

## Accuracy and Discrete Energy Behaviour of L1 and L2-1 $\sigma$ Time-Stepping Schemes for Caputo Fractional Diffusion Equations

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### Abstract

Time-fractional diffusion equations combine a nonlocal memory operator with diffusion and therefore require time-stepping methods that are accurate without losing the qualitative stability of the underlying problem. This paper provides a controlled computational comparison of the classical L1 formula and the second-order L2-1 $\sigma$  formula for a Caputo diffusion equation. The study is designed as a baseline for the development of energy-stable high-order schemes. A standard one-dimensional model is discretised in space by centred differences and in time by the two fractional formulas. Accuracy is assessed with the manufactured solution  $u(x,t)=t^3 \sin(\pi x)$  for fractional orders  $\alpha=0.5$  and  $\alpha=0.7$ . For  $\alpha=0.5$ , the observed L1 order approaches 1.47 while the L2-1 $\sigma$  method gives approximately second-order convergence. For  $\alpha=0.7$ , the corresponding orders are about 1.29 and 2.03. A second experiment considers the unforced problem with  $u(x,0)=\sin(\pi x)$  and monitors the discrete L2 energy. Both methods produce monotone energy decay for the tested step sizes, with the L2-1 $\sigma$  trajectory closely matching the L1 baseline. The results confirm the expected accuracy advantage of the high-order formula and show why energy diagnostics should accompany convergence tests. They also identify initial regularity and history cost as the principal issues that must be addressed in subsequent high-order scheme development.

**Keywords:** Caputo derivative; fractional diffusion equation; L1 scheme; L2-1 $\sigma$  scheme; energy stability; time stepping; error analysis

### 1. Introduction

Fractional diffusion equations are now a standard mathematical model for transport processes in which the present state depends on the past. In contrast with the classical heat equation, where the first time derivative is local, a time-fractional model contains a history-dependent operator. This feature is useful for anomalous transport, trapping, viscoelastic relaxation and heterogeneous media, but it also changes the numerical problem fundamentally. Every new time level contains information from all earlier levels, and the solution frequently has reduced temporal regularity near  $t=0$ . These two properties make accuracy, stability and computational cost inseparable design questions [1–3].

The PhD research framework from which this paper is developed is concerned with energy-stable high-order time-stepping schemes for fractional diffusion equations. That framework identifies four linked tasks: construction of higher-order temporal discretisations, derivation of

a discrete energy structure, rigorous stability and error analysis, and numerical comparison against established methods. The present paper addresses the comparison stage first. This is deliberate. A new scheme can only be evaluated meaningfully when its behaviour is measured against reference formulas whose convergence and stability properties are well understood.

The L1 formula remains the most widely used reference method. It is simple, robust and based on piecewise-linear interpolation of the solution inside the Caputo history integral. For a sufficiently smooth solution on a uniform mesh its local consistency leads to a temporal rate close to  $2-\alpha$ , although weak initial singularities can reduce that rate substantially [6,7]. The L2- $1\sigma$  method proposed by Alikhanov [4] uses a higher-order reconstruction and evaluates the derivative at an off-step point  $t_{n+\sigma}$ . With  $\sigma = 1 - \alpha/2$ , it gives second-order time accuracy under appropriate regularity and has become an important building block for high-order fractional solvers [5,8,9].

A difficulty in discussing 'stability' is that several notions are used in the fractional literature. Norm stability means that numerical errors do not grow uncontrollably. Energy stability is stronger and more structural: the discretisation should preserve, bound or appropriately mimic a continuous dissipation law. For gradient-flow models this issue is explicit, and recent work has shown that positivity or positive-semidefiniteness properties of discrete fractional operators can be used to derive energy laws for L2-type methods [10–13]. For a linear diffusion problem, a practical preliminary diagnostic is the decay of a discrete L2 energy. Such a diagnostic does not replace a theorem, but it can quickly expose a time integrator that produces nonphysical growth.

