Parallelization

PALM group

Institute of Meteorology and Climatology, Leibniz Universität Hannover

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Basics of Parallelization

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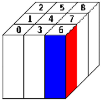

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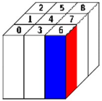

program loops are parallelized, i.e. each processor solves for a subset of the total index range

```
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   .
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```

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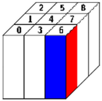

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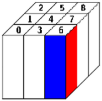

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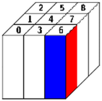

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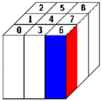

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shared memory model (OpenMP)
accelerator model (OpenACC)

Basic Architectures of Massively Parallel Computers

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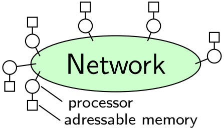

distributed memory

(Cray-XC30)

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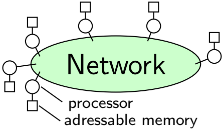

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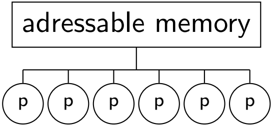

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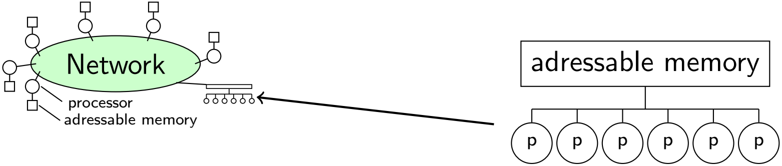

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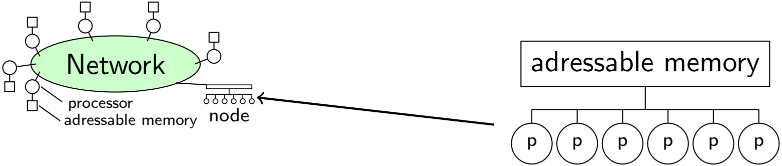

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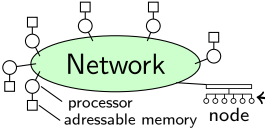

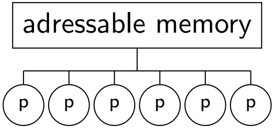

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clustered systems

(IBM-Regatta, Linux-Cluster, NEC-SX, SGI-ICE, Cray-XC)

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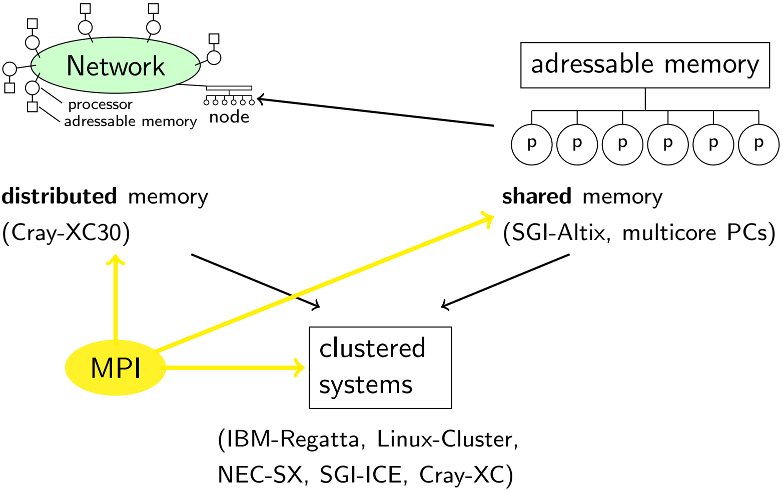

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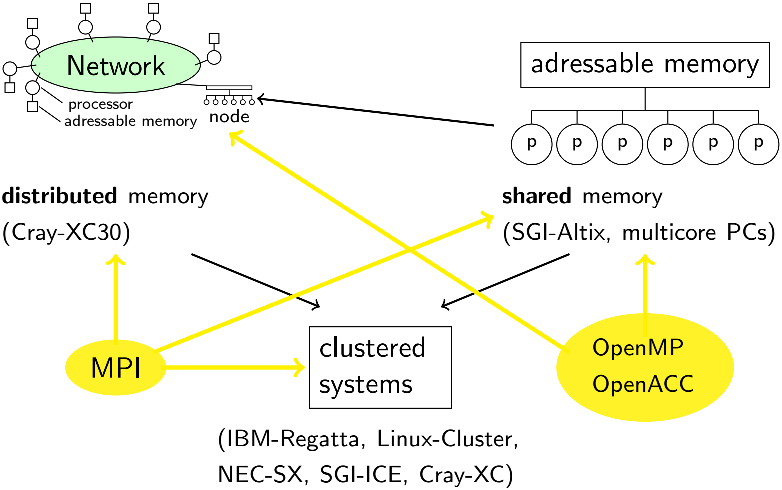

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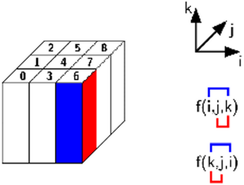

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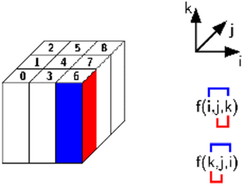

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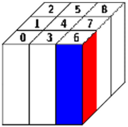

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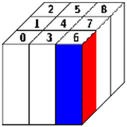

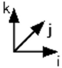

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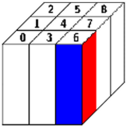

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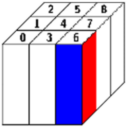

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- OpenMP parallelization as well as mixed usage of OpenMP and MPI is realized.

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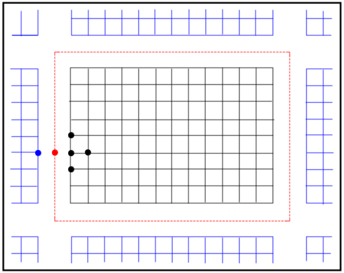

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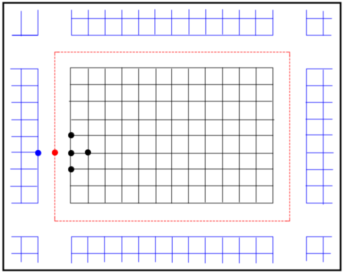

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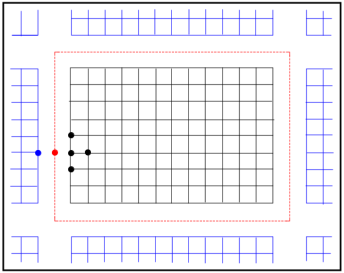

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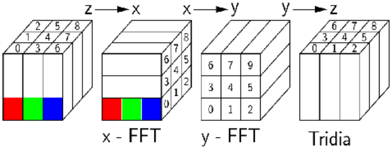

Example: transpositions for solving the Poisson equation

How to Use the Parallelized Version of PALM

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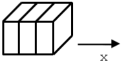

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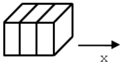
- Using the Open-MP parallelization does not yield any advantage over using a pure domain decomposition with MPI (contrary to expectations, it mostly slows down the computational speed), but this may change on cluster systems for very large number of processors (>10000?) or with Intel-Xeon-Phi accelerator boards.



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- All MPI calls must be within

