Sediment Quality Sampling Design for Darwin Harbour

Richard Brinkman and Murray Logan
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Cover photo:
‘RV Solander in Darwin Harbour’. Image: AIMS
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ACKNOWLEDGEMENT

This project was funded by INPEX-operated Ichthys LNG Project with equal co-investment from the Australian Institute of Marine Science. It is an output of a pilot project with the Sediment Quality sub-program of the Darwin Harbour Integrated Marine Monitoring and Research Program (IMMRP).
1 EXECUTIVE SUMMARY

Many toxicants do not have long residence times in water but will readily attach to suspended particulate matter and ultimately accumulate in benthic sediments. Modelling studies have shown that changes in land-use have the potential to significantly degrade the condition of Darwin Harbour. Some parts of the Harbour are poorly flushed and the tidal asymmetry and complex circulation near embayments and headlands means that much of the fine-sediment that is delivered by rivers is trapped internally within the Harbour arms. This fine fraction of sediment is easily transported and readily accessible to filter feeders and deposit feeders, and thus poses significant threats to fauna if contaminants are bioavailable/bioaccessible.

In the context of increasing development and associated pressures, this project aims to inform the development of a first systematic, long-term, sediment monitoring program for Darwin Harbour. The rationale for the program is that seabed and estuarine sediments are both an extensive habitat and the ultimate repository for many contaminants that enter waterways.

A suite of hydrodynamic, wave and sediment transport models were applied to Darwin Harbour to define a set of physical constraints on sediment mobility and to compartmentalise the Harbour into spatial units that reflect broad-scale fine-sediment dynamics. Additional data on sediment chemical composition from a harbour-wide survey provided background information to predict the full spatial distribution of sediment chemicals and help tune and evaluate sampling designs. These physical (grain size, etc) and chemical (metal(loids) and nutrients) data sets informed the development of spatial statistical models to recreate the complete coverage of the physical and chemical attributes in the Harbour. In turn, these chemical coverages and sediment dynamics layers underpin statistical approaches (e.g. random sites, structured grid, Conditional Latin Hypercube Sampling, spatially balanced design) for generating candidate sampling configurations, for which an optimum sampling size and configuration is determined.

Overall, 2D spatially balanced sampling designs for both Outer Harbour and East Arm would seem most appropriate. These designs are immune to any uncertainty in previous physicochemical data and spatial modelling and should yield well balanced spatial configurations. A total of 100 samples collected from both East Arm and Outer Harbour is likely to yield representative samples from which to construct a variety of spatio-temporal models into the future.

Knowledge of the dominant processes controlling sediment transport within the Harbour has enabled the development of a conceptual model of sediment movement within the Harbour. The proposition for the conceptual model of sediment transport is that fine sediment typically enters the Harbour during wet season flow events. This sediment is easily suspended and remains in suspension, due to large tidal currents, within the central section of the Harbour until it is moved into more quiescent regions, via flood dominated tidal asymmetry, where it deposits. This system represents a mechanism of nett fine sediment movement into depositional areas in the upper reaches of the Harbour arms. Understanding the net sediment movement within the Harbour will
facilitate identifying potential accumulation locations for contaminants arising from development in Darwin Harbour.

2 INTRODUCTION

Many toxicants do not have long residence times in water, but will readily attach to suspended particulate matter and ultimately accumulate in benthic sediments. Modelling studies have shown that changes in land-use have the potential to significantly degrade the condition of Darwin Harbour. Some parts of the Harbour are poorly flushed and the tidal asymmetry and complex circulation near embayments and headlands means that much of the fine-sediment that is delivered by rivers is trapped internally within the Harbour. This fine fraction of sediment is easily transported and readily accessible to filter feeders and deposit feeders, and thus may pose potential threats to fauna if contaminants in the sediment are bioavailable/bioaccessible. Due to the role oceanographic processes play in the movement of sediment within the Harbour it is critical to consider these factors when designing a monitoring program to ensure sampling locations capture areas that are potential accumulation locations for contaminated sediment.

In the context of increasing development and associated pressures, this project aims to inform the development of a first systematic, long-term, sediment monitoring program for Darwin Harbour which takes into consideration the physicochemical nature of Darwin Harbour sediment and the oceanographic processes which will influence the movement of contaminated sediment in the Harbour. The rationale for the program is that seabed and estuarine sediments are both an extensive habitat and the ultimate repository for many contaminants that enter waterways. In addition, monitoring of contaminants in sediment may facilitate the identification of increasing contaminant loads in the Harbour which may not be detected by water monitoring programs due to the high flushing rate within Darwin Harbour and infrequent water sample collection.

3 METHODS

3.1 Overview of methodology

The scientific challenge of sediment sampling lies in designing a sampling program that is spatially comprehensive, targets zones of consistent deposition and is statistically randomised and robust. The methodology for this project uses outputs from the hydrodynamic, sediment transport and wave models to define physical constraints on sediment mobility and to describe the broad-scale patterns of sediment dynamics (Table 1). Additional data on sediment chemical composition from a harbour-wide survey provides background information to predict the full spatial distribution of sediment chemicals and help tune and evaluate sampling designs. These physical (grain size, etc) and chemical (metal(loids) and nutrients) data sets (Table 2) informed the development of spatial
statistical models to recreate the complete coverage of the physical and chemical attributes in the Harbour. In turn, these chemical coverages and sediment dynamics layers from modelling underpin statistical approaches for generating candidate sampling configurations, for which an optimum sampling size and configuration is determined. An optimum sampling design is a configuration of sites that collectively represent the broader area as efficiently as possible, and in this context, efficiency is a compromise between complete representation (resulting from saturating the spatial domain with sites) and minimising sampling effort.

Table 1: Model outputs used to inform the design of sediment sampling program for Darwin Harbour

<table>
<thead>
<tr>
<th>Model</th>
<th>Output/spatial parameter in map</th>
<th>Characteristic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrodynamic (RMA)</td>
<td>Seabed shear stress</td>
<td>Sediment resuspension due to current</td>
</tr>
<tr>
<td>Wave model (SWAN)</td>
<td>Wave induced orbital velocity</td>
<td>Sediment resuspension due to waves</td>
</tr>
<tr>
<td>Sediment transport (RMA)</td>
<td>Sediment deposition and erosion</td>
<td>Spatial description of likelihood of accumulation or erosion.</td>
</tr>
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Table 2: Sediment physical and chemical data (Munskgaard et al., 2013) used for developing full spatial map (modelled) of sediment characteristics in Darwin Harbour

<table>
<thead>
<tr>
<th>Physical or chemical* parameter</th>
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<tbody>
<tr>
<td>Grain size</td>
</tr>
<tr>
<td>Total Kjeldahl nitrogen</td>
</tr>
<tr>
<td>Total organic carbon</td>
</tr>
<tr>
<td>Phosphorous</td>
</tr>
<tr>
<td>Sulfur</td>
</tr>
<tr>
<td>Aluminium</td>
</tr>
<tr>
<td>Chromium</td>
</tr>
<tr>
<td>Iron</td>
</tr>
<tr>
<td>Manganese</td>
</tr>
<tr>
<td>Cobalt</td>
</tr>
<tr>
<td>Nickel</td>
</tr>
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<td>Copper</td>
</tr>
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<td>Zinc</td>
</tr>
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<td>Arsenic</td>
</tr>
<tr>
<td>Cadmium</td>
</tr>
<tr>
<td>Lead</td>
</tr>
<tr>
<td>Calcium</td>
</tr>
<tr>
<td>Vanadium</td>
</tr>
<tr>
<td>Gallium</td>
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<tr>
<td>Molybdenum</td>
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</table>

* metal(loids) measured in 2mm fraction
This analysis of existing physicochemical data, and hydrodynamic information has focused on the Outer Harbour and East Arm. The East Arm region was selected for the sediment monitoring program due to it being the centre for development in Darwin Harbour (https://denr.nt.gov.au/water/water-management/darwin-harbour/darwin-harbour-region-report-cards/2018-report-cards/zone-2-east-arm-2018). For the purpose of the sediment monitoring program, East Arm is defined as the region including East Arm, Elizabeth River and a section of the Middle Harbour adjacent the city of Darwin. The Outer Harbour has been defined as Outer Harbour and Shoal Bay. These areas are presented in Figure 1.

![Figure 1 Map of Darwin Harbour highlighting the Outer Harbour and East Arm sections.](image-url)
Each of the major elements of the study methodology are described in sections 3.2 – 3.5.

### 3.2 Tidal Hydrodynamics

A numerical model of the broader study region was established using the RMA-2 hydrodynamic modelling software to simulate tidal currents and water levels. RMA-2 is a two-dimensional depth averaged finite element hydrodynamic numerical model (King 2016). It computes water surface elevations and horizontal velocity components for subcritical, free-surface two-dimensional flow fields. RMA-2 is a general-purpose model designed for far-field problems in which vertical accelerations are negligible and velocity vectors, generally, point in the same direction over the entire depth of the water column at any instant of time. It expects a vertically homogeneous fluid with a free surface. Several studies by the Australian Institute of Marine Science (AIMS) have shown that the vertical distribution of currents over the Harbour are regular and without stratification so that a 2D assumption is valid. The hydrodynamic field simulated is then used to drive the sediment transport model. RMA-2 computes a finite element solution of the Reynolds and Navier-Stokes equations for turbulent flows, solving the depth-integrated equations of fluid mass and momentum conservation in two horizontal directions. Friction is calculated with the Manning’s or Chezy equation, and eddy viscosity coefficients are used to define turbulence characteristics. Both steady and unsteady (dynamic) problems can be analysed. The model uses an implicit time step scheme and for this implementation the model was run with a timestep of 15 minute which adequately captures the tidal signature.

The finite element mesh established for the study area (shown in Figure 2) includes Beagle Gulf in order to accurately model circulation seaward of the Harbour entrance. The underpinning bathymetry for the model grid was derived from a 10m bathymetric survey grid compiled from both the latest available bathymetry data for the region (Siwabessy et al., 2019).

The model boundaries to the west and east of the mode grid coincide with co-tidal lines derived by the Bureau of Meteorology (BOM) National Tide Facility and have been based on a suite of tidal observations. The western boundary is taken as the recorded tides at Forth Hill wharf in Darwin minus 30 minutes and the eastern boundary has been derived based on the harmonic constituent data for Cape Hotham. The tides at Cape Hotham have range of 4.5 metres and the tides at the eastern boundary have a range of up to 8 metres. Mean sea level for both tide data sets were calculated and the tide data adjusted to Chart Datum for Darwin.

