Real-time monitoring of water quality through a holistic approach to particle characterization: ‘Particle-omics’

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Monitoring for pathogens often involves time-intensive or expensive laboratory analyses

- **COST**: requires accurate identification through microscopy or molecular techniques

- **EXPERTISE**: requires extensive training in the use of advanced techniques

- **RISKS**: look for one thing at a time, therefore other potential risks or emerging threats not identified

- **RELIABLE INDICATOR**: Real-time monitoring can assist in identifying particular organisms only if a diagnostic feature or probe is available
Goal

Develop rapid and cost-effective tools for the detection of threats to water quality

In situ sensors are ideally suited for rapid detection; however, they are often not very specific

Specific techniques are often labor intensive and/or expensive to implement
Particles are closely tied to water quality

A drop of seawater

David Liittschwager, National Geographic

R. Noble
An –*omics* approach to particle characterization

**Genome** → the holistic characteristics of a set of genes corresponding to an organism

**No one gene operates in isolation**

*Particleome*: The sum total of all particles (biotic and abiotic) in a given environment.
Why use an –omics approach?

• Difficult to identify a single property that defines water quality
• Changes in holistic properties might be more sensitive and less expensive to track
• Move from a biomarker approach to a fingerprinting approach to identify threats to water quality
• Apply multivariate statistical techniques to real-time data, borrowing from bioinformatics
A variety of techniques are used to characterize particles
FlowCAM

- Detects individual cells by scatter and/or fluorescence induced by laser light excitation;
- Rapidly counts and photographs individual particles;
- Distinguishes the shape and unique fluorescence properties of each cell in a sample;
- Provides a suite of particle properties (35 variables) as well as a set digital images of the particles.
Data Analysis

• Data reduction: Principal Component Analysis, (=Empirical Orthogonal Function analysis)
• Correlation analysis: correlate EOFs to environmental variables or to presence of pathogen of interest
• Example data set: Columbia River (Land Ocean Biogeochemical Observatory, LOBO)
4/20/2011: spring bloom (pre-freshet)
PCA case scores: 3/23/2011

Axis 1

Axis 2

Vector scaling: 0.84
PCA case scores: 10/29/2010

Vector scaling: 2.62
Axis 2 = PC 2: blue, transparency (hetero vs. autotroph?)
Axis 3 = phycoerythrin fluorescence/chl fluorescence
chl
turbidity

%O₂ sat
scattering
Variance

EOF 1 (PC1) 
- $r = 0.56, p = 0.05$

EOF 2 (PC2) 
- Hetero vs. autotroph?

EOF 3 (PC3) 
- $r = -0.44, p = 0.03$

Turbidity (NTU)

% $O_2$ Saturation

Hetero vs. autotroph?
Challenges

• Large size range of particles in the natural environment
• Different size ranges often requires different technique to measure particles → Data interfacing
• Obtaining comprehensive and representative databases/libraries that provide meaningful diagnostics
Summary and ongoing work

• Through particle-omics, we seek to characterize holistic properties of the particle load in water to identify meaningful changes or qualities

• Goal 1: perform laboratory tests using perturbations to assess sensitivity of the approach

• Goal 2: build a library of data and images for the lower Columbia River

• Goal 3: develop a standardized workflow for data processing
PCA variable loadings: 3/23/2011
PCA variable loadings: 4/20/2011

Axis 3

Axis 4
PCA case scores: 4/20/2011

Vector scaling: 0.86