

## Notes from 10 March

Logo design continues apace.

Discussion of current MCMC test code. Text from Scott's previous email:

To start off, here's a summary of the modules in my test code (or at least pieces I think could be spun into their own models), where they stand now, and some of the variations we could try to incorporate. Seems like we're focusing on 1 and 2 now. Let me know, and I can try to encapsulate any of these parts and share.

1. Load and parse data
  - Currently input fields hard coded for two test datasets + synthetics created within script
2. Load and parse prior information (parameter search range, instrument info, standards...)
  - All currently hard coded, could be set by user, read from file...
3. Parameterize model (includes isotope ratio, intensity, instrument gain, noise parameters, etc.)
  - Again, toggle is set for two test options.
  - Several potential parametrizations for time-dependent variables. Currently piecewise linear, but splines or transdimensional version possible.
4. Determine initial model values
  - Currently roughly approximated from data, could be input by user, or based on prior.
5. Set up forward modeling relationship between data and model
  - Dependent on input data and model parameterization
6. Build ensemble through Monte Carlo iterations
  - Many subroutines involved in this one (below)
  - Output is ensemble of models (~10,000 models)
  - Ensemble written to disk, either during iterations or at end
  - We will at least test a few algorithms here (adaptive, reversible jump) which may be mutually exclusive but overlap in functions needed.
7. Produce ensemble statistics – mean, covariance, etc.
  - This and the following steps are often done separately following MC iterations. I expect we will want to be a part of the normal process, and even do calculate statistics during iterations.
  - May get a lot of ideas and user requests here.
8. Visualize results
  - I imagine we'll use a few of the concepts from my scripts, but completely remake for Tripoli.

And within the Monte Carlo iterations, there are a few additional functions/modules to consider:

1. Proposing updated model

- How will model be changed from previous iteration? Algorithm dependent - either one parameter at a time for rjMCMC or all at once for Adaptive.
2. Calculating data based on new model
  3. Evaluating acceptance criteria
    - How does new model compare to old in terms of data fit and adherence to prior information?
    - Also several possibilities here, very algorithm dependent.

Scott will pull out one of the test cases to liberally comment and send out as an example.