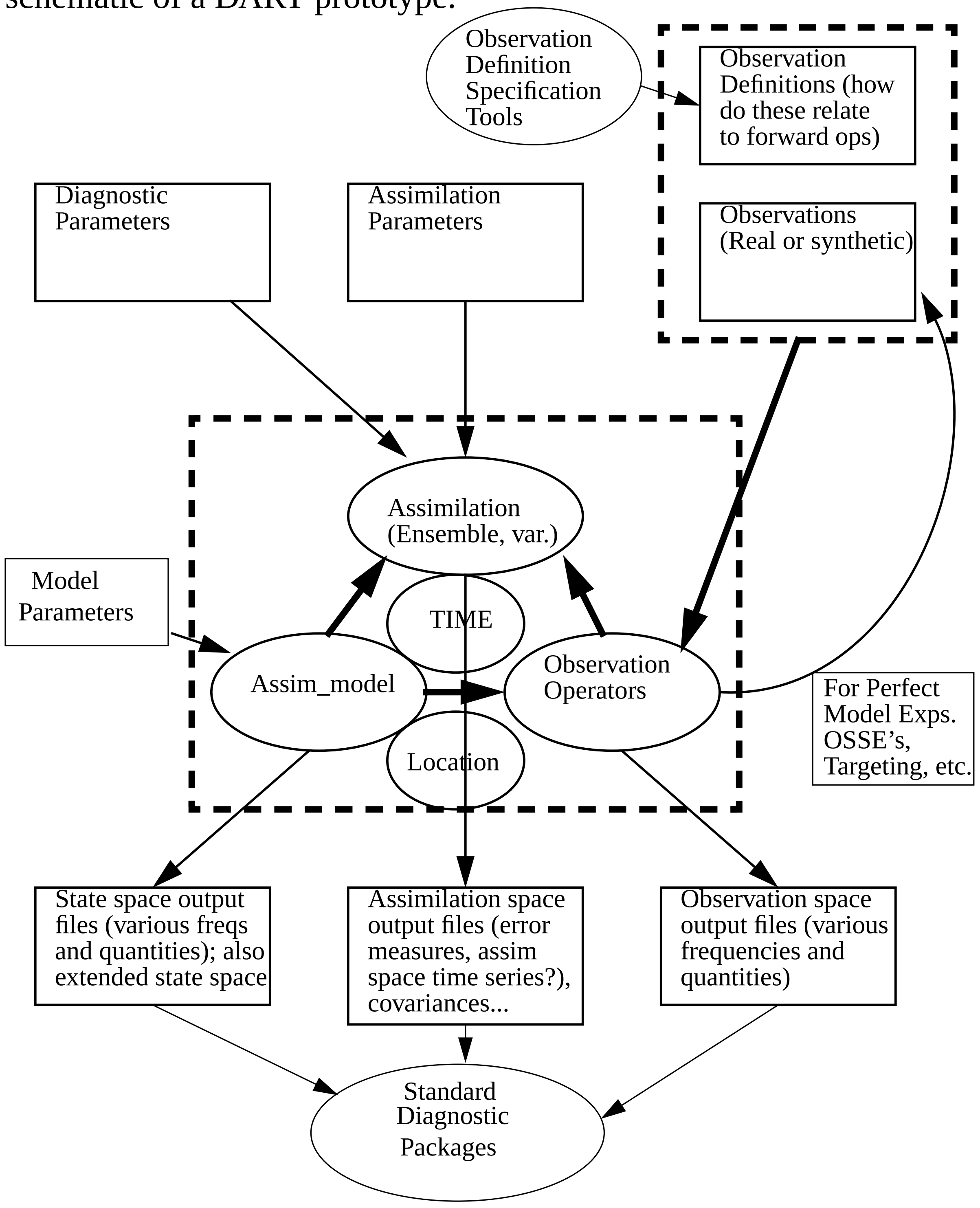
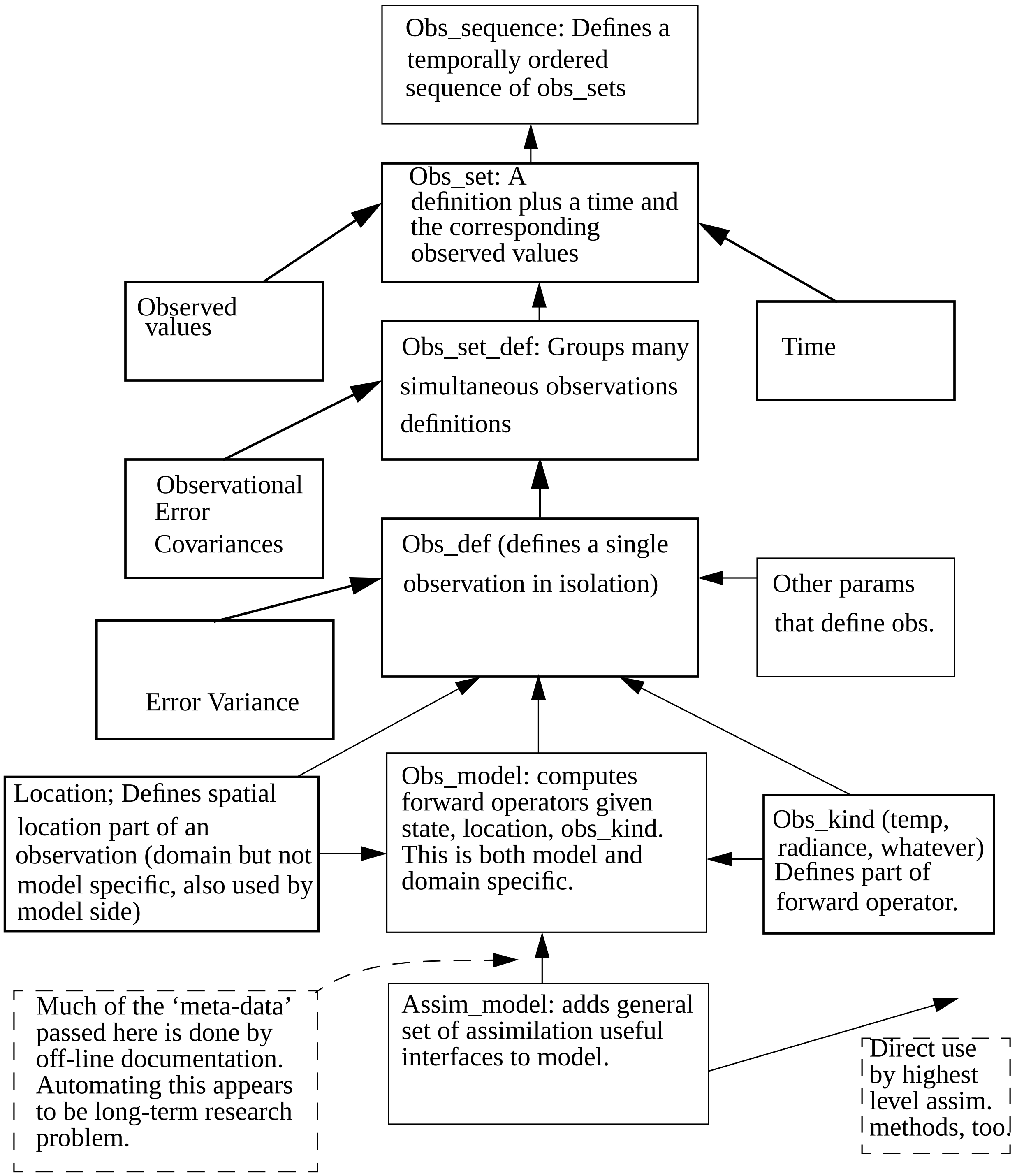
A schematic of a DART prototype.