The purpose of this paper is therefore threefold. First, it states the L1 and L2- $1\sigma$  discretisations in a common notation. Secondly, it quantifies their temporal accuracy on a smooth manufactured solution while keeping the spatial error small. Thirdly, it examines the discrete energy history for the homogeneous problem. The paper does not claim a new fractional formula. Its contribution is a clean, reproducible benchmark and an analytical interpretation that can serve as the control case for subsequent development of corrected, variable-step or genuinely higher-order energy-stable methods.

## 2. Model problem and analytical setting

Consider the one-dimensional time-fractional diffusion equation on  $\Omega=(0,1)$  and  $0 < t \leq T$ :

$$CD_t^\alpha u(x,t) - \kappa u_{xx}(x,t) = f(x,t), \quad 0 < \alpha < 1, \quad \kappa > 0$$

with homogeneous Dirichlet conditions  $u(0,t)=u(1,t)=0$  and initial value  $u(x,0)=u_0(x)$ . The Caputo derivative is defined by

$$CD_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} u'(s) ds$$

The kernel  $(t-s)^{-\alpha}$  is weakly singular and gives non-negligible weight to the complete solution history. This is the source of the memory cost in direct algorithms. For the continuous homogeneous diffusion problem, multiplication by  $u$  and integration over space leads to a dissipative structure. Fractional time differentiation complicates the exact form of the energy identity, but the diffusion operator still acts as a positive spatial dissipation mechanism. A

credible numerical method should therefore avoid artificial growth in a suitable norm when  $f=0$ .

Space is discretised on  $x_i = ih$ ,  $i=0, \dots, M$ , using the centred second difference. If  $U^n$  denotes the vector of interior values, the spatial operator is the positive definite matrix  $A_h$  corresponding to  $-\kappa\delta_{xx}$ . The fully discrete problem can then be written as a fractional time approximation plus  $A_h U$  at the appropriate time level. In the accuracy experiment  $\kappa=1$  and the mesh uses  $M=1000$  subintervals. This spatial resolution is intentionally fine so that the reported differences mainly reflect the temporal method.

### 3. Time-stepping formulas

3.1 L1 approximation. Let  $t_n = n\tau$  on a uniform mesh. The L1 approximation at  $t_n$  is

$$D_\tau^\alpha U^n = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{k=0}^{n-1} b_k (U^{n-k} - U^{n-k-1})$$

where  $b_k = (k+1)^{1-\alpha} - k^{1-\alpha}$ . The coefficients are positive and decreasing. At each step, only the newest increment contains  $U^n$ , so the implicit diffusion equation requires the solution of one symmetric positive definite linear system. The history sum, however, contains  $O(n)$  terms; without fast convolution the total work grows quadratically with the number of time levels.

For smooth solutions the L1 formula is expected to show an order close to  $2-\alpha$  on a uniform mesh. That expectation must be used with care. Time-fractional diffusion solutions commonly contain terms such as  $t^\alpha$  near the initial point, even for smooth spatial data. In that case the nominal uniform-mesh rate may not be realised globally [6,7,14]. This regularity issue is isolated in the second paper of the pair, where graded meshes are examined directly.

3.2 L2-1 $\sigma$  approximation. The Alikhanov formula evaluates the Caputo derivative at  $t_{n+\sigma}$ , where  $\sigma = 1-\alpha/2$ . On a uniform grid it can be expressed as

$$D_{\tau,\sigma}^\alpha U^{n+\sigma} = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{k=0}^n c_{n-k}^{(n)} (U^{k+1} - U^k)$$

The coefficients are constructed from power differences generated by a quadratic interpolation of the solution history. In the present implementation,  $a_0 = \sigma^{1-\alpha}$ ,  $a_j = (j+\sigma)^{1-\alpha} - (j-1+\sigma)^{1-\alpha}$ , and the auxiliary  $b_j$  coefficients contain the corresponding  $(2-\alpha)$ -power differences. The  $c_j$  weights are then formed from  $a_j$  and successive  $b_j$  values, with the usual special treatment of the first and last coefficient [4]. The diffusion term is evaluated at  $U^{n+\sigma} = \sigma U^{n+1} + (1-\sigma)U^n$ .

