

Program Control by Physical Parameters

PALM group

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Steering of PALM and Interpreting the Output

- ▶ This section describes how to steer the model and how to interpret the model output (**it does not explain, how to start and control model runs**).

Steering of PALM and Interpreting the Output

- ▶ This section describes how to steer the model and how to interpret the model output (**it does not explain, how to start and control model runs**).
- ▶ It gives a general overview of the input and output files and explains the contents of the most important files in some detail.

PALM Input/Output Overview (I)

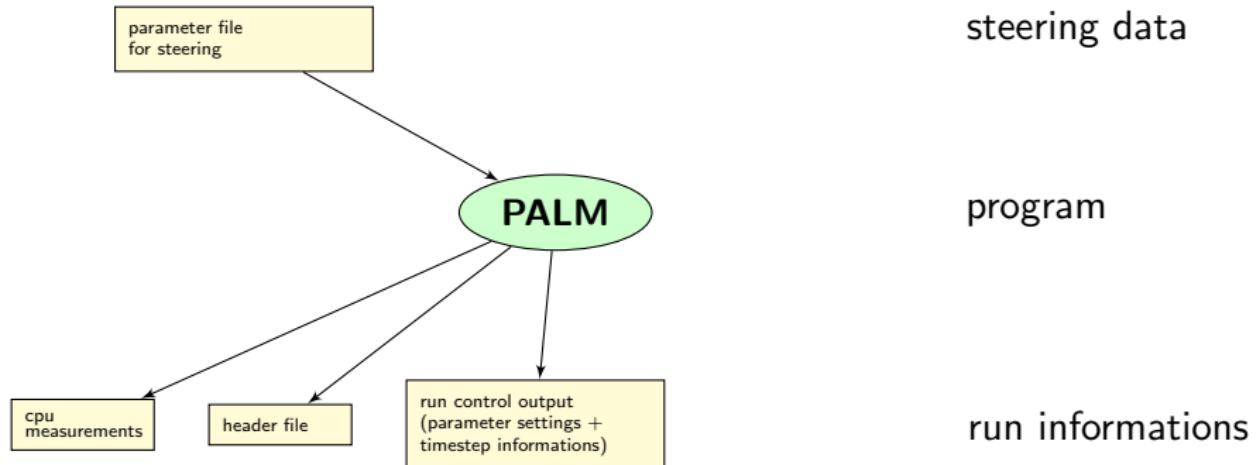


program

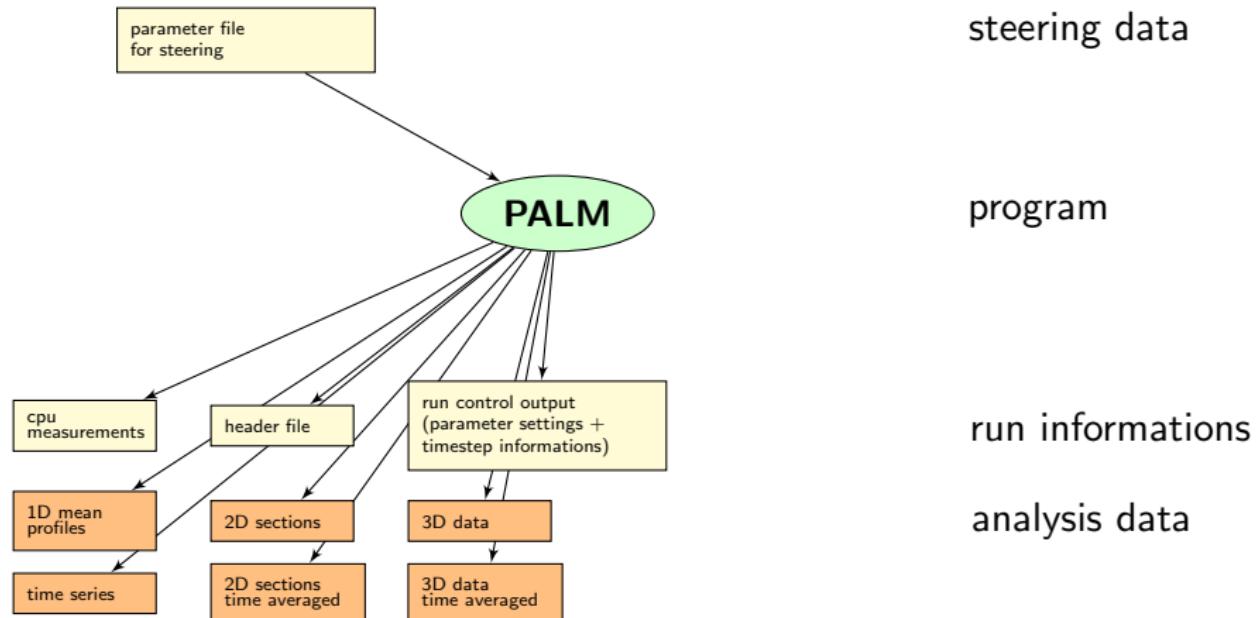
PALM Input/Output Overview (I)



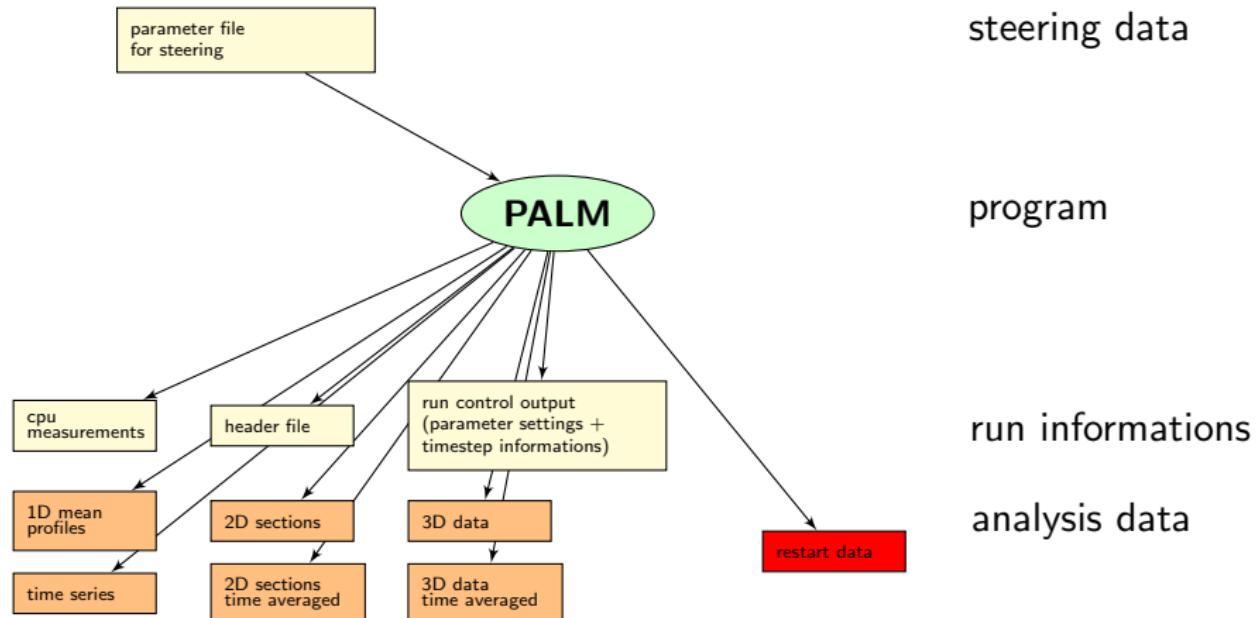
PALM Input/Output Overview (I)



