Supplementary Note:
Positive Recurrence for Single-Linkage Bimolecular Weakly Reversible Stochastic Reaction Networks

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Abstract

This supplementary note collects edge-case clarifications and reproducibility interfaces supporting the main manuscript. The finite-trace and embedded-chain-to-continuous-time propositions, including their proofs, remain in the main manuscript.

1 Trace-chain and physical-time details

1.1 Labelled-channel marking

The augmented state records the target of the actual labelled channel that fired. If two channels have the same population displacement but different sources or targets, their post-jump populations can agree while their carried targets or transition probabilities differ. They therefore remain separate. Only channels with identical source and target may be aggregated.

1.2 Nonemptiness of the Foster set

The finite set K in the episode-drift construction is nonempty, not merely finite. The global-minimum argument is pathwise: the residual log-factorial potential has a global minimum, and every possible episode endpoint has potential at least that minimum. No optional-stopping or integrability claim is needed at this step because every episode has uniformly bounded finite length.

1.3 Hitting versus positive return

The trace-chain proof distinguishes first hitting from positive return. From $k \in K$, one ordinary jump is taken before the next hit of K, so the resulting return time is positive. There are only finitely many successors of states in K, and the endpoint-chain drift estimate gives finite expected hitting of K from each successor. The finite trace chain is considered only after this step. A uniform finite-block chance of reaching one selected trace state gives finite expected positive trace return; the random trace excursions are then expanded into ordinary embedded jumps using the strong Markov property and Tonelli's theorem.

1.4 Stationary occupation balance

The return construction gives a finite expected number of embedded jumps and a finite expected amount of physical time before the positive return to the selected state x_*. During a complete return cycle, the number of arrivals at any state $y \neq x_*$ equals the number of departures from y pathwise. At x_* the initial departure and terminal arrival also balance. Taking expectations and weighting each visit by its exponential holding-time mean gives the statewise stationary balance equations for the normalized mean occupation measure displayed in the manuscript. This is the elementary cycle-level interface behind the cited regenerative occupation theorem.

1.5 Nonexplosion in physical time

The population embedded chain is constructed before nonexplosion is known. The finite-mean return result for that embedded chain supplies a population state x_* visited infinitely often. At each visit, the following holding time has the same exponential law with one fixed finite rate. The strong Markov construction makes these holding times independent copies, and their infinite sum diverges almost surely. Total physical time dominates this subseries, so jump times cannot accumulate at a finite time. This recovers nonexplosion for the present subclass; broader bimolecular weakly reversible nonexplosion is already known, as cited in the main manuscript. Once nonexplosion is established, the uniform positive lower bound on total rates and the finite mean embedded return give finite expected physical return by Tonelli's theorem.

1.6 Absorbing singletons

Absorbing singleton reachability classes are handled before channel augmentation and carry their point-mass stationary laws. In a nonabsorbing irreducible class every population state enables a genuine channel; otherwise that state would itself be absorbing, and symmetry of accessibility would force its reachability class to be the singleton.

2 Computational verification boundary

The accompanying dependency-free Python package performs deterministic, exact-arithmetic checks of the falling-factorial identity and source-probability rewrite. It also tests state-cycle lifting and accessibility symmetry on finite calibration networks, scalar-envelope branch conditions and monotonicity, the bimolecular top-complex classification with certificate-validated witnesses, absorbing-singleton handling, the corrected $\kappa_2 \downarrow 0$ rate-example limit, the exact logarithmic coefficient, the exact Anderson–Cappelletti–Kim Example 4.1 comparison included in the paper, and the stationary return-cycle normalization on a finite chain.

The reproducer runs the complete test suite, emits the canonical report twice, requires those reports to be byte-identical, and compares the result with the committed report. Environment information is recorded separately so that it does not destabilize the canonical JSON. The canonical report is verified on CPython 3.11 through 3.14; no claim is made for future interpreter versions until they are added to the test matrix.

These computations are falsification and regression aids. No finite atlas proves the universal theorem, no random test proves recurrence, and no computation enumerates the analytic Foster set K or certifies a useful bound on its cardinality, location, or diameter. Those universal conclusions come only from the manuscript's analytic argument.

3 Reproduction pointers

From the tagged Version 1.2.4 release directory, run:

```
cd code
./reproduce.sh
```

The canonical output is `code/verification_report.json`; an identical durable copy is retained as `supplement/verification_report.json`. The reproducibility environment, release identifiers, and complete clean-checkout replay procedure are recorded in `REPRODUCIBILITY.env` and `validation/`; the release manifest is `supplement/MANIFEST.sha256`. The package archive is created deterministically by `supplement/build_release_archive.py` and checked byte-for-byte in continuous integration.