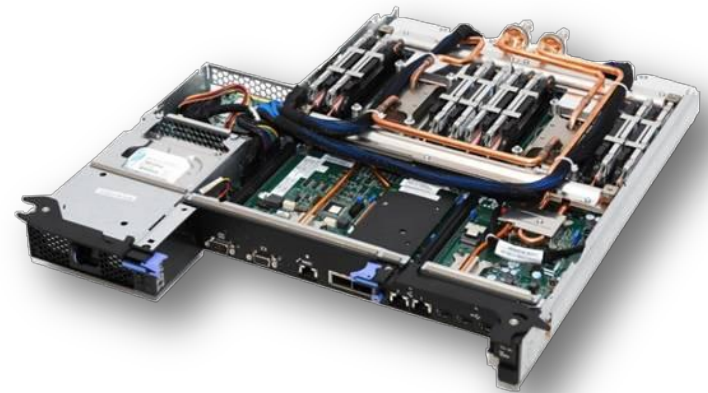


SuperMUC – Peak Performance

- Peak performance: 3 Peta Flops = $3 \cdot 10^{15}$ Flops
 - Mega 10^6 million
 - Giga 10^9 billion
 - Tera 10^{12} trillion
 - Peta 10^{15} quadrillion
 - Exa 10^{18} quintillion
 - Zetta 10^{21} sextillion
- Flops: Floating Point Operations per Second

SuperMUC – Distributed Memory Architecture

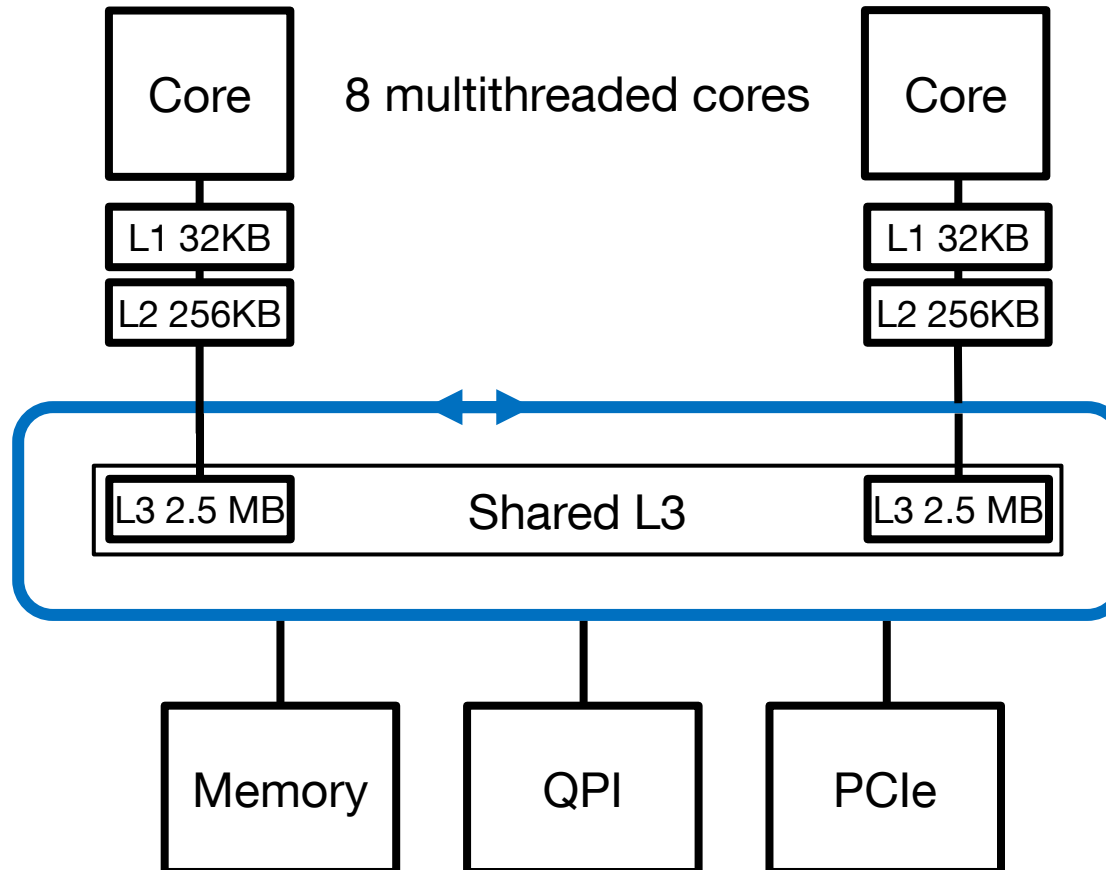
- 18 partitions (*islands*) with 512 nodes each
- One node is a shared memory system with 2 processors
 - Sandy Bridge-EP Intel Xeon E5-2680 8C
 - 2.7 GHz (Turbo 3.5 GHz)
 - 32 GByte memory
 - Infiniband network interface
- Each processor has 8 cores
 - 2-way hyperthreading
 - 21.6 GFlops @ 2.7 GHz per core
 - 172.8 GFlops per processor