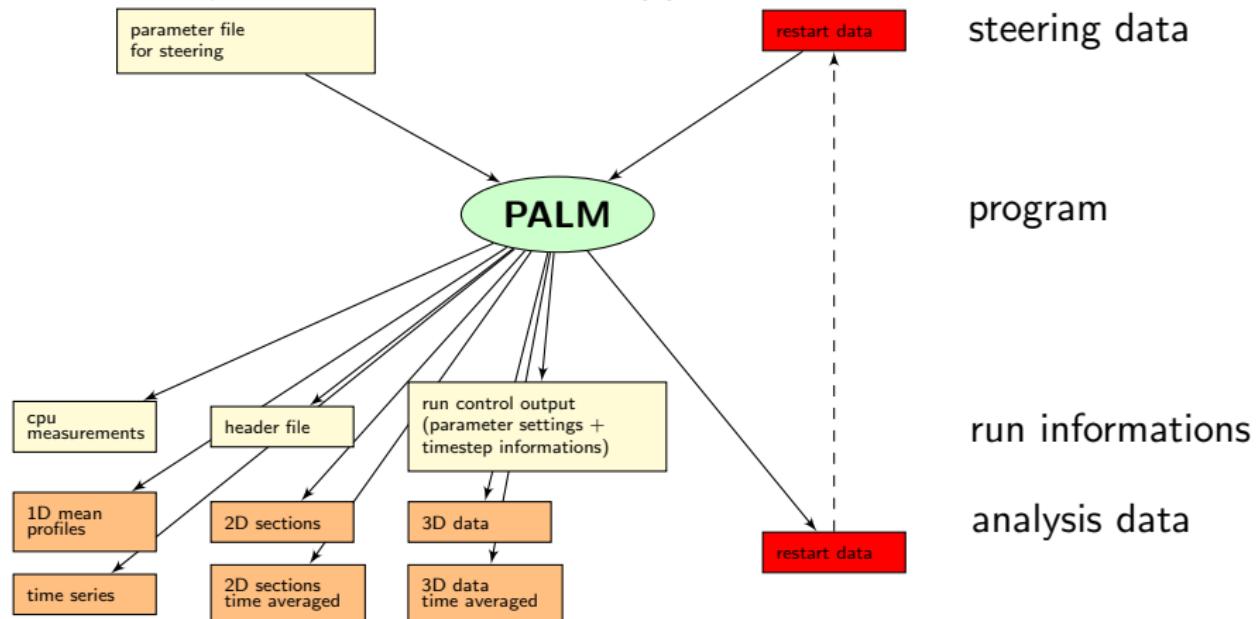
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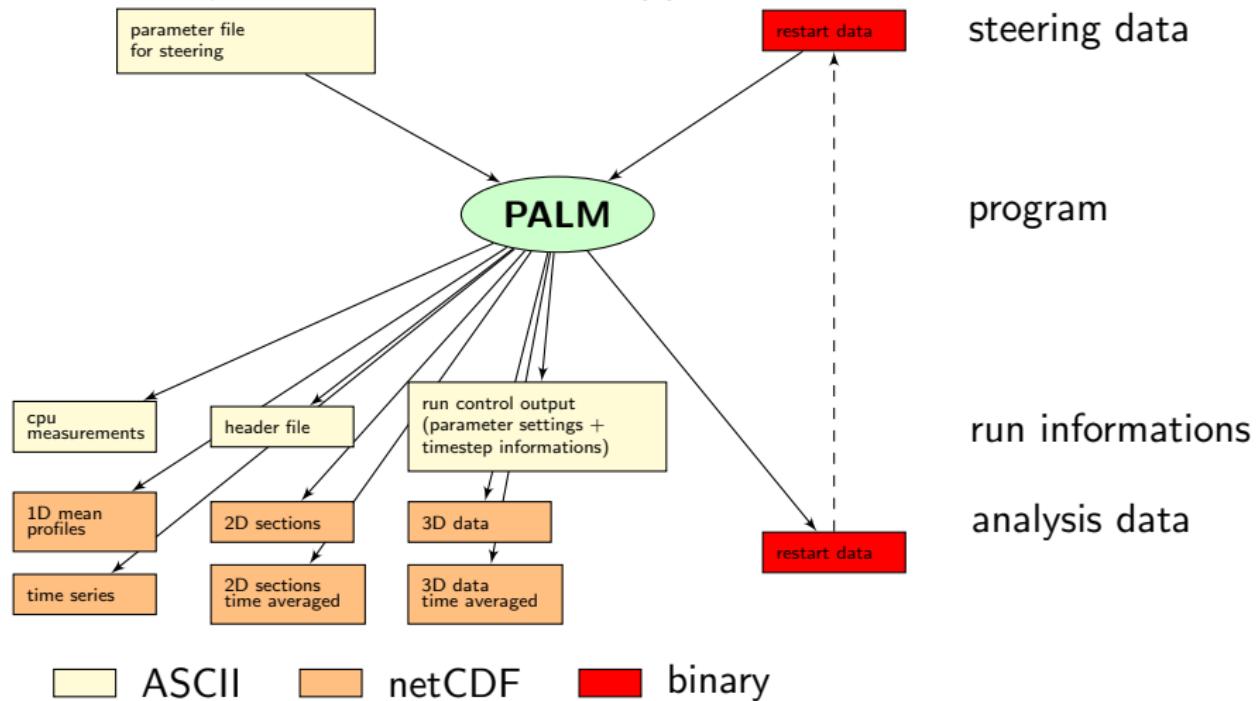
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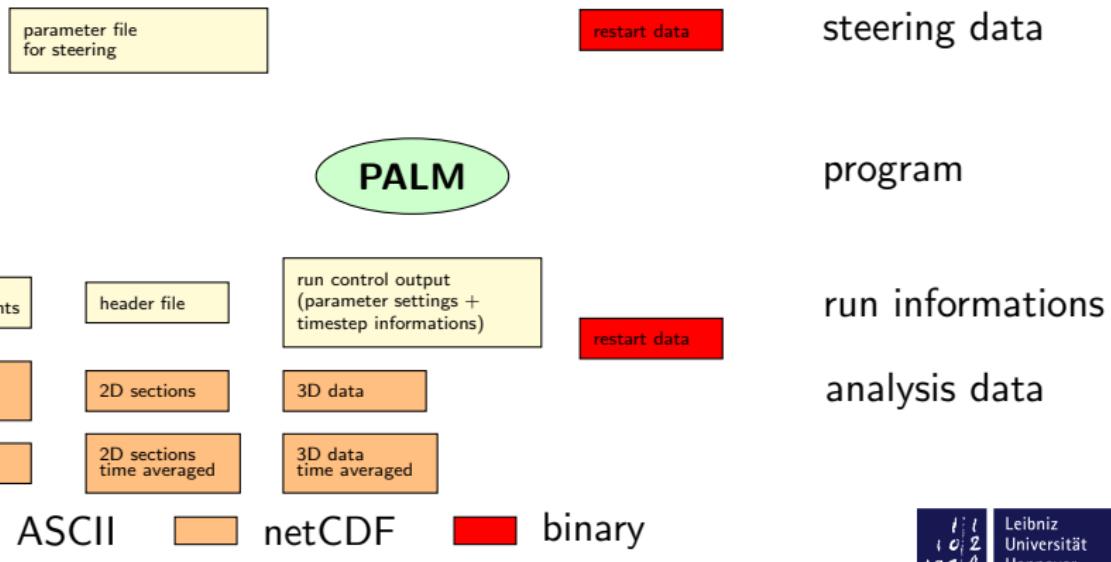
PALM Input/Output Overview (I)



