

# Full year simulations vs scenarios simulations in the SZE pollution model

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# Unsteady microscale simulations

# Dispersion model in **OpenFOAM**

1. Wind field computation: URANS with k-eps turbulence model for incompressible fluids

$$\begin{aligned} \nabla \cdot (\rho \mathbf{u}) &= 0\\ \frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) &= \mathbf{g} + \nabla \cdot \overline{(\tau)} - \nabla \cdot (\rho \mathbf{R})\\ \frac{D}{Dt}(\rho k) &= \nabla \cdot (\rho D_k \nabla k) + P - \rho \epsilon\\ \frac{D}{Dt}(\rho \epsilon) &= \nabla \cdot (\rho D_\epsilon \nabla \epsilon) + \frac{C_1 \epsilon}{k} \left(P + C_3 \frac{2}{3} k \nabla \cdot \mathbf{u}\right) - C_2 \rho \frac{\epsilon^2}{k} \end{aligned}$$

- Steady simulations are also used (e.g. for the initial state)
- Boundary conditions: inlet conditions based on interpolated, time-dependent ECMWF wind data or generated from logarithmic wind profile, zero-gradient outflow.

2. Dispersion computation:

• s: NOx concentration from emission calculated with scalar transport with volumetric source  $S_s$ 

$$rac{\partial}{\partial t}s + \, 
abla \, \cdot ({f u} s) - \, 
abla \, \cdot (D_s \, 
abla s) = S_s$$

•  $D_s$  (mixing coeff.): Function of turbulent viscosity (from URANS) and PBL-height (from ECMWF met. sim.):

$$D_s = D_0 + b \cdot \nu_t h_{PBL}, \qquad D_0, b \text{ const.}, \ \nu_t = C_\mu \frac{k^2}{\epsilon}$$

- NOx value = *s* + background concentrations (which is given by the user or from CAMS CDS data)
- NOx is converted to NO2 by multiplying NOx and reference time series of meas. for the NO2 / NOx ratio



### Unsteady microscale simulations

# Parallel performance in **OpenFOAM**

#### Benchmarking for scalability for the NO2 simulation to Győr

- Computer: Hawk, HLRS (5632 x 2 x 64 core AMD Rome 7702), 1 node=128 core
- Mesh sizes 728k, 3.4M, 14M, which mean 4 meter, 2 meter, 1 meter ground level resolution, resp.
- Code is optimized (in collab. with EXCELLERAT CoE): ca.10 times faster than the initial settings



Mesh size   resolution	Time for simulation of 1 physical day	Time for simulation of 1 physical year	Estimated Sim. Cost on Hawk (1 node hour = €1.13)
728k (Gyor)   4 meter	0.4 hour (on 4 nodes)	5.6 days (on 4 nodes)	€540
3.4M (Gyor)   2 meter	1.5 hours (on 16 nodes)	22.7 days (on 16 nodes)	€8.800
14M (Gyor)   1 meter	6.5 hour (on 256 nodes)		



# Unsteady microscale simulations

Accuracy and performance characteristics for a full year

Participation in the CT4 Antwerp intercomparison exercise with OpenFOAM

The simulation, including evaluations of the indicators

- done consecutively, 12 times one month
- Hardware: Solyom (local cluster in Győr) and on Irene (PRACE cluster in France)
- Simulation time for 1 month: 34.4 hours (on Solyom), 25 hours (on Irene)
- Antwerp, #cells = 3.3M octree, mesh resolution = 2 m (at ground level)
- PBL height from ECMWF (coupled through Polytope API)
- Output data size = 120GB per month, 1.4 TB in total

Simulation re-done mid-October 2022 due to failure in some input data.

• Accuracy from the hourly values of the computations for January 2016: median of the relative errors is 13% (backgr. station) and 30% (street station).



