Distributed Memory Parallelization in NGSolve

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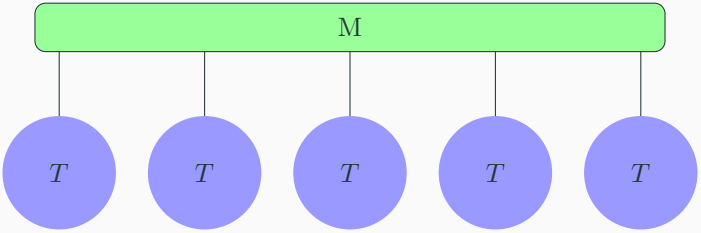
From Shared to Distributed Memory

Shared Memory

Parallelization via **threads** ($\rightarrow$ unit for **scheduling**).
Programming model:



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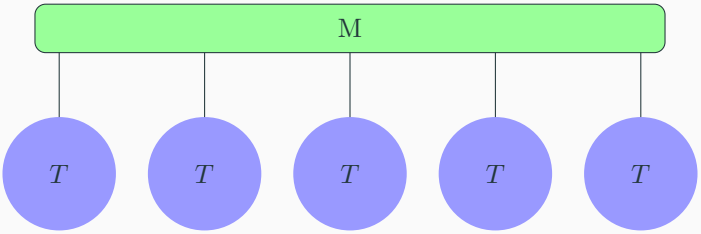

Assumption:
All threads can access **all** parts of the memory equally fast.

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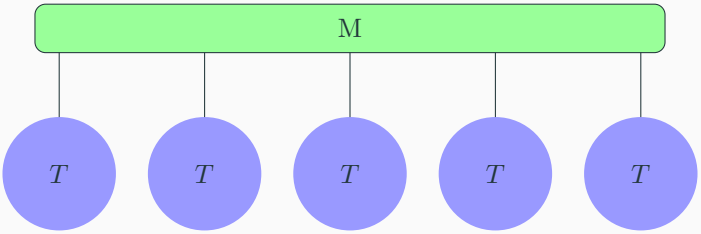

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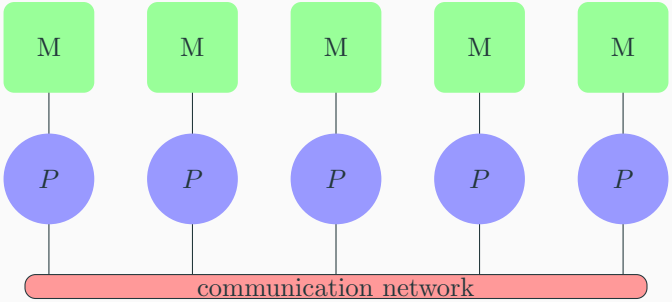

Distributed Memory

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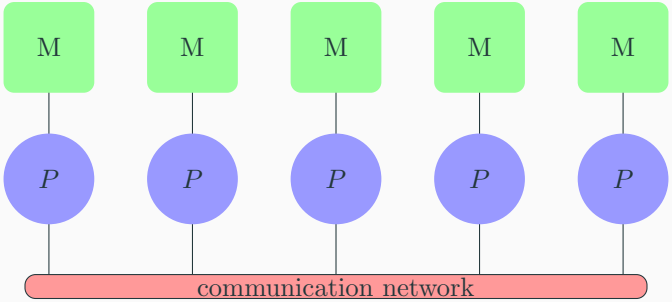


Parallelization via **procs** ($\rightarrow$ unit for scheduling **and memory management**).

Outline

MPI

Message Passing Interface

A **standard** for message-passing **between independent processes**; implemented in multiple libraries.

De facto standard for numerical computations.

It features functions for Point-to-Point communication between procs, by sending and receiving of ”messages”.

Portability is a huge aspect - write it once, run it on a laptop or a supercomputer!

Also: collective communication, one-sided comunication, ...

Point-to-Point communication

Process identified by **rank**, a number from 0 to NP.

To exchange message, one has to specify: pointer to data, amount of data, type of data, source/destination, ...

On the sending end:

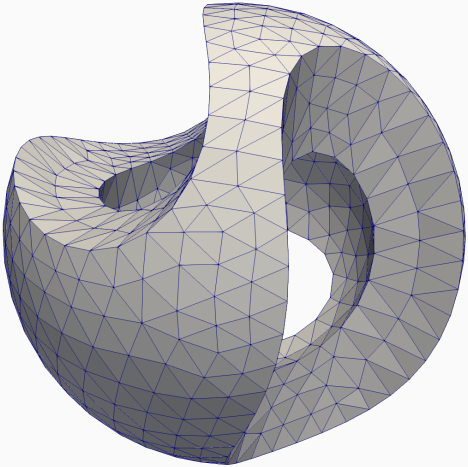
```
Array<double> send_values(len);
MPI_Send(&send_values[0], len, MPI_DOUBLE, recv_proc, ...);
```

