Ural Federal University
named after the first President of Russia B.N.Yeltsin

Teaching Heart Modeling and Simulation on Parallel Computing Systems

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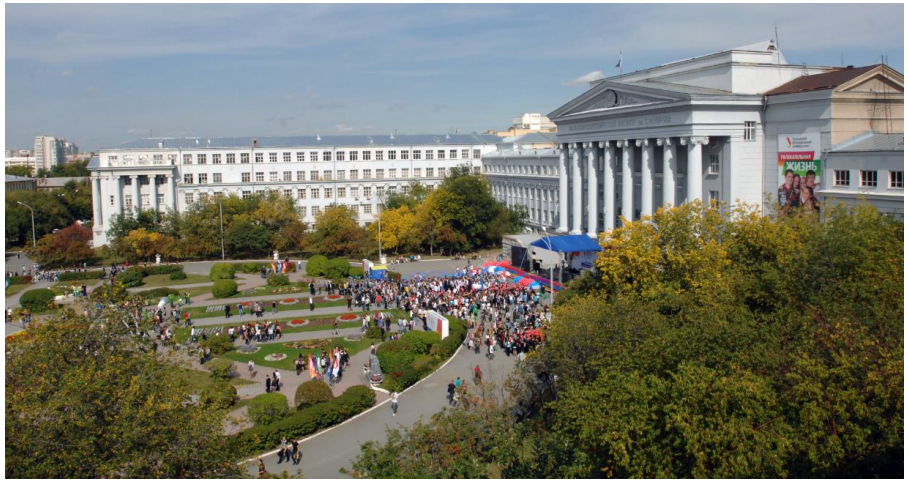
1st European Workshop on Parallel and Distributed Computing Education for Undergraduate Students (Euro-EDUPAR), Vienna, August 24, 2015

Ural Federal University



Ekaterinburg, Russia

One of the largest universities in Russia:

- 30 000 students from 60 countries
- 2000 faculty members
- 13 Institutes

IT and Computer Science Activities:

- 2014 ACM ICPC Global Programming Championship World Final
- Best Cisco Academy in Europe, 2013
- IT security Hackerdom team won the Nuit du Hack (Paris) CTF competition, 2012 and 2013

High Performance Computing Department

Jointly organized in 1997 by:

- Ural State University (now Ural Federal University)
- Institute of Mathematics and Mechanics UrB RAS

The department was created specifically to teach Parallel Computing

Computational resources:

- Supercomputer "URAN" of Institute of Mathematics and Mechanics UrB RAS, 240 TFLOPS, 370 GPU NVIDIA Tesla, 800 Intel Xeon CPU Cores
- Educational cluster of Ural Federal University, 24 TFlops, 12xIntel Xeon Phi, 12xGPU NVIDIA Tesla, 144 CPU Cores

HPC Courses

Parallel and distributed computing:

- Introductory course
- Architecture of parallel computing systems
- Multithreading programming
- Vectorization (SIMD)
- OpenMP
- MPI
- MapReduce

Advanced courses:

- GPU Programming
- Xeon Phi Programming

Target audience:

- Master students in Computer Science

The problem

Students think that parallel programming is easy!

One OpenMP directive:

- #pragma omp parallel for
- Similar OpenACC directive for GPU

Six MPI functions:

- MPI_Init, MPI_Finalize, MPI_Comm_size, MPI_Comm_rank, MPI_Send, MPI_Recv (or MPI_Bcast, MPI_Reduce)

By the end of the traditional HPC courses students:

- Know the basic parallel computing technologies
- Able to solve simple problems using HPC
- Not able to tackle real-world scientific problems

Programming technology progress

Serial Code

Single CPU Core Performance: ***1x***

```
.
.
.
.
for(int j=1;j<ny-1;j++) {
 for(int k=i1;k<nz-1;k++) {
  for(int i=1;i<nx-1;i++) {
   Anext[Index3D (nx,ny,i,j,k)] =
    (A0[Index3D (nx,ny,i,j,k+1)] +
       A0[Index3D (nx,ny,i,j,k-1)] +
       A0[Index3D (nx,ny,i,j+1,k)] +
       A0[Index3D (nx,ny,i,j-1,k)] +
       A0[Index3D (nx,ny,i+1,j,k)] +
       A0[Index3D (nx,ny,i-1,j,k)])*c1
       -A0[Index3D (nx,ny,i,j,k)]*c0;
   }
  }
}
```

