


## Tensor approximation of functional differential equations

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Functional differential equations (FDEs) play a fundamental role in many areas of mathematical physics, including fluid dynamics (Hopf characteristic functional equation), quantum field theory (Schwinger-Dyson equations), and statistical physics. Despite their significance, computing solutions to FDEs remains a longstanding challenge in mathematical physics. In this paper we address this challenge by introducing approximation theory and high-performance computational algorithms designed for solving FDEs on tensor manifolds. Our approach involves approximating FDEs using high-dimensional partial differential equations (PDEs), and then solving such high-dimensional PDEs on a low-rank tensor manifold leveraging high-performance (parallel) tensor algorithms. The effectiveness of the proposed approach is demonstrated through its application to the Burgers-Hopf FDE, which governs the characteristic functional of the stochastic solution to the Burgers equation evolving from a random initial state.

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### I. INTRODUCTION

Functional differential equations (FDEs) are equations involving operators (nonlinear functionals) and derivatives/integrals of such operators with respect to functions (functional derivatives) and other independent variables such as space and time [1,2]. FDEs arise naturally across a spectrum of mathematical physics disciplines. A classical example in fluid dynamics is the Hopf-Navier-Stokes equation [3–6]

$$\frac{\partial \Phi([\theta], t)}{\partial t} = \sum_{k=1}^d \int_{\Omega} \theta_k(\mathbf{x}) \left( i \sum_{j=1}^d \frac{\partial}{\partial x_j} \frac{\delta^2 \Phi([\theta], t)}{\delta \theta_k(\mathbf{x}) \delta \theta_j(\mathbf{x})} + \nu \nabla^2 \frac{\delta \Phi([\theta], t)}{\delta \theta_k(\mathbf{x})} \right) d\mathbf{x}, \quad (1)$$

which governs the temporal evolution of the characteristic functional

$$\Phi([\theta], t) = \mathbb{E} \left\{ \exp \left[ i \int_{\Omega} \mathbf{u}(\mathbf{x}, t) \cdot \boldsymbol{\theta}(\mathbf{x}) d\mathbf{x} \right] \right\}. \quad (2)$$

Here  $\Omega \subseteq \mathbb{R}^d$  is the spatial domain ( $d = 1, 2, 3$ ),  $\mathbf{u}(\mathbf{x}, t)$  represents a stochastic solution of the Navier-Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u}, \quad (3)$$

$$\nabla \cdot \mathbf{u} = 0,$$

corresponding to a random initial velocity distribution [7,8],  $\mathbb{E}\{\cdot\}$  is the expectation over the probability measure of such

random velocity distribution, and  $\boldsymbol{\theta}(\mathbf{x})$  is a divergence-free test function. Equation (1) involves derivatives of the functional  $\Phi([\theta], t)$  with respect to the functions  $\theta_i(\mathbf{x})$ , i.e., functional derivatives  $\delta/\delta\theta_i(\mathbf{x})$  [2], and derivatives with respect to the independent variables  $x_j$  and  $t$ .

As is well known, the characteristic functional (2) encodes the full statistical information of the random field  $\mathbf{u}(\mathbf{x}, t)$  that solves the Navier-Stokes equations (3), including multipoint statistical moments, cumulants, and multipoint joint probability density functions. For instance, by taking functional derivatives of  $\Phi$  we can immediately express the mean and autocorrelation function of  $\mathbf{u}(\mathbf{x}, t)$  as

$$\mathbb{E}\{u_k(\mathbf{x}, t)\} = \frac{1}{i} \frac{\delta \Phi([\theta], t)}{\delta \theta_k(\mathbf{x})} \Big|_{\theta=0},$$

$$\mathbb{E}\{u_k(\mathbf{x}, t) u_j(\mathbf{y}, t)\} = \frac{1}{i^2} \frac{\delta^2 \Phi([\theta], t)}{\delta \theta_k(\mathbf{x}) \delta \theta_j(\mathbf{y})} \Big|_{\theta=0}. \quad (4)$$

Similarly, by evaluating (2) at  $\theta_i(\mathbf{x}) = a_i \delta(\mathbf{x} - \mathbf{y})$  yields the one-point characteristic function of the solution  $\mathbf{u}(\mathbf{y}, t)$  at an arbitrary spatial location  $\mathbf{y} \in \Omega$  as

$$\phi(\mathbf{a}, \mathbf{y}, t) = \mathbb{E} \left\{ \exp \left[ i \int_{\Omega} \mathbf{u}(\mathbf{x}, t) \cdot \mathbf{a} \delta(\mathbf{x} - \mathbf{y}) d\mathbf{x} \right] \right\}$$

$$= \mathbb{E}\{e^{i\mathbf{a} \cdot \mathbf{u}(\mathbf{y}, t)}\}. \quad (5)$$

The inverse Fourier transform (in the sense of distributions) of  $\phi(\mathbf{a}, \mathbf{y}, t)$  with respect to the variable  $\mathbf{a}$  is the probability density function PDF of the solution  $\mathbf{u}(\mathbf{y}, t)$  at the spatial location  $\mathbf{y} \in \Omega$  and time  $t$ . Any other statistical property of  $\mathbf{u}(\mathbf{x}, t)$  can be derived from the characteristic functional (2). For this reason, the FDE (1) was deemed by Monin and Yaglom ([4], Ch. 10) to be “the most compact formulation of the general turbulence problem,” which is the problem of determining the statistical properties of the velocity and the pressure fields of

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the Navier-Stokes equations given statistical information on the initial state.

Another well-known classical example of functional differential equation is the Schwinger-Dyson (SD) equation of quantum field theory [9,10]. The SD equation describes the dynamics of the generating functional of the Green functions of a quantum field theory, allowing us to propagate quantum field interactions in a perturbation setting (e.g., with Feynman diagrams) or in a strong coupling regime. The usage of FDEs saw rapid growth in the 1970s, driven by the realization that techniques originally developed for quantum field theory by Dyson, Feynman, and Schwinger could be, at least formally, extended to other branches of mathematical physics. A pivotal contribution to this evolution was the ground-breaking work by Martin, Siggia, and Rose [11]. This work served as a landmark in the field, showcasing the possibility of applying quantum field theoretic methods, such as functional integrals and diagrammatic expansions [12–15], to problems in classical statistical physics.

More recently, FDEs have appeared in both mean-field games and mean-field optimal control [16,17]. Mean-field games are optimization problems involving a large (potentially infinite) number of interacting players. In some cases, it is possible to reformulate such optimization problems in terms of a nonlinear Hamilton-Jacobi-Bellman FDE in a Wasserstein space of probability measures. The standard form of such equation is (see [18], p. 1)

$$\frac{\partial F([\rho], t)}{\partial t} + \mathcal{W}\left([\rho], \left[\frac{\delta F([\rho], t)}{\delta \rho(\mathbf{x})}\right]\right) = 0, \quad F([\rho], 0) = F_0([\rho]), \quad (6)$$

where  $\rho(\mathbf{x})$  is a  $d$ -dimensional probability density function supported on  $R \subseteq \mathbb{R}^d$ ,  $\delta F/\delta \rho(\mathbf{x})$  is the first-order functional derivative of  $F$  relative to  $\rho(\mathbf{x})$ , and  $\mathcal{W}$  is the Hamilton functional

$$\mathcal{W}\left([\rho], \left[\frac{\delta F([\rho], t)}{\delta \rho(\mathbf{x})}\right]\right) = \int_R \Psi\left(\mathbf{x}, \nabla \frac{\delta F([\rho], t)}{\delta \rho(\mathbf{x})}\right) \rho(\mathbf{x}) dx + \mathcal{J}([\rho]). \quad (7)$$

Here  $\Psi$  is the Hamilton’s function and  $\mathcal{J}([\rho])$  is an interaction potential. Mean-field theory is also useful in optimal feedback control of nonlinear stochastic dynamical systems and in deep learning. For instance, E and collaborators [17] established the mathematical groundwork for the population risk minimization problem in deep learning by framing it as a mean-field optimal control problem. This yields a generalized version of the Hamilton-Jacobi-Bellman equation in a Wasserstein space of probability measures, which is a nonlinear FDE of the form (6), e.g., Eq. (20) in [17] and Eq. (1.1) in [19].

In this paper we develop approximation theory and high-performance computational algorithms designed for solving FDEs on tensor manifolds. Our approach involves first approximating FDEs in terms of high-dimensional partial differential equations (PDEs), and then computing the solution to such high-dimensional PDEs on a low-rank tensor manifold leveraging high-performance (parallel) tensor algorithms. To this end, we will build upon our recent work on tensors, i.e., on step-truncation tensor methods [20,21], and demonstrate convergence to functional approximations of FDEs. In

particular, we study the Burgers-Hopf characteristic functional equation [22–24]

$$\frac{\partial \Phi([\theta], t)}{\partial t} = \int_0^{2\pi} \left[ \frac{i}{2} \frac{\partial}{\partial x} \frac{\delta^2 \Phi([\theta], t)}{\delta \theta(x)^2} + \gamma \frac{\partial^2}{\partial x^2} \frac{\delta \Phi([\theta], t)}{\delta \theta(x)} + \alpha \sum_{k=1}^{\infty} \frac{(-\pi)^k}{(2k+1)! i^{2k}} \frac{\delta^{2k+1} \Phi([\theta], t)}{\delta \theta(x)^{2k+1}} \right] \theta(x) dx, \quad (8)$$

which governs the Hopf characteristic functional of the solution to the Burgers equation on the unit circle  $\Omega = [0, 2\pi]$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \gamma \frac{\partial^2 u}{\partial x^2} + R(u), \quad (9)$$

where  $R(u) = \alpha \sin(\pi u)$  is a nonlinear reaction term. The Burgers-Hopf equation (8) has the same structure as the Hopf-Navier-Stokes equation (1). In fact, by setting  $\alpha = 0$ , (8) becomes identical to (1) when  $d = 1$ .

This paper is organized as follows. In Sec. II we briefly review necessary and sufficient conditions for existence and uniqueness of solutions to FDEs. In Sec. III we discuss functional approximation of FDEs in terms of high-dimensional PDEs. In Sec. IV we briefly review numerical tensor methods approximate the solution of high-dimensional PDEs on tensor manifolds. In Sec. IV we demonstrate our functional approximation methods for FDEs to the Burgers-Hopf equation. The main findings are summarized in Sec. VI. In the Appendix A we describe the high-performance (parallel) tensor algorithms we developed to solve high-dimensional PDEs on tensor manifolds.

