PR- PLPM (Plume Rise Photochemical Lagrangian Particle Model): Formulation and validation of the new plume rise scheme

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A Lagrangian Dispersion Model: PLPM

(Photochemical Lagrangian Particle Model) - Bellasio et Al., 1999

- Single particle's trajectory:

$$\vec{x}(t+\Delta t) = \vec{x}(t) + \Delta t(\vec{u} + \vec{u}')$$

Deterministic term (wind mean velocity)

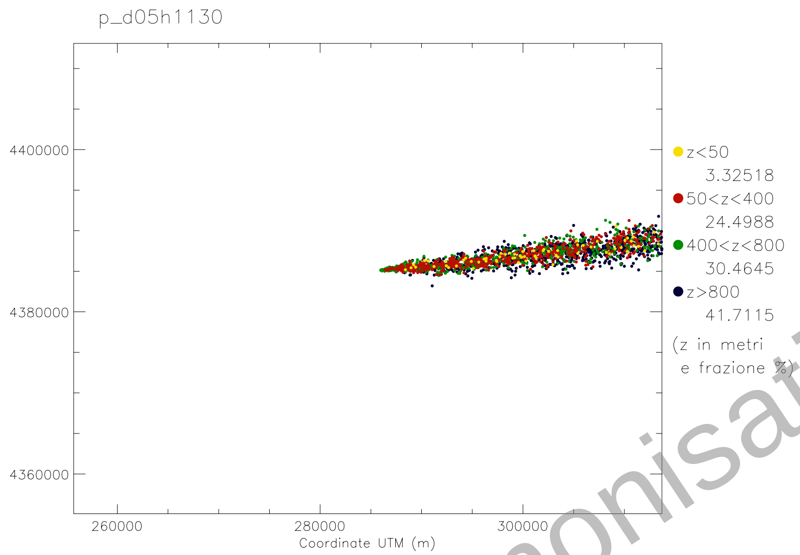
Stochastic term (turbulence)

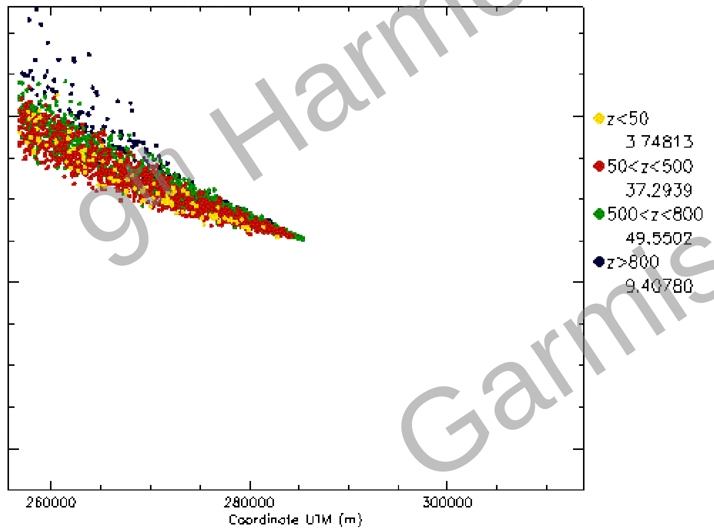
- u' achieved from Langevin equation (Thomson, 1987):

$$du_i' = a_i(\underline{x},\underline{u}',t)\,dt + b_{ij}(\underline{x},\underline{u}',t)\,d\xi_j(t)$$

Luhar and Britter (1989), Hurley and Physick (1993), Bianconi et al. (1999)

