A NOVEL METHOD AVOIDING INVERSE CRIME IN SOLVING INVERSE PROBLEMS OF PARABOLIC TYPE USING MODEL REDUCTION METHODS*

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5 Abstract. In this paper, we propose novel proper orthogonal decomposition (POD)-based 6 methods that effectively address the issue of inverse crime when solving parabolic inverse problems 7 using model reduction methods. We study inverse source and initial value problems using our new 8 methods. By exploiting the low-dimensional structures inherent in the solution space of parabolic 9 equations and constructing POD basis functions, our methods significantly reduce computational 10 costs while maintaining accuracy in solving parabolic inverse problems. In addition, we provide 11 the convergence analysis of the proposed methods for solving these two types of parabolic inverse problems. Finally, we conduct numerical experiments to demonstrate the accuracy and efficiency of 12 13 the proposed method. The results show that our method efficiently solves parabolic inverse problems 14and overcomes the inverse crime issues associated with traditional model reduction methods for such 15 problems.

Key words. Parabolic inverse problem; Regularization method; Model reduction method;
 17 Inverse crime; Convergence analysis.

18 MSC codes. 35R30, 65J20, 65M12, 65N21, 78M34.

1. Introduction. Inverse problems associated with parabolic equations have 19garnered significant attention in mathematics and engineering research fields [25, 19]. 20 These problems can be broadly categorized into several types: recovering source terms 21 in the PDEs, determining the system's initial state, identifying physical parameters, 22 and determining the boundary conditions. In this paper, we focus on the first two 23 types of inverse problems and leave the other types as future work. We will refer 24 to the first two types of inverse problems as inverse source problems and backward 25problems, respectively. 26

27 Inverse source problems, which involve reconstructing the source from final time observation, have attracted much attention from researchers in recent decades [23] 28 and references therein. These problems have been extensively studied in the litera-29 ture and applied to various physical and engineering source identification problems, 30 such as groundwater migration, groundwater pollution detection, pollution source 31 control, and environmental protection [8, 12, 16, 11, 23] and references therein. Ac-32 33 curately recovering pollutant sources is crucial for ensuring environmental safeguards in densely populated cities [9]. The estimation of the strength of acoustic sources 34 from measurements can be found in e.g. [23, 13, 31]. Given the importance of inverse 35 source problems in practical applications, numerous numerical methods have been 36 extensively explored [8, 6, 29, 15, 16] and references therein. 37

For inverse source problems, iteration optimization methods are typically used to determine the true source term [6, 10, 24]. The forward parabolic equation must be solved one or two times in each iteration. However, as the size of discrete problems

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^{*}Submitted to the editors DATE.

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increases (e.g. using the finite element method (FEM) or finite difference method
(FDM)), the computational time increases rapidly, especially for time-evolution problems. As a result, the computation of the forward equation will consume the most
time throughout the entire process.

To address the computational challenges associated with solving parabolic inverse 45 source problems, we propose a data-driven model reduction method [35]. Our method 46 consists of offline and online stages. In the offline stage, we exploit the low-dimensional 47 structures in the solution space of parabolic equations in the forward problem, given 48 a class of source functions, and construct a small number of POD basis functions 49to achieve significant dimension reduction. With the POD basis functions, we can 50rapidly solve the forward problem in the online stage. Consequently, we developed 52 a fast algorithm called the POD algorithm to solve the optimization problem in the parabolic inverse source problems. Moreover, we derive an error estimate for the POD 53 algorithm in parabolic inverse source problems. Numerical results demonstrate that 54the POD algorithm offers significant computational savings compared to the FEM while maintaining the same level of accuracy. However, we have to point out that 56 our POD algorithm has a limitation: it requires assuming that the true source term belongs to a known function class, leading to the inverse crime [25, 22]. In this paper, 58 we aim to develop novel model reduction methods to solve parabolic inverse problems 59and eliminate the inverse crime issue. 60

Backward problems are another important type of parabolic inverse problem that 61 has been extensively studied in physics and engineering, particularly in the field of 63 heat transfer. The main focus of these problems is to determine the initial condition from transient temperature measurements at the final time T. The main difficulty in 64 solving the backward problems arises from the exponential decay of forward solutions 65 of the parabolic equations with respect to the initial data. Therefore, backward 66 problems are also ill-posed in the sense of Hadamard [23, 18], as the eigenvalues of 67 elliptic operators decay exponentially fast, making them particularly unstable with 68 respect to measurement data uncertainties. This lack of stability poses a significant challenge for numerical inversions, as even small changes in the data can lead to 70substantial differences in the reconstructed source strength. 71

In response to these challenges, many regularization techniques have been devel-72oped for solving backward problems. For instance, in [26], Sobolev error estimates 73 and a prior parameter selection for semi-discrete Tikhonov regularization were de-74rived. A backward problem for the one-dimensional heat conduction equation, with 75 the measurements on a discrete set, was considered in [7], and the uniqueness of recov-76ering the initial value was proved using the analytic continuation method. It is worth 77 noting that in [30], a comparison of various inverse methods for estimating the initial 7879 condition of the heat equation was studied, demonstrating that explicit approaches to the backward problem yield disastrous results unless some form of regularization 80 is utilized. 81

In our recent work [36], we study the stochastic convergence of regularized solu-82 tions for backward problems. We derive an error estimate for the least-squares reg-83 84 ularized minimization problem within the framework of stochastic convergence. Our analysis reveals that the optimal error of the Tikhonov-type least-squares optimization 85 86 problem depends on the noise level, the number of sensors, and the underlying ground truth. Additionally, we propose a self-adaptive algorithm to identify the optimal reg-87 ularization parameter for the optimization problem without requiring knowledge of 88 the noise level or any other prior information, which would be highly practical in ap-89 plications. Numerical results demonstrate the effectiveness of our method in solving 90

91 backward problems. By assuming the initial condition belongs to a known function 92 class, it is straightforward to develop a POD method to solve backward problems 93 using the stochastic convergence developed in [36]. However, the corresponding POD 94 method also suffers from the issue of inverse crime [25, 22]. Once again, this motivates 95 us to develop new model reduction methods to solve parabolic backward problems and 96 eliminate the inverse crime issue.

As we have discussed, the issue of inverse crime arises when we develop the POD method for solving inverse problems [35], where the forward model used for generating the data is identical to the one employed for solving the inverse problem. This scenario can lead to overly optimistic results and underestimates the uncertainties associated with the solution. The inverse crime poses a significant challenge in inverse problem solving, as it fails to account for model errors and uncertainties that are inherent in real-world applications.

Motivated by an interesting observation in our previous work on numerical simulation of parabolic equations, we propose a novel POD-based model reduction method to address the issue of inverse crime encountered in solving inverse problems associated with parabolic equations. Specifically, we aim to develop a novel POD methodology that can be applied to both the inverse source problems and backward problems of the parabolic type. To start with, we consider a generic parabolic equation as follows:

111 (1.1)
$$\begin{cases} u_t + \mathcal{L}u = f(x) & \text{in } \Omega \times (0, T), \\ u(x, t) = 0 & \text{on } \partial \Omega \times (0, T), \\ u(x, 0) = g(x) & \text{in } \Omega, \end{cases}$$

112 where $\Omega \subset \mathbb{R}^d$ (d = 1, 2, 3) is a bounded domain with a C^2 boundary or a convex 113 domain satisfying the uniform cone condition, \mathcal{L} denotes a second-order elliptic oper-114 ator given by $\mathcal{L}u = -\nabla \cdot (q(x)\nabla u) + c(x)u$, f(x) is the source term, and g(x) is the 115 initial condition. We assume the elliptic operator \mathcal{L} is uniform elliptic, i.e., there exist 116 $q_{\min}, a_{\max} > 0$ such that $q_{\min} < q(x) < q_{\max}$ for all $x \in \Omega$. Additionally, we assume 117 $q(x) \in C^1(\overline{\Omega}), c(x) \in C(\overline{\Omega})$ and $c(x) \ge 0$.

118 Let *u* represent the solution of the parabolic equation (1.1). We define the forward 119 operator $S: S(f,g) = u(\cdot,T)$. The forward problem involves computing the solution 120 $u(\cdot,t)$ for t > 0 given the source term f(x) and initial condition g(x). The inverse 121 problem, on the other hand, aims to reconstruct f(x) or g(x) from the final time 122 measurement $m = u(\cdot,T)$. We will solve two types of inverse problems as follows:

123 1. Inverse source problem: recover the source term f(x) using the final time 124 measurement $m = u(\cdot, T)$ and the known initial term g(x).

125 126

2. Backward problem: recover the initial term g(x) using the final time measurement $m = u(\cdot, T)$ and the known source term f(x).

