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Title:

Bitwise Reproducibility as an Incomplete Correctness Signal: A Structural Audit for Parallel Spectral GCMs

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Bitwise Reproducibility as an Incomplete Correctness Signal: A Structural Audit for Parallel Spectral GCMs

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ABSTRACT

Bitwise reproducibility of an OpenMP-parallelized scientific code is usually verified by checksumming a short run—an inductive leap with no guarantee at longer integration lengths. We study it instead as a deductive, diagnostic property of the source text, using a legacy spectral atmospheric general circulation model whose time step is a reduction over a partitioned latitude dimension. We isolate four source-level conditions, (C0)–(C3): determinism of the inner transform reductions, a fixed-order outer reduction, per-iteration state isolation, and disjoint per-thread writes—two ordering and two independence conditions. Under them and an IEEE-754 determinism assumption, the output is bit-identical across all thread counts up to the number of parallel latitude iterations on a fixed binary for arbitrary integration length—strictly stronger than the fixed-thread-count rerun determinism a single checksum verifies; we prove this as a lemma. Its per-iteration factorization yields the diagnostic point: an across-thread reproducibility check detects an inter-iteration state-leakage fault only when the fault’s effect on the checksum varies with the thread count. Driving the model to bit-identity exposed a real, long-undetected leak in its vertical-exchange cache for that reason; but it is, by construction, blind to a thread-count-invariant leak—one that stays bit-identical while corrupting the physics—whatever reproducible-summation algorithm produces the checksum. A structural audit of the state-isolation condition detects such leaks directly, so bitwise reproducibility is a sound but incomplete correctness signal the audit complements rather than replaces. We give (C0)–(C3) as a reusable audit checklist for any partitioned-reduction OpenMP loop—five historical faults from the model’s engineering log map onto the conditions—and demonstrate the diagnostic on an open synthetic kernel whose released sweep harness confirms the asymmetry over 108 parameter scenarios with no counterexample in the validity region.

1. Introduction

The bitwise non-reproducibility of parallel scientific simulation under OpenMP [6, 25] is well known but has received little theoretical treatment. Its mechanism—the non-associativity of floating-point summation under reordering—is standard textbook material, yet the conditions under which it can be excluded in practice have not, to the author’s knowledge, been stated in deductive form. The community has accumulated decades of empirical evidence [14, 27] that the issue is pervasive in atmospheric general circulation models (AGCMs): a single rounding-sized perturbation, injected anywhere in the integration loop, is amplified by the chaotic dynamics of the flow [22]; in atmospheric integrations it grows rapidly, driven primarily by the physical parameterizations rather than by the resolved dynamics [27]. Common verification practices—for example, a checksum comparison on a one-month integration window—are inductive: a passing check is taken as evidence that bit identity will hold at all integration lengths, although this extrapolation is mathematically unsupported. The IEEE-754 standard [17] fixes the result of each individual floating-point operation, but does not constrain the order in which operations are issued; bit reproducibility is therefore not a property of arithmetic but of the source-code structure that determines

that order. It is, in the strict sense, a *structural* property of the implementation. A spectral atmospheric GCM is the concrete domain in which we develop and verify the formalism; the four conditions formulated below are properties of the source text. By the same structural argument the result is conjectured to extend to other parallel scientific simulations in which an inner reduction is performed over a partitioned geometric or geographic dimension by a kernel that may carry procedure-local persistent state; Section 12 develops this point, without empirical verification.

An established line of prior work establishes bit reproducibility through algorithmic means. Demmel and Nguyen [7] introduce a pre-rounding reproducible summation that makes the addition operator associative by construction. Collange et al. [5] extend the idea to multi-core machines through high-precision integer superaccumulators capable of absorbing the full IEEE-754 exponent (dynamic) range, and Iakymchuk et al. [16] generalize the construction to mixed MPI+OpenMP linear solvers. Closest in spirit to the present work is the reproducible-summation construction of Arteaga et al. [1], whose error-free transformation makes a parallel reduction independent of evaluation order. A related but distinct program is the COSMO work of Schär et al. [28], which attains bit reproducibility not by an order-independent reduction but by fixing the source-level operand order—a preprocessor that parenthesizes every expression, together with portable transcendental functions—and reports residual discrepancies in some modules relevant for long and restarted simulations. All of these methods reliably guarantee bit

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reproducibility in production use. What they do not do is diagnose the host code: by absorbing non-associativity into reproducibility-preserving arithmetic they fix the *order* of a reduction, but they say nothing about the *values* being reduced. A latent inter-iteration state leak in the host code corrupts those values. Whether an across-thread reproducibility check then catches the corruption depends only on whether the leak's effect varies with the thread partition, not on which summation algorithm is in use. The canonical mechanism by which such leaks arise in legacy Fortran is the `SAVE` attribute [24], a language feature that preserves a procedure-local variable across invocations of its enclosing procedure—used heavily in legacy F77 AGCMs for caching of state between time steps, but unsafe across the iterations of a parallel loop unless explicitly converted to thread-private storage. Such bugs are common in legacy Fortran AGCMs, and whether an across-thread reproducibility check even detects one turns on the axis the leak spans—the asymmetry this paper makes precise (Section 7). A structural approach to bit reproducibility—guaranteed by audit of the source text rather than by reproducibility-preserving arithmetic—is therefore complementary, not a substitute: it answers the question the checksum cannot, whether such hidden cross-iteration state exists at all.

The contribution of this paper is to make that structural perspective precise and to draw a diagnostic conclusion from it. We formalize four conditions on the parallel implementation of a spectral AGCM time step—(C0) a fixed evaluation order for the inner transform reductions, (C1) a fixed evaluation order for the outer per-latitude reduction, (C2) per-call isolation of state in the physical parameterizations, and (C3) disjoint per-thread writes to shared arrays—and we establish, as a lemma (Section 5), that their simultaneous satisfaction implies bitwise identity of the model output across thread counts on a fixed binary. The proof proceeds in two stages: a single-time-step argument establishes the base case, and induction over the time axis, exploiting closure of the per-step factorization under the conditions, extends the result to integration lengths beyond what is feasibly verified by measurement. The lemma's per-iteration factorization frames the paper's diagnostic point (Observation 1): a source-level audit that discharges the conditions detects every inter-iteration state-leakage fault carried by the persistence channels it enumerates (precisely the faults a violation of (C2) admits), whereas an across-thread reproducibility check detects only those whose manifestation depends on the thread partition—and is blind to a leak that corrupts the physics identically at every thread count. The conditions thus double as a reusable audit checklist (Section 11). A companion empirical paper [33] verifies them in the MGO T42L25 spectral AGCM, reporting MD5 identity of the monthly `tabm` history file across thread counts $N \in \{1, 2, 4, 8, 12, 16\}$ on AMD Zen 5 (84991763. . .) and $\{1, 2, 4, 8, 12, 16, 24\}$ on Intel Ivy Bridge-EP (1322f6da. . .). The present paper's contribution is distinct within that series: where the companion study [33] *measures* the bit-identity, and the supporting information of the preprint of the climate-impact study [31]

states it in compact form (there as a theorem) for that single model under three conditions, the diagnostic asymmetry developed here—what an across-thread check can and cannot certify—is new, as is the standalone four-condition form of the lemma. Section 9 returns to the structural-versus-algorithmic comparison and develops the trade-offs of the two routes.

The paper is organized as follows. Section 2 situates this work with respect to three threads of prior work—the foundations of parallel summation, algorithmic reproducibility constructions, and climate-modeling reproducibility frameworks—and the distinctive position of the present result. Section 3 introduces notation for the spectral state, the per-time-step factorization, and the parallel execution model. Section 4 states the four structural conditions; Section 5 states the bit-identity lemma and Section 6 proves it. Section 7 draws out the diagnostic asymmetry developed as the paper's principal result, and Section 8 delimits the scope. Section 9 contrasts the structural and algorithmic routes, Section 10 demonstrates the observation on an open synthetic kernel, and Section 11 distills the conditions into an audit checklist. Section 12 discusses theoretical applicability to other spectral atmospheric GCMs, and Section 14 concludes.

2. Related work

The question of bitwise reproducibility under parallel floating-point summation has a substantial and rapidly growing literature. We discuss three threads of prior work, then the distinctive role of the present result with respect to each.

Foundations and parallel summation algorithms. Compensated summation [21] fixes a sequential order and is not directly applicable to the parallel case. Rosinski and Williamson [27] characterized the growth of rounding-sized initial errors in the NCAR CCM2 atmospheric circulation model and introduced a port-validation strategy for atmospheric general circulation models, identifying physical parameterizations as the source of fast error amplification. He and Ding [14] documented floating-point divergence in parallel climate simulations and proposed a double-double reduction operator to suppress it, but did not characterize source-level conditions for bitwise identity.

