Transient Algorithm

1. Set *m* = 0 and run an unthrottled KMC snapshot. Increment *m* by 1.
2. Gather all observed event frequencies (oEFs) and rank the processes:
   1. Calculate unthrottled event frequencies (uEFs) from the oEFs and the old aggregate throttling factors (ATFs) by

uEF = oEF / ATF

* 1. The processes are ranked with paired ranking according to the fastest uEF in the pair. If a process is irreversible, then its reverse process is assumed to have an EF of zero.
     1. For each process rank, the uEF of that process rank is the higher of the two uEFs within that process pair.
  2. Classify each process pair as fast frivolous processes (FFPs), the fastest rate determining process (FRP), slow processes (SPs), or negligibly slow processes (NSPs).
     1. The FRP (if it exists) is the fastest process pair that is not in quasi-equilibrium.
     2. FFPs are the set of process pairs that are quasi-equilibrated and faster than the FRP.
     3. SPs are the set of non-negligible process pairs that are slower than the FRP and may or may not be quasi-equilibrated.
     4. NSPs are process pairs where each process in the pair has rates low enough that they are not expected to occur during the maximum relevant simulation time (MRST, which is “max\_time”).
        1. Any processes pair with a rate below Nsites/MRST is excluded.
        2. MRST is user supplied. During most applications, this would be of the same order of magnitude as the specified simulation cutoff\_time.
     5. Any process in a pair that is negligibly slow is not throttled, and is not considered in the below algorithmic steps.

1. Calculate ATFs for the required compression scale. Iterate over the compression scales to try to make EF\_range\_fast\_actual ≤ EF\_range\_fast and EF\_range\_slow\_actual ≤ EF\_range\_slow or EF\_range\_actual ≤ EF\_range\_full, starting with no compression (0, 0) and increasing up to the maximum (3, 3) if the compression criteria are not met. (The first index in the 2-tuple (f, s) is the fast process compression level, and the second index is the slow process compression level.)
   * When setting the compression level and staggering factors (SF) during the below steps:
     + The fast process compression level always proceeds through each of its levels before the next slow process compression level is tested. (In other words, the fast/slow compression level is the inner/outer variable in a doubly-nested loop.)
     + Each compression level sets a target SF for each pair of adjacent processes.
       - If at least one of the processes in the pair is throttled, the actual SF is the smaller of the target SF or the actual ratio between the uEFs.
       - If both processes are unthrottled, the actual SF is the actual ratio between the uEFs (i.e., no compression/throttling).
   1. Always attempt to step down the predicted throttled event frequency (ptEF) of the slowest FFP (sFFP) from the previous oEF toward the minimum FFP rate FFP\_floor.
      1. The sFFP is the slowest process pair with uEFs above FFP\_floor.
      2. The default target ptEF of the sFFP is determined by the formula

sFFP\_ptEF = oEF \* SU / SD

where oEF is the oEF from the previous snapshots, SU is a step-up factor (this is for cases where the sFFP is *already* more aggressively throttled than other FFPs, in which case we bring the sFFP in-line with other FFPs before the stepdown), and SD is the step-down factor which attempts to gradually bring the sFFP closer to the floor.

* + - 1. Make a set of the prior snapshot ATFs for the current set of FFPs (but excluding the FQPs). SU is then obtained by taking the largest of this set (or 1, whichever is lesser) and dividing this factor by the previous ATF for the current sFFP. By definition, the SU should always be > 1. The restriction of the numerator being < 1 is to prevent the SU from stepping up the ptEF of the sFFP above the uEF prior to step-down.
      2. SD is a user-defined/adjustable parameter. A conservative value is 10.
    1. During this stepping down of the sFFP, the ptEF of the sFFP is subject to several constraints.
       1. The sFFP ptEF is larger than or equal to FFP\_floor; and
       2. The sFFP ptEF is larger than or equal to the product of Nsites and the ptEF of the FRP; and
       3. The sFFP ptEF is at least the product of the SF for the current compression level and the ptEF of the next slower process, if it exists; and
       4. The sFFP ptEF is never larger than the corresponding uEF.
       5. If the sFFP is within Nsites of the Floor, then (during stepdown) we constrain it to also not being throttled closer than the *current compression* *staggering factor* relative to the fastest FQP. If the compression level is 0, then this factor is Nsites (this is *different* from other parts of the code, where a compression level of 0 has no restriction). The sFFP can of course *naturally* be closer than Nsites to the fastest FQP, in which case it would not be stepped down further.
  1. Compress the FFPs
     1. Any FFPs with uEFs below FFP\_floor are not compressed (we refer to these as FQPS)
     2. Iterate over the FFPs, starting with the sFFP and moving to the fastest FFP (fFFP).
        1. The ptEF of the next faster process (if it exists) is the ptEF of the current process multiplied by the SF between the current and next process for the current compression level.
        2. The ATF is then calculated by

ATF = ptEF / uEF

* 1. Compress the SPs.
     1. The fastest throttled slow process (fSP) is the fastest SP that has a rate less than or equal to oEF\_FRP / Nsites.
     2. Iterate over the throttled SPs, starting with the fSP and moving to the slowest SP (sSP).
        1. The ptEF for the next slower process (if it exists) is the ptEF of the current process divided by the SF between the current and next process for the current compression level.
        2. The ATF is then calculated by

ATF = ptEF / uEF

* 1. Calculate the achieved compression ratio(s) and determine if they meet the compression criteria.
     1. If split range compression is employed:
        1. For fast processes, if the sFFP is within Nsites of an adjacent FQP such that

FQP\_ptEF \* Nsites > sFFP\_ptEF

then

EF\_range\_fast\_actual = fFFP\_ptEF / FFP\_floor

Otherwise,

EF\_range\_fast\_actual = fFFP\_ptEF / sFFP\_ptEF

* + - 1. For slow processes,

EF\_range\_slow\_actual = FRP\_ptEF / sSP\_ptEF

* + 1. If full range compression is employed, then EF\_range\_full\_actual is the ratio of the ptEFs for the fastest and slowest processes ranks (for each process rank, the ptEF of that process rank is the higher of the two ptEFs within that process pair).
    2. The compression criteria are met if the actual compression ratio(s) are less than the target compression ratios.
  1. Check if the target compression is achieved. If the achieved compression ratios are not sufficient (based on Step 2e) and the current compression level is less than the maximum allowed, go to Step 2a and try the next compression level. Otherwise, continue.
  2. If *m*/*M* is an integer, unthrottle the slow processes by setting their ATFs to 1.

1. Apply the calculated ATFs to the transition rate constants. Run a snapshot, and increment *m* by 1.
2. Repeat steps 1-3 until steady-state is reached.