Numerical Solution of PDEs Using the Finite Element Method

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Goals

- How to use deal.II for Finite Element computations
- Refresh numerical PDE knowledge
- Also:
  - Software best practices
  - C++, Debugging, IDEs, Visualization
  - Parallel computations with MPI

Schedule

	Monday	Tuesday	Wednesday	Thursday	Friday
09:30-10:45	Intro	Dimension independence			
11:15-12:30	First Steps				
					END
14:00-15:15	Seminar (14:30)		Hands-on		
15:45-17:00	Hands-on		Seminar (16:00)		

- Today:
  - What is deal.II?
  - Compiling, using an IDE
  - Overview about FEM
  - Basic tutorials (create mesh, solve Poisson's equation, visualization)
- Tuesday:
  - Finite Element Analysis (refinement, computing errors)
- Wednesday/Thursday/Friday:
  - Advanced topics
  - Time for projects

The plan

- Slides, some lectures on blackboard
- Many live demonstrations
- Exercises:
  - Work in groups of two!
  - Ask questions!
- Projects:
  - Required for MHPC students
  - Groups of two

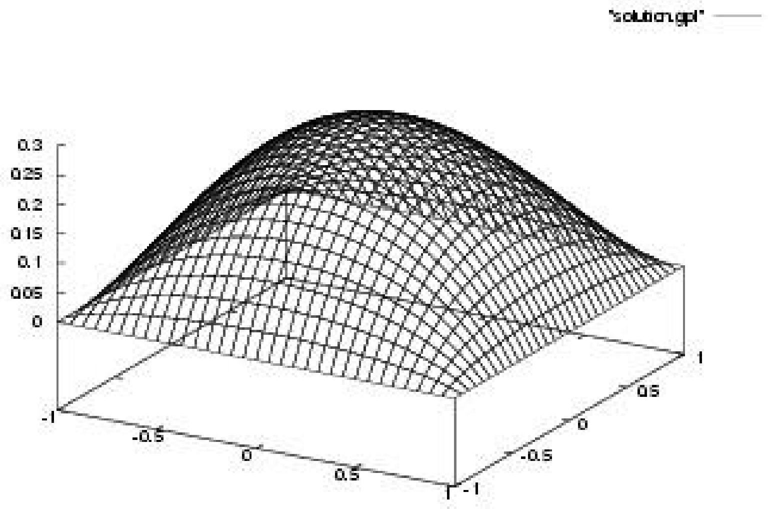
Resources

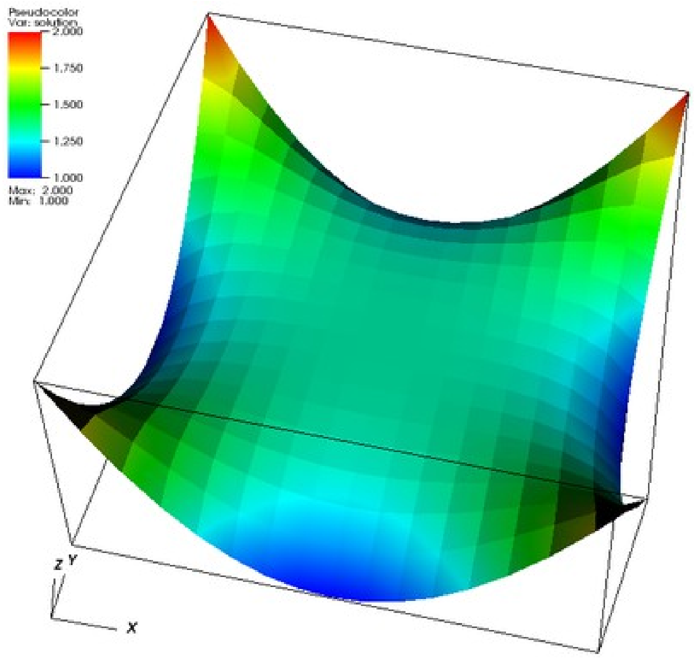
- http://indico.ictp.it/event/7751/overview
  - Schedule, Rooms, etc.
- http://dealii.org
  - Manual
  - Tutorial steps
  - Tutorial videos
- On your machine: folder /scratch/smr1909/
  - Slides
  - Example programs
  - Exercises
  - Other files

Finite Element Method

- Solve partial differential equations numerically
- Example:

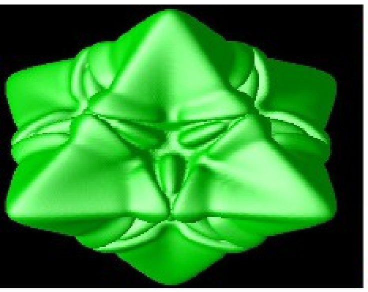
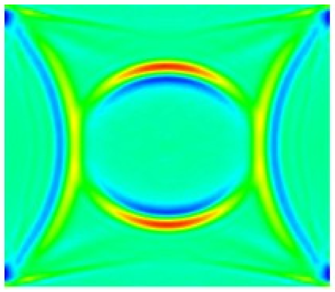
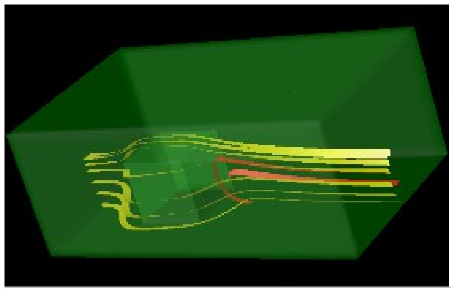
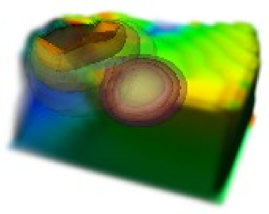
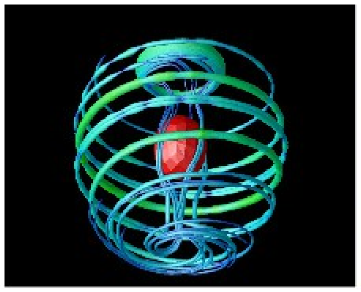
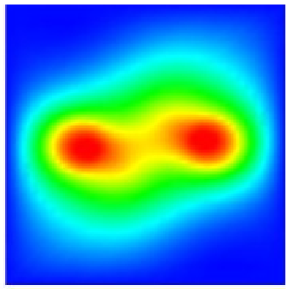
$$\begin{aligned} -\Delta u &= f && \text{in } \Omega, \\ u &= 0 && \text{on } \partial\Omega. \end{aligned}$$





deal.II

- “A Finite Element **D**ifferential **E**quations **A**nalysis **L**ibrary”
- Open source, c++ library
- I am one of the four maintainers
- One of the most widely used libraries:
  - 900+ papers using and citing deal.II
  - ~600 downloads/month
  - 100+ people have contributed in the past 15 years
  - ~500,000 lines of code
  - 10,000+ pages of documentation
- Website: www.dealii.org