Algorithmic reproducibility constructions. Demmel and Nguyen [7] present reproducible summation algorithms via pre-rounding that guarantee order-independence by making the operator associative. Collange et al. [5] introduce super-accumulators for multi-core reproducibility, absorbing the full exponent (dynamic) range into a high-precision integer; Iakymchuk et al. [16] extend this approach to MPI+OpenMP linear solvers. The order-independent reproducible summation of Arteaga et al. [1] carries the pre-rounding family into the distributed setting; the closest relative in spirit to the structural conditions developed here is instead the COSMO bit-reproducibility program of Schär et al. [28], which attains reproducibility by fixing the source-level operand order (forced parenthesization and portable transcendentals), with

discrepancies remaining in some modules relevant for long and restarted simulations. The detailed comparison between algorithmic and structural approaches is the subject of Section 9.

Climate-modeling reproducibility frameworks. A separate strand of literature addresses reproducibility at the level of climate-modeling workflows. Baker et al. [2] introduce ensemble-based consistency tests for the Community Earth System Model, motivated by the observation that common events in a model’s development life cycle routinely break bit-for-bit identity. Massonnet et al. [23] establish a statistical replicability protocol for EC-Earth3, adopted by a consortium of 27 institutions. Schär et al. [28] measure the performance cost of enforcing bit reproducibility in COSMO, quantified in Section 9. Zeman and Schär [38] document that, in part because of such costs, bit reproducibility is generally not enforced in operational weather and climate models.

The distinctive role of the present result. The literature above is largely empirical or algorithmic. The present result occupies a different position: it gives a *deductive structural characterization* of the conditions under which bit-reproducibility is guaranteed by construction. It is complementary to the algorithmic approaches—where they absorb non-associativity into reproducibility-preserving arithmetic, the present result identifies structural code properties whose audit catches latent inter-iteration state-leakage bugs, including the thread-count-invariant ones that no reproducibility check can see (Section 9). The result is also complementary to the empirical climate-modeling literature: it renders the checksum equality reported in works such as Vokhmintsev [33] a deductive consequence of four named conditions, rather than an inductive extrapolation from a short integration window. Methodologically, establishing what a verification check provably cannot certify—independently of how often the missed class is met—is itself a recognized mode of contribution: the fault-detecting ability of test-adequacy criteria has been analyzed in exactly these terms [11], and the limits of a method are routinely established by a constructed instance rather than a field one [3]. The diagnostic asymmetry developed below is a result of that kind.

3. Setting and notation

This section states the notation, assumptions, and conditions on which the lemma rests; the lemma is proved in Section 6. A compact version of the bit-identity result, specialized to the single model studied in the companion climate-impact study, appears in the supporting information of the preprint of that study [31] under three conditions (C1)–(C3). The present development is self-contained, broadened to the general spectral-AGCM setting, and adds the inner-reduction determinism condition (C0) together with the IEEE-754 hardening of (A0); the labels Lemma 1/Lemma 2 here mark the result’s supporting role to the diagnostic Observation that is this paper’s principal contribution (Section 7). The two formulations express the same instrumental result; the

strengthening from three to four conditions is additive, not in tension.

3.1. The model in abstract form

We describe the model state at the level of its spectral representation. Writing $\mathbf{S}_t$ for the state carried from one time step to the next, it is the finite collection of spectral coefficients

$$\mathbf{S}_t = (c_{\ell,m}^{(q)}(t))_{\ell,m,q}, \quad (1)$$

in which the superscript q ranges over the five prognostic fields (ζ , D , T , ℓ_z , ℓ_p)—respectively vorticity, divergence, temperature, the model’s water-vapor variable, and the log-surface-pressure $\ell_p = \ln p_s$; the index ℓ runs from 0 to the triangular-truncation limit M , and the zonal wavenumber m from 0 to ℓ , the coefficients for $m < 0$ being fixed by the conjugate symmetry of the real physical fields. We fix $M = 42$ wherever a concrete value aids the exposition, but nothing in the argument depends on that choice, and every statement carries over to any other triangular truncation. Each coefficient is complex and is stored as a pair of finite-length IEEE-754 double-precision numbers (REAL*8 real and imaginary parts), so the entire state is a fixed-width bit pattern. The state vector may also be extended by documented per-latitude persistent module state: each slot indexed by its latitude J , restored deterministically at the start of the J -th iteration, and independent of the thread partition; every per-latitude tendency introduced below then remains a deterministic function of $(J, \mathbf{S}_t)$ with $\mathbf{S}_t$ read in this extended sense.

3.2. The per-time-step update

One time step of the model factors as

$$\mathbf{S}_{t+1} = \mathcal{F}(\mathbf{S}_t) = \mathcal{L}(\mathbf{S}_t) + \sum_{J=1}^{J_M} \Delta^{(J)}(\mathbf{S}_t). \quad (2)$$

Here $\mathcal{L}(\mathbf{S}_t)$ gathers the spectral-space terms that are evaluated once per step and carry no dependence on the latitude index—horizontal diffusion, the pressure-gradient term, the Coriolis term, and the semi-implicit treatment of gravity waves—so that, by construction, it is a deterministic IEEE-754 function of $\mathbf{S}_t$. Each $\Delta^{(J)}(\mathbf{S}_t)$ supplies the grid-space tendency originating at latitude row J : it bundles the column-physics output (radiation, convection, vertical exchange, turbulence), maps it back into spectral space through a longitudinal FFT followed by a direct Legendre transform, and accumulates the result into the shared coefficient array. The limit J_M is one half of the Gaussian-grid row count, the saving coming from equatorial symmetry; at T42 this fixes $J_M = 32$. The latitude sum $\sum_{J=1}^{J_M}$ in Eq. (2) is what we call the *spectral-analysis reduction*—the forward (grid-to-spectral) transform that accumulates each latitude’s contribution into the coefficient array, whose parallel structure is classical [10]—and the order in which its terms are combined is precisely what the lemma constrains.

3.3. The parallel execution model

Parallelism enters through the latitude loop. Given a thread count N drawn from $\{1, 2, \dots, J_M\}$, the OpenMP runtime distributes the J_M latitude iterations over the N threads. We write $\mathcal{P}_N(J) \in \{0, \dots, N-1\}$ for the index of the thread to which iteration J is assigned under a static schedule. Threads are pinned to physical cores (OMP_PROC_BIND=close, OMP_PLACES=cores) for timing stability, but the lemma nowhere relies on which thread lands on which core: the binding affects timing, not the computed bits.

3.4. IEEE-754 determinism (assumption A0)

Throughout we take it as given that the compiled executable runs in a single fixed IEEE-754 rounding mode (round-to-nearest, ties-to-even) and that neither the compiler nor the processor introduces any reordering that the IEEE-754 reading of the source text would not already permit. Spelled out, this is four stipulations.

- The build uses `-O2 -march=native` [13]; fused multiply-add is contracted where the target ISA provides it [9, 19]—an FMA path on Zen 5, separate mul and add on Ivy Bridge-EP, which has no FMA3 [9]. An FMA folds $a \cdot b + c$ into a single rounding, distinct from an isolated mul followed by an add; in either case the contraction is fixed *per binary*: a fixed source expression compiles to the same instruction sequence on every build and every run of that binary. The property claimed is bit-stability across thread counts on *one* such binary, not bit-identity to a differently optimized or differently targeted build.
- No reassociating or “fast-math” optimization is in effect: `-ffast-math` and `-fassociative-math` [13], which would legalize reassociation of a reduction, are absent, so the compiler may not re-order the operands of a sum; and the latitude loop runs under an OpenMP static schedule [25] with a fixed thread-to-latitude map $\mathcal{P}_N$. These are what keep the source-level operand order—fixed by (C0) and (C1)—intact in the emitted code.
- Micro-architectural reordering (out-of-order issue, re-order buffers) changes when an instruction retires, never the value it produces.
- Each library transcendental the model calls (sin, cos in the Fourier and Legendre transforms, exp, log in the physics) is evaluated by a fixed scalar libm implementation [12] (the gfortran build links no SVML [18, 20]). IEEE-754 does not mandate correctly rounded transcendentals, so their determinism is a property of the pinned library version and is part of “the same hardware-compiler configuration”. Remaining external non-determinism is excluded by construction: the reproducibility runs use no random-number generator, all forcing inputs (SST/SIC fields, aerosol data) are byte-identical from run to run, and clocks are read only in non-reducing paths that never re-enter $\mathbf{S}$.