Density reconstruction



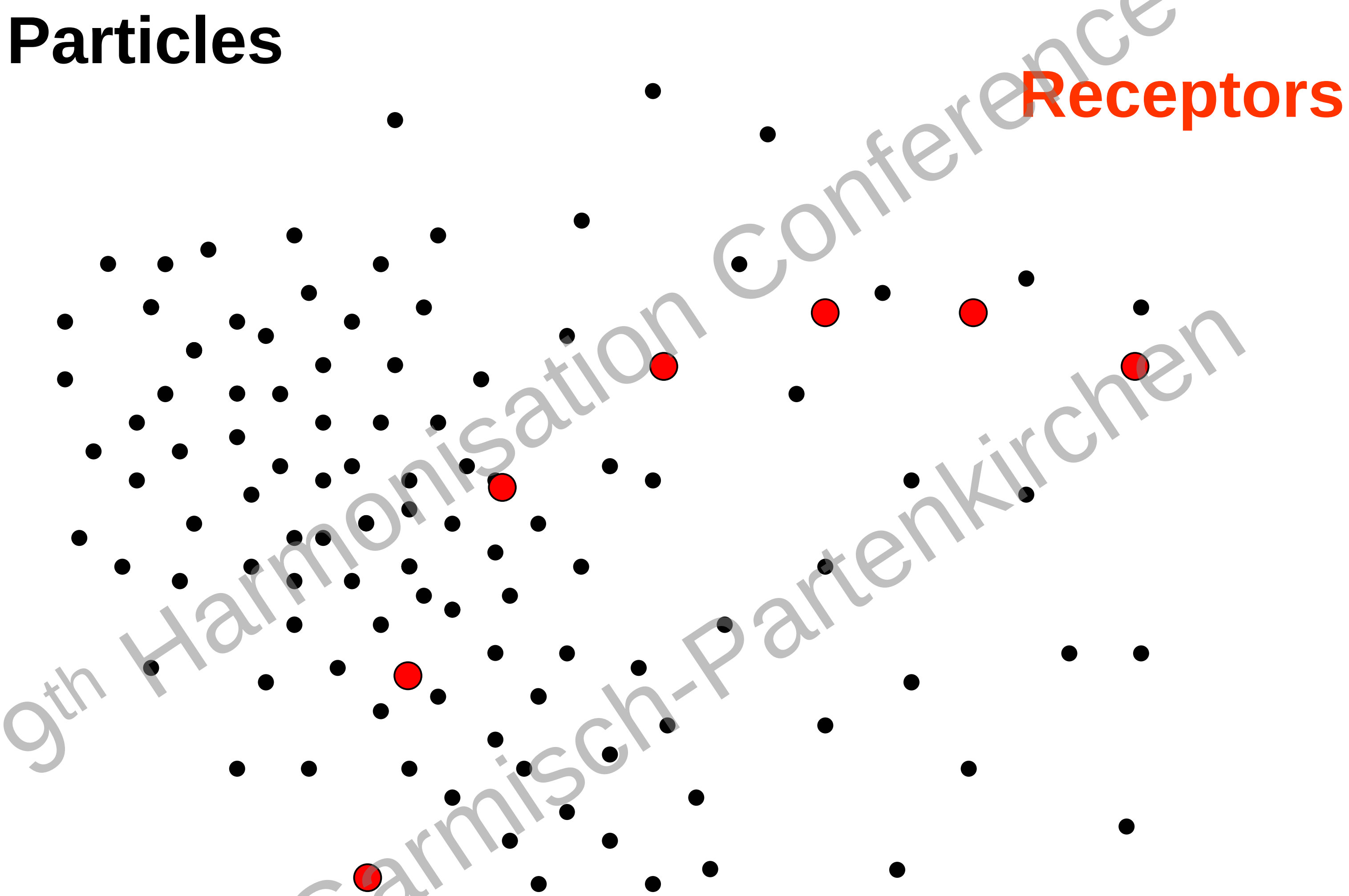


Particles positions $\mathbf{X_i}$

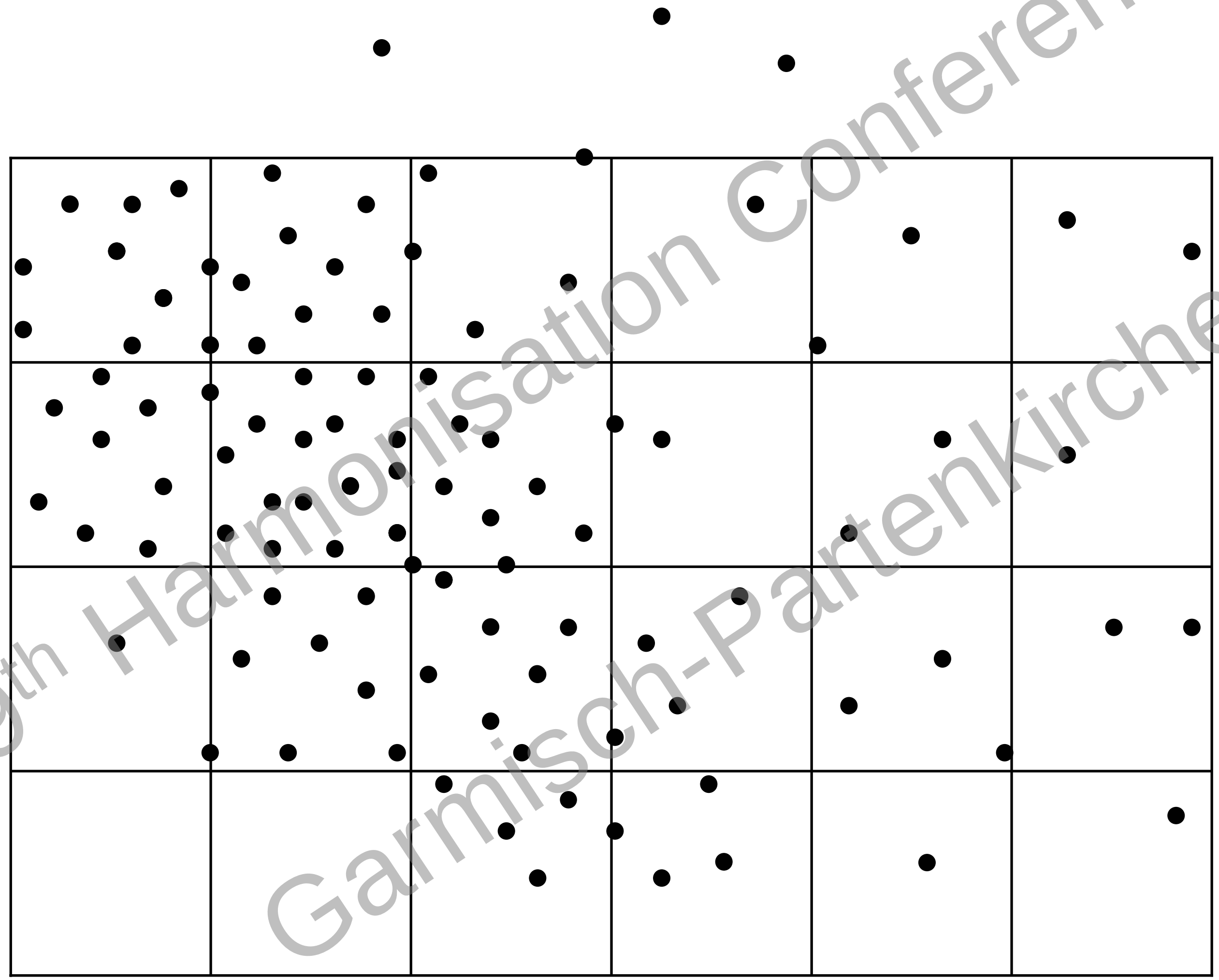
Particles masses M_i

Concentration field $C(x,y,z)$

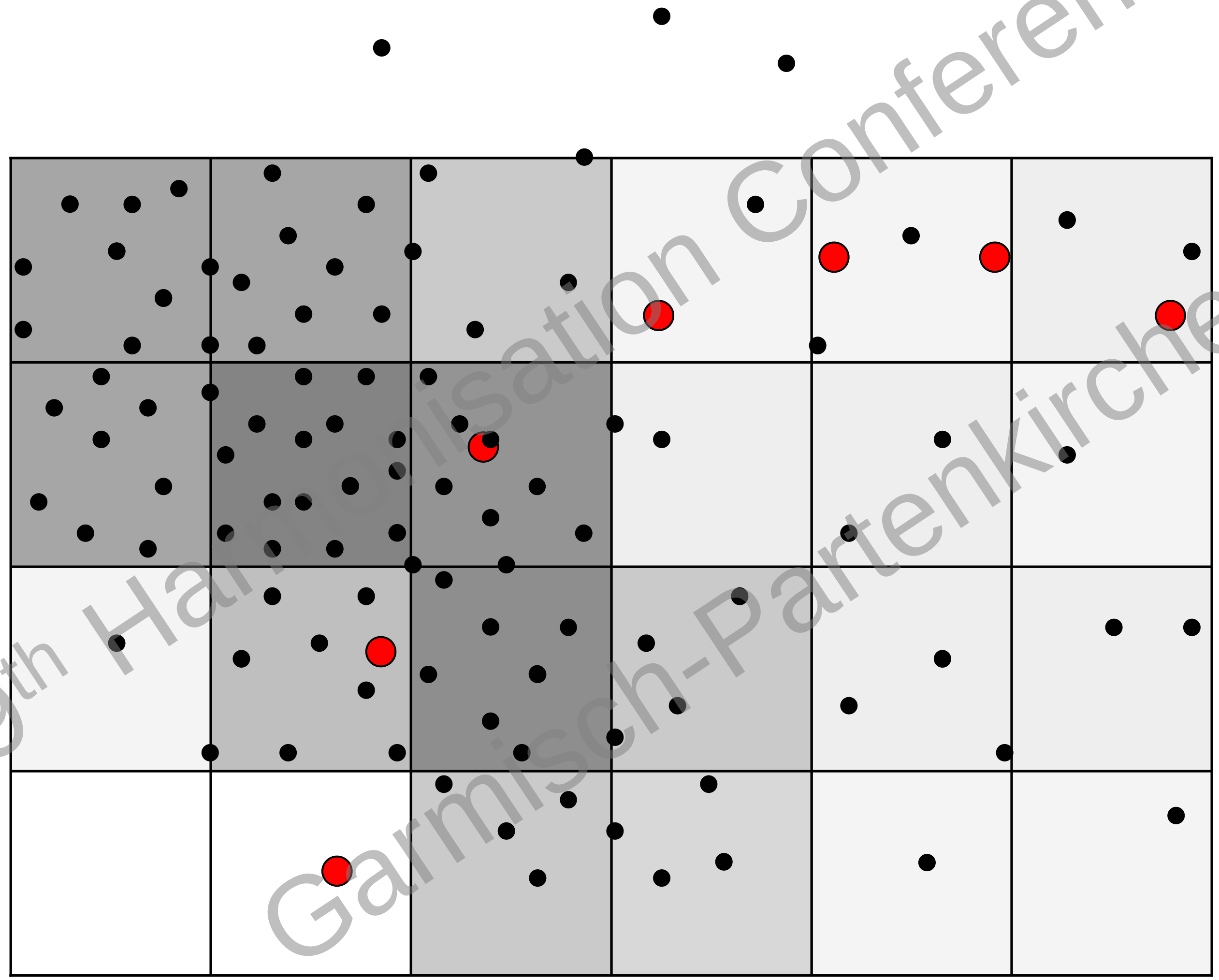
Density reconstruction



Density reconstruction – Box Counting



Density reconstruction – Box Counting



Density reconstruction - Kernel

Particles mass is distributed in space by means of a **kernel function**

$$c(x,y,z,t) = \sum_{i=1}^{n} \frac{m_i}{\lambda_x \lambda_y \lambda_z} K\left(\left|\frac{x_i - x}{\lambda_x}\right|\right) K\left(\left|\frac{y_i - y}{\lambda_y}\right|\right) K\left(\left|\frac{z_i - z}{\lambda_z}\right|\right)$$