Features

- 1d, 2d, 3d computations, adaptive mesh refinement (on quads/hexes only)
- Finite element types:
  - Continuous and DG Lagrangian elements
  - Higher order elements, hp adaptivity
  - Raviart-Thomas, Nedelec, …
  - And arbitrary combinations
- PDEs on surfaces embedded in higher dimensions

Features, part II

- Linear Algebra
  - Own sparse and dense library
  - Interfaces to PETSc, Trilinos, UMFPACK, BLAS, ..
- Parallelization
  - Laptop to supercomputers
  - Multi-threading on multi-core machines
  - MPI: 64,000+ processors
- Output in many visualization file formats

Development of deal.II

- Professional-level development style
- Development in the open, repository on github.com
- Mailing lists for users and developers
- Test suite with 8,700+ tests after every change
- Platform support:
  - Linux/Unix
  - Mac
  - Windows
- Hope to see you on github.com or the mailing list!

Lab Setup

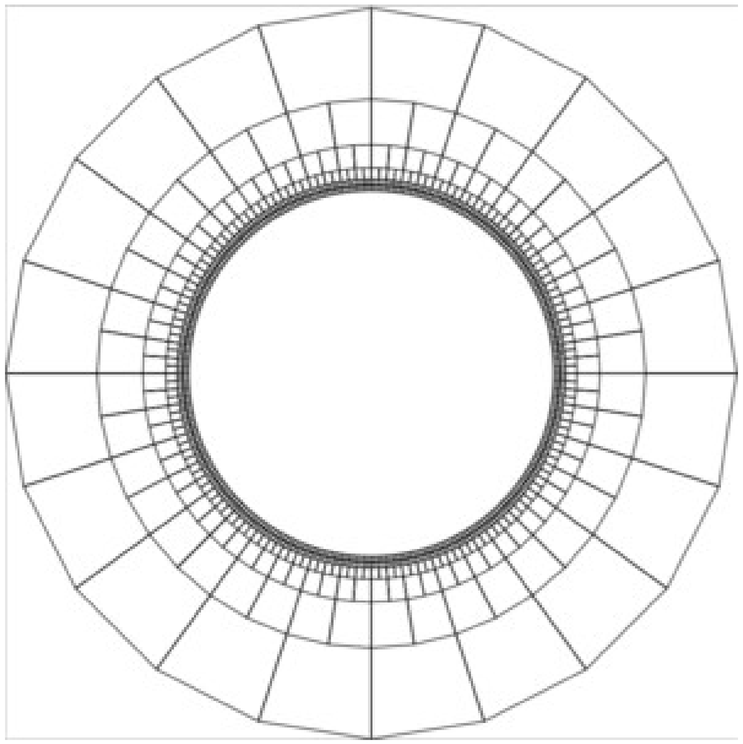
- deal.II and all required dependencies are already installed at

  /scratch/smr2909/

- (Demo, show lab01.pdf and run included step 1)

Lab 1 (step-1)

- See lab01.pdf
- Topic: creating meshes



Running examples

- In short:

```
cd examples/step-1
cmake .
make run
```

- cmake:
  - Detect configuration, only needs to be run once!
  - Input: CMakeLists.txt
  - Output: Makefile, (other files like CMakeCache.txt)
- make:
  - Code compilation
  - Tool to execute commands in Makefile, do every time you change your code
  - Input: step-1.cc, Makefile
  - Output: step-1   (the binary executable file)

- Run your program with

```
./step-1
```

- Or (compile and run):

```
make run
```

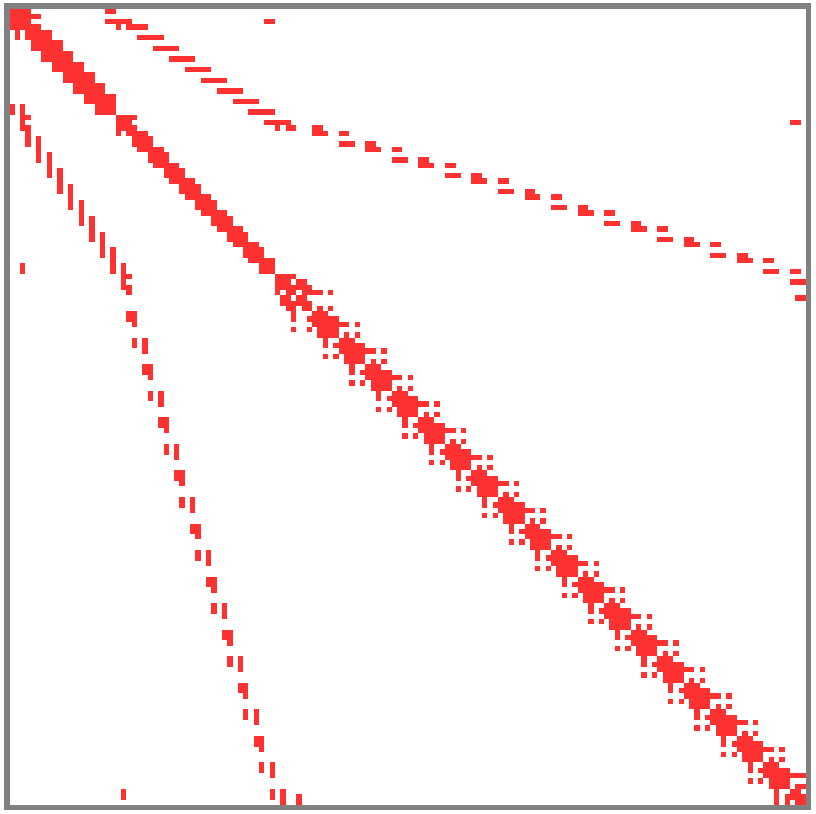
- Open in qtcreator IDE:

```
qtcreator .
```