Granting (A0), each elementary floating-point operation (add, multiply, FMA, divide, square root) returns the unique correctly-rounded value fixed entirely by its operands—this is the correctly-rounded-result contract for the basic operations in IEEE-754 [17, §5.1, §5.4.1], the one part of the standard whose determinism is unconditional rather than implementation-defined. The open synthetic kernel of Section 10 exhibits the same property empirically: in its CLEAN regime, where all arithmetic is restricted to deterministic IEEE-754 add/multiply/divide on a fixed binary, the output MD5 is bit-identical across $N \in \{1, 2, 4, 8, 16, 32\}$. Pinning down which operands enter each primitive, and in what order, then fixes the entire bitstream of results.

4. The four structural conditions

The four conditions fall into two families. The two *ordering* conditions, (C0) and (C1), fix the order in which the inner and the outer reductions sum their operands; the two *independence* conditions, (C2) and (C3), keep working state from coupling across iterations and keep concurrent writes from racing. Assumption (A0) of Section 3.4 sits beneath both families rather than inside either: it fixes the *value* each arithmetic primitive returns, leaving the *order* in which those values combine to the ordering conditions and the *isolation* of the state they read to the independence conditions.

4.1. (C0) Determinism of the inner reductions (ordering condition)

Condition (C1) below fixes the order of the *outer* latitude sum $\sum_J \Delta^{(J)}$, but each tendency $\Delta^{(J)}$ is itself the product of a chain of floating-point reductions: the longitudinal fast Fourier transform, the Gaussian-quadrature sum over the points of latitude row J , the direct (forward) associated-Legendre transform, and the combination of the northern row with its mirror-image southern row implied by the equatorial symmetry that halves the Gaussian grid. We require that every one of these *inner* reductions be evaluated in a fixed operation order—*independent* of the thread count N and of the OpenMP schedule—by the single thread $\mathcal{P}_N(J)$ that owns iteration J . Granting this, each $\Delta^{(J)}(\mathbf{S}_t)$ is a deterministic function of $(J, \mathbf{S}_t)$ alone. Condition (C0) is to the inner transforms what assumption (A0) is to the individual arithmetic primitives: (A0) fixes the result of each isolated operation, (C0) fixes the order in which the inner reductions combine those results, and (C1) fixes the order of the outer accumulation across latitudes. In the MGO realization (C0) holds structurally: the longitudinal FFT (INFFT/FFT) and the associated-Legendre routines (ALPM/ALPMN) are serial, hand-coded kernels—FFT invoked from inside the latitude loop by the owning thread; INFFT precomputing the transform tables and ALPM/ALPMN the associated-Legendre polynomials at initialization; the in-loop direct Legendre transform running as inline code over the precomputed polynomial arrays—with no nested parallel region and no multithreaded vendor transform library. We state this inner-reduction determinism as an explicit named condition, so that (C0) joins (C1)–(C3)

as an auditable property of the source text and a precise failure surface in the diagnostic of Section 7.

4.2. (C1) Ordered per- J reduction (ordering condition)

Condition (C1) requires that the spectral-analysis reduction be carried out in one fixed, N -independent order. Any such order suffices; the realization that motivates the lemma combines the per-latitude contributions as one prescribed serial accumulation,

$$c_{\ell,m} \leftarrow c_{\ell,m}^{\text{LIN}} \oplus \Delta c_{\ell,m}^{(1)} \oplus \Delta c_{\ell,m}^{(2)} \oplus \dots \oplus \Delta c_{\ell,m}^{(J_M)}, \quad (3)$$

where $\oplus$ denotes IEEE-754 addition applied strictly left to right, so that the bracketing $((a \oplus b) \oplus c) \oplus d$ is forced rather than incidental. What (C1) demands is not this particular left-to-right sequence but that *some* fixed order be used independently of N : a deterministic fixed-shape tree reduction would satisfy it equally. The MGO realization secures that fixed order in the simplest way—the accumulation runs on one thread alone, the OpenMP master, within an `!$OMP MASTER` region—and only after every worker thread has finished its assigned latitudes and written its $\Delta c_{\ell,m}^{(J)}$ into a private slot of the per- J buffer arrays. Because the master then walks those slots in the fixed order $J = 1, 2, \dots, J_M$ regardless of how many threads produced them, the summation sequence—and hence its rounded result—does not depend on N .

In the MGO T42L25 implementation that motivates the lemma, the code modules implementing (C1) are `COMSPE_PREJ_REDUCE` (a serial ordered sum of five spectral fields over J), `CVDDR_ACC_FINALIZE` (a serial ordered sum of vertical-diffusion diagnostics), and `SPH_ACC_FINALIZE` (a serial ordered sum of `AIN_MOD` scalar diagnostics together with seven `REAL*4` arrays). Condition (C1) is, however, a property of the algorithm, not of any specific Fortran realization: the same condition can be satisfied by an explicit reduction kernel in any parallel programming model.

4.3. (C2) State isolation (independence condition)

For every J -iteration, all `THREADPRIVATE` (or thread-private equivalent) working arrays of every subroutine called inside the J -loop are reset to a deterministic initial state before the J -th evaluation. The initial state is either zero (for accumulators) or a designated neutral value of physical significance. A deterministic per- J restoration of documented prior-step state—the snapshot/restore variant of the companion climate-impact study [31]—is an admissible reset rule, provided that state is included in the specified state vector (Section 3); what (C2) forbids is persistence outside the specified state and reset rule: any carry-over between J -iterations within a time step, and any cross-step carry-over not part of the documented state.

The substantive content of (C2) is that no information may persist in working state across J -iterations within the same time step. Working arrays that the column-physics codes treat as scratch space must *behave* as scratch space: their contents at the entry of the J -th call must be a function of J and the

deterministic reset rule alone, never a function of the values left behind by the $(J - 1)$ -th, $(J - 2)$ -th, ... calls.

In the audited revision of MGO T42L25 (the revision on which the companion measurements were taken), condition (C2) is implemented by an explicit per- J -reset code block in the vertical-exchange kernel (`VE_JRESET`), which zeroes the kernel's per-call work arrays at the top of every entry into the vertical-exchange parameterization. A twelve-array subset of these carries what the source annotates as `MEMORISED` state—a memoization cache: each array holds an expensive intermediate quantity (level geometry, turbulence length scales, and the like) computed once and reused on subsequent calls to spare the recomputation. This caching is a design decision about *what* is retained for reuse; the Fortran `SAVE` attribute is merely the storage mechanism that makes the retention possible. The reset zeroes the twelve *memorized* cache arrays of the kernel; separately, two non-memoized work arrays are reset to unity rather than zero, a neutral value consistent with a known idiom in the legacy vertical-exchange code. These per- J resets are complemented by module-level `*_INIT` subroutines: the per- J buffer initializers run before the parallel region is opened, and the per-thread allocation initializers run at the top of the parallel region, before the worksharing latitude loop. The companion empirical study [33] documents the discovery that the cache spanned the wrong axis: the twelve *memorized* cache arrays carried their values from one latitude into the next, rather than only from one time step to the next as the memoization intended, with the `SAVE` storage making the unintended cross-latitude carry-over possible. That discovery was the immediate motivation for formulating (C2) explicitly.

4.4. (C3) Disjoint writes (independence condition)

Within a single J -iteration, the set of memory addresses written by thread $\mathcal{P}_N(J)$ is disjoint from the set of memory addresses written by any other thread $\mathcal{P}_N(J')$ with $J' \neq J$. In particular:

- per- J buffer arrays (`COMSPE_PREJ_MOD::YLPC_J(:, J)`, `CVDDR_ACC_MOD::GRM2_J(J)`, `SPH_ACC_MOD::EK_J(J)`, etc. in the MGO implementation) are indexed by the latitude J of the writing thread; no other thread writes to the same J -slice;
- `THREADPRIVATE` arrays are, by definition, distinct memory per thread;
- shared read-only data (grid constants, input boundary conditions) is not written.

Condition (C3) is enforced structurally rather than verified empirically. In the MGO implementation, the parallel region is opened by an `!$OMP PARALLEL DEFAULT(NONE)` directive carrying an explicit `SHARED/PRIVATE/FIRSTPRIVATE` classification of every variable in scope (over three hundred classified names, with `THREADPRIVATE` module state declared at its point of definition), and the latitude loop runs under `!$OMP DO SCHEDULE(STATIC)`. The `DEFAULT(NONE)` clause forces an explicit data-sharing attribute for every variable referenced in the

region, so an unclassified variable is a compile-time error rather than a silently shared one; misclassification remains possible, but it is confined to the explicit, auditable clause lists of a single directive, and it is this explicit classification that makes the write-disjoint property a structural property of the source code rather than an accident of optimization.