The implementation of the RMA-2 model to Darwin Harbour has been used for previous investigations of hydrodynamic circulation, water quality, and sediment transport assessments. Over the years the model has been refined to assist in understanding the general movement of cohesive and non-cohesive sediments and nutrients in the Harbour. It has been enhanced with data from Multibeam Echo Sounder (MBES) surveys conducted in 2011 and 2015-16 and from Acoustic Doppler Current Profiler (ADCP) measurements in 2015 (Williams 2016).

The model was ‘spun-up’ from an initial condition of static water levels, and then run for a 30-day period to capture a characteristic month-long tidal cycle. At each model element, tidal velocities and tidally generated seabed shear stress were calculated and analysed.
Figure 2 Finite Element mesh established for the numerical hydrodynamic model of Beagle Gulf and Darwin Harbour.
3.3 Wave Dynamics

Wave propagation within Beagle Gulf and Darwin Harbours was modelled with the SWAN shallow water wave model (Ris et al., 1999). SWAN is a third-generation spectral model that contains implicit shallow water routines to allow for shoaling, frictional dissipation, wave breaking and refraction. The model grid was a regular, rectilinear mesh with 100m spatial resolution, with bathymetry at model grid points interpolated from a 10m bathymetric survey grid compiled from both previously reported and new survey data (Siwabessy et al., 2019).

The wave climate in the region is dominated by locally generated waves, with little incident swell entering the Harbour from the west, except under monsoonal cyclone/tropical low events (Rigby et al., 2014). For the purposes of this report, the modelling focuses on typical wind conditions, and does not consider episodic wet season wind events that are responsible for longer-frequency swell. An analysis of 20 years of hourly wind observations the BOM tide gauge site on Fort Hill wharf suggests that a wind speed of 10 m/s is a characteristic of a typical strong wind in the region (see Figure 3). As such, surface wave simulations were performed with wind forcing of at 10 m/s from directions of 0, 90, 140, 270 and 315 degrees. Maps of wave-derived bed orbital velocity and wave bed shear stress were calculated and used to assess wave derived bottom orbital velocity shear stress.
Figure 3 Analysis of 3 p.m. wind velocity from Darwin Airport (Australia Bureau of Meteorology)
3.4 Sediment Modelling

The dynamics of sediment in the Harbour was investigated through application of the RMA-11 water quality and sediment transport model, with underlying hydrodynamic field being provided by the RMA-2 Hydrodynamic model described above.

The sediment RMA11 model simulated the movement of non-cohesive sediment (sand – grainsize 62µm – 2mm) transport and the cohesive (fines – grainsize < 62µm) transport model. The sediment transport rates were simulated using the transport potential method based on Van Rijn’s computation (Van Rijn 1984a, 1984b).

In order to understand the regional characteristics of erosion and deposition, the model was initiated with a uniform layer of fine sediment and run for a period of 6 weeks (re-cycling the month-long hydrodynamic inputs) to assess the nett changes in sediment thickness throughout the Harbour. Areas of positive nett changes indicated areas of deposition; areas of negative change indicated areas of erosion. Sediment characteristics used in the simulations were guided by previous sediment sampling in the Harbour (Streten, Tsang and Harries 2017).

Key parameters used in the mode were:

<table>
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<td>Critical shear stress for erosion</td>
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</tr>
<tr>
<td>Critical shear stress for deposition</td>
<td>0.1 N/m²</td>
</tr>
<tr>
<td>Fine sediment settling velocity</td>
<td>0.0006 m/s</td>
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<tr>
<td>Sediment bulk density</td>
<td>1400 kg/m³</td>
</tr>
<tr>
<td>Sediment initial condition</td>
<td>10 kg/m²</td>
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3.5 Sediment sampling design analysis

The spatial design of the sediment monitoring program was intended to identify candidate sampling configurations, for which an optimum sampling size and configuration could be determined, with a target of 100 locations, to be sample in addition to 20 designated sites.

The following physical and chemical data sets informed the development of spatial statistical models to recreate the complete coverage of the physical and chemical attributes in the Harbour, from which sampling configurations were determined.

1. Hydrodynamic modelling of the entire Darwin Harbour (as described above) comprising tidal bed shear and velocity as well as wave-induced orbital velocities. Field from the models were provided as Raster datasets, and sub-sampled at 10m resolution. Together, the hydrodynamic and wave data was used to isolate areas likely to experience persistent conditions that were more conducive to deposition (rather than erosion) of sediments.

2. Munksgaard sediment chemical survey from 2012. These data provide background information that assisted in predicting the full spatial distribution of a range of sediment chemicals. These spatial distributions then supported tuning and evaluating a range of sampling designs.
3. Offset shallow Outer Harbour sediment. Similar to the Munksgaard et al. (2013), these data provided background information for the Outer Harbour.

4. The probability of ‘hard’ seabed based on multibeam mapping (Siwabessy 2019) was also used as a mask to constrain sampling locations.

Specific details of the procedure are presented in Appendix 1, but in summary, it involved the following steps:

- Fit barrier spatial models to each of the Munksgaard et al. (2013) sediment chemicals to isolate the analysis to the relevant subregion and predict/develop spatial layers for the East Arm section
- Fit a barrier spatial model to each of the Offset shallow Outer Harbour sediment chemicals to isolate the analysis to the relevant subregion and predict/develop spatial layers for the Outer Harbour.
- Develop masks out of the hydrodynamic model data and use them to exclude areas of likely erosion from the chemical spatial layers
- Use spatial layers representing hard seabed, shipping channels, ports, and other exclusion zones to establish additional masks to apply alongside hydrodynamic modelling masks to further restrict the sampling domains and prevent sampling configurations containing sites in the exclusion zones.
- Explore three different sample generation routines for a range of sample sizes to establish an optimal sampling design. The five routines will be:
  - Using the masked chemical spatial layers to inform Conditioned Latent Hypercube Sampling - this will generate samples of nominated sizes that are located in a manner that most represents the underlying patterns in the chemical spatial layers.
  - Completely random sampling - this will select the nominated number of samples from within the masked area and is completely naive to any underlying spatial patterns (and hence is only likely to be representative of the underlying patterns when the number of samples is large).
  - A regular sampling grid - this will select approximately the nominated number of samples configured in a regular grid within the masked area. Like the completely random sampling, the regular sampling grid is completely naive to the underlying spatial patterns, yet it does guarantee a more even spatial coverage.
  - A spatially balanced design - this will yield a spatially balanced design in which sampling sites are spread out throughout the spatial domain.
  - A high dimensional spatially balanced design - this will yield a design in which sampling sites are spread in multiple dimensions (spatial and according to patterns in the underlying chemical distribution)

In addition to the 100 long-term monitoring sites, there are 20 designated sites. These sites provide information on areas of interest including (but not limited to) known or potential contaminant hotspots, key habitats, established monitoring sites, compliance monitoring sites etc. Although these sites are additional to the long-term samples, they form part of the overall design and thus need consideration in the candidate configurations.
4 RESULTS

4.1 Tidal and wave driven hydrodynamic processes.

Tidal velocity percentiles and accompanying percentiles of tidal bed shear stress produced from the hydrodynamic model show increased velocities in deeper channels and along salient topographic features with large depth gradients, such as hard headlands and large benthic features. The model domain includes mangrove areas, and lower bed shear values are predicted in these regions, although there is often higher shear within the channels leading to mangrove systems.

Figure 4 shows the synoptic distribution of the 50th percentile of tidally generated seabed shear stress within Darwin Harbour and the Outer Harbour. A threshold for sediment erosion of 0.1 Newton/m² (force per square meter) for fine sediment was determined based on the sediment characteristics observed in the Harbour (Streten, Tsang and Harries 2017), and from previous observational studies (D. Williams – pers. Comms.). Areas of high sediment erosion can be seen in West and Middle Arms (Figure 4) as well patches throughout the Middle Harbour. East Arm did not have the high bed shear stress identified in West and Middle Arm.
Wave modelling was undertaken for a range of typical wind directions, with a wind velocity of 10 m/s (36 km/hr). Maps of the synoptic distribution of wave-derived bed orbital velocity (as an indicator of wave-driven resuspension) were calculated for a wind speed of 10 m/s from directions of 0, 90, 140, 270 and 315 degrees. These distributions are shown in Figure 5, with a composite of maximum wave-orbital velocity (from all directions) shown in Figure 6, demonstrate that wave induced bed orbital velocity within the Harbour is generally low, with locally generated waves dominating the local wave energy budget. Thus, unlike bed shear stress, wave derived bed orbital velocity did not show high levels in regions such as Middle and West Arms (Figure 6). Instead areas of high maximum wave induced bed orbital velocity occurred at the mouth of the arms. The northward/north-westward facing shorelines at the entrances to Darwin are also exposed to significant wave energy (Figure 6). Wave energy within the Harbour is limited (Figure 6), due to limited wave energy transmission into the Harbour from offshore and small fetch within most harbour regions.

The modelling results present a broad description of the synoptic patterns of the primary hydrodynamic drivers with the Inner and Outer Harbour, which is dominated by tidal energy, with only episodic contributions from river inputs during the wet season, and limited influence of wave energy on the overall circulation.
Figure 5 Wave induced Maximum Orbital Velocity (m/s) generated from sustained winds of 10m/s (36km/hr) from dominant wind directions (indicated in each sub-figure).
Figure 6 Composite dataset of maximum Wave induced Orbital Velocity (m/s) generated from sustained winds of 10m/s (36km/hr) from dominant wind directions. Contour shows 0.1, 0.2, 0.3 m/s.

4.2 Sediment transport modelling

The spatial distribution of estimated sedimentation rate (um/day) within the Harbour and Harbour entrance based on the cohesive fine-sediment transport model, after a 6 weeks simulation is shown in Figure 7. The general patterns of sedimentation (deposition) correlate with the general patterns of bed-shear.
Figure 7 Estimated sedimentation rate (um/day) based on the cohesive fine - sediment transport model, after a 6 weeks simulation, in which the Harbour bottom was initiated with a uniform layer of fine sediment. Negative numbers indicate erosion.

4.3 Sediment characteristics from previous sampling programs

Particle size distributions from previous sampling programs are shown in Figure 8 and Figure 9. The figures demonstrate a sand-dominated environment in the Outer Harbour and a higher prevalence of fine sediments in the Inner Harbour.