```
CALL MPI_INIT( ierror )
:
:
CALL MPI_FINALIZE( ierror )
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- Communication is needed for
  - exchange of ghost points
  - transpositions (FFT-poisson-solver)
  - calculating global sums (e.g. for calculating horizontal averages)
- Additional MPI calls are required to define the so-called virtual processor grid and to define special data types needed for more comfortable exchange of data.

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pdims(1) = npex   !  # of processors along x
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- The ids of the neighbouring PEs are determined by:

```
CALL MPI_CARD_SHIFT( comm2d, 0, 1, pleft, pright, ierr )
CALL MPI_CARD_SHIFT( comm2d, 1, 1, psouth, pnorth, ierr )
```

Exchange of ghost points

- Ghost points are stored in additional array elements added at the horizontal boundaries of the subdomains, e.g.

```
u(:,:,nxl-nbgp), u(:,:,nxr+nbgp) !  left and right boundary
u(:,nys-nbgp,:), u(:,nyn+nbgp,:)  !  south and north boundary
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  The actual code uses `nxlg=nxl-nbgp`, etc...

Exchange of ghost points

- Ghost points are stored in additional array elements added at the horizontal boundaries of the subdomains, e.g.

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- The exchange of ghost points is done in file `exchange_horiz.f90`
  Simplified example: synchroneous exchange of ghost points along x (yz-planes, send left, receive right plane):

```
CALL MPI_SENDRECV( ar(nzb,nysg,nxl), ngp_yz, MPI_REAL, pleft, 0,
                   ar(nzb,nysg,nxr+1), ngp_yz, MPI_REAL, pright, 0,
                   comm2d, status, ierr )
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- In the real code special MPI data types (vectors) are defined for exchange of *yz*/*xz*-planes for performance reasons and because array elements to be exchanged are not consecutively stored in memory for *xz*-planes:

```
ngp_yz(0) = (nzt - nzb + 2) * (nyn - nys + 1 + 2 * nbgp )
CALL MPI_TYPE_VECTOR( nbgp, ngp_yz(0), ngp_yz(0), MPI_REAL, type_yz(0), ierr )
CALL MPI_TYPE_COMMIT( type_yz(0), ierr ) !  see file init_pegrid.f90

CALL MPI_SENDRECV( ar(nzb,nysg,nxl), 1, type_yz(grid_level), pleft, 0, ...
```

Transpositions

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```
!
!-- in SUBROUTINE transpose_xy:
CALL MPI_ALLTOALL( f_inv(nys_x,nzb_x,0),   sendrecvcount_xy, MPI_REAL, &
                   work(1,nzb_y, nxl_y,0), sendrecvcount_xy, MPI_REAL, &
                   comm1dy, ierr )
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- The data resorting before and after the calls of MPI_ALLTOALL is highly optimized to account for the different processor architectures and even allows for overlapping communication and calculation.