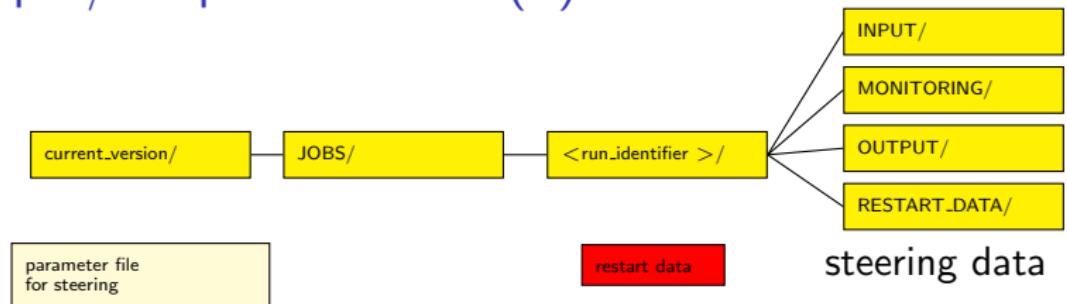
PALM Input/Output Overview (I)



PALM Input/Output Overview (II)



PALM Input/Output Overview (II)

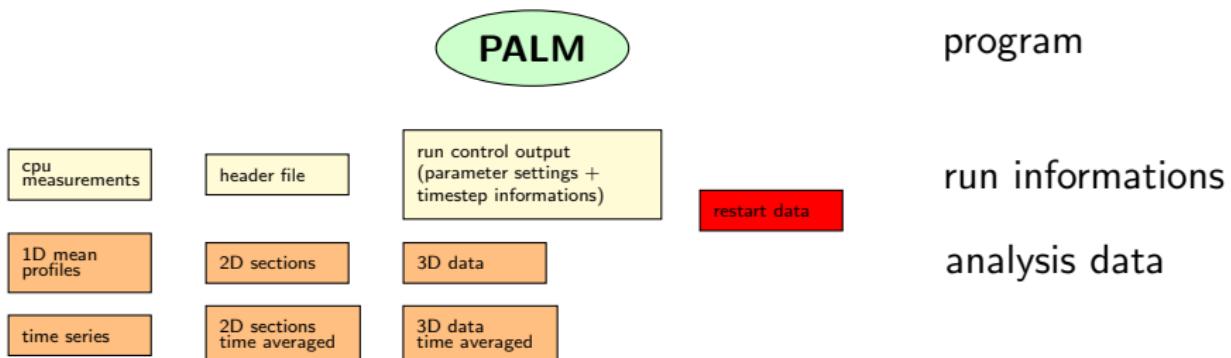


steering data

program

