Notes for PACE Uncertainty Group meeting 25 January 2021

1. Overall Goals of working group
   1. Need common terminologies. This is evident from the survey.
   2. Suggest methods for developing a standardized uncertainty estimate (or at least a framework)
   3. Each team should provide a common minimum set of uncertainty metrics
   4. ID when we report data with uncertainty vs. flagging retrievals
   5. Coordinate consistent assumptions between groups regarding noise and sources of said noise
   6. Can we reduce uncertainty?
   7. Think about level 3 products
2. Overview of Survey responses
   1. Most responses say they will provide uncertainty estimates with some standard procedures
      1. Analytical Error Propagation, Optimal Estimation, Post launch validation, Bootstrapping
      2. We still need a common formulation of uncertainties. There didn’t seem to be a common propagation of uncertainty analysis.
      3. There will be difficulties with forward vs. reverse uncertainty propagations.
      4. Matteo: Shouldn’t we be avoiding bootstrapping? (ZTT model discussion for Mike Twardowski)
   2. Where are the gaps in the uncertainty budget?
      1. Modeling uncertainties (physics assumptions ,clouds, machine learning training data uncertainty), Noise covariance matrix (systematic errors), Computational resources for the error propagation, Prior covariance matrix, Field observations (post-launch data), Uncertainty in field observations (ac-9/s, radiometry, profiler, etc.), Gridding uncertainty (Alexi?)
         1. For Alexei’s: spatial binning – algorithm specific
   3. How will these uncertainties be communicated?
      1. Discrete quality flags based on threshold unc. (or chi2), Error bars (1 sigma), Bias, Spatial/temporal bin products after considering all uncertainty budgets, Posterior error covariance matrix, MAPE or RMSE
   4. What are the main stat metrics for alg performance?
      1. Median symmetric accuracy, symmetric signed percentage bias.(Morley et al. 2018), R2, bias, mean absolute error, and root mean square error, (x\_ret -x\_true)/sigma to check covariance matrix assumptions, Posterior error covariance matrix, MAPE or RMSE
      2. Morley 2018 paper link: <https://agupubs.onlinelibrary.wiley.com/doi/full/10.1002/2017SW001669>
3. After-discussion
   1. Do we have instrument specs on the website? A: not yet, but being accumulated
   2. What’s the objective of this subgroup? Guidance for the rest of the group? Short-term vs. long-term?
      1. Amir: intro slide, but focus on understanding how the uncertainty is calculated from each group, settle on common terminology and metrics
      2. Possible white paper?
      3. Jeremy: I can envision this group generating a position white paper [tech memo] on defining and assessing uncertainties for PACE. This would accomplish: (1) getting the current SAT on the same page and moving forward similarly and (2) providing guidance on other algorithm and performance related assessments for the future (as Heidi suggested).
      4. Andy: My feeling is this is also useful for the SOB for algorithm selection.
   3. How do you deal with categorical variables? These seem to be continuous variables
      1. Need more responses from ocean biology folks
   4. Snorre was requesting uncertainty from the instrument on a level 1c common grid
      1. Andy: this will likely be provided
      2. Bryan: might increase the data size, we just provide models
      3. Xu: Good to have a coordinated effort or website or something to get each team’s model out there (like a white paper or something [ATBD?]) instead of having to go to each team to ask for it. We still need to focus on IDing the source of these errors (random vs systematic), and what Snorre was talking about, which was actually co-locating the different instrument uncertainties. Need more interaction between Algorithm teams and Instrument teams
         1. Bryan: instrument uncertainties (SNR, etc) is being aggregated now. Also, Bryan points out that post-launch there will be additional unknown uncertainties
         2. Lachlan: Error covariance matrix “supply chain” to go from instrument through algorithm, but we need to poke the instrument teams to provide these numbers
            1. This group should tell instrument team what they’d like to see and what form
            2. But also we need to understand systemic things like stray light corrections, environmental variables, etc that will go on top of instrument uncertainties, so this won’t include everything they characterize in lab.
            3. Xu: Each team can likely artificially create these uncertainties for use in their own algorithm uncertainties, but this might be too much post-launch work for now
      4. Heidi: can we do per-pixel uncertainties? This might be a very different problem open-ocean versus coastal. Some places (e.g. no validation data in Southern Ocean) it's hard to know if your retrieval/uncertainty are reasonable: suggest adopting quality flags. So no “global” value
         1. Lachlan: If we focus on individual variable uncertainty, we might be able to be region-agnostic, but this will take a lot of work
         2. Amir: this is algorithm-dependent, and teams should focus on how they deal with their assumptions. But we can still learn from algorithms that are “wrong” in certain regions. Need to understand bias.
         3. Lorraine: aren’t we doing uncertainty validation? Or are we just trusting the math?
            1. Andy: we are, and they’re sometimes not great, but better than nothing   
               (brings us back to analyzing uncertainties in in situ datasets as a group goal)
            2. Ocean data: we can probably scale stats up temporally and see if we can account for seasonal variability instead of a one data point in the satellite footprint as “truth”
   5. Next time will invite Frédéric Mélin who authored white paper on uncertainty propagation in the IOCCG dataset (this will likely be a full PACE team meeting)
      1. Link to IOCCG report: https://ioccg.org/wp-content/uploads/2020/01/ioccg-report-18-uncertainties-rr.pdf
   6. Amir will send out a summary of the meeting and a survey for the next meeting time

**Action points:**

* Document uncertainties on validation field data so groups can use these consistently (Andy, Heidi, Lachlan make a first pass, later present to wider group).
* Document uncertainties inherent in the matchup process due to spatiotemporal mismatch (Andy is trying for aerosols).
* Document uncertainties on model parameterizations (common in ocean color forward models); tedious but needed to move forward with meaningful uncertainty propagation.
* Heidi will Invite Frédéric Mélin for full PACE SAT meeting.