iCLM4 -- key physics spots

Essentially, whenever water moves around (h2osoi_liq/_ice, h2ocan, h2osno), isotopic/tracer water must move around too. In many places this is straightforward, but when phase changes occur, equilibrium and kinetic fractionation factors must be considered.

The tracking of water within leaves (its isotope ratio) is a key addition, and necessary for resolving the canopy isotopic water balance.

Apologies for verbosity and length. Some of the notes below may seem obvious or silly, but I erred on the side of too helpful.

BareGroundFluxesMod.F90

- As soil water or canopy water -> 0 during evaporation/sublimation, at some point (??? in iCLM4) must evaporate/sublimate all tracer water, otherwise isotope ratios distill -> infinity
- CLM evaporates out of the top soil layer, so the isotope ratio of the top layer is the natural choice, but sometimes there is not enough water to supply the evaporation demand. The "searchforwater" loop is needed to find the first soil layer with enough water to supply the evaporation. This may not be an issue in the BeTR version, because the below-ground transport could potentially supply evaporation from the top ~30 cm (or thereabouts) of soil moisture, as occurs in the real world (Wang et al., 2014). This is a major drawback in iCLM4 and hopefully will look much better in iCLM5. I'm very excited and optimistic about this one.
- Need to be careful to have 3 cases for evaporation, for the fractionation factors:
    - (1) evap>0, T_grnd>T_frz -- equilibrium (Horita and Wesolowski, 1994) and kinetic (Merlivat and Jouzel, 1979; or Merlivat, 1978; or Mathieu and Bariac, 1996) fractionation factors
    - (2) evap>0, T_grnd<T_frz -- sublimation (no fractionation factors)
    - (3) evap<0 -- same case as #1
    - And make sure you use the appropriate coefficients for equilibrium fractinoation for ice versus liquid (Horita and Wesolowski, 1994)
- Need to insert fill values into some of the arrays (e.g., ecosystem resistances and leaf water isotope ratios) so that the averaging across PFTs works out (can't have NaNs)

Biogeophysics1Mod.F90

- Similarly to BareGroundFluxes' soil evaporation, for the isotope ratio of the surface vapor, assign the isotope ratio of the highest soil layer with enough water (>h2otiny).

Biogeophysics2Mod.F90

- At the first-order Euler evaporation step:
    - If evap<0, assign RFlux=canopy vapor isotope ratio to the first-order correction term

    - Otherwise, RFlux=isotope ratio of j=snl(c)+1 (top snow/soil layer), since that's where the evaporate coming from. And be sure to use a weighted average of the soil liquid and ice water's isotope ratios.
    - Here, there may also be trouble if the RFlux ends up as 0 for some reason (e.g., too little bulk water in the evaporation source water pool), but there's still bulk evaporation going on. In this case, need to set RFlux to Rstnd (1, or Rsmow, or some deeper soil layer, or GNIP ratios)

BiogeophysicsLakeMod.F90

- Use Merlivat and Jouzel (1979) for lake evaporation. They developed this formulation for evaporation over open water, so it's quite appropriate here. Plus, we determined that treating lake water with no isotopic fractionation leads to wacky isotope ratios around lakes in a coupled model set-up (far too enriched d18O and too depleted dxs).

CanopyFluxesMod.F90

- Same points as in BareGroundFluxesMod (aside from setting fill values for veg. components of arrays)
- How to parameterize a kinetic fractination factor for rlitter (leaf liter layer resistance) is an open question. Global sensitivitiy experiments Jesse and I have done have shown that using alpk=1 (no kinetic fractionation) for litter resistance is a fine place to start.
- Back out conductances for isotopic transpiration (T) and evaporation of canopy-intercepted water (Ec) (as in the geotrace code)
- HydrologyTracerCanopy subroutine -- critical step, to calculate isotope ratios of leaf water and canopy vapor, then the modified Craig-Gordon model is used in CanopyFluxes to calculate the isotopic flux streams.
    - First calculate steady state isotope ratios, where the transpiration isotope ratio is equal to the xylem water (root-weighted) isotope ratio
    - Optional Peclet effect and non-steady state
- If the transpiration is looking funky, you can always just hard-code steady state in as:
    - isotope_T = R_xylem*bulk_T

Hydrology1Mod.F90

- During first order Euler update of h2ocan, need a check to make sure that if there's no bulk h2ocan, the tracer h2ocan is set to 0 as well.

HydrologyLakeMod.F90

- Evaporation (sublimation) of snow on lakes can be troublesome. Be careful when setting the isotope ratio of the snow evaporation/sublimation, and melt, especially when there is very little evaporate/melt.

HydrologyTracer.F90

- Critical tracer module. Among other things, contains the HydrologyTracerSoilWater (soil substepping routines) and HydrologyTracerCanopy (5-way tracer mass balance between sunlit/shaded transpiration, ground evaporation, canopy evaporation, and total ET).
- Possibly, HydrologyTracerSoilWater may not be needed in BeTR, if you already have algorithms to maintain numerical stability when moving around tiny amounts of tracer mass?
- Also important: get_wratio function -- calculates isotope ratios, but (the important part) below a certain cutoff for the denominator (bulk mass/flux/whatever) the ratio is set to 0. (This is for stability)

SoilHydrologyMod.F90

- SurfaceRunoff -- for surface runoff, use the isotope ratio of qflx_top_soil (since it's what is incident on the surface).
- SoilWater -- isotopic water is not moved around in here, since it depends on the final change in bulk soil moisture once all of the checks and updates are done (Some of them are in Drainage, e.g.).
- Drainage -- as it stands, the changes in moisture content for each soil layer after the tridiagonal system is solved for the bulk water soil update are used to determine fluxes between each soil layer (starting from the first layer, where we know the infiltration, the upper boundary condition). Then these fluxes are moved between the relevant layers, in a series of substeps (1 second currently, for stability).
- Drainage -- just like the fixes for when the tridi solve finds h2osoi<0 as a solution, we have to fix negative tracer water sometimes. Jesse and I settled on:
    - If layer j has negative tracer water, fill with water from layer j+1
    - If bottom layer has negative tracer water, fill by reducing the tracer drainage flux

SoilTemperatureMod.F90

- PhaseChange --
    - Make sure if all the snow melts, all the tracer/isotopic snow does too.
    - No fractionation factors for snow melt
    - Isotope ratio of freezing water should be the ratio of the *liquid* mass

UrbanMod.F90

- Never got the fractionation factors and Craig-Gordon model to work well for urban landunits, so this module has always been constant ratio (non-fractionating).
- Considering that some 30% or so of the land surface contained urban landunits (I think it was a 2-degree run?), it would certainly be nice to get this working. We always had this on a back burner, however, because most folks with a dataset didn't stick a Picarro on a skyscraper collect rainwater off their gutters (though that would be interesting…); most data sets folks would use with iCLM are not from an Urban setting.