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Sensitivity of local air quality to the interplay between small- and large-scale circulations: a large-eddy simulation study

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S1 Description of the modifications to PALM for the treatment of heterogeneous surface boundary conditions

The heterogeneous fields for H_s and T_s are specified via separate ASCII files, containing arrays with the same dimension as the computational domain (*Maronga and Raasch* (2013), Björn Maronga personal communication). The files are read into the model in the beginning of each simulation. The arrays contain the value 1 if a specific heat flux or surface temperature should be used for the corresponding model grid-cell and 0 otherwise. The values of H_s and T_s for all grid-cells are then prescribed for a freely chosen number of times during the run via a separately read ASCII list. The use of mixed BC is reached by running the model with the Dirichlet BC and correcting H_s back to the prescribed value over the land surface area for every time step, including a correction of the calculation of the friction velocity and temperature in the Prandtl layer routine. At each grid-point, either H_s or T_s have to be prescribed.

S2 Second order statistics from resolution sensitivity runs.

The vertical kinematic heat fluxes are calculated for two sub-areas of the computational domain, over the fjord and over the valley land surface (Fig. S1). The area over the fjord for case 3 shows a well developed convective ABL (Fig. S2). The subgrid-scale heat flux decreases rapidly over the fjord surface and is already smaller than the resolved-scale flux at the first vertical level above the surface centred at 5 m height. Over the valley land surface the subgrid-scale fluxes are decaying fast as well but the signal does not show a clearly developed inversion ABL. The reason for this is that the surface is not flat like over the fjord. Only 1 % of area 2 has a surface elevation of 0 m. The most frequent surface elevation in area 2 is 30 m with 38 % prevalence. The highest surface elevation is 60 m with 1 % prevalence again. For the higher/lower resolution simulations the distribution of surface height is slightly different dependent on the discretisation of the surface height within PALM. This also makes a comparison of the simulations with different resolutions difficult. Over the fjord, the profiles with the three different resolutions are similar above 50 m height with some minor differences in the fluxes below. Over the land fraction there is a distinct difference in the minimum of the resolved-scale heat fluxes possibly due to the different surface heights. Above 100 m, however, the profiles are fully collapsed on top of each other for the simulations with 5 and 10 m resolution, whereas they remain different for the lowest resolution of 20 m. This indicates that a 10 m resolution can be seen as a reasonable compromise between the highest possible resolution and computational costs, whereas a resolution of 20 m might be too low, especially also when considering the shallow inversions that are to be resolved.