Sediment characteristics of the outer Harbour indicate that most particles are classified as sand with particle sediment particles size between 0.1mm and 1mm (based on results from Offsets Outer Harbour sampling program). Depth-averaged velocity to initiate motion and suspension for sand of this grainsize is approximately 0.3 m/s (Van Rijn 1984a). For fine sediment in the Inner Harbour, the threshold for sediment movement is <0.1 m/s.
Figure 8 Inner Harbour - Particle size distribution (as percentage abundance) of different sediment grain sizes observed across the Munksgaard sediment sampling program.

Figure 9 Outer Harbour - Particle size distribution (as percentage abundance) of different sediment grain sizes observed across the Offsets Outer Harbour sediment sampling program.

4.4 Sediment sampling design analysis

4.4.1 Existing chemical sediment data, Outer Harbour sediment monitoring data, and designated sampling sites

The spatial configuration of the Munksgaard 2012 sediment sampling sites are illustrated in Figure 10 (circular points). Primarily, only the sites within the Outer Harbour and East Arm will be used to inform the current exploration of future sampling designs.

Note, while the coverage of East Arm sites is extensive, the Outer Harbour sites are clustered together in the south east corner of the Outer Harbour. The use of these Munksgaard 2012 Outer Harbour sediment data to estimate the underlying patterns throughout the entire Outer Harbour is not appropriate. Any modelling patterns are only reliable within the spatial bounds of the available data. Any attempts to extrapolate to a broader area (e.g. the rest of the Outer Harbour), is not appropriate.

The spatial configuration of the Offset Outer Harbour sediment sampling sites is illustrated in Figure 10 (square points). These data will be used to inform the selection of Outer Harbour sites.
In addition to the long-term monitoring sites, a number of designated sites have been provided. These sites form additional sites and need consideration in the candidate configurations and are illustrated in Figure 10 as red points.

![Map of Darwin Harbour indicating the spatial configuration of Munksgaard 2012 sediment monitoring sites (dots). Solid dots signify sites within the Outer Harbour and East Arm focal areas. Black circular points represent Munksgaard 2012 sediment sampling sites, square points represent Offset Outer Harbour sediment sites and red points represent designated sites.](image)

4.4.2 Hydrodynamic modelling layers

The seabed shear stress products provide spatial modelling of the expected forces acting on the seabed and provide proxies for the likelihood for sediment erosion, transportation and deposition. These products were used to create masks that exclude areas of high erosive or transportation potential. Masks for East Arm and the Outer Harbour are shown in Figure 11 and Figure 12,
respectively. Sites outside areas of high seabed shear stress are good candidates for sample site allocation.

Figure 11 East Arm mask derived from the combination of 50th percentile seabed shear stress and each of the wave derived seabed shear stresses. The blue areas indicate areas of predicted relatively low erosion and transport potential and thus good candidate areas for sample site allocation. The black dots illustrate the position of Munksgaard 2012 sediment sampling sites.

Figure 12 Outer Harbour mask derived from the combination of 50th percentile seabed shear stress and each of the wave derived seabed shear stresses. The blue areas indicate areas of predicted relatively low
erosion and transport potential and thus good candidate areas for sample site allocation. The black dots illustrate the position of Munksgaard 2012 sediment sampling sites.

4.4.3 Exclusion zone masks

In addition to using hydrodynamic modelling masks to exclude areas that might be considered unsuitable for sediment monitoring, there are areas throughout Darwin Harbour that are not practical or appropriate for monitoring. These include areas of high probability of hard seaded (Siwabessy, 2019), shipping channels, port exclusion zones as well as other exclusions zones associated with major infrastructure e.g. military bases. These additional masks were developed from spatial layers provided (DENR). Maps in Figure 13 and Figure 14 illustrate the sampling masks associated with numerous exclusion zones for East Arm and Outer Harbour respectively.

Figure 13 East Arm mask derived from numerous exclusion zone shapefiles. The blue areas represent the spatial domain available for sampling. The black dots illustrate the position of Munksgaard 2012 sediment sampling sites. Red dots represent the designated sites. Open black and red circles represent samples that are outside of the East Arm area.
Figure 14  Additional Outer Harbour mask derived from numerous exclusion zone shapefiles. The blue areas represent the spatial domain available for sampling. The black dots illustrate the position of Outer Harbour sediment sampling sites. Open black circles represent samples that are outside of the Outer Harbour area.

4.5  Spatial Model fitting.

A target or set of targets is required against which the effectiveness and accuracy of candidate sampling designs can be tuned or gauged. This target should represent the full underlying metal(loid) and nutrient concentrations and in essence represents a saturated sampling design - a sampling design in which all possible locations/sites are sampled. Whilst this is logistically not possible, given an adequate set of baseline data, statistical spatial models can be generated to estimate the underlying patterns. The resulting predicted layers can be used to represent the targets.

Spatial models are complex statistical models that attempt to recreate the full feature space from which a limited set of samples were collected. In so doing, they attempt to incorporate two-dimensional patterns and correlations to allow prediction to areas in between samples. In the simplest cases, simple surfaces can be derived by linear interpolation between all the sampling points. However, when samples are distributed unevenly, there are strong spatial dependencies and/or the bounding domain is not a simple rectangle, more complex methodologies are required.

Ecological and environmental process are often correlated through space. To account for these spatial dependencies within a spatial model, it is useful to incorporate a Gaussian Random Field (GRF) which specifies a spatially dependent covariance structure in which locations that are closer to one another in space will in general be more highly correlated to one another than locations that are further apart.

Large or complex spatial models soon become intractable using a traditional frequentist modelling framework. By contrast, equivalent Bayesian models are typically very computationally expensive. Integrated Nested Laplace Approximation (INLA: Rue, Martino, and Chopin 2009) is a Bayesian approximation framework that offers the philosophical advantages of a full Bayesian approach, yet
with the computational efficiency of frequentist approaches. We can consider a GRF to be stationary if the degree of correlation between two points is dependent only on the distance between the points, or non-stationary if we allow the correlation function to vary over the landscape.

In a boundary model, two different range parameters are applied. One of the range parameters is applied to the boundary area (in this case land) and the other to the focal area (in this case Harbour). By setting the boundary range smaller (and close to zero) than the focal area range, the dependency structure across boundaries is disrupted and approaches zero.

The random field was approximated via a Constrained Refined Delaunay Triangulation (CRDT) mesh. The mesh comprises an inner region that surrounded all the Munksgaard et al. (2013) sediment monitoring sites as well as an outer mesh provides a buffer to help ensure estimates close to the inner mesh boundary are robust, in doing so, the maximum permissible triangle edge length for the inner and outer mesh regions was set to 0.01 and 0.04 (units of lat long projection) respectively. The smaller the values, the finer the mesh. This mesh is then projected onto the location of the observed sample location. The above models were fit for each of the sediment chemical recorded in the Munksgaard 2012 sediment sampling program. See Appendix 1 for more details.

Figure 15 provides an example of one of the chemical (zinc) spatial models. Figure 15a depicts the random field mesh with the Munksgaard et al. (2013) sampling sites and Harbour boundary overlayed. Figure 15b illustrates the boundary used for the barrier in the spatial model and Figure 15c illustrates the final predicted spatial layer (with original sample data overlayed) for zinc within the East Arm area. For comparison, both predicted (model output) and observed (Munksgaard et al. 2013 samples) are presented on the same colour scale. Figure 15c and d illustrate the final predicted spatial layer for zinc within the East Arm area and where the colour scale is based purely on the range of predicted values.
4.5.1 Background on statistical techniques for designing sediment sampling program

This section provides a summary of the methods used for sample design, the above techniques are explained in more detail in Appendix 1.

4.5.1.1 Naive sample design methods

Random sampling

The simplest approach to generating a spatial sampling design is to repeatedly simulate sampling from the spatial domain with a range of sample sizes and use the above metric to help determine the optimum sampling size and configuration. Given a sufficiently large sample size, random sampling should provide an unbiased and representative sampling design. However, it is highly likely that at low sample sizes, this approach will not yield highly representative samples (high Error), yet,
increasing the sample size should result (on average) in lower Error (= greater accuracy). To counter the natural stochasticity associated with simulation, we will repeat each sample size five times.

**Sampling on a regular grid**

In the simple random sampling approach described above, each simulated random draw is independent of all other draws. As a result, all configurations are possible - even those in which multiple samples are aggregated together in close proximity. In the absence of any prior knowledge about the underlying environmental conditions and heterogeneity, an even and regular spread of samples can ensure that the sampling design does offer general representativeness. Regular grid sampling generates a regular spread of samples. Grids of increasing sample size offer progressively finer granularity and thus the ability to detect smaller scale perturbations in space.

4.5.1.2 **Informed sampling design methods**

**Conditioned Latin Hypercube Sampling**

In drawing both random samples and regular grid samples, the process is completely naive to the underlying environmental conditions. Consequently, they will only likely to be representative once a large number of samples have been collected. Conditional Latin Hypercube Sampling (cLHS) is a robust and efficient statistical sampling procedure that generates samples based on the variability within a multidimensional covariate feature space. Since the sampling process is supervised by the underlying conditions (or proxies thereof), for a given sample size, the resulting candidate sampling configurations are more likely to yield samples that are representative of the complex underlying conditions. In this project particle size distribution, metalloid and nutrient concentrations in sediment were used as the underlying conditions.

**Spatially balanced design**

Whilst regular grid sampling designs do space samples out throughout the spatial domain, they do have the potential to introduce biases due to any underlying systematic processes that might align with the design (albeit unintentionally) and do not necessarily provide good representation. On the other hand, random sampling designs offer some degree of protection from those biases, the shear nature of randomization means that it is possible that some sampling locations can be clustered in very close proximity. When this is the case, not only does it waste valuable sampling effort (as there is no need to provide multiple estimates of the same location), it introduces another bias. Any resulting estimates in the distribution of element concentrations from this sampling design will be biased towards the metalloid and nutrient concentrations measured in the samples clustered together as those conditions are effectively weighted higher by virtue of the greater sampling effort.

The ideal design is to be able to have a random configuration that still prevents the clustering of samples. In effect, a way to generate random locations whose probability of selection is proportional to the distance from all already selected sites. This is the inspiration behind spatially balanced designs.

There are numerous spatially balanced designed techniques. Some such as Generalized Random-Tessellation Stratified (GRTS), map the full two-dimensional spatial domain into a single dimension (in a way that preserves the spatial ordering) before applying a systematic psps sampling technique to ensure a balanced distribution of samples throughout the spatial domain.