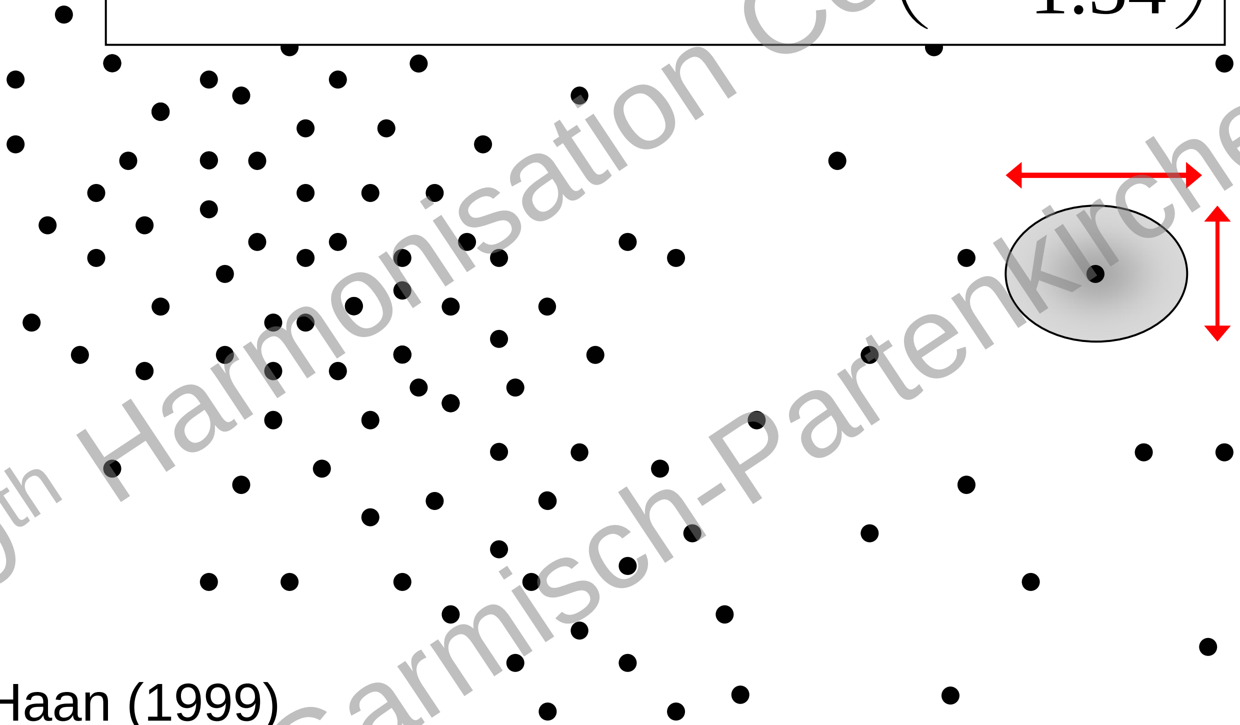
$K(x) = 0.75(1-x^2)$ if $|x| < 1$

$K(x) = 0$ otherwise

Bandwidths are crucial for density estimation

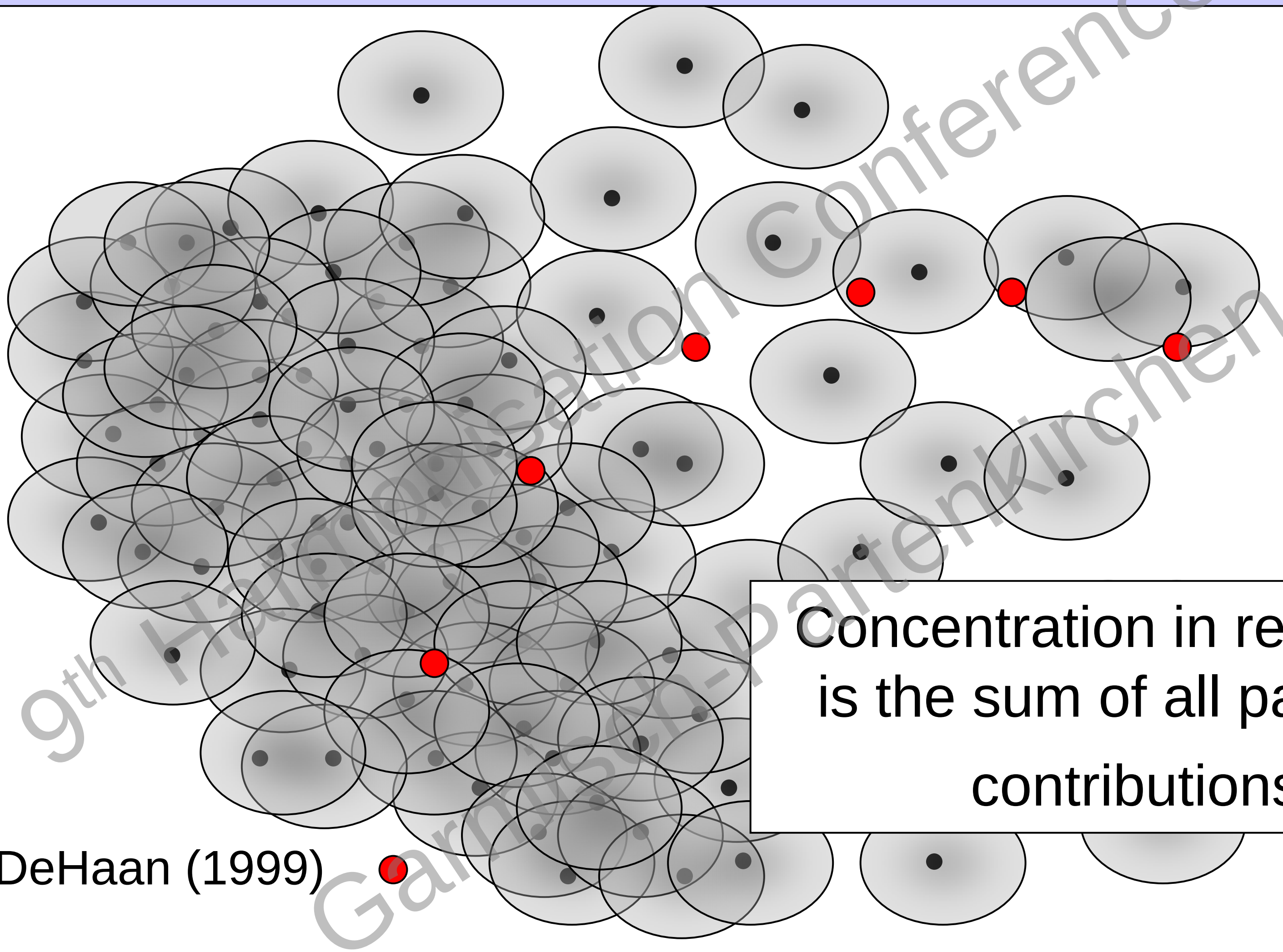
Particles-based Global (PG)

$$\lambda_i = \alpha \cdot A(K) \cdot n^{-\frac{1}{d+4}} \cdot \min\left(\sigma_i, \frac{R_i}{1.34}\right)$$



DeHaan (1999)

Particles-based Global (PG)

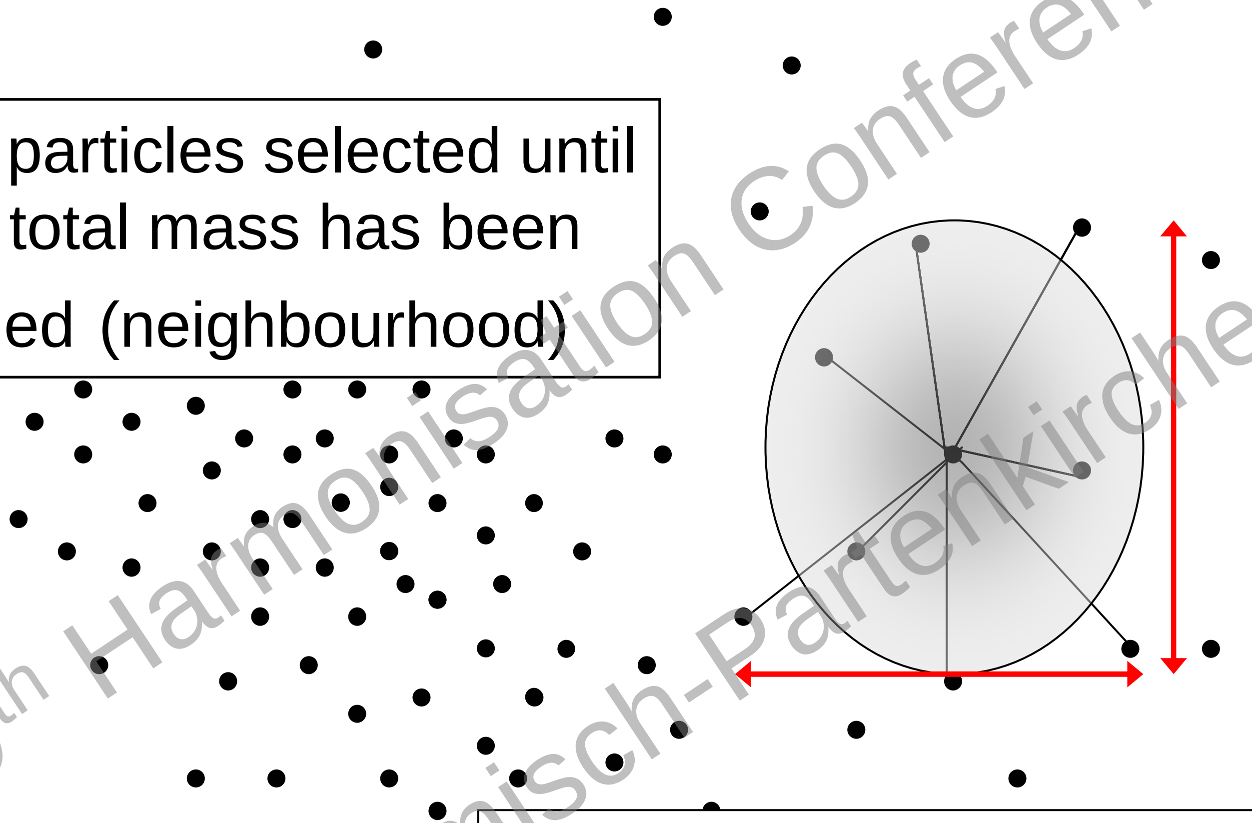


Concentration in receptors is the sum of all particles contributions

DeHaan (1999)

Particles-based Local 3-D (PL3)