## II. EXISTENCE AND UNIQUENESS OF SOLUTIONS TO THE HOPF EQUATION

Back in 1972 Monin and Yaglom stated [4], p. 773 that “When we tried to develop a complete statistical description of turbulence with the aid of the Hopf equation for the characteristic functional we found that no general mathematical formalism for solving linear equations in functional derivatives was available. There are also no rigorous theorems on the existence and uniqueness of the solution to such equations.”

Since then, there were advancements in the theory of existence and uniqueness of solutions to the FDE (1). In particular, it was found the existence of a solution to (1) is strongly related to the existence of a Hopf-Leray weak solution for the Cauchy problem of the Navier–Stokes equations, which is a well-established result for both two- and three-dimensional Navier-Stokes equations [25–28] (see also [29], Theorem 3.1). A Hopf-Leray solution is a specific class of weak solutions to the Navier-Stokes equations (3) defined in an appropriate function space (see, e.g., [25], Sec. 3), for an initial condition  $\mathbf{u}_0$  that is divergence-free in the sense of distributions. Additionally, Hopf-Leray solutions satisfy the energy inequality

$$\|\mathbf{u}(\mathbf{x}, t)\|_{L^2(\Omega)}^2 + 2\nu \int_0^t \|\nabla \mathbf{u}(\mathbf{x}, s)\|_{L^2(\Omega)}^2 ds \leq \|\mathbf{u}_0\|_{L^2(\Omega)}^2.$$

It can be shown that if there exists a Hopf-Leray solution to the Navier-Stokes equations, then there exists a statistical solution to the Hopf-Navier-Stokes equation (1) (see [30], Sec. 5 in

Ch. 4). A similar results was obtained by Foias in [8], p. 254 for initial velocity conditions described by probability measures with finite second moments.

Regarding uniqueness of the solution to the Hopf-Navier-Stokes equation (1), it turns out that this is again connected to the uniqueness of Hopf-Leray weak solutions to the Navier-Stokes equation. Indeed, Vishik and Fursikov proved in [30], Theorem 6.1 that if there exists a unique Hopf-Leray solution to the Navier-Stokes equation, then any space-time statistical solution of the Hopf-Navier-Stokes equation is uniquely determined by the initial probability measure (see also [8], pp. 323–344). In two spatial dimensions it is well known that there exists a unique global Hopf-Leray solution, and therefore a unique statistical solution. The proof was formalized by Gishlarkaev in [31] for the Hopf-Navier-Stokes equation using techniques developed in [30]. The uniqueness of the Hopf-Leray solution for the three-dimensional Navier-Stokes equations is still an open problem, and a rather active area of research. For example, it can be shown that the Hopf-Leray solution is unique within at least a short-time integration period if we choose the initial condition in nonconventional function spaces [26–28,32,33]. Also, the Hopf-Leray solution is unique and global in time if we choose the initial data small enough [28,34]. Recently, Galdi proved [35] that very weak solutions to the Cauchy problem for the Navier-Stokes equations must be Hopf-Leray solutions if their initial data are solenoidal with finite kinetic energy. A smooth (mild or strong) solution of the Navier-Stokes equations is of course also a Hopf-Leray (weak) solution. More precisely, it can be shown that a mild solution to Navier-Stokes in  $H^s$  agrees with a weak Hopf-Leray solution almost everywhere in  $[0, T^*)$ . This result, which belongs to the so-called weak-strong uniqueness methods [36], implies that weak Hopf-Leray solutions are unique as long as a mild (or a strong) solution exists. In particular, Leray-Hopf solutions are unique whenever they are regular enough to be strong solutions. Once the strong solution is integrated past  $t \sim T^*$  (maximum Cauchy development), there is no further guarantee of uniqueness [28,37]. We also recall that if the energy inequality that characterizes Hopf-Leray weak solutions is dropped, then it is possible to construct multiple weak solutions of the Navier-Stokes equations with finite kinetic energy [38]. On the other hand, weak solutions obeying the energy inequality are necessarily unique and smooth if they lie in  $L^p([0, T]) \otimes L^q(\Omega)$  with  $2/p + 3/q = 1$  and  $q > 3$ . These conditions are known as Prodi-Serrin-Ladyzhenskaya conditions, and they have been recently generalized in various ways (see [26,39,40]).

Regarding the existence and uniqueness of solutions to Hopf characteristic functional equations corresponding to PDEs other than Navier-Stokes, this can be established on a case-by-case basis by generalizing the results of Theorem 1.1 and Theorem 1.2 in [30], Chapter 5.

### III. APPROXIMATION OF FDEs BY HIGH-DIMENSIONAL PDEs

Consider a well-posed initial/boundary value problem for an FDE, i.e., a problem that admits a unique solution in some function space as discussed in Sec. II. How do we compute

the solution? This is a longstanding problem in mathematical physics and a rather new research area of computational mathematics.

The FDEs (1) and (6) can be seen as PDEs in an infinite number of independent variables. Such infinite-dimensional PDEs may be approximated by PDEs in a finite (though possibly extremely large) number of variables using the functional analytic methods described in [1,2,18,19]. For instance, we have shown in [1,2] that Eq. (1) can be approximated by the high-dimensional linear PDE

$$\frac{\partial \phi}{\partial t} = \sum_{p=1}^n a_p \left( v \sum_{k=1}^n B_{pk} \frac{\partial \phi}{\partial a_k} + i \sum_{j,k=1}^n A_{pj k} \frac{\partial^2 \phi}{\partial a_k \partial a_j} \right), \quad (10)$$

where

$$\begin{aligned} a_p &= \int_{\Omega} \boldsymbol{\theta} \cdot \boldsymbol{\Gamma}_p d\mathbf{x}, & B_{pk} &= \int_{\Omega} \boldsymbol{\Gamma}_p \cdot \nabla^2 \boldsymbol{\Gamma}_k d\mathbf{x}, \\ A_{pj k} &= \int_{\Omega} \boldsymbol{\Gamma}_p \cdot [(\boldsymbol{\Gamma}_k \cdot \nabla) \boldsymbol{\Gamma}_j] d\mathbf{x}, \end{aligned} \quad (11)$$

$\{\boldsymbol{\Gamma}_1(\mathbf{x}), \dots, \boldsymbol{\Gamma}_n(\mathbf{x})\}$  is a divergence-free basis, and  $\phi(a_1, \dots, a_n, t)$  is the characteristic function approximating the characteristic functional  $\Phi([\boldsymbol{\theta}], t)$  in the following sense:

$$\phi(a_1, \dots, a_n, t) = \Phi([P_n \boldsymbol{\theta}], t), \quad (12)$$

where  $P_n$  is an orthogonal projection onto  $\{\boldsymbol{\Gamma}_1, \dots, \boldsymbol{\Gamma}_n\}$ . The divergence-free basis  $\{\boldsymbol{\Gamma}_1, \dots, \boldsymbol{\Gamma}_n\}$  can be constructed in terms of div-free wavelets [41,42], radial basis functions [43], trigonometric polynomials [44], or eigenvalue problems for the Stokes operator with appropriate boundary conditions [25]. Approximating the FDE (1) using the PDE (10) bears a resemblance, in a certain aspect, to what is known as the “method of lines” for discretizing a nonlinear partial differential equation into a high-dimensional system of nonlinear ordinary differential equations (ODEs). However, in the context of FDEs, the “lines” are determined by a hyper-dimensional PDE instead of a system of ODEs.

In [2], Theorem 7.1 we proved that if we choose the test function  $\boldsymbol{\theta}(\mathbf{x})$  in a Sobolev sphere  $\mathcal{S}(\Omega)$  of  $H^1(\Omega)$ -div functions [which is a compact subset of  $L^2(\Omega)$ -div], then  $\phi$  converges uniformly to the characteristic functional  $\Phi$  as the number of independent variables  $n$  goes to infinity:

$$\lim_{n \rightarrow \infty} \sup_{\substack{\boldsymbol{\theta} \in \mathcal{S}(\Omega) \\ t \in [0, T]}} |\phi(a_1, \dots, a_n, t) - \Phi([\boldsymbol{\theta}], t)| = 0. \quad (13)$$

Moreover, convergence of the high-dimensional PDE to the FDE can be exponential. The result (13) leverages the Trotter-Kato approximation theorem [45], p. 210 for abstract evolution equations in Banach spaces [46].

Gangbo *et al.* [19] proved a similar result for the nonlinear functional HJB equation (6). Specifically, by evaluating the functional equation (6) on the Wasserstein space  $\mathcal{P}_2(\mathbb{R}^d)$  (space of probability densities in  $\mathbb{R}^d$  with finite second-order moment) with elements

$$\rho_n(\mathbf{x}) = \frac{1}{n} \sum_{k=1}^n \delta(\mathbf{x} - \mathbf{x}_k) \quad \mathbf{x}, \mathbf{x}_i \in \mathbb{R}^d, \quad (14)$$

then we can write the FDE (6) as a hyper-dimensional nonlinear PDE

$$\frac{\partial f}{\partial t} + \frac{1}{n} \sum_{k=1}^n \Psi \left( \mathbf{x}_i, \frac{\partial f}{\partial \mathbf{x}_k} \right) + j(\mathbf{x}_1, \dots, \mathbf{x}_n) = 0, \quad (15)$$

where  $f(\mathbf{x}_1, \dots, \mathbf{x}_n, t) = F([\rho_n], t)$  (see [19], Eq. (1.2)). Moreover, if we choose the empirical measure (14) in a bounded subset  $B$  of the Wasserstein space  $\mathcal{P}_2(\mathbb{R}^d)$ , then  $f(\mathbf{x}_1, \dots, \mathbf{x}_n, t)$  converges uniformly to the (unique) solution of (6) as  $n$  goes to infinity ([19], Theorem 1.2):

$$\lim_{n \rightarrow \infty} \sup_{\substack{\rho_n \in B \\ t \in [0, T]}} |f(\mathbf{x}_1, \dots, \mathbf{x}_n, t) - F([\rho_n], t)| = 0. \quad (16)$$

The boundedness assumption of  $B$  is essential for convergence. Similarly, the compactness assumption of the function space  $S$  in (13) is essential for convergence (see [2], Theorems 7.1 and 8.3).

To solve high-dimensional PDEs such as (10) and (15) numerically, we need a computational paradigm for PDEs that can handle tens, hundreds, or thousands of independent variables efficiently. Such computational paradigm is discussed in the next section.