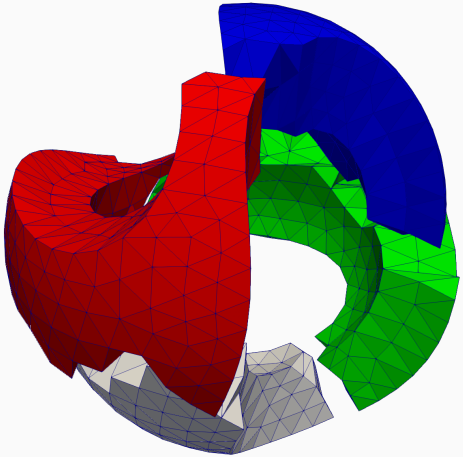
On the receiving end:

```
Array<double> recv_values(len);
MPI_Recv(&recv_values[0], len, MPI_DOUBLE, send_proc, ...);
```

NGS+MPI

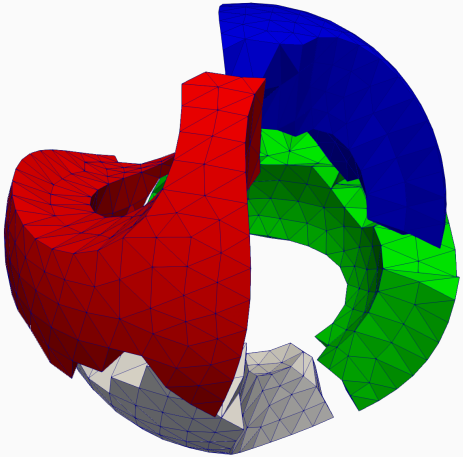
Distributing the Mesh





Distributing the Mesh

- **non-overlapping** partition (no ghost-elements)
- shared interface-nodes (edges in 2d, faces & edges in 3d)
- proc 0 (master proc) gets nothing!



Distributing the FESpace

A finite element consists of a space $V_{h,i}$ and a basis of its dual space $(\phi_{i,j})_j$.

The FESpace is then "glued together":

$$V_h = \left\{ u \in \Pi_i V_{h,i} : \phi(u_i) = \phi(u_k) \quad \forall \phi \in V'_{h,i} \cap V'_{h,j} \right\}$$

$\rightarrow$ Treat each subdomain as a "makro - Finite Element"!

Subdomain-spaces are glued together by functionals corresponding to nodes on interfaces.

Parallel Matrices

- Assemble element-matrices to submatrices A_i on each subdomain.
- The global Matrix $A = \sum_i E_i A_i E_i^T$ (with embeddings E_i) is never assembled.
- No communication needed to assemble matrices!

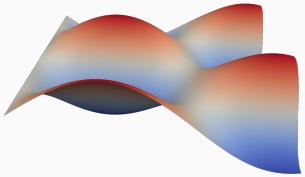
Parallel Vectors

- Local vector on each subdomain
- Can be CUMULATED (consistent values) or DISTRIBUTED (partial values)

$$x_j^{(C)} = E_j^T \sum_i E_i x_i^{(D)}$$

- DISTRIBUTED $\rightarrow$ CUMULATED requires communication!

Parallel Vectors - Visualized



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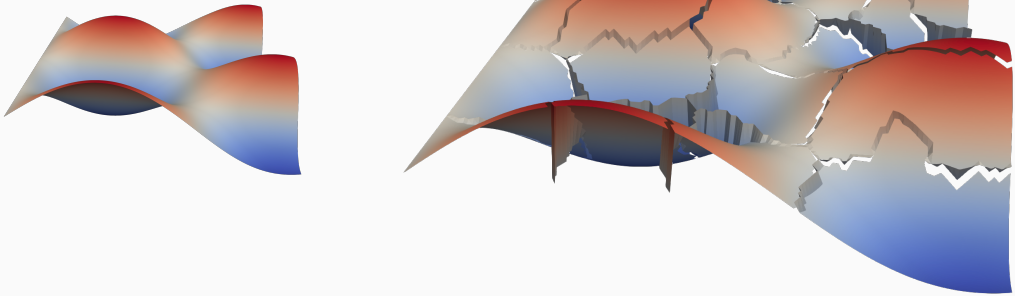