# Steady microscale simulations

Scenario setups and simulations

- 128 scenario setup:
  - 32 wind directions, 4 wind speeds: 1, 2, 5, 10
- Two types of scenario setups:
  - Constant velocity scenarios, mapped to 5m/s in 4, 8, 16, 32 directional tiling
  - Variable velocity scenarios mapped to 1, 2, 5 and 10 m/s with 4, 8, 16 or 32 directions
- Scenario evaluation and NO2 calculation:



$$NO2_{approx} = F_w(t) \cdot F_m(t) \cdot F_h(t) \cdot NOx_{scenario} \cdot \frac{V_{scenario}}{V(t)} \cdot \frac{NO2_{station}(t)}{NOx_{station}(t)} + BackGroundNO2(t)$$

$$AVG(NO2_{approx}) = AVG\left(F_w(t) \cdot F_m(t) \cdot F_h(t) \cdot NOx_{scenario} \cdot \frac{V_{scenario}}{V(t)} \cdot \frac{NO2_{station}(t)}{NOx_{station}(t)} + AVG(BackGroundNO2(t))\right)$$



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# Results – Stage1 – May 6th – Urban Background

	NO	2 - Compa	aring to M	easureme	ents	1.00
Jnsteady -	0.15	0.20	1.00	0.95	0.60	- 1.00
C4C -	0.20	0.25	1.00	0.96	1.11	- 0.75
C8C -	0.22	0.26	1.00	0.96	1.11	- 0.50
C16C -	0.22	0.25	1.00	0.96	1.11	- 0.25
C32C -	0.21	0.25	1.00	0.96	1.12	- 0.00
V4V -	-0.02	0.20	0.96	0.85	0.56	0.25
V8V -	0.01	0.20	1.00	0.87	0.51	0.50
V16V -	0.03	0.18	1.00	0.86	0.51	0.75
V32V -	0.04	0.18	1.00	0.85	0.53	- 1.00
	MFB	MFE NO2 - Con	FAC2	Corr Unstead	Target Y	-1.00
- C4C	0.05	0.19	1.00	0.96	0.52	
- 80	0.07	0.18	1.00	0.96	0.51	
- C16C	0.07	0.18	1.00	0.97	0.51	
- C32C	0.07	0.18	1.00	0.96	0.52	
- 747	-0.17	0.21	0.96	0.81	0.71	
- V8V	-0.14	0.19	0.96	0.83	0.66	
79LV	-0.12	0.16	0.96	0.83		
V32V	-0.11	0.16	0.96	0.82	0.65	
	MEB	MEE	FAC2	Corr	Target	



Date



Unsteady

C4C ·

C8C

C16C -

C32C

V4V

V8V

V16V

V32V

C4C

CBC

C16C

C32C

V4V

V8V

V16V

V32V

# Results – Stage1 – May 6th – Urban Streetside



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# 1-day results, 7th and 8th of May **Urban Streetside Station**



NO2 - Comparing to Measurements									
Unsteady -	0.14	0.34	0.92	0.80	0.65	1.00			
C4C -	0.29	0.33	0.96	0.83	1.16	- 0.75			
C8C -	0.31	0.34	0.92	0.84	1.16	- 0.50			
C16C -	0.30	0.33	0.92	0.84	1.16	- 0.25			
C32C -	0.30	0.33	0.92	0.84	1.17	- 0.00			
V4V -	-0.17	0.39	0.88	0.20	1.02	0.25			
V8V -	-0.07	0.34	0.88	0.20	1.02	0.50			
V16V -	-0.08	0.35	0.88	0.20	1.02	0.75			
V32V -	-0.08	0.34	0.88	0.20	1.02	-0.75			
	MFB	MFE	FAC2	Corr	Target	1.00			

Scenarios for NO2 concentration [ug/s] from 2016-05-08 00:00:00 for X42R802: Urban Streetside station



#### NO2 - Comparing to Measurements

15.03.2023

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# Results – Stage1 – May 6th – AOI



Stage 1 AOI NO2 - compare to measurements										
Unsteady -	0.00	0.00	1.00	1.00	0.00	- 1.00				
C4C -	0.09	0.09	1.00	0.98	1.11	- 0.75				
C8C -	0.10	0.10	1.00	0.99	1.28	- 0.50				
C16C -	0.10	0.10	1.00	0.99	1.22	- 0.25				
C32C -	0.10	0.10	1.00	0.99	1.28	- 0.00				
V4V -	-0.15	0.15	1.00	0.98	0.42	0.25				
V8V -	-0.12	0.12	1.00	0.99	0.35	0.50				
V16V -	-0.09	0.10	1.00	0.99	0.29	0.75				
V32V -	-0.09	0.09	1.00	0.99	0.28	0.75				
	MEB	MEE	FAC 2	Corr	Target	1.00				