A further (and perhaps alternative) ideal is to be able to have a balanced design not only based on spatial proximity, but also on the basis of dissimilarity of underlying conditions. Spatial areas that are homogeneous with respect to some underlying sampling conditions require fewer sampling
locations to characterize the underlying patterns than areas that are relatively heterogeneous. The spatially balanced design via pivotal method allows any number of dimensions to determine the inclusion probabilities.

### 4.5.1.3 Metrics to assess sampling design

Ideally, a good sampling design should comprise a configuration of sites that collectively represent the broader area as efficiently as possible. In this context, efficiency is a compromise between complete representation (resulting from saturating the spatial domain with sites) and minimizing sampling effort. There are numerous approaches for generating candidate sampling configurations. Irrespective of the approach, there must be a metric by which the suitability of the configuration can be gauged. If we assume that full saturation must provide maximum representation, then all other configurations can be gauged relative to the full saturation. Hence a measure of how well a configuration is likely to represent the full spatial domain is the difference between some empirical property calculated from the candidate configuration and full saturation. For example, we could calculate the difference between the estimated mean zinc concentration from a candidate configuration and the equivalent mean calculated from the full saturation sampling of the spatial domain with sites. The magnitude of this difference is thus a measure of the inaccuracy and thus suitability of the candidate configuration.

In the current application, there are numerous metal(loid) and nutrient concentrations in the sediment that can be used to describe the underlying conditions within the spatial domain. Consequently, the metric needs to incorporate the differences across concentrations of each of the metal(loid)s and nutrients. There are three metrics presented to capture three broad characteristics of the ‘accuracy’ of the candidate sampling designs:

- **MeanError** - this is a measure of the average deviation between the estimated zone mean (from the candidate model) and target mean concentration for all the metal(loid)s and nutrients.

- **MaxError** - this is a measure of the maximum deviation between the estimated zone mean (from the candidate model) and the target mean concentration for all the metal(loid)s and nutrients. As a maximum, it can be used to compare the worst performing aspects of each candidate sampling configuration and thus acts as a worst-case scenario.

- **MinError** - this is a measure of the minimum deviation between the estimated zone mean (from the candidate model) and the target mean concentration for all the metal(loid)s and nutrients. As a minimum, it can be used to compare the best performing aspects of each candidate sampling configuration and thus acts as a best-case scenario.

#### 4.5.1.4 Selection of statistical method based on sampling program objective

A key determinant of which of the above techniques to adopt is what the purpose of the sampling design is for. If for example, the purpose is to characterize the overall mean concentration of metal(loid)s and nutrients, then a 2D spatially balanced design is arguably most appropriate as it should represent the general metal(loid) and nutrient concentrations in the sediment in the study area (spatial boundaries). If on the other hand, the purpose is to be able to model the underlying patterns in metal(loid)s and nutrient concentrations and understand where any changes in these patterns occur, then arguably a design that has been optimized around measured elemental...
4.5.2 Results from statistically derived sampling design - East Arm

For a range of sample sizes (5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 120, 200, 1000), for East Arm, each of the above sampling approaches was repeated five times. For each run, the error metric was calculated. The results are presented in Figure 16 (mean error). As expected, as the sample sizes increase, the error declines. Of the informed sampling design techniques, cLHS had the lowest mean error, it had the lowest mean error of all the techniques used to design a sediment sampling program for East Arm (Figure 16). The simple random sampling design performs worst having the highest error at sample sizes >50 (Figure 16). The regular grid sampling is better than the random sampling. Whilst clusters of samples might be appropriate for representing the metalloid and nutrient concentrations in sediment when the measured concentrations of these elements cluster correspondingly, totally random samples are highly unlikely to resemble the correct cluster configuration. The non-uniform distribution of cLHS on the other hand is directly due to the clustering patterns in the underlying metalloid and nutrient concentrations and thus it is not surprising that this technique has the least error. A more detailed discussion is presented in Appendix 1.

![Figure 16 Comparison of the mean Error conditional on sample size and sampling method for the East Arm](image)

On the basis of Figure 16 we could conclude that a sample size of 100 within East Arm is a sound choice, although it is likely that as few as 50 could still potentially yield similar overall patterns, particularly if the sediment sampling site selection is based on cLHS. The spatial representation of the two dimensional spatially balanced sampling configuration for the East Arm (100 samples) is shown in Figure 17.

The sample size of 100 also accommodates a buffer against sample loss. Nevertheless, this entire simulation process is contingent on several unverifiable assumptions:

1. that the Munksgaard 2012 sediment sampling data are representative of the typical conditions and spatial patterns.
2. all Munksgaard 2012 sediment chemicals are equally useful and informative

3. the INLA models are able to fully represent the true metal(loid) and nutrient concentrations in sediment in the area of interest

4. the costs and logistics of sampling are equal irrespective of location

Figure 17 Two dimensional spatially balanced sampling configuration for the East Arm (100 samples)

4.5.3 Results from statistically derived sampling design – Outer Harbour

For a range of sample sizes (5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 120, 200, 1000), for Outer Harbour, each of the above sampling approaches was repeated five times. For each run, the error metric was calculated. The results are presented in Figure 18 (mean error). As like East Arm, as the sample sizes increase, the error declines and the simple random sampling design performs worst (Figure 18). Contrary to the situation for the East Arm area, the conditioned latin hypercube sampling technique only outperforms the other techniques at very low sample sizes (Figure 18). After a sample size of approximately 30, the 2D spatially balanced design has better Minimum and Maximum Error (Figure 18). Also of interest is the finding that the multidimensional spatially balanced design is consistently worse than both a regular grid and 2D spatially balanced design and on par with a totally random design (Figure 18). This might suggest that there are fewer distinct patterns in the underlying sediment chemical data as observed in the Offset Outer Harbour sampling program. A more detailed discussion is presented in Appendix 1.
On the basis of Figure 18 we could conclude that a sample size of 100 within Outer Harbour is a sound choice, although it is likely that as few as 50 could still potentially yield similar overall patterns particularly if the sediment sampling site selection is based on cLHS. If the purpose of the sampling design is to provide an unbiased representative sample of the general conditions across the spatial domain, then it could be argued that the 2D spatially balanced design is most appropriate for the Outer Harbour - particularly if there is any doubt in the assumptions below. Therefore, the spatial representation of the two dimensional spatially balanced sampling configuration for the Outer Harbour (100 samples) is shown in Figure 19.

The sample size of 100 also accommodates a buffer against sample loss. Nevertheless, this entire simulation process is contingent on a number of unverifiable assumptions:

1. that the Outer Harbour sediment sampling data are representative of the typical conditions and spatial patterns.
2. all Outer Harbour sediment chemicals are equally useful and informative
3. the INLA models are able to fully represent the true metal(loid) and nutrient concentrations in sediment in the area of interest
4. the costs and logistics of sampling are equal irrespective of location

With the 2D spatially balanced design most of sediment sampling sites are in Shoal Bay (Figure 19), the underrepresentation of sites closer to Darwin city may decreases the power of the monitoring to detect changes associated with development of Darwin city. The exclusion of sites closer to Darwin city is controlled by the application of spatial masks of areas of high hydrodynamic energy.

**Figure 18** Comparison of the mean Error conditional on sample size and sampling method for the Outer Harbour

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4.5.4 Representation of sampling sites mapped with hydrodynamic and sediment modelling parameters

The sampling sites generated through spatial modelling of sediment chemistry and sampling design evaluation through statistical models are presented as maps overlaid on the modelled hydrodynamic and sedimentation parameters to visualise sampling sites in relation to underlying modelled oceanographic processes. These are presented below for tidal shear stress and wave orbital velocity in Figure 20 and Figure 21, and Figure 22 displays the proposed sampling locations overlaid on the spatial distribution of zones of nett deposition and erosion of fine sediments.

Outer Harbour:
The oceanographic regime of the Outer Harbour is characterised by relatively weak tidal currents, but moderate wave energy. The sediments in the Outer Harbour are dominated by sand (Figure 9), which has a higher velocity threshold for motion and suspension than the finer sediment of the Inner Harbour. Sampling locations proposed for the Outer Harbour in general fall outside of the regions of higher wave-induced orbital velocity (Figure 21), and tidal currents (Figure 20) required to initiate motion (>0.3 m/s).

Inner Harbour:
The oceanographic regime within the Inner Harbour is a spatially complex combination of areas of strong tidal currents in deep channels, areas of lower velocity in vegetated intertidal areas, and low wave energy under most meteorological regimes. The sediment particle size distribution in the Inner Harbour (Figure 8) matches this diversity of energy regimes, with a predominance of fine sediments (silt and fine sands) typical of low energy environments, together with a mix of coarse sand and gravel, typical of more energetic environments. Sampling locations proposed within the Inner are overall located in areas of low tidal and wave energy and coincide with areas of nett deposition of fine sediments (Figure 22).

For the modelling results representing sedimentation, the spatial distribution of sedimentation was analysed to identify zones of nett deposition and nett erosion. This map overlaid with sampling sites is presented in Figure 22.

![Figure 20 50th percentile of tidally generated seabed shear stress (N/m²). Contour shows 0.1 N/m² (approx. threshold for erosion of fine sediment). Coloured circles indicate locations of statistically derived sampling sites.](image-url)
Figure 21 Composite dataset of maximum Wave induced Orbital Velocity (m/s) generated from sustained winds of 10m/s (36km/hr) from dominant wind directions. Contour shows 0.1, 0.2, 0.3 m/s. Coloured circles indicate locations of statistically derived sampling sites.
Figure 22  Zonation of the Inner Harbour into areas of nett Deposition and nett Erosion. Derived from cohesive fine sediment transport model, and only applicable to the Inner Harbour where fine sediment is the dominant sediment class. Coloured circles indicate locations of statistically derived sampling sites.
4.6 Harbour Sediment Zonation, and conceptual representation:

The combination of a macrotidal environment and the incised nature of Darwin Harbour results in complex oceanographic features characterised by large tidal flows constrained to deeper channels, bordered by more quiescent regions which extend into the numerous arms and embayments. The circulation is dominated by tidal energy, with episodic contributions from river inputs during the wet season, and limited influence of wave energy on the overall circulations due to the limited fetch. Within the harbour, there is significant tidal energy to keep fine sediment in suspension and the region is therefore naturally turbid due to the continual remobilisation of fine sediments from shallow Harbour seafloors and intertidal mudflats. Turbidity values range from 5 Nephelometric Turbidity Units (NTU) in the dry season to in excess of 400 NTU during wet season storms, suggesting a significant contribution of fine sediments is delivered into the Harbour from terrestrial sources draining into the Harbour via the reaches of West, Middle and East Arms. Coarser sand has been shown to primarily originate from offshore areas, with a net import into the Harbour (Tonyes, 2018).