In this paper, we develop a novel POD-based model reduction method, called the 127 adjoint-POD method, for solving inverse problems of parabolic types. We begin by 128 developing the adjoint-POD method to solve the inverse source problem and construct 129130basis functions for this problem. Specifically, we study the convergence of the POD basis functions obtained by our adjoint-POD method and prove their approximation 131132 property in Theorem 2.3. By leveraging this property, we derive the convergence analysis of the adjoint-POD method in solving inverse parabolic source problems 133in Theorem 2.4 and Theorem 2.5. We then extend our approach to the parabolic 134backward problem, where we construct the POD basis functions by solving the adjoint 135136 equation with the given final time measurement as the initial condition. We also prove

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the approximation property of the corresponding POD basis functions in Theorem 3.2 and the convergence analysis of the adjoint-POD method in solving the parabolic backward problem in Theorem 3.3 and Theorem 3.4. Finally, we present numerical experiments that demonstrate the effectiveness of our adjoint-POD method in solving parabolic inverse problems and its ability to overcome inverse crime.

The rest of the paper is organized as follows. In Section 2, we introduce the adjoint-POD method for solving parabolic inverse source problems and provide the error estimate for the proposed methods. Similarly, in Section 3, we propose the adjoint-POD method for solving parabolic backward problems and provide the corresponding error estimate. In Section 4, we present numerical results to demonstrate the accuracy of our methods. Finally, concluding remarks are made in Section 5.

2. Adjoint-POD method for parabolic inverse source problems. Regularization methods are commonly used to solve inverse problems, where one applies iterative methods to solve the forward problem one or more times in each iterative step. As a result, most computational time is spent on solving the forward problem. To address this issue, it is natural to develop model reduction methods to decrease the computational cost of solving the forward problems.

One of the model reduction ideas in solving time-evolution problems is the POD 154155 method [33, 4]. The POD method uses data from an experiment or an accurate numerical simulation and extracts the most energetic modes in the system by using the 156singular value decomposition. This approach generates low-dimensional structures 157that can approximate the solutions to the time-evolution problem with high accu-158racy. The POD method has been applied successfully to solve many types of PDEs, 159including linear parabolic equations [34, 27], Navier-Stokes equations [27], viscous 160 G-equations [17], Hamilton–Jacobi–Bellman (HJB) equations [28], and optimal con-161 trol problems [2]. The interested reader is referred to [32, 3, 20] for a comprehensive 162 introduction to the model reduction methods. 163

The traditional POD method has a significant drawback: to construct the POD basis functions, one must know the source term f(x) or the initial condition g(x). Therefore, directly using the POD method to solve inverse problems may result in the inverse crime issue. In our previous work [35], we mitigated this issue by assuming that the true source term belongs to a known function class. However, this approach does not fully address the issue of the inverse crime.

To tackle this challenge, we propose a novel method for model reduction in inverse problems: the adjoint-POD method. Unlike the traditional POD method, our method does not require any prior knowledge of the source or initial term. By integrating the adjoint method with the model reduction capabilities of the POD method, we will show that the adjoint-POD method can efficiently solve inverse problems while avoiding the inverse crime issue.

2.1. Adjoint POD method. To demonstrate the idea of the adjoint-POD method, we will first apply it to solve the inverse source problem. This problem involves recovering the unknown source term f(x) of the parabolic equation, given the final time measurement $m(x) = S(f) = u(\cdot, T)$. Here, u satisfies the following equation:

181 (2.1)
$$\begin{cases} u_t + \mathcal{L}u = f(x) & \text{in } \Omega \times (0, T), \\ u(x, t) = 0 & \text{on } \partial \Omega \times (0, T), \\ u(x, 0) = 0 & \text{in } \Omega. \end{cases}$$

Here we assume that u(x,t) = 0 and u(x,0) = 0 for simplicity, otherwise, one just needs to subtract the background solution from the measurement m(x). Since the source term f(x) is unknown, we cannot use the traditional POD method to obtain snapshots. Instead, we will obtain the snapshots from the following equation:

186 (2.2)
$$\begin{cases} \tilde{u}_t + \mathcal{L}\tilde{u} = m(x) & \text{in } \Omega \times (0, T), \\ \tilde{u}(x, t) = 0 & \text{on } \partial\Omega \times (0, T), \\ \tilde{u}(x, 0) = 0 & \text{in } \Omega. \end{cases}$$

We denote the snapshots as $\tilde{y}_k = \tilde{u}(\cdot, t_{k-1}), k = 1, \dots, M+1$ with $M = \frac{T}{\Delta t}$, and $\tilde{y}_k = \overline{\partial} \tilde{u}(\cdot, t_{k-M-1}), k = M+2, \dots, 2m+1$. Here, $\overline{\partial} \tilde{u}(\cdot, t_k) = \frac{\tilde{u}(\cdot, t_k) - \tilde{u}(\cdot, t_{k-1})}{\Delta t}$ for $k = 1, \dots, M$. We then construct the new POD basis functions $\{\psi_1, \dots, \psi_{N_{\text{pod}}}\}$ using the 187 188 189 method described in Appendix A from the adjoint equation (2.2). Finally, we denote 190the linear space spanned by the POD basis functions as $V_{\text{POD}} = \text{span}\{\psi_1, ..., \psi_{N_{\text{pod}}}\}$. 191 We can use these new POD basis functions $\{\psi_1, ..., \psi_{N_{\text{pod}}}\}$ to approximate the 192forward problem and speed up the computation. We construct the fully discrete 193scheme on V_{pod} , and we denote the solution by U_k for $k = 1 \cdots M$. Specifically, we 194 seek numerical solutions U_k such that: 195

196 (2.3)
$$(\bar{\partial}U_k,\psi) + a(U_k,\psi) = (f,\psi), \quad \forall \psi \in V_{\text{pod}}.$$

Here the bilinear form $a(u, v) = (q\nabla u, \nabla v) + (cu, v)$. We define the solution operator from the source term f to the final time solution U_M as S_{pod} , such that $S_{\text{pod}}f = U_M$. By using the new POD basis functions and the reduced-order model represented by S_{pod} , we can efficiently solve the forward problem for each time step. This significantly reduces the computational cost compared to using the full-scale model. This approach is particularly useful when solving inverse problems, where multiple forward problem evaluations are required.

204 **2.2.** Convergence of the adjoint-POD method. We will first revisit an im-205 portant property of the eigenvalue distribution for the classical elliptic operator \mathcal{L} 206 [1, 14].

207 PROPOSITION 2.1. Suppose Ω is a bounded domain in \mathbb{R}^d and $a(x), c(x) \in C^0(\overline{\Omega})$, 208 $c(x) \geq 0$. Then, the eigenvalue problem

209 (2.4)
$$\mathcal{L}\psi = \mu \psi \quad \text{with} \quad \psi_{\partial\Omega} = 0$$

has a countable set of positive eigenvalues $\mu_1 \leq \mu_2 \leq \cdots$, with corresponding eigenfunctions $\{\phi_k\}_{k=1}^{\infty}$ forming an orthogonal basis of $L^2(\Omega)$. Moreover, there exist positive constants $C_1, C_2 > 0$ such that $C_1 k^{2/d} \leq \mu_k \leq C_2 k^{2/d}$ for all $k = 1, 2, \cdots$.

According to the Proposition above, the eigenfunction set $\{\phi_k\}_{k=1}^{\infty}$ forms an orthogonal basis of $L^2(\Omega)$. Thus, for any $f \in L^2(\Omega)$, we can write $f = \sum_{k=1}^{\infty} f_k \phi_k$, where f_k 's are coefficients. Similarly, let $u = \sum_{k=1}^{\infty} u_k(t)\phi_k$ be the solution of the problem (2.1). Substituting these expressions of f and u into the first equation of (2.1) and noting that $\mathcal{L}\phi_k = \mu_k\phi_k$, we can compare the coefficients of ϕ_k on both sides of the equation to obtain $u_k(0) = 0$ and

219 (2.5)
$$u'_k(t) + \mu_k u_k = f_k \quad \text{in } (0,T).$$

This equation expresses the time evolution of the coefficients $u_k(t)$ in terms of the coefficients f_k of the source term f. We can write the solution as $u_k(T) = \alpha_k f_k$, where $\alpha_k = e^{-\mu_k T} \int_0^T e^{\mu_k s} ds = \frac{1}{\mu_k} (1 - e^{-\mu_k T})$. Noting that $Sf = u(\cdot, T) = \sum_{k=1}^{\infty} u_k(T)\phi_k$, we can formally write

224
$$S\left(\sum_{k=1}^{\infty} f_k \phi_k\right) = \sum_{k=1}^{\infty} \alpha_k f_k \phi_k$$

This representation of the solution operator S provides a convenient way to compute the solution $u(\cdot, T)$ using the eigenfunctions ϕ_k and the coefficients α_k . To simplify the problem, we approximate the source term f(x) by truncating it to a finite-dimensional space, i.e.