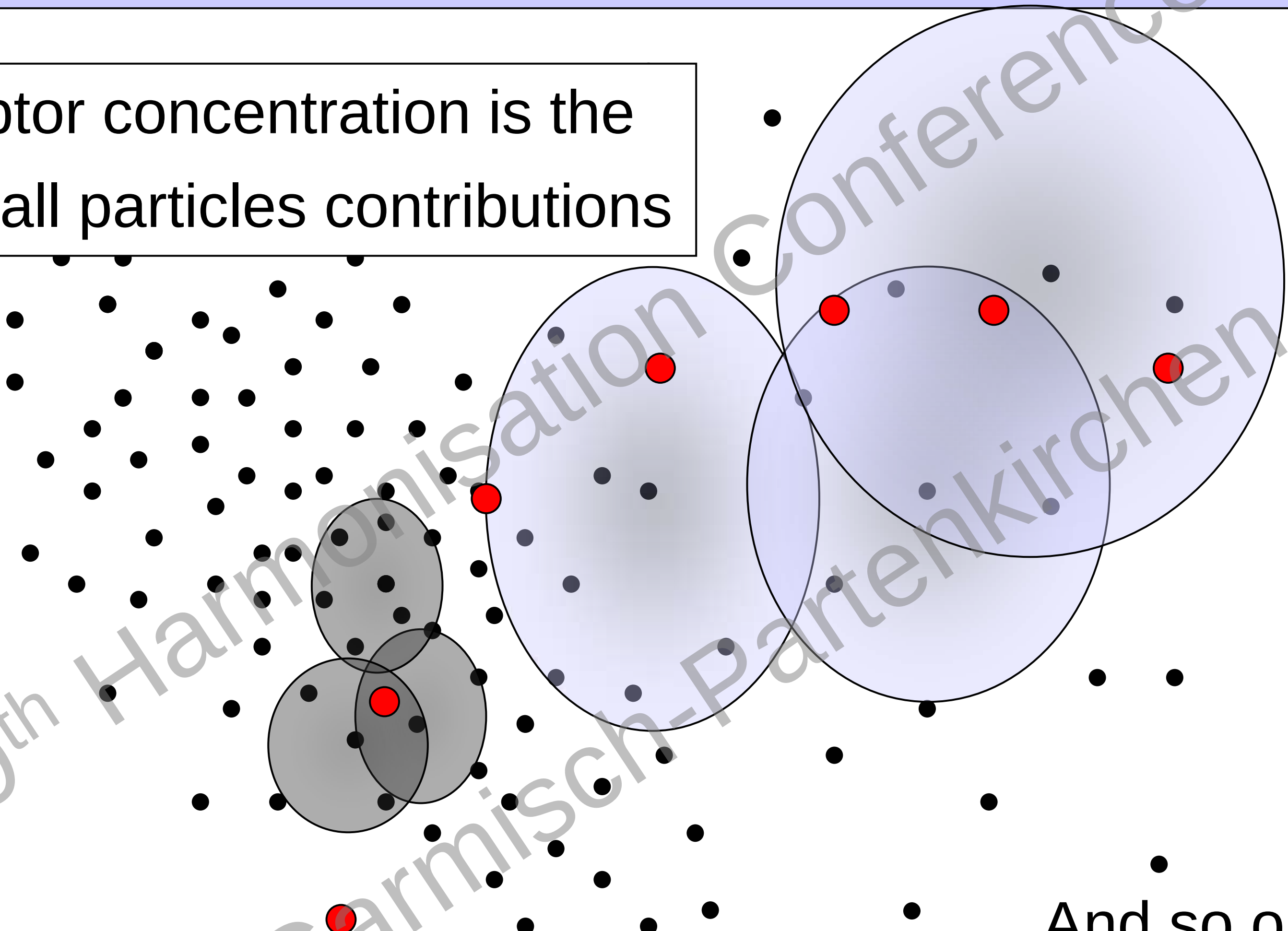
Closest particles selected until 1/8 of total mass has been reached (neighbourhood)



BWs are set as maximum projected distance of neighbours

Particles-based Local 3-D (PL3)

Receptor concentration is the sum of all particles contributions



And so on…

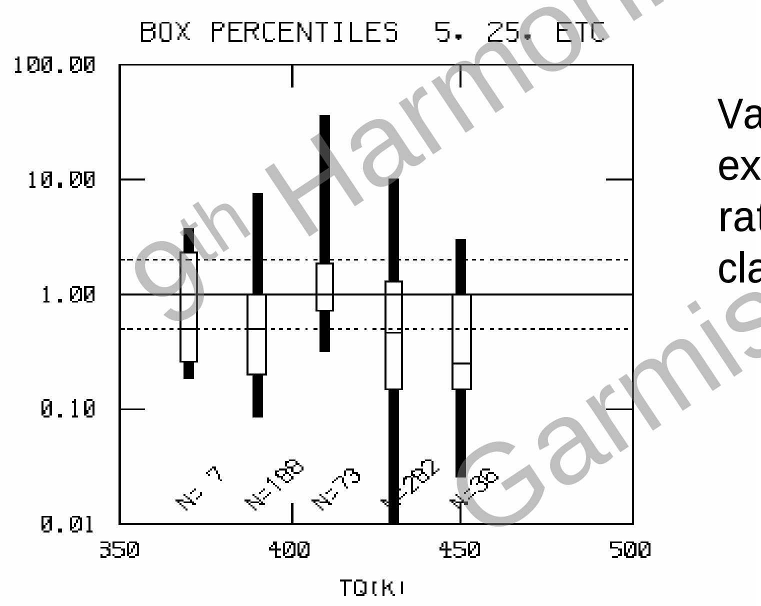
Limits of PLPM (Harmo 8)

- Plume rise empirical model (Briggs Formulae):