run informations

analysis data



ASCII

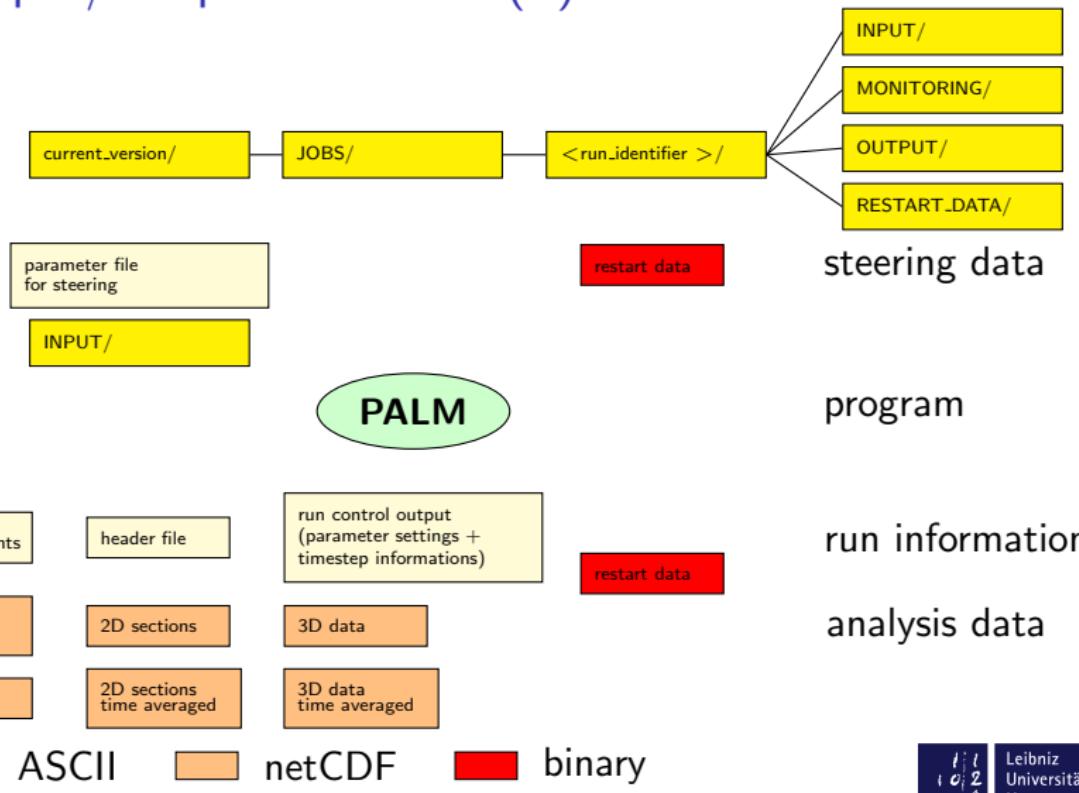


netCDF

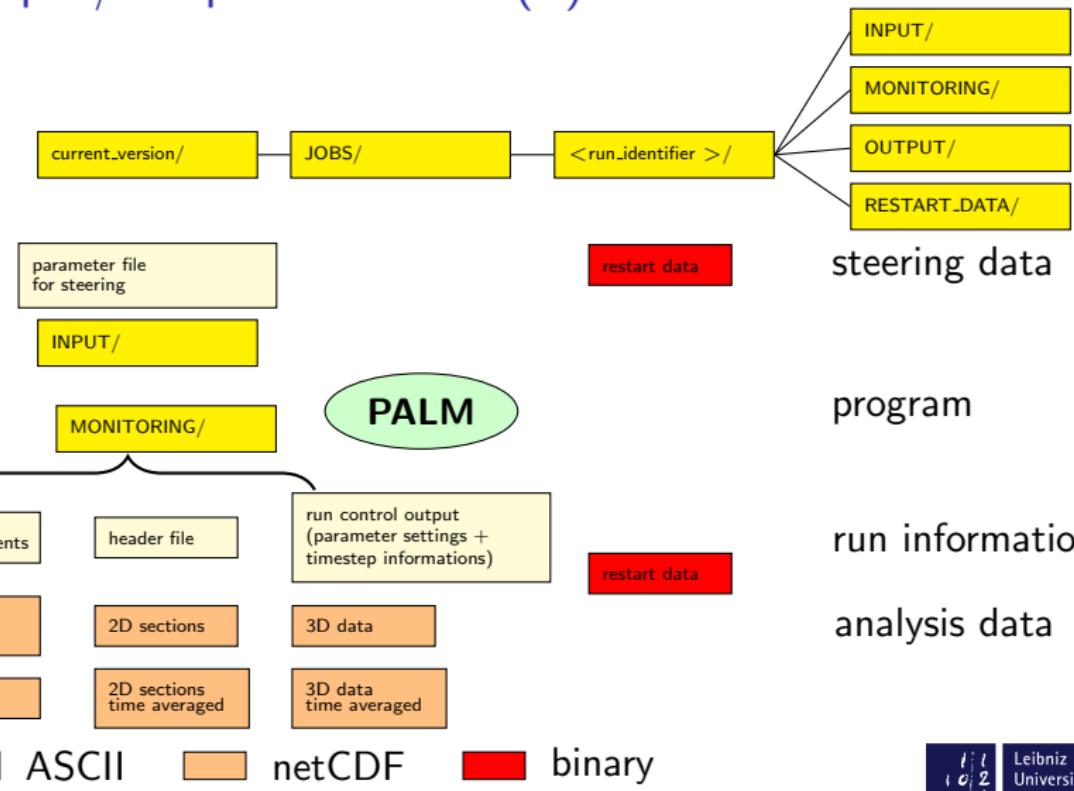


binary

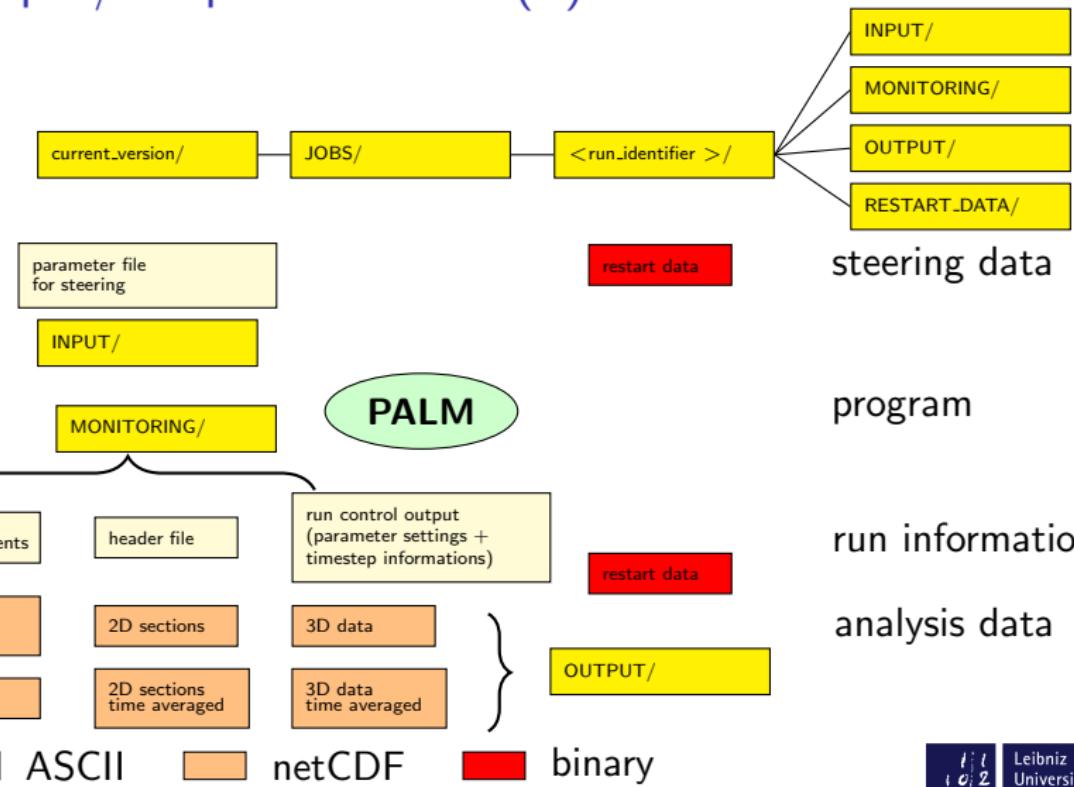
PALM Input/Output Overview (II)