Tides within the Harbour increase in asymmetry with distance upstream, with the flood tide of shorter duration but greater velocity than the ebb. Trapping of fine suspended sediment occurs in the more quiescent areas of the Harbour as tides flowing into these regions can carry relatively higher loads of sediment due to the higher flooding tidal velocities, but a proportion of the suspended sediment is deposited as flow decelerates, and lower velocity ebb tides do not remobilise a proportion of the newly settled sediment. Water residence times within the upper reaches of the system can be of the order of 20 days, with increased flushing in deeper channels closer to the Harbour mouths (Williams et al., 2006). This high residence time of suspended matter in some reaches of the Harbour, coupled with the flood dominated tidal asymmetry, results in a net movement of fine sediments into the lower energy regions within the Harbour, and retention in these areas (Williams et al., 2006). The proposition for the conceptual model of sediment transport is that fine sediment typically enters the Harbour during wet season flow events. This sediment is easily suspended and remains in suspension, due to large tidal currents, within the central section of the Harbour and deeper sections of the Harbour arms until it is moved, via flood dominated tidal asymmetry, into more quiescent regions where it deposits. This system represents a mechanism of net fine sediment movement into depositional areas in the upper reaches of the Harbour arms. This conceptual description of fine sediment transport in the Harbour is presented in Figure 23.

The combination of oceanographic features and distinct origin and behaviours of different sediment classes (fine sediments versus sand transport) result a complex sedimentary system. In relation to fine sediments, numerical modelling results suggest that the large tidal energy and homogenisation of fine sediments within the Middle Harbour and deeper sections of the Harbour arms result in a sediment pool that is well mixed, prior to redistribution overtime into less energetic regions of the Harbour. As such, it is unlikely that sediment zonation within the depositional zones will strongly reflect changes in sediment provenance at the spatial scale representing fine sediment inputs into the Harbour. The exception to this is the distinction between Inner and Outer Harbour sediments, with grain size analysis demonstrating a higher proportion of fine sediments in the Inner and a
greater proportion of larger grainsizes in the Harbour sediments, with these coarser sediments originating from offshore areas (Tonyes, 2018).

Our understanding of sediment movement within the Harbour translates into a sediment zonation pattern summarised as follows:

- Fine sediment is delivered into the Harbour from various sources including lateral inflow and river inputs during wet season flows.
- High tidal energy in the deep channels of the Middle Harbour and in the centreline of the East, Middle and Western Arms keeps fine sediment from various sources in homogenous suspension and well mixed within the Middle Harbour, and deeper sections of the arms.
- Under Neap conditions, the suspended sediment may settle out, but is easily resuspended as tidal energy increases during the spring phases of the spring-neap tidal cycle.
- The pool of suspended sediment and easily resuspended sediment in the Middle Harbour and arms is a source for tidal pumping into the more quiescent areas and mangrove habitats lining the edges of the Harbour arms.
- Due to the high level of mixing of fine sediment within the Middle Harbour, there is no clear nett pathway of sediment through the Middle Harbour and between the various arms.
- The Middle Harbour acts to homogenise sediment that is resuspended locally and delivered via inputs from the arms and other sources, and such it is difficult to determine a clear, nett transport.
- Areas close to potential sources of inputs and contaminants and with low tidal energy (e.g. east of the East Arm Wharf and Fort Hill and Stokes Hill wharf precinct), are likely to have an increased signature of sediment signals associated with industrial activities, due to proximity to the source, and the propensity for tidal pumping of fine sediment into quiescent zones.
- There is a nett import of sand into the Harbour, where it remains within, or close to the more highly energetic areas of the Middle Harbour, and deposits on conspicuous sand bars.

This understanding of sediment zonation pattern is presented in Figure 24.

The movement of sand transport within the Harbour has been investigated through a CDU Post Graduate student (S Toynes). This work found that most coarse sand in the Harbour is derived from offshore, and the Harbour is a nett importer of sand of offshore origin. The conceptual understanding of sand transport is shown in Figure 25.
Figure 23 Conceptual diagram of fine sediment transport pathways within Darwin Harbour.
Figure 24 Conceptual diagram of sediment zonation within Darwin Harbour.

- Middle Harbour: High tidal energy keeps fine sediment from various sources in suspension and well mixed. Pool of suspended sediment is a source for tidal pumping into Harbour Arms. No clear net pathway of sediment through the Middle Harbour.

- East Arm/Port Precinct: Due to the proximity of industrial activities, this area is likely to have an increased signature of sediment signals associated with port operations.

- East Arm/Elizabeth River: Fine sediment delivered during wet season inflows. High velocity in deep channels keep fine sediment in suspension. Suspended sediment in the deeper channels is a source for tidal pumping and settlement into mangrove areas.

- Middle and West Arms: Fine sediment delivered during wet season inflows. High velocity in deep channels keep fine sediment in suspension. Suspended sediment in the deeper channels is a source for tidal pumping and settlement into mangrove areas.
A suite of hydrodynamic, wave and sediment transport models were applied to Darwin Harbour to define a set of physical constraints on sediment mobility and to describe the broad-scale patterns of sediment dynamics. Additional data on sediment chemical composition from a harbour-wide survey provided background information to predict the full spatial distribution of nutrient and metal(loid) concentrations in sediment and help tune and evaluate sampling designs. These physical and chemical data sets informed the development of spatial statistical models to recreate the complete coverage of the physical and chemical attributes in the Harbour. In turn, these coverages underpin statistical approaches (e.g. random sites, structured grid, Conditional Latin Hypercube Sampling,

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**Figure 25** Sand transport pathways in Darwin Harbour. From Tonyes (2018) - Sand dynamics in Darwin Harbour: a tool for coastal management. A thesis submitted for the degree of Doctor of Philosophy, CDU (currently unpublished)
spatially balanced design) for generating candidate sampling configurations, for which an optimum sampling size and configuration is determined.

Overall, 2D spatially balanced sampling designs for both Outer Harbour and East Arm would seem most appropriate. These designs are immune to any uncertainty in previous data and spatial modelling and should yield well balanced spatial configurations. A total of 100 samples collected from both East Arm and Outer Harbour is likely to yield representative samples from which to construct a variety of spatio-temporal models into the future.

Knowledge of the dominant processes controlling sediment transport within the Harbour has enable the development of conceptual model of sediment movement within the Harbour. The proposition for the conceptual model of sediment transport is that fine sediment typically enters the Harbour during wet season flow events. This sediment is easily suspended and remains in suspension, due to large tidal currents within the central section of the Harbour until it is moved into more quiescent regions, via flood dominated tidal asymmetry, where it deposits. This system represents a mechanism of nett fine sediment movement into depositional areas in the upper reaches of the Harbour Arms. The movement of the fine sediment which has higher binding affinity for contaminants than sand, can be used to guide the selection of sediment sampling sites as depositional zones are potential sinks for contaminants within Darwin Harbour.
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APPENDIX 1.
1. Synopsis

The purpose of this work was to inform the spatial component of the Darwin Harbour Sediment Monitoring sampling design. In particular, to determine the ‘best’ location for 100 sediment monitoring sites in the East Arm and Outer Harbour sections of Darwin Harbour.

To help inform this process, there were three broad sources of data available:

1. Hydrodynamic modelling of the entire Darwin Harbour. These data (availed via geoTiffs), comprise broadly tidal bed shear and velocity as well as wave driven forces at 10m resolution and will be used to isolate areas likely to experience deposition (rather than erosion) of sediments.

2. Munksgaard sediment chemical survey from 2012 provided by Lynda Radke (as an Excel workbook). These data provided background information that was used to predict the full spatial distribution of a range of sediment chemicals. These spatial distributions then helped tune and evaluate a range of sampling designs.

3. Offset shallow Outer Harbour sediment survey provided by Lynda Radke (as an Excel workbook). Similar to the Munksgaard, data these data provided background information for the Outer Harbour.

The basic procedure involved the following steps:

1. Read in a process the data sources.
2. Fit a barrier spatial model to each of the Munksgaard sediment chemicals and predict/develop spatial layers for the East Arm section.

3. Fit a barrier spatial model to each of the Offset shallow Outer Harbour sediment chemicals and predict/develop spatial layers for the Outer Harbour.

4. Develop masks out of the hydrodynamic model data and use them to exclude areas of likely erosion from the chemical spatial layers.

5. Use spatial layers representing shipping channels, ports and other exclusion zones to establish additional masks to apply alongside hydrodynamic modelling masks to further restrict the sampling domains and prevent sampling configurations containing sites in the exclusion zones.

6. Explore three different sample generation routines for a range of sample sizes to establish an optimal sampling design. The five routines will be:
   
   a) Using the masked chemical spatial layers to inform Conditioned Latent Hypercube Sampling - this will generate samples of nominated sizes that are located in a manner that most represents the underlying patterns in the chemical spatial layers.
   
   b) Completely random sampling - this will select the nominated number of samples from within the masked area and is completely naive to any underlying spatial patterns (and hence is only likely to be representative of the underlying patterns when the number of samples is large).
   
   c) A regular sampling grid - this will select approximately the nominated number of samples configured in a regular grid within the masked area. Like the completely random sampling, the regular sampling grid is completely naive to the underlying spatial patterns, yet it does guarantee a more even spatial coverage.
   
   d) A spatially balanced design - this will yield a spatially balanced design in which sampling sites are spread out throughout the spatial domain.
   
   e) A high dimensional spatially balanced design - this will yield a design in which sampling sites are spread in multiple dimensions (spatial and according to patterns in the underlying chemical distributions).

In addition to the 100 long-term monitoring sites, there are 20 designated sites. These sites are to be sampled more regularly and are for the purpose of compliance monitoring specific areas. Although these sites are additional to the long-term samples, they do form part of the overall design and thus need to be considered when considering candidate configurations.