Condition (C3) is the bitwise restatement of a classical parallelization criterion: the disjointness of the per-iteration write sets is exactly Bernstein’s output-set condition $O_i \cap O_j = \emptyset$ for two iterations to execute concurrently without altering the result [4]. The analogy stops there, and the gap is instructive. Bernstein’s conditions certify that a parallel execution yields the *same value* as the serial one regardless of the order in which independent work is interleaved—they are deliberately order-agnostic. Bitwise reproducibility is the opposite regime: because floating-point summation is non-associative, the *same bits* are obtained only if the reduction order is itself fixed—precisely what the ordering conditions (C0) and (C1) add and what a value-equivalence criterion such as Bernstein’s neither needs nor supplies.

5. The bit-identity lemma

The reproducibility result of this section is stated as a lemma rather than as the paper’s central result, by design. Its role is instrumental: it supplies the per- J factorization on which the diagnostic Observation 1 is built—the Observation analyzes what an across-thread check can and cannot detect when condition (C2) is violated, a question on which the lemma’s positive (C0–C3-hold) direction is silent. The two forms below—single-step and its inductive extension—state the bit-identity result. All four conditions, (C0) included, are carried explicitly as hypotheses, because the proof (Section 6) uses each of them.

5.1. Single-step version

Lemma 1 (Single-step bitwise reproducibility). *Let S_t be the state at time step t . Under assumption (A0) of IEEE-754 determinism and conditions (C0), (C1), (C2), and (C3), the state at time step $t + 1$ computed by the parallelized binary is bit-identical for every thread count $N \in \{1, 2, \dots, J_M\}$ on the same hardware-compiler configuration:*

$$\forall N, N' \in \{1, \dots, J_M\} : S_{t+1}^{(N)} = S_{t+1}^{(N')}. \quad (4)$$

5.2. Inductive version

Lemma 2 (Multi-step bitwise reproducibility). *Under the same assumptions, if $S_0^{(N)} = S_0^{(N')}$ (identical initialization, typically from the same restart file), then*

$$\forall t \geq 0, \forall N, N' \in \{1, \dots, J_M\} : S_t^{(N)} = S_t^{(N')}. \quad (5)$$

It follows that any file obtained from S_t by a fixed, deterministic post-processing step inherits the property. The byte-identity actually measured across thread counts is that of the `tabm` history file [33]; the `tabv` and `tabcltm` diagnostics follow deductively, as deterministic functions of the same state. The 1st logs are not claimed bit-identical: that would

additionally require suppressing per-thread initialization messages.

5.3. Scope of “the same hardware-compiler configuration”

Lemmas 1 and 2 are predicated on a single executable: a fixed binary, fixed `libgomp` and `libm` [12, 25], a fixed CPU micro-architecture, and a fixed memory subsystem, jointly yielding one IEEE-754 result per arithmetic primitive. Within that fixed configuration the lemmas hold for every admissible N . What they do not assert is bit-identity between distinct binaries—comparing, say, AMD Zen 5 against Intel Ivy Bridge-EP, each built with the same `-O2 -march=native` flag string, which resolves to a different instruction-set target on each host—because the two compilations emit different instruction streams (an FMA path on Zen 5, separate `mul` and `add` on Ivy Bridge), and IEEE-754 alone does not equate the two. Read in this light, the cross-platform checksums of the companion empirical study [33]—84991763. . . on Zen 5 and 1322f6da. . . on Ivy Bridge-EP, differing between platforms yet bit-stable across the tested thread counts on each—are exactly what Lemma 2 predicts, not a counterexample to it. Section 13 adds measured cross-configuration evidence from a second legacy code: pinning the two divergence mechanisms named here restores bit-identity even across the CPU–GPU instruction-set boundary within one configuration.

6. Proof of the lemma

6.1. Proof of Lemma 1

Proof. Fix a thread count N and a state S_t . We show that $S_{t+1}^{(N)}$ coincides with $S_{t+1}^{(1)}$, the reference serial trajectory. Bit-identity then follows for every pair (N, N') by transitivity.

The linear update $\mathcal{L}$. $\mathcal{L}(S_t)$ is evaluated in serial code outside the J -loop, using the same source expressions in every run. By (A0), its output is deterministic. In particular, the reference value $c_{\ell,m}^{\text{LIN}} = \mathcal{L}_{\ell,m}(S_t)$ is identical for N and $N = 1$.

The per- J contributions $\Delta c^{(J)}$. Fix a latitude J . The tendency $\Delta^{(J)}(S_t)$ is computed by evaluating the column physics (vertical exchange, convection, radiation, condensation), the FFT along longitude, the Gaussian quadrature, and the direct Legendre transform over that J . By condition (C0) each of these inner reductions runs in a fixed, N -independent operand order, so all of them are deterministic IEEE-754 computations on inputs drawn from:

- S_t (shared, read-only during the parallel region);
- grid constants (shared, read-only);
- per- J forcings (shared, read-only; e.g. SST at latitude J);
- the initial state of any `THREADPRIVATE` work array, *reset by condition (C2)* to a deterministic value before the J -evaluation.

Therefore $\Delta c_{\ell,m}^{(J)}$ is a function only of J and $\mathbf{S}_t$, not of the thread that happens to compute it, not of other threads' concurrent activity, and not of the history of previous J -iterations.

Formally, let $f_{\ell,m} : \{1, \dots, J_M\} \times \text{State} \rightarrow \text{IEEE-754}$ be defined by $f_{\ell,m}(J, \mathbf{S}) := \Delta c_{\ell,m}^{(J)}(\mathbf{S})$. Condition (C0) guarantees that the inner reductions producing $\Delta c_{\ell,m}^{(J)}$ combine in a fixed order, so that the value of $f_{\ell,m}(J, \mathbf{S})$ is independent of the thread count and schedule; conditions (C2) and (C3) together make $f_{\ell,m}$ a pure function—(C2), applied across the enumerated persistence channels, excludes any within-thread dependence on the history of previous iterations, and (C3) excludes any cross-thread side channel, so that no other thread overwrites the inputs of $f_{\ell,m}$ during its evaluation. Under (A0), the value of $f_{\ell,m}(J, \mathbf{S}_t)$ is byte-identical in every run, for every N .

The reduction. Condition (C1) guarantees that the update

$$c_{\ell,m}(t+1) = c_{\ell,m}^{\text{LIN}} \oplus f_{\ell,m}(1, \mathbf{S}_t) \oplus f_{\ell,m}(2, \mathbf{S}_t) \oplus \dots \oplus f_{\ell,m}(J_M, \mathbf{S}_t) \quad (6)$$

is evaluated in this left-to-right order, in a single thread, for every N . IEEE-754 addition with a fixed operand order, under (A0), is a deterministic function of its operand sequence. Therefore $c_{\ell,m}(t+1)$ is bit-identical for every N .

Conclusion. Every coefficient of $\mathbf{S}_{t+1}^{(N)}$ equals the corresponding coefficient of $\mathbf{S}_{t+1}^{(1)}$, byte for byte. Since $\mathbf{S}_{t+1}$ is a finite tuple of such coefficients, $\mathbf{S}_{t+1}^{(N)} = \mathbf{S}_{t+1}^{(1)}$. $\square$

6.2. Proof of Lemma 2

Proof. By induction on t . The base case is $t = 0$ by assumption. Conditions (C0)–(C3) are properties of the source text rather than of the state, so they hold at every step, and Lemma 1 applies at each step. The inductive step is therefore Lemma 1: if $\mathbf{S}_t^{(N)} = \mathbf{S}_t^{(N')}$, then $\mathbf{S}_{t+1}^{(N)} = \mathbf{S}_{t+1}^{(N')}$ by applying Lemma 1 to $\mathbf{S}_t^{(N)}$ (which equals $\mathbf{S}_t^{(N')}$ by induction). $\square$

Crucially, the single-step guarantee does not weaken as t grows. There is nothing for chaos to amplify: at each step the trajectory $\mathbf{S}_t^{(N)}$ already agrees bit-for-bit with the serial reference $\mathbf{S}_t^{(1)}$, so the next step departs from an identical state rather than from a state perturbed by some ϵ . The well-known sensitivity of a chaotic atmospheric circulation to its starting point speaks to runs begun from *different* initial states; here the inductive hypothesis makes the states *the same*, and the sensitivity argument simply does not apply.

7. The diagnostic asymmetry

The lemma does not prove that any specific implementation *is* reproducible; it proves that, *if* the conditions hold, reproducibility follows. Used in contrapositive form it becomes a diagnostic: a bit-reproducibility failure cannot

occur while (A0), (C0), (C1), (C2), and (C3) all hold, so every observed failure must violate at least one of them.¹ This structure made the debugging tractable during the MGO T42L25 refactoring that motivated the present work. The five historically discovered violations in the engineering log map as listed in Table 1.

Each fix corresponded to restoring a specific condition. The conditions are in this sense a sufficient specification of reproducibility: an implementation that satisfies (A0) and (C0)–(C3) is reproducible by construction, and—within that sufficiency—a reproducibility failure is evidence that one of them has been violated. The checksum that tests reproducibility is, however, a weaker instrument than that specification suggests—an incomplete signal of *correctness*, blind to a whole class of faults. We now make that gap precise.