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# Results – Stage2 – Samplers





#### Samplers NO2 - Compare to measurements

Measurement -	0.00	0.00	1.00	1.00	0.00	
Unsteady -	0.11	0.15	1.00	0.74	0.81	
C4C -	0.13	0.16	1.00	0.74	0.90	
C8C -	0.14	0.17	1.00	0.74	0.96	
C16C -	0.14	0.17	1.00	0.74	0.96	
C32C -	0.14	0.17	1.00	0.73	0.95	
V4V -	-0.40	0.40	0.87	0.75	1.22	
V8V -	-0.34	0.34	0.87	0.74	1.14	
V16V -	-0.35	0.35	0.87	0.74	1.16	
V32V -	-0.34	0.34	0.87	0.74	1.14	
	MFB	MFE	FAC2	Corr	Target	

Samplers NO2 - Compare to Unsteady									
Measurement -	-0.11	0.15	1.00	0.74	1.13	- 1.00			
Unsteady -	0.00	0.00	1.00	1.00	0.00	- 0.75			
C4C -	0.02	0.03	1.00	0.99	0.18	- 0.50			
C8C -	0.03	0.04	1.00	0.99	0.24	- 0.25			
C16C -	0.03	0.03	1.00	1.00	0.22				
C32C -	0.03	0.03	1.00	1.00	0.22	- 0.00			
V4V -	-0.50	0.50	0.91	0.99	1.24	0.25			
V8V -	-0.45	0.45	0.92	0.99	1.14	0.50			
V16V -	-0.46	0.46	0.92	1.00	1.16	0.75			
V32V -	-0.45	0.45	0.92	1.00	1.14	1.00			
_	MFB	MFE	FAC2	Corr	Target	1.00			

1.00

0.75

- 0.50

- 0.25

- 0.00

- -0.25

-0.50

-0.75

-1.00

60

- 55

- 50

- 45

- 40

- 35



# Results – Stage2 – AOI



	Stage 2	AOI NO2 -	compare	to measu	irements	
Unsteady -	0.00	0.00	1.00	1.00	0.00	1.00
C4C -	0.08	0.08	1.00	0.98	0.76	- 0.75
C8C -	0.09	0.09	1.00	0.99	0.81	- 0.50
C16C -	0.09	0.09	1.00	0.99	0.81	- 0.25
C32C -	0.09	0.09	1.00	0.99	0.85	- 0.00
V4V -	-0.15	0.15	1.00	0.98	0.42	0.25
V8V -	-0.13	0.13	1.00	0.99	0.34	0.50
V16V -	-0.12	0.12	1.00	0.99	0.34	0.75
V32V -	-0.12	0.12	1.00	0.99	0.32	0.75
	MFB	MFE	FAC2	Corr	Target	

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- 80

60

- 40

- 20

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# Results – Stage2 – Station 801

NO2 concentration [ug/s] from 2016-04-30 00:00:00 for X42R801: Urban Background station



NO2 - Comparing to Measurements

NO2 - Comparing to Measurements								
Unsteady -	-0.01	0.18	0.99	0.88	0.49	- 1.00		
C4C -	-0.01	0.18	0.99	0.88	0.67	- 0.75		
C8C -	0.01	0.18	0.99	0.89	0.68	- 0.50		
C16C -	0.01	0.18	1.00	0.89	0.67	- 0.25		
C32C -	0.01	0.18	1.00	0.89	0.67	- 0.00		
V4V -	-0.23	0.31	0.89	0.26	0.98	0.25		
V8V -	-0.19	0.28	0.91	0.25	0.98	0.50		
V16V -	-0.19	0.28	0.91	0.26	0.98	0.75		
V32V -	-0.18	0.28	0.91	0.25	0.98			
	MFB	MFE	FAC2	Corr	Target	<u> </u>		

						- 1.00
- C4C	0.00	0.11	0.99	0.90	0.60	- 0.75
- 80	0.02	0.10	0.99	0.91	0.60	-0.75
- C16C	0.02	0.10	0.99	0.91	0.59	- 0.50
- C32C	0.02	0.10	0.99	0.92	0.60	- 0.00
- V4V	-0.22	0.24	0.94	0.36	0.97	- 0.00
V8V -	-0.18	0.21	0.96	0.36	0.97	0.25
V16V	-0.18	0.20	0.96	0.35	0.97	0.50
V32V	-0.18	0.20	0.96	0.35	0.97	0.75
	MEB	MFE	FAC2	Corr	Target	