The attraction of L2-1 $\sigma$  is not simply a smaller error constant. It changes the order regime. Under sufficient regularity, the method is second order in time for  $0 < \alpha < 1$ , while retaining an implicit structure compatible with standard elliptic solvers. Extensions to nonuniform meshes, fast history evaluation and energy-stable phase-field schemes have been developed in recent work [10–13,15,17]. These advances make L2-1 $\sigma$  a useful reference point for any proposed high-order method.

#### 4. Numerical design

Two experiments are used. The first is an accuracy test with an exact solution. We choose

$$u(x, t) = t^3 \sin(\pi x)$$

The forcing term is obtained analytically from the identity  $CD_t^\alpha t^\beta = \frac{\Gamma(\beta+1)}{\Gamma(\beta+1-\alpha)} t^{\beta-\alpha}$ . Hence, with  $\beta=3$  and  $\kappa=1$ ,

$$f(x, t) = \left[ \frac{\Gamma(4)}{\Gamma(4-\alpha)} t^{3-\alpha} + \pi^2 t^3 \right] \sin(\pi x)$$

The initial and boundary conditions are then satisfied exactly. Errors are measured at  $T=1$  in the discrete  $L_2$  norm. Temporal step numbers  $N=20, 40, 80, 160$  are used for  $\alpha=0.5$  and  $\alpha=0.7$ , and the observed order is  $\log_2(e_N/e_{2N})$ .

The second experiment uses  $f=0$ ,  $T=2$  and initial value  $u_0(x)=\sin(\pi x)$ . The purpose is not to estimate a convergence order but to inspect qualitative dissipation. The diagnostic energy is  $E^n = \frac{1}{2} h \sum_i (U_i^n)^2$ . Both methods use  $N=100$  time steps and  $M=400$  spatial subintervals. A monotone decrease of this quantity is treated as a necessary computational check, not as a substitute for a formal fractional energy inequality. This distinction is important because a sequence can have decreasing  $L_2$  norm without satisfying the stronger energy law required by a particular physical model.

#### 5. Results

Table 1 reports the smooth-solution convergence results. For  $\alpha=0.5$ , the  $L_1$  rate increases from 1.45 to about 1.47, close to the theoretical  $2-\alpha=1.5$ . The  $L_2$ - $1\sigma$  rate is essentially 2.00 and reaches 2.04 on the finest tested temporal mesh. The absolute error is also substantially smaller at  $N=160$ : about  $1.35 \times 10^{-5}$  for  $L_2$ - $1\sigma$  against  $4.36 \times 10^{-5}$  for  $L_1$ . The result is consistent with the role of the Alikhanov formula as a genuinely second-order temporal discretisation for smooth data.

For  $\alpha=0.7$ , the same pattern is clearer because the expected  $L_1$  order is only 1.3. The measured values range from 1.27 to 1.29, whereas  $L_2$ - $1\sigma$  remains very close to order two. At  $N=160$ , its final-time error is approximately  $1.65 \times 10^{-5}$ , compared with  $1.70 \times 10^{-4}$  for  $L_1$ . Thus, for this benchmark, the high-order method reduces the temporal error by roughly one order of magnitude without changing the spatial discretisation.

The energy experiment gives a complementary result. Starting from  $E^0=0.25$ , both schemes show monotone decay for  $\alpha=0.5$  and  $\alpha=0.7$ . At  $\alpha=0.5$  the  $L_1$  energies at  $t=0.5, 1$  and  $2$  are  $1.63 \times 10^{-3}$ ,  $8.17 \times 10^{-4}$  and  $4.08 \times 10^{-4}$ . The  $L_2$ - $1\sigma$  values are  $1.61 \times 10^{-3}$ ,  $8.11 \times 10^{-4}$  and  $4.07 \times 10^{-4}$ . For  $\alpha=0.7$  the corresponding final values are  $1.21 \times 10^{-4}$  and  $1.20 \times 10^{-4}$ . No positive energy increment was observed across the computed histories.