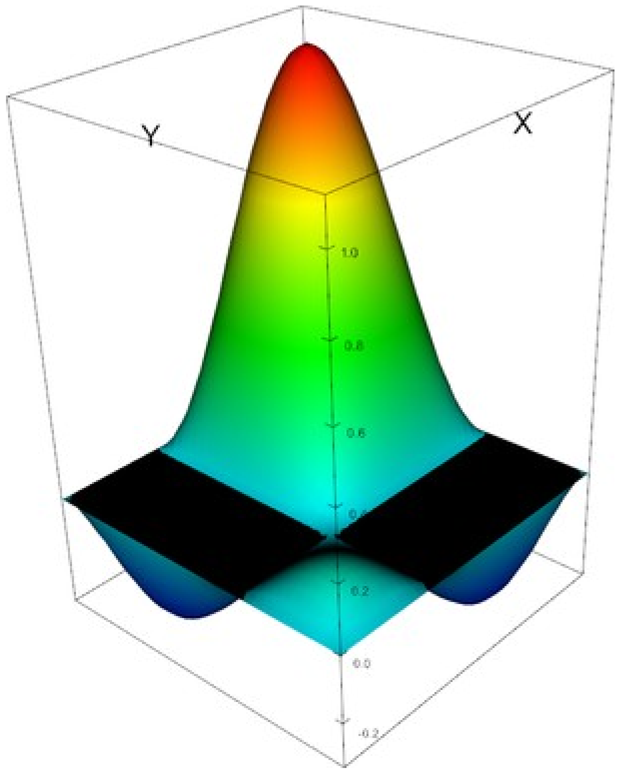
- Learn to use an IDE! (not vim, emacs, …)
- Copy into home directory required!
- [Demo the above and open project in qtcreator]

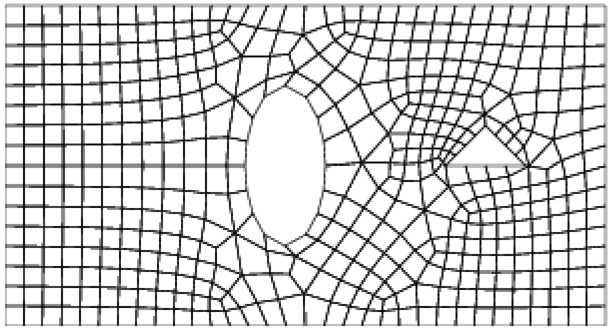
Lab 2 (step-2)

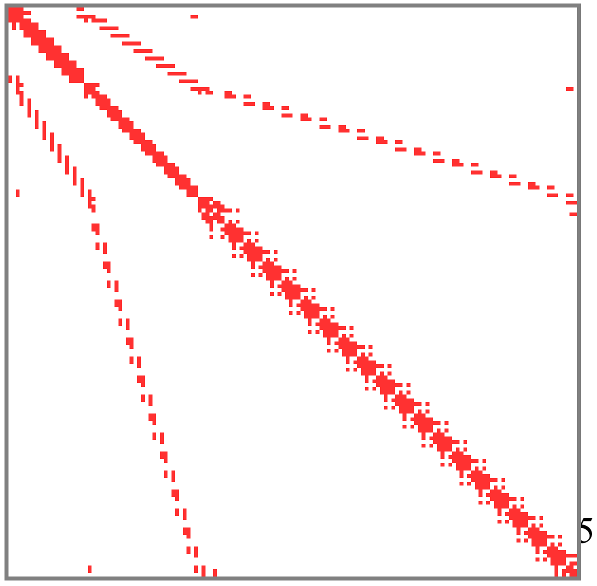
- See lab02.pdf
- Topic: sparsity patterns of matrices



Finite Element Assembly







$$A_{ij} = (\nabla\phi_i, \nabla\phi_j)$$

$$A_{ij} \approx \sum_K \sum_q J_K^{-1}(x_q)\nabla\phi_i(x_q) \cdot J_K^{-1}(x_q)\nabla\phi_j(x_q) \cdot |detJ(x_q)|w_q$$

in pseudo-code:

```
for i=0,...,N-1:
 for j=0,...,N-1:
  for all K:
    A_ij += \sum_q grad_phi(i,q) grad_phi(j,q) JxW(q)
```

But most of these contribution are zero. So we switch the order of the loops to get

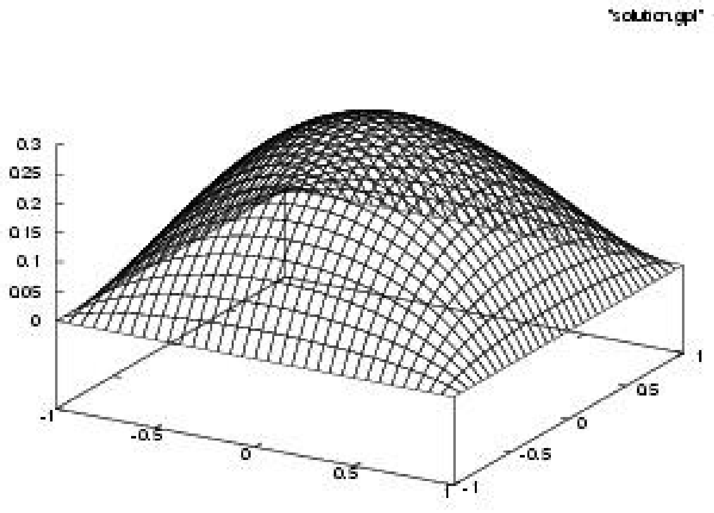
```
for all K:
 for i = 0,...,N-1:
  for j = 0,...,N-1:
    A_ij += \sum_q grad_phi(i,q) grad_phi(j,q) JxW(q)
```

which I can simplify to only look at non-zero basis functions:

```
for all K:
 a = 0
 for alpha = 0,...,n_local_dofs:
  for beta = 0,...,n_local_dofs:
   for q:
    a_{alpha,beta} += grad_phi(alpha,q) grad_phi(beta,q) JxW(q)
 A_ij += a
```