Parallel Code for GPU

Add One OpenACC Directive
Tesla K40 Perf: ***13.6x***

```
.
.
.
#pragma acc parallel loop collapse(3)
for(int j=1;j<ny-1;j++) {
 for(int k=i1;k<nz-1;k++) {
  for(int i=1;i<nx-1;i++) {
   Anext[Index3D (nx,ny,i,j,k)] =
    (A0[Index3D (nx,ny,i,j,k+1)] +
       A0[Index3D (nx,ny,i,j,k-1)] +
       A0[Index3D (nx,ny,i,j+1,k)] +
       A0[Index3D (nx,ny,i,j-1,k)] +
       A0[Index3D (nx,ny,i+1,j,k)] +
       A0[Index3D (nx,ny,i-1,j,k)])*c1
       -A0[Index3D (nx,ny,i,j,k)]*c0;
   }
  }
}
```

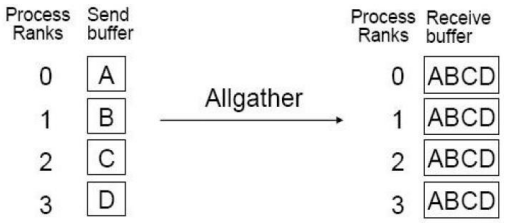
Dual socket E5-2698 v3 @2.3GHz (Haswell), 16 cores per socket, 256 GB memory, 1x Tesla K40
Benchmark: Parboil Stencil from University of Illinois with 1000 iterations
Source code for Parboil: http://impact.crhc.illinois.edu/Parboil/parboil.aspx

https://developer.nvidia.com/openacc

The problem

Introductory course exercises:

- Computing PI, Monte-Carlo Simulation, Matrix Multiplication, Mandelbrot Set, Conwey's Game of Life, k-Means Clustering, Canny Edge Detection, Jacoby Simulation
- Could be solved using simple techniques
- Short simulation time (seconds, minutes, seldom hours)



Real-world application requires much more:

- Advanced MPI: non-blocking point-to-point communication, advanced collective communication, overlapping computation with sending/receiving data, virtual topologies
- Hybrid parallelization: MPI+OpenMP+SIMD (+GPU, +Xeon Phi, +FPGA)
- Optimal domain decomposition: 1D, 2D, 3D, etc.
- Data locality optimizations

First solution: advanced exercises

Include advanced exercises into the introductory courses:

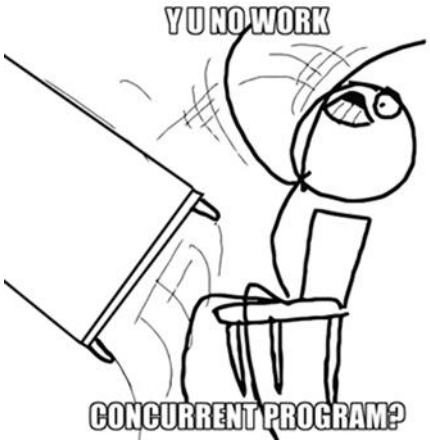
- Optional
- Mandatary

Negative results:

- Almost no one chose the optional advanced exercises
- Almost everyone failed the mandatary advanced exercises

Reasons of failure:

- Technical difficulties: advanced exercises requires much more studying and practicing than the basic ones
- Lack of students' motivation
- Lack of math or domain area knowledge



Second solution: real-world tasks

Give the students big real-world scientific tasks to solve

High motivation

- Students solve real problems instead of boring exercises
- Parallel programing is studied not for its own sake, but as a useful tool for research

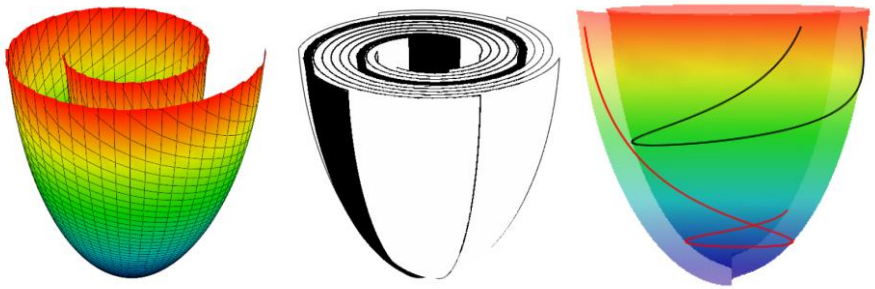
Teach parallel computing together with domain science:

- Introductory course on parallel computing
- Theoretical course on domain science
- Advanced course on using parallel computing in the domain science
- Big projects in domain science (real-world problems)

Heart modeling

Cooperation with the laboratory "Modeling of living systems on supercomputers"