These results should be interpreted in the correct hierarchy. The convergence table verifies the implementation against known formal orders. The energy table demonstrates that the high-order method does not introduce an obvious artificial growth mode in the tested linear problem. It does not prove unconditional energy stability. A proof would require a discrete identity or inequality based on positivity, monotonicity or positive-semidefiniteness of the fractional

convolution operator, followed by control of the spatial bilinear form. Recent L2 analyses show how such arguments can be developed [10–13].

**Table 1. Final-time discrete L2 errors and observed temporal orders for the smooth benchmark**

| $\alpha$ | N   | L1 error  | L1 order | L2-1 $\sigma$ error | L2-1 $\sigma$ order |
|----------|-----|-----------|----------|---------------------|---------------------|
| 0.5      | 20  | 9.109e-04 | —        | 8.904e-04           | —                   |
| 0.5      | 40  | 3.331e-04 | 1.451    | 2.227e-04           | 2.000               |
| 0.5      | 80  | 1.207e-04 | 1.465    | 5.531e-05           | 2.009               |
| 0.5      | 160 | 4.362e-05 | 1.468    | 1.346e-05           | 2.039               |
| 0.7      | 20  | 2.448e-03 | —        | 1.090e-03           | —                   |
| 0.7      | 40  | 1.013e-03 | 1.273    | 2.720e-04           | 2.002               |
| 0.7      | 80  | 4.162e-04 | 1.283    | 6.758e-05           | 2.009               |
| 0.7      | 160 | 1.704e-04 | 1.288    | 1.652e-05           | 2.032               |

**Table 2. Discrete L2 energy E(t) for the homogeneous diffusion test (E(0)=0.25)**

| $\alpha$ | t   | L1 energy | L2-1 $\sigma$ energy | Difference |
|----------|-----|-----------|----------------------|------------|
| 0.5      | 0.5 | 1.635e-03 | 1.611e-03            | 2.35e-05   |
| 0.5      | 1.0 | 8.170e-04 | 8.113e-04            | 5.67e-06   |
| 0.5      | 2.0 | 4.085e-04 | 4.071e-04            | 1.39e-06   |
| 0.7      | 0.5 | 1.010e-03 | 9.774e-04            | 3.25e-05   |
| 0.7      | 1.0 | 3.421e-04 | 3.373e-04            | 4.79e-06   |
| 0.7      | 2.0 | 1.210e-04 | 1.202e-04            | 7.78e-07   |

## 6. Discussion: implications for high-order energy-stable scheme development

The benchmark highlights three design requirements for the wider research programme. The first is regularity robustness. The attractive second-order result for L2-1 $\sigma$  was obtained with  $u = t^3 \sin(\pi x)$ , which is deliberately smooth at  $t=0$ . Real subdiffusion solutions are often much less regular. High order derived under classical differentiability assumptions can therefore be misleading unless the starting layer is treated explicitly. Starting corrections, graded meshes and nonuniform formulations are not optional refinements; they are central to practical error control [6,7,9,14].

The second requirement is a rigorous energy mechanism. For linear diffusion, positive spatial dissipation and a well-behaved fractional convolution are usually sufficient to obtain stable norms. For nonlinear gradient flows, however, the physical energy may contain a potential term and the time-fractional derivative can make the discrete dissipation law nonlocal. Work by Quan and Wang, Liao and co-authors, and Zhang and Liao shows that reformulation of high-order L2-type operators, discrete gradient structures and auxiliary-variable strategies can recover meaningful energy laws [10–12,16]. A new scheme should therefore be designed around an energy estimate rather than tested for stability only after its coefficients have been fixed.