Observation Definition Specification Tools
Observation Definitions (how do these relate to forward ops)
Observations (Real or synthetic)
Diagnostic Parameters
Assimilation Parameters
Assimilation (Ensemble, var.)
Model Parameters
TIME
Assim_model
Observation Operators
Location
For Perfect Model Exps. OSSE's, Targeting, etc.
State space output files (various freqs and quantities); also extended state space
Assimilation space output files (error measures, assim space time series?), covariances...
Observation space output files (various frequencies and quantities)
Standard Diagnostic Packages

Obs_sequence and other classes defining observation operators component


Obs_sequence: Defines a temporally ordered sequence of obs_sets
Obs_set: A definition plus a time and the corresponding observed values
Observed values
Time
Obs_set_def: Groups many simultaneous observations definitions
Observational Error Covariances
Obs_def (defines a single observation in isolation)
Other params that define obs.
Error Variance
Location; Defines spatial location part of an observation (domain but not model specific, also used by model side)
Obs_model: computes forward operators given state, location, obs_kind. This is both model and domain specific.
Obs_kind (temp, radiance, whatever) Defines part of forward operator.
Much of the 'meta-data' passed here is done by off-line documentation. Automating this appears to be long-term research problem.
Assim_model: adds general set of assimilation useful interfaces to model.
Direct use by highest level assim. methods, too.

1. Rough class specifications for DART below assimilation level

Each class begins with a crude type definition and is followed by a series of Fortran class interface descriptions. The interfaces are roughly ordered by class with initialization, calls to get data from the class, calls to set data in the class, logical queries, input, output, and finally termination.

I. obs_sequence (Called obs stream by operational folks)

This is the highest level class on the observations side.