- The laboratory develops various heart models on different levels (cell – tissue - organ)
- Distinguished feature: anatomical models of heart left ventricle (LV) with an analytic description of its shape and fibre orientation
- Simulation of 1 heart bit (1 second of physical time) requires 3 day on personal computer



Existing theoretical course:

- Simulation of Living Systems
- Olga E. Solovyova, Head of the laboratory

Proposed course:

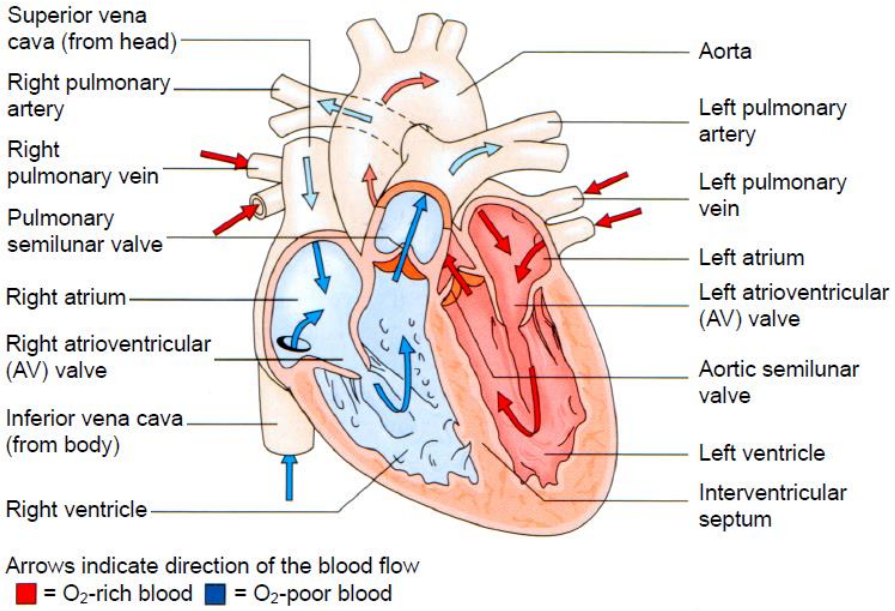
- Modeling Heart Dynamics on Parallel Computing Systems

Heart modeling on PCS course

Simulation of electromechanical function of the mammal heart LV on parallel computing systems

Lecture topics:

- Structure and physiology of the mammal heart
- Various methods and models of heart LV digital representation
- Numerical methods: mass-spring system, finite element method (FEM)
- Simulation of the heart LV electrodiusion
- Simulation of heart LV mechanical contraction

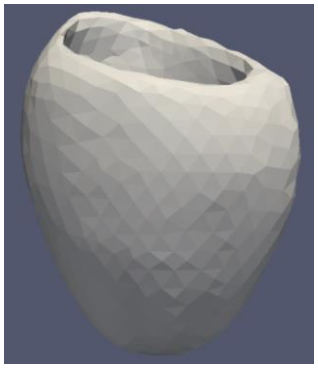


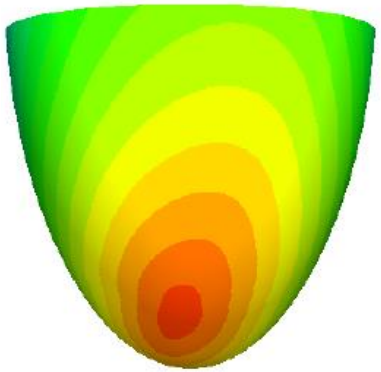
L. Sherwood, Human physiology : from cells to systems. Australia ; United Kingdom: Thomson Brooks/Cole, 2004.

Heart modeling on PCS course

Workshop topics:

- Building the model of LV using the tetrahedral 3D-network with the help of “GMsh” library
- Studying the FEM implementation for MPI clusters from the “FEniCS” library
- Optimization of the FEM application on parallel computing systems
- Simulation of the muscle cube on MPI cluster using the “FEniCS” library
- Visualization of simulation results using Paraview

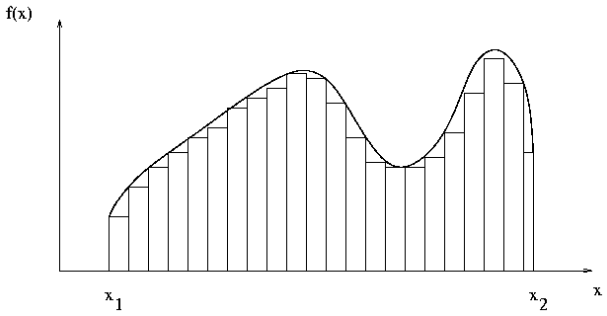




Parallel Numerical Methods Course

Compute-intensive tasks:

- Linear algebra
- Numerical integration and differentiation
- Numerical solving of mathematical physics equations
- Finite element method



Data-intensive tasks:

- Processing of large graphs

Techniques of effective parallelization:

- Efficient cache usage
- Data partitioning among the processes
- Reducing the inter-process communication

Parallel Numerical Methods Course

Course mission:

- Teach students how to choose algorithmic building blocks for scalable parallel application
- Explain to students how to avoid performance degradation of parallel programs

Home programming assignments requirements:

- Implement several version of parallel algorithms
- Carry out research on their performants and scalability
- Choose the most efficient algorithm and implementation

Positive outcome:

- Students started to learn advanced parallel computing techniques to create efficient implementation for home programming assignments

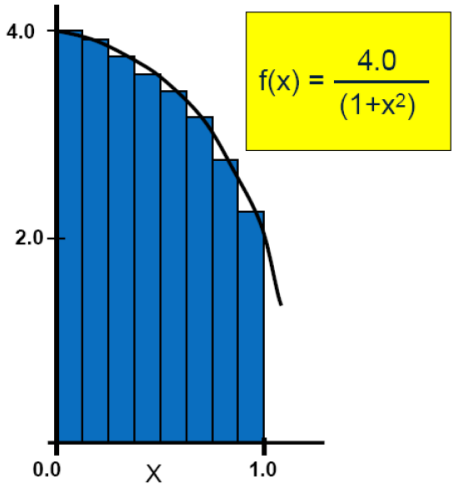
Parallel Numerical Methods Course

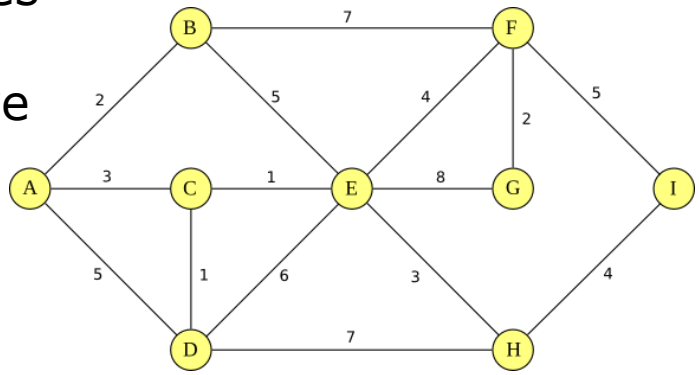
First programming assignment:

- Numerical integration
- Point-to-point communications (MPI_Send, MPI_Recv)

Advanced programming assignment:

- Single source shortest paths (SSSP) graph problem
- Point-to-point communications provides small speedup
- Students investigates various collective communications
- Efficient solution requires usage of MPI_Allgather (despite the big overhead of the function)



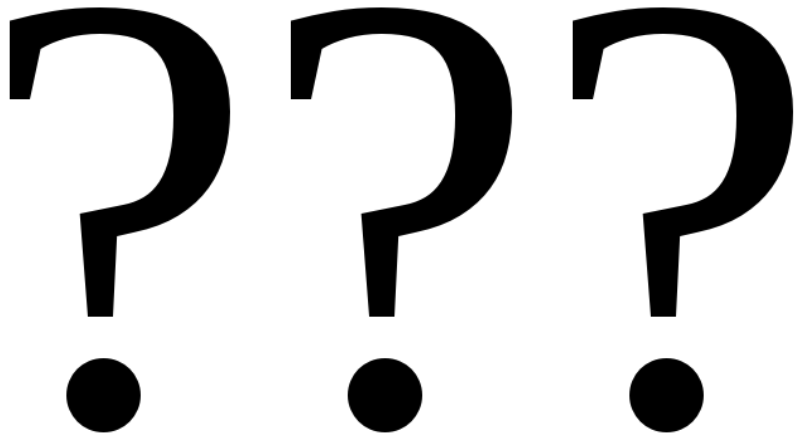


Modules of the course track

Three modules:

- Parallel and distributed computing
- Parallel numerical methods
- Heart modeling

Will the students be able to solve real-world scientific problems on parallel computer systems?



More time with teachers!

Three modules:

- Parallel and distributed computing
- Parallel numerical methods
- Heart modeling

Will the students be able to solve real-world scientific problems on parallel computer systems?

No!