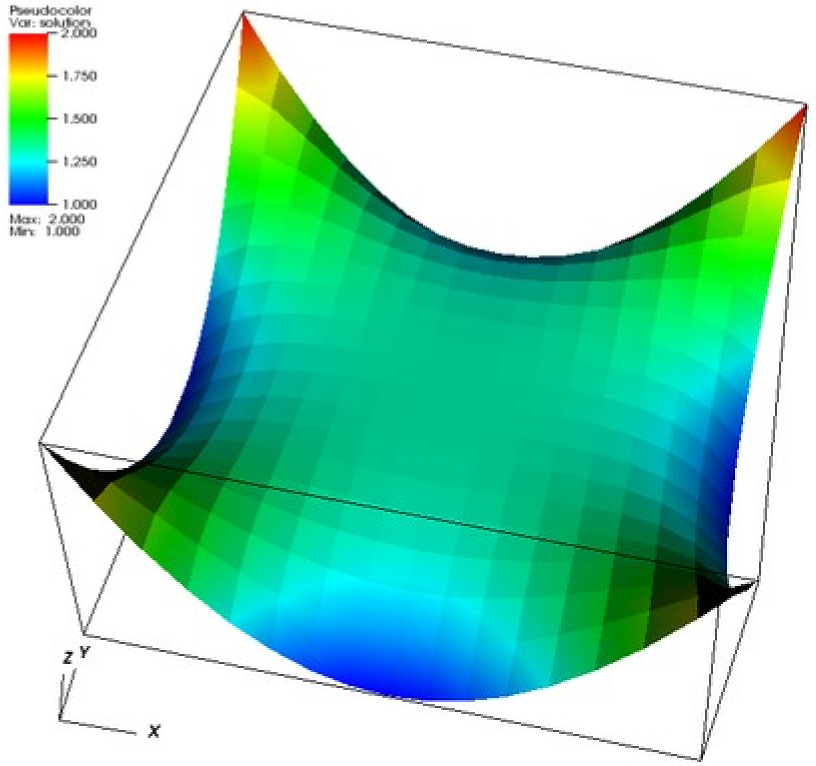
Lab 3 (step-3)

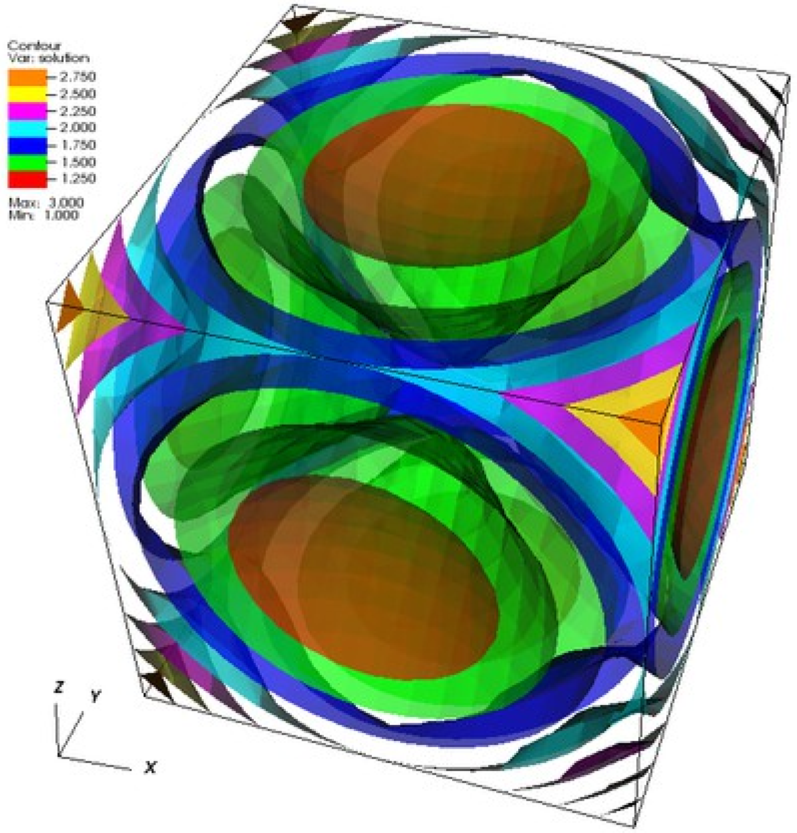
- See lab03.pdf
- Topic: solving Poisson's equation



Towards Lab 4 (step-4)

- Goals:
  - Dimension independent programming
  - Need: C++ templates





Templates in C++

- "blueprints" to generate functions and/or classes
- Template arguments are either numbers or types
- No performance penalty!
- Very powerful feature of C++: difficult syntax, ugly error messages, slow compilation
- More info: http://www.cplusplus.com/doc/tutorial/templates/

  http://www.math.tamu.edu/~bangerth/videos.676.12.html
- Demos in /scratch/smr2909/lab-04/

Why used in deal.II?

- Write your program once and run in 1d, 2d, 3d:

```
DoFHandler<dim>::active_cell_iterator
    cell = dof_handler.begin_active(),
    endc = dof_handler.end();

for (; cell!=endc; ++cell)
 { ...

  cell_matrix(i,j) += fe_values.shape_grad (i, q_point)
                    * fe_values.shape_grad (j, q_point)
                    * fe_values.JxW (q_point));
```

- cell->face () is a quad in 3d but a line in 2d
- Also: large parts of the library independent of dimension:
  - hyper_cube (square vs box), etc.