Observation 1 (Diagnostic asymmetry: an across-thread checksum is a sound but incomplete leakage detector). Let B denote the class of unintended inter-iteration state-leakage faults: a procedure-local value that persists across iterations—of the latitude loop or of the time-step loop—outside the specified state and reset rule, and makes some $\Delta^{(J)}$ depend on processing history rather than on $(J, \mathbf{S}_t)$ alone. Call the *output manifestation* of a fault the change it induces in the byte content of the checksummed history file. Fix a tested set $\mathcal{N}$ of thread counts. The across- N reproducibility check—MD5 equality of the output over all $N \in \mathcal{N}$ on one fixed binary—relates to B as follows.

1. *Blind spot (necessary condition for a flag).* The check flags a fault only if its output manifestation differs for some $N, N' \in \mathcal{N}$; equivalently, it cannot flag any fault whose output is identical across $\mathcal{N}$. This includes every leak confined to the cross-time-step axis (invariant in N by construction), and any cross-latitude leak whose N -dependence cancels in the output or first separates at a thread count outside $\mathcal{N}$.
2. *Detection (sufficient condition for a flag).* The check flags a fault if, for some $N, N' \in \mathcal{N}$, the partition changes the set of latitudes processed before an affected iteration and the resulting difference in $\Delta^{(J)}$ reaches the output without cancellation. Under a static schedule a

¹We claim sufficiency, not necessity: there may be reproducibility mechanisms these conditions do not capture. In the MGO T42L25 refactoring that motivated this work, however, every reproducibility failure we encountered—taken to mean a bit-level divergence of an otherwise well-formed binary—was traceable to the violation of exactly one of them. Build-level defects that abort or miscompile the binary rather than let a well-formed run silently diverge—Fortran storage-association mismatches and dummy-argument type mismatches of the kind endemic to F77-to-OpenMP modernization—violate the premise of a single well-formed IEEE-754 binary and so fall beneath assumption (A0) rather than within (C0)–(C3); they lie outside the scope of this claim. One entry deserves clarification: the spectral-coefficient accumulation itself was protected by construction throughout the refactoring—first by an ordered pipeline, later by a per- J term-split—and never ran under REDUCTION; the order-varying REDUCTION violation of (C1) listed in Table 1 arose instead in the global diagnostic accumulators and was resolved by an ordered per- J sum. Condition (C0) is the one condition for which the engineering log records no historical violation; its realistic failure surface—a multithreaded vendor FFT or BLAS call nested inside a latitude iteration—does not arise in the MGO implementation.

Table 1

Historical bit-reproducibility violations encountered during refactoring of the MGO atmospheric general circulation model and the structural condition each one violated.

Historical bug	Violated condition
SAVE-persistent accumulators in the convective-adjustment routine carrying state between J iterations	(C2)
Vertical-exchange kernel's twelve <i>memorized</i> cache arrays leaking across J (motivating VE_JRESET)	(C2)
Order-varying REDUCTION(+:) on global diagnostic accumulators (module scalars and REAL*4 accumulation arrays), combined in thread-arrival order	(C1)
Shared writable scratch space in the radiation-diagnostics output routine	(C3)
Uninitialized THREADPRIVATE arrays on secondary threads	(C2)

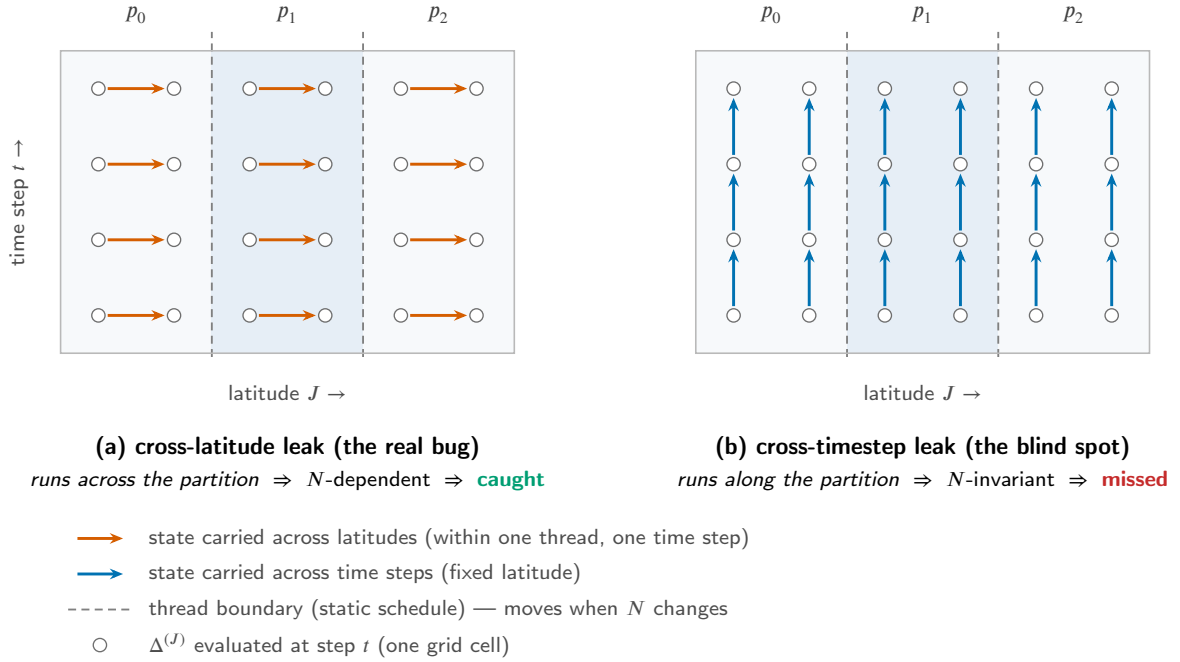


Figure 1: The diagnostic asymmetry of Observation 1, on the latitude–time-step plane, with the OpenMP threads p_0, p_1, p_2 drawn as vertical bands under a static schedule. **(a)** A cross-latitude leak runs *across* the partition: its contamination chain is segmented by the band boundaries, so it changes when the thread count N changes—hence N -dependent and flagged by the across- N checksum (the real vertical-exchange bug). **(b)** A cross-time-step leak runs *along* the partition, parallel to the boundaries and so untouched by them: identical at every N —hence N -invariant and invisible to any across- N check (the blind spot), realized by regime B of the synthetic kernel of Section 10. The geometry is the result: a fault can be caught only when its arrows cross a boundary that N can move.

cross-latitude leak meets this for a suitable pair, which is why the MGO vertical-exchange bug was caught.

A structural audit of state isolation (C2), by contrast, inspects the reset policy of every enumerated persistence channel and so removes or exhibits every fault in B that those channels carry, independently of N .

Stated this abstractly, the asymmetry is immediate: a check keyed to variation across N cannot register a fault that is invariant across N . Its content lies elsewhere—in the leak's exact axis (cross-time-step) and the condition it violates (C2); in the fact that the gap survives *any* reproducible-summation arithmetic (Section 9); and in a real bug, in the audited code, that sat one axis away from it. Figure 1 renders this geometry:

a leak *across* the partition (panel a) varies with the thread count and is caught, whereas a leak *along* it (panel b) does not and is missed. We take the two sides in turn—the check's *blind spot* and the audit's completeness for B —then exhibit both in the one cache that motivated the work.

The audit side. Discharging (C2) over the parallel scope forces the analyst to read every SAVE and THREADPRIVATE declaration reachable from the J -loop and to give each a reset rule fixed by J and the specified state alone. A genuine carrier of cross-latitude state is therefore either removed or exhibited—the audit cannot terminate while one remains unexamined—so the audit is complete for B relative to the persistence channels it enumerates (SAVE, THREADPRIVATE,

COMMON, DATA, EQUIVALENCE); a leak carried by a channel outside that list, such as library-internal static state, is a coverage obligation rather than a guarantee. Soundness runs in the matching direction as a conservative bound: an array whose (C2) reset erases every cross-iteration dependence is not in B and is not flagged; a declaration the audit does flag marks persistent state that must either be given a reset rule fixed by J alone or be shown to leave every $\Delta^{(J)}$ a function of (J, S_i) alone—a flag resolved by inspection, not a confirmed fault. This completeness is largely immediate, B being by definition the class of (C2) violations whose effect reaches some $\Delta^{(J)}$; what is not immediate is the contrast with the checksum’s incompleteness in part (1). Each (C2) violation of Table 1 was localized to its persistence channel by exactly this reading of reset policies.