Defines type obs_sequence_type
Has file_id
file_pointer
status is in or out or both
obs and defs or just defs

1. function init_output_obs_sequence(file_name, additional file level meta_data, number of copies of obs associated with each obs_set, meta_data for the individual copies ...) returns an obs_sequence_type that is initialized and ready for output. The global metadata for the output file is written. At this level it must not be model or observation type dependent. the third argument specifies the number of values of actual observations that will be output with the file, with zero indicating it will just be observation definitions. This is useful for setting up observation definition files for synthetic observation type experiments. Need to decide on action if the file_name already exists. For initial implementation, the file level meta_data is just a string describing the file. The meta_data for the individual copies of the obs should also initially be just a string describing the individual observations sets meanings, for instance ensemble member number, prior, posterior, truth, regular obs, or whatever.

2. function init_input_obs_sequence(file_name) returns an obs_sequence_type which is attached to the obs_sequence format file with file_name. Things are initialized so that the obs_sequence_type is ready to return the first obs_set in the file. If the file does not exist or if its initial global metadata is invalid execution should terminate through the error handler.

3. function init_inout_obs_sequence(file_name, global meta_data, number of copies of obs associated with each obs_set, meta_data for the individual copies) returns an obs_sequence_type but this one can have stuff dynamically appended (required for targeted observations etc.). Not recommended for initial implementation but must be supported in final product.

4. function number_of_data(obs_sequence_type) returns an integer, 0 if no data, otherwise number of copies of obs data (for ensembles, prior, posterior, etc) at each time. This returns the number of observation values associated with each obs_set.

5. function get_global_meta_data(obs_sequence_type) returns the global metadata associated with an obs_sequence. For initial implementation this is just a descriptive string.

6. function get_num_obs_copies(obs_sequence_type) returns the number of copies of observation data associated with each observation set. For just a specification this is 0, for a standard obs_sequence file it is 1, but it might be larger for files that contain truth, noisy obs, prior, posterior, ensemble members, etc.

7. function get_copy_meta_data(obs_sequence_type, index) returns the meta-data associated with the indexth copy of the observations. Error if index exceeds number of copies. For initial implementation meta-data is just a text string describin what this particular copy contains.

8. function get_next_obs_set(obs_sequence_type, optional prev_obs_set???, optional index) : Returns the next obs_set from the obs_sequence. The obs_sets are ordered sequentially by the end of the time interval that they span. In the simple case, they are simply ordered by the scalar time at which observations are taken. The obs_sequence module is assumed to have some global state that keeps track of what was the last observation set returned. However, an optional argument that gives an obs_set and asks for the next obs_set might also be supported. If this is implemented, need to document what doing this does to the global state pointer (probably best to reset it to this point?). The optional index allows access to sequences associated with different copies of the observations. An index of 0 returns only the obs_set_def information and no data, no index or a value of 1 returns the data associated with the first copy, an index greater than 1 returns data associated with the corresponding copy (error if number available is exceeded).

9. function get_first_obs_after(obs_sequence_type, time_type) returns obs_sequence with pointer set to the first observation in this obs_sequence whose observation interval begins after the time_type. Not needed for initial implementation.

10. function get_last_obs_before(obs_sequence_type, time_type) returns obs_sequence with pointer set to last observation in this obs_sequence whose observation interval ends before the time_type. Need to clarify action if no such obs_set exists. Not needed for initial implementation.

10. function add_obs_set_def(obs_seq, obs_set_def) returns a handle (for now an integer index) to identify this obs_set_def.

11. function add_obs_set(obs_seq, obs_set) should this return a handle of some sort or just be a subroutine?

11. Additional search and query options might be needed eventually.

12. function end_of_sequence(obs_sequence_type) returns true if the pointer is at the end of the file.

13. subroutine output_obs_set(obs_sequence_type, obs_set_type, optional index) writes the obs_set to the file associated with this obs_sequence_type. An error occurs if this obs_set is not in proper time order for this sequence; need to determine exactly what action should be taken. If only the obs_set_def is to be output, index should have the value 0. If index is not included, it is assumed that the data (time and observation values) are for the first copy. If an index > 1 is included, it indicates that data is for this copy. For initial implementation, insist that calls to

output_obs_set be in index order (1, 2, ...n) and that all calls for a particular obs_set be made before calls for any other obs_set. Should check for compliance, but for initial implementation may just trust to users care.

14. function terminate_obs_sequence(obs_sequence_type) terminates output or input, closes files.

II. Obs_set

Defines a set of observations that are all associated with the same time interval and the associated observation values. This pushes time interpolation to this rather high level. This should be re-evaluated at design review. The higher level assimilation algorithms would need to keep states at different times if model won’t return stuff at required time. In mature implementation, time must be general and the lower level assim_model class must return info on the interval over which an observation is taken (weighted time interval with delta function as simplest case, followed by average, weighted average, etc.). The higher level assimilation will have to decide what to do with observation sets that are defined over more generalized time intervals.