All code for this project is available on github https://github.com/AIMS/darwin-harbour-sampling.git

2. Data processing

2.1. GIS data

A shapefile of Darwin Harbour (see Figure 1) was utilized in order to define the initial sampling domain(s). This project focused on the Outer Harbour and East Arm. For the purpose of the sediment monitoring program, East Arm was defined as East Arm, Elizabeth River and a section of the Middle Harbour adjacent the city of Darwin. The Outer Harbour was defined as Outer Harbour and Shoal Bay.
2.2. Munksgaard 2012 chemical sediment data

Munksgaard 2012 chemical sediment data were provided by Lynda Radke in the form of an Excel workbook. These data were consolidated together into a single flat csv text file to support analyses. The spatial configuration of the Munksgaard sediment sampling sites are illustrated in Figure 2 (circular points). Primarily only the sites within the Outer Harbour and East Arm will be used to inform the current exploration of future sampling designs.

Note: while the coverage of East Arm sites was extensive, the Outer Harbour sites were clustered together in the south east corner of the Outer Harbour (see Figure 2). The use of these Munksgaard 2012 Outer Harbour sediment data to estimate the underlying patterns throughout the entire Outer Harbour was not appropriate. Any modelling patterns are only reliable within the spatial bounds of the available data. Any attempts to extrapolate to a broader area (e.g. the rest of the Outer Harbour), is not appropriate. Consequently, and unfortunately, the Munksgaard sediment data were of little utility for designing a sampling program for the Outer Harbour.
2.3. Offset Outer Harbour sediment monitoring data

Offset Outer Harbour sediment monitoring data were provided by Lynda Radke in the form of an Excel workbook. These data were consolidated together into a single flat csv text file to support analyses. The spatial configuration of the Offset Outer Harbour sediment sampling sites are illustrated in Figure 2 (square points). These data were used to inform the selection of Outer Harbour sites.

2.4. Designated sampling sites

In addition to the long-term monitoring sites, a number of more regularly sampled designated sites were provided by Lynda Radke in the form of an Excel workbook. These sites formed additional sites, yet they needed to be considered in the formulation on site configurations and are illustrated in Figure 2 as red points. Note: none of the designated sites fall in the defined Outer Harbour and East Arms regions and thus they were not considered further.

Figure 2: Map of Darwin Harbour indicating the spatial configuration of Munksgaard 2012 sediment monitoring sites (dots). Solid dots signify sites within the Outer Harbour and East Arm focal areas. Black circular points represent Munksgaard 2012 sediment sampling sites, square points represent Offset Outer Harbour sediment sites and red points represent designated sites.
2.5. Hydrodynamic and wave modelling

When designing a sediment monitoring program, it is important to consider the erosive, transportation and deposition forces operating on the seabed. Ideally all, if not most, of the sampling sites should be located in areas that are more likely to experience sediment deposition than erosion or transportation.

Various hydrodynamic and wave modelling products were made available by Dr. Richard Brinkman (AIMS) that provide estimates of erosive, transportation and deposition likelihoods and include:

- **current velocity** (50th and 75 percentiles - these were calculated from a 30 day characteristic spring-neap tidal cycle. Higher velocity equates to higher likelihood of sediment transport and erosion and thus lower probability of sediment deposition.

- **seabed shear stress** (50th and 75 percentiles - these were derived from the current velocity and are a measure of the shear forces likely to be experienced on the sea bed due to tidal movement. Higher bed shear stress equates to higher likelihood of sediment transport and erosion and thus lower probability of sediment deposition.

- **wave derived orbital velocity magnitude at seabed** - a shallow water wave model was applied using a 10 m/s wind forcing from a range of directions (0, 90, 140, 270 and 315 degrees) to simulate the likely orbital velocity experienced by the seabed. Higher orbital velocity equates to a higher likelihood of sediment transport and erosion and thus lower probability of sediment deposition.

- **wave derived seabed shear stress** - the same shallow water wave model was expressed in terms of wave bed shear stress. Higher shear stress equates to higher likelihood of sediment transport and erosion and thus lower probability of sediment deposition.

Visual representations of each of the above products within the Outer Harbour and East Arm focal areas are depicted in Figures 3 – 6.

Figure 3: *Outer Harbour extract of four hydrodynamic modeling tidal products.*
Figure 4: East Arm extract of four hydrodynamic modeling tidal products.
Figure 5: Outer Harbour extract of five hydrodynamic modeling wave products. The different products represent different wind angles (0, 90, 140, 270 and 315 degrees).
2.5.1. Masks

The seabed shear stress products provided spatial modelling of the expected forces acting on the sea bed during a typical spring-neap tidal cycle. In so doing, they provided proxies for the likelihood for sediment erosion, transportation and deposition. These products were used to create masks that exclude areas of high erosive or transportation potential.
To establish a mask (to focus only on deposition areas), thresholds need to be established for what represent the critical values below which deposition is likely. Figures 7 and 8 provide these for a range of sediment particle sizes for water velocity and sea bed stress respectively.

Figure 7: Hjulstrom Curve linking sediment size and the velocity needed to erode, transport or deposit (from https://www.thegeoroom.co.zw/hydrology/hjulstrom-curve.php).
Figure 8: Critical bed shear stress for erosion and particle settling velocity of a range of particle sizes from Thomsen (2002)

East Arm sampling domain

Figure 9 illustrates the distribution of percentage abundance of a range of particle sizes class categories from the Munksgaard sampling program. On average, particles in the size classes 4-62µm (Silt) and 62-250µm (fine sand) made up 25.4 and 43.4 percent of the sediment samples respectively. Hence, it was important that future East Arm sampling designs focus on sites that will ensure deposition of particles of these sizes. According to Figures 7 and 8, particles at or above 29µm (middle of the silt range) correspond to critical deposition values of approximately 0.2 m/s velocity and 0.1 seabed shear stress.

The hydrodynamic modeling seabed shear stress products represent the 50th and 75th percentile values. In the case of the 50th percentile, this means that 50 percent of the time, seabed shear stress was estimated to be above this value and 50 percent of values where below. If a mask was based on setting the threshold to correspond to the 50th percentile, then the masked layer represents areas where sediment deposition is likely to occur more regularly than erosion and transport.

Nevertheless, it was important to also establish the distribution of seabed shear stress across the seabed in order to better understand the distribution of values. Figures 10 and 11 illustrate the frequency of seabed shear stresses (and velocity) for the East Arm area. The 50th percentiles for seabed shear stress appear to drop off the peak at around 0.2 m/s, hence this appears to be a sensible threshold value.
Figure 9: The percentage abundance of different sediment grain sizes observed across the Munksgaard sediment sampling program.

Figure 10: Frequency distributions of hydrodynamic products in the East Arm area.
Figure 11: Frequency distributions of wave modelling seabed shear stress products in the East Arm area.
Both current velocity and seabed shear stress were derived from the same model and were thus closely correlated. Similarly, both wave derived orbital velocity and wave derived seabed shear stress were correlated. In each case, the shear stress proxies are intended to be expressions of the forces that are likely to be acting on the seabed (from tides and waves respectively). Hence only the seabed shear stress versions of the hydrodynamic and wave models were used as the proxy estimates of tidal and wave forces.

Figure 12 illustrates the resulting masks for the East Arm area using a threshold of 0.2 m/s (or 0.3 m/s for the 75th percentiles). Each of the wave derived seabed shear masks were added together and then joined with the 50 percentile hydrodynamic seabed shear mask. The resulting mask is illustrated in Figure 13. This mask represents (in blue shading) the areas most likely to experience more deposition than erosion and thus suitable areas for sediment monitoring. When we compared this mask to the spatial extent of the Munksgaard 2012 sediment monitoring site configuration, it was evident that while they broadly overlap, there was substantially less suitable area in the region adjacent to the City and substantially more in the East Arm reaches.

**Figure 12:** Individual East Arm masks from various hydrodynamic (bedShear_) and wave (beagle_) models categorised using a threshold values of 0.2 for all other than the 75th percentile products with use a threshold of 0.3 m/s. The blue areas indicate areas of predicted relatively low erosion and transport potential and thus good candidate areas for sample site allocation. The black dots illustrate the position of Munksgaard 2012 sediment sampling sites.
2.6. Outer Harbour sampling domain

Figure 14 illustrates the distribution of percentage abundance of a range of particle sizes class categories from the Offsets Outer Harbour sampling program. The majority of particles were classified as sand. Based on Figures 7 and 8, it is likely that the majority of the sediment particles were between 0.1mm and 1mm and that this corresponds to critical deposition values of approximately 1 m/s to 5 m/s and 0.2-0.3 seabed shear stress.
The distribution of hydrodynamic seabed shear stress and velocity (Figure 15) had an initial valley at 0.3. The distribution of wave derived seabed shear stress and velocity is illustrated in Figure 16, however, and suggests that the majority of the Outer Harbour was un-affected by high erosive wave shear forces.
Figure 15: Frequency distributions of hydrodynamic products in the Outer Harbour area.
Figure 16: Frequency distributions of wave modelling seabed shear stress products in the Outer Harbour area.
Figure 17: Individual Outer Harbour masks from various hydrodynamic (bedShear__) and wave (beagle__) models categorised using a threshold values of 0.2 for all other than the 75th percentile products with use a threshold of 0.3 m/s. The blue areas indicate areas of predicted relatively low erosion and transport potential and thus good candidate areas for sample site allocation. The black dots illustrate the position of Munksgaard 2012 sediment sampling sites.

A single combined mask, incorporating the 50th percentile seabed shear stress and each of the wave derived seabed shear stresses is illustrated in Figure 18 for Outer Harbour.
2.7. Exclusion zone masks

In addition to using hydrodynamic modelling masks to exclude areas that might be considered unsuitable for sediment monitoring, there are areas throughout Darwin Harbour that are not practical or appropriate for monitoring. These include the areas of a high probability of hard seabed (Siwabessy 2019), shipping channel and port exclusion zones as well as other exclusions zones associated with major infrastructure of military bases. Hence additional masks were developed from spatial layers provided by Lynda Radke.

