The use of Monte Carlo Simulations of georeferenced information to evaluate composition trends in oceanic waters

Carlos Borges[1], Carla Palma[1], Ricardo Silva[2]

[1] Instituto Hidrográfico, R. Trinas 49, 1249-093 Lisboa, Portugal

[2] Centro de Química Estrutural, Faculdade de Ciências, Universidade de Lisboa, Campo Grande, 1749-016 Lisboa, Portugal

Problem Identification:

The assessment of large oceanic areas' environmental status and evaluation of temporal trends is demanding. Impacting factors are: seasonality, heterogeneity and size.

Until recently, uncertainty associated with representative sampling was omitted from these evaluations.

Methodology:

Sampling:

Portuguese Continental Platform, between 40.12° N and 40.46° N and 8.96° W and 9.30° W
Sampling dates: October 2018 and April 2019
Number of samples, n = 20
Grid of 15 x 20 nautical miles
Distance between samples, d = 5 x 5 nautical miles
Sampling level: 25 m

Analysis:

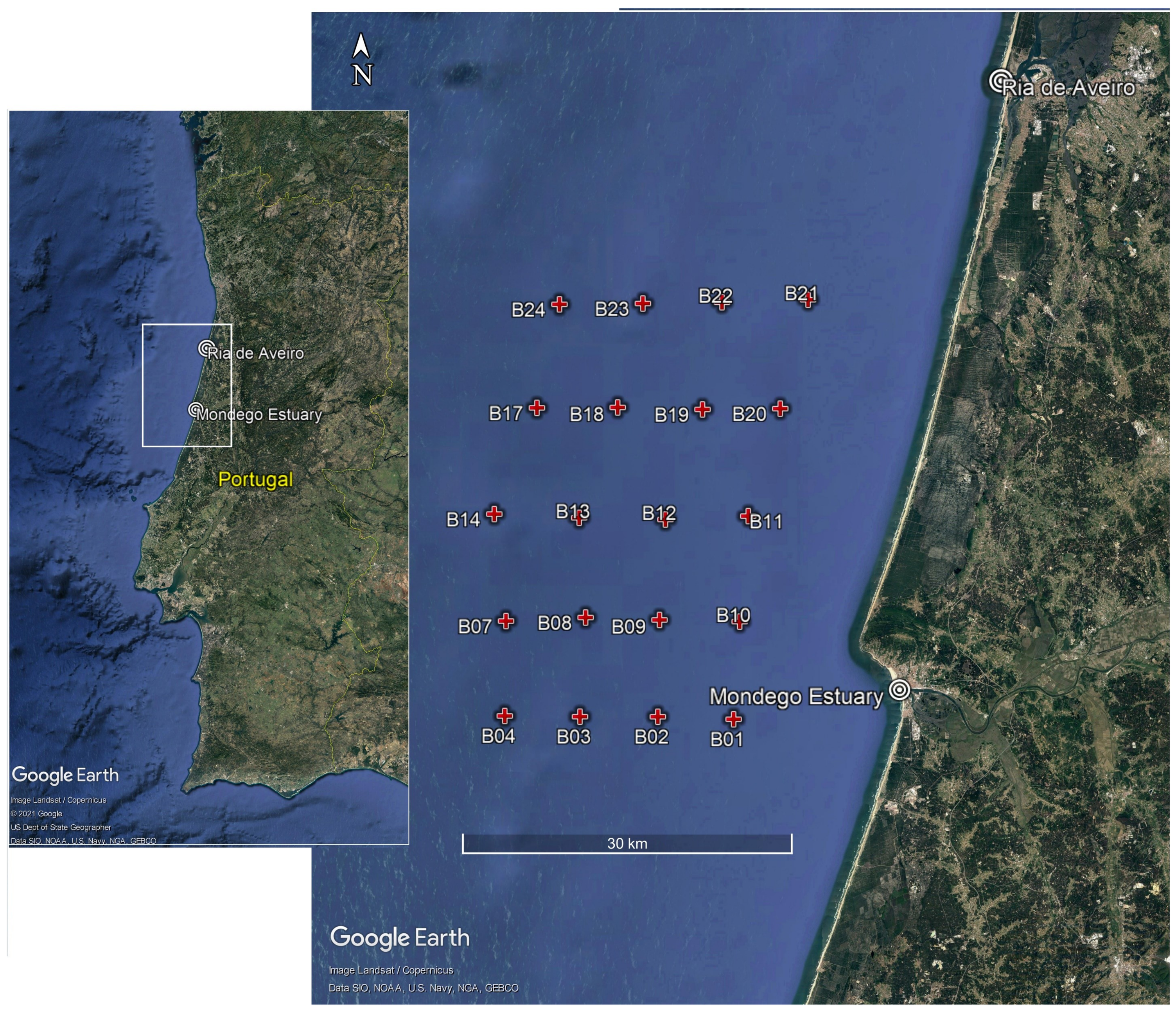
Segmented Flow Analysis

Uncertainty Modelation:

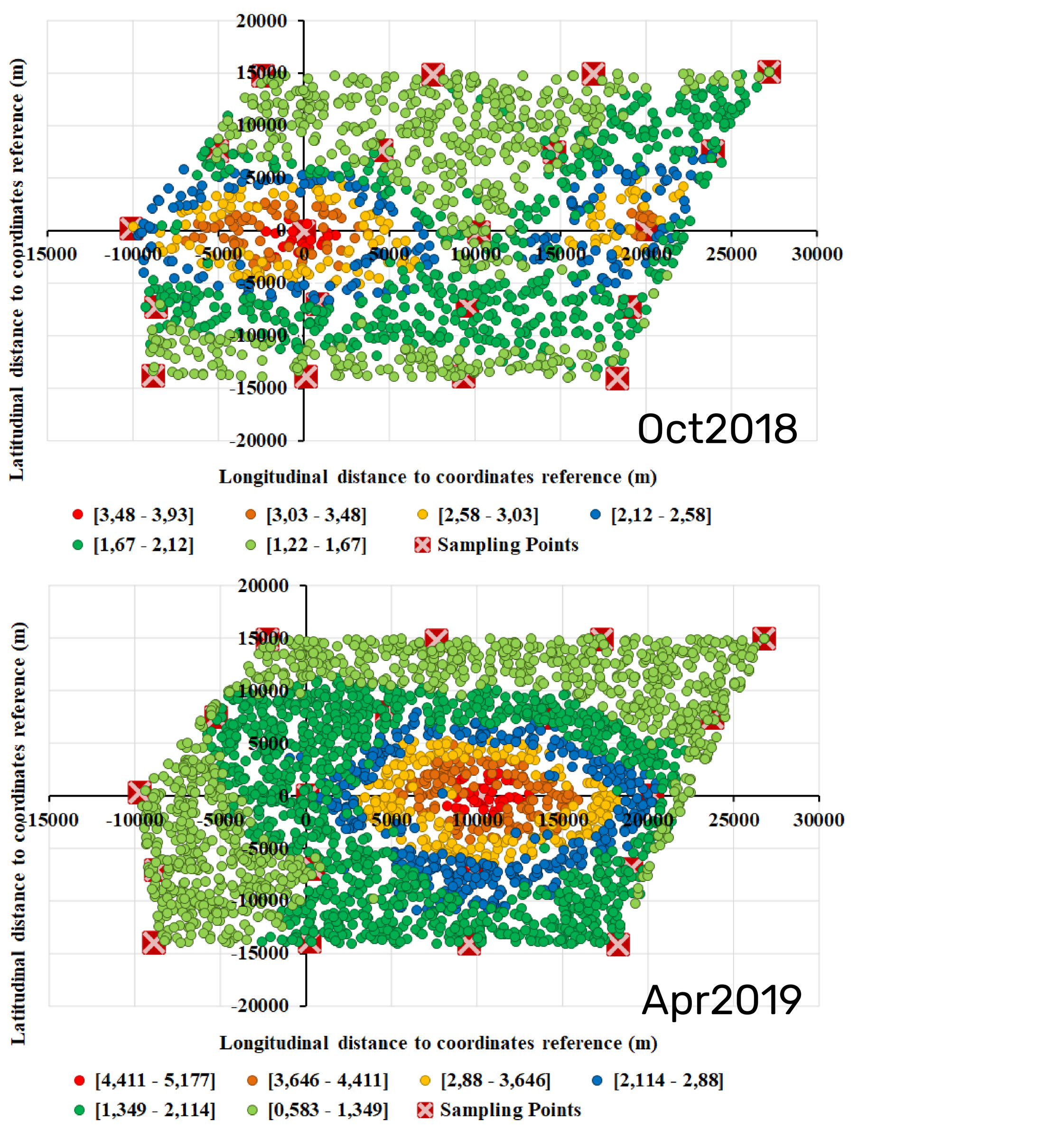
Monte Carlo Simulations of georeferenced information applied to the nutrient Silicate
Single Sampling (SS) modeling strategy used