Defines type obs_set_type

composed of
values of observations
flag indicating whether observations are present or if this is just definition
generalized_time representing interval over which observation is taken
obs_set_def_type

1. function init_obs_set(obs_set_def, num_copies): Initializes the storage for an obs_set associated with the obs_set_def and with num_copies of the associated data. Num_copies is optional with a default value of 1.

1. function get_obs_set_time(obs_set_type :: set): Returns a generalized_time_type that describes the characteristics of this set of observations.

2. subroutine get_obs_values(obs_set_type :: set, obs, index??) : Returns a vector of ‘real’ values that came from the instrument(s). Some value might be returned if the data is missing for certain elements, but this is not defined. If integer or other types of obs were happening might have to extend or overwrite this, but can’t think of a relevant case.

3. function copy_obs_set(obs_set_type) returns a copy of the obs_set, overloaded to =.

4. subroutine set_obs_set_time(obs_set_type, generalized_time_type) sets the time interval associated with a particular observation.

5. subroutine set_obs_set_values(obs_set_type, vector of values) : Sets the observation values for an obs_set. Possibly used for setting up assimilation system simulation experiments as an example.

6. subroutine set_obs_set_missing(obs_set_type, vector of logicals): The observations corresponding to any true elements are set to missing.

7. function contains_data(obs_set_type) returns logical, true if this set has observations and false if it only has a definition.

8. function obs_value_missing(obs_set_type) returns a logical array with false for all entries where an observation exists and true if observation is missing.

9. function read_obs_set(file pointer), reads an obs set from file with this pointer (can just be an index for now)

10. function read_obs_set_data(file pointer), reads only the data values for an obs set.

11. subroutine write_obs_set(file, pointer, obs_set), writes an obs_set to file with this pointer.

12. subroutine write_obs_set_data(file_pointer, obs_set), writes only the data values for an obs set the the file.

ALSO INHERITS the calls from obs_set_def which should act directly on the obs_set_def in the obs_def structure.

IIB. Set_def_index

Provides permanent storage with indexing and retrieval for obs_set_def structures. This is between the obs_set_def and the obs_sequence. Only obs_set_def structures that have been registered in the index can be used as subsets or can be referenced in an obs_set.

Defines type set_def_index_type

An ordered list of set_defs (can be in an array for right now)

max_set_defs
num_set_defs

1. function init_set_def_index(max_set_defs) returns a set_def_index (suppose one could have more than one

2. function add_set_to_index(set_def_index_type, obs_set_def) returns the unique integer key for this set.

3. function add_subset_to_set(index_of_superset, index_of_subset) Need to bump up all the things from the current obs_set_def that concern subsets to this level.

III. obs_set_def

Defines a set of associated observations. A definition only includes information about the spatial aspects of the set of observations (the values and the time interval are added by obs_set).

Defines type obs_set_def_type

contains information on the
error_covariance / error correlation
list of obs_set_defs
list of obs_set sizes
---
list of obs_defs
num of obs_defs

Should have a unique key for assimilation algorithm caching

As currently envisioned, obs_set_defs are viewed as being recursive. Each obs_set_def is composed of zero or more obs_set_defs (called obs_subsets in description) plus zero or more individual scalar observations. The abstraction is also associated with an ordered set of unitary observations obtained by recursively descending the subsets.

1. function init_obs_set_def(num_subsets, num_obs) returns a handle to a structure for an obs_set_def. Specifying the number of subsets and num_obs for the single obs is annoying but precludes the need for dynamic data structures at this point. Might want to make them optional at a much later time.

2. subroutine get_diag_obs_err_cov(obs_set_def :: set, cov) : Returns the diagonal of the observation error covariance matrix for this set in a one dimensional array.

3. function get_obs_err_cov(obs_set_def :: set) : Returns a two dimensional array containing the observational error covariance for this set. Not needed in initial implementation.

4. function get_expected_obs(obs_set_def :: set, model_state_vector or extended model state vector:: state) : Returns a one dimensional array containing the expected values for this observation set given the model state. Need to give more thought to how the extended state is passed around if it is required and whether it is of fixed or variable composition (probably variable for big models). For initial implementation need only implement raw state part.

5. function get_obs_set_def_key(obs_set_def) returns the unique integer key associated with this set. May want interfaces to access obs_set_defs by key from an obs_sequence at some later point.

6. function get_total_num_obs(obs_set_def :: set): Returns the total number of observations in a set, including the observations included recursively in all subsets. This is easily computed as sets are built up recursively.

7. function get_obs_def(obs_set_def, index) returns handle to the the index-th observation (this may be a problem for efficiency with obs sets being built up recursively) in the set. The order is established by the recursive search of the set. Need error action if index exceeds total number of obs in set.

8. function get_number_single_obs(obs_set_def), returns the number of observation definitions in the set that are not included in other subsets; not clear that this is necessary as a public interface.

9. function get_number_obs_subsets(obs_set_def), returns the number of observations sets that are contained in the current set; not clear that this is necessary as a public inteface.