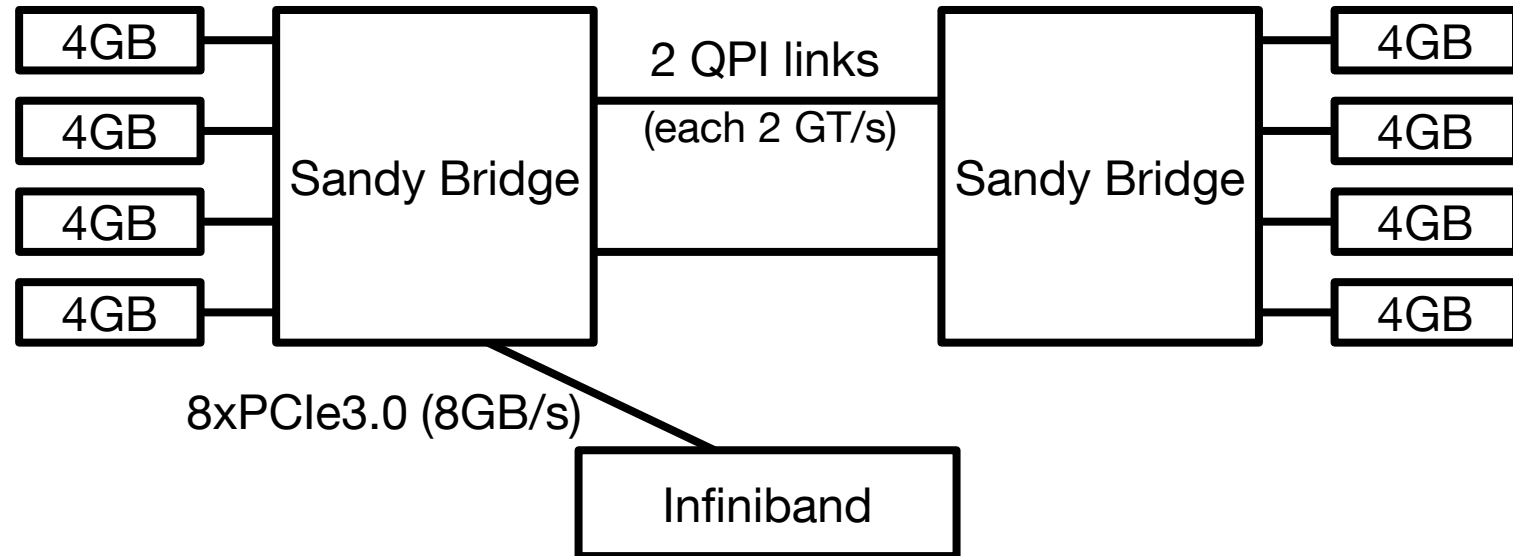
Sandy Bridge Processor

Latency:

- 4 cycles
- 12 cycles
- 31 cycles



SuperMUC – NUMA Node



- 2 processors with 32 GB of memory
- Aggregate memory bandwidth per node 102.4 GB/s
- Latency
 - local ~50ns (~135 cycles @2.7 GHz)
 - remote ~90ns (~240 cycles)

SuperMUC – Access

- Accounts per Email after TUMOnline registration
first of all, change your password by visiting the ID-Portal of LRZ:
<http://idportal.lrz.de/r/entry.pl?Sprache=en>
- SSH-only access (login / data transfer):
connection only allowed from trusted DNS (e.g. lxhalle)

```
ssh -Y <username>@supermuc.lrz.de
```

- Details and info:
http://www.lrz.de/services/supermuc/access_and_login/

SuperMUC – Job scheduling

- LoadLeveler batch system
<http://www.lrz.de/services/compute/supermuc/loadleveler/>
 - build a job command file – plain text file
 - submit with `llsubmit`
 - check status with `llq`
- Interactive jobs
 - used in general for testing
 - have limited resources
- Never run measurements on the login node