Class Templates for Functions

- Blueprint for a function
- One type called "number"
- You can use "typename" or "class"

```
template <typename number>
number square (const number x)
{ return x*x; };

int x = 3;
int y = square<int>(x);
```

- Sometimes you need to state which function you want to call:

```
template <typename T>
void yell ()
 { T test;
test.shout("HI!"); };

// cat is a class that has
shout()
yell<cat>();
```

Value Templates

- Template arguments can also be values (like int) instead of types:

```
template <int dim>
void make_grid (Triangulation<dim>
&triangulation) { …}

Triangulation<2> tria;
make_grid<2>(tria);
```

- Of course this would have worked here too:

```
template <typename T>
void make_grid (T &triangulation)
{ …// now we can not access “dim” though
```

Class templates

- Whole classes instead of functions built from a blueprint
- Same idea:

```
template <int dim>
class Point
{
  double elements[dim];
  // ...
}

Point<2> a_point;
Point<5> different_point;
```

```
namespace std
{
  template <typename
number>
  class vector;
}

std::vector<int>
list_of_ints;
std::vector<cat> cats;
```

Example

```
template <unsigned int N>
double norm (const Point<N> &p)
{
 double tmp = 0;
 for (unsigned int i=0; i<N; ++i)
   tmp += square(v.elements[i]);
 return sqrt(tmp);
}
```

- Value of N known at compile time, never stored!
- Compiler can optimize (unroll loop)
- Fixed size arrays faster than dynamic (dealii::Point<dim> vs dealii::Vector<double>)

Examples in deal.II

- Step-4:

```
template <int dim>
void make_grid (Triangulation<dim> &triangulation) {...}
```

- So that we can use Vector<double> and Vector<float>:

```
template<typename number>
class Vector< number > { number [] elements; ...};
```

- Default values (embed dim-dimensional object in spacedim):

```
template<int dim, int spacedim=dim>
class Triangulation< dim, spacedim > { ... };
```

- Already familiar:

```
template<int dim, int spacedim>
void GridGenerator::hyper_cube  (Triangulation< dim, spacedim
> &  tria, const double left, const double right) {...}
```

Explicit Specialization

- different blueprint for a specific type T or value

```
// store some information
// about a Triangulation:

template <int dim>
struct NumberCache
{};

template <>
struct NumberCache<1>
{
  unsigned int n_levels;
  unsigned int n_lines;
};
```

```
template <>
struct NumberCache<2>
{
  unsigned int n_levels;
  unsigned int n_lines;
   unsigned int n_quads;
}

// more clever:
template <>
struct NumberCache<2>:
public NumberCache<1>
{
      unsigned int
n_quads;
}
```

Lab 4 (step-4)

- Dimension independent Laplace problem
- Triangulation<2>, DoFHandler<2>, ...

  replaced by

  Triangulation<dim>, DoFHandler<dim>, …
- Template class:

```
template <int dim>
class Step4 { … };
```

Lab 5

- Modified step-4 to check correctness
- Using the method of manufactured solutions
- Computing L2 and H1 errors and check order

Computing Errors

- Important for verification!
- See step-7 for an example
- Set up problem with analytical solution and implement it as a Function<dim>
- Quantities or interest:

$$e = u - u_h$$

$$\|e\|_0 = \|e\|_{L_2} = \left(\sum_K \|e\|_{0,K}^2 \right)^{1/2} \qquad \|e\|_{0,K} = \left(\int_K |e|^2 \right)^{1/2}$$

$$|e|_1 = |e|_{H^1} = \|\nabla e\|_0 = \left(\sum_K \|\nabla e\|_{0,K}^2 \right)^{1/2}$$

$$\|e\|_1 = \|e\|_{H^1} = \left(|e|_1^2 + \|e\|_0^2 \right)^{1/2} = \left(\sum_K \|e\|_{1,K}^2 \right)^{1/2}$$

- Break it down as one operation per cell and the “summation” (local and global error)
- Need quadrature to compute integrals

Computing Errors

- Example:

```
Vector<float> difference_per_cell (triangulation.n_active_cells());
VectorTools::integrate_difference (dof_handler,
                                   solution, // solution vector
                                   Solution<dim>(), // reference solution
                                   difference_per_cell,
                                   QGauss<dim>(3), // quadrature
                                   VectorTools::L2_norm); // local norm
const double L2_error = difference_per_cell.l2_norm(); // global norm
```

- Local norms:

  `mean, L1_norm, L2_norm,Linfty_norm, H1_seminorm, H1_norm, ...`

- Global norms are vector norms: `l1_norm(), l2_norm(), linfty_norm(), ...`

Lab 6

- Higher order mappings, see step-10/step-11
- Start with lab-6. Find a solution so that higher order mapping gives correct convergence order!

More features of deal.II

- Adaptive mesh refinement, including dual-weighted error estimators (step-6, step-7)
- Linear solvers: direct solvers, iterative solvers, preconditioners, multigrid, etc.
- Parallel computing: multithreading (step-9), MPI (step-40)
- Vector-valued problems: step-8, step-20, …
- Other FE spaces: DG, RT, Nedelec, ...
-

More features of deal.II b)

- Non-homogeneous Neumann conditions, boundary integrals: step-7
- Systems of PDEs: step-8, step-20
- Nonlinear problems: step-15
- Time dependent problems: step-18, ...
- Fluid flow (Stokes, Navier-Stokes, …): step-22, step-32, ...
- Complicated meshes: step-49
- Matrix-free computations: step-37, step-48

Resources

- Tutorials (by topic, graph, etc.): https://www.dealii.org/developer/doxygen/deal.II/Tutorial.html
- Video lectures:

  http://www.math.tamu.edu/~bangerth/videos.html
- Manual: https://www.dealii.org/developer/doxygen/deal.II/index.html
- Mailing list: https://groups.google.com/forum/#!forum/dealii
-

Fixing lab 6

- Yesterday we saw optimal 3rd order convergence of the L2 norm on the circle even with a linear mapping
- It turns out we applied the correct boundary conditions for Omega_h and only computed the error on Omega_h. In essence, we were solving on a piece-wise linear Omega on each refinement level.
- Take a look at lab06.pdf...