229 (2.6)
$$f_{\rm app} = \sum_{k=1}^{L} f_k \phi_k.$$

Using this truncation, the solution u(x,t) of the parabolic equation can be written as:

232 (2.7)
$$u(\cdot,T) = \sum_{k=1}^{L} \frac{1}{\mu_k} (1 - e^{-\mu_k T}) f_k \phi_k.$$

After simple calculation, we will also derive that

234 (2.8)
$$\tilde{u}(x,t) = \sum_{k=1}^{L} \frac{1}{\mu_k} (1 - e^{-\mu_k T}) (1 - e^{-\mu_k t}) f_k \phi_k.$$

It is worth noting that the POD basis (A.4) is simply the singular value decomposition of the matrix $\tilde{A} = (\tilde{y}_1, ..., \tilde{y}_M)$, where $\tilde{y}_j = (\tilde{u}(x_1, t_j), ..., \tilde{u}(x_N, t_j))^T$ and $x_1, ..., x_N$ are the finite element nodes in Ω . Specifically, if A has the singular value decomposition $A = U\Sigma V$, then the first M columns of U correspond exactly to the POD basis $\{\psi_k\}_{k=1}^M$.

Let us denote $A = (y_1, ..., y_M)$, $\tilde{A} = (\tilde{y}_1, ..., \tilde{y}_M)$, the matrix $\Phi = (\phi_1(\vec{x}, t_1), ..., \phi_L(\vec{x}, t_1))$, $F = \text{diag}(f_1, ..., f_L)$, and $D = \text{diag}(\frac{1}{\mu_k}(1 - e^{-\mu_k T}), ..., \frac{1}{\mu_L}(1 - e^{-\mu_L T}))$. In addition, let J be an $L \times M$ matrix with entries $J(i, j) = \frac{1}{\mu_i}(1 - e^{-\mu_i t_j})$. Φ is a column orthogonal matrix due to the normal orthogonality of the eigenfunctions ϕ_k . Using the formulations of u and \tilde{u} , we can represent the matrices A and \tilde{A} as follows: 245

246 (2.9)
$$A = \Phi F J$$
, and $\tilde{A} = \Phi D F J$.

Proposition A.1 shows that the low-rank space V_{pod} provides the best N_{pod} rank approximation of the column space of \tilde{A} . Our objective is to demonstrate that V_{pod} is also a good approximation of the column space of A, which will validate the effectiveness of the new POD method. To begin, we need to establish the relationship between the matrices A and \tilde{A} .

252 LEMMA 2.2. If $L \leq M$, then $span\{y_1, ..., y_M\} = span\{\tilde{y}_1, ..., \tilde{y}_M\}$, i.e. $C(A) = C(\tilde{A})$.

Proof. We will provide a concise proof for the case when the eigenvalues μ_i are 254distinct from each other. The proof for the case of repeated eigenvalues follows a 255similar approach. To demonstrate the desired results, we need to show that there 256exist matrices P and \tilde{P} such that 257

258 (2.10)
$$\Phi DFJP = \Phi FJ$$
, and $\Phi DFJ = \Phi FJP$.

We will only present a brief proof for the first equality, as the second can be 259derived similarly. Since the columns of Φ are independent and the diagonal matrix F 260 is invertible, we can show the existence of a matrix P by proving that the following 261equation holds 262

263 (2.11)
$$JP = DJ.$$

First, we will prove that the matrix $J'_{L\times L}$ with entries $J'(i,j) = 1 - e^{-\mu_i t_j}$ is invertible. To do this, we introduce the vector $\mathbf{e} = (1, ..., 1)^T$. It follows that we can 264 265write J' as the difference between the outer product of **e** and its transpose, ee^T , and 266the Vandermonde matrix V_L , where $V_L(i, j) = e^{-\mu_i t_j}$. Namely, we have $J' = \mathbf{e}\mathbf{e}^T - V_L$. 267Next, we aim to show the invertibility of J' by contradiction. Suppose that J' is 268singular, which implies that there exists a nonzero vector $\mathbf{c} = (c_1, ..., c_L)^T$ satisfying 269 $J'\mathbf{c} = 0$. Equivalently, we can express this as $V_L \mathbf{c} = \mathbf{e} \mathbf{e}^T \mathbf{c}$. Let us consider the function $f(x) = \sum_{j=1}^{L} c_j e^{xt_j}$. With this assumption, we have 270

271272that

273 (2.12)
$$f(0) = f(\mu_1) = f(\mu_2) = \dots = f(\mu_L),$$

which implies that the function f has L + 1 distinct zeros. Therefore, its derivative 274 $f'(x) = \sum_{i=1}^{L} c_i t_j e^{xt_j}$ must has L distinct zeros. Since **c** is nonzero, and all μ_j s are 275also nonzero, this implies that the Vandermonde matrix V_L is singular. However, 276this contradicts the fact that V_L is an invertible matrix. Consequently, J' must be a 277nonsingular matrix. 278

Since the invertibility of J', the first L columns of J are independent and thus 279form a basis for \mathbb{R}^L . Similarly, the matrix DJ also has independent columns that form 280a basis for \mathbb{R}^L . Therefore, there must exist a matrix P such that JP = DJ. This 281 result establishes that the spaces spanned by the sets $\{y_1, ..., y_M\}$ and $\{\tilde{y}_1, ..., \tilde{y}_M\}$ are 282 equivalent, i.e., span $\{y_1, \ldots, y_M\}$ = span $\{\tilde{y}_1, \ldots, \tilde{y}_M\}$. This completes the proof. 283

Proposition A.1 suggests that the new POD basis provides an effective approxi-284 mation of the set $\{\tilde{y}_1, ..., \tilde{y}_M\}$. Given the previous results, we can now show that the 285new POD basis also serves as a good approximation for the original set $\{y_1, \dots, y_M\}$. 286

THEOREM 2.3. Using the same notation as in Proposition A.1, we can derive 287 an approximation error bound if a sufficient number of snapshots are available, i.e. 288 $L \leq M$. In this case, the following error bound holds: 289

290 (2.13)
$$\frac{\sum_{i=1}^{M} ||y_i - P_{pod}y_i||_{L^2(\Omega)}^2}{\sum_{i=1}^{M} ||y_i||_{L^2(\Omega)}^2} \le CL^{4/d}\rho_i$$

. .

where P_{pod} is the projection operator onto the adjoint-POD space span{ $\psi_1, \ldots, \psi_{N_{pod}}$ } 291and $\rho = \frac{\sum_{k=N_{pod}+1}^{2M+1} \lambda_k}{\sum_{k=1}^{2M+1} \lambda_k}$ is a parameter that depends on the decay speed of the eigenvalues 292

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of the correlation matrix. 293

294*Proof.* In the following proof, we assume L = M for simplicity. For the case L < M, the proof is similar. Using the same notation of Lemma 2.2, Φ and J are 295296 both invertible square matrices. Then there exists a unique matrix P such that,

297 (2.14)
$$\Phi DFJP = \Phi FJ,$$

where $P = J^{-1}D^{-1}J$. 298

Hence, we have $y_j = \sum_{i=1}^{L} P_{ij} \tilde{y}_i$. Using the Cauchy-Schwarz inequality, we can show that for any $1 \leq j \leq L$, 299 300

301 (2.15)
$$\|y_j - P_{\text{pod}}y_j\|^2 \le \sum_{i=1}^L P_{ij}^2 \sum_{i=1}^L \|\tilde{y}_i - P_{\text{pod}}\tilde{y}_i\|^2.$$

Moreover, we can get that 302

303 (2.16)
$$\sum_{j=1}^{L} \|y_j - P_{\text{pod}}y_j\|^2 \le \sum_{i,j=1}^{L} P_{ij}^2 \sum_{i=1}^{L} \|\tilde{y}_i - P_{\text{pod}}\tilde{y}_i\|^2 = \|P\|_F^2 \sum_{i=1}^{L} \|\tilde{y}_i - P_{\text{pod}}\tilde{y}_i\|^2$$

The rest is to estimate the Frobenius norm of P. Since $P = J^{-1}D^{-1}J$, we can 304 define $||P||_d = ||D^{-1}||_2$. It is easy to verify that $||\cdot||_d$ is a matrix norm. Then, we 305have 306

307 (2.17)
$$||P||_F \le C||P||_d = C||D^{-1}||_2 \le C\mu_L.$$

On the other hand, since Φ is an orthogonal matrix, we have, 308

309 (2.18)
$$\sum_{j=1}^{L} \|\tilde{y}_j\|^2 = \|\Phi DFJ\|_F^2$$

310 (2.19)
$$= \|DFJ\|_F^2 \le \|D\|_F^2 \|FJ\|_F^2$$

311 (2.20)
$$\leq C \|FJ\|_F^2 \leq C \sum_{j=1}^{L} \|y_j\|^2$$

312 Aligning with Proposition A.1, we can combine the previous inequalities to obtain

313 (2.21)
$$\frac{\sum_{i=1}^{M} ||y_i - P_{\text{pod}}y_i||_{L^2(\Omega)}^2}{\sum_{i=1}^{M} ||y_i||_{L^2(\Omega)}^2} \le C ||P||_F^2 \frac{\sum_{i=1}^{M} ||\tilde{y}_i - P_{\text{pod}}\tilde{y}_i||_{L^2(\Omega)}^2}{\sum_{i=1}^{M} ||\tilde{y}_i||_{L^2(\Omega)}^2}$$

314 (2.22)
$$\leq \mu_L^2 \rho.$$

The conclusion follows from the estimation $\mu_i \leq C i^{2/d}$. 315

2.3. Convergence of inverse parabolic source problem. To solve this in-316 verse source problem, we use the well-established Tikhonov regularization method, 317 which is expressed as 318

319 (2.23)
$$\min_{f \in X} \|\mathcal{S}(f) - m\|_{L^2(\Omega)}^2 + \lambda \|f\|_{L^2(\Omega)}^2$$

320 However, in the conventional application of the POD method, the source term fmust be determined initially to generate snapshots and obtain the POD basis func-321 tions. In the context of inverse problems, the only available information is the mea-322 surement m(x). This predicament, referred to as the inverse crime, makes the conven-323324 tional POD method impossible to implement in practice. Our new method overcomes this vital drawback by using the POD forward solver as the forward solver in the Tikhonov regularization method.