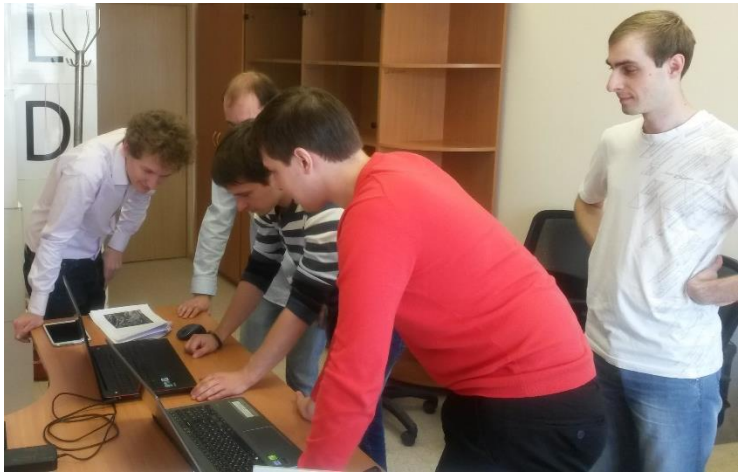
For complex projects students need much more assistance from the teachers than for introductory exercises:

- Complex projects require a broad knowledge of various parallel programming technologies
- Few information in the Internet about solving complex tasks on the parallel computing systems

Science Hackathon

Course aim:

- Provide the students with opportunity to work together with the tutor for a long time



Course format:

- Conducted on Saturdays
- Lasts all the day
- Group of students works on one project together with a tutor to produce usable software
- Students choose the topic of the projects

Examples of projects:

- Using auto-vectorization for Xeon Phi
- Evaluating Intel VML performance on Xeon Phi
- "FEniCS" library
- Simulating the heart muscle cube using FEM and mass-spring methods

Science Hackathon

Benefits for students:

- Tutor quickly corrects mistakes in the students code
- Tutor suggests the performance optimization techniques suitable for the projects
- Tutor provides quick feedback on the projects and further guidance

Positive outcome:

- Significant speedup of students' projects

Additional positive outcome for students:

- Team software development
- Problem solving skills
- Professional confidence
- Leadership (some students work as tutors with other students)

Heart modeling course track

No	Course name	Credits
1	***Parallel and distributed computing module***	
1.1	Parallel and distributed computing	4
1.2	GPU programming	2
1.3	Xeon Phi programming	2
2	***Numerical methods module***	
2.1	Parallel numerical methods	2
2.2	Science hackathon	4
3	***Heart modeling module***	
3.1	Simulation of living systems	4
3.2	Modeling heart dynamics on parallel computing systems	2

Heart modeling course track

Target audience

- Master students in Computer Science
- Bachelor Computer Science students and Master students in other majors are also eligible

Every course in the track is elective

- Students are not required to take all the courses
- Each student can choose courses according to his/he individual needs

Typical enrollment

- 10-15 students

Recommended sequence of study

Semester	Course name
1	Parallel and distributed computing Simulation of living systems
2	GPU programming Parallel numerical methods Modeling heart dynamics on parallel computing systems
3	Xeon Phi programming Science Hackathon

Positive results

Key success points

- Interesting real-world scientific tasks to solve
- The tasks simulation on personal computers takes long time
- Knowledge in the three area: parallel computing, numerical methods, and domain science
- Coherent courses programs
- Large amount of time with teachers/tutors

The reason of success

- High students' motivation
- Long simulation time force students to learn advanced parallel computing techniques in order to decrease it
- Students work in groups and share their knowledge
- Teachers/tutors provide quick feedback and project guidance

Student's success story

Second year Computer Science Master student

Project topics

- Building the analytical model of LV shape using the ultrasonic data (personalized model)
- Electrophysiological simulation of LV with the personalized analytical model

Student's achievements

- Ultrasonic data was imported into the LV simulation software
- Performance of the LV electrophysiological simulation software was improved
- Work with other students during Science hackathon

Student obtained research position at the laboratory "Modeling of living systems on supercomputers"

Future works

English version of the track courses

Short-term English-language internship program (1-3 months)

- Parallel computing internship program is already exists http://iie.urfu.ru/en/article/student-internships
- Include heart modeling courses into the internship program

MOOC “Modeling heart dynamics on parallel computing systems” on EdX.org

- Ural Federal University is the first Russian university that signed an agreement with EdX.org

Interdisciplinary courses in different domain areas:

- Molecular dynamics simulation
- Astronomy

Thank you!

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Non Computer Science Students

Master students with non Computer Science Bachelor Degree are highly welcomed

- Physics, mathematics, biology
- Have broad domain knowledge
- Lack of the software development skills

Additional courses

- Scientific computing in C
- Software performance optimization

Best group of students for successful project

- One or two students with Computer Science Bachelor Degree
- One student with Domain Science Bachelor Degree