Figures 19 and 20 illustrate the sampling masks associated with East Arm and Outer Harbour respectively.
Figure 19: East Arm mask derived from numerous exclusion zone shapefiles. The blue areas represent the spatial domain available for sampling. The black dots illustrate the position of Munksgaard 2012 sediment sampling sites. Red dots represent the designated sites. Open black and red circles represent samples that are outside of the East Arm area.
Figure 20: Outer Harbour mask derived from numerous exclusion zone shapefiles. The blue areas represent the spatial domain available for sampling. The black dots illustrate the position of Outer Harbour sediment sampling sites. Open black circles represent samples that are outside of the Outer Harbour area.
3. Spatial Model fitting

A target or set of targets is required against which the effectiveness and accuracy of candidate sampling designs can be tuned or gauged. This target should represent the full underlying conditions and in essence represent a saturated sampling design - a sampling design in which all possible locations/sites are sampled. Whilst this is logistically not possible, given an adequate set of baseline data, statistical spatial models can be generated to estimate the underlying patterns. The resulting predicted layers can be used to represent the targets.

Spatial models are complex statistical models that attempt to recreate the full feature space from which a limited set of samples were collected. In so doing, they attempt to incorporate two-dimensional patterns and correlations to allow prediction to areas in between samples.

In the simplest cases, simple surfaces can be derived by linear interpolation between all the sampling points. However, when samples are distributed unevenly, there are strong spatial dependencies and/or the bounding domain is not a simple rectangle, more complex methodologies are required.

Ecological and environmental processes are often correlated through space. To account for these spatial dependencies within a spatial model it is useful to incorporate a Gaussian Random Field (GRF) which specifies a spatially dependent covariance structure in which locations that are closer to one another in space will in general be more highly correlated to one another than locations that are further apart.

Large or complex spatial models soon become intractable using a traditional frequentist modelling framework. By contrast, equivalent Bayesian models are typically very computationally expensive. Integrated Nested Laplace Approximation (INLA: Rue, Martino, and Chopin 2009) is a Bayesian approximation framework that offers the philosophical advantages of a full Bayesian approach, yet with the computational efficiency of frequentist approaches.

We can consider a GRF to be stationary if the degree of correlation between two points is dependent only on the distance between the points, or non-stationary if we allow the correlation function to vary over the landscape. An extreme form of non-stationary model occurs when there are physical barriers that disrupt or block the flow of contagious processes. In such cases, just because two locations are in close proximity, does not necessarily mean that they will be highly correlated. Consider a simple example of the diffusion of a dye in water throughout a tank. The dye will spread out from the source and gradually disperse throughout the tank. Consequently, the correlation between the concentration of dye at any two locations during dispersion will be dependent on the distance between the two locations. If however, the tank had a partial barrier that restricted the flow of dye molecules, then two locations either side of the barrier might have very different dye concentrations despite being in close proximity. Barrier models are able to account for these obstructions.

\[
y_i \sim \Gamma(\mu_i, \alpha) \\
\log(\mu_i) = \beta_0 + u(s_i) + \epsilon_i \\
\beta_0 \sim N(0, 1000) \\
u(s_i) \sim GRF(r, \sigma_u) \\
\epsilon_i \sim N(0, \sigma^2) \\
\pi(\sigma_e) \sim \lambda_e e^{-\lambda_e \sigma_e} \\
\pi(\sigma_u) \sim \lambda_0 e^{-\lambda_0 \sigma_u} \\
\pi\left(\frac{1}{r}\right) \sim \lambda_1 e^{-\lambda_1 \frac{1}{r}}
\]

where \( y_i \) is the \( i \)th observation of the target chemical variable, \( \epsilon_j \) is the independent and individually variable random effect used to model the very short range erratic dependencies and \( u(s_i) \) is the Gaussian Random Field and is used to model the long-range structural (autocorrelation) dependencies. A diffuse prior is applied to the intercept (\( \beta_0 \)) and \( \epsilon_i \) a vector of independent Gaussians. The Matern family spatial random
effect \(u(s_i)\) and its covariance is defined by two parameters: the range \((r:\) represents the length scale of the spatial dependencies) and standard deviation \(u:\) representing the ratio of spatial to independent noise). The smaller the range, the lower the correlation between two proximal locations.

In a boundary model, two different range parameters \((r)\) are applied. One of the range parameters is applied to the boundary area (in this case land) and the other to the focal area (in this case Harbour). By setting the boundary range smaller (and close to zero) than the focal area range, the dependency structure across boundaries is disrupted and approach zero.

Hyper-parameter priors for the random effects \((\sigma_e, \sigma_u)\) as well as \(r\) are defined in terms of a \(\lambda\) parameter which is determined by the scale of the response (on the log scale in this case). Both \(\lambda_e\) and \(\lambda_0\) were set to the median value of the target response (on a log scale). and the focal area \(r\) was set to half the width of the spatial domain after (Bakka et al. 2016).

The random field was approximated via a Constrained Refined Delaunay Triangulation (CRDT) mesh. The mesh comprised of an inner region that surrounded all the Munksgaard sediment monitoring sites as well as an outer mesh provides a buffer to help ensure estimates close to the inner mesh boundary are robust. In doing so, the maximum permissible triangle edge length for the inner and outer mesh regions was set to 0.01 and 0.04 (units of latlong projection) respectively. The smaller the values, the finer the mesh. This mesh was then projected onto the location of the observed sample location.

The above models were fit for each of the sediment chemical recorded in the Munksgaard 2012 sediment sampling program. Figure 49 provides an example of the major elements of one of the chemical (Zinc) spatial models. Equivalent figures for the other chemicals are presented in Appendix A.

Figure 49a depicts the random field mesh with the Muksgaard 2012 sampling sites and Harbour boundary overlayed. Figure 49b illustrates the boundary used for the barrier in the spatial model and Figure 49c illustrates the final predicted spatial layer (with original sample data overlayed) for Zinc within the East Arm area. For comparison, both predicted (model output) and observed (Munksgaard samples) are presented on the same colour scale. Figure 49c illustrates the final predicted spatial layer for Zinc within the East Arm area and where the colour scale is based purely on the range of predicted values.
Although the shrinkage in models is a little high (there is a tendency for the magnitude of change over space to be dampened), generally the models do a very good job of depicting the relative patterns of change in space. For this application, the absolute scale of the changes in patterns are not important (only the relative patterns), since in order to gauge the accuracy of any candidate sampling designs, it is necessary to standardize the patterns anyway. Hence it is more important that the model depict the general patterns in the observed data than the exact values of the observed data.
4. Sampling

Ideally, a good sampling design should comprise a configuration of sites that collectively represent the broader area as efficiently as possible. In this context, efficiency is a compromise between complete representation (resulting from saturating the spatial domain with sites) and minimizing sampling effort.

There are numerous approaches for generating candidate sampling configurations. Irrespective of the approach, there must be a metric by which the suitability of the configuration can be gauged. If we assume that full saturation must provide maximum representation, then all other configurations can be gauged relative to the full saturation. Hence a measure of how well a configuration is likely to represent the full spatial domain is the difference between some empirical property calculated from the candidate configuration and full saturation. For example, we could calculate the difference between the estimated mean Magnesium from a candidate configuration and the equivalent mean calculated from the full saturation. The magnitude of this difference is thus a measure of the inaccuracy and thus suitability of the candidate configuration.

In the current application, there are numerous sediment chemicals that can be used to describe the underlying conditions within the spatial domain. Consequently, the metric needs to incorporate the differences across each of the chemicals. The following metric will be adopted.

\[
\begin{align*}
\text{MeanError} & = \frac{1}{n} \sum_{i=1}^{n} \frac{\text{abs}(\bar{c}_i - \bar{s}_i)}{r_i} \\
\text{MaxError} & = \max_{i=1}^{n} \frac{\text{abs}(\bar{c}_i - \bar{s}_i)}{r_i} \\
\text{MinError} & = \min_{i=1}^{n} \frac{\text{abs}(\bar{c}_i - \bar{s}_i)}{r_i}
\end{align*}
\]

where \( \bar{c} \) and \( \bar{s} \) are the estimated domain means of the \( i \)th chemical (out of \( n \)) from the candidate and full saturation configurations respectively and the normalizing constant \( r_i \) is the difference between maximum and minimum predicted values for the \( i \)th chemical. There are three metrics presented so capture three broad characteristics of the ‘accuracy’ of the candidate sampling designs:

- MeanError - this is a measure of the average deviation between the estimated zone mean (from the candidate model) and target mean from across all chemical species.
- MaxError - this is a measure of the maximum deviation between the estimated zone mean (from the candidate model) and the target mean from across all chemical species. As a maximum, it can be used to compare the worst performing aspects of each candidate and thus acts as a worst case scenario.
- MinError - this is a measure of the minimum deviation between the estimated zone mean (from the candidate model) and the target mean from across all chemical species. As a minimum, it can be used to compare the best performing aspects of each candidate and thus acts as a best case scenario.

Random sampling

The simplest approach to generating a spatial sampling design is to repeatedly simulate sampling from the spatial domain with a range of sample sizes and use the above metric to help determine the optimum sampling size and configuration. Given a sufficiently large sample size, random sampling should provide an unbiased and representative sampling design. However, it is highly likely that at low sample sizes this approach will not yield highly representative samples (high Error). Yet increasing the sample size should result (on average) in lower Error (= greater accuracy). To counter the natural stochasticity associated with simulation, we repeat each sample size five times.
Sampling on a regular grid

In the simple random sampling approach above, each simulated random draw was independent of all other draws. As a result, all configurations are possible - even those in which multiple samples are aggregated together in close proximity. In the absence of any prior knowledge about the underlying environmental conditions and heterogeneity, an even and regular spread of samples can ensure that the sampling design does offer general representativeness. Grids of increasing sample size offer progressively finer granularity and thus the ability to detect smaller scale perturbations in space.

Conditioned Latin Hypercube Sampling

In drawing both random samples and regular grid samples, the process is completely naive to the underlying environmental conditions. Consequently, they were only likely to be representative once a large number of samples were been collected. Conditional Latin Hypercube Sampling (cLHS) is a robust and efficient statistical sampling procedure that generates samples based on the variability within a multidimensional covariate feature space (Minasny and McBratney 2006a). Since the sampling process is supervised by the underlying conditions (or proxies thereof), for a given sample size, the resulting candidate sampling configurations are more likely to yield samples that are representative of the complex underlying conditions.

In introducing the procedure, Minasny and McBratney (2006a) provided a real world example of a soil mapping project in which relatively small samples sizes generated by cLHS closely represented the original distribution of a set of environmental covariates. Furthermore, Minasny and McBratney (2006b) found cLHS superior (in terms of accuracy) to a range of alternative sampling procedures including random and stratified random sampling.