The blind-spot side. The MGO vertical-exchange bug lies in the N -dependent part of B , and that is exactly why the push for bitwise reproducibility exposed it. Under the static schedule the twelve *memorized* cache arrays carried state from each latitude into the next within a thread, so the inherited cache—and with it $\Delta^{(J)}$ —differed between thread counts; the symptom was a checksum that changed with N , and the check caught it. Restoring (C2) with `VE_JRESET` recovered bit-identity across the tested thread counts [33].

The same cache marks the limit of the check. Had the identical leak run along the cache’s intended axis—persisting wrongly from one time step to the next at a fixed latitude rather than across latitudes—its effect would have been the same at every thread count. The run would then be bit-identical across N and physically wrong at once, and no across- N check, by any arithmetic, could distinguish it from a correct one: the check tests invariance under repartitioning, not correctness. Only the state-isolation audit, which reads the reset policy directly, separates the two cases. We did not encounter such an N -invariant leak in the MGO refactoring—every violation in the engineering log (Table 1) was N -dependent and was therefore caught—so the blind spot is established here *by construction* and by the near-miss just described (the same cache, leaking along its other axis), and is exhibited empirically on regime B of the open synthetic kernel (Section 10); it is a structurally entailed failure mode, not one we observed in the field.

What the algorithmic route changes, and what it does not. An algorithmic reproducibility regime is sometimes expected to hide such faults; it does not, for a reason worth stating precisely. A superaccumulator [5] or a pre-rounded reduction [7] fixes the *order* of the latitude sum $\sum_J \Delta^{(J)}$; it does not touch the *computation* of the individual $\Delta^{(J)}$, which is where a state leak acts. An exact sum of N -dependent summands is still N -dependent, so such a regime would *not* have concealed the N -dependent vertical-exchange bug—the reproducibility check would still have failed on it. What no reproducibility regime of any kind can surface is the N -invariant fault just described; that gap is closed by the structural audit, not by a change of arithmetic. The

algorithmic route answers “does the parallel run match the serial one?”; the structural route answers “can any procedure-local state cross an iteration boundary?”. A production refactoring would use both—algorithmic determinism for cheap verification, the audit for the race detection it alone provides—and bitwise reproducibility, however obtained, must not be read as correctness.

Why not simply compare against a trusted reference?

A regression test against a byte-exact serial reference would indeed flag the N -invariant fault, since regime B differs from the correct output. That route, however, presumes what a port or a refactoring cannot assume: a serial reference already known to be correct on the same binary configuration. When the goal is precisely to establish a first trustworthy baseline—a new model, or a legacy code under modernization—no such oracle exists; and a pre-existing reference can itself be physically wrong, as it was here, where the latent vertical-exchange leak had contaminated the model’s own serial history before the drive to bitwise reproducibility exposed it. In that regime the across- N check and the state-isolation audit add information a baseline comparison cannot, precisely because the baseline is the object in question.

Nor can two computed answers certify each other. The limitation is not specific to the reproducibility check: it holds for any mutual comparison of two computed results. Agreement between two runs bounds their *difference*, not their common error—both may carry the same wrong physics, as the leaky serial history above did. For linear-algebra kernels the point is quantitative: two implementations that are each backward stable may return results whose difference is of the order of the condition number times the backward error, so their agreement measures conditioning, not correctness—a direct consequence of the forward-error rule of thumb of Higham [15, §1.6]. Discriminating between two uncertain answers requires a third, independently trusted reference—an analytic or manufactured solution [26], or a conserved quantity whose residual is checkable without any second implementation.

A deterministic fault outside B: a caution from the audited code’s own history. The blind spot is not exhausted by state leaks. During the same refactoring, resolving a storage-association construct in the surface-albedo path exposed an indexing defect in the legacy code: a two-dimensional surface mask was addressed as `MAS(I*J)` where the linearized index `MAS(I + (J-1)*KM2)` was intended. The defect is deterministic—identical at every thread count by construction—and, measured on the one-month verification window, it has no output manifestation at all: the corrected and the defective code produce byte-identical January output, the fault evidently lying on a path whose contribution is insensitive at that season and horizon. Every instrument discussed so far is blind to it: the across- N check (nothing varies with N), the fixed- N regression against the frozen baseline (the bytes are equal), and the (C2) audit (no persistence channel is involved). It was found by reading the code, and it delimits

Table 2

What each verification instrument certifies, and the fault classes it can and cannot see. The first three rows factor the diagnostic asymmetry of Observation 1 together with the deterministic-fault caution above; the last row is the only one that speaks to correctness against ground truth.

Instrument	Certifies	Detects	Blind to
Across- N reproducibility check (one binary)	Thread-count invariance of the output	Faults whose output manifestation varies with N (cross-latitude leaks under a static schedule)	N -invariant leaks; any fault without output manifestation on the tested horizon; deterministic faults outside B
Fixed- N regression against a frozen baseline	Bit-equality with a prior run of the same configuration	Any fault that changes the output at the tested horizon	Faults with no manifestation at that horizon (the indexing defect above); wrong physics inherited by the baseline itself
Structural audit of (C0)–(C3)	The lemma's premises, hence bit-identity across $N \leq J_M$ by construction	Every leak in B on the enumerated persistence channels; races; order-varying reductions	Deterministic faults outside B : indexing, constants, order-invariant wrong physics
Independent reference (analytic or manufactured solution; conservation residuals)	Proximity of the computed answer to ground truth, within the reference's scope	Deterministic wrong physics, including faults invisible to all rows above	Whatever the reference does not constrain

the present framework honestly: the audit is complete for the leak class B , not for correctness at large.

Table 2 factors these observations into a single decision grid: what each verification instrument certifies, what it detects, and what it cannot see. The instruments are complementary contracts, not substitutes: the across- N check and the baseline regression are cheap *regression* contracts—they certify invariance, never truth; the structural audit turns reproducibility from an observation into a construction and closes the leak class B ; and correctness at large closes only against an independent reference—an analytic or manufactured solution where one exists [26], or conservation residuals, which need no second implementation. A systematic treatment of reference-based correctness criteria for legacy ports is beyond the scope of this paper.

8. Limitations of the lemma

The lemma characterizes a precisely scoped property. Four limitations bound this scope explicitly.

- **Same-binary scope.** Bit-identity across *different* binaries (different compilers, different `-march`, different optimization levels) is not claimed and cannot be claimed under IEEE-754 alone: FMA contraction, instruction scheduling, and libm implementations differ [9, 12]. The companion empirical study [33] measures distinct MD5 checksums on Zen 5 (with FMA) and Ivy Bridge-EP (without FMA), both internally bit-stable across the tested thread counts.
- **Same-hardware scope.** Bit-identity across CPUs with different FMA or extended-precision behavior (rare in modern hardware, but some x87 legacy paths can differ) requires additional conditions on the instruction set beyond (A0).

- **No guarantee against external non-determinism.** If a diagnostic write path records a wall-clock timestamp and feeds it back into the state S , assumption (A0) is violated. In the MGO implementation we audited the code to confirm that no such path exists; in general, this is an audit obligation on the implementer.
- **Not a statement about $N > J_M$.** Oversubscription (more threads than latitudes) produces idle threads but does not change the reduction order; the lemma remains valid, but the argument applies only vacuously.

9. Comparison with algorithmic approaches

A natural question is why source-level structural refactorings were chosen rather than an algorithmic route—for example, deploying a superaccumulator library [5, 16] or a pre-rounded reduction [7] as a transparent replacement for the model's floating-point summations. The two families of approaches are not exclusive; they address slightly different goals, and the present discussion is intended to clarify what each one establishes; the diagnostic difference between the two routes was drawn out in Section 7.

9.1. The algorithmic approach

Algorithmic approaches achieve reproducibility through changes to the arithmetic itself.

Pre-rounded reductions. Demmel and Nguyen [7] show that, by pre-rounding each summand to a common exponent before accumulation, the resulting summation operator becomes associative under IEEE-754 semantics. Order-independence then follows automatically; any parallel evaluation order produces the same result. The cost is a small,

bounded loss of accuracy—comparable to that of conventional (non-reproducible) summation—together with the algorithmic overhead of the pre-rounding step.

Superaccumulators. Collange et al. [5] introduce a different mechanism: a high-precision integer accumulator wide enough to absorb the full exponent (dynamic) range of double-precision inputs without intermediate rounding. Iakymchuk et al. [16] extend this to MPI+OpenMP solvers; the superaccumulator becomes a thread-local data structure that is later merged in a deterministic order. The cost is a sizable memory and instruction overhead per operation, with the exact factor depending on the accumulator width and the architecture.