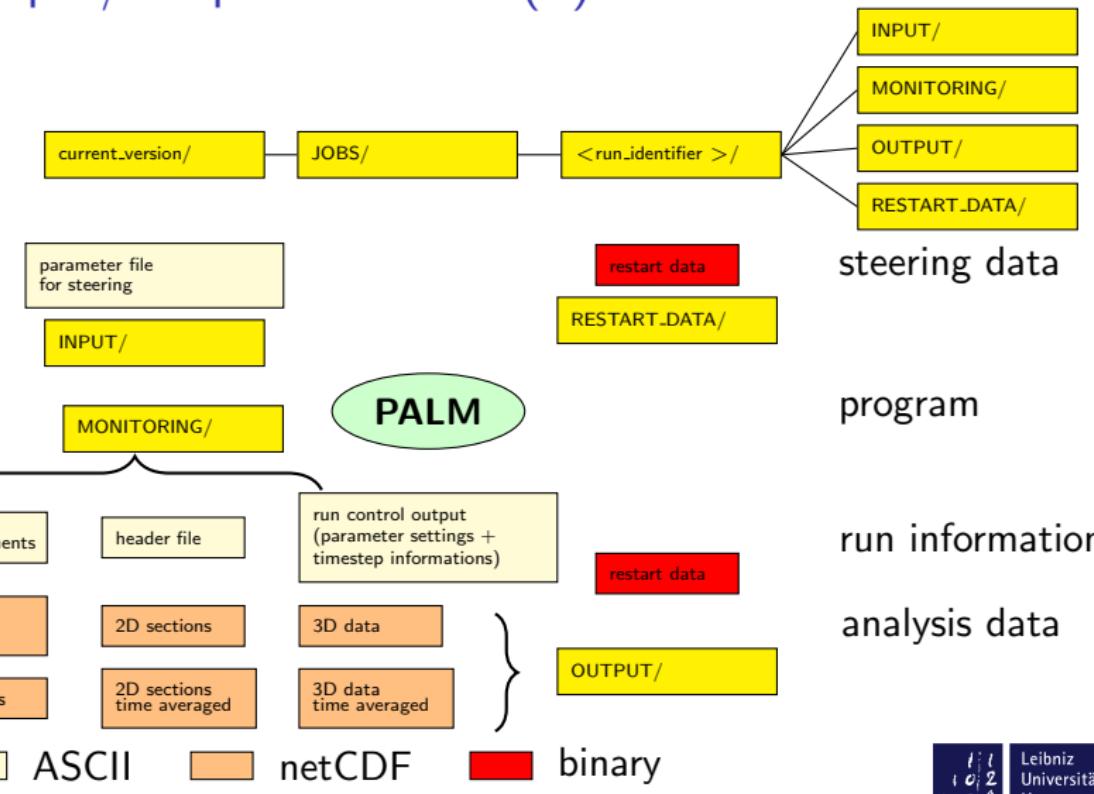
PALM Input/Output Overview (II)



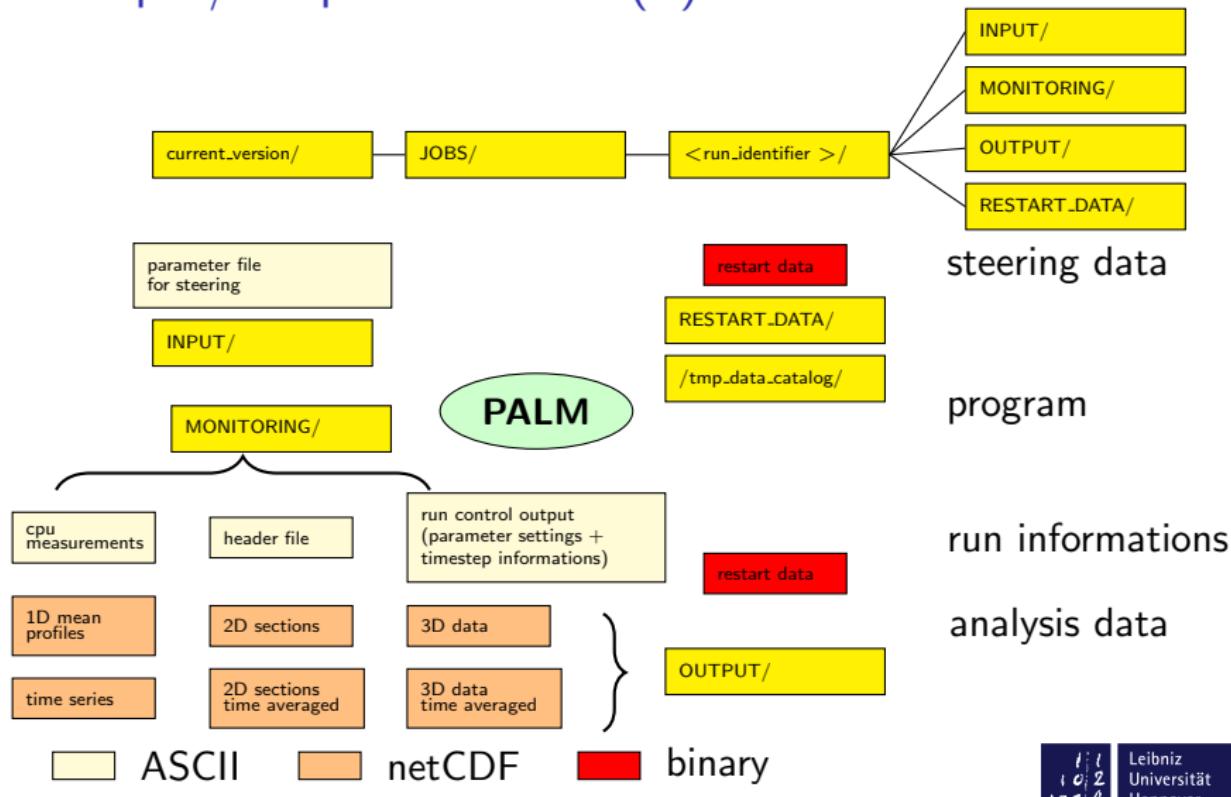
PALM Input/Output Overview (II)