10. function get_single_obs_def(obs_set_def, index), returns the index-th observation from the single observations in this set. May not be necessary. Need an error action if index exceeds number of single obs in set.

11. function get_obs_subset(obs_set_def, index), returns the index-th obs subset handle; not clear if this needs to be a public interface. Need an error return if index exceeds the number of subsets.

12. function copy_obs_set_def(obs_set_def) copies the obs_set_def (this will be involved). Overloaded to =.

Following 3 interfaces push up obs_def functions to this level (inherited)

13. subroutine get_obs_locations(obs_set_def, locations) returns ordered set of locations for the observations in the set.

14. subroutine get_close_states(obs_set_def, radius, number, indices) returns array of numbers plus 2D array of indices for state variables close to each ob in the set.

15. subroutine get_num_close_states(obs_set_def, radius, number) returns array of number of close states for each of the observations in the set.

16. subroutine add_obs(obs_set_def, obs_def) adds the obs_def to this obs_set as a single observation. Need error return if the number of single obs would be exceeded by this insertion.

17. subroutine set_err_cov(obs_set_def, obs_subset_index, obs_subset_index, obs_index1, obs_inces2, cov) sets error covariance between two obs subsets/obs. Only two of the subset / obs indices can be set in the call. The covariance is a two dimensional matrix with the covariance values. Error is required if the indices are outside the range for this set or if the covariance matrix is not the correct size for the pair. Not needed in initial implementation.

18. subroutine add_obs_subset(obs_set_def, obs_set_def (subset)) adds the second set as a subset of the first. Need error returns if the first set is already full.

19. function diag_obs_err_cov(obs_set_def :: set) : Returns true if error covariance for this obs set is diagonal, false otherwise. Initial implementation can support only diagonal covariances with great simplification.

20. function read_obs_set_def(file_pointer), returns an obs_set_type with contents read in from a standard file format (this may be relatively sophisticated as it will have to allocate storage, etc. Should make use of calls defined above.

21. subroutine write_obs_set_def(file_pointer, obs_set_def) outputs an obs_set_def in standard file format.

Need to push up obs_def functions to this level

IV. obs_def

Defines a single scalar observations spatial characteristics and kind.

Defines type obs_def_type

contains information on
error variance
params associated with observation
location (a location type)
'kind' (says something about forward operator)

unique key for caching

1. function init_obs_def(obs_kind, obs_location, error_variance) returns an obs_def with this kind, location and error variance.

2. function get_expected_obs(obs_def, model_state_vector / extended state vector), returnsexpected value given state or extended state vector. For initial implementation only need to deal with raw state.

3. function get_error_variance(obs_def), returns observational error variance of observation definition.

4. function get_obs_location(obs_def), returns a location_type for this observation. For some more complex types of observations the definition of location may involve additional parameters, but let's avoid that complexity for this stage.

5. function get_obs_def_kind(obs_def), returns the kind of this observation, this probably needs to itself be a class (obs_kind class) although it could just be some fixed text string representation for now.

6. function get_obs_def_key(obs_def) returns integer key to this definition.

7. function get_num_close_states(obs_def, radius) this assumes that the model class data is global (only one type of model in use). At some point it would be nice to generalize this, but not now.

8. subroutine get_close_states(obs_def, radius, number, close_state_list) See above.
9. function copy_obs_def(obs_def) returns obs_def overloaded to =.

10. function set_obs_location(obs_def, location)

11. function set_error_variance(obs_def, err_var)

12. function set_obs_def_kind(obs_def, obs_kind)

13. function read_obs_def(file_pointer) reads an obs_def from standard format off the file. Will need error returns if read fails.

14. function write_obs_def(file_pointer, obs_def) writes an obs_def in standard format to the file.

V. location

This is the level at which the details of the spatial representation come into play. There will be different location data representations for different spaces (sort of like the one and twod loc and dist mods but more general).

Defines type location_type

1. function get_dist(loc1, loc2), returns some metric of distance between two locations.

2. function get_location(location_type) returns values of the location in the arguments; inverse of set_loc.

3. function set_loc(space model specific arguments, for instance, lat, lon, height) returns a location type with these values.

4. subroutine write_location(file_pointer, location_type) writes the location to the file in a standard format.

5. function read_location(file_pointer) reads the location from the file in a standard format. Need error return if read fails.

VI. generalized_time

For early implementations, let’s just assume all times are discrete and use the standard FMS time manager package to do this. However, need to keep possibility of a weighted observation time interval in mind. Need to be able to output and input a time.

VII. obs_kind

This is specific to a particular model and some notion of externally defined observation type. For a model, need to be able to get a forward operator to generate this quantity in conjunction with spatial (and possibly temporal, currently pushed to highest level) interpolation. For now, the obs_kind is just a string.

1. function get_obs_kind(obs_kind) returns string (integer for now) specifiying the obs_kind.