Purpose:

Determine if mean concentration differences are meaningful and cannot be justified by system heterogeneity and/or analytical uncertainty



Location of the sampling positions (B01 to B24) where water samples were collected, at 25 m depth, on two sampling occasions (October 2018 and May 2019), implanted over Google Earth images.



Simulated variability of silicate concentration by application of the Single Sampling modulation strategy

Results:

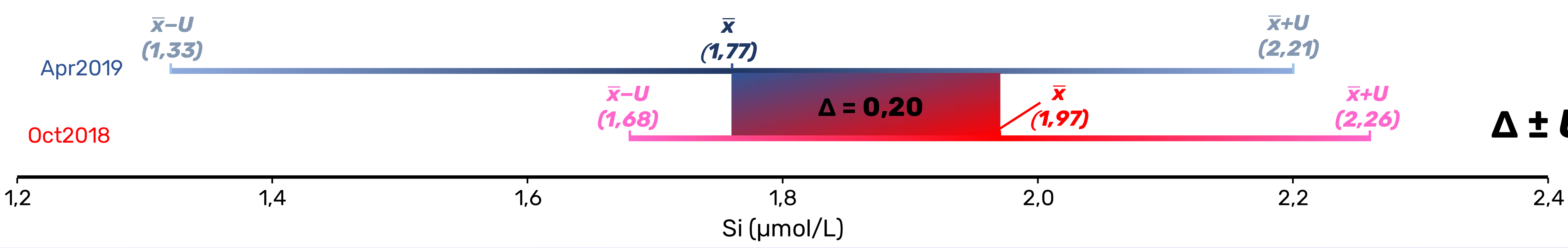
Simulated mean mass concentrations of silicate and estimated sampling and combined expanded uncertainties using different sampling strategies (SS, RS and LS – Single, Random and Linear Random Sampling). (§ - Value obtained by the Monte Carlo Method; s'_r= 2.95%, s'_I= 2.51% and u'_T= 3.09%)

	October 2018			May 2019		
Sampling	Mean §	s'_S (%) §	U' (%)	Mean §	s'_S (%) §	U' (%)
SS	**1.97**	**27.03**	**55.0**	**1.77**	**52.11**	**104.7**
RS(2)	-	19.11	39.5	-	36.85	74.4
RS(4)	-	13.52	28.8	-	26.06	53.0
RS(7)	-	10.22	22.7	-	19.70	40.6
LS(2; 15000)	1.91	6.61	16.5	2.76	5.90	15.4
LS(4; 5000)	1.91	13.89	29.5	2.60	10.80	23.8
LS(7; 2500)	1.92	16.71	34.9	2.55	12.88	27.6
Mean (n=20)	**1.97**	**6.04**	**14.5**	**1.77**	**11.65**	**24.7**

s'_r – repeatability relative standard deviation;
s'_I – intermediate precision relative standard deviation;
u'_T – trueness relative standard uncertainty;
s'_S – representative sampling relative standard deviation;
U'– relative expanded uncertainty for 95% confidence level

$$U_{mean} = 2 \times \sqrt{(s_S^2/n)+s_r^2+s_I^2+u_T^2}$$

Conclusions:



Concentration difference not meaningful ⇒ no trend can be observed

Δ ± *U* (k=3)= (-0.20 ± 0.78) µmol L^{-1}

References

Borges, C.; Palma, C.; Silva, R. B. Optimization of river sampling: application to nutrients distribution in Tagus river estuary, Anal. Chem. 2019, 91, 5698–5705. https://doi.org/10.1021/acs.analchem.8b05781

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