#### IV. TENSOR APPROXIMATION OF HIGH-DIMENSIONAL PDEs

We have seen in Sec. III that FDEs can be approximated by high-dimensional PDEs of the form

$$\frac{\partial f(\mathbf{x}, t)}{\partial t} = \mathcal{G}(f(\mathbf{x}, t), \mathbf{x}), \quad f(\mathbf{x}, 0) = f_0(\mathbf{x}), \quad (17)$$

where  $f : D \times [0, T] \rightarrow \mathbb{R}$  is an  $n$ -dimensional time-dependent scalar field defined on the domain  $D \subseteq \mathbb{R}^n$ ,  $T$  is the period of integration, and  $\mathcal{G}$  is a nonlinear operator which may depend on the variables  $\mathbf{x} = (x_1, \dots, x_n) \in D$  and may incorporate boundary conditions. For simplicity, we assume that the domain  $D$  is a Cartesian product of  $n$  one-dimensional domains  $D_i$

$$D = D_1 \times \dots \times D_n. \quad (18)$$

This factorization holds, e.g., for  $n$ -dimensional hyper-cubes, or for  $n$ -dimensional tori (topologically equivalent to hyper-cubes with periodic boundary conditions). We also assume that  $f$  is an element of a Hilbert space  $H(D; [0, T])$ . In these hypotheses, we can leverage the isomorphism

$$H(D; [0, T]) \cong H([0, T]) \otimes H(D_1) \otimes \dots \otimes H(D_n) \quad (19)$$

and represent the solution of (17) as

$$f(\mathbf{x}, t) \approx \sum_{i_1=1}^{m_1} \dots \sum_{i_n=1}^{m_n} f_{i_1 \dots i_n}(t) h_{i_1}(x_1) \dots h_{i_n}(x_n), \quad (20)$$

where  $h_j(x_j)$  are one-dimensional orthonormal basis functions of  $H(D_i)$ . Substituting (20) into (17) and projecting onto an appropriate finite-dimensional subspace of  $H(\Omega)$  yields the

semidiscrete form

$$\frac{d\mathbf{f}}{dt} = \mathbf{G}(\mathbf{f}), \quad \mathbf{f}(0) = \mathbf{f}_0, \quad (21)$$

where  $\mathbf{f} : [0, T] \rightarrow \mathbb{R}^{m_1 \times m_2 \times \dots \times m_n}$  is a multivariate array with coefficients  $f_{i_1 \dots i_n}(t)$ , and  $\mathbf{G}$  is the finite-dimensional representation of the nonlinear operator  $\mathcal{G}$ . The number of degrees of freedom associated with the solution to the Cauchy problem (21) is  $N_{\text{dof}} = m_1 m_2 \dots m_n$  at each time  $t \geq 0$ , which can be extremely large even for moderately small dimension  $n$ . For instance, the solution of the Boltzmann-BGK equation on a six-dimensional ( $n = 6$ ) flat torus [47,48] with  $m_i = 128$  basis functions in each position and momentum variable yields  $N_{\text{dof}} = 128^6 = 4\,398\,046\,511\,104$  degrees of freedom at each time  $t$ . This requires approximately 35.18 terabytes per temporal snapshot if we store the solution tensor  $\mathbf{f}$  in a double precision IEEE 754 floating point format. Several general-purpose algorithms have been developed to mitigate such an exponential growth of degrees of freedom, the computational cost, and the memory requirements. These algorithms include, e.g., sparse collocation methods [49–51] and techniques based on deep neural networks [52,53].

In a parallel research effort that has its roots in quantum field theory and quantum entanglement, researchers have recently developed a new generation of algorithms based on tensor networks and low-rank tensor techniques to compute the solution of high-dimensional PDEs [54–58]. A tensor network is a factorization of an entangled object such as a multivariate function or an operator into simpler objects, e.g., low-dimensional functions or separable operators, which are amenable to efficient representation and computation. A tensor network can be visualized in terms of graphs (see Fig. 1). The vast majority of tensor algorithms currently available to approximate functions, operators and PDEs on tensor spaces is based on canonical polyadic (CP) decompositions [47,56,58,60], Tucker tensors, or tensors corresponding to binary trees such as tensor train (TT) [61–63] and hierarchical Tucker (HT) tensors [64–67]. A compelling reason for using binary tensor trees is that they allow us to construct the tensor expansion by leveraging the spectral theory for linear operators, in particular the hierarchical Schmidt decomposition [61,68–71].

In particular, if we represent  $\mathbf{f}(t)$  in (21) using the tensor train (TT) format discussed in the Appendix A at a fixed time  $t$ , we obtain

$$\begin{aligned} f[i_1, i_2, \dots, i_n] &= \sum_{j_1=1}^{r_1} \dots \sum_{j_{n-1}=1}^{r_{n-1}} \mathbf{C}_1[1, i_1, j_1] \\ &\quad \times \mathbf{C}_2[j_1, i_2, j_2] \dots \mathbf{C}_d[j_{n-1}, i_n, 1], \quad (22) \end{aligned}$$

where  $\mathbf{r} = (r_1, \dots, r_{n-1})$  denotes the multilinear rank. Hence, to represent  $\mathbf{f}$  in a TT format we just need to store the so-called tensor cores  $\mathbf{C}_i$ . Similarly, to perform arithmetic operations on a TT tensor, we manipulate the values stored in the cores. To apply a distributed memory parallelization of this data format (see Appendix A 2), we separate the cores across many compute units along the  $i_1, i_2, \dots, i_n$  indices. This results in a one-dimensional domain decomposition along the second tensor index for each core.



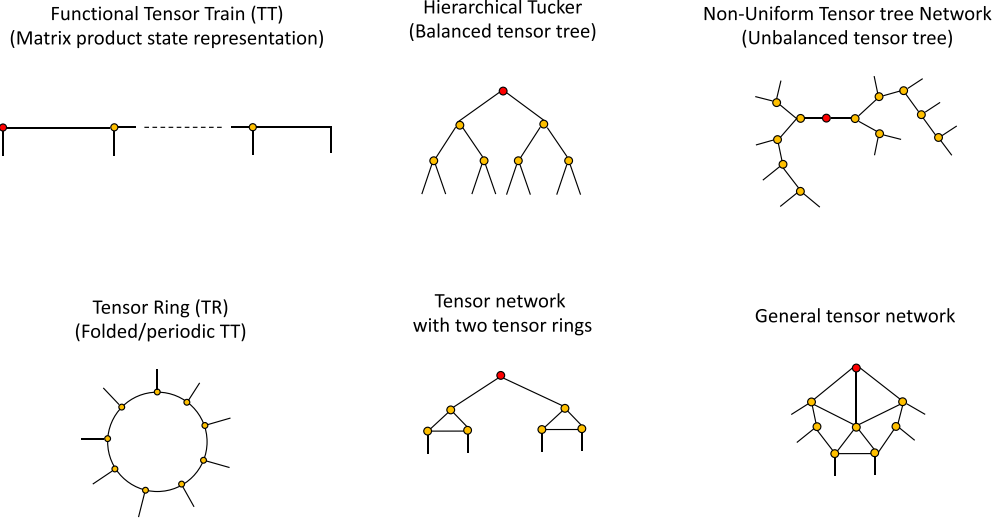


FIG. 1. Examples of tensor networks. The vertices represent tensor modes (functions) used in the decomposition. The edges connecting to vertices represent summation over an index (contraction) between two modes. The free edges represent input variables  $x_j$  ( $j = 1, \dots, n$ ).

### A. Step-truncation tensor methods

A new class of algorithms to integrate (21) on a low-rank tensor manifold was recently proposed in [20,21]. These algorithms are known as *step-truncation methods*, and they are based on integrating the solution  $f(t)$  of the ODE (21) off the tensor manifold for a short time using any conventional explicit time-stepping scheme, and then mapping it back onto the manifold using a tensor truncation operation. To briefly describe these methods, let us discretize the ODE (21) in time with a one-step method on an evenly-spaced temporal grid as

$$f_{k+1} = \Psi_{\Delta t}(\mathbf{G}, f_k), \quad f_0 = f(0), \quad (23)$$

where  $f_k$  denotes an approximation of  $f(k\Delta t)$  for  $k = 0, 1, \dots$ , and  $\Psi_{\Delta t}$  is an increment function. To obtain a step-truncation integrator, we simply apply a truncation operator  $\mathfrak{T}_s(\cdot)$ , i.e., a nonlinear projection onto a tensor manifold  $\mathcal{M}_s$  of HT (or TT) tensors with multilinear rank  $s$  [67], to the scheme (23) (see Fig. 2). This yields

$$f_{k+1} = \mathfrak{T}_s[\Psi_{\Delta t}(\mathbf{G}, f_k)]. \quad (24)$$

The need for tensor rank-reduction when iterating (23) can be easily understood by noting that tensor operations such as the application of an operator to a tensor and the addition between two tensors naturally increase tensor rank [72].

We now present the rank-adaptive step-truncation algorithms used here to integrate FDEs on tensor manifolds. The first one is a truncated version of the Euler forward scheme,

$$f_{k+1} = \mathfrak{T}_r[f_k + \Delta t \mathfrak{T}_s[\mathbf{G}(f_k)]]. \quad (25)$$

We have shown that this scheme is convergent to first-order in  $\Delta t$  provided the rank  $r$  is properly updated at each time step (see [20] for details). The second step-truncation scheme is derived from the explicit midpoint rule, and it is defined as

$$f_{k+1} = \mathfrak{T}_\alpha \left[ f_k + \Delta t \mathfrak{T}_\beta \left[ \mathbf{G} \left( f_k + \frac{\Delta t}{2} \mathfrak{T}_\gamma(\mathbf{G}(f_k)) \right) \right] \right], \quad (26)$$

where  $\alpha$ ,  $\beta$ , and  $\gamma$  are once again selected adaptively as time integration advances.

Both (25) and (26) are *explicit* step-truncation methods. These schemes are very simple to implement and have proven successful in integrating initial value problems for a variety of PDEs [20]. However, the combination of dimensionality, nonlinearity, and stiffness may introduce time-step restrictions which could make explicit time integration on tensor manifolds computationally infeasible. To overcome this problem, we recently developed a class of *implicit* rank-adaptive step-truncation algorithms for temporal integration PDEs on tensor manifolds [21]. These algorithms are based on an inexact Newton's method with tensor train GMRES iterations [59] to

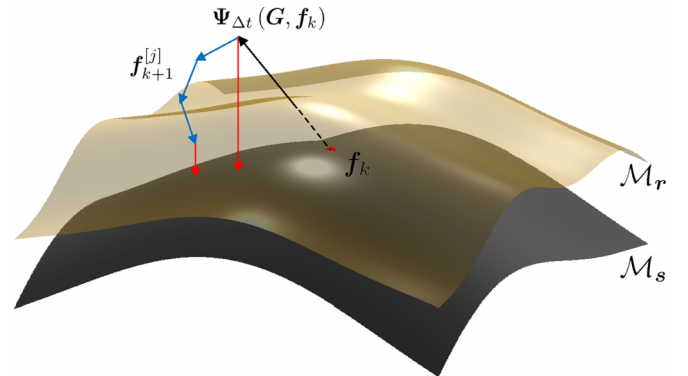


FIG. 2. Sketch of implicit and explicit step-truncation integration methods. Given a tensor  $f_k$  with multilinear rank  $s$  on the tensor manifold  $\mathcal{M}_s$ , we first perform an explicit time step with any conventional time-stepping scheme. The explicit step-truncation integrator then projects  $\Psi_{\Delta t}(\mathbf{G}, f_k)$  to a tensor manifold with rank  $s$ . The multilinear rank  $s$  is chosen adaptively based on desired accuracy and stability constraints [20]. On the other hand, the implicit step-truncation method takes  $\Psi_{\Delta t}(\mathbf{G}, f_k)$  as input and generates a sequence of fixed-point iterates  $f^{[j]}$  shown as dots connected with blue lines. The last iterate is then projected onto a low-rank tensor manifold, illustrated here also as a red line landing on  $\mathcal{M}_s$ . This operation is equivalent to the compression step in the HT/TT-GMRES algorithm described in [59].

solve the algebraic equation arising from time discretization on the tensor manifold.