The third requirement is efficiency. Direct L1 and L2-1 $\sigma$  history evaluation needs  $O(N^2)$  arithmetic over N time levels and  $O(N)$  stored solution history. This is acceptable for the

present benchmark but not for long-time or multidimensional simulations. Sum-of-exponentials approximations can reduce the effective memory and work of the history term, as demonstrated for fast high-order L2-type schemes [15]. Any new high-order method intended for practical use should be assessed not only by asymptotic order but also by error per unit computational cost and by its compatibility with fast convolution.

A sensible next stage is therefore a corrected or variable-step high-order method with four properties checked in parallel: consistency on smooth solutions, restored accuracy under weak initial singularity, a provable discrete energy inequality, and a fast history implementation. The present results provide the numerical control case for that work. In particular, an improved method should beat the  $L_2$ - $1\sigma$  error level under comparable spatial resolution while retaining or strengthening the observed dissipation and avoiding restrictive time-step ratios where possible.

### **7. Error sources, reproducibility and limitations**

A comparison of fractional time-stepping methods can be distorted easily if spatial, temporal and algebraic errors are not separated. The present calculations therefore used a deliberately fine centred-difference grid in the manufactured-solution test. The spatial truncation error is second order in  $h$ , whereas the temporal error varies between approximately  $\tau^{2-\alpha}$  and  $\tau^2$ . With  $M=1000$ , further spatial refinement changed the reported temporal trends only in the last digits. This separation is important because a high-order time method can otherwise appear to stop converging simply because the spatial mesh has become the dominant error source.

The implementation also uses the formulas in their direct history-summation form. At step  $n$ , every previous solution increment contributes to the Caputo approximation. This choice makes the algorithm transparent and is suitable for verification, but it is not the recommended form for large production runs. Fast convolution can introduce an additional approximation tolerance through kernel compression. A fair future comparison should therefore distinguish three errors: discretisation error, fast-history approximation error and linear-solver error. The fast tolerance should be set low enough that the convergence slope of the underlying time discretisation remains visible.

Reproducibility requires more than listing the differential equation. For the smooth benchmark, the exact solution, forcing, spatial interval, final time, spatial grid, temporal levels, error norm and order formula have all been stated explicitly. The first time-stepping coefficient is treated separately where required by the  $L_2$ - $1\sigma$  formula. At each step the resulting tridiagonal linear system is solved to numerical precision. These details are sufficient for the tables to be reproduced independently in MATLAB, Python, Julia or another numerical environment without relying on proprietary data.

The energy calculation also has a specific scope.  $E^n = \frac{1}{2} \|U^n\|_h^2$  is a diagnostic norm for the linear homogeneous diffusion problem. Its monotonic decrease is consistent with a dissipative numerical trajectory, but this quantity is not presented as the unique fractional energy of the continuous equation. In time-fractional gradient-flow analysis, energy can involve memory-dependent corrections or auxiliary variables, and different schemes may satisfy different but

asymptotically compatible energy laws [10,13]. Consequently, the present energy table should be used as a screening test: any proposed high-order extension should at least avoid spurious growth here before a stronger theorem is attempted.

Another limitation is that the comparison uses uniform time steps. Uniform meshes are appropriate for the smooth manufactured solution but are not representative of the weak initial regularity encountered in many subdiffusion models. A method that looks excellent in Table 1 can suffer substantial order reduction on a solution proportional to  $t^\alpha$ . This is not a defect specific to  $L2-1\sigma$ ; it is a general regularity issue for high-order time discretisations. The companion paper therefore changes the test function deliberately and uses graded temporal meshes to expose this mechanism.

The present study also restricts attention to one space dimension and constant diffusivity. Neither restriction is fundamental to the time-stepping formulas. In several space dimensions,  $A_h$  would be replaced by the corresponding finite-difference, finite-element or spectral stiffness operator. Variable coefficients alter the spatial bilinear form and can make energy estimates more technical, but the temporal convolution remains the central nonlocal component. A later paper can therefore reuse the current temporal baseline while replacing the spatial discretisation with a higher-order compact, finite-element or discontinuous Galerkin method.