$$\Delta H(x) = const \cdot F_b^{\ \alpha} \overline{u}^{(-\beta)} x^{\gamma}$$

$$F_b = f(u_p, T_p, T_a, d)$$

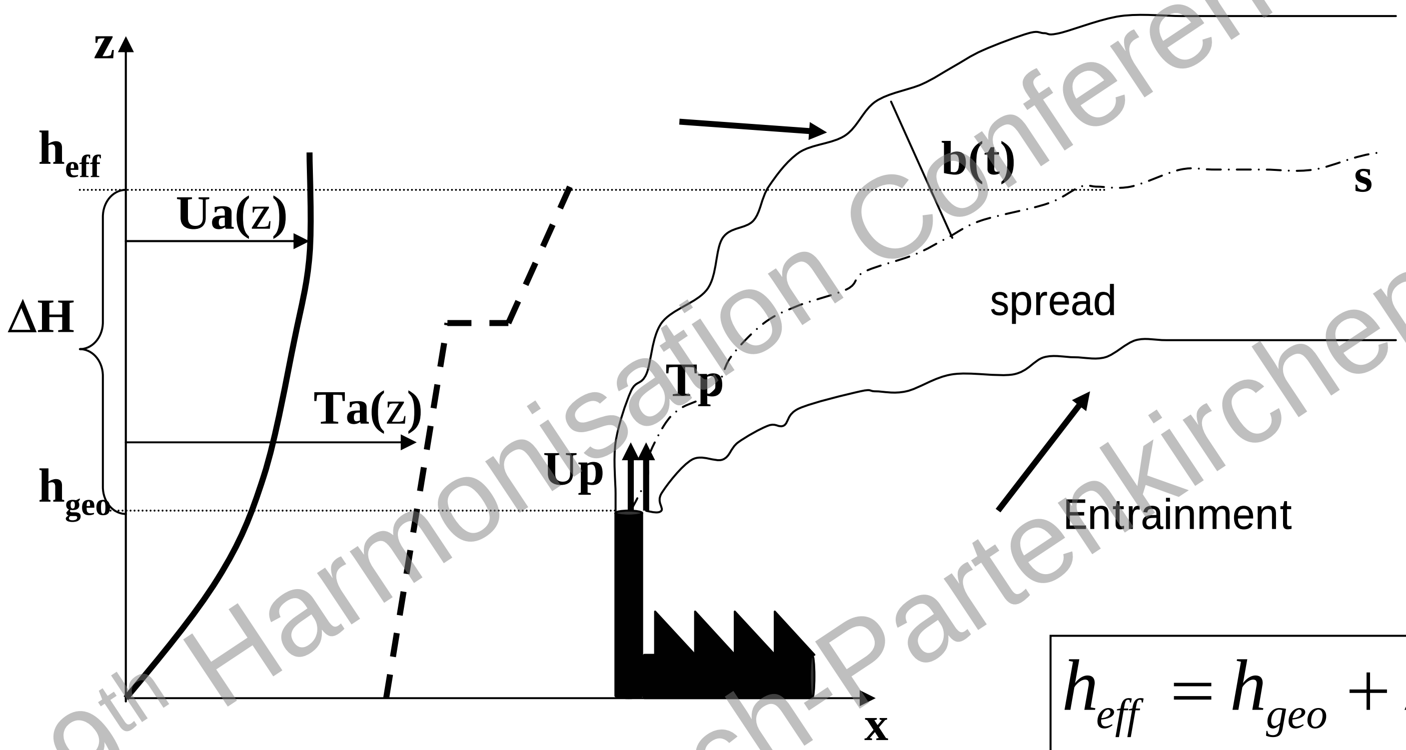
- Worse performances when T_p increases (underestimation of the ground concentration values)



Validation of PLPM based on Kincaid experiment: residual analysis of the ratios C_p/C_o. Data distribution within classes of temperature (x axis).

PLUME RISE DESCRIPTION

The Plume Rise Effect



$$h_{eff} = h_{geo} + \Delta H$$

The plume rise effect is ruled by:

- **Buoyancy** force due to hot pollutant emitted ($Tp > Ta$)→ ΔH of plume axis
- **Entrainment** of air mass at lower temperature ($Tp \rightarrow Ta$ in a finite time)
- **Spread** of the plume due to internal turbulence
- **Wind transport** ($Up \rightarrow Ua$)

The new PR-PLPM model

- Implementation of the Ooms plume rise model
  - ➢ Eulerian ODE conservation system (Ooms 1972, Ooms and Mahieu 1981, Robins et Al. 1999):

- $$\frac{d}{ds}\begin{pmatrix} F_m \\ F_{Mx} \\ F_{My} \\ F_{Mz} \\ F_h \end{pmatrix} = \begin{pmatrix} E_m \\ -F_m(du_a/ds) - D_x \\ -F_m(dv_a/ds) - D_y \\ -F_m(dw_a/ds) + B - D_z \\ -F_m c_p (d\theta_a/ds) \end{pmatrix}$$

- $P_i = \rho_i \cdot RT_i$
  $i = a, p$

Mass, momentum and enthalpy conservation equations referred to a plume control volume; perfect gas law

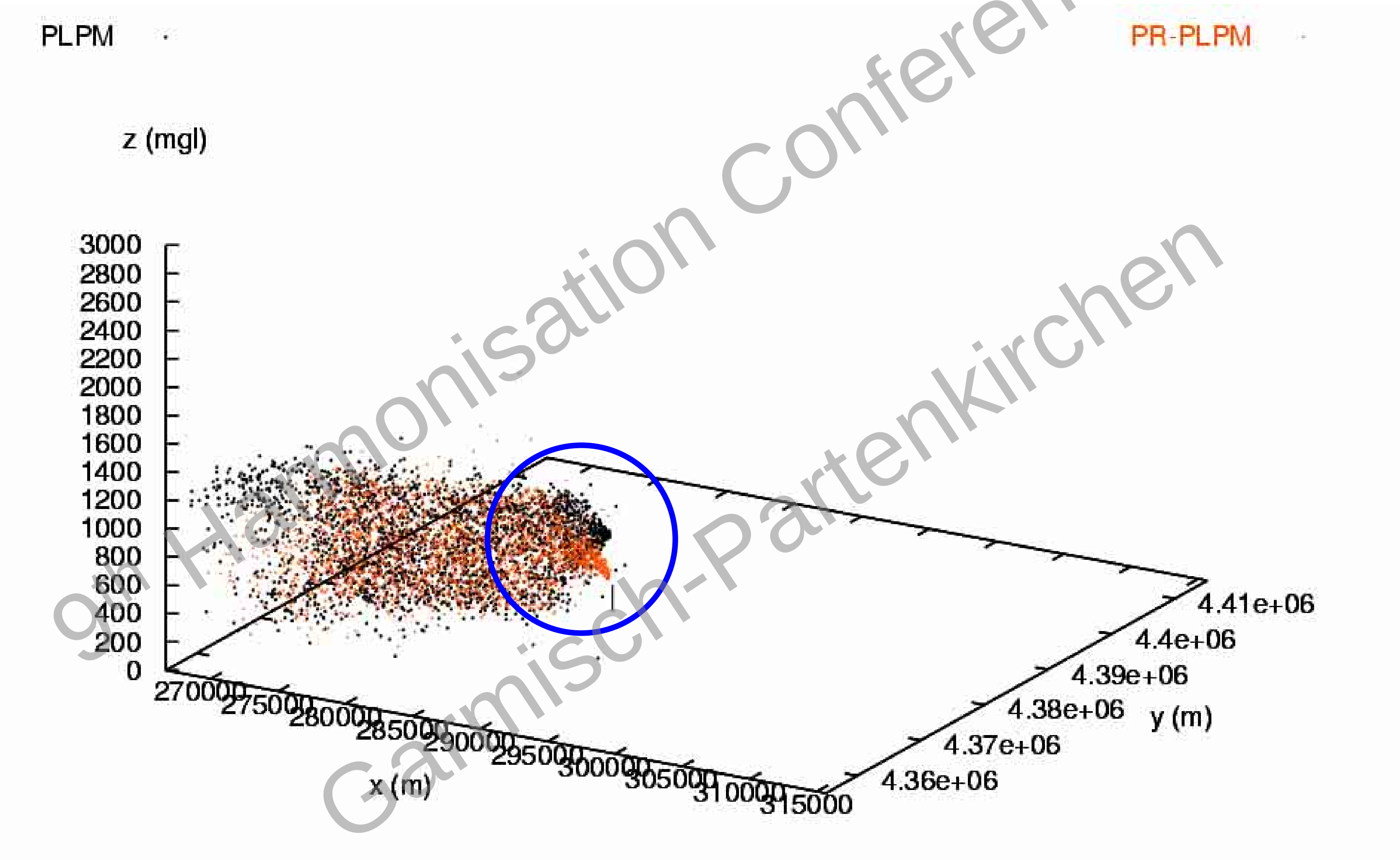
- Integration within PLPM
  - ➢ Introduction of the concept of the ***plume-particle***
  - ➢ New expression of the particle trajectory (Webster and Thomson, 2002):