To describe these methods, let us consider the standard Euler backward scheme

$$\mathbf{f}_{k+1} = \mathbf{f}_k + \Delta t \mathbf{G}(\mathbf{f}_{k+1}), \quad (27)$$

and the associated root-finding problem

$$\mathbf{H}_k(\mathbf{f}_{k+1}) = \mathbf{f}_{k+1} - \mathbf{f}_k - \Delta t \mathbf{G}(\mathbf{f}_{k+1}) = \mathbf{0}. \quad (28)$$

If  $\mathbf{G}$  is linear, e.g., for PDEs of the form (10), this reduces to a linear inversion problem

$$(\mathbf{I} - \Delta t \mathbf{G})\mathbf{f}_{k+1} = \mathbf{f}_k. \quad (29)$$

To solve the linear system (29) in a tensor format, we apply the TT-GMRES method proposed by Dolgov in [59]. For the implicit midpoint method, the logic is identical. We apply the above steps to the linear system

$$(\mathbf{I} - \frac{1}{2} \Delta t \mathbf{G})\mathbf{f}_{k+1} = (\mathbf{I} + \frac{1}{2} \Delta t \mathbf{G})\mathbf{f}_k. \quad (30)$$

For the fully nonlinear case, one may couple the TT-GMRES iteration to an inexact Newton method and retain all convergence properties (see [21], Appendix A for further details). In [21] we have recently show that under mild conditions on the tensor truncation error, the implicit step-truncation Euler and implicit step-truncation midpoint converge, respectively, with order one and order two in  $\Delta t$ .

### V. BURGERS-HOPF FDE

Consider Burger’s equation on the unit circle  $\Omega = [0, 2\pi]$ ,

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \gamma \frac{\partial^2 u}{\partial x^2} + R(u), \quad (31)$$

with a reaction term  $R(u) = \alpha \sin(\pi u)$  and random ( $2\pi$ -periodic) initial condition  $u(x, 0)$ .

In our simulations we set  $\alpha = 10$ . Let

$$\Phi([\theta(x)], t) = \mathbb{E} \left\{ \exp \left[ i \int_0^{2\pi} u(x, t) \theta(x) dx \right] \right\} \quad (32)$$

be the characteristic functional of the stochastic solution to (31). It is straightforward to show that  $\Phi([\theta(x)], t)$  satisfies the following Burgers-Hopf FDE:

$$\begin{aligned} \frac{\partial \Phi([\theta], t)}{\partial t} &= \int_0^{2\pi} \left[ \frac{i}{2} \frac{\partial}{\partial x} \frac{\delta^2 \Phi([\theta], t)}{\delta \theta(x)^2} + \gamma \frac{\partial^2}{\partial x^2} \frac{\delta \Phi([\theta], t)}{\delta \theta(x)} \right. \\ &\quad \left. + \alpha \sum_{k=1}^{\infty} \frac{(-\pi)^k}{(2k+1)! i^{2k}} \frac{\delta^{2k+1} \Phi([\theta], t)}{\delta \theta(x)^{2k+1}} \right] \theta(x) dx, \end{aligned} \quad (33)$$

which admits a unique solution due to the uniqueness of the solution to the weak form of the Burgers equation (see Sec. II).

Approximating the FDE (33) in terms of a high-dimensional PDE of the form of (10) and taking the inverse Fourier transform (in the sense of distributions) yield the

Liouville-type linear hyperbolic conservation law

$$\begin{aligned} \frac{\partial p}{\partial t} &= - \sum_{i=1}^N \frac{\partial}{\partial u_j} \left[ \sum_{j=1}^N (-u_i D_{ij}^{(1)} u_j \right. \\ &\quad \left. + \delta_{ij} R(u_j) + \gamma D_{ij}^{(2)} u_j \right) p \right], \end{aligned} \quad (34)$$

where  $\delta_{ij}$  is the Kronecker delta and  $p(u_1, u_2, \dots, u_N, t)$  is the joint probability density function of the solution to (31) at all evenly spaced grid points  $x_j = 2\pi(j-1)/N$  ( $j = 1, \dots, N$ ), i.e.,  $u_j = u(x_j, t)$ .

In Eq. (34),  $D_{ij}^{(1)}$  and  $D_{ij}^{(2)}$  are differentiation matrices. In our numerical experiments, we use the second-order finite difference matrix on a periodic domain. From here, it is straightforward to write a step-truncation tensor method to solve the high-dimensional PDE (34).

However, this may not yield an accurate scheme due to the properties of the solution. In fact, it is well known that PDF equations of the form (34) can develop shocks [73] or can have solutions converging to Dirac delta functions if the time asymptotic solution is deterministic. In these cases, it is convenient to first transform the kinetic equation into a cumulative distribution function (CDF) equation via an integral transform [74], and then solve such CDF equation. This allows us to transform PDF shocks into CDF ramps and PDF Dirac deltas into CDF shocks. In other words, the CDF equations produces solutions with features that are well known to the numerical analysis community (shocks, ramps, and solutions with range bounded in  $[0,1]$ ) and therefore can be handled with numerical schemes for hyperbolic conservation laws [75].

By integrating Eq. (34) with respect to the phase variables  $\{u_1, \dots, u_N\}$  we obtain the following CDF equation:

$$\begin{aligned} \frac{\partial F}{\partial t} &= \sum_{i,j=1}^N (u_i D_{ij}^{(1)} u_j - \gamma D_{ij}^{(2)} u_j - \delta_{ij} R(u_j)) \frac{\partial F}{\partial u_i} \\ &\quad - \sum_{\substack{i,j=1 \\ i \neq j}}^N (D_{ij}^{(1)} u_i - \gamma D_{ij}^{(2)}) \int_{-\infty}^{u_j} \frac{\partial F}{\partial u_i} du_j \\ &\quad - \alpha \sum_{j=1}^N \sin(\pi u_j) \frac{\partial F}{\partial u_j}, \end{aligned} \quad (35)$$

where

$$F(u_1, \dots, u_n, t) = \int_{-\infty}^{u_1} \dots \int_{-\infty}^{u_n} p(v_1, \dots, v_n, t) dv_1 \dots dv_n. \quad (36)$$

With the CDF  $F(u_1, \dots, u_N, t)$  available it is straightforward to compute the PDF

$$p(u_1, \dots, u_N, t) = \frac{\partial^n F(u_1, \dots, u_N, t)}{\partial u_1 \dots \partial u_N}. \quad (37)$$

To apply the proposed step-truncation tensor methods to Eq. (35), we discretize the phase space in terms of a  $N$ -dimensional hypercube centered at the origin which covers the support of  $p(u_1, u_2, \dots, u_N, t)$ . For the specific application at hand such a hypercube is  $\Sigma = [-1.3, 1.3]^N$ . On the boundary of  $\Sigma$ , it is straightforward to show that the derivative of  $F$

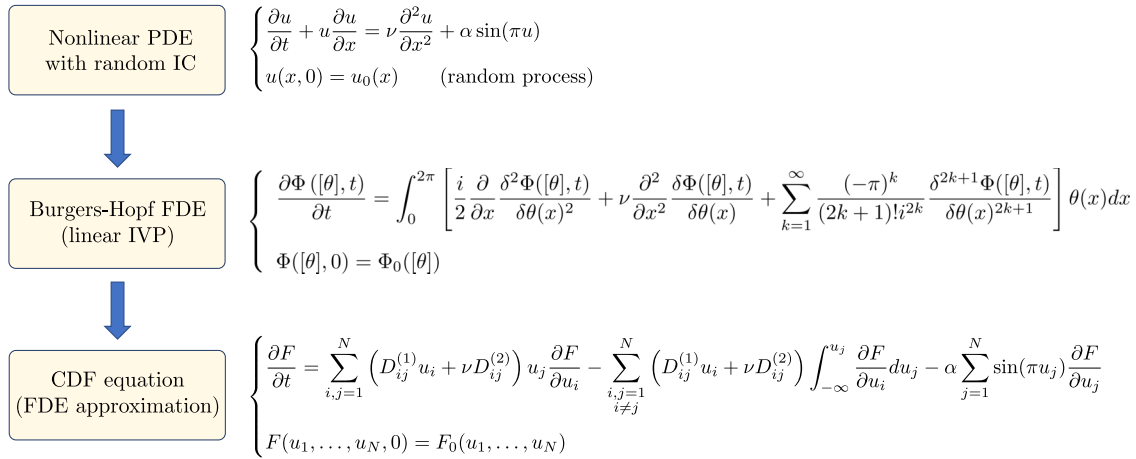


FIG. 3. Sketch of the logical flow to transform a random nonlinear initial value problem (IVP) for the Burgers equation into the (linear) Burgers-Hopf FDE, which is linear. The Burgers-Hopf FDE is subsequently approximated using the methods outlined in Sec. III. This yields an  $N$ -dimensional characteristic function equation of the form (10). By taking the inverse Fourier transform of such characteristic function equation and integrating it with respect to the phase variable we obtain the  $N$ -dimensional CDF equation shown above. The CDF equation is then solved using the proposed step-truncation tensor methods.

normal to the hypercube boundary is zero. Therefore we may apply outflow boundary conditions, i.e., set  $\partial F / \partial u_j = 0$  at the boundary of  $\Sigma$ . We discretize each variable  $u_i$  in  $\Sigma$  on an evenly spaced grid with  $n_i = 64$  points. Also, we approximate the integrals in (35) using the trapezoidal rule, and the partial derivatives with centered second-order finite differences. For the initial condition, we set the CDF to be a product of  $N$  zero-mean Gaussian CDFs with standard deviation  $\sigma = 0.25$ , i.e.,

$$F(u_1, \dots, u_N, 0) = \prod_{k=1}^N g(u_k), \quad (38)$$

where

$$g(u) = \frac{1}{2} \left[ 1 + \operatorname{erf} \left( \frac{u}{\sigma \sqrt{2}} \right) \right] \quad (39)$$

and  $\operatorname{erf}(x)$  is the standard error function.