Order-independent reproducible reductions. Arteaga et al. [1] build on the pre-rounding construction: an error-free transformation yields a reduction independent of evaluation order, so that any parallel summation order produces the same result without fixing that order at the source level. Fixed ordering is used only for intra-thread non-associative expressions, not for the distributed reduction itself; in this respect the mechanism belongs with the pre-rounding and superaccumulator constructions above rather than with our structural condition (C1). The COSMO program of Schär et al. [28] is, by contrast, *not* an order-independent reduction: a preprocessor automatically parenthesizes every mathematical expression of the source code, and custom portable transcendental functions replace the intrinsics, so the compiler cannot reorder operands—that is, it enforces a fixed source-level operand order, the same structural family as conditions (C0)–(C1), realized as a build-system discipline. The COSMO realization is integrated into a specific code base and its build system, rather than stated as a portable specification.

Performance cost. Schär et al. [28] report the measured cost of enforcing bit reproducibility between CPU and GPU implementations of COSMO: 37 % on CPU and 13 % on GPU, against the non-bit-reproducible counterparts. The cost is non-trivial enough that Zeman and Schär [38] document that bit reproducibility is generally not enforced in operational weather and climate models, citing the performance penalty as a leading reason.

9.2. The structural approach (present result)

The lemma developed in this paper takes a complementary route: rather than modifying the arithmetic, it identifies four structural conditions on the existing code—(C0) fixed-order inner reductions, (C1) deterministic outer reduction order, (C2) per-call state isolation, (C3) disjoint per-thread writes—and establishes them by source-level audit and refactoring.

The trade-offs run in opposite directions.

Library dependency. The structural approach requires no specialized arithmetic library: the bit-reproducibility property is achieved with stock IEEE-754 operations. By contrast, the algorithmic approaches inherently require the

implementation to use a library (ExBLAS [16], FAST2SUM-based pre-rounding, COSMO’s custom preprocessor) that is itself a maintenance and verification burden.

Performance overhead. The structural approach imposes no per-operation arithmetic overhead: every addition, multiplication, and FMA in the refactored code is the same IEEE-754 primitive as in the non-reproducible version. The performance cost is therefore localized in the reduction step (which becomes sequential rather than tree-style) and in the per- J memory cost of the buffer arrays. In our MGO implementation, both costs are measured: a 73 MB memory pool for the per- J buffers (0.1 % of the 64 GB test system’s memory), and a fixed-order serial reduction profiled at 1.9 % of single-thread wall time in the companion study [33], its execution dominated by memory bandwidth rather than arithmetic; the refactored model attains 93.9 % of its profiled algorithmic Amdahl limit at 16 threads.

Audit burden. The structural approach requires an exhaustive audit of all `SAVE` and `THREADPRIVATE` working state in every subroutine that may be entered from within the J -loop. For a legacy Fortran 77 codebase such as MGO, this audit is labor-intensive: the source-level OMP directive in the refactored MGO model contains over three hundred classified names in the parallel scope alone, and the discovery of the inter-latitude state leakage in the vertical-exchange kernel (a twelve-array *memorized* cache) required reading the unrefactored source to identify the latent race. The labor is precisely what algorithmic approaches absorb into their machinery.

10. An open synthetic demonstration

Observation 1 and the conditions behind it were drawn from one proprietary model. To make the claim checkable without that source, we provide a small, open Fortran/OpenMP program that reproduces the diagnostic on code anyone can compile and run. It is a miniature of the spectral time step: a contribution $\Delta^{(J)}$ is computed for each of $J_M = 32$ partitions under an OpenMP `schedule(static)` loop, the per-partition results are written to disjoint slots (C3) and combined by a fixed-order serial reduction (C1), and the state is advanced a fixed number of steps before its raw bytes are checksummed. The three runs differ in one respect only—the reset policy of two memoization caches, the analogue of the vertical-exchange arrays of Section 4:

- `CLEAN` resets both caches every iteration (condition (C2) satisfied);
- A lets a `THREADPRIVATE` cache persist across partitions within a thread—an inter-*partition* leak;
- B lets a per-partition cache persist across time steps—an inter-*step* leak.

All arithmetic is deterministic IEEE-754 (no random numbers, no wall-clock, no transcendentals) and the time map is

Table 3

Synthetic-kernel demonstration of Observation 1: the MD5 of the output state across thread counts for the three cache-reset regimes, on one `-O2 -march=native` binary. An across- N reproducibility check flags regime A (an N -dependent leak) and is blind to regime B (an N -invariant leak that is bit-identical across threads yet physically wrong); the state-isolation reset of `CLEAN` removes both.

Regime	Cache leak	Output across $N \in \{1, 2, 4, 8, 16, 32\}$	Diagnosis
CLEAN	none (C2 holds)	one MD5, identical	reproducible <i>and</i> correct (reference)
A	cross-partition (N -dependent)	a distinct MD5 at each tested N	non-reproducible $\Rightarrow$ caught
B	cross-step (N -invariant)	one MD5, $\neq$ CLEAN	reproducible but wrong $\Rightarrow$ missed

contractive, so the state stays bounded and a fixed binary is bit-stable across thread counts by construction in `CLEAN`.

Table 3 reports the MD5 of the output for thread counts $N \in \{1, 2, 4, 8, 16, 32\}$ on one binary (`gfortran -fopenmp -O2 -march=native` [13]). The pattern is exactly the one Observation 1 predicts. `CLEAN` is bit-identical across N and is the correct reference. A, whose leak is N -dependent under the static partition, yields a different checksum at every N and is therefore caught. B, whose leak is N -invariant, yields a single checksum across all N —it passes the reproducibility check—yet that checksum differs from `CLEAN`, so the run is bit-identical across threads while being physically wrong. The across- N check sees A and is blind to B; only the (C2) reset policy of `CLEAN` removes both. The literal checksums depend on the compiler and `-march` target—a different binary emits different bytes, exactly as the two MGO platforms do—while the three-way pattern is the prediction of Observation 1 for any IEEE-754 platform; it is measured here on one x86-64 platform and one compiler, and the harness regenerates the table with a single command. Beyond the canonical configuration, the released harness sweeps 108 parameter scenarios (324 logged scenario–mode runs): leak amplitude across fourteen orders of magnitude (10^{-15} – 10^{-1}), contraction factor through the contractive boundary, partition count 4–64, state width 2–64, and integration length 10–1000 steps. The three-way pattern of Table 3 holds in every scenario that completes without numerical blowup, with a single expected degenerate exception—at zero leak amplitude the leaking regime collapses onto the reference—and the artifact logs every scenario and carries a standing counterexample-reporting pledge [35].

11. A reusable audit checklist

The conditions are not specific to a climate model. They apply to any OpenMP loop that reduces per-iteration contributions—computed from shared read-only inputs by a kernel that may carry procedure-local state—into a shared accumulator over a partitioned geometric or geographic dimension. Table 4 restates (C0)–(C3) as a checklist a practitioner can run against such a loop: for each condition it names the property to establish, a source-level (static) test that establishes it, the fault a violation produces, and the concrete instantiation in the MGO realization.

The checklist makes the diagnostic point of Observation 1 operational: running it forces the analyst to read exactly the

declarations where inter-iteration state leakage hides, whereas adopting an algorithmic-reproducibility library discharges none of (C0)–(C3) and leaves the (C2) fault class—the one that can corrupt the physics while preserving the checksum—entirely unexamined.

12. Applications to other spectral atmospheric GCMs

The conditions were derived from one model, but they are stated as properties of the spectral-transform time step rather than of any particular code, so they transfer to any spectral atmospheric model whose latitude accumulation matches Section 3. ECHAM6 is a concrete example: it uses a spectral-transform dynamical core at triangular truncations from T63 to T127 [29], so its inner FFT and Legendre transforms fall under (C0), its coefficient accumulation under (C1), and the per-column physics state under (C2) and (C3); on its hybrid distributed/shared-memory implementation the conditions would govern the shared-memory (OpenMP) level. The mapping is not uniform across models: a spectral-element core such as CAM-SE replaces the global Legendre transform with element-local operations, so (C1) must be re-stated per element [8, 37]; in the IFS, which uses hybrid distributed/shared-memory parallelization [36], (C0)–(C3) govern the intra-node reduction while the cross-rank MPI sum is a separate order-of-reduction question; and a grid-point model such as COSMO has no (C1) analogue, though (C2) and (C3) still apply and the bit-reproducibility program already carried out for it [28]—forbidding expression re-association and supplying portable transcendentals—is the grid-point counterpart of (A0) and (C0). These mappings are theoretical: the parallelization architectures above are drawn from the cited model-description papers, whereas the assignment of (C0)–(C3) to each model’s components is our own inference from its published architecture, not a property verified against its source. Verifying the assignment on an openly distributed spectral code is the first of the open directions listed in Section 14.