$$x(t+\Delta t) = x(t) + (\bar{u} + u')\Delta t$$

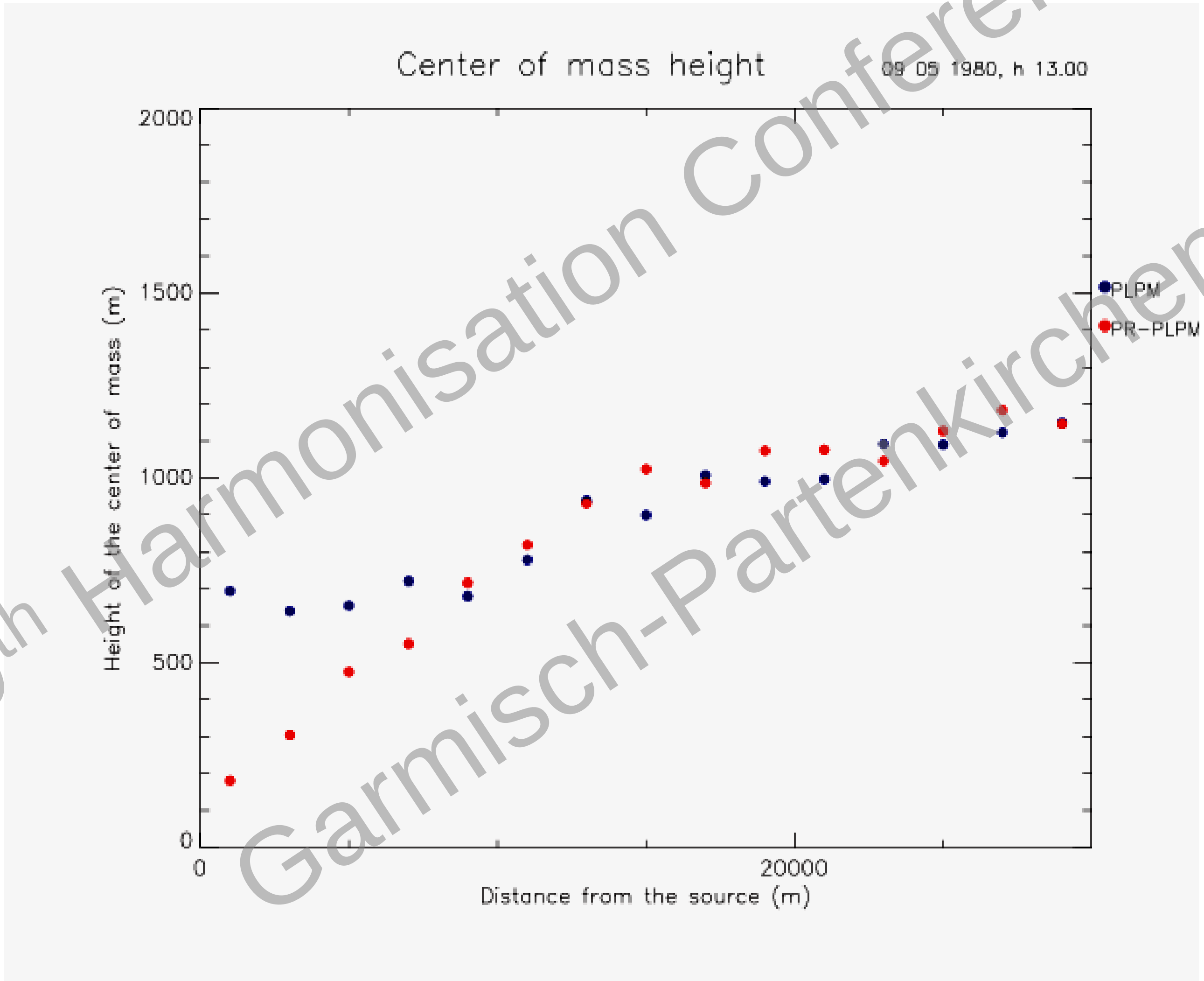
U_p
IF [$(t+\Delta t) <= 1\ h$
OR $(U_{pz} - U_{az}) >= 0.1\ m/s$]