### Numerical results

To solve the high-dimensional CDF equation (35) approximating the Burgers-Hopf FDE (33) we developed a high-performance (parallel) tensor code implementing the step truncation tensor methods discussed in Sec. IV A.

We first perform a numerical study to verify temporal accuracy of order one and order two of the proposed step-truncation tensor methods applied to the high-dimensional CDF equation (35) (see Fig. 3). To stabilize explicit step-truncation methods, we add a numerical diffusion term proportional to the round-off error in  $\Delta t$  to the right-hand side of (35), in a similar manner to the Lax-Wendroff method [76]. To guarantee that we are accurately capturing second- and first-order errors in time, we must ensure that the semidiscrete PDE we are solving for our reference solution matches that of our step-truncation integrators. To this end, we compute the local truncation errors of each scheme by computing its difference with a Richardson extrapolation (see [77], II.4) of it to one order higher; i.e., we take two steps of size  $\Delta t/2$  and

combine it with a step of size  $\Delta t$  to create a more accurate estimate for the purposes of comparing it to a single step of size  $\Delta t$ . To this end, we calculate the local truncation errors by computing the difference between the prediction of each scheme and a Richardson extrapolation of one order higher (as outlined in [77], II.4). In other words, we take two steps of size  $\Delta t/2$  and integrate them with a step of size  $\Delta t$  to generate a more precise estimation for comparison with a single step of size  $\Delta t$ . The results are shown in Fig. 4. It is seen that the explicit/implicit Euler and explicit/implicit midpoint step-truncation integrators have accuracy of order one and order two, respectively. To quantify the errors, we constructed a benchmark CDF via Monte Carlo simulation. In practice, we sampled  $5 \times 10^6$  initial conditions  $u(x, 0)$  from the Gaussian distribution described above, computed the solution  $u(x, t)$  of (31) using the Fourier pseudospectral method [78], and then used a kernel density estimator (KDE) [79] to obtain the one-point and the two-points CDFs. This allows us to study convergence of the solutions to the CDF equation (35) as we increase the dimension  $N$  of the PDE. This convergence study is *crucial* for establishing convergence of the solution of the CDF equation (35) to the solution of the Burgers-Hopf FDE. For this analysis, we selected the explicit step-truncation midpoint tensor method as the temporal integrator, due to its favorable performance and ease of implementation.

In Fig. 5 we plot the joint CDF of  $u(0, t)$  and  $u(\pi, t)$  at  $t = \{0, 0.04, 0.08, 0.12\}$  computed with Monte Carlo, and the proposed step-truncation midpoint tensor method applied to a 20-dimensional ( $N = 20$ ) CDF equation (35). Clearly there is visual agreement between the results from the tensor simulation and the results from Monte Carlo simulation. In Fig. 6 we demonstrate convergence of the solution to the CDF equation (35), the Burgers-Hopf FDE, as we increase the dimension  $N$  from 8 to 20. The error plot in Fig. 6 represents the  $L^2$  error between the joint CDFs shown in Fig. 5. Run time increases considerably with dimension though, especially for moderately high solution ranks. For example, once rank surpasses 100, the  $N = 20$  case requires approximately 45 minutes per

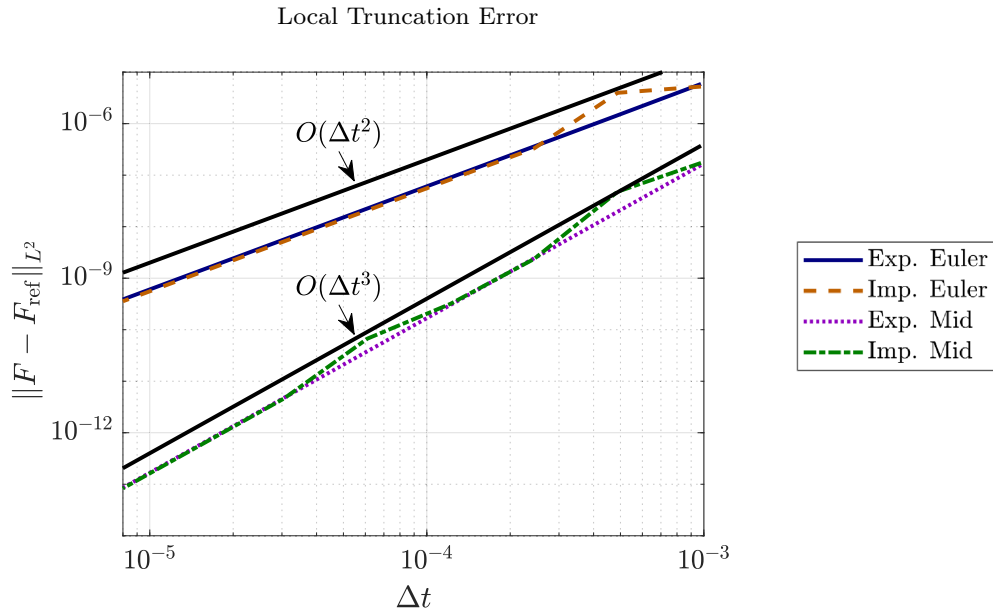


FIG. 4. Local truncation errors [calculated as  $O(\Delta t^{p+1})$  for an order  $p$  method] of the proposed step-truncation tensor methods. These errors are computed by comparing one time step of step-truncation method with its Richardson extrapolation. It is seen that explicit/implicit Euler and explicit/implicit midpoint step-truncation methods have accuracy of order one and order two, respectively.

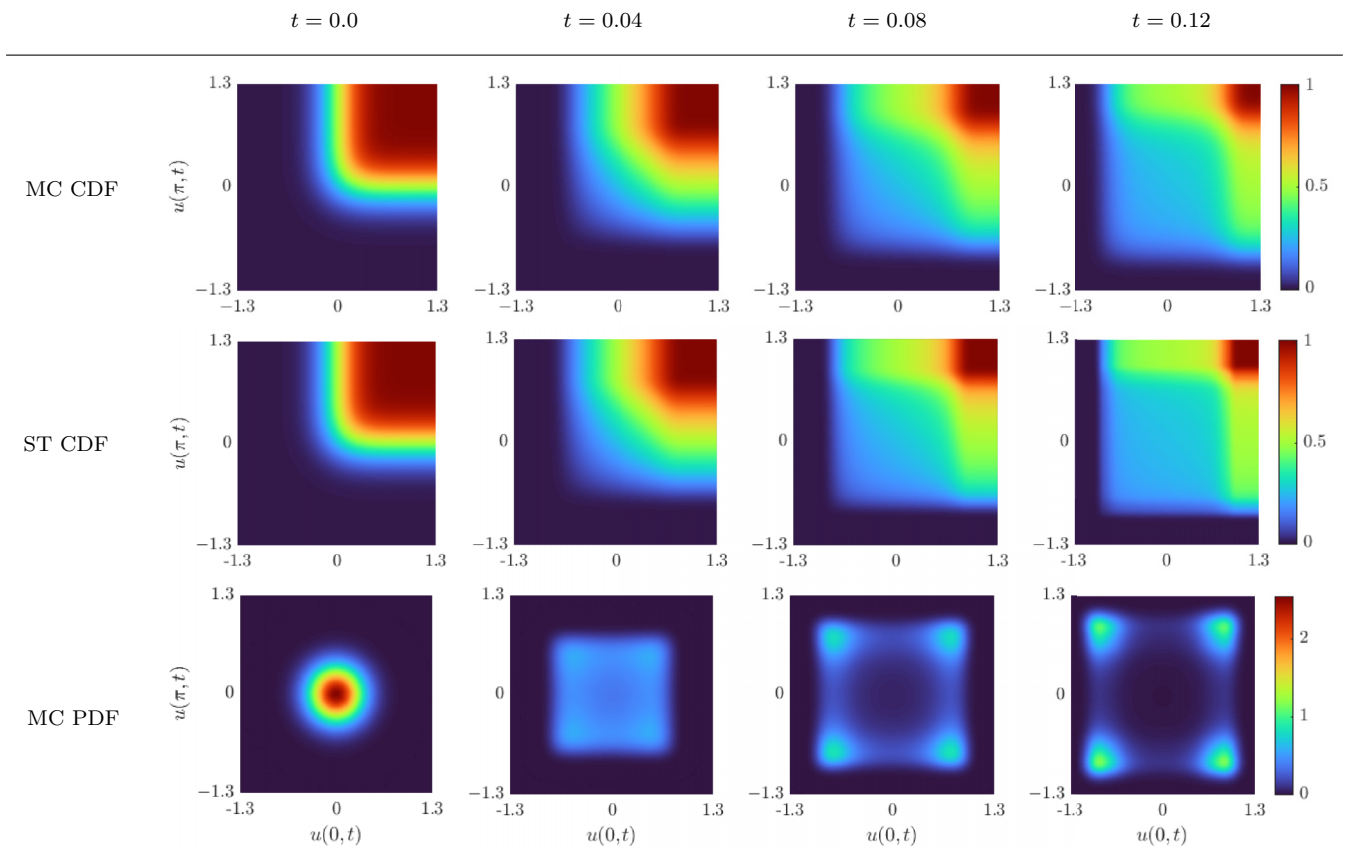


FIG. 5. Two joint CDF of  $u(0, t)$  and  $u(\pi, t)$ . The CDF is computed by generating numerical solutions to (35) for  $N = 20$  using the proposed step-truncation tensor methods, and then marginalizing the solution in the remaining 18 variables. We also show a Monte Carlo estimate of the joint CDF obtained by sampling  $5 \times 10^6$  solutions to (31).



