Evaluation of the sampling uncertainty from the Monte Carlo Simulation of georeferenced information

Carlos Borges[1],
Carla Palma[1] ,
Tony Dadamos[2] ,
Ricardo Bettencourt da Silva[3]

MU2019 Workshop

[1] Instituto Hidrográfico, Portugal
[2] IQSC-USP - Universidade de São Paulo, Brazil
[3] CQE@FCUL - Universidade de Lisboa, Portugal

Overview

- Introduction
- Assessment of pollution trends
- Transitional vs oceanic waters
- Sampling Uncertainty Modelling
- Application examples:
  - Phosphate levels in the Tagus Estuary
  - Phosphate levels in oceanic coastal waters
- Conclusions

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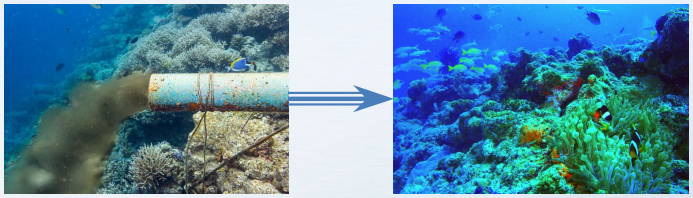
Introduction

- Environmental protection aims to:
  - preserve the existing natural environment
  - to repair damage and reverse trends, when possible
- How?
  - Identifying and characterizing pollution sources
  - Limiting or eliminating its effects



- Monitoring plays a major role in environmental protection policies
- The assessment of trends is essential, which requires long term monitoring (e.g. ocean acidification or eutrophication studies)

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Assessment of pollution trends

The assessment of pollution trends is affected by environment heterogeneity.

The mean value of a component in a large environmental area is robust to system heterogeneity (…)

The modelling of system heterogeneity depends on:
» Number and positions from where samples are collected;
» Determined concentration values that express concentration profiles;
» Uncertainty of position coordinates;
» Uncertainty of sample analysis;
(defines system models uncertainty)

Evaluated MU depends on available information and the detail of their modelling.

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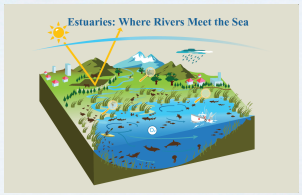
Transitional vs oceanic waters

A comparison

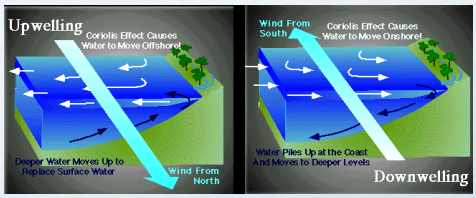
Estuarine Water

- Seasonality – freshwater flow and temperature
- Low scale spatial gradients
- Anthropogenic activities
- Tidal effects



Ocean Water

- Seasonality – currents and wind
- Large scale spatial gradients
- Nutrient poor/depleted superficial water layers



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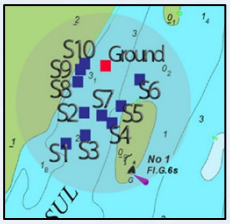
Sampling Uncertainty Modelling

Methodology:

1) **Collect samples at a defined depth and known GPS coordinates**



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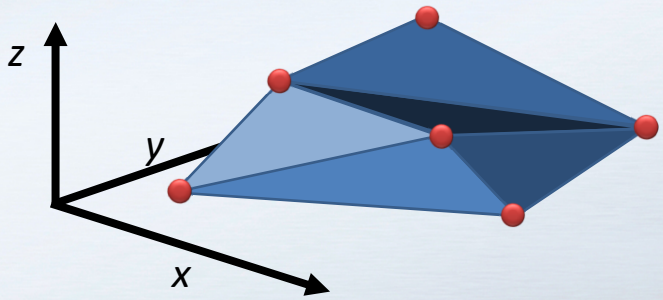
Sampling Uncertainty Modelling