In the general discrete approximation of problem (2.23), we seek to solve the following least-squares regularized optimization problem:

329 (2.24)
$$\min_{f \in V_{\text{pod}}} \|\mathcal{S}_{\text{pod}}(f) - m\|_{L^2(\Omega)}^2 + \lambda \|f\|_{L^2(\Omega)}^2.$$

Consider the functional $\mathcal{J}_{\text{pod}}[f] = \|\mathcal{S}_{\text{pod}}f - m\|_{L^2(\Omega)}^2 + \lambda \|f\|_{L^2(\Omega)}^2$. By computing the Fréchet derivative of $\mathcal{J}_{\text{pod}}[f]$, we can derive the subsequent iterative scheme:

$$332 \quad (2.25) \qquad \qquad f_{k+1} = f_k - \beta d\mathcal{J}_{\text{pod}}[f_k], \quad \forall k \in \mathbb{N},$$

where β is the step size, $d\mathcal{J}_{\text{pod}}[f] = S^*_{\text{pod}}(S_{\text{pod}}f - m) + \lambda f$ denotes the Fréchet derivative, and f_0 is an initial guess [35].

The above theory is based on the noise-free case, where the final time measurement $m = u(\cdot, T)$ is assumed to be precisely known. However, in practical applications, measurement data often contains uncertainties. We assume that the measurement data is blurred by noise and takes the discrete form

339 (2.26)
$$m_i^n = u(d_i, T) + e_i, \quad i = 1, \cdots, n,$$

where d_i s represent the positions of detectors, and $\{e_i\}_{i=1}^n$ are independent and identically distributed (i.i.d.) random variables on an appropriate probability space $(\mathfrak{X}, \mathcal{F}, \mathbb{P})$.

Based on [6] and the analysis therein, we know that $\|u\|_{C([0,T];H^2(\Omega))} \leq C \|f\|_{L^2(\Omega)}$. According to the embedding theorem of Sobolev spaces, we know that $H^2(\Omega)$ is continuously embedded into $C(\overline{\Omega})$ so that $u(\cdot,T)$ is well defined point-wisely for all $d_i \in \Omega$. Without loss of generality, we assume that the scattered locations $\{d_i\}_{i=1}^n$ are uniformly distributed in Ω . That is, there exists a constant B > 0 such that $d_{\max}/d_{\min} \leq B$, where d_{\max} and d_{\min} are defined by

349 (2.27)
$$d_{\max} = \sup_{x \in \Omega} \inf_{1 \le i \le n} |x - d_i|$$
 and $d_{\min} = \inf_{1 \le i \ne j \le n} |d_i - d_j|.$

We will first use the technique developed in [5] to recover the final time measurement $u(\cdot, T)$ from the noisy data m_i^n , for i = 1, ..., n. We approximate $u(\cdot, T)$ by solving the following minimization problem:

353 (2.28)
$$m = \underset{u \in X}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} (u(x_i) - m_i^n)^2 + \alpha |u|_{H^2(\Omega)}^2.$$

The choice of the optimal parameter α typically depends on both the noise level and the unknown function u^* . In the case of measured data with uncertainty, an a posteriori method has been proposed and discussed in previous literature [5, 6, 36]. We list the algorithm below.

Assuming the pointwise noise e_i has a bounded variance σ , which is referred to as the noise level, [5] analyzed this problem and provided optimal convergence results. Moreover, they proposed an a posteriori algorithm to obtain the best approximation without knowing the true solution m and noise level σ . Here, we list their main results. If one chooses the optimal regularization parameter

363 (2.29)
$$\alpha^{1/2+d/8} = O(\sigma n^{-1/2} \| u(\cdot, T) \|_{H^2(\Omega)}^{-1}),$$

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Algorithm 2.1 A self-consistent algorithm for finding the optimal α Given an initial guess of α_0 ; for $j = 0, 1, \cdots$, do the following Solve (2.28) for u_h with α replaced by the current value of α_j on the mesh; Update α_{j+1} : $\alpha_{j+1}^{1/2+d/8} = n^{-1/2} ||u_h - m^n||_n |u_h|_{H^2(\Omega)}^{-1}$. The algorithm stops if $|\alpha_j - \alpha_{j+1}| < 10^{-10}$.

then the solution m of (2.28) achieves the optimal convergence

365 (2.30)
$$\mathbb{E}\left[\|u(\cdot,T) - m\|_{L^2(\Omega)}\right] \le C\alpha^{1/2} \|u(\cdot,T)\|_{H^2(\Omega)}.$$

If the noise $\{e_i\}_{i=1}^n$ are independent Gaussian random variables with variance σ , we further have,

368 (2.31)
$$\mathbb{P}(\|u(\cdot,T) - m\|_{L^2(\Omega)} \ge \alpha^{1/2} \|u(\cdot,T)\|_{H^2(\Omega)} z) \le 2e^{-Cz^2}.$$

Using this recovered function m(x), we generate the adjoint POD basis functions in Section 2.1. It can be easily shown that, with uncertainty, the POD basis functions are still a good low-rank approximation of the snapshots $\{y_1, ..., y_M\}$. Combining Theorem 2.3 and (2.30), we have that for any $1 \le i \le M$,

373 (2.32)
$$||y_i - P_{\text{pod}}y_i||_{L^2(\Omega)}^2 \le C(ML^{4/d}\rho + \alpha)||f||_{L^2(\Omega)}^2.$$

Since we replace the source term by a finite truncation (2.6) and if $f \in H^1(\Omega)$, we have

376 (2.33)
$$\|f - f_{\text{app}}\|_{L^2} \le C \frac{\|\nabla f\|_{L^2}}{\sqrt{\mu_L}} \le C \frac{\|\nabla f\|_{L^2}}{L^{1/d}}.$$

377 If $f \in L^2(\Omega)$, then $f_{app} \to f$ as $L \to +\infty$. We assume

378 (2.34)
$$||f - f_{app}||_{L^2}^2 \le \varepsilon,$$

where ε depends on *L*. With these results, using a similar technique to prove Theorem 4.1 in [35], we can obtain the following convergence results.

THEOREM 2.4. Let $\{e_i\}_{i=1}^n$ be independent random variables satisfying $\mathbb{E}[e_i] = 0$ and $\mathbb{E}[e_i^2] \leq \sigma^2$ for $i = 1, \dots, n$. Set $\alpha^{1/2+d/8} = O(\sigma n^{-1/2} \| u^*(\cdot, T) \|_{H^2(\Omega)}^{-1})$ in (2.28), and $\lambda = O(ML^{4/d}\rho + \alpha)$. Then, we have the following error estimates

384 (2.35)
$$\mathbb{E}\left[\|\mathcal{S}f^* - \mathcal{S}_{pod}f_{pod}\|_{L^2(\Omega)}^2\right] \le C\lambda \|f^*\|_{L^2(\Omega)}^2 + C\varepsilon,$$

385

386 (2.36)
$$\mathbb{E}\left[\|f^* - f_{pod}\|_{L^2(\Omega)}^2\right] \le C \|f^*\|_{L^2(\Omega)}^2 + C\varepsilon,$$

387 and

388 (2.37)
$$\mathbb{E}\left[\|f^* - f_{pod}\|_{H^{-1}(\Omega)}^2\right] \le C\lambda^{1/2} \|f^*\|_{L^2(\Omega)}^2 + C\varepsilon.$$

Furthermore, if we assume the noise $\{e_i\}_{i=1}^n$ are independent Gaussian random variables with variance σ , we can obtain a stronger type of convergence. A similar proof can be found in [6]. We list the results here for completeness. THEOREM 2.5. Let $\{e_i\}_{i=1}^n$ be independent Gaussian random variables with variance σ . Set $\alpha^{1/2+d/8} = O(\sigma n^{-1/2} \| u^*(\cdot, T) \|_{H^2(\Omega)}^{-1})$ in (2.28), and $\lambda = O(ML^{4/d}\rho + \alpha)$. Then, there exists a constant C, for any z > 0, such that