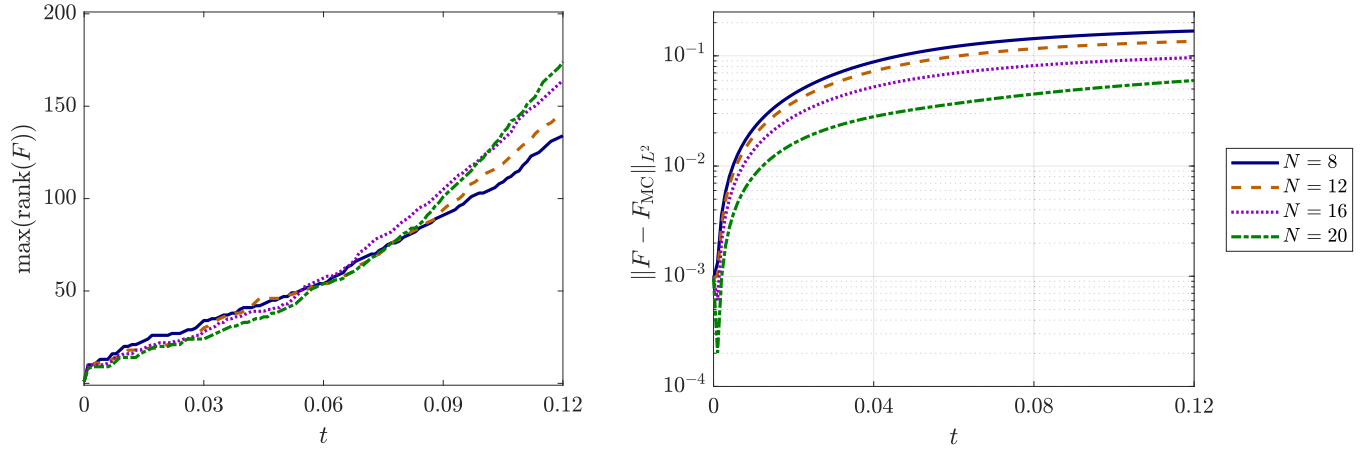


FIG. 6. Left: Highest rank of the tensor train cores for tensor solutions of the CDF to Eq. (35) computed with the explicit step-truncation midpoint method for dimension  $N = \{8, 12, 16, 20\}$ . Right: Convergence of the solution to the CDF equation (35) the Burgers-Hopf FDE as we increase the dimension  $N$  from 8 to 20. The error plot represents represents the  $L^2$  error between the joint CDFs shown in Fig. 5.

time step on an Intel i9-7980xe workstation. The storage of the CDF tensor solution in 20 dimensions requires approximately 690 megabytes per temporal snapshot for tensor ranks of the order of 150. This is a significant compression of a multidimensional double precision floating point array of size  $64^{20}$ , which would normally require approximately  $10^{22}$  petabytes. That is to say that we capture  $O(10^{-2})$  accuracy of the data while achieving a data compression ratio of  $1.44 \times 10^{26}\%$  and data space savings of approximately 100%. Of course, 690 megabytes is not negligible on practical computing systems. It is essentially nothing compared to the decompressed data though. In Fig. 7 we compare the CDF of  $u(0, t)$  computed by solving the CDF equation (35) with  $N = \{8, 12, 16, 20\}$  and then marginalizing, with a benchmark CDF obtained by Monte Carlo simulation of (31). It is seen that as we increase the dimension  $N$  the marginal of the CDF tensor solution approaches the Monte Carlo benchmark.

While our numerical tensor schemes are accurate and provably convergent, they may not preserve important properties of the CDF solution, such as positivity, monotonicity, and range in  $[0, 1]$ . The development of a structure-preserving tensor integration schemes is indeed a rather unexplored research area. One possibility is to enforce structure at the level of the tensor truncation operation, i.e., perform rounding conditional to some required property. For instance, if we are interested in enforcing non-negativity in a step-truncation tensor scheme, then we can simply replace the truncation operator based on recursive QR decomposition (see the Appendix A), with the distributed non-negative tensor truncation discussed in [80]. Another approach to enforce structure can be built directly at the level of the tensor equations. This approach was recently proposed by Einkemmer *et al.* [81–83] in the context of Vlasov and Vlasov-Poisson kinetic equations. The resulting dynamical low-rank algorithm conserves mass, momentum, and energy.

## VI. SUMMARY

In this paper, we developed approximation theory and high-performance computational algorithms to solve functional differential equations (FDEs) on tensor manifolds. Our

approach involves initially approximating the given FDE with a high-dimensional partial differential equation (PDE) using the functional methods described in [1, 2, 19]. Subsequently, we compute the numerical solution of such PDE using parallel (rank-adaptive) step-truncation methods [20, 21]. This is an effective strategy for tackling the long-standing problem of computing numerical solutions to FDEs, opening avenues for further research and practical applications in computational mathematics and physics. We demonstrated the effectiveness of the proposed approach through its application to the Burgers-Hopf FDE, which governs the characteristic functional of the stochastic solution to the Burgers equation evolving from a random initial state. Our numerical results and convergence studies indicate that tensor methods, while computationally intensive, represent a tractable way to solve functional differential equations.

The code for material in this paper can be found at our GitHub repository [84].

## ACKNOWLEDGMENTS

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## APPENDIX A: TENSOR ALGORITHMS

In this Appendix, we describe the high-performance (parallel) tensor algorithms we developed to solve high-dimensional PDEs on tensor manifolds, in particular the CDF equation discussed in Sec. V. To this end, we begin with a brief review of the algebraic representation of the tensor train (TT) format [85].

### 1. Tensor train (TT) format

A tensor in  $\mathbf{f} \in \mathbb{R}^{n_1 \times n_2 \times \dots \times n_d}$  is in TT format if there is an array of positive integers (called the TT rank)  $\mathbf{r} = (r_0, r_1, r_2, \dots, r_{d-1}, r_d)$  with  $r_0 = 1 = r_d$  and a list of order three tensors (called the TT cores)  $\mathbf{C} = (\mathbf{C}_1, \mathbf{C}_2, \dots, \mathbf{C}_d)$

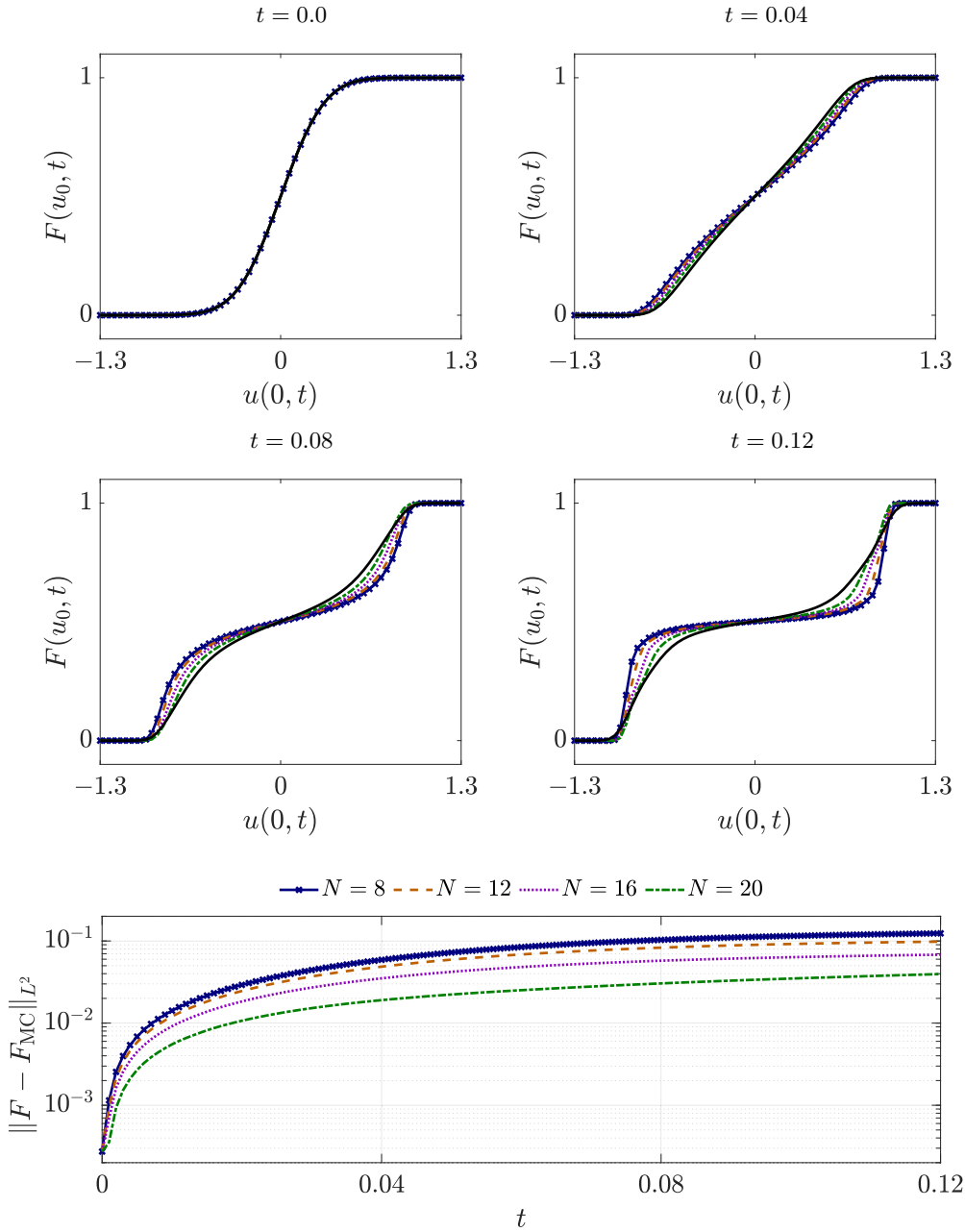


FIG. 7. CDF of  $u(0, t)$  computed by solving Eq. (35) with the proposed step-truncation tensor method. It is seen that as we increase the dimension  $N$  [number of independent variables in the CDF equation (35)] the tensor solution converges to the Monte Carlo benchmark (black continuous line).

where  $C_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$  such that the entries of  $f$  may be written as the iterated matrix product

$$f[i_1, i_2, \dots, i_d] = \sum_{j_1=1}^{r_1} \dots \sum_{j_{d-1}=1}^{r_{d-1}} C_1[1, i_1, j_1] \times C_2[j_1, i_2, j_2] \dots C_d[j_{d-1}, i_d, 1]. \quad (\text{A1})$$

Though rather involved at first glance, the above expression may be derived by writing a multivariate function series expansion by the method of separation of variables, rearranging the expression into a finite sequence of infinite matrix

products, truncating the series so that the matrix products are finite, then discretizing in space so that the multivariate function is sampled on a tensor product grid. From this perspective, it becomes apparent that the tensor train cores represent a two-dimensional array of functions of a single variable and the ranks are the number of functions present in a series expansion approximation. A more concrete exploration of this perspective is given in [61,86].