Finally, the word 'high-order' should be used carefully in fractional computation.  $L2-1\sigma$  is second order in time, which is high relative to the classical  $L1$  formula but lower than corrected BDF or  $L2$  formulas that can attain orders above two for sufficiently smooth data. The value of the present comparison is that it establishes a reliable intermediate benchmark. A newly constructed method should demonstrate a clear advantage over both  $L1$  and  $L2-1\sigma$ , and that advantage should persist after initial singularity, energy structure and computational memory are considered together.

There is also a methodological reason for retaining both reference methods in later experiments.  $L1$  supplies a conservative benchmark with simple positive weights, while  $L2-1\sigma$  supplies a more demanding accuracy benchmark. If a proposed scheme improves only on  $L1$  but not on  $L2-1\sigma$ , the case for using the additional algebra may be weak. Conversely, if it improves accuracy over  $L2-1\sigma$  but produces oscillatory energy histories or severe step-ratio restrictions, it may not satisfy the stability objective of the thesis. Reporting both references therefore creates a balanced evaluation in which accuracy, robustness and structural behaviour are visible at the same time.

For publication-quality numerical evidence, future tables should also include at least two spatial resolutions at a fixed fine temporal mesh. This verifies that the spatial solver has entered its expected asymptotic regime. Where exact solutions are unavailable, a highly resolved reference solution should be generated with a method of demonstrably higher accuracy. These controls become especially important for variable-coefficient and multidimensional problems, because spatial anisotropy or iterative-solver tolerances can otherwise be mistaken for temporal

instability. A clear separation of error sources will make the eventual energy-stable high-order contribution easier to defend analytically and numerically.

## 8. Conclusion

This paper compared the  $L1$  and  $L2-1\sigma$  formulas for a Caputo time-fractional diffusion equation using a common finite-difference framework. On the smooth manufactured solution,  $L1$  reproduced the expected order near  $2-\alpha$ , while  $L2-1\sigma$  delivered approximately second-order convergence for both  $\alpha=0.5$  and  $\alpha=0.7$ . In the homogeneous diffusion test, both methods produced monotone decay of the discrete  $L2$  energy over the computed interval. The  $L2-1\sigma$  method therefore provides a strong high-order baseline: it improves accuracy substantially without producing a visible loss of dissipative behaviour in the tested case.

The main limitation is equally clear. Smooth-data accuracy and numerical energy decay are not sufficient to establish a general energy-stable high-order theory. Fractional diffusion solutions may be weakly singular at the initial time, and direct history summation is expensive. The next methodological step should combine nonuniform or corrected starting treatment with a discrete energy proof and fast memory evaluation. These requirements are taken up explicitly in the companion paper on graded temporal meshes and weak initial singularities.

From a thesis-development perspective, the benchmark also clarifies what would count as a substantive new contribution. Merely increasing the formal order on a smooth example would not be enough. A stronger scheme should retain its advantage for low-regularity data, admit an energy estimate that is stated in a precise discrete norm, and remain computationally viable when the number of time levels is large. Ideally, the proof should identify explicit conditions on coefficients or step ratios rather than relying only on numerical evidence. The computational study should then verify those analytical conditions across several fractional orders and compare the method against both  $L1$  and  $L2-1\sigma$  at matched accuracy. This combination of theorem, singular-data robustness and cost-aware validation would connect the numerical experiments directly to the approved research objectives and provide a defensible basis for a later journal paper centred on the genuinely new method.

The two benchmark values of  $\alpha$  used here are also useful for later sensitivity analysis. The case  $\alpha=0.5$  represents stronger memory and a larger separation between  $L1$  and second-order behaviour, whereas  $\alpha=0.7$  gives a milder but still clearly fractional regime. Adding  $\alpha$  close to one and  $\alpha$  below one-half in future work would test whether a proposed method remains reliable across both weak-memory and strongly singular limits. The same benchmark can then be reused unchanged, which makes cross-method comparisons more transparent and statistically unnecessary because the outputs are deterministic numerical errors.

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