2. function set_obs_kind(string) returns and obs_kind with this string (integer for now) as its definition.

3. subroutine write_kind(file, kind) outputs a kind to file.

4. function read_kind(file) reads a kind from a file.

Can this whole level just be dropped for initial implementation?

VIII. obs_model class

This is the level at which classes become model dependent on the observation taking side of things. This class needs to know considerable detail about how the model data is laid out, how to interpolate, how to do forward operators for different types of observations, etc. Probably the biggest chunks of code someone will have to write in order to get things going? Maybe there should be one more layer that just does interpolation and knows about the model?

1. function take_obs(model state vector or extended model state vector, location, obs_kind_id) there may be a variety of different algorithms. Making use of interpolation if needed from assim_model, this computes the observation given the state and returns the value.

IX. assim_model

This is the interface needed to a model by the assimilation algorithms and observation networks. This is model specific and tries to abstract away the model details. Because of F90 limitations, seems appropriate to think of only being able to work with one model type (class) at a time, i.e. one couldn't work on a separate atmosphere and ocean model at once with these interfaces. Assim_model is a class for a particular kind of model and the instances are the state (including some indexed time). Initialization and end calls are for the class data (for instance setting up transform stuff for a spectral model). Smart choices about timestepping can be pushed into calls at this level. Extended state should not be viewed as part of the class data, but is instead the return from some functions operating on the state. May want a concept of static extended state (things that can be obtained by operating on the state variables without time integration) and extended state that requires integration. For initial implementation, assume that model timestep is fixed at a particular delta_t and that all observations will be specified as falling exactly on one of these timesteps. The general timestepping computations can probably be pushed into an auxiliary module since they will be used for all models.

Defines type assim_model_type
time type with associated global base time that defines model time
state vector
meta data describing state vectors

1. function initialize_assim_model() initializes the class data for the model, for instance transform data for spherical harmonics. Returns the size of the models state vector.

2. function init_diag_output(file_name, global_meta_data, copies_of_fields_per_time, meta_data_per_copy) returns file_id for an output diagnostic file that will output a given number of copies (say posterior, prior, truth, ensembles, etc) of fields at each time. For now the global meta-data is a text string describing the file contents and the meta_data_per_copy is an array of text strings describing the contents of each copy of data.

3. function get_model_size() returns integer size of model state vector; need to be very careful to understand multiple time-level state interactions. Note that this is class data.

4. function get_max_dt()

5. function get_min_dt()

6. function get_other_dt_stuff()

7. function get_last_state_time_before(time)

8. function get_first_state_time_after(time)

9. function get_closest_state_time_to(assim_model, time) given a model state in assim_model and a time, finds the closest time to which the model state can be advanced to this time.

10. function get_next_state_time(time)

11. function get_prev_state_time(time)

12. function get_initial_condition() returns an assim_model_type to start from. This might come from a file or from something else, controlled by model runtime paramerters??? This needs to be given some help through some runtime interface I think. One option is that a 'restart' file is available in some standard place, this is read in and the corresponding state returned (watch out for multi-level timestepping stuff here). Another option is just some basic spin-up state. The assim_model_type returned has a time associated with it. For now, this time needs to just come in with whatever is read from file or generated and is probably controlled by a runtime input. Coordinating the time between the model and observation set areas should be automated eventually but can be pushed to runtime for now.

13. subroutine get_state_meta_data(index, location, optional kind) returns metadata for the indexed state variable as a location plus a kind (if the model has more than one kind of variable).

14. subroutine get_extended_state_meta_data(index, location, optional kind) returns metadata for the indexed extended state variable. May need to further refine this for large models with a large number of possible extended state types.

15. subroutine get_close_states(location_type, radius, number, indices) returns list of state indices within radius of the given location and the number of such state variables. May want to make kind an optional input. Need error handling if there is a storage issue. Should probably implement with a clean extensible list. Note that these are class functions that don't depend on a particular state instantiation.

16. function get_num_close_states(location_type, radius) returns the number of state variables within radius distance of this location.

17. function get_model_time(assim_model_type) returns time type that is the time for this state.

18. function get_static_extended_state(assim_model_type, optional field specifier) returns static extended state variables computed from model state. Not needed in initial implementation.

19. function get_model_state_vector(assim_model_type, plus additional arguments to specify a portion?)

20. function copy_assim_model(assim_model_type) returns assim_model_type overloaded to =.

21. function advance_state(assim_model_type, target_time, extended state requests optional) returns state and optionally extended state vector advanced in time to the target_time. If the model has flexibility to do so, it will be advanced to exactly target_time. If it has a fixed time_step,

target_time should be within some small tolerance (for floating point stuff) of a time to which the model can go or an error should be returned. The philosophy here is that the requisite time computations should be done first and then the model should be advanced. For initial implementation, assume that model has single dt and that all observations will fall exactly on a dt interval.