(2.38)
$$\mathbb{P}(\|S_{pod}f_{pod} - Sf^*\|_{L^2(\Omega)} \ge (\lambda^{1/2} \|f^*\|_{L^2} + \varepsilon)z) \le 2e^{-Cz^2},$$

397 (2.39)
$$\mathbb{P}(\|f_{pod} - f^*\|_{L^2(\Omega)} \ge (\|f^*\|_{L^2} + \varepsilon)z) \le 2e^{-Cz^2},$$

398 and

399 (2.40)
$$\mathbb{P}(\|f_{pod} - f^*\|_{H^{-1}(\Omega)} \ge (\lambda^{1/4} \|f^*\|_{L^2} + \varepsilon)z) \le 2e^{-Cz^2}.$$

400 Theorems 2.4 and 2.5 provide the stochastic convergence rate for the error $\|\mathcal{S}f^* - \mathcal{S}_{\text{pod}}f_{\text{pod}}\|_{L^2(\Omega)}^2 = O_p(\lambda \|f^*\|_{L^2(\Omega)}^2 + \varepsilon)$, and $\|f^* - f_{\text{pod}}\|_{H^{-1}(\Omega)}^2 = O_p(\lambda^{1/2} \|f^*\|_{L^2(\Omega)}^2 + \varepsilon)$ 402 in terms of the values λ and ε . These results provide useful guidance for practical 403 numerical simulations.

3. Parabolic backward problem. For the backward problem of the parabolic equation, our goal is to recover the initial condition g(x), given the final time measurement $m = S(g) = u(\cdot, T)$. In this case, u satisfies the following equation:

407 (3.1)
$$\begin{cases} u_t + \mathcal{L}u = 0 & \text{in } \Omega \times (0, T), \\ u(x, t) = 0 & \text{on } \partial\Omega \times (0, T), \\ u(x, 0) = g(x) & \text{in } \Omega, \end{cases}$$

Unlike the traditional POD method, we obtain the snapshots from the adjoint equation as follows:

410 (3.2)
$$\begin{cases} \tilde{u}_t + \mathcal{L}\tilde{u} = 0 & \text{in } \Omega \times (0, T), \\ \tilde{u}(x, t) = 0 & \text{on } \partial\Omega \times (0, T), \\ \tilde{u}(x, 0) = m(x) & \text{in } \Omega, \end{cases}$$

In this case, the snapshots are generated by solving the adjoint equation (3.2) with the given final time measurement m(x) as the initial condition.

Following the standard procedure in section 2.2, we generate the new POD basis functions ψ_k 's from the snapshots $\{\tilde{u}(\cdot, t_0), \tilde{u}(\cdot, t_1), \ldots, \tilde{u}(\cdot, t_M)\}$, where $t_k = k\Delta t$ with $\Delta t = \frac{T}{M}$ and $k = 0, \ldots, M$. Then, we obtain the following error formula, similar to Proposition A.1:

417 (3.3)
$$\frac{\sum_{i=1}^{2M+1} \left\| \tilde{y}_i - \sum_{k=1}^{N_{\text{pod}}} \left(\tilde{y}_i, \psi_k(\cdot) \right)_{L^2(\Omega)} \psi_k(\cdot) \right\|_{L^2(\Omega)}^2}{\sum_{i=1}^{2M+1} \left\| \tilde{y}_i \right\|_{L^2(\Omega)}^2} = \rho,$$

418 where the number N_{pod} is determined according to the decay of the ratio $\rho = \frac{\sum_{k=N_{\text{pod}}+1}^{2M+1} \lambda_k}{\sum^{2M+1} \lambda_k}$.

⁴¹⁹ $\sum_{k=1}^{2M+1} \lambda_k$. ⁴²⁰ We consider using these new POD basis functions to approximate the forward ⁴²¹ problem to accelerate the computation. The fully discrete scheme is constructed on ⁴²² V_{pod} , and the solution is denoted by U_k for $k = 1 \cdots M$ with $M = \frac{T}{\Delta t}$. Specifically, ⁴²³ we seek numerical solutions U_k such that

(3.4)
$$(\bar{\partial}U_k,\psi) + a(U_k,\psi) = 0, \quad \forall \psi \in V_{pod},$$

with $U_0 = g(x)$. We define the solution operator from the initial condition g(x) to the final time solution U_M as S_{pod} , i.e., $S_{\text{pod}}g = U_M$. 427 **3.1. Convergence of the adjoint-POD method.** For any $g \in L^2(\Omega)$, we 428 can write $g = \sum_{k=1}^{\infty} g_k \phi_k$ for a set of coefficients g_k . Let $u = \sum_{k=1}^{\infty} u_k(t)\phi_k$ be the 429 solution of the problem (2.1). Substituting these two expressions of g and u into the 430 first equation of (2.1), we get, by noting the fact that $L\phi_k = \mu_k\phi_k$ and comparing 431 the coefficients of ϕ_k on both sides of the equation, that $u_k(0) = g_k$ and

432
$$u'_k(t) + \mu_k u_k = 0$$
 in $(0, T)$.

433 We can write the solution as $u_k(T) = \alpha_k g_k$, with $\alpha_k = e^{-\mu_k T}$. Noting that 434 $Sg = u(\cdot, T) = \sum_{k=1}^{\infty} u_k(T)\phi_k$, we can formally write

435
$$S\Big(\sum_{k=1}^{\infty} g_k \phi_k\Big) = \sum_{k=1}^{\infty} \alpha_k g_k \phi_k.$$

This representation shows the relationship between the initial condition g and the solution $u(\cdot, T)$ at the final time T. The operator S maps the initial condition to the solution at time T through the coefficients α_k , which depend on the eigenvalues μ_k of the operator L and the final time T. This relationship can be used to analyze the properties of the solution and the backward problem.

441 For simplicity, we approximate the source term g(x) by a finite-dimensional trun-442 cation, i.e.

443 (3.5)
$$g_{\rm app} = \sum_{k=1}^{L} g_k \phi_k.$$

444 Then, the solution u(x,t) of the parabolic equation has the form: $u(\cdot,T) = \sum_{k=1}^{L} e^{-\mu_k T} f_k \phi_k$. After simple calculation, we can also have that $\tilde{u}(x,t) = \sum_{k=1}^{L} e^{-\mu_k T} e^{-\mu_k T} f_k \phi_k$. Constructing the POD basis functions is equivalent to computing the 446 singular value decomposition of the matrix $\tilde{A} = (\tilde{y}_1, ..., \tilde{y}_M)$, where $\tilde{y}_j = (\tilde{u}(x_1, t_j), ...$ 448 $, \tilde{u}(x_N, t_j))^T$. Here $x_1, ..., x_N$ are the finite element nodes in Ω . Suppose A has the 449 singular value decomposition: $A = U\Sigma V$, then the $\psi_k s$ are exactly the first M columns 450 of U.

Let us denote $A = (y_1, ..., y_M)$ and $\tilde{A} = (\tilde{y}_1, ..., \tilde{y}_M)$, the matrix $\Phi = (\phi_1(\vec{x}, t_1), ...$ $\phi_L(\vec{x}, t_1)), F = \text{diag}(f_1, ..., f_L)$ and $D = \text{diag}(e^{-\mu_1 T}, ..., e^{-\mu_L T})$. We also define the $L \times M$ matrix J with entries $J(i, j) = e^{-\mu_i t_j}$. Since the normal orthogonality of the eigenfunctions ϕ_k 's, Φ is a column orthogonal matrix. Using the formulations of uand \tilde{u} , we can represent the matrix A and \tilde{A} as follows:

456 (3.6)
$$A = \Phi F J$$
, and $\tilde{A} = \Phi D F J$.

The matrix representations of A and \tilde{A} provide a concise way to express the relationship between the coefficients of the eigenfunctions ϕ_k and the solutions u(x,t)and $\tilde{u}(x,t)$.

460 Proposition A.1 shows that the low-rank space V_{pod} provides the best N_{pod} -rank 461 approximation of the column space of \tilde{A} . We aim to prove that V_{pod} is also a good 462 approximation of the column space of A, which will confirm the effectiveness of the 463 new POD method. To begin, we establish the connection between the matrices A and 464 \tilde{A} .

LEMMA 3.1. If $L \leq M$, it follows that $span\{y_1, ..., y_M\} = span\{\tilde{y}_1, ..., \tilde{y}_M\}$. Consequently, the column spaces of A and \tilde{A} are identical, i.e., $C(A) = C(\tilde{A})$.