Parallel I/O

- PALM writes and reads some of the input/output files in parallel, i.e. each processor writes/reads his own file. **Each file then has a different name!**

  Example: binary files for restart are written into a subdirectory of the PALM working directory:

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General comment:

- Parallel I/O on a large number of files (>1000) currently may cause severe file system problems (e.g. on Lustre file systems).
  Workaround: reduce the maximum number of parallel I/O streams (see `mrun`-option `-w`)

PALM Parallel I/O for 2D/3D Data

- 2D- and 3D-data output is also written in parallel by the processors (2D: by default, 3D: generally).

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- `combine_plot_fields.x` is automatically executed by `mrun`.
- The executable `combine_plot_fields.x` is created during the installation process by the command

```
mbuild -u -h <host identifier>
```

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- d3par-parameter `netcdf_data_format=5` has to be set in the parameter file

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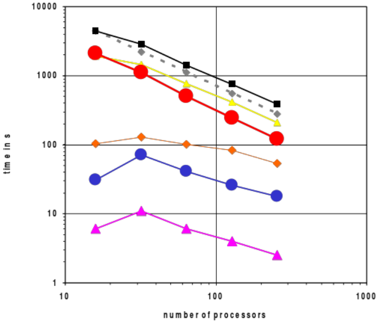
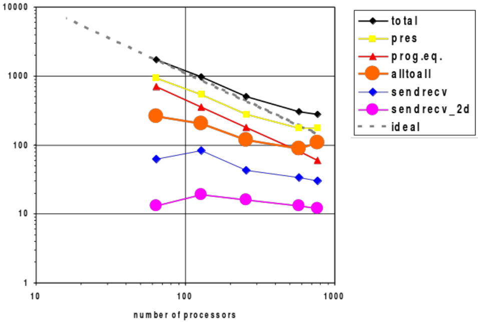
- d3par-parameter `netcdf_data_format=5` has to be set in the parameter file
- `combine_plot_fields.x` is not required in this case

Performance Examples (I)

- Simulation using 1536 * 768 * 242 grid points ($\sim$ 60 GByte)



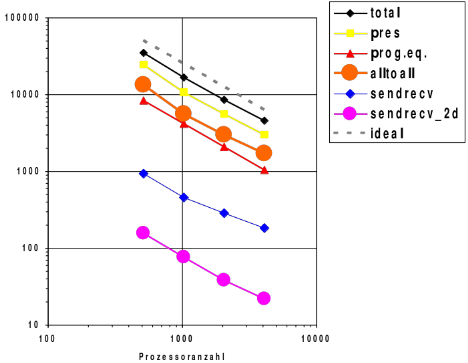
IBM-Regatta, HLRN, Hannover
(1D domain decomposition)



Sun Fire X4600, Tokyo Institute of Technology
(2D domain decomposition)

Performance Examples (II)

- Simulation with 2048^3 grid points ($\sim$ 2 TByte memory)



SGI-ICE2, HLRN-II, Hannover
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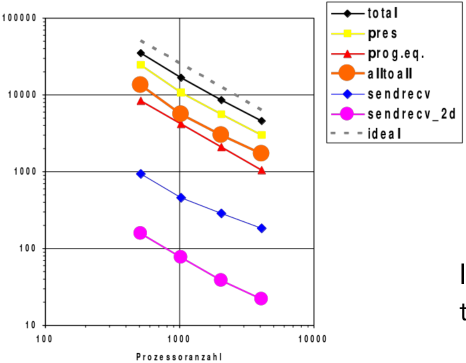


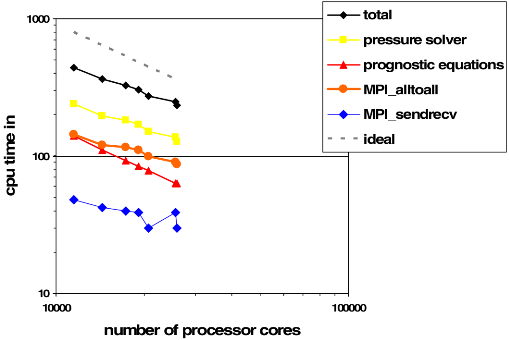
SGI-ICE2, HLRN-II, Hannover
(2D-domain decomposition)

largest simulation feasible on that system:

4096^3 grid points

Performance Examples (III)

- Simulation with 4320^3 grid points ($\sim$ 13 TByte memory)



Cray-XC40, HLRN-III, Hannover
(2D-domain decomposition)

Performance Examples (III)

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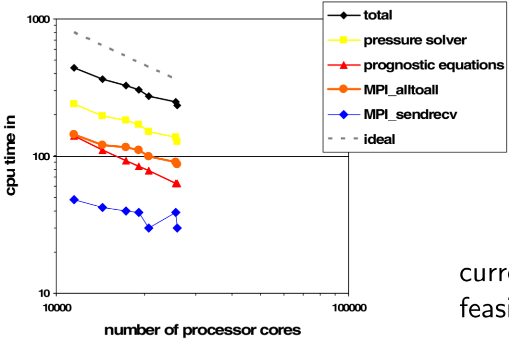

Cray-XC40, HLRN-III, Hannover
(2D-domain decomposition)

currently largest simulation feasible on that system:

5600^3 grid points