Lab 7

- Based on step-38 (Laplace-Beltrami)
- Compute L2 and H1 errors for a half-sphere

Lab 8 & 9

- See maple spreadsheets for references
- Lab-8:
  - Start with lab-7 code and solve on torus
- Lab-9:
  - Start with lab-9 and solve on parametric surface

Adaptive Mesh Refinement

- Typical loop:
  - Solve
  - Estimate
  - Mark
  - Refine/coarsen
- Estimate is problem dependent:
  - Approximate gradient jumps: `KellyErrorEstimator` class
  - Approximate local norm of gradient: `DerivativeApproximation` class
  - Or something else
- Mark:

  `GridRefinement::refine_and_coarsen_fixed_number(...)` or
  `GridRefinement::refine_and_coarsen_fixed_fraction(...)`
- Refine/coarsen:
  - `triangulation.execute_coarsening_and_refinement ()`
  - Transferring the solution: `SolutionTransfer` class (maybe discussed later)

Constraints

- Used for hanging nodes (and other things!)
- Have the form:

$$x_i = \sum_j \alpha_{ij} x_j + c_j$$

- Represented by class ConstraintMatrix
- Created using `DoFTools::make_hanging_node_constraints()`
- Will also use for boundary values from now on:

```
VectorTools::interpolate_boundary_values(...,
constraints);
```

- Need different SparsityPattern (see step-6):

```
DoFTools::make_sparsity_pattern (...,
constraints, ...)
```

Constraints II

- Old approach (explained in video):
  - Assemble global matrix
  - Then eliminate rows/columns: `ConstraintMatrix::condense(...)`

    (similar to `MatrixTools::apply_boundary_values()` in step-3)
  - Solve and then set all constraint values correctly: `ConstraintMatrix::distribute(...)`
- New approach (step-6):
  - Assemble local matrix as normal
  - Eliminate while transferring to global matrix:

```
constraints.distribute_local_to_global (cell_matrix, cell_rhs,
                                         local_dof_indices,
                                         system_matrix,
system_rhs);
```

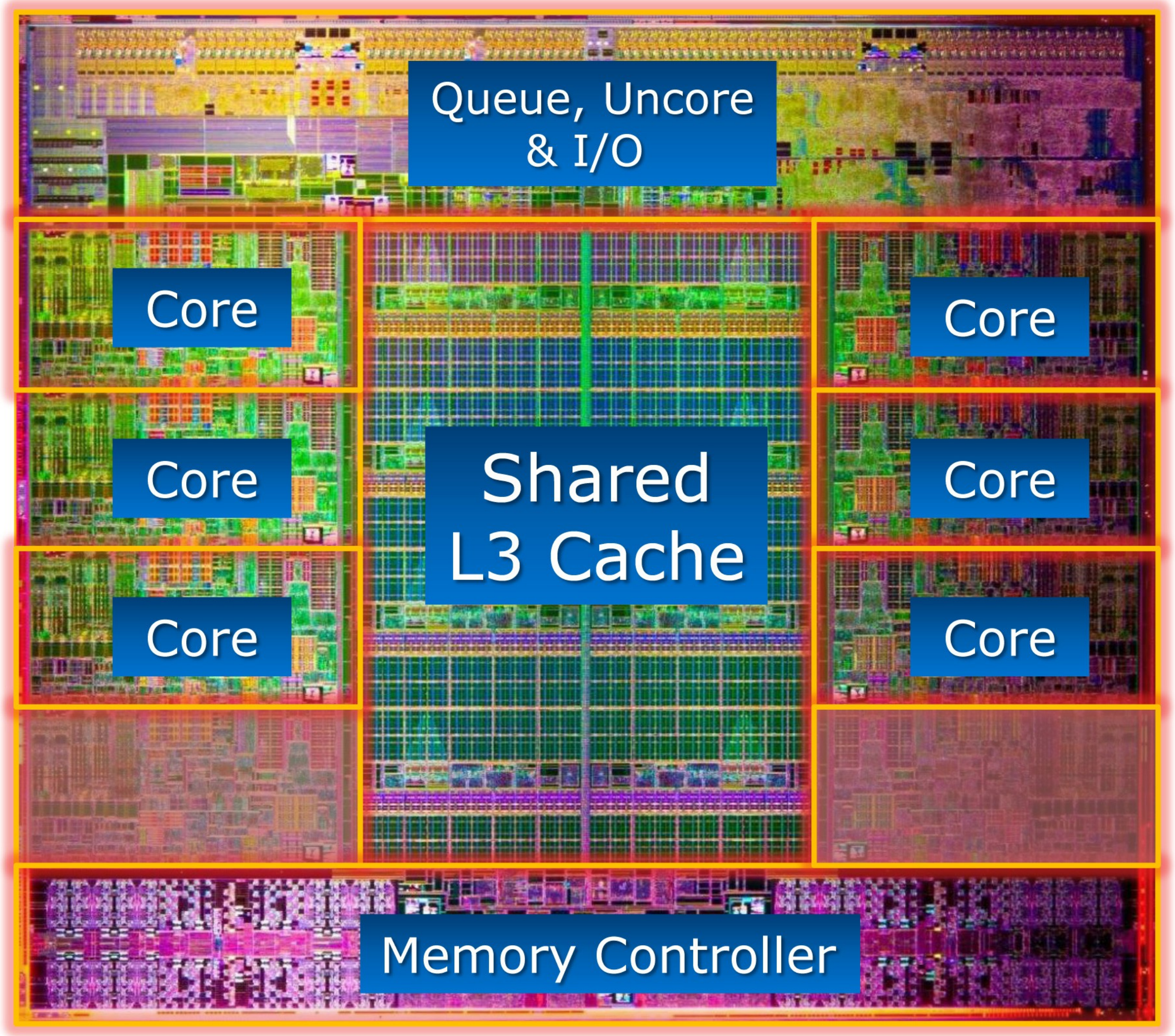
  - Solve and then set all constraint values correctly: `ConstraintMatrix::distribute(...)`