Methodology:

1) Collect samples at a defined depth and known GPS coordinates
2) Describe collected information as a 3D surface (*x*, *y*, *z*), where *x* and *y* are GPS coordinates and *z* samples concentrations



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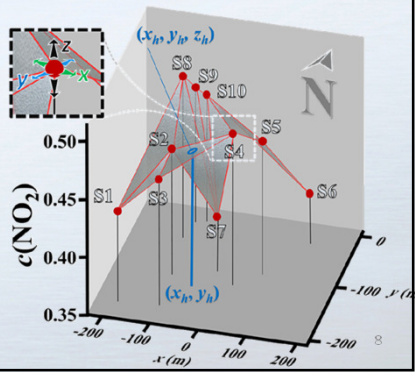
3) Randomization of the 3D surface given GPS coordinates and sample analysis precision



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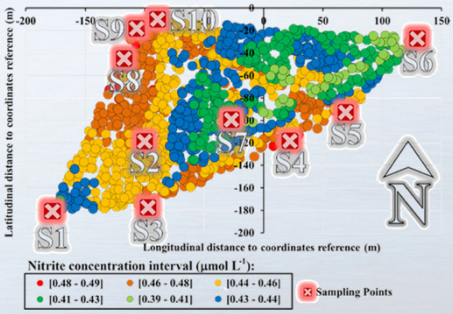
4) **Random scanning of the randomised surfaces to model concentration variation (Single Sampling)**



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Sampling Uncertainty Modelling

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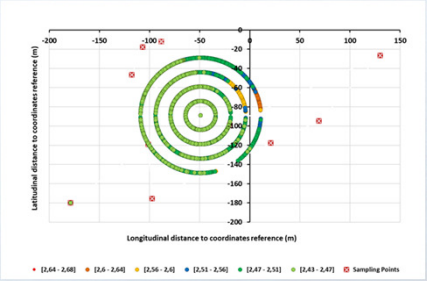
3) Randomization of the 3D surface given GPS coordinates and sample analysis precision
4) Random scanning of the randomised surfaces to model concentration variation (Single Sampling)
5) **Simulate other types of sampling strategies**



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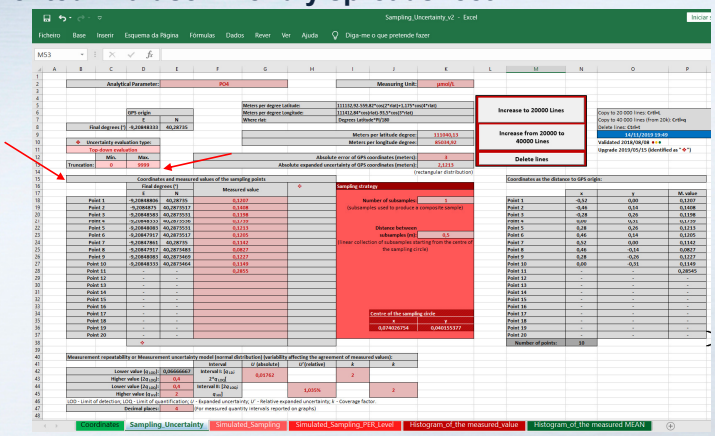
Sampling Modelation

The sampling modelling was based on Monte Carlo Simulations implemented in a user-friendly spreadsheet:



C. Borges, C. Palma, R. J. N. Bettencourt da Silva, *Optimization of river sampling: application to nutrients distribution in Tagus river estuary*, Anal. Chem. **91** (2019) 5698-5705.