Proof. The proof of this statement is analogous to that of Lemma 2.2, using the 467 fact that the matrix J is a Vandermonde matrix. 468 Π

Using (3.3), we observe that the new POD basis provides a good approximation 469 of $\{\tilde{y}_1, ..., \tilde{y}_M\}$. With the preceding analysis, we aim to demonstrate that the new 470POD basis is also an effective approximation of $\{y_1, ..., y_M\}$. 471

THEOREM 3.2. Using the same notation in this section, we note that if a sufficient 472 number of snapshots are available, i.e., $L \leq M$, then we have 473

474 (3.7)
$$\frac{\sum_{i=1}^{M} ||y_i - P_{pod}y_i||_{L^2(\Omega)}^2}{\sum_{i=1}^{M} ||y_i||_{L^2(\Omega)}^2} \le C e^{2\mu_L T} \rho,$$

where P_{pod} denotes the projection operator on the adjoint-POD space $span\{\psi_1, ..., \psi_n\}$ 475 $\psi_{N_{pod}}$, and $\rho = \frac{\sum_{k=N_{pod}+1}^{M} \lambda_k}{\sum_{k=1}^{M} \lambda_k}$. 476

Proof. In the following proof, we assume L = M for simplicity. For the case 477 L < M, the proof is similar. Using the same notation of Lemma 3.1, Φ and J are 478both invertible square matrices. Then, there exists a unique matrix P such that, 479

$$480 \quad (3.8) \qquad \qquad \Phi DFJP = \Phi FJ,$$

481

where $P = J^{-1}D^{-1}J$. Therefore, we have $y_j = \sum_{i=1}^{L} P_{ij}\tilde{y}_i$. Using the Cauchy-Schwarz inequality, we obtain the following estimate for any 482 $1 \leq j \leq L$, 483

484 (3.9)
$$||y_j - P_{\text{pod}}y_j||^2 \le \sum_{i=1}^L P_{ij}^2 \sum_{i=1}^L ||\tilde{y}_i - P_{\text{pod}}\tilde{y}_i||^2.$$

Hence, we can obtain that 485

486 (3.10)
$$\sum_{j=1}^{L} \|y_j - P_{\text{pod}}y_j\|^2 \le \sum_{i,j=1}^{L} P_{ij}^2 \sum_{i=1}^{L} \|\tilde{y}_i - P_{\text{pod}}\tilde{y}_i\|^2 = \|P\|_F^2 \sum_{i=1}^{L} \|\tilde{y}_i - P_{\text{pod}}\tilde{y}_i\|^2.$$

The remaining part is to estimate the Frobenius norm of P. Since $P = J^{-1}D^{-1}J$, 487 we define that $||P||_d = ||D^{-1}||_2$. It is easy to verify that $|| \cdot ||_d$ is a matrix norm. Then, 488 we obtain 489

490 (3.11)
$$||P||_F \le C||P||_d = C||D^{-1}||_2 \le Ce^{\mu_L T}$$

On the other hand, since Φ is an orthogonal matrix, we have 491

492 (3.12)
$$\sum_{j=1}^{L} \|\tilde{y}_j\|^2 = \|\Phi DFJ\|_F^2 = \|DFJ\|_F^2 \le \|D\|_F^2 \|FJ\|_F^2$$

493 (3.13)
$$\leq C \|FJ\|_F^2 \leq C \sum_{j=1}^L \|y_j\|^2.$$

Aligned with the equation (3.3), we can derive the following estimate: 494

495 (3.14)
$$\frac{\sum_{i=1}^{M} ||y_i - P_{pod}y_i||^2_{L^2(\Omega)}}{\sum_{i=1}^{M} ||y_i||^2_{L^2(\Omega)}} \le C ||P||^2_F \frac{\sum_{i=1}^{M} ||\tilde{y}_i - P_{pod}\tilde{y}_i||^2_{L^2(\Omega)}}{\sum_{i=1}^{M} ||\tilde{y}_i||^2_{L^2(\Omega)}}$$

496 (3.15)
$$\leq C e^{2\mu_L T} \rho.$$

Therefore, we can conclude the inequality with the estimated value of $\mu_i \leq C i^{2/d}$. 497

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3.2. Stochastic convergence of backward problem. To solve this backward
 problem, we use the traditional Tikhonov regularization method,

500 (3.16) $\min_{g \in X} \|\mathcal{S}(g) - m\|_{L^2(\Omega)}^2 + \lambda \|g\|_{L^2(\Omega)}^2,$

501 where λ is the regularization parameter.

502 In the discrete approximation of the regularization problem (3.16), we solve the 503 following least-squares regularized optimization problem:

504 (3.17)
$$\min_{g \in V_{\text{pod}}} \|\mathcal{S}_{\text{pod}}(g) - m\|_{L^2(\Omega)}^2 + \lambda \|g\|_{L^2(\Omega)}^2.$$

We define the functional $\mathcal{J}_{\text{pod}}[g] = \|\mathcal{S}_{\text{pod}}g - m\|_{L^2(\Omega)}^2 + \lambda \|g\|_{L^2(\Omega)}^2$. We can compute the Fréchet derivative of $\mathcal{J}_{\text{pod}}[g]$ and obtain the following iterative scheme:

507 (3.18)
$$g_{k+1} = g_k - \beta d\mathcal{J}_{pod}[g_k], \quad \forall k \in \mathbb{N},$$

where β is the step size, $d\mathcal{J}_{\text{pod}}[g] = \mathcal{S}^*_{\text{pod}}(\mathcal{S}_{\text{pod}}g - m) + \lambda f$, and g_0 is an initial guess. 508 The above theory is based on the assumption of a noise-free case, where the final 509 510time measurement $m = u(\cdot, T)$ is known exactly. However, in practical applications, the measurement data often contains uncertainty. To account for this uncertainty, we assume that the measurement data takes the discrete form $m_i^n = u(d_i, T) + e_i$ for $i = 1, \dots, n$, where e_i denotes the measurement error at the *i*-th point. Based on the 513properties of parabolic equations [36], we know that $||u||_{C([0,T];H^2(\Omega))} \leq C||g||_{L^2(\Omega)}$. 514515Furthermore, according to the embedding theorem of Sobolev spaces, we know that 516 $H^2(\Omega)$ is continuously embedded into $C(\overline{\Omega})$, ensuring that $u(\cdot, T)$ is well-defined pointwise for all $d_i \in \Omega$. 517

518 We repeat the procedure of (2.28) in section 2.3. If we choose the optimal regu-519 larization parameter $\alpha^{1/2+d/8} = O(\sigma n^{-1/2} || u(\cdot, T) ||_{H^2(\Omega)}^{-1})$ (in practice, we chose the 520 optimal parameter using Algorithm 2.3), then the denoised solution *m* achieves the 521 optimal convergence with noise of bounded variance σ^2 given by

522 (3.19)
$$\mathbb{E}\left[\|u(\cdot,T) - m\|_{L^{2}(\Omega)}\right] \leq C\alpha^{1/2} \|u(\cdot,T)\|_{H^{2}(\Omega)}.$$

Assuming that the noise $\{e_i\}_{i=1}^n$ are independent Gaussian random variables with a variance of σ , we can obtain a further result. Specifically, we have:

525 (3.20)
$$\mathbb{P}(\|u(\cdot,T) - m\|_{L^2(\Omega)} \ge \alpha^{1/2} \|u(\cdot,T)\|_{H^2(\Omega)} z) \le 2e^{-Cz^2}$$

In practice, the noise level and the true initial term may be unknown. To determine the optimal regularization parameter α for denoising, we can apply Algorithm 2.3. This algorithm will select a value of α that balances the trade-off between reducing noise and preserving important features of the solution. Using the recovered function m(x), we generate the adjoint POD basis in Section 2.1. It can be shown that, even with uncertainty, the POD basis still provides a good low-rank approximation of the snapshots $\{y_1, ..., y_M\}$. Combining Theorem 3.2 and (3.19), we can deduce that for any $1 \le i \le M$, the following inequality holds:

534 (3.21)
$$||y_i - P_{\text{pod}}y_i||_{L^2(\Omega)}^2 \le C(Me^{2\mu_L T}\rho + \alpha)||g||_{L^2(\Omega)}^2.$$

535 Since we replace the source term with a finite truncation (3.5), we make the 536 assumption that:

537 (3.22)
$$\|g - g_{app}\|_{L^2}^2 \le \varepsilon(L).$$

Using similar techniques to those employed in the proof of Theorem 3.7 in [36], we can derive the following convergence results based on the aforementioned assumptions.

540 THEOREM 3.3. Let $\{e_i\}_{i=1}^n$ be independent random variables satisfying $\mathbb{E}[e_i] = 0$ 541 and $\mathbb{E}[e_i^2] \leq \sigma^2$ for $i = 1, \dots, n$. If we set $\alpha^{1/2+d/8} = O(\sigma n^{-1/2} \|u(\cdot, T)\|_{H^2(\Omega)}^{-1})$ in 542 (2.28) and $\lambda = O(Me^{2\mu_L T}\rho + \alpha)$, then we obtain:

543 (3.23)
$$\mathbb{E}\left[\left\|\mathcal{S}g^* - \mathcal{S}_{pod}g_{pod}\right\|_{L^2(\Omega)}^2\right] \le C\lambda \|g^*\|_{L^2(\Omega)}^2 + C\varepsilon,$$

544 and

545 (3.24)
$$\mathbb{E}\left[\|g^* - g_{pod}\|_{L^2(\Omega)}^2\right] \le C \|g^*\|_{L^2(\Omega)}^2 + C\varepsilon$$

546 Furthermore, if we assume that the noise $\{e_i\}_{i=1}^n$ are independent Gaussian ran-547 dom variables with a variance of σ , we can obtain a stronger type of convergence. A 548 similar proof can be found in [36]. Here, we only present the resulting convergence 549 results.