# Results – Stage2 – Station 802

NO2 concentration [ug/s] from 2016-04-30 00:00:00 for X42R802: Urban Streetside station



- 1.00

- 0.75

- 0.50

- 0.25

- 0.00

- -0.25

-0.50

-0.75

- -1.00

Unsteady -	0.11	0.27	0.94	0.81	0.66	
C4C -	0.11	0.25	0.98	0.84	0.88	
C8C -	0.12	0.25	0.97	0.85	0.91	
C16C -	0.12	0.25	0.97	0.85	0.90	
C32C -	0.12	0.25	0.98	0.85	0.90	
V4V -	-0.13	0.36	0.88	0.23	0.99	
V8V -	-0.10	0.35	0.88	0.23	0.98	
V16V -	-0.10	0.34	0.88	0.23	0.99	
V32V -	-0.10	0.34	0.88	0.23	0.98	
	MFB	MFE	FAC2	Corr	Target	

	NO2 - Comparing to Unsteady									
- 66	-0.00	0.13	0.99	0.88	0.67	- 1.00				
- 80	0.01	0.12	0.99	0.89	0.67	- 0.75				
-	0.01	0.12	0.99	0.89	0.67	- 0.50				
- C	0.01	0.12	0.99	0.89	0.67	- 0.25				
V4V -	-0.25	0.27	0.92	0.37	0.98	- 0.00				
V8V -	-0.22	0.25	0.93	0.37	0.97	0.25				
V16V	-0.22	0.24	0.94	0.37	0.97	0.50				
V32V	-0.22	0.24	0.94	0.37	0.97	0.75				
-	MFB	MFE	FAC2	Corr	Target	1.00				



# Results – Stage3 – AOI



	Stage 3	AOI NO2 -	compare	to measu	irements	1 00
Unsteady -	0.00	0.00	1.00	1.00	0.00	1.00
C4C -	0.09	0.09	1.00	0.97	1.00	- 0.75
C8C -	0.10	0.10	1.00	0.98	1.21	- 0.50
C16C -	0.10	0.10	1.00	0.99	1.19	- 0.25
C32C -	0.10	0.10	1.00	0.99	1.22	- 0.00
V4V -	-0.10	0.10	1.00	0.98	0.32	0.25
V8V -	-0.07	0.08	1.00	0.99	0.25	0.50
V16V -	-0.08	0.08	1.00	0.99	0.24	0.75
V32V -	-0.07	0.08	1.00	0.99	0.25	0.75
	MFB	MFE	FAC2	Corr	Target	1.00

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# Results – Stage3 – Stations – Statistics only

