Journal of Computational Physics 292 (2015) 43–55

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Semi-implicit integration factor methods on sparse grids for high-dimensional systems

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ARTICLE INFO

Article history:
Received 7 October 2014
Received in revised form 5 February 2015
Accepted 17 March 2015
Available online 24 March 2015

Keywords:
Reaction–diffusion equations
Implicit method
Sparse grids
High-dimension
Fokker–Planck equation
Stiffness

ABSTRACT

Numerical methods for partial differential equations in high-dimensional spaces are often limited by the curse of dimensionality. Though the sparse grid technique, based on a one-dimensional hierarchical basis through tensor products, is popular for handling challenges such as those associated with spatial discretization, the stability conditions on time step size due to temporal discretization, such as those associated with high-order derivatives in space and stiff reactions, remain. Here, we incorporate the sparse grids with the implicit integration factor method (IIF) that is advantageous in terms of stability conditions for systems containing stiff reactions and diffusions. We combine IIF, in which the reaction is treated implicitly and the diffusion is treated explicitly and exactly, with various sparse grid techniques based on the finite element and finite difference methods and a multi-level combination approach. The overall method is found to be efficient in terms of both storage and computational time for solving a wide range of PDEs in high dimensions. In particular, the IIF with the sparse grid combination technique is flexible and effective in solving systems that may include cross-derivatives and non-constant diffusion coefficients. Extensive numerical simulations in both linear and nonlinear systems in high dimensions, along with applications of diffusive logistic equations and Fokker–Planck equations, demonstrate the accuracy, efficiency, and robustness of the new methods, indicating potential broad applications of the sparse grid-based integration factor method.

1. Introduction

Consider the following partial differential equation:

$$\frac{\partial u(\mathbf{x},t)}{\partial t} = Pu(\mathbf{x},t) + f(u(\mathbf{x},t)), \mathbf{x} = (x_1,\ldots,x_d) \in (0,1)^d, t \in [0,T], \tag{1}$$

where P is an elliptic differential operator with respect to the spatial variable $\mathbf{x}$. This equation has been extensively studied because of its wide application in certain fields. For instance, the formation of the morphogen gradient during the development of the embryo is modeled using reaction–diffusion systems [1], where P denotes the Laplacian operator with respect to $\mathbf{x}$. The stochastic behavior of a gene network can be described using the Fokker–Planck equation [2], also known as the backward Kolmogorov equation, where P is a second-order differential operator containing cross-derivatives. In finance, the

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http://dx.doi.org/10.1016/j.jcp.2015.03.033

Black–Scholes equation adopts a similar form when used to estimate the price of options under several risk factors [3]. In population genetics, the site-frequency spectrum can be modeled using such equations as well [4].

From the numerical perspective, solving Eq. (1) in high dimensions can be extremely challenging. Due to the "curse of dimensionality", achieving good accuracy of $O(1/N_{\mathbf{x}}^{\alpha})$ (for example, $\alpha = 2$ by a second-order central difference formula) usually requires an $O(N_{\mathbf{x}}^{d})$ number of points in uniform grids. The storage and operations on this large number of grid points can be prohibitively expensive when d is large. In addition, spatial discretization due to high-order spatial derivatives and stiff reactions leads to severe stability constraints on the time step for temporal integration. For the explicit methods, such as Runge–Kutta or Euler methods, a severe constraint is placed on the time step, whereas for implicit methods, such as the Crank–Nicolson method, large nonlinear systems are solved at each time step, leading to excessive computational costs.

The sparse grid technique has been shown to be an efficient approach for dealing with high spatial dimensions [5]. The discretization for this approach involves an $O(N \cdot (\log N)^{d-1})$ number of points along with an accuracy of $O((\log N)^{d-1}/N^2)$ when the one-dimensional piecewise linear hierarchical basis is applied. Such an approach may be extended to the general piecewise d-linear hierarchal basis by a tensor product construction in d-dimensional spaces [6,5]. Other hierarchical bases, e.g., high-order polynomials, interpolets, wavelets, have also been developed for a higher order of accuracy [7–9]. Moreover, sparse grids have been recently applied to stochastic simulations and parameter estimations [10–12].