THEOREM 3.4. Let $\{e_i\}_{i=1}^n$ be independent Gaussian random variables with a variance of σ . If we set $\alpha^{1/2+d/8} = O(\sigma n^{-1/2} ||u(\cdot,T)||_{H^2(\Omega)}^{-1})$ in (2.28) and $\lambda = O(Me^{2\mu_L T}\rho + \alpha)$, then for any z > 0, there exists a constant C such that:

553 (3.25)
$$\mathbb{P}(\|S_{pod}g_{pod} - Sg^*\|_{L^2(\Omega)} \ge (\lambda^{1/2} \|g^*\|_{L^2(\Omega)} + \varepsilon)z) \le 2e^{-Cz^2},$$

554 and

555 (3.26)
$$\mathbb{P}(\|g_{pod} - g^*\|_{L^2(\Omega)} \ge (\|g^*\|_{L^2(\Omega)} + \varepsilon)z) \le 2e^{-Cz^2}.$$

Theorem 3.3 and Theorem 3.4 provide the stochastic convergence rate as $\|Sg^* - S_{\text{pod}}g_{\text{pod}}\|_{L^2(\Omega)}^2 = O_p(\lambda \|g^*\|_{L^2(\Omega)}^2 + \varepsilon)$ in terms of the values λ and ε . These results also provide useful guidance for practical numerical simulations.

4. Numerical examples. This section presents several numerical examples to demonstrate the reconstruction results for the inverse source problem and the backward problem discussed in this paper. Specifically, we consider a parabolic equation as follows:

563 (4.1)
$$\begin{cases} u_t - \Delta u = f(x) & \text{in } \Omega \times (0, T), \\ u(x, t) = 0 & \text{on } \partial \Omega \times (0, T), \\ u(x, 0) = g(x) & \text{in } \Omega, \end{cases}$$

where the domain $\Omega = [0, \pi]^2$, f(x) is the source term, and g(x) is the initial condition. For each observation data set, we first use the backward Euler scheme in time and the linear finite element method (specifically, the P1 element) in space with a mesh size of h = 1/50 and a time step of $\Delta t = T/400$. We use 9 POD basis functions (usually less basis is enough) to compute the inverse problems unless otherwise specified. For the FEM, there are approximately 2500 basis functions.

In [35], the authors have already compared the efficiency of the POD method and the finite element method for solving this inverse problem. They have demonstrated that the POD method achieves a speed-up of at least 6 times, even with 400 finite element basis functions. Therefore, we do not include a comparison with the finite element method in this paper. However, it is worth noting that as the number of finite element basis functions increases, the potential for the POD method to achieve greater speed-up also grows correspondingly. 4.1. Numerical results for inverse source problems. In the following examples, we use the adjoint POD method to recover the source term f as described in Section 2. We obtain the data for the forward problem with the exact source term fat the final time T = 1.

Example 4.1 We first demonstrate the importance of choosing the appropriate POD basis functions. For the same source term, we apply different right-hand sides of equation (2.1) to obtain the POD basis functions. Subsequently, we solve the inverse source problem using these different POD basis functions.

Figure 1 illustrates this process. The true source term is $\sin(2x)\sin(2y)e^{\frac{x+y}{\pi}}$, and its surface plot is shown in Figure 1 (a). Figure 1 (b) presents the reconstruction result obtained using the adjoint POD method proposed in this paper, indicating that our new method effectively and efficiently recovers the source term. Figure 1 (c) displays the result when an incorrect right-hand side is used to generate the POD basis functions. In this case, we use $\sin(x)\sin(y)$ as the right-hand side in (2.1) to generate the POD basis functions. Figure 1 (d) shows the result when we use an *A*-shaped function as the right-hand side to derive the POD basis.

As can be seen, Figure 1 (b) provides a good reconstruction, whereas Figures 1 (c) and (d) yield inaccurate results. The result in Figure 1 (d) is particularly striking, as the recovered image deviates significantly from the exact source term.

In this example, we demonstrate the importance of selecting appropriate basis functions for solving inverse problems. Using an unsuitable set of basis functions can lead to incorrect results. Our proposed adjoint POD method offers a set of suitable basis functions for such problems. In the following examples, we will compare our adjoint POD basis functions with the original true POD basis to validate Theorem 2.3.



(c) Using the POD basis geneerated with the right hand side ated with the right hand side of $\sin(x)\sin(y)$ A shaped function

FIG. 1. The importance of choice of POD basis

Example 4.2 In this example, we first use the true source term as the right-hand 602 side in (2.1) to generate the POD basis. Then, we generate the POD basis using our 603 proposed adjoint POD method. To validate Theorem 2.3, we compare both sets of 604 basis functions and assess their similarity. Figure 2 shows the results when using the 605 exact source term $f^* = \sin(2x)\sin(2y)$. Figure 2 (b) and Figure 2 (c) show that both 606 the traditional POD method and our adjoint POD method recover the true source 607 term accurately. However, our adjoint POD method does not require prior knowledge 608 of the exact source term, while the traditional POD method does, leading to the 609 so-called inverse crime. 610

Figure 3 presents the results for an exact source term f^* in the form of a Z-shaped function. This example also illustrates the efficiency of the POD method in solving inverse problems compared to the finite element method. Figure 3 (c) and Figure 3 (e) show that both traditional POD and our adjoint POD method yield basis functions that contain critical information about the exact source term we aim to recover. In contrast, the basis functions of the finite element method do not contain any prior





(b) Recovered result by tradi- (c) Result by the adjoint POD tional POD with exact right hand side

FIG. 2. Comparison of basis between traditional POD and the adjoint POD for $f = \sin(2x)\sin(2y)$.



FIG. 3. Comparison of basis between traditional POD and the adjoint POD for f^* of Z-shaped function.

In the previously mentioned cases, all measured data were noise-free. We will now examine highly challenging cases with noise levels ranging from 10% to 50% to test the denoising method described in Section 2.3. Example 4.3 In this example, we will evaluate the robustness of the adjoint POD method in the presence of noise. We consider the measurement data to be $m_i^n = u(d_i, T) + \sigma e_i, i = 1, \dots, n$, where d_i represents positions within the domain Ω , and $\{e_i\}_{i=1}^n$ are independent standard normal random variables. We will take 2500 positions d_i uniformly distributed over the domain Ω .

Figure 4 demonstrates the robustness of our method in the presence of significant noise. Even with a 50% noise level, where the measured data is entirely obscured by noise as shown in Figure 4 (c), our method is still able to recover the source term as depicted in Figure 4 (f).



FIG. 4. Robustness of the adjoint POD against the noise for $f = \sin(2x)\sin(2y)e^{\frac{x+y}{\pi}}$.

Example 4.4 In this example, we demonstrate the effect of choosing different 630 numbers of our new POD basis and verify the convergence of our POD method. Figure 631 5 illustrates this test. We see that as the number of our POD basis increases, the 632 reconstruction error decays rapidly; see Figure 5 (f). We observe exponential decay 633 from our numerical experiments. Even for a complicated function with a 'Z' shape, we 634 can obtain satisfactory results with just 10 POD basis functions. As the number of our 635 POD basis increases, the reconstruction becomes increasingly accurate, as depicted 636 in Figure 5 (a) - (e). 637

4.2. Numerical results for backward problems. In this subsection, we apply the new POD method to recover the initial condition g, as discussed in Section 3. We collect the data at the time T = 0.05. Since most of the examples are similar to what we did in section 4.1, we may not explain the setting of numerical examples in detail.

Example 4.5 In this example, we demonstrate the importance of POD basis,
 similar to what we did in Example 4.1. We solve the backward problem using different
 POD basis functions.



FIG. 5. Effects of the numbers of POD basis.

Figure 6 illustrates the corresponding results. The true initial condition is $\sin(2x)$ sin $(2y)e^{\frac{x+y}{\pi}}$, and its surface plot is shown in Figure 6 (a). Figure 6 (b) presents the reconstruction result using our adjoint POD method. Figure 6 (c) shows the result when we use an incorrect initial condition to generate the POD basis functions, and Figure 6 (d) displays the result when we use an A-shaped function as the initial condition to generate the POD basis functions.

Example 4.6 In the following two examples, we adopt the approach of example
4.2. We first use the true initial condition as the initial condition in Eq. (3.1) to
generate the POD basis functions. Then, we generate the POD basis functions using
our proposed adjoint POD method.