	NO2 - Comparing to Measurements					1.00	NO2 - Comparing to Unsteady						1.00
Unsteady -	-0.04	0.17	0.99	0.85	0.53	- 1.00	- <del>6</del>	0.03	0.09	0.99	0.92	0.58	- 1.00
C4C -	-0.01	0.15	0.99	0.91	0.48	- 0.75	28 -	0.04	0.09	0.99	0.92	0.60	- 0.75
C8C -	-0.00	0.15	1.00	0.91	0.47	- 0.50	- 19 1	0.04	0.09	0.99	0.92	0.60	- 0.50
C16C -	-0.00	0.15	1.00	0.91	0.47	- 0.25	- 2C	0.04	0.09	0 99	0.92	0.60	- 0.25
C32C -	-0.00	0.15	1.00	0.91	0.47	- 0.00	0 \	0.01	0100	0.55			- 0.00
V4V -	-0.19	0.28	0.92	0.22	0.99	0.25	- V4	-0.16	0.18	0.96	0.32	0.97	0.25
V8V -	-0.17	0.26	0.93	0.22	0.99	0.50	V8V -	-0.13	0.16	0.97	0.31	0.96	0.50
V16V -	-0.17	0.26	0.93	0.23	0.98	-0.50	716V	-0.13	0.16	0.97	0.32	0.96	-0.50
V32V -	-0.17	0.25	0.93	0.23	0.98	0.75	/ J2V	-0.13	0.16	0.97	0.33	0.96	0.75
	MFB	MFE	FAC2	Corr	Target	1.00	>	MFB	MFE	FAC2	Corr	Target	1.00
NO2 - Comparing to Measurements						NO2 - Comparing to Unsteady							
	NO	2 - Compa	aring to M	easureme	ents	1.00		ı	NO2 - Con	nparing to	Unstead	У	1.00
Unsteady -	NO2 0.08	2 - Compa 0.23	aring to M 0.97	easureme 0.78	ents 0.63	- 1.00	- C4C	0.03	NO2 - Com 0.11	nparing to 0.99	Unstead 0.89	<b>y</b> 0.72	- 1.00
Unsteady - C4C -	NO2 0.08 0.11	2 - Compa 0.23 0.20	aring to M 0.97 0.99	easureme 0.78 0.87	ents 0.63 0.66	- 1.00 - 0.75	C8C C4C	0.03 0.04	NO2 - Com 0.11 0.10	nparing to 0.99 0.99	0 Unstead 0.89 0.89	y 0.72 0.73	- 1.00 - 0.75
Unsteady - C4C - C8C -	NO2 0.08 0.11 0.12	2 - Compa 0.23 0.20 0.20	aring to M 0.97 0.99 0.99	easureme 0.78 0.87 0.87	ents 0.63 0.66 0.67	- 1.00 - 0.75 - 0.50	16C C8C C4C	0.03 0.04 0.04	NO2 - Com 0.11 0.10 0.10	nparing to 0.99 0.99 0.99	0 Unstead 0.89 0.89 0.89	y 0.72 0.73 0.73	- 1.00 - 0.75 - 0.50
Unsteady - C4C - C8C - C16C -	NO2 0.08 0.11 0.12 0.12	2 - Compa 0.23 0.20 0.20 0.20	aring to M 0.97 0.99 0.99 0.99	easureme 0.78 0.87 0.87 0.87	ents 0.63 0.66 0.67 0.67	- 1.00 - 0.75 - 0.50 - 0.25	2C CI6C C8C C4C	0.03 0.04 0.04 0.04	NO2 - Com 0.11 0.10 0.10 0.10	nparing to 0.99 0.99 0.99 0.99	0 Unstead 0.89 0.89 0.89 0.89	y 0.72 0.73 0.73 0.73	- 1.00 - 0.75 - 0.50 - 0.25
Unsteady - C4C - C8C - C16C - C32C -	NO: 0.08 0.11 0.12 0.12 0.12	2 - Compa 0.23 0.20 0.20 0.20 0.20	aring to M 0.97 0.99 0.99 0.99 0.99	easureme 0.78 0.87 0.87 0.87 0.88	ents 0.63 0.66 0.67 0.67 0.66	- 1.00 - 0.75 - 0.50 - 0.25 - 0.00	V C32C C16C C8C C4C	0.03 0.04 0.04 0.04	NO2 - Con 0.11 0.10 0.10 0.10	nparing to 0.99 0.99 0.99 0.99	0 Unstead 0.89 0.89 0.89 0.89	y 0.72 0.73 0.73 0.73	- 1.00 - 0.75 - 0.50 - 0.25 - 0.00
Unsteady - C4C - C8C - C16C - C32C - V4V -	NO2 0.08 0.11 0.12 0.12 0.12 0.12	2 - Compa 0.23 0.20 0.20 0.20 0.20 0.32	aring to M 0.97 0.99 0.99 0.99 0.99	easureme 0.78 0.87 0.87 0.87 0.88 0.88	ents 0.63 0.66 0.67 0.67 0.66	- 1.00 - 0.75 - 0.50 - 0.25 - 0.00 0.25	V4V C32C C16C C8C C4C	0.03 0.04 0.04 0.04 -0.17	NO2 - Com 0.11 0.10 0.10 0.10 0.21	nparing to 0.99 0.99 0.99 0.99 0.94	0 Unstead 0.89 0.89 0.89 0.89 0.89	y 0.72 0.73 0.73 0.73 0.73	- 1.00 - 0.75 - 0.50 - 0.25 - 0.00 0.25