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PALM Input/Output Overview (II)



The Parameter File

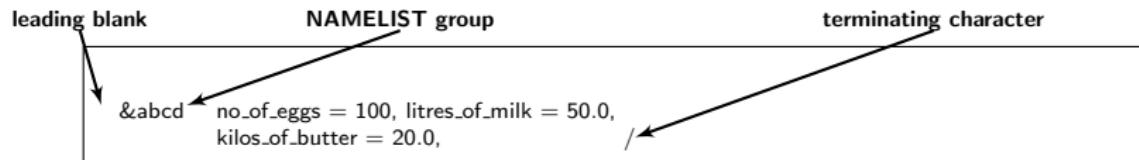
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- ▶ General structure of a FORTRAN-NAMELIST file

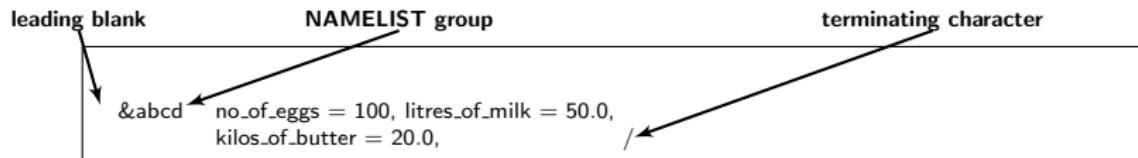
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The Parameter File

- ▶ Physical and numerical features of a PALM run (e.g. initial and boundary conditions, numerical methods) are controlled by a so called **parameter file** which uses FORTRAN-NAMELIST syntax.
- ▶ General structure of a FORTRAN-NAMELIST file



- ▶ This file can be read from a FORTRAN program in the following way:

```

INTEGER :: no_of_eggs = 30
REAL ::      litres_of_milk = 0.0, kilos_of_butter, kilos_of_cream = 33.0

NAMELIST /abcd/    no_of_eggs, litres_of_milk, kilos_of_butter, kilos_of_cream

OPEN ( 1, FILE='Filename' )

READ ( 1, abcd )
  
```

An Example of PALM - NAMELIST Input

```
&inipar nx = 39, ny = 39, nz = 40,  
dx = 50.0, dy = 50.0, dz = 50.0,  
  
initializing_actions = 'set_constant_profiles',  
ug_surface = 0.0, vg_surface = 0.0,  
  
pt_vertical_gradient      = 0.0, 1.0,  
pt_vertical_gradient_level = 0.0, 800.0,  
  
surface_heatflux = 0.1, bc_pt_b ='neumann', /  
  
&d3par end_time = 3600.0,  
  
dt_dopr = 900.0, averaging_interval_pr = 600.0,  
data_output_pr = 'pt', 'u', 'v', /
```

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- ▶ There are two NAMELIST groups (&inipar and &d3par).

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```

- ▶ There are two NAMELIST groups (`&inipar` and `&d3par`).
- ▶ Assignments to parameters in `&inipar` are ignored within restart runs (exception: `initializing_actions = 'read_restart_data'` is obligatory for restart runs).

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&d3par end_time = 3600.0,  
  
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- ▶ There are two NAMELIST groups (`&inipar` and `&d3par`).
- ▶ Assignments to parameters in `&inipar` are ignored within restart runs (exception: `initializing_actions = 'read_restart_data'` is obligatory for restart runs).
- ▶ Values of `&d3par` parameters can be changed for restart runs.

The Run Control File

- ▶ For initial runs, the parameter settings and many additional informations about the run (header informations) are printed at the beginning of this file.

```
***** Rev: 1648 ***** atmosphere = 3D - run without ID = prerus
***** Run control output: *****

RUN   ITER. HH:MM:SS.DS DT(E)    UMAX    VMAX    WMAX    U*     W*     THETA*    Z_I     ENERG.    DISTENERG    DIVOLD    DIVREW    UMAX(KJ)    VMAX(KJ)    WMAX(KJ)    ADVECX    ADVECY    MGCGC
      0       00:00:20.00 20.0000A -0.2192 -0.2169 -0.1214 0.001 0.69 -0.124E+03 100. 0.105E-02 0.948E-03 0.491E-05 0.355E-15 11 32 5 5 37 29 4 26 0 0.000 0.000 0
      0       2 00:00:40.00 20.0000D -0.2151 -0.2176 -0.1209 0.001 0.69 -0.125E+03 100. 0.104E-02 0.940E-03 0.802E-05 0.359E-15 11 32 5 5 37 29 4 26 0 0.000 0.000 0
:
```

The Run Control File

- ▶ For initial runs, the parameter settings and many additional informations about the run (header informations) are printed at the beginning of this file.
- ▶ The parameter settings are followed by values of specific model variables for certain timesteps (one line for each timestep, the output intervall can be controlled by run parameter `dt_run_control`).

```
***** Rev: 1648 ***** atmosphere = 3D - run without ID = prerus
***** Date: 15-09-18 Run: example_cbl *****
***** Time: 17:34:44 Run-No.: 00 *****
Run on host: lcnmk
Number of PE's: 4 Processor grid (x,y): ( 2, 2) calculated

Run-control output:
RUN ITER HH:MM:SS DT(E) UMAX VMAX WMAX U* W* THETA* Z_I ENERG. DISTENERG DIVOLD DIVREW UMAX(KJ) VMAX(KJ) WMAX(KJ) ADVECX ADVECY MGCYC
0 0 00:00:00 20.00000 -0.2192 -0.2169 -0.1214 0.001 0.69 -0.124E+03 100. 0.105E-02 0.948E-03 0.491E-05 0.355E-15 11 32 5 5 37 29 4 26 0 0.000 0.000 0
0 1 00:00:20 20.00000 -0.2192 -0.2169 -0.1214 0.001 0.69 -0.124E+03 100. 0.105E-02 0.948E-03 0.491E-05 0.355E-15 11 32 5 5 37 29 4 26 0 0.000 0.000 0
0 2 00:00:40 20.00000 -0.2151 -0.2176 -0.1209 0.001 0.69 -0.125E+03 100. 0.104E-02 0.940E-03 0.802E-05 0.359E-15 11 32 5 5 37 29 4 26 0 0.000 0.000 0
:
```

The Run Control File

- ▶ For initial runs, the parameter settings and many additional informations about the run (header informations) are printed at the beginning of this file.
- ▶ The parameter settings are followed by values of specific model variables for certain timesteps (one line for each timestep, the output intervall can be controlled by run parameter `dt_run_control`).