Figure 7 shows the results obtained by using the exact source term $g^* = \sin(2x)$ sin $(2y)e^{\frac{x+y}{\pi}}$. Figures 7 (b) and 7 (c) demonstrate that both the traditional POD and our adjoint POD methods work well in recovering the true initial condition. However, our adjoint POD method does not require prior knowledge of the exact initial condition. Figure 8 shows the results using the exact initial condition g^* of the A-shaped function.

In the above numerical examples in this subsection, all the measured data are noise-free. Now, we test the denoising method discussed in Section 3.2 by examining very challenging cases with noise levels ranging from 10% to 50%.

Example 4.7 Similar to Example 4.3, we test the robustness of the adjoint POD method against noise. We take the measurement data as $m_i^n = u(d_i, T) + \sigma e_i$, for $i = 1, \dots, n$, where d_i s represent the positions inside Ω , $\{e_i\}_{i=1}^n$ are independent standard normal random variables, and σ is the noise level. We use 2500 positions d_i uniformly distributed over the domain Ω . Figure 9 demonstrates that our method is robust even in the presence of significant noise. Remarkably, even with 50% noise, when the measured data is completely obscured by noise as shown in Figure 9 (c), we



(c) Using the POD basis geneerated with the initial term ated with the initial term of A-sin(x)sin(y) shaped function

FIG. 6. The importance of choice of POD basis



FIG. 7. Comparison of basis between traditional POD and the adjoint POD for $f = sin(2x)sin(2y)e^{\frac{x+y}{\pi}}$.

672 can still recover the initial condition, as seen in Figure 9 (f).

Example 4.8 Finally, we study a more interesting case. Although the inverse 673 source problem and the backward problem are two distinct problems, we have ob-674served from the previous numerical examples that they share some commonalities. 675Specifically, the POD basis functions for both problems contain critical information 676 about the functions one wants to recover. As a result, we employ the POD basis 677 678 functions derived from the inverse source problem to solve the backward problem. Please refer to Figure 10 for the reconstruction results. This example also shows that 679 the inverse source problem and the backward problem share similar basis functions 680 from the point of view of the POD method. This similarity can also be explained by 681682 the theory of semi-groups and spectral analysis.



(a) Exact initial condition

(b) Recovered result by tradi- (c) Result by the adjoint POD tional POD with exact initial term

FIG. 8. Comparison of basis between traditional POD and the adjoint POD for f^* of A shaped function.



FIG. 9. Robustness of the adjoint POD against the noise for g = sin(2x)sin(2y).

5. Conclusion. In this paper, we have developed a novel POD-based model re-683 duction method for solving parabolic inverse problems, specifically focusing on inverse 684 source and inverse initial value problems. By leveraging the intrinsic low-dimensional 685 structures in the parabolic equations, we have successfully developed POD basis func-686 tions that reduce computational costs while maintaining accuracy in solving parabolic 687 688 inverse problems. Our primary contribution is the effective addressing of the inverse crime issue associated with traditional model reduction methods for solving PDEs, 689 690 which is a common challenge encountered by traditional POD methods for solving inverse problems. Furthermore, we have provided convergence analysis for our proposed 691 method and demonstrated its accuracy and efficiency through numerical examples. 692 The results show that our proposed method overcomes the inverse crime issue and 693 694 produces superior results compared to traditional methods. Therefore, our proposed



FIG. 10. Solve the backward problem using the basis from the inverse source problem.

695 method provides a promising avenue for solving parabolic inverse problems with high 696 accuracy and computational efficiency.

Acknowledgement. The research of W. Zhang is supported by the National
Natural Science Foundation of China under grant numbers 12371423 and 12241104.
The research of Z. Zhang is supported by the National Natural Science Foundation
of China under grant number 12171406, Hong Kong RGC grant projects 17307921
and 17304324, Seed Funding for Strategic Interdisciplinary Research Scheme 2021/22
(HKU), and Seed Funding from the HKU-TCL Joint Research Centre for Artificial
Intelligence.

Appendix A. Proper orthogonal decomposition (POD) method. 704 Assuming that $u \in H^1_0(\Omega)$ is the solution to the weak formulation of the parabolic 705equation (1.1), the construction of POD basis functions requires solution snapshots. 706 These solution snapshots can be obtained through various technological means related 707 to a specific application, such as experimental data or numerical methods. For in-708 stance, one can measure the solution at different times using sensors in experimental 709710 settings to obtain the solution snapshots. Alternatively, one can use FEM to solve the parabolic equation numerically and obtain the solution snapshots. 711

Given a set of solutions at different time instances $\{u(\cdot,t_0), u(\cdot,t_1), \ldots, u(\cdot,t_M)\}$, where $t_k = k\Delta t$ with $\Delta t = \frac{T}{M}$ and $k = 0, \ldots, M$, we first obtain the solution snapshots $\{y_1, \ldots, y_{M+1}, y_{M+2}, \ldots, y_{2M+1}\}$, where $y_k = u(\cdot, t_{k-1}), k = 1, \ldots, M + 1$, and $y_k = \overline{\partial} u(\cdot, t_{k-M-1}), k = M + 2, \ldots, 2m + 1$ with $\overline{\partial} u(\cdot, t_k) = \frac{u(\cdot, t_k) - u(\cdot, t_{k-1})}{\Delta t}, k = 1, \ldots, M$. The POD basis functions $\{\psi_k\}_{k=1}^{N_{\text{pod}}}$ are constructed by minimizing the following projection error:

718 (A.1)
$$\frac{1}{2m+1} \left(\sum_{j=0}^{M} \| u(t_j) - \sum_{k=1}^{N_{\text{pod}}} (u(t_j), \psi_k)_{L^2(\Omega)} \psi_k \|_{L^2(\Omega)}^2 \right)$$

719 (A.2)
$$+ \sum_{j=1}^{M} \left\| \overline{\partial} u(t_j) - \sum_{k=1}^{N_{\text{pod}}} (\overline{\partial} u(t_j), \psi_k)_{L^2(\Omega)} \psi_k \right\|_{L^2(\Omega)}^2 \right)$$

subject to the constraints that $(\psi_{k_1}(\cdot), \psi_{k_2}(\cdot))_{L^2(\Omega)} = \delta_{k_1k_2}, 1 \le k_1, k_2 \le N_{\text{pod}}$, where $\delta_{k_1k_2} = 1$ if $k_1 = k_2$, otherwise $\delta_{k_1k_2} = 0$. Here, N_{pod} denotes the number of POD basis functions that will be extracted from solution snapshots. Let $V_{\text{pod}} = \text{span}\{\psi_1, \dots, \psi_{N_{\text{pod}}}\}$ denote the finite-dimensional space spanned by the POD basis functions. Using the method of snapshot proposed by Sirovich [33], we know that the minimizing problem can be reduced to the following eigenvalue problem:

727 (A.3)
$$Kv = \mu v$$

where the correlation matrix K is computed from the solution snapshots $\{y_1, y_2, \ldots, y_{2M+1}\}$ with entries $K_{ij} = (y_i, y_j)_{L^2(\Omega)}, i, j = 1, \ldots, 2M+1$, and K is symmetric and semi-positive definite. We sort the eigenvalues in a decreasing order as $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{2m+1}$ and the corresponding eigenvectors are denoted by $v_k, k = 1, \ldots, 2M+1$. It can be shown that if the POD basis functions are constructed by

733 (A.4)
$$\varphi_k(\cdot) = \frac{1}{\sqrt{\lambda_k}} \sum_{j=1}^{2M+1} (v_k)_j u(\cdot, t_j), \quad 1 \le k \le N_{\text{pod}},$$

where $(v_k)_j$ is the *j*-th component of the eigenvector v_k , they minimize the projection error.

The approximation error for the POD method has been studied extensively in the literature, particularly in the works [21] and [3].

PROPOSITION A.1 (Section 3.3.2, [21] or p. 502, [3]). Let $\lambda_1 \geq \lambda_2 \geq ... \geq$ 739 $\lambda_{2M+1} \geq 0$ denote the non-negative eigenvalues of the correlation matrix K in the r40 eigenvalue problem (A.3). Then, $\{\psi_k\}_{k=1}^{N_{pod}}$ constructed according to the method of r41 snapshots (A.4) is the set of POD basis functions, and we have the following error r42 formula:

743 (A.5)
$$\frac{\sum_{i=1}^{2M+1} \left\| \tilde{y}_i - \sum_{k=1}^{N_{pod}} \left(\tilde{y}_i, \psi_k(\cdot) \right)_{L^2(\Omega)} \psi_k(\cdot) \right\|_{L^2(\Omega)}^2}{\sum_{i=1}^{2M+1} \left\| \tilde{y}_i \right\|_{L^2(\Omega)}^2} = \frac{\sum_{k=N_{pod}+1}^{2M+1} \lambda_k}{\sum_{k=1}^{2M+1} \lambda_k},$$

744 where the number N_{pod} is determined by the decay of the ratio $\rho = \frac{\sum_{k=N_{pod}+1}^{2M+1} \lambda_k}{\sum_{k=1}^{2M+1} \lambda_k}$.

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