A popular approach for addressing the problem associated with dimensionality is the sparse grid finite element method using the Galerkin technique [13,14] constructed on piecewise linear element using weak formulas. Another approach is the sparse grid finite difference method [15], which employs the regular second-order central difference approximation on the diffusion terms. The finite volume method [16] and the spectral method [17,18] can also be integrated with the sparse grid technique. Another interesting approach is the so-called *sparse grid combination technique* [19] that uses multi-level regular uniform grids such that the final solution is constructed using a linear combination of the intermediate solutions at the uniform grids, leading to a straightforward implementation, similar to the standard uniform grid approach.

For temporal integration, the integration factor (IF) and exponential time differencing (ETD) methods are effective ways to deal with the temporal stability constraints arising from high-order spatial derivatives on uniform meshes [20–22]. The IF and ETD methods usually treat linear operators of the highest-order derivatives exactly, and hence, they provide good temporal stability by allowing larger sizes of time step in temporal updates [23,24,20]. For addressing the stiffness in reactions, a class of semi-implicit integration factor (IIF) methods, which integrate the differential operators exactly like the IF schemes while treating the reaction terms implicitly, have been developed [25]. In IIF, the calculation of the diffusion and implicit treatment of the reaction is decoupled such that the size of the nonlinear system that needs to be solved at each time step is the same as that of the original continuous PDEs. This property results in good efficiency, in addition to excellent stability conditions (e.g., the second-order IIF is linearly unconditionally stable). Moreover, the IIF method can handle reaction–convection–diffusion equations through an operator splitting technique [26] and can be incorporated with the adaptive meshes and general curvilinear coordinates [27]. Because the exact treatment of the diffusion terms requires computing exponentials of matrices resulting from the discretization of the linear differential operators, a compact representation of IIF (cIIF) [28,27] and an array representation of IIF (AcIIF) [29] for systems with high spatial dimensions have been introduced. In the compact or array representations, the discretized functions in high spatial dimensions can be represented using multi-dimensional arrays rather than vectors or matrices so that the cost and storage associated with the calculation of the exponentials are significantly reduced.

In this paper, we integrate the sparse grids with the IIF methods to take the advantages provided by both methods to solve temporal PDEs (e.g., Eq. (1)) in high spatial dimensions. In particular, we combine the two temporal schemes, the IIF and AcIIF methods, with the three different sparse grid discretization techniques: finite element, finite difference, and sparse grid combination technique. The combination technique is found to be especially effective in terms of incorporating various implicit integration factor methods, particularly when dealing with systems that include cross-derivatives and non-constant diffusion coefficients.

The paper is organized as follows. In Section 2, we construct the IIF method on sparse grids based on the finite element and Galerkin technique. In Section 3, we construct the AcIIF method on sparse grids using the finite difference approximation. In Section 4, we apply the AcIIF method to the sparse grid combination technique. In Section 5, we describe numerical tests to demonstrate the accuracy, efficiency, and applications of these methods.

2. Semi-implicit integration factor method with finite element method on sparse grids

In this section, we consider the following reaction–diffusion equation:

$$\frac{\partial u}{\partial t}(\mathbf{x}, t) = \Delta_{\mathbf{x}} u(\mathbf{x}, t) + f(u), \tag{2}$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_d)$ and $\Delta_{\mathbf{x}}$ is the Laplacian operator with respect to $\mathbf{x}$. For simplicity of presentation, we assume the spatial domain to be $(0, 1)^d$ and zero Dirichlet boundary conditions at the boundaries for u. We only focus on the piecewise d-linear hierarchical basis on the sparse grids.