Vector Valued Problems

- (video 19&20)
- FESystem: list of FEs (can be nested!)
- Will give one FE with N shape functions
- Use FEValuesExtractors to do `fe_values[velocities].divergence (i, q), ...`
- Ordering of DoFs in system matrix is independent
- See module “handling vector valued problems”
- Non-primitive elements (see fe.is_primitive()):

  shape functions have more than one non-zero component, example: RT

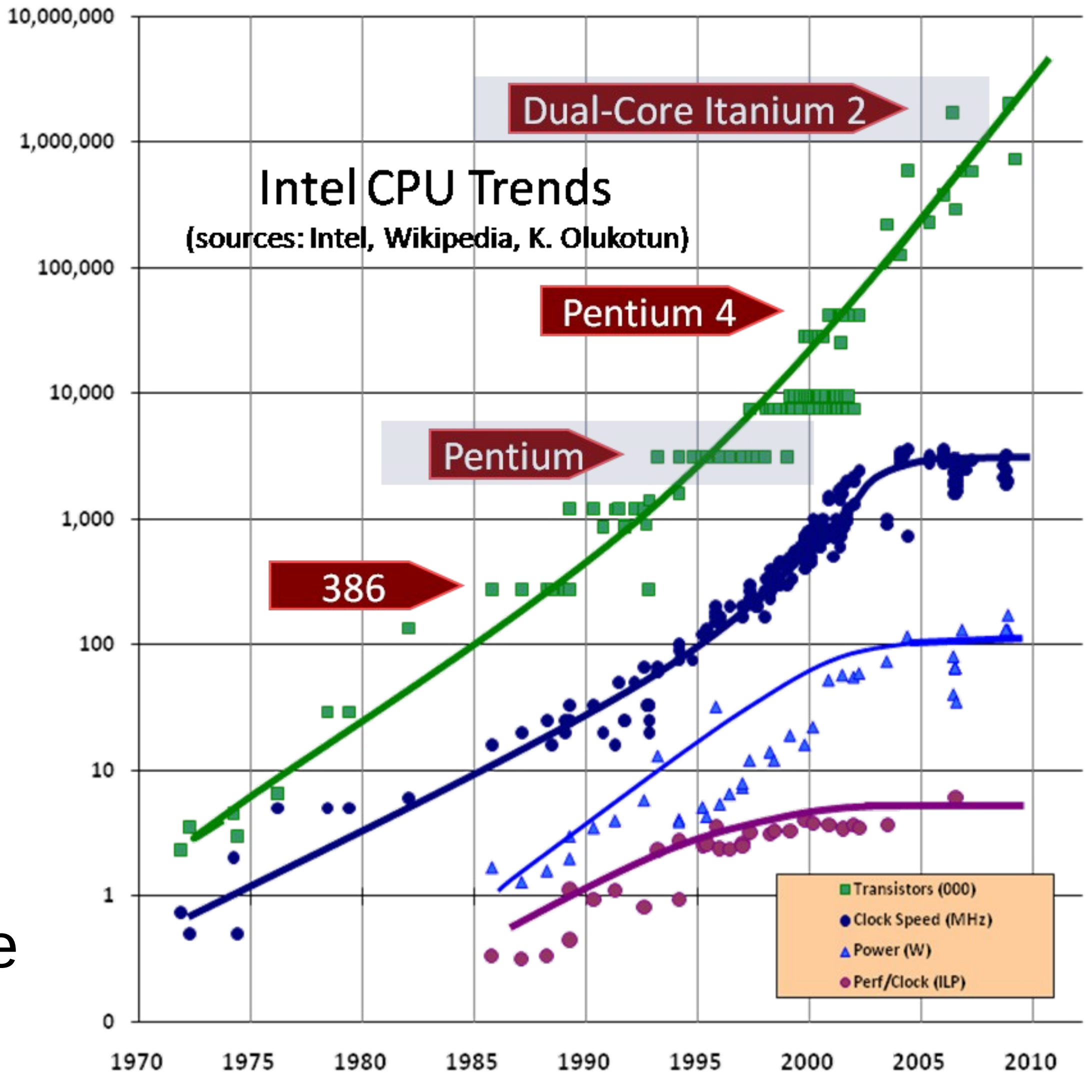
Parallel Computing: Introduction



A modern CPU: Intel Core i7

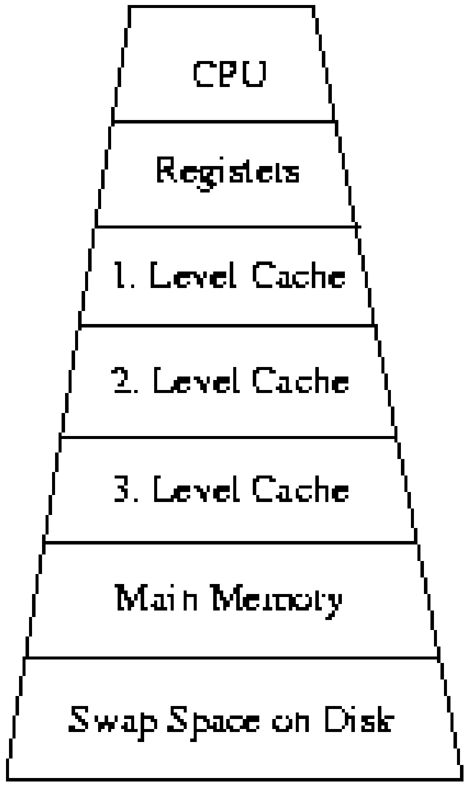
Basics

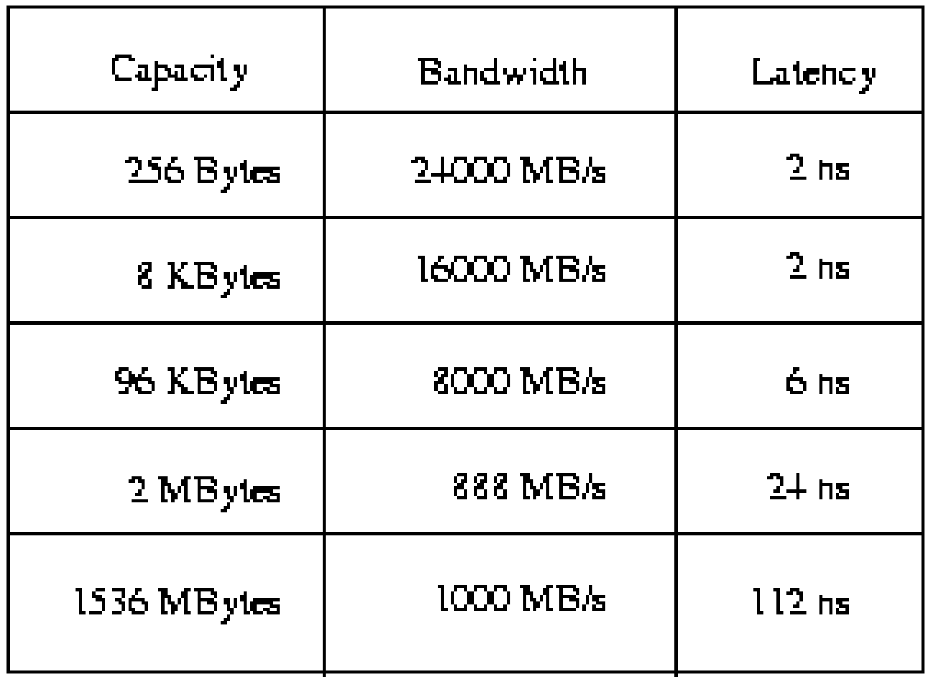
- Single cores are not getting (much) faster
- “the free lunch is over”: http://www.gotw.ca/publications/concurrency-ddj.htm
- Concurrency is only option:
  - SIMD/vector instructions
  - Several cores
  - Several chips in one node
  - Combine nodes into supercomputer