22. function interpolate(state vector / extended state vector, location, field_id) returns value for this field interpolated to the location. Need to be very clear here. What is a field_id and how is it obtained. What about 2D fields in 3d models, etc. For now, only implement for state vector and add extended state at later date. Field_id needs to be associated with some sort of string i.d. that is part of the model metadata.

23. subroutine set_model_time(assim_model_type, time_type)

24. subroutine set_model_state_vector(assim_model_type, state_vector, plus additional arguments to specify a portion?

5. subroutine write_state_restart(assim_model_type, file_name) writes out the state vector and the time in a form with machine precision so that time integration can be resumed without evidence of interruption.

26. function read_state_restart(file_name) reads a machine precision restart from file_name including the time and state vector.

27. subroutine output_diagnostics(file_id, state vector, time, copy_index optional) outputs diagnostic state information for this time for the copy_index copy. If copy_index is not present it is assumed to be 1. For now, the copies at a given time must be called sequentially and no other calls for output for this file_id may be made until all copies are output at this time.

28. subroutine end_assim_model() shuts down and cleans up class data for model.

2. Contents of diagnostic output and control input files:

I. State space output files: Contain metadata and data for output of state space quantities. These are arranged into a (set of) file(s) with different associated time axes (in the NetCDF sense). Things that may be here include the ensemble members before and after each observation (prior and posterior), and the ensemble mean. Might also want extended state to be available from model which would have to output the appropriate extended state and its associated metadata. Might also want variance of prior and posterior state (more consistent with non-ensemble methods). If available, the truth for state variables should be in a file of this format (but would be generated ahead of time) if output is for a synthetic run. In all cases, the assim_model level is required to provide calls that output metadata for the appropriate output variables to a file.

II. Observation space output files: Contain prior and posterior (ensemble) values for the observations, truth for the observation would also be in a file like this. Could also include variance, etc., if desired. These variables are apt to be irregularly spaced in space and time with potentially very complex metadata. While it is desirable in the long run to attempt to use some standard metadata format to express this, doing this correctly appears to be a difficult research problem. For the initial implementation, it is acceptable to use a customized ascii based format which can be plotted for some subset of metadata types by standard matlab based interfaces. For efficiency, it will be necessary to compact this ascii metadata at the head of the output file as per NetCDF. However, for ease of initial implementation may want to generate two output files, one with metadata and one with data and combine them after execution is completed.

There is significant overlap between the observation definition/observation input files and the observation space diagnostic output files. For the initial implementation, these should use identical basic metadata although the diagnostic output may contain additional instances of the data.

III. Assimilation space output files: Measures of global error, detailed time series of individual assimilation variables (do this for efficiency?), covariance output between state/obs variables. This output is generated directly by the assimilation level which is responsible for generating the appropriate metadata. However, in many simple cases, the majority of this output may in fact be in model space and the model interfaces could be used to generate metadata and output the data. In more general cases, this metadata may be even more messy than that for the observation space files since it will combine observation and model space output along with statistical products between these spaces. Again, it would be desirable to use a standard metadata format, but this is probably impossible at present and a custom metadata format with associated extraction and plotting will be required.

IV. Observation definition/observation input files: These contain efficient metadata describing observations and sets of observations as well as data (time plus observation value(s)) describing the associated observations. Eventually, want to be able to stream real observation sets from some community standard data servers through this interface. Also need a capability to generate observation sets on the fly (i.e. need random access files with read and write pointers) so that targeted observation types of OSSEs can be performed without modifying the configuration of an assimilation.

V. Parameter control input files: A number of different files are needed to control run-time behavior of different components of the assimilation system. Traditionally, this type of input has tended to be done through F90 namelists but this has proved to be somewhat limited. For now, DART will allow the use of either namelists or more general control input files to be read at run-time. Standard naming convention for input control files will be the module name followed by an appropriate extension.

3. Different views of DART for different users:

I. Diagnostics users (general diagnostics interfaces)

Want to be able to select the output files associated with a particular experiment. The experiment was generated by a particular model, set of observations, assimilation method, and parameterizations associated with the model and the assimilation method. These different aspects will control to some extent how the diagnostics appear, although diagnostics in most cases should be relatively independent of this.