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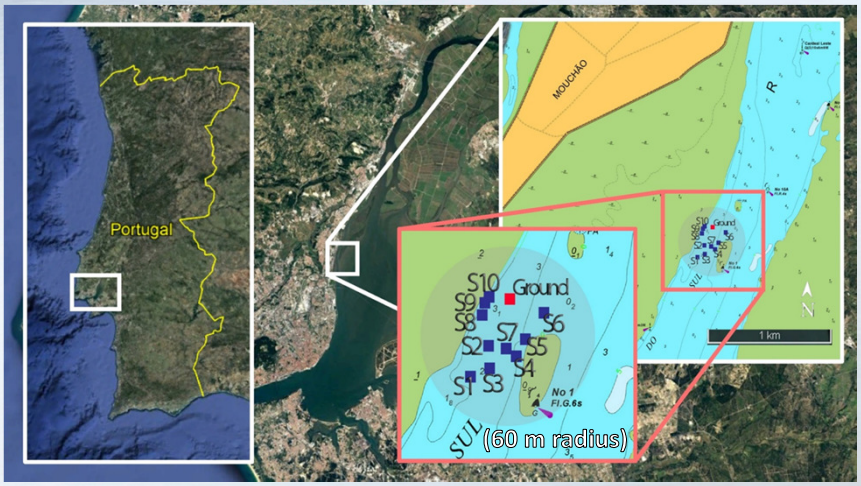
Sampling Procedure

Estuarine Waters (Tagus River)

Collection of 10 samples in a sampling circle of the river:



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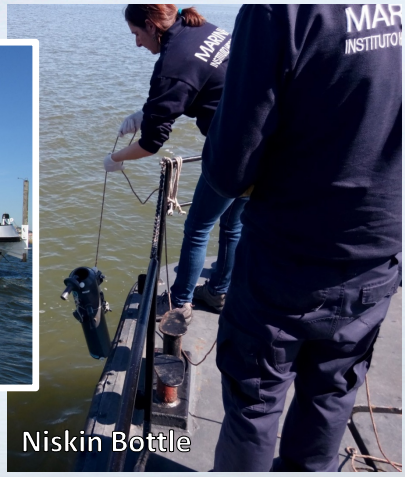

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Sampling Procedure

Ocean Waters (Portuguese Continental Platform)

Collection of 9 samples within a 10 x 10 nm grid;

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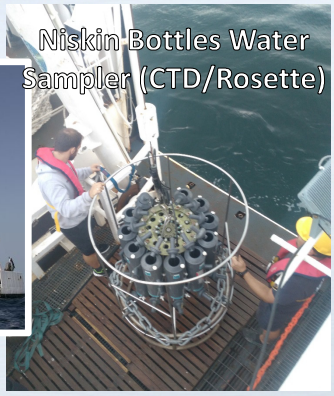
Sampling Procedure

Ocean Waters (Portuguese Continental Platform)

Collection of 11 samples within a 1 m radius



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Results

The case of Phosphate

Simulated variability of the mass concentration and estimated sampling and combined expanded uncertainties using different sampling strategies.

Sampling	Mean §	s'_r (%)	s'_v (%) §	s'_I (%)	u'_T (%)	U' (%)
Tagus Estuary						
SS	3.08	0.52	2.26	2.35	3.21	9.21
RS(5)	-	0.52	1.01	2.35	3.21	8.28
LS(5; 15)	3.07	0.52	0.51	2.35	3.21	8.09
Ocean Water (large scale)						
SS	0.186	4.73	17.37	7.13	3.21	39.25
RS(5)	-	4.73	7.77	7.13	3.21	23.98
LS(5; 2000)	0.185	4.85	7.86	7.13	3.21	24.20
Ocean Water (small scale)						
SS	0.123	7.17	9.59	7.13	3.21	28.60
RS(5)	-	7.17	4.29	7.13	3.21	22.88
LS(5; 0.20)	0.123	7.15	4.47	7.13	3.21	23.00

§ - Value obtained by the Monte Carlo Method; SS - Single sampling; RS(m) - Random composite sampling from m subsamples; LS(m; d) - Linear composite sampling from m subsamples positioned at d meters.