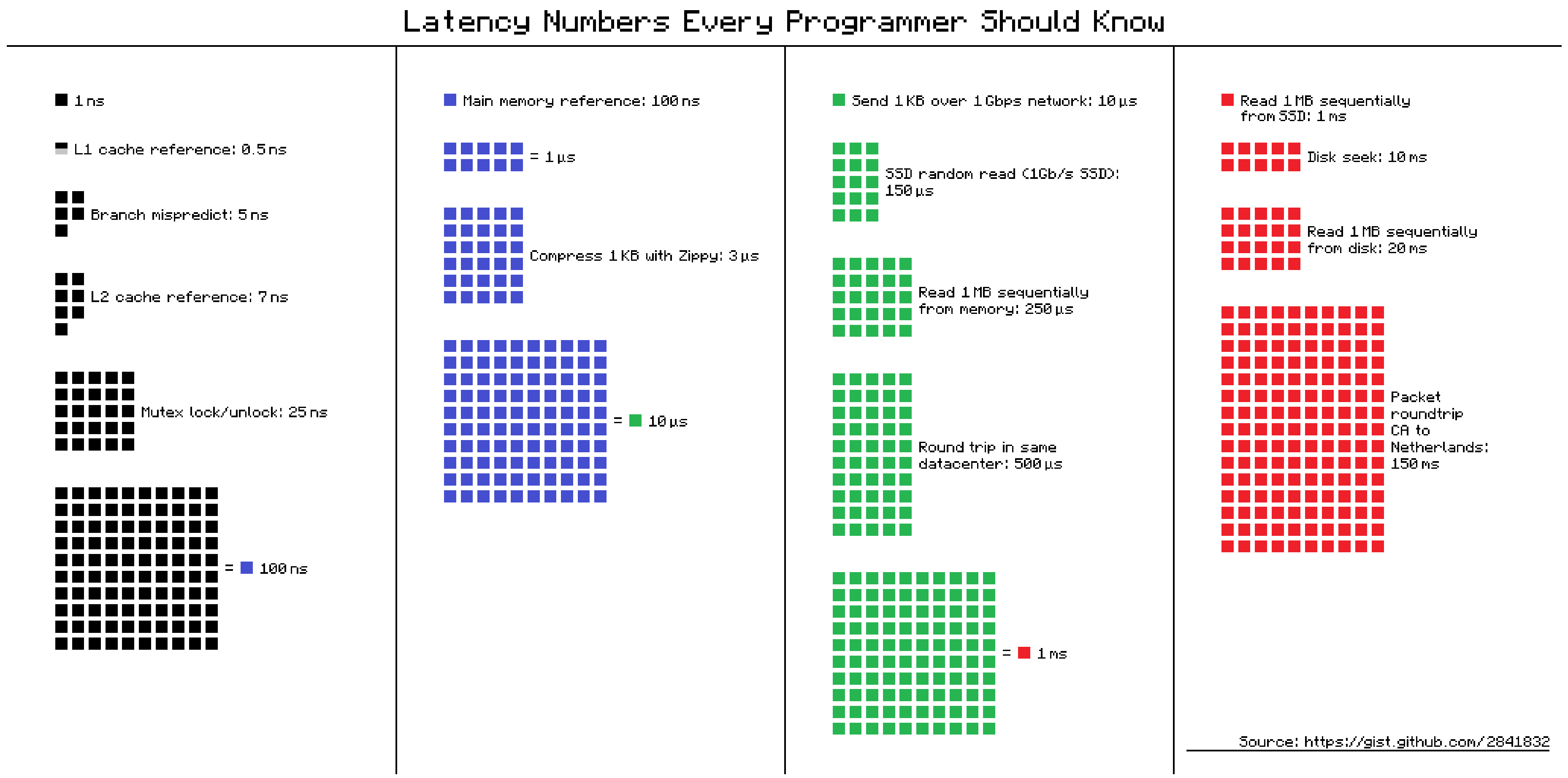
Hierarchy of memory

- Latency: time CPU gets data after requesting
- Bandwidth: how much data per second?
- prefetching of data, “cache misses” are expensive
- automatically managed by processor





Capacity	Bandwidth	Latency
256 Bytes	24000 MB/s	2 ns
8 KBytes	16000 MB/s	2 ns
96 KBytes	8000 MB/s	6 ns
2 MBytes	888 MB/s	24 ns
1536 MBytes	1000 MB/s	112 ns



https://gist.github.com/hellerbarde/2843375

Amdahl's Law

- Task: serial fraction s, parallel fraction p=1-s
- N workers (whatever that means)
- Runtime: T(N) = (1-s)T(1)/N + sT(1)
- Speedup T(1)/T(N), N to infinity:

  max_speedup = 1/ s
- http://en.wikipedia.org/wiki/Amdahl%27s_law
- Reality: T(N) = (1-s)T(1)/N + sT(1) + aN + bN^2

Summary

- Computing much faster than memory access
- Parallel computing required: no free lunch!
- Communication is serial fraction (or worse when increasing with N!)
- Communication in Amdahl's law is main challenge in parallel computing