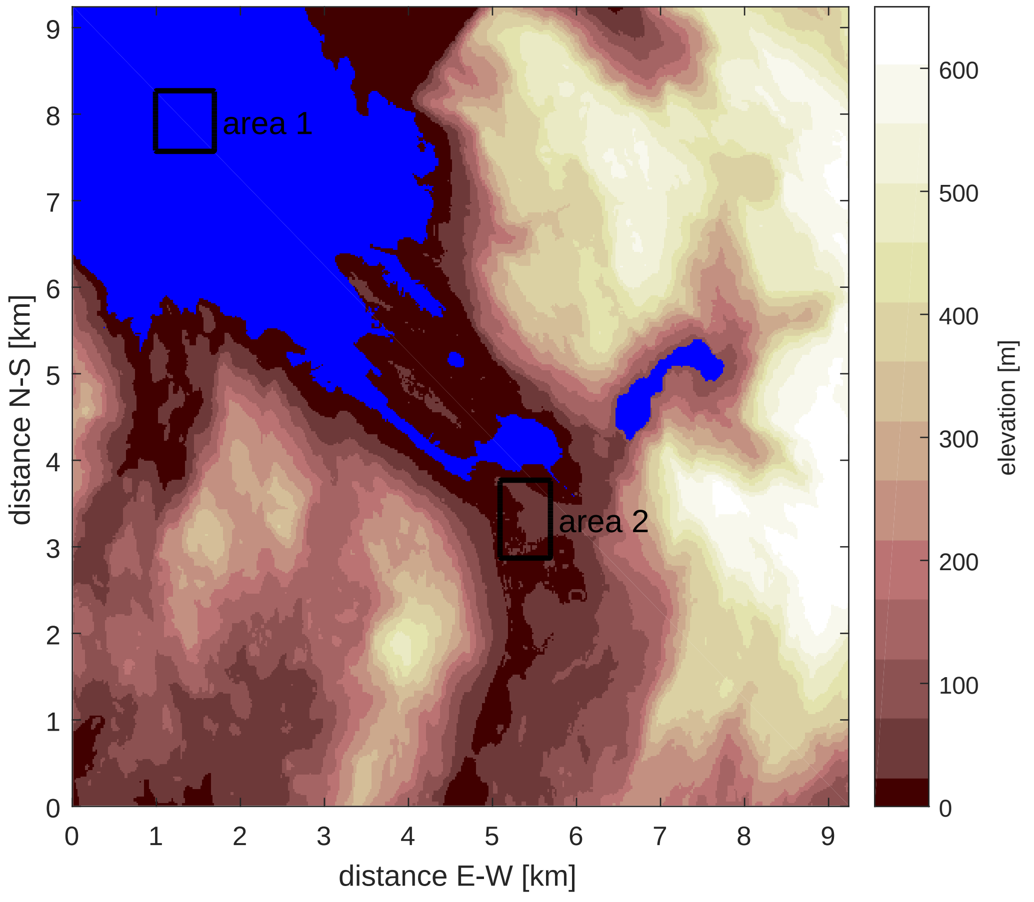

Fig. S1: Areas for calculation of second order statistics.

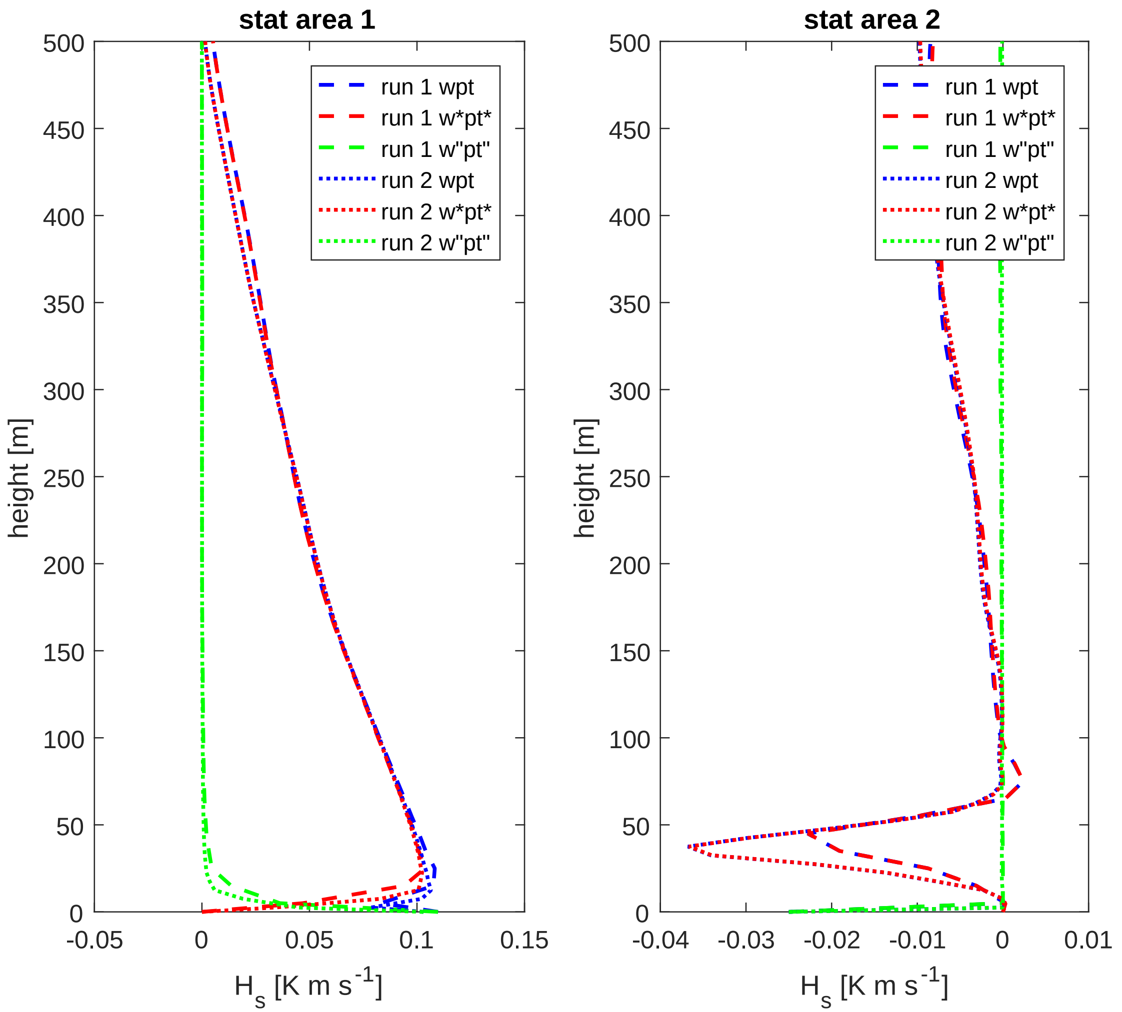

Fig. S2: Vertical heat fluxes over the fjord (left panel) and the valley surface (right panel) as indicated in Fig. S1. Run 1 refers to the baseline simulation Case 3. Run 2 refers to a test-simulation with the same setup but double resolution (5 m). The variables w“pt” and w*pt* are the subgrid- and resolved-scale heat fluxes and wpt are the total heat fluxes.