13. Cross-configuration evidence from a second legacy code

The same-configuration scope drawn in Section 5 admits a direct test: if the cross-configuration divergence of the checksums is really attributable to the mechanisms named

Table 4

The (C0)–(C3) audit checklist for a partitioned-reduction OpenMP loop. Each condition is established by a source-level test; a violation produces the indicated reproducibility or correctness fault. An order-independent algorithmic reduction (superaccumulator, pre-rounded sum) discharges none of these conditions and so leaves the (C2) fault class—which can corrupt the physics while preserving the checksum—unexamined.

Cond.	Source-level test	Violation produces	MGO instantiation
(C0)	Every inner reduction (FFT, quadrature, transform, symmetry combine) runs in fixed order on one thread; no nested-parallel or threaded-library call in the loop body.	Thread- or schedule-dependent inner sums; $\Delta^{(J)}$ not single-valued.	Serial hand-coded <code>INFFT/FFT</code> and <code>ALPM/ALPMN</code> kernels.
(C1)	The outer accumulation uses a fixed, N -independent order—a serial <code>!\$OMP MASTER</code> walk or a fixed-shape tree—after a barrier.	A reduction whose order varies with N (atomic, or a tree whose shape depends on the thread count); non-reproducible across thread counts.	Ordered per- J reduction in <code>COMSPE_PREJ</code> .
(C2)	Every <code>SAVE/THREADPRIVATE</code> array entered from the loop is reset to a value fixed by J alone; audit all persistence channels (<code>SAVE</code> , <code>DATA</code> , <code>COMMON</code> , <code>EQUIVALENCE</code>).	Inter-iteration state leakage: a physically wrong run that may still reproduce bit-for-bit.	<code>VE_JRESET</code> zeroing the vertical-exchange kernel's work arrays.
(C3)	Per-iteration writes address disjoint slots; enforce with <code>DEFAULT(NONE)</code> plus an explicit data-sharing clause on every name.	Data races on the shared accumulator; non-deterministic output.	>300 classified names under <code>DEFAULT(NONE)</code> ; latitude loop under <code>SCHEDULE(STATIC)</code> .

there—FMA contraction and the platform-native transcendental implementations—then pinning those mechanisms should extend bit-identity beyond a single instruction stream. A second proprietary legacy code of the same institutional provenance—a limited-area (regional) *gridpoint* atmospheric model (Fortran 77, 183×381 horizontal grid, 37.5 s time step)—provides that test in an ongoing GPU port: the dynamical core and the longwave-radiation block are offloaded with OpenACC (`nvfortran` on both configurations tested), and every port increment is gated on MD5 equality of the model's one-day output file (a fixed 14 223 508-byte record set) across three executions: the multitarget binary on the accelerator, the same binary in host fallback, and a separately compiled no-offload CPU reference. Three ingredients pin the arithmetic: FMA contraction disabled on both host and device compilations; a portable single-source double-precision exponential—argument reduction, a truncated Taylor series, and exact power-of-two scaling, built from correctly rounded basic operations—evaluated identically on host and device and rounded to single precision at the call site, replacing the platform-native single-precision intrinsic whose host and device implementations differ by 1–2 ULP (its source is included in the archived protocol); and round-trip data movement for offloaded units whose shared outputs are read downstream on the host. Under this recipe the three executions produce one hash per configuration—all three executions in each case: `800c6e04`. . . on an AMD Zen 5 host with an RTX A2000, and `095bf63f`. . . on an Intel Ivy Bridge-EP host with a Tesla V100—while the hash differs between the two configurations, and, on one and the same host, merely changing the compiler (`gfortran` to `nvfortran`, native intrinsics and FMA permitted) changes the

bytes (`084ec782`. . . versus `98efc2bf`. . .) while preserving the domain statistics of every output field.

This is the converse of the same-configuration scope statement, now measured: bit-identity is a property of the full compilation configuration, not of the hardware alone, and when the divergence mechanisms are pinned it extends even across the CPU–GPU instruction-set boundary within one configuration—*within-configuration bit-identity*, *cross-configuration divergence*. The evidence is deliberately scoped: the second code is a gridpoint model under an offload decomposition, so the partitioned-reduction condition (C1) has no analogue exercised here, and the gate is a one-day integration applied at every increment, not a long-horizon envelope; what transfers is the same-configuration contract and the pinning route of the (A0)/(C0) family. The full protocol—output byte layout, build lines, and checksum tables—is archived openly [30]; the port itself and its performance engineering are reported separately.

14. Conclusions

We have recast the bit-reproducibility of a parallel spectral atmospheric model as a deductive property of its source text. Four source-level conditions—(C0) determinism of the inner reductions, (C1) a fixed-order outer reduction, (C2) per-iteration state isolation, and (C3) disjoint per-thread writes—together with an IEEE-754 determinism assumption imply *thread-count-invariant bitwise reproducibility*: bit-identical output across all thread counts $N \leq J_M$ on a fixed binary for arbitrary integration length, replacing the customary inductive checksum test with a guarantee (the bit-identity lemma). That lemma is resolution-agnostic: it transfers to

any triangular truncation—T63L25, T106L25, and beyond—without change. Extension to a coupled configuration requires one additional premise: the fields the coupler supplies at each step must be deterministic from run to run and remain read-only during the parallel region, exactly as the prescribed forcing fields are in the audited configuration. Its role, however, is instrumental. The central point is diagnostic (Observation 1): a structural audit of (C0)–(C3)—through its state-isolation condition (C2)—detects every inter-iteration state-leakage fault on the audited persistence channels, whereas an across-thread reproducibility check detects only those whose effect depends on the thread count and is blind to the rest—a class established here by construction rather than by observed field frequency—no matter which summation algorithm produces the checksum. A companion empirical study [33] confirms the predicted bit-identity across the tested thread counts ($N \in \{1, 2, 4, 8, 12, 16\}$) on AMD Zen 5 and $N \in \{1, 2, 4, 8, 12, 16, 24\}$ on Intel Ivy Bridge-EP. The corrected configurations of the second companion study [31], bit-reproducible across thread counts by the same conditions, have since produced its multi-decadal ensemble integrations. Three directions remain open: verifying the conditions on a second legacy spectral model of independent provenance, most directly one with openly distributed source; extending (C1) to the grid-point setting in the manner of the canonical-order constructions for finite-difference models [1]; and combining the two routes in production—algorithmic determinism for cheap verification, the structural audit for the race detection it alone provides. The two are complementary, never substitutes, and reproducibility alone must not be read as correctness.

Data and Software Availability

Apart from the open synthetic kernel of Section 10—a self-contained Fortran/OpenMP program with its build-and-check harness, released as this paper’s own open replication artifact [35] (Zenodo, [10.5281/zenodo.21070991](https://zenodo.org/record/21070991))—and the cross-configuration verification protocol of Section 13 (output byte layout, build lines, and checksum tables; no third-party source), archived separately [30], the article is a theoretical contribution and reports no new data of its own. The MGO atmospheric general circulation model that motivates the conditions analyzed here is proprietary legacy code whose source is not publicly redistributable, and the present author, working as an independent researcher without institutional access, is not in a position to grant access to it. The empirical bit-reproducibility evidence underlying the lemma—MD5 checksum tables establishing byte-identical tabm output across thread counts on two hardware platforms, together with the verification scripts and build-environment manifests—is archived in the replication package of the first companion paper [32] (Zenodo, [10.5281/zenodo.19653300](https://zenodo.org/record/19653300)), and the derived products of the second companion paper in its own package [34] (Zenodo, [10.5281/zenodo.21196560](https://zenodo.org/record/21196560)). Consistent with the access constraint above, the first archive documents the conditions (C0)–(C3) through this verification

evidence—the checksum tables, scripts, and environment manifests—rather than through redistributable model source.

CRedit authorship contribution statement

Dmitrii Vokhmintsev: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Resources, Data curation, Writing – original draft, Writing – review & editing, Visualization, Project administration.

Declaration of Competing Interest

The author was previously employed at the Voeikov Main Geophysical Observatory (Saint Petersburg, Russia), where parallelization of the MGO model was begun; that employment concluded in July 2025, and the structural audit and the results reported here were carried out subsequently as independent, self-funded work. The author holds one issued Rospatent computer-program registration and has two related Rospatent patent applications under examination on the parallel-reduction and thread-safety methodology; these are derivative works that do not cover the proprietary MGO model. The author declares no other competing interests.

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Declaration of generative AI and AI-assisted technologies in the manuscript preparation process

During the preparation of this work the author used generative AI tools as a writing assistant, limited to copy-editing, structural revision of selected passages, and identification of editorial inconsistencies (notation, terminology, cross-reference accuracy). These tools were not used to generate scientific content: the lemma and its proof, the diagnostic-asymmetry observation, the analysis, and any figures were produced by the author, who has reviewed and edited all assisted text and takes full responsibility for the entire content of this work, including any material prepared with the aid of such tools.

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