Unsteady - C4C - C8C - C16C - C32C - V4V - V8V -	NO2 0.08 0.11 0.12 0.12 0.12 -0.09 -0.07	2 - Compa 0.23 0.20 0.20 0.20 0.20 0.32 0.31	aring to M 0.97 0.99 0.99 0.99 0.99 0.90 0.91	easureme 0.78 0.87 0.87 0.87 0.88 0.19 0.19	ents 0.63 0.66 0.67 0.67 0.66 0.99	- 1.00 - 0.75 - 0.50 - 0.25 - 0.00 0.25 0.50	V8V V4V C32C C16C C8C C4C	0.03 0.04 0.04 0.04 -0.17 -0.16	NO2 - Com 0.11 0.10 0.10 0.10 0.21 0.19	nparing to 0.99 0.99 0.99 0.99 0.94 0.96	0 Unstead 0.89 0.89 0.89 0.89 0.89 0.33	y 0.72 0.73 0.73 0.73 0.73 0.96	- 1.00 - 0.75 - 0.50 - 0.25 - 0.00 0.25 0.50
Unsteady - C4C - C8C - C16C - C32C - V4V - V8V - V8V -	NO2 0.08 0.11 0.12 0.12 0.12 -0.09 -0.07 -0.07	2 - Compa 0.23 0.20 0.20 0.20 0.20 0.32 0.31 0.31	aring to M 0.97 0.99 0.99 0.99 0.99 0.90 0.91 0.92	easureme 0.78 0.87 0.87 0.87 0.88 0.19 0.19 0.19	ents 0.63 0.66 0.67 0.67 0.66 0.99 0.99	- 1.00 - 0.75 - 0.50 - 0.25 - 0.00 0.25 0.50	V16V V8V V4V C32C C16C C8C C4C	0.03 0.04 0.04 0.04 -0.17 -0.16	NO2 - Com 0.11 0.10 0.10 0.10 0.21 0.19 0.19	nparing to 0.99 0.99 0.99 0.99 0.94 0.96 0.96	Unstead 0.89 0.89 0.89 0.89 0.33 0.33	y 0.72 0.73 0.73 0.73 0.96 0.96	- 1.00 - 0.75 - 0.50 - 0.25 - 0.00 0.25 0.50
Unsteady - C4C - C8C - C16C - C32C - V4V - V8V - V16V - V16V -	NO2 0.08 0.11 0.12 0.12 0.12 -0.09 -0.07 -0.07	2 - Compa 0.23 0.20 0.20 0.20 0.32 0.31 0.31 0.31	aring to M 0.97 0.99 0.99 0.99 0.99 0.90 0.91 0.92 0.92	easureme 0.78 0.87 0.87 0.87 0.88 0.19 0.19 0.20	ents 0.63 0.66 0.67 0.66 0.99 0.99 0.99	-1.00 $-0.75$ $-0.50$ $-0.25$ $-0.00$ $0.25$ $-0.50$ $0.75$	V32V V16V V8V V4V C32C C16C C8C C4C	0.03 0.04 0.04 0.04 -0.17 -0.16 -0.16	NO2 - Com 0.11 0.10 0.10 0.10 0.21 0.19 0.19 0.19	1paring to 0.99 0.99 0.99 0.94 0.96 0.96 0.96	Unstead 0.89 0.89 0.89 0.33 0.33 0.33 0.33	y 0.72 0.73 0.73 0.73 0.96 0.96 0.96	-1.00 -0.75 -0.50 -0.25 -0.00 0.25 0.50 0.75



- 1. We have done unsteady CFD simulation for a full year with OpenFOAM for NO2 for Antwerp 2m resolution at ground level (3M cells)
  - 1. Accuracy has been tested in the CT4 intercomparison exercise
  - 2. Running time: 12\*1.5 days on a cluster and 12\*1 days on PRACE HPC
  - 3. Computational time costs on Hawk: €9.000
  - 4. The code is now 10-20 times faster than at the start of the HiDALGO-project
- 2. We have compared steady scenario simulations with the full year unsteady simulation and the measurements.
  - 1. Unsteady produce best results most of the time
  - 2. Unable to determine which scenario is best with constant wind speed.
  - 3. More investigation needed for low speed accuracy of scenario modells.

# Thank you!

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