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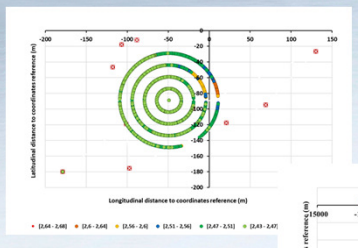
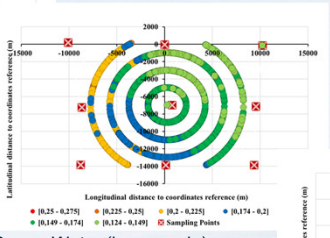
Results

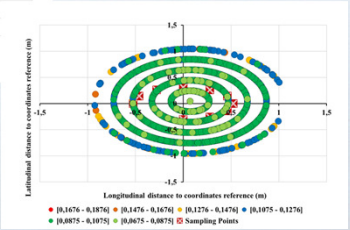
5-points Linear Composite Sampling (LS5)



Tagus Estuary



Ocean Water (large scale)



Ocean Water (small scale)

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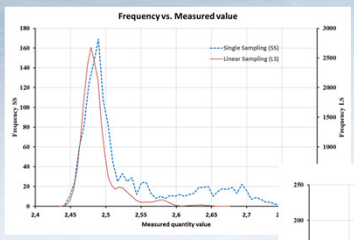
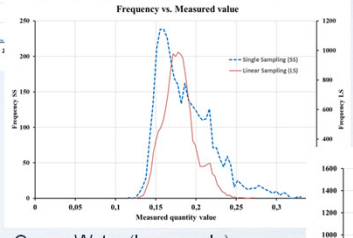
Results

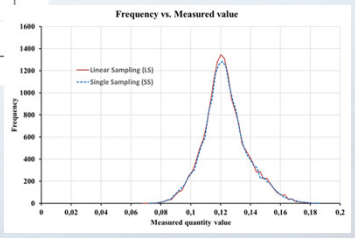
Histograms of the measured values (MC Simulations)



Tagus Estuary



Ocean Water (large scale)



Ocean Water (small scale)

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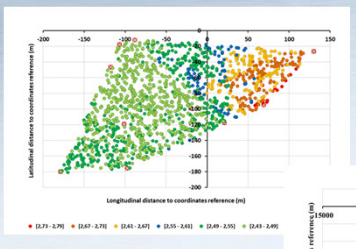
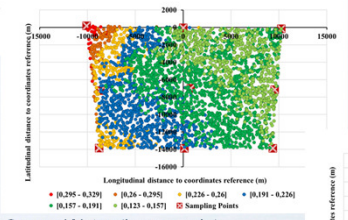
Results

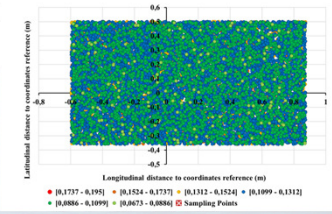
Random Sampling



Tagus Estuary



Ocean Water (large scale)



Ocean Water (small scale)

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Conclusions

The developed methodology for uncertainty modelling and optimisation was successfully applied to marine systems sampling;

Major Features:

- Case 1 (Tagus Estuary):
  - Duplicate or triplicate composite sampling (random or linear with 30 m distances) allow a useful reduction of the measurement uncertainty.
- Case 2 (Ocean Waters, large scale):
  - LS can not be applied to estimate sampling uncertainty due to system□s heterogeneity
  - The use of the tool can be used to assess trends e detect abnormalities in large systems behaviour
- Case 3 (Ocean Water, small scale):
  - Duplicate or triplicate composite sampling (from distinct bottles) allow a useful reduction of the measurement uncertainty
- Special Feature:
  - Application of sampling uncertainty to establish different cargo capabilities scenarios

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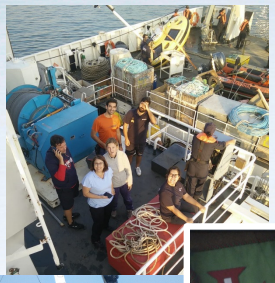

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