Due to the iterated matrix product definition of the format, it becomes apparent that a number of arithmetic operations may be represented in the format by producing a new TT tensor with different ranks. In particular if  $f, g$  have TT core

## ALGORITHM 1. Left orthogonalization.

**Data:** A tensor  $\mathbf{f}$  in TT format with cores  $(\mathbf{C}_1, \mathbf{C}_2, \dots, \mathbf{C}_d)$ .  
**Result:** A tensor  $\mathbf{g} = \mathbf{f}$  in TT format with left orthogonal cores.

Reserve memory for each core  $\mathbf{D}_c$  with sizes of  $\mathbf{C}_c$ .  
 $\mathbf{D}_1 = \mathbf{C}_1$   
**for**  $c = 1, 2, \dots, d-1$  **do**  
      $[\mathbf{Q}_c, \mathbf{R}_c] = QR(\mathcal{V}(\mathbf{D}_c))$   
      $\mathbf{H}_{c+1} = \mathbf{R}_c \mathcal{H}(\mathbf{C}_{c+1})$   
      $\mathbf{D}_c = \text{reshape}(\mathbf{Q}_c)$   
      $\mathbf{D}_{c+1} = \text{reshape}(\mathbf{H}_{c+1})$   
**end**  
 Set the cores of  $\mathbf{g}$  as  $(\mathbf{D}_1, \mathbf{D}_2, \dots, \mathbf{D}_d)$

lists  $\mathbf{C}, \mathbf{D}$ , then by a simple inductive argument, we have

$$\begin{aligned} & \mathbf{f}[i_1, i_2, \dots, i_d] + \mathbf{g}[i_1, i_2, \dots, i_d] \\ &= \sum_{j_1=1}^{r_1} \cdots \sum_{j_{d-1}=1}^{r_{d-1}} [\mathbf{C}_1[1, i_1, j_1] \mid \mathbf{D}_1[1, i_1, j_1] \\ & \quad \times \left[ \begin{array}{c|c} \mathbf{C}_2[j_1, i_2, j_2] & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_2[j_1, i_2, j_2] \end{array} \right] \cdots \left[ \begin{array}{c|c} \mathbf{C}_1[:, i_d, 1] \\ \mathbf{D}_1[:, i_d, 1] \end{array} \right]]. \end{aligned} \quad (\text{A2})$$

Thus the sum  $\mathbf{w} = \mathbf{f} + \mathbf{g}$  is a TT tensor with cores obtained by concatenating those of  $\mathbf{f}$  and  $\mathbf{g}$ . Scalar multiplication by a number  $\alpha$  is straightforward and can be implemented by just scaling any of the cores

$$\begin{aligned} \alpha \mathbf{f}[i_1, i_2, \dots, i_d] &= \sum_{j_1=1}^{r_1} \cdots \sum_{j_{d-1}=1}^{r_{d-1}} (\alpha \mathbf{C}_1[1, i_1, j_1] \\ & \quad \times \mathbf{C}_2[j_1, i_2, j_2] \cdots \mathbf{C}_d[j_{d-1}, i_d, 1]). \end{aligned} \quad (\text{A3})$$

In order to perform more sophisticated operations such as tensor truncations, we must frequently reshape the tensor cores into lower dimensional arrays. Two particularly useful reshaping are the horizontal flattening

$$\mathcal{H} : \mathbb{R}^{a \times b \times c} \longrightarrow \mathbb{R}^{a \times (bc)} \quad \mathbf{C}[i, j, k] \longmapsto \mathbf{H}[i, j + bk],$$

and the vertical flattening,

$$\mathcal{V} : \mathbb{R}^{a \times b \times c} \longrightarrow \mathbb{R}^{(ab) \times c} \quad \mathbf{C}[i, j, k] \longmapsto \mathbf{V}[i + aj, k].$$

The above maps are two-dimensional array analogs of the vectorization of a tensor, in which we have the coordinates listed as  $\mathbf{C}[i, j, k] = \mathbf{v}[i + aj + bk]$ . Note that when the entries of a tensor are stored contiguously in computer memory, no memory movement or copying needs to be done to interpret a tensor as its flattening or vectorization. To undo the flattening in an algorithm, we denote copying all the entries as  $\mathbf{C} = \text{reshape}(\mathbf{H})$  or  $\mathbf{C} = \text{reshape}(\mathbf{V})$ .

## ALGORITHM 2. Truncation of a TT Tensor.

**Data:** A tensor  $\mathbf{f}$  in TT format with cores  $(\mathbf{C}_1, \mathbf{C}_2, \dots, \mathbf{C}_d)$  and a desired accuracy  $\varepsilon$ .  
**Result:** A tensor  $\mathbf{g}$  so that  $\|\mathbf{g} - \mathbf{f}\| \leq \varepsilon$  in TT format with right orthogonal cores.

Reserve memory for each core  $\mathbf{D}_c$  with sizes of  $\mathbf{C}_c$ .  
 Set  $(\hat{\mathbf{C}}_1, \hat{\mathbf{C}}_2, \dots, \hat{\mathbf{C}}_d)$  as orthogonal by Alg. 1.  
 $\hat{\varepsilon} = \varepsilon / \sqrt{d-1}$   
 $\mathbf{D}_1 = \hat{\mathbf{C}}_1$   
**for**  $c = d, d-1, \dots, 2$  **do**  
      $[\mathbf{U}_c, \mathbf{\Sigma}_c, \mathbf{V}_c^\top] = \text{SVD}(\mathcal{H}(\mathbf{D}_c), \hat{\varepsilon})$  (Truncated SVD)  
      $\mathbf{H}_{c-1} = \mathcal{V}(\hat{\mathbf{C}}_{c-1}) \mathbf{U}_c \mathbf{\Sigma}_c$   
      $\mathbf{D}_c = \text{reshape}(\mathbf{U}_c)$   
      $\mathbf{D}_{c-1} = \text{reshape}(\mathbf{H}_{c-1})$   
**end**  
 Set the cores of  $\mathbf{g}$  as  $(\mathbf{D}_1, \mathbf{D}_2, \dots, \mathbf{D}_d)$

The general procedure of truncating the ranks of a TT tensor comes in two phases. The first phase is to collect all the norm of the tensor into a single core through a sequence of matrix factorizations, leaving all other cores to have Frobenius norm 1. Then a sequence of SVDs are applied, multiplying a nonunitary factor from a tensor train core to its neighboring cores. The first phase is called orthogonalization of a TT tensor, and we now present an algorithm for it.

There are two variants of orthogonalization we will discuss. One is Left-to-Right orthogonalization and the other Right-to-Left orthogonalization. They are the same algorithm mirrored across the middle core of the tensor train, and each step in one is a transpose of its counterpart in the other. A TT tensor is left orthogonal if for  $c = 1, 2, \dots, d-1$ , we have  $\mathcal{V}(\mathbf{C}_c)^\top \mathcal{V}(\mathbf{C}_c) = \mathbf{I}$ . Similarly, a TT tensor is right orthogonal if for  $c = 2, 3, \dots, d$ , we have  $\mathcal{H}(\mathbf{C}_c) \mathcal{H}(\mathbf{C}_c)^\top = \mathbf{I}$ . One may transform the cores of a TT tensor to be left orthogonal while the full tensor is unchanged by applying iterated matrix factorizations. All we must do is sequentially flatten, orthogonalize by QR decomposition, then unflatten each core, until the final one is reached. This process is summarized in Algorithm 1. For the right orthogonal case, the procedure is largely identical, though we use LQ factorization, the lower-triangular orthogonalizing decomposition, instead.

We now describe one algorithm for truncation of a tensor train given an orthogonalized TT tensor. The process is essentially the same as orthogonalization: we apply a sequence of orthogonal matrix factorizations to each core, multiplying one of the terms into that core's left or right neighbor. We then replace the current core with the entries of an orthogonal factor. The difference in this algorithm is that we apply an SVD rather than QR or LQ factorization. The term "truncation" comes from truncating the singular value decomposition series expansion of a matrix up to a desired tolerance. This truncation is described as the rounding algorithm in [63]. We present the right orthogonal variant of it here as Algorithm 2. There is no clear general rule for preferring one left or right variant truncation algorithm. They have identical computational costs and similar formulations. It is possible that differing runtime will occur based on row-major versus col-

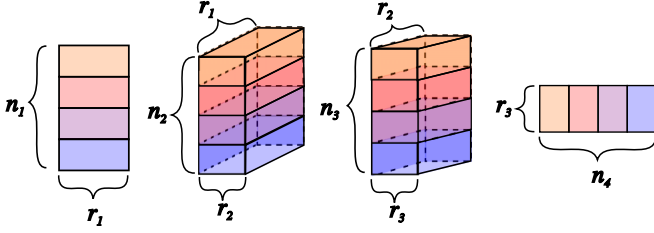


FIG. 8. Parallel memory layout for the tensor train format. This graphic shows a visualization of the data layout described by equation (A4) with  $d = 4$  tensor cores and  $P = 4$  compute nodes. Each tensor core is split up into blocks which store a contiguous segment of memory, depicted here in different shades.

umn major layout of the matrices, though this is highly dependent on the specific memory mapping and workspaces used in the SVD, QR, and LQ calls.

## 2. Parallel algorithms for tensor train arithmetic

Among the arithmetic operations performed on the tensor train during the evolution of the solution to a differential equation, the most costly is the truncation. This is due to the fact that it requires data access and editing of every core twice. Due to the sequential nature of the loops in Algorithms 1 and 2 we see that parallelizing the inner loop would be most effective. To this end, we follow the approach of [87]. Our extension of the algorithms presented in [87] can be found at our GitHub repository [84]. Since the rank of the tensor train is expected to change frequently during program execution, we must split the memory stored on a total of  $P$  compute nodes in a manner independent of the tensor rank. To this end, we introduce a  $P \times d$  memory partition matrix  $\mathbf{M}$  with positive integer values so that for each core  $\mathbf{C}_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$ , we have  $\sum_{p=1}^P \mathbf{M}[p, k] = n_k$ . This matrix describes a block-tensor storage layout for the tensor train core list. More precisely, for each core  $\mathbf{C}_k$ , we define an array of core blocks  $(\mathbf{C}_k^1, \mathbf{C}_k^2, \dots, \mathbf{C}_k^P)$  with array sizes defined via  $\mathbf{C}_k^p \in \mathbb{R}^{r_{k-1} \times \mathbf{M}[p, k] \times r_k}$  so that

$$\mathbf{C}_k[i, (1, \dots, n_k), j] = \begin{bmatrix} \mathbf{C}_k^1[i, (1, \dots, \mathbf{M}[1, k]), j] \\ \mathbf{C}_k^2[i, (1, \dots, \mathbf{M}[2, k]), j] \\ \vdots \\ \mathbf{C}_k^P[i, (1, \dots, \mathbf{M}[P, k]), j] \end{bmatrix}. \quad (\text{A4})$$

In other words, each distributed memory compute node with index  $p$  stores the core list  $(\mathbf{C}_1^p, \mathbf{C}_2^p, \dots, \mathbf{C}_d^p)$ . These cores are treated as being “stacked” on top of each other, with the process index denoting the “top” of the tensor core. This is depicted in Fig. 8. This memory layout is designed so that

$$\mathcal{V}(\mathbf{C}_k) = \begin{bmatrix} \mathcal{V}(\mathbf{C}_k^1) \\ \mathcal{V}(\mathbf{C}_k^2) \\ \vdots \\ \mathcal{V}(\mathbf{C}_k^P) \end{bmatrix} \quad \text{and} \quad \mathcal{H}(\mathbf{C}_k) = [\mathcal{H}(\mathbf{C}_k^1) \mid \mathcal{H}(\mathbf{C}_k^2) \mid \dots \mid \mathcal{H}(\mathbf{C}_k^P)].$$

We may therefore compute a flattening of the cores without any memory movements or cross-node communications by reinterpreting the array storage offsets in column major layout. Additionally, sums and scalar multiplications of tensors may also be computed in parallel without communications. We may simply repeat the serial summation and scalar multiplication algorithms, but applied to the distributed memory core list  $(\mathbf{C}_1^p, \mathbf{C}_2^p, \dots, \mathbf{C}_d^p)$ .