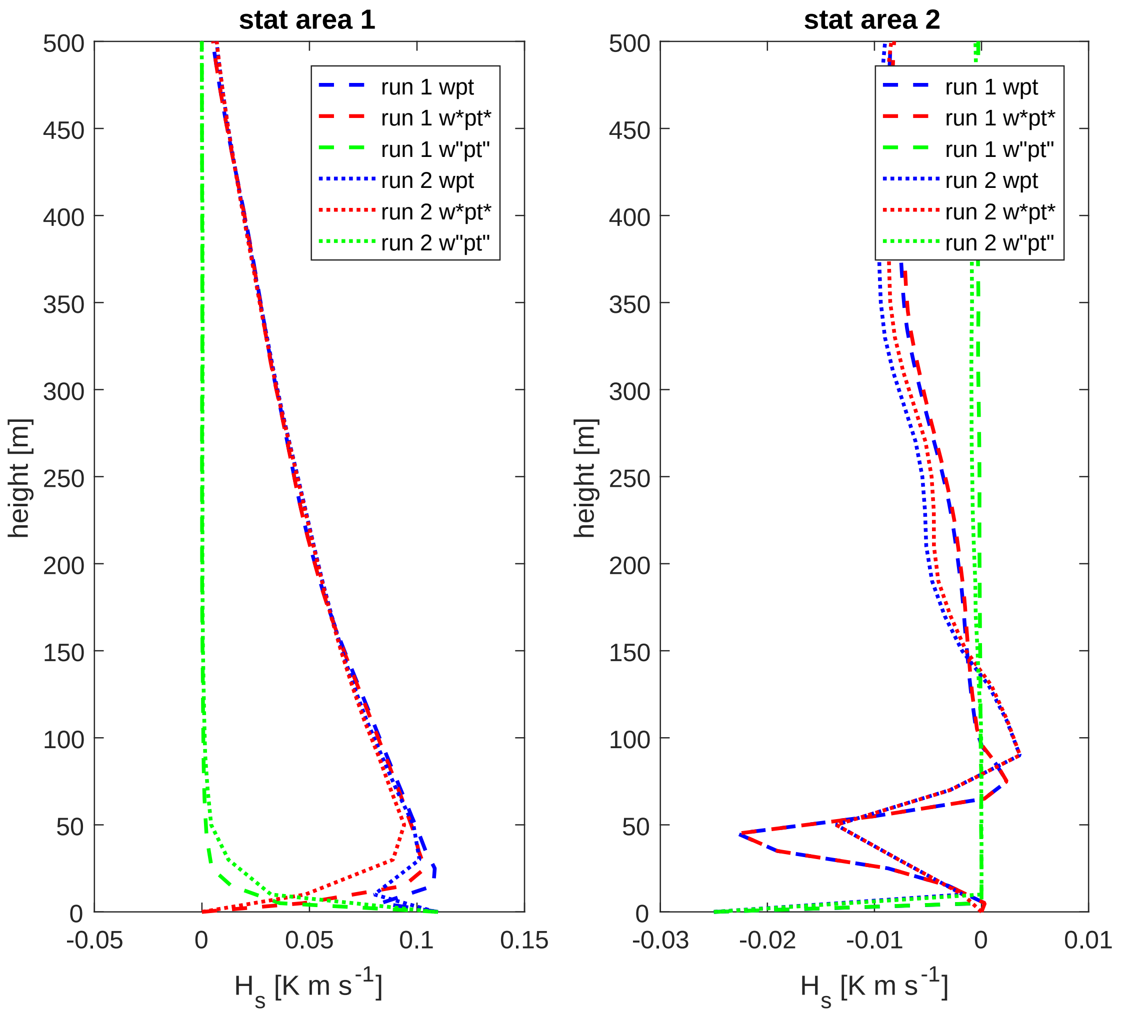

Fig. S3: Same as Fig. S2 but for a test-simulation with the same setup as Case 3 with half resolution (20 m)