Some example diagnostics that one might like to have readily accessible by a simple GUI. Initially, many of these will be front-end wrappers for Matlab diagnostic routines. Some examples of diagnostics that would be nice to have standardized:

a. Plots of overall RMS, spread, etc. as function of assimilation time
b. Plots of ensemble behavior for individual variables
c. Order statistic histograms for selected variables, for both truth or observations, if observations need to correct for error
d. A catalog of which variables are available and a way to relate them to what they represented in the model
e. Plots or animations of model state (or slabs / hyperslabs of model state) as function of lead time
f. Plots of error as above
g. Plots of spread as above
h. Plots of mean bias as above
i. Plots of individual ensemble members as above
j. Plots of error for individual members as above
k. Diagnostic plot of where the observations are
l. For non-perfect cases can’t do all of the quantities above, may often be limited to working at observation locations which may not be regularly gridded
m. Mean value of innovations, time series of innovations, etc.
n. Plots of prior and/or posterior correlations of variables

In order to do this in the most general form, the output file must contain the following items:

1. Values of observations, along with description of location and error, plus possibly h's?a. Plots of overall RMS, spread, etc. as function of assimilation time
b. Plots of ensemble behavior for individual variables
c. Order statistic histograms for selected variables, for both truth or observations, if observations need to correct for error
d. A catalog of which variables are available and a way to relate them to what they represented in the model
e. Plots or animations of model state (or slabs / hyperslabs of model state) as function of lead time
f. Plots of error as above
g. Plots of spread as above
h. Plots of mean bias as above
i. Plots of individual ensemble members as above
j. Plots of error for individual members as above
k. Diagnostic plot of where the observations are
l. For non-perfect cases can't do all of the quantities above, may often be limited to working at observation locations which may not be regularly gridded
m. Mean value of innovations, time series of innovations, etc.
n. Plots of prior and/or posterior correlations of variables
a. Plots of overall RMS, spread, etc. as function of assimilation time
b. Plots of ensemble behavior for individual variables
c. Order statistic histograms for selected variables, for both truth or observations, if observations need to correct for error
d. A catalog of which variables are available and a way to relate them to what they represented in the model
e. Plots or animations of model state (or slabs / hyperslabs of model state) as function of lead time
f. Plots of error as above
g. Plots of spread as above
h. Plots of mean bias as above
i. Plots of individual ensemble members as above
j. Plots of error for individual members as above
k. Diagnostic plot of where the observations are
l. For non-perfect cases can't do all of the quantities above, may often be limited to working at observation locations which may not be regularly gridded
m. Mean value of innovations, time series of innovations, etc.
n. Plots of prior and/or posterior correlations of variables

In order to do this, output files must contain the following:
1. Values of observations, along with description of location and error, plus possibly representation of forward operators
2. Prior ensembles for observations
3. Model state variables, ensemble members and mean
4. Model state variables before and after each assimilation time (can get innovations from this)
5. Truth state variables along with the ensemble if this is a simulated observations case.

II. University type educational user (student):

This type of user wants to do new runs with existing models (or modified models) and design their own observation set or use previously defined observation sets. Divide this into two categories: Making a run with existing observational set and model but changing some parameters of the run like model or assim parameters and generating output

OR, designing a particular observational set and running either synthetic obs or real obs with this configuration

Will need tools to build observation sets, in particular to build sets of relatively regular observations or small number of irregularly spaced.

III. Sophisticated model developer: Put in a new model and some associated metadata and plotting routines etc. Will need to write the assim_model class, the obs_model class, and the location type if the domain is something new. While this should be much more straightforward than in a naive modeling setup, this is not going to be trivial and will require lots of expertise on DART.

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4. Sophisticated assim person: Put in a new assimilation scheme.

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5. Sophisticated data set person, put in a new data set for use with one or more models. This may be relatively straightforward if the forward operator is simple, but could be extremely complicated in the case of the most general forward operators.

Some notes on DART usage in prototype:

Given a model, etc.

1. Observation definitions, observations set definitions, result is a file containing an observations definition set (set_def_list); can end up with an array of set_def_lists associated with a particular spatial dicretization (and model because of obs_kind?)

2. Observation sequence definitions: define a sequence of observations through time, result is a file containing an observation sequence (obs_sequence): have an array of obs_sequence files available for a particular spatial discretization (and model?). These may or may not have some sort of observation values associated with them, but for this purpose those are not relevant.

3. Perfect model output files: given an observation sequence definition (with no obs values required) one can run the model (given some initial state). Have output to a state file which receives the true values of the (extended) state. Also have output to an obs_sequence file which includes not only the same definition, but also adds in the true value of the observation variables and the synthetically generated observations that have samples of the observation error added onto the true observation variables.

4. Assimilation experiments: take as input an obs_sequence with at least one copy of data associated to act as observations. Outputs are assim, state and obs output files. The state output has the values of the state ensemble members both prior and posterior. The obs outputs are another obs_sequence file, this time with the prior and posterior values for the observations associated. The assim output files can be postponed for development for now.

5. Doing analysis: Analysis is done by taking input from a set of files. For observation space analysis, input files might include one that has the perfect obs (if available), the actual obs (always available) and for a filter a file with the prior and posterior obs. In the long run want to be able to sub-sample so that files don't get huge, but that's an add-on. For state, might have truth (if available), plus a second file with prior and posterior ensembles. Analysis programs need to be told what file name (and what copy or metadata tag within the file) are associated with the truth, the obs (for obs files), and the ensembles. They can then provide an array of plotting options.