This parallel layout also allows for straightforward applications of finite difference stencils. Consider a finite difference stencil which requires  $s$  many points where the number of one-dimensional ghost cells required is  $g = (s - 1)/2$ . Let  $\mathbf{D}_{FD}$  be the linear operator for this stencil. To apply a partial derivative in variable  $k$  to a TT tensor, we replace the entries of core  $\mathbf{C}_k$  with the entries of  $\mathbf{D}_{FD}$  applied to Eq. (A4) for each  $i, j$ . To perform the parallel version of this stencil, we first perform a nonblocking communication to deliver the ghost cells of compute node  $p$  to their neighboring nodes  $p \pm 1$ . For nodes  $p = 1$  or  $p = P$ , we instead rely on discrete boundary condition formulas, communicating again between nodes  $p = 1$  and  $p = P$  if periodic boundary conditions are required. After boundary condition communications, every processor has an appropriate local version of the finite difference stencil, which is identical save for the definition of the ghost cells.

Numerical integration is similar, though instead of sharing ghost cells of compute node  $p$  with compute node  $p \pm 1$ , we need only pass the data with compute node  $p + 1$ , due to the one-sided stencil of a cumulative summation formula.

### a. Parallel tall-skinny QR factorization

In order to truncate a TT tensor with the described block memory layout, we must perform a distributed memory QR factorization on a matrix of the form

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_1 \\ \mathbf{A}_2 \\ \vdots \\ \mathbf{A}_P \end{bmatrix},$$

#### ALGORITHM 3. Parallel left orthogonalization.

**Data:** A tensor  $\mathbf{f}$  in distributed memory TT format with cores  $([\mathbf{C}_1^p], [\mathbf{C}_2^p], \dots, [\mathbf{C}_d^p])$ .  
**Result:** A tensor  $\mathbf{g} = \mathbf{f}$  in distributed memory TT format with left orthogonal cores.

Reserve memory for each block  $\mathbf{D}_c^p$  with sizes of  $\mathbf{C}_c^p$ .  
 $\mathbf{D}_1^p = \mathbf{C}_1^p$   
**for**  $c = 1, 2, \dots, d - 1$  **do**  
      $[\mathbf{Q}_c^p, \mathbf{R}_c] = \text{TSQR}(\mathcal{V}(\mathbf{D}_c^p))$   
      $\mathbf{H}_{c+1}^p = \mathbf{R}_c \mathcal{H}(\mathbf{C}_{c+1}^p)$   
      $\mathbf{D}_c^p = \text{reshape}(\mathbf{Q}_c^p)$   
      $\mathbf{D}_{c+1}^p = \text{reshape}(\mathbf{H}_{c+1}^p)$   
**end**  
 Set the cores of  $\mathbf{g}$  as  $([\mathbf{D}_1^p], [\mathbf{D}_2^p], \dots, [\mathbf{D}_d^p])$



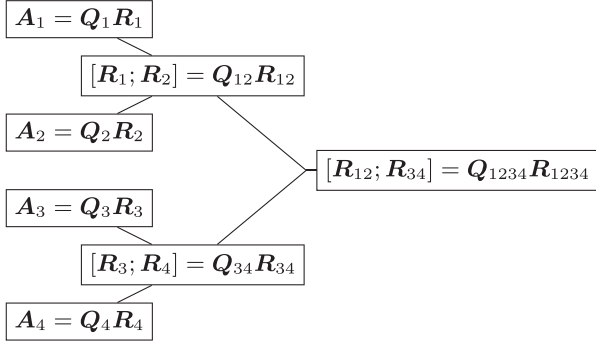


FIG. 9. Parallel TSQR algorithm with 4 compute nodes. A binary tree is formed which outlines the communication pattern for calculating the  $\mathbf{R}$  factor. At each level, the node with larger ID sends its  $\mathbf{R}$  factor to the tree sibling it connects to. The sibling then does a QR factorization with a concatenated pair of child  $\mathbf{R}$  factors. This process repeats until the final  $\mathbf{R}$  factor is found at the root of the tree stored on processor  $p = 1$ . We then broadcast this matrix to all other processors. To get the  $\mathbf{Q}$  factor, we store the orthogonal  $\mathbf{Q}_i$  for each tree node  $i$  and multiply the parent's  $\mathbf{Q}_i$  on the right side of the child's  $\mathbf{Q}$  factor, traversing the tree from the root to the leaves. This results in a distributed memory orthogonal matrix  $\mathbf{Q} = [\mathbf{Q}_1; \mathbf{Q}_2; \mathbf{Q}_3; \mathbf{Q}_4]$ .

or equivalently, perform an LQ factorization on the horizontally concatenated transpose of  $\mathbf{A}$ . For mathematical simplicity, we present only the QR variant, though our GitHub code available at [84] has both variants. One such factorization amenable to this layout is the Tall-Skinny QR (TSQR) factorization [88]. This algorithm uses a binary tree structure to define a communication pattern for decomposing the QR factorization of  $\mathbf{A}$  into a collection of smaller QR factorizations, avoiding communications if possible. By factoring the blocks into their own QR factorizations, we see that the  $\mathbf{Q}$  factor may be presented as a sequence of products of block diagonal matrices. This process is then applied to a recursive binary tree to track the nesting of the orthogonal  $\mathbf{Q}$  factor. The final result is an orthogonal matrix  $\mathbf{Q} = [\mathbf{Q}_1; \mathbf{Q}_2; \dots; \mathbf{Q}_P]$  distributed in the same block layout as  $\mathbf{A}$  and an upper triangular matrix  $\mathbf{R}$  copied across all compute nodes. See Fig. 9 for a visual representation of the binary tree storage structure for the case  $P = 4$ . The transposed version of this algorithm is called the Wide-Fat LQ (WFLQ) factorization and has the same tree data storage structure, but every matrix factorization is transposed.

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#### ALGORITHM 4. Parallel TT truncation.

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**Data:** A tensor  $\mathbf{f}$  in distributed memory TT format with cores  $([\mathbf{C}_1^p], [\mathbf{C}_2^p], \dots, [\mathbf{C}_d^p])$  and a desired accuracy  $\varepsilon$ .  
**Result:** A tensor  $\mathbf{g}$  so that  $\|\mathbf{g} - \mathbf{f}\| \leq \varepsilon$  in TT format with right orthogonal cores.

Reserve memory for each block  $\mathbf{D}_c^p$  with sizes of  $\mathbf{C}_c^p$ .  
 Set  $([\hat{\mathbf{C}}_1^p], [\hat{\mathbf{C}}_2^p], \dots, [\hat{\mathbf{C}}_d^p])$  as orthogonal by Alg. 3.

$$\hat{\varepsilon} = \varepsilon / \sqrt{d - 1}$$

$$\mathbf{D}_d^p = \hat{\mathbf{C}}_d^p$$

for  $c = d, d - 1, \dots, 2$  do

$$\begin{aligned} [\mathbf{L}_c, \mathbf{Q}_c^p] &= WFLQ(\mathcal{H}(\mathbf{D}_c^p)) \\ [\mathbf{U}_c, \mathbf{\Sigma}_c, \mathbf{V}_c^\top] &= SVD(\mathbf{L}_c, \hat{\varepsilon}) \quad (\text{Truncated SVD}) \end{aligned}$$

$$\mathbf{H}_{c-1}^p = \mathcal{V}(\hat{\mathbf{C}}_{c-1}^p) \mathbf{U}_c \mathbf{\Sigma}_c$$

$$\hat{\mathbf{Q}}_c^p = \mathbf{V}_c^\top \mathbf{Q}_c^p$$

$$\mathbf{D}_c^p = \text{reshape}(\hat{\mathbf{Q}}_c^p)$$

$$\mathbf{D}_{c-1}^p = \text{reshape}(\mathbf{H}_{c-1}^p)$$

end

Set the cores of  $\mathbf{g}$  as  $([\mathbf{D}_1^p], [\mathbf{D}_2^p], \dots, [\mathbf{D}_d^p])$

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#### b. Parallel orthogonalization and truncation

We now introduce a parallelization of Algorithms 1 and 2. It can be seen that parallelizing the orthogonalization algorithms is as simple as replacing the QR factorizations with their TSQR variants. However, the truncation requires a bit of manipulation. In order to parallelize this, we first note the following relationship of the SVD and QR factorizations:

$$\begin{aligned} \mathbf{QR} &= \mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^\top, \\ \mathbf{R} &= \mathbf{Q}^\top \mathbf{U} \mathbf{\Sigma} \mathbf{V}^\top. \end{aligned}$$

Thus,  $\mathbf{R}$  has the same singular values as  $\mathbf{A}$ , and so truncating an SVD of  $\mathbf{R}$  produces the same approximation error as truncating  $\mathbf{A}$  directly. Since the TSQR algorithm is designed to produce a copy of  $\mathbf{R}$  on each compute node, we apply a shared memory SVD redundantly on this copied  $\mathbf{R}$  to determine the truncated tensor. This process is formalized in Algorithms 3 and 4.

These algorithms are designed so that the only communications required are those that are involved in the computation of the QR or LQ factorizations. Each algorithm is mathematically equivalent to its serial counterpart. The core difference is the use of a superscript  $p = 1, 2, \dots, P$ , to denote which matrices take on different values within the different compute nodes. Matrices which are numerically identical across all nodes lack this superscript.

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