U_a
ELSE

Results: particle distribution

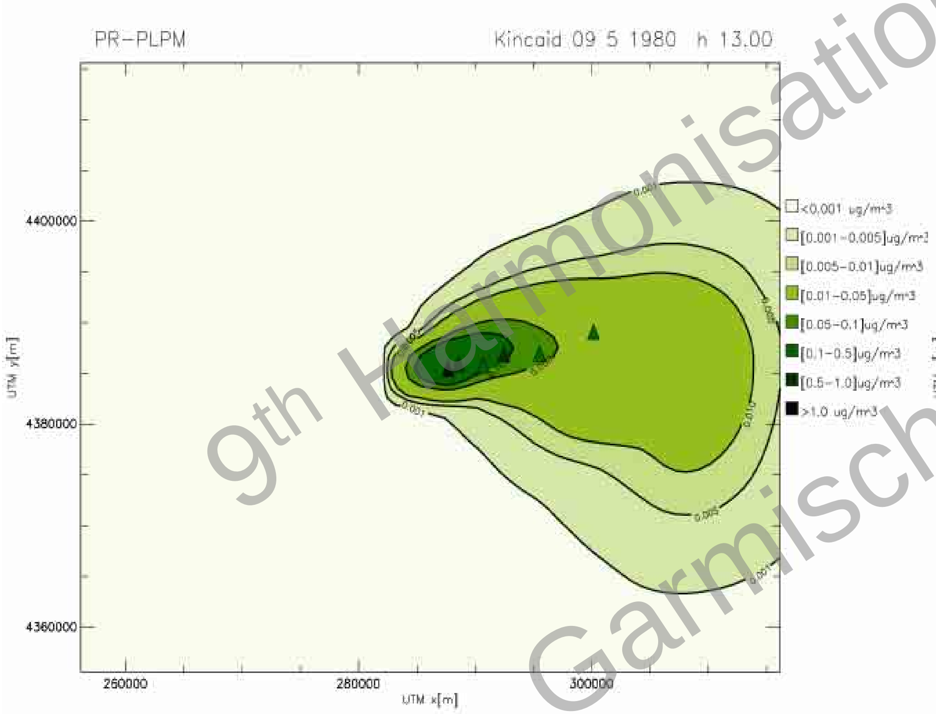


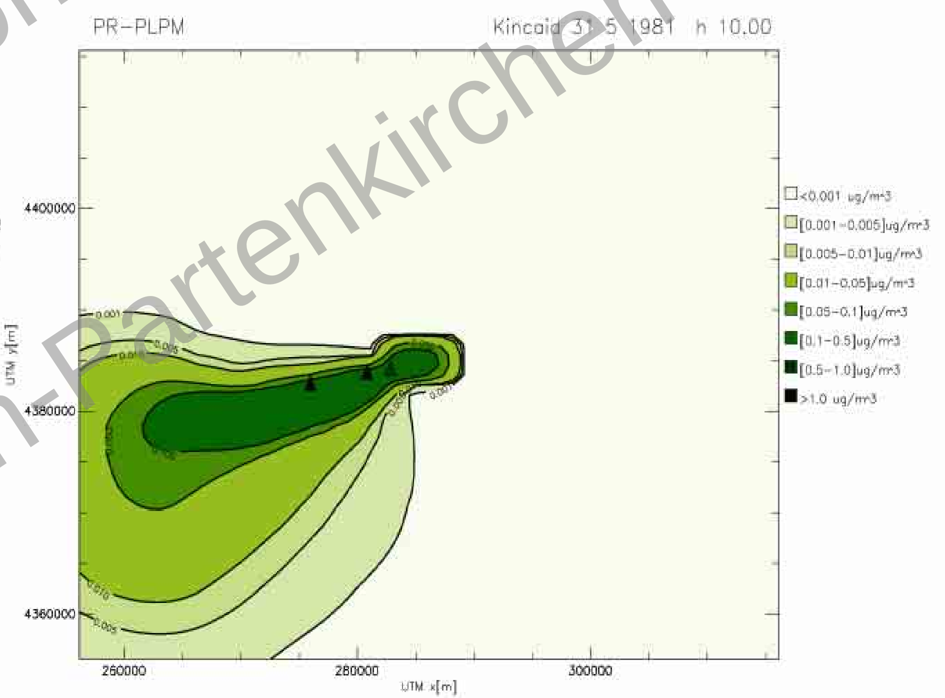
Results: height of the centre of mass



Results: Density Reconstruction (PL3)

Ground concentration maps: comparison with measured data

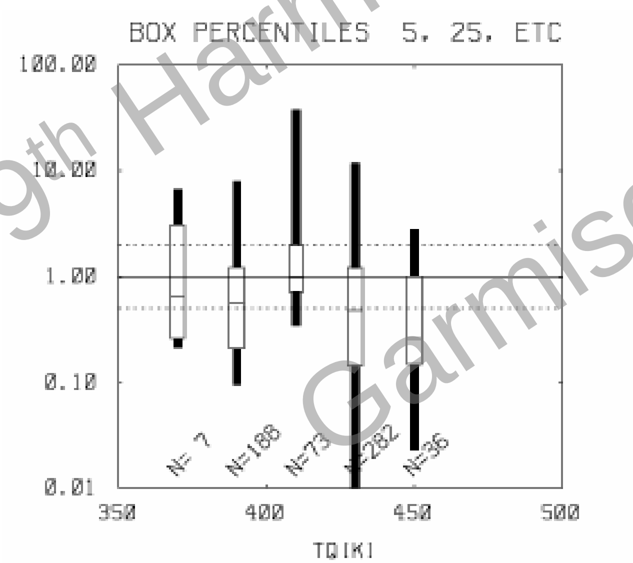


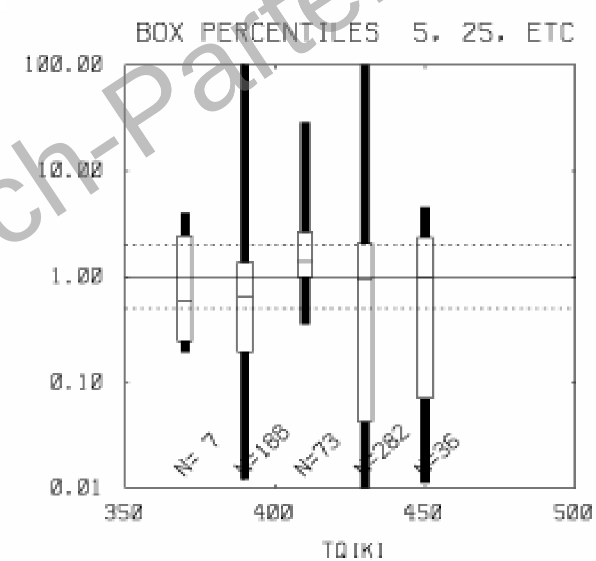


PR-PLPM Validation Results

Q=2,3 N=586	mean [(ng/m³)/(g/s)]	sigma [(ng/m3)/(g/s)]	bias [(ng/m3)/(g/s)]	NMSE	R	FAC2	FB	FS
MIS	40.96	39.26	0	0	1	1	0	0
PLPM	23.89	28.96	17.07	2.65	0.036	0.319	0.526	0.302
PR-PLPM	34.41	42.43	6.55	2.38	0.007	0.332	0.174	-0.077

Q=3 N=338	mean [(ng/m³)/(g/s)]	sigma [(ng/m3)/(g/s)]	bias [(ng/m3)/(g/s)]	NMSE	R	FAC2	FB	FS
MIS	54.34	40.25	0	0	1	1	0	0
PLPM	22.85	25.18	31.49	2.57	0.029	0.302	0.816	0.461
PR-PLPM	32.02	39.26	22.31	2	0.056	0.361	0.517	0.025





Conclusions and work in progress

- A plume rise scheme enhancing PLPM performance has been implemented and validate on the “classic” Kincaid data set.
- Full inert validation of PLPM on MVK in progress
- Tests are in progress for chemical reactions (box models and active plumes)

Chemical reactions

- Concentrations C_i in particle locations are computed every chemical step.
- Chemical mechanism computes “new” concentrations C'_i
- Particles chemical composition is reassigned proportionally to C'_i/C_i and new mass is added if necessary

Chemical reactions – in progress tests

- Dynamic time step and chemical time step.
- Is the kernel best performing in the inert case also the best performing in complex reactions?
- How complex is to use “local” inertia ellipsoid axis as kernel axis?