Contents of this timestep output should be carefully checked after each run, because it allows a first control, if the model had run correctly, or if any errors have occurred!

atmosphere = 3D - run without 1D - prerun																					
Date:	15-09-18	Run:	example_cbl																		
Time:	17:34:44	Run-No.:	00																		
Run on host:	lcmak																				
Number of PE's: 4 Processor grid (x,y): (2, 2) calculated																					
Run-control output:																					
RUN	ITER.	HH:MM:SS.SS	DT(E)	UMAX	VMAX	WMAX	U*	W*	THETA*	Z_I	ENERG.	DISTENERG	DIVOLD	DIVREW	UMAX(KJ1)	VMAX(KJ1)	WMAX(KJ1)	ADVECX	ADVECY	MGCYC	
0	0	00:00:20.00	20.0000	-0.2192	-0.2169	-0.1214	0.001	0.69	-0.124E+03	100	0.105E-02	0.948E-03	0.491E-05	0.355E-15	11	32	5	37	29	4 26 0	0.000 0.000 0
0	1	00:00:40.00	20.0000	-0.2151	-0.2176	-0.1209	0.001	0.69	-0.125E+03	100	0.104E-02	0.940E-03	0.802E-05	0.359E-15	11	32	5	37	29	4 26 0	0.000 0.000 0
0	2	00:00:40.00	20.0000	-0.2151	-0.2176	-0.1209	0.001	0.69	-0.125E+03	100	0.104E-02	0.940E-03	0.802E-05	0.359E-15	11	32	5	37	29	4 26 0	0.000 0.000 0

The Header File

- ▶ The header file contains nearly the same informations as the header of the run control file of the initial run.

```
:
:
Run time and time step information:
-----
Timestep:           variable      maximum value: 20.000 s    CFL-factor: 0.90
Start time:          0.000 s
End time:           3600.000 s

Time reached:       3601.930 s
CPU-time used:     4.391 s      per timestep:                 0.017 s
                           per second of simulated time: 0.001 s

Computational grid and domain size:
-----
Grid length:        dx =      50.000 m    dy =      50.000 m    dz =      50.000 m
:
:
```

The Header File

- ▶ The header file contains nearly the same informations as the header of the run control file of the initial run.
- ▶ It is generated for **every run** (initial run as well as restart runs).

```
:
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Timestep:           variable      maximum value: 20.000 s    CFL-factor: 0.90
Start time:          0.000 s
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Grid length:        dx =      50.000 m    dy =      50.000 m    dz =      50.000 m
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The Header File

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- ▶ It is generated for **every run** (initial run as well as restart runs).
- ▶ It is created at the beginning **and** at the end of a run (overwrites the file created at beginning).

```
:
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Timestep:           variable      maximum value: 20.000 s    CFL-factor: 0.90
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Computational grid and domain size:
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Grid length:        dx =      50.000 m    dy =      50.000 m    dz =      50.000 m
:
:
```

The Header File

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- ▶ It is generated for **every run** (initial run as well as restart runs).
- ▶ It is created at the beginning **and** at the end of a run (overwrites the file created at beginning).
- ▶ Only at the end, cpu time information is included!

```
:
:
Run time and time step information:
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Timestep:           variable      maximum value: 20.000 s    CFL-factor: 0.90
Start time:          0.000 s
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                           per second of simulated time: 0.001 s