Spatially balanced design

Whilst regular grid sampling designs do space samples out throughout the spatial domain, they do have the potential to introduce biases due to any underlying systematic processes that might align with the design (albeit unintentionally) and do not necessarily provide good representation. On the other hand, random sampling designs offer some degree of protection from those biases. The shear nature of randomization means that it is possible that some sampling locations can be clustered in very close proximity. When this is the case, not only does it waste valuable sampling effort (as there is not need to provide multiple estimates of the same location), it introduces another bias. Any resulting estimates from the sampling design will be biased towards the clustered sample conditions as those conditioned are effectively weighted higher by virtue of the greater sampling effort.

The ideal design is to be able to have a random configuration that still prevents the clustering of samples. In affect, a way to generate random locations whose probability of selection is proportional to the distance from all already selected sites. This is the inspiration behind Spatially balanced designs.

There are numerous spatially balanced designed techniques. Some such as Generalized Random-Tessellation Stratified (GRTS), map the full two dimensional spatial domain into a single dimension (in a way that preserves the spatial ordering) before applying a systematic πps sampling technique to ensure a balanced distribution of samples throughout the spatial domain. Grafström, Lundström, and Schelin (2012) introduced an alternative technique in which unequal inclusion probabilities are generated via a pivotal method.

A further (and perhaps alternative) ideal is to be able to have a balanced design not only based on spatial proximity, but also on the basis of dissimilarity of underlying conditions. Spatial areas that are homogeneous with respect to some underlying sampling conditions require fewer sampling locations to characterise the underlying patterns than areas that are relatively heterogeneous. The spatially balanced design via pivotal method allows any number of dimensions to determine the inclusion probabilities.

A key determinant in selecting which of the above techniques to adopt is based on an evaluation of the purpose of the sampling design. If for example, the purpose is to characterise the overall condition
mean, then a 2D spatially balanced design is arguably most appropriate as it should represent the general underlying conditions. If on the other hand, the purpose is to be able to model the underlying patterns and understand where any changes in these patterns occur, then arguably a design that has been optimised around the underlying conditions (such as a n-dimensional spatially balanced design or conditioned latin hypercube sampling technique) is arguably more appropriate.

4.1. East Arm

For a range of sample sizes (5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 120, 200, 1000), for East Arm, each of the above sampling approaches was repeated five times. For each run, the Error metric was calculated. The results are presented in Figures 22 (mean error) and 23 (max error). As expected, as the sample sizes increase, the error declines. The simple random sampling design performs worst. The regular grid sampling is better than the random sampling. Whilst clusters of samples might be appropriate for representing conditions when the conditions cluster correspondingly, totally random samples are highly unlikely to resemble the correct cluster configuration. The non uniform distribution of cLHS on the other hand was directly due to the clustering patterns in the underlying conditions and thus it was not surprising that this technique had the least error.

Interestingly, the reduction in error after a sample size of 50 is relatively mild (notwithstanding that the figure is presented on a log-y scale). For each of sample sizes 50, 60, 70, 80 and 100, the best (based on lowest error) cLHS configuration is presented in Figure. Comma delimited text files are also available with the Latitude and Longitudes of these coordinates.

Figure 22: Comparison of the mean Error conditional on sample size and sampling method for the East Arm
On the basis of Figures 22, 23 and 24 we could conclude that a sample size of 100 within East Arm is a sound choice, although it is likely that as few as 50 could still potentially yield similar overall patterns. The sample size of 100 also accommodates a buffer against sample loss. Nevertheless, this entire simulation process is contingent on a number of unverifiable assumptions:

1. that the Munksgaard 2012 sediment sampling data are representative of the typical conditions and spatial patterns.
2. all Munksgaard 2012 sediment chemicals are equally useful and informative.
3. the INLA models are able to fully represent the true underlying conditions.
4. the costs and logistics of sampling are equal irrespective of location.
The conditioned latin hypercube sampling technique consistently outperforms the other techniques. Interestingly, there was very little difference between the 2D and nD Spatially balanced designs. This suggests that either the sediment chemicals were relatively homogeneous over space or else patterns in one chemical species was countered by patterns in another chemical species.

The conditioned latin hypercube sampling technique appeared to be able to tune its design on the underlying sediment chemical patterns better than the spatially balanced designs. Thus if the above assumptions are reasonable and the main intention of the sampling was to be able to describe the patterns in the sediment chemicals, then the sampling design derived from this technique seems most appropriate.

If however, the purpose of the sampling design was to provide an unbiased representative sample of the general conditions across the spatial domain, then it could be argued that the 2D spatially balanced design was most appropriate - particularly if there was any doubt in the above assumptions.
Figure 25: Sampling configurations associated with the lowest mean Error for each sample size for cLHS for the East Arm
Figure 26: Sampling configurations associated with the lowest mean Error for each sample size for Regular grid sampling for the East Arm
Figure 27: Sampling configurations associated with the lowest mean Error for each sample size for nD Spatially balanced sampling for the East Arm
Figure 28: Sampling configurations associated with the lowest mean Error for each sample size for 2D Spatially balanced sampling for the East Arm
4.2. Outer Harbour

For a range of sample sizes (5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 120, 200, 1000), for Outer Harbour, each of the above sampling approaches was repeated five times. For each run, the Error metric was calculated. The results are presented in Figures 30 (mean error) and 31 (max error). As expected, as the sample sizes increase, the error declined. The simple random sampling design performs worst. The regular grid sampling was better than the random sampling. Whilst clusters of samples might be appropriate for representing conditions when the conditions cluster correspondingly, totally random samples are highly unlikely to resemble the correct cluster configuration. The non uniform distribution of cLHS on the other hand was directly due to the clustering patterns in the underlying conditions and thus it is not surprising that this technique had the least error.

Interestingly, the reduction in error after a sample size of 50 was relatively mild (notwithstanding that the figure is presented on a log-y scale). For each of sample sizes 50, 60, 70, 80 and 100, the best (based on lowest error) cLHS configuration is presented in Figure... Comma delimited text files are also available.
with the Latitude and Longitudes of these coordinates.

Figure 30: Comparison of the mean Error conditional on sample size and sampling method for the Outer Harbour

Figure 31: Comparison of the maximum Error conditional on sample size and sampling method for the Outer Harbour
On the basis of Figures 30, 31 and 32 we could conclude that a sample size of 100 within Outer Harbour was a sound choice, although it is likely that as few as 50 could still potentially yield similar overall patterns. The sample size of 100 also accommodates a buffer against sample loss. Nevertheless, this entire simulation process is contingent on a number of unverifiable assumptions:

1. that the Offset Outer Harbour sediment sampling data are representative of the typical conditions and spatial patterns.
2. all Offset Outer Harbour sediment chemicals are equally useful and informative.
3. the INLA models are able to fully represent the true underlying conditions.
4. the costs and logistics of sampling are equal irrespective of location.

Contrary to the situation for the East Arm area, the conditioned latin hypercube sampling technique only outperformed the other techniques at very low sample sizes. After a sample size of approximately 30, the 2D spatially balanced design had better Minimum and Maximum Error. Also of interest is the finding that the multidimensional spatially balanced design was consistently worse than both a regular grid and 2D spatially balanced design and on par with a totally random design. This might suggest that there were fewer distinct patterns in the underlying sediment chemical data as observed in the Offset Outer Harbour sampling program.

Again, if however the purpose of the sampling design was to provide an unbiased representative sample of the general conditions across the spatial domain, then it could be argued that the 2D spatially balanced design was most appropriate - particularly if there was any doubt in the above assumptions.
Figure 33: Sampling configurations associated with the lowest mean Error for each sample size for cLHS for the Outer Harbour
Figure 34: Sampling configurations associated with the lowest mean Error for each sample size for Regular grid sampling for the Outer Harbour
Figure 35: Sampling configurations associated with the lowest mean Error for each sample size for nD Spatially balanced sampling for the Outer Harbour
Figure 36: Sampling configurations associated with the lowest mean Error for each sample size for 2D Spatially balanced sampling for the Outer Harbour
Figure 37: Two dimensional spatially balanced sampling configuration for the Outer Harbour (100 samples)

5. Conclusions

Overall, 2D spatially balanced sampling designs for both Outer Harbour and East Arm would seem most appropriate. These designs are immune to any uncertainty in previous data and spatial modelling and should yield well balanced spatial configurations. A total of 100 samples collected from both East Arm and Outer Harbour was likely to yield representative samples from which to construct a variety of spatio-temporal models into the future.
6. Appendix A

Figure 38: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Aluminium. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 39: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Phosphorus. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 40: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Sulfur. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 41: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Calcium. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 42: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Vanadium. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 43: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Chromium. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 44: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Iron. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 45: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Manganese. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 46: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Cobult. The diagram illustrates 
a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) 
the resulting predicted 2D surface scaled to the range of predictions.
Figure 47: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Nickel. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 48: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Copper. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 49: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Zinc. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 50: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Gallium. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 51: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Arsenic. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 52: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Selenium. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 53: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Molybdenum. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 54: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Cadmium. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 55: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Lead. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 56: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Aluminium. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 57: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Arsenic. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 58: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Cerium. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 59: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Chromium. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 60: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Copper. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 61: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Iron. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 62: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Manganese. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 63: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Nickel. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 64: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Lead. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 65: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Antonium. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 66: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Vanadium. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 67: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Zn. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 68: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Total organic Carbon. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.
Figure 69: Integrated Nested Laplace Approximation (INLA) barrier spatial modelling of Total Nitrogen. The diagram illustrates a) the mesh, b) the barrier mask, c) the resulting predicted 2D surface (and observed training data as points) and d) the resulting predicted 2D surface scaled to the range of predictions.

This document was produced from markdown using knitr on R version 3.6.1 (2019-07-05) on a x86_64-pc-linux-gnu system.

```{r}
sessionInfo()
```

R version 3.6.1 (2019-07-05)
Platform: x86_64-pc-linux-gnu (64-bit)
Running under: Arch Linux

Matrix products: default
BLAS: /usr/lib/libopenblas-r0.3.7.so
LAPACK: /usr/lib/liblapack.so.3.8.0

locale:
[1] LC_CTYPE=en_AU.utf8    LC_NUMERIC=C    LC_TIME=en_AU.UTF-8
attached base packages:
[1] stats graphics grDevices utils datasets methods base

other attached packages:
[1] knitr_1.25

loaded via a namespace (and not attached):
[1] compiler_3.6.1 magrittr_1.5 tools_3.6.1 stringi_1.4.3 stringr_1.4.0 xfun_0.10
[7] evaluate_0.14

7. References

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