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1st assignment

- General facts
 - Get to know the machine you are using
 - Reproducible results – at least 3 runs for each configuration
 - Code instrumentation using the PAPI hw counters library
- Different runtime behavior in different application phases
 - Initialization: read input data files
 - Computation: efficient usage of resources
 - Finalization: output the results
- Carry out performance experiments using different compiler optimization flags
- Metrics: execution time, MFlops, L2/L3 cache miss rate



PAPI Instrumentation

- Library for accessing the performance counter hardware on microprocessors
 - main website: <http://icl.cs.utk.edu/papi/>
 - User's Guide: http://icl.cs.utk.edu/projects/papi/files/documentation/PAPI_USER_GUIDE_23.htm
- Requires user instrumentation of applications
- Available on SuperMUC: `module load papi`
- Supported events and counters: `papi_avail`
 - check which counters you can use on SuperMUC
- High-Level API vs. Low-Level API

PAPI Instrumentation – High-Level API HW Counters

```
#include <papi.h>
#define NUM_EVENTS 2

void main( ) {
    int Events[NUM_EVENTS] = { PAPI_TOT_INS, PAPI_TOT_CYC };
    long_long values[NUM_EVENTS];

    // Start counting events
    if ( PAPI_start_counters( Events, NUM_EVENTS ) != PAPI_OK ) handle_error( 1 );

    // Do some computation here

    // Read the counters
    if ( PAPI_read_counters( values, NUM_EVENTS ) != PAPI_OK ) handle_error( 1 );

    // Do some more computation here

    // Read again the counters and stop counting events
    if ( PAPI_stop_counters( values, NUM_EVENTS ) != PAPI_OK ) handle_error( 1 );
}
```


PAPI Instrumentation – Low-Level API HW Counters

```
int EventSet = PAPI_NULL;
if ( PAPI_library_init( PAPI_VER_CURRENT ) != PAPI_VER_CURRENT ) exit(1);

// Create an EventSet
if ( PAPI_create_eventset( &EventSet ) != PAPI_OK ) handle_error( 1 );

// Add Total Instructions Executed to the EventSet
if ( PAPI_add_event( &EventSet, PAPI_TOT_INS ) != PAPI_OK ) handle_error(1);

// Start counting
if ( PAPI_start( EventSet ) != PAPI_OK ) handle_error(1);

// Do some computation here

// Read the counters
if ( PAPI_read( values ) != PAPI_OK ) handle_error( 1 );

// Read again the counters and stop counting events
if ( PAPI_stop( EventSet, values ) != PAPI_OK ) handle_error( 1 );
```

PAPI Instrumentation – Timers

```
long_long start_cycles, end_cycles, start_usec, end_usec;

if ( PAPI_library_init( PAPI_VER_CURRENT ) != PAPI_VER_CURRENT ) exit(1);

start_cycles = PAPI_get_real_cyc(); // Gets the starting time in clock cycles
start_usec = PAPI_get_real_usec(); // Gets the starting time in microseconds

// Do some computation here

end_cycles = PAPI_get_real_cyc(); // Gets the ending time in clock cycles
end_usec = PAPI_get_real_usec(); // Gets the ending time in microseconds

printf ( "Wall clock time in usecs: %lld\n", end_usec - start_usec );
```

I/O – ASCII vs. Binary Data Files

- Change initial data format: ASCII → binary
- Compare execution time in both cases
- Analyze storage space
- Discuss the differences

Visualization with ParaView

- ParaView visualization software
 - open-source product: www.paraview.org
 - load the module on SuperMUC

```
module load paraview
```
 - you can download & install it locally on your computer
- Uses VTK file format
 - use the supplied functions to convert the data prior to export
 - export the vector values using the provided function
- Visualize the resulting VTK files for tjunc.dat for the VAR, CGUP and SU arrays
- Store the images in jpeg format

Submission

- Deadline: 1. Nov 2012 @ 08:00 CET
- Plan for unscheduled maintenances & overbooked job queues!!!
- Choose a team-mate until Monday, 21st Oct. and announce your group at berariu@in.tum.de
- Git repositories are prepared for each group and access details will be sent via email.
- Repository structure:
 - Folder **A1/code/** : *.c, *.h, Makefile
 - Folder **A1/data/** : Data.ods /.xlsx
 - Folder **A1/report/** : Report.pdf
 - Folder **A1/plots/** :
 - SU.jpeg & SU.vtk (input: tjunc.dat)
 - VAR.jpeg & VAR.vtk (input: tjunc.dat)
 - CGUP.jpeg & CGUP.vtk (input: tjunc.dat)

Thank You

and good luck with your first assignment!