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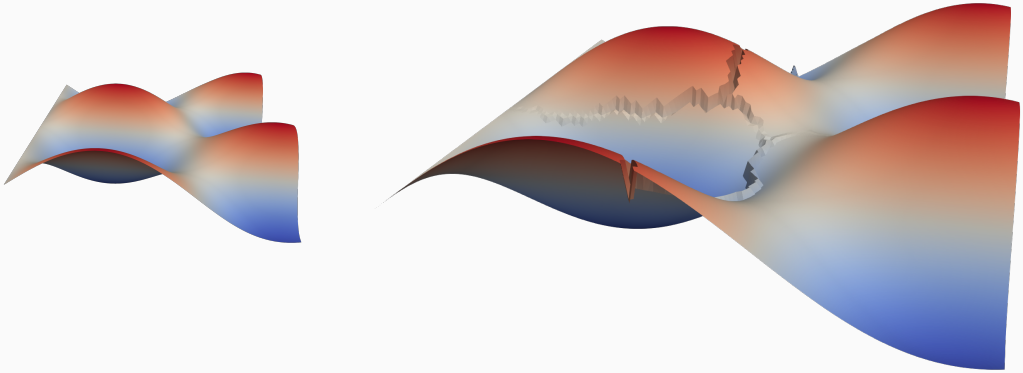


$$(Ax)_j^{(C)} = E_j^T \sum_i E_i A_i x_i^{(C)} = E_j^T \sum_i E_i (Ax)_i^{(D)}$$

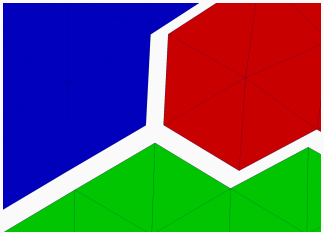
$$A_i x_j^{(C)} = (Ax)_j^{(D)}$$

Multiplication with local matrices takes a C-vector and returns a D-vector, to make it a C-vector again, we need communication!

We want to **apply** a (possibly nonlinear) operator involving dg-jumps, e.g:

```
a = BilinearForm(V)
a += SymbolicBFI( (u-u.Other())*(v-v.Other()),
skeleton=True)
a.Apply(u.vec, res)
```

remember: **no ghost elements** → what is ".Other()" on a subdomain interface??



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- We know "both sides" have the same expression
- Need trace values in IPs of all trial-proxies "from the other side"!
- "Other side" needs trace values of all trial-proxies from me!

→ Exchange trial-proxy traces!

Parallel DG III

```
Table<double> tv_send; //np rows
Table<double> tv_recv; //np rows
for(facet : mpi_facet)
        CalcTraceValues(facet, tv_send[p][facet_part])
for(p : Range(0,np) ) {
        MPI_Isend(tv_send[p],p,...) // send trace values
        MPI_Irecv(tv_recv[p],p,...) // recv trace values
}
MPI_Waitall(...) // wait for communication to finish
for(facet : mpi_facet)
        ApplyFromTraceValues(my_el, tv_recv[p][facet_part])
```

Under the hood - bottom line

Typical for programing with MPI:

- understand the problem
- understand the exact data dependencies
- simplify & reformulate to minimize those
- implement

Using MPI-parallel NGSolve

Setting up MPI-parallel NGSolve

Ideally, only need to switch on MPI with CMake option -DUSE_MPI=ON.

In fact, on clusters, this can be a bit more messy.

Generally, we try to hide MPI as well as possible, however, in fact, the user has to do **some stuff** differently.

Things to consider:

- **meshing is sequential only**
- **the netgen-ui is shm-parallel only** ($\rightarrow$ use VTK+ParaView)
- **you** have to take care of parallelizing anything that happens outside the ngsolve-libraries (e.g shell in- and output)
- any other considerations for running large jobs (e.g workload-manager)
- not quite as feature rich as shm-parallel version

MPI+Python-Interface

ngspy - wrapper around python3 In the simplest case:

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```
$ sbatch job_script
```

```
#!/usr/bin/bash
#
#SBATCH --job-name=ngs_phi
#SBATCH --partition=phi
#SBATCH  -N 10
#SBATCH --ntasks 640
#SBATCH --ntasks-per-node=64
#SBATCH --ntasks-per-core=1

mpirun ngspy mpi_poisson.py
```

Python Files

Solvers and Preconditioners

Own solvers/preconditioners :

- BDDC
- "Soon": Own AMG ($\rightarrow$ Bernd Schwarzenbacher, tomorrow)

Interfaces for:

- MUMPS
- HYPRE BoomerAMG
- HYPRE AMS

Switch on with -DUSE_MUMPS=ON / -DUSE_HYPRE=ON; superbuild downloads and builds the libraries automatically.

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Does definitely NOT work (yet): multigrid, Block-jacobi, Block-GS

Experiences

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Works well on 2000 cores across 100 nodes.

- 3d-poisson, p2, 450M NDOF, 40 sec. setup + 13 sec solve (CG+AMG)

Works on 10 xeon phi's (640 mpi-procs).

- 3d-poisson, p1, 36M NDOF, 28 sec. setup + 6.5 sec solve (CG+BoomerAMG)

Bonus slide; VTK + Paraview