Computational grid and domain size:
-----
Grid length:        dx =      50.000 m    dy =      50.000 m    dz =      50.000 m
:
:
```

CPU Measurements File

- Contains informations about the CPU requirements of single parts of the program.

PALM 4.0 Rev: 1648 run: example_cbl.00 host: lcmuk 15-09-15 17:34:44						
CPU measures for 4 PEs (2(x) * 2(y) tasks * 1 threads):						
gridpoints (x/y/z): 40 * 40 * 40						
nr of timesteps: 253						
cpu time per grid point and timestep: 0.57070 * 10***-6 s						
place:	mean	counts	min	max	rms	
	sec.	%	sec.	sec.	sec.	sec.
total	9.241	100.00	1	9.241	9.241	0.000
all progn.equations	5.899	63.83	759	5.827	5.977	0.056
pres	1.508	16.32	760	1.506	1.508	0.002
diffusivities	0.632	6.84	759	0.624	0.642	0.006
exchange-horiz-progn	0.412	4.45	759	0.333	0.441	0.056
flow_statistics	0.270	2.92	254	0.269	0.271	0.001
calculate_timestep	0.205	2.21	253	0.150	0.223	0.031
prandtl_fluxes	0.150	1.63	759	0.148	0.153	0.002
sum_up_3d_data	0.016	0.17	146	0.016	0.016	0.000
initialisation	0.014	0.15	1	0.014	0.014	0.000
disturb_field	0.006	0.06	10	0.005	0.006	0.001
data_output_2d	0.004	0.04	10	0.003	0.004	0.000
data_output_tseries	0.003	0.04	253	0.000	0.000	0.006
run_control	0.003	0.03	254	0.000	0.000	0.005
swap_timelevel	0.001	0.01	759	0.001	0.001	0.000
last_actions	0.001	0.01	1	0.000	0.001	0.000
average_3d_data	0.000	0.00	2	0.000	0.000	0.000
user_actions	0.000	0.00	759	0.000	0.000	0.000
data_output_profiles	0.000	0.00	4	0.000	0.000	0.000
special measures:						
timesteps	9.222	99.80	253	9.222	9.222	0.000
poisfft	0.871	9.42	760	0.868	0.873	0.002
exchange_horiz	0.588	6.37	6866	0.505	0.619	0.058
divergence	0.259	2.81	1520	0.258	0.261	0.001
fft_y	0.239	2.59	760	0.236	0.244	0.003
fft_x	0.238	2.58	760	0.236	0.243	0.002
transpo forward	0.195	2.12	760	0.187	0.202	0.006
mpi_alltoall	0.162	1.75	4560	0.148	0.169	0.008
transpo invers	0.113	1.22	760	0.109	0.114	0.002
tridia	0.083	0.90	760	0.082	0.084	0.000
exchange_horiz_2d	0.040	0.44	3795	0.034	0.046	0.005

CPU Measurements File

- ▶ Contains informations about the CPU requirements of single parts of the program.
- ▶ It should be inspected regularly in order to find out, if the code is still well optimized (e.g. load balance).

PALM 4.0 Rev: 1648 run: example_cbl.00 host: lcmuk 15-09-15 17:34:44						
CPU measures for 4 PEs (2(x) * 2(y) tasks * 1 threads):						
gridpoints (x/y/z): 40 * 40 * 40						
nr of timesteps: 253						
cpu time per grid point and timestep: 0.57070 * 10***-6 s						

place:	mean		counts		min	
	sec.	%	sec.	sec.	sec.	rms sec.
total	9.241	100.00	1	9.241	9.241	0.000
all progn.equations	5.899	63.83	759	5.827	5.977	0.056
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flow_statistics	0.270	2.92	254	0.269	0.271	0.001
calculate_timestep	0.205	2.21	253	0.150	0.223	0.031
prandtl_fluxes	0.150	1.63	759	0.148	0.153	0.002
sum_up_3d_data	0.016	0.17	146	0.016	0.016	0.000
initialisation	0.014	0.15	1	0.014	0.014	0.000
disturb_field	0.006	0.06	10	0.005	0.006	0.001
data_output_2d	0.004	0.04	10	0.003	0.004	0.000
data_output_tseries	0.003	0.04	253	0.000	0.000	0.006
run_control	0.003	0.03	254	0.000	0.000	0.005
swap_timelevel	0.001	0.01	759	0.001	0.001	0.000
last_actions	0.001	0.01	1	0.000	0.001	0.000
average_3d_data	0.000	0.00	2	0.000	0.000	0.000
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special measures:						
timesteps	9.222	99.80	253	9.222	9.222	0.000
poisfft	0.871	9.42	760	0.868	0.873	0.002
exchange_horiz	0.588	6.37	6866	0.505	0.619	0.058
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- ▶ It should be inspected regularly in order to find out, if the code is still well optimized (e.g. load balance).
- ▶ Prognostic-equations and pressure solver (pres) should be the main consumer.

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initialisation	0.014	0.15	1	0.014	0.014	0.000
disturb_field	0.006	0.06	10	0.005	0.006	0.001
data_output_2d	0.004	0.04	10	0.003	0.004	0.000
data_output_tseries	0.003	0.04	253	0.000	0.000	0.006
run_control	0.003	0.03	254	0.000	0.000	0.005
swap_timelevel	0.001	0.01	759	0.001	0.001	0.000
last_actions	0.001	0.01	1	0.000	0.001	0.000
average_3d_data	0.000	0.00	2	0.000	0.000	0.000
user_actions	0.000	0.00	759	0.000	0.000	0.000
data_output_profiles	0.000	0.00	4	0.000	0.000	0.000

special measures:						
timesteps	9.222	99.80	253	9.222	9.222	0.000
poisfft	0.871	9.42	760	0.868	0.873	0.002
exchange_horiz	0.588	6.37	6866	0.505	0.619	0.058
divergence	0.259	2.81	1520	0.258	0.261	0.001
fft_y	0.239	2.59	760	0.236	0.244	0.003
fft_x	0.238	2.58	760	0.236	0.243	0.002
transpo forward	0.195	2.12	760	0.187	0.202	0.006
mpi_alltoall	0.162	1.75	4560	0.148	0.169	0.008
transpo invers	0.113	1.22	760	0.109	0.114	0.002
tridia	0.083	0.90	760	0.082	0.084	0.000
exchange_horiz_2d	0.040	0.44	3795	0.034	0.046	0.005

CPU Measurements File

- ▶ Contains informations about the CPU requirements of single parts of the program.
- ▶ It should be inspected regularly in order to find out, if the code is still well optimized (e.g. load balance).
- ▶ Prognostic-equations and pressure solver (pres) should be the main consumer.
- ▶ For larger grids (1024^3 points), pres may need up to 50% of the total time or more.

PALM 4.0 Rev: 1648 run: example_cbl.00 host: lcmuk 15-09-15 17:34:44						
CPU measures for 4 PEs (2(x) * 2(y) tasks * 1 threads):						
gridpoints (x/y/z): 40 * 40 * 40 nr of timesteps: 253 cpu time per grid point and timestep: 0.57070 * 10***-6 s						
place:	mean sec.	counts %	min sec.	max sec.	rms sec.	
total	9.241	100.00	1	9.241	9.241	0.000
all progn.equations	5.899	63.83	759	5.827	5.977	0.056
pres	1.508	16.32	760	1.506	1.508	0.002
diffusivities	0.632	6.84	759	0.624	0.642	0.006
exchange-horiz-progn	0.412	4.45	759	0.333	0.441	0.056
flow_statistics	0.270	2.92	254	0.269	0.271	0.001
calculate_timestep	0.205	2.21	253	0.150	0.223	0.031
prandtl_fluxes	0.150	1.63	759	0.148	0.153	0.002
sum_up_3d_data	0.016	0.17	146	0.016	0.016	0.000
initialisation	0.014	0.15	1	0.014	0.014	0.000
disturb_field	0.006	0.06	10	0.005	0.006	0.001
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- ▶ Prognostic-equations and pressure solver (pres) should be the main consumer.
- ▶ For larger grids (1024^3 points), pres may need up to 50% of the total time or more.
- ▶ Time needed for communication (sum of `exchange_horiz(_2d)` and `mpi_alltoall`) should not exceed about 10-15% of the total time.

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Other Files

- ▶ Data output files (1D profiles and timeseries, 2D cross sections, 3D volume data) are by default in **netCDF** format which is suitable to be processed by public domain graphics software like **ncview**, **ferret**, **ncl** (used by PALM group), **IDL**, etc.

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- ▶ **ncdump** can be used to display the netCDF file contents in ASCII format (**ncdump -c** displays only header informations).
- ▶ The simple viewer for netCDF-data - **ncview** - as well as **ncl** graphic software is available on the notebooks and on the IMUK-cluster.

Steering by Unix Environment Variables

Most features of PALM are controlled by the parameter file but a few are exclusively controlled by unix environment variables. The most important one is `write_binary`.

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Variable	Meaning	Value set by <code>mrun</code> -option
<code>host</code>	host identifier that <code>mrun</code> is using for the host on which the job is running	<code>-h</code>
<code>maximum_cpu_time_allowed</code>	cpu time allowed for the job	<code>-t</code>
<code>run_identifier</code>	identification string for the run	<code>-d</code>
<code>tasks_per_node</code>	number of MPI tasks to be started on each node	<code>-T</code>
<code>write_binary</code>	switch for writing binary data to be used for restart runs	<code>-r (+setting in configuration file .mrun.config)</code>

PALM / netCDF Documentation

- ▶ A detailed description of how to use PALM and a complete list of steering parameters and their meaning can be found on the PALM-server:

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- ▶ General information about the netCDF data format can be found under

<http://www.unidata.ucar.edu/software/netcdf/>