

Adjoint-based gradient estimation for gray-box solutions of unknown conservation laws

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1 Abstract

Many engineering applications can be formulated as optimizations constrained by conservation laws. Such optimizations can be efficiently solved by the adjoint method, which computes the gradient of the objective to the design variables. Traditionally, the adjoint method has not been able to be implemented in many “gray-box” conservation law simulators. In gray-box simulators, the analytical and numerical form of the conservation law is unknown, but the full solution of relevant flow quantities is available. In this paper, we consider the case where the flux function is unknown. This article introduces a method to estimate the gradient by inferring the flux function from the solution, and then solving the adjoint equation of the inferred conservation law. This method is demonstrated in the sensitivity analysis of two flow problems.

2 Background

Optimization problems are of great interest in the engineering community. We consider an optimization problem to be constrained by conservation laws. For example, oil reservoir simulations may employ PDEs of various flow models, in which different fluid phases and components satisfy a set of conservation laws. Such simulations can be used to facilitate the oil reservoir management, including optimal well placement [3] and optimal production control [1, 2]. Another example is the cooling of turbine airfoils. We are interested in optimizing the interior flow path of turbine airfoil cooling to minimize pressure loss [4, 5].

In many cases, such simulations can be computationally costly, potentially due to the complex computational models involved, and large-scale time and space discretization. Furthermore, the dimensionality of the design space, d , can be high. For example, in oil reservoir simulations, the well pressure can be controlled at each well individually, and they can vary in time. To parameterize the well pressure, we require Nm number of design variables, where N is the number of wells, and m is the number of parameters, to describe the variation in time for each well. Similarly, in turbine airfoil cooling, the geometry of the internal flow path can also be parameterized by many variables. Optimizing a high-dimensional design, c , can be challenging. A tool to enable efficient high-dimensional optimization is adjoint sensitivity analysis [8-11], which efficiently computes the gradient of the objective to the design variables. The continuous adjoint method solves a continuous adjoint equation derived from the conservation law, which requires the PDE of the conservation law. The discrete adjoint method solves a discrete adjoint equation derived from the numerical implementation of the conservation law, which requires the simulator's numerical implementation. Adjoint automatic differentiation applies the chain rule to every elementary arithmetic operation of the simulator, which requires accessing and modifying the simulator's source code.

We are interested in gray-box simulations. By gray-box, we mean a conservation law simulation without the adjoint method implemented. Furthermore, we are not able to implement the adjoint method when the governing PDE for the conservation law and its numerical implementation is unavailable: for example, when the source code is proprietary or legacy. Another defining property of gray-box simulation is that it can provide the space-time solution of the conservation law. If the simulation solves for time-independent problems, a gray-box simulation should be able to provide the steady state solution. In contrast, we define a simulator to be a blackbox, if neither the adjoint nor the solution is available. The only output of such simulations is the value of the objective function to be optimized. If the adjoint method is implemented or is able to be implemented, we call such simulations open-box. We summarize their differences in Table 1.

Table 1: Comparison of black-box, gray-box, and open-box simulations

	PDE and implementation	Space (or space-time) solution	Adjoint
Black-box	✗	✗	✗
Gray-box	✗	✓	✗
Open-box	✓	✓	✓

Depending on the type of simulation involved, we may choose different optimization methods. If the simulation is black-box, we may use derivative-free optimization methods. Derivative-free methods require only the availability of the objective function value, but not the derivative information [14]. Such methods are popular because they are easy to use. However, when the dimension of the design space increases, derivative-free methods may suffer from the curse of dimensionality. The curse of dimensionality refers to problems caused by the rapid increase in the search volume associated with adding an extra dimension in the search space. The resulting increase of search volume increases the number of objective evaluation required. It is not uncommon to encounter tens or hundreds of dimensions in real life engineering problems, making derivative-free methods computationally expensive.

If the simulation is open-box, we may use gradient-based optimization methods. Such methods use the gradient information to locate a local optimum. A well-known example is the quasi-Newton method [13]. When the design space is high-dimensional, gradient-based methods can require fewer objective evaluations to converge than derivative-free methods. Let c be the design variables, u be the flow solution, and J be the objective value. Gradient-based optimization methods require $\frac{dJ}{dc} = \frac{\partial J}{\partial c} + \frac{\partial J}{\partial u} \frac{du}{dc}$, the total derivative of the objective to the design variables. The term $\frac{dJ}{dc}$ can be evaluated efficiently by using adjoint methods. The continuous adjoint method derives the continuous adjoint equation from the PDE of the simulation through the method of the Lagrange multiplier; therefore, it requires knowing the PDE of the simulator. The discrete adjoint method applies variational analysis to the discretized PDE, and it requires knowing the discretized PDE of the simulator. The discrete adjoint method can be implemented by using automatic differentiation (AD). AD decomposes the simulation into elementary arithmetic operations and functions, and then applies the chain rule to compute the gradient. Because adjoint methods require access to the PDE and its discretization, they cannot be directly applied to

gray-box simulations.

If the simulation is gray-box, we cannot apply the adjoint method to the gray-box conservation law to compute the gradient. In current practice, gray-box simulations are often treated as black-box simulations, to which adjoint-based optimization is not applicable. The gray-box simulation is viewed as a calculator for the objective, while its space-time solution is neglected. This paper introduces a method to enable adjoint-based optimization on gray-box simulations. We propose a two-step procedure to estimate the objective’s gradient by using the gray-box simulation’s space-time solution. In the first step, we infer the conservation law governing the simulation by using its space-time solution. In the second step, we apply the adjoint method to the inferred conservation law to estimate the gradient.

In the remainder of the paper, Section 3 defines the particular type of gray-box models considered in this paper. Section 4 explains why it can be feasible to infer the governing PDE from the output of the gray-box model, i.e. the space-time solution. Section 5 describes how the PDE can be inferred. Section 7 demonstrates that our method works on a 1-D porous media flow problem and a 2-D Navier-Stokes flow problem.

3 Optimization constrained by gray-box conservation laws

3.1 Problem definition

We consider the optimization problems which are constrained by the solution of two types of conservation laws. The first type of problems is the space-time solution of conservation laws

$$\dot{\mathbf{u}} + \nabla \cdot \mathbf{F}(\mathbf{u}) = \mathbf{q}(\mathbf{u}, c) \quad (1)$$

where \mathbf{u} is a vector representing flow quantities, $\dot{\mathbf{u}}$ is the derivative of \mathbf{u} with respect to time, c represents the design variables, $t \in [0, T]$ is time; and $x \in \Omega \subseteq \mathbb{R}^n$ is the spatial coordinate. Ω may depend on the design variables, c . \mathbf{F} is the flux tensor. \mathbf{q} is a source vector that may also depend on c . The boundary and initial conditions are known. The discretized space-time solution of Eqn.(1) given by a gray-box simulation is written as $\hat{u}(t_i, \mathbf{x}_i; c), i = 1, \dots, N$, where $t = \{t_1, \dots, t_N\}$ indicates the discretized time,

and \mathbf{x}_i indicates the spatial discretization at time t_i .

The second type is the steady state solution of conservation laws

$$\nabla \cdot \mathbf{F}(\mathbf{u}_\infty) = \mathbf{q}_i(\mathbf{u}_\infty, c) \quad (2)$$

where \mathbf{u}_∞ is the converged solution of Eqn.(1) at $t \rightarrow \infty$.

For both types of solutions, we assume \mathbf{F} in Eqns.(1) or (2) are unknown, so the simulations that generate the solutions are gray-box.

We are interested in estimating the gradient of

$$J = \int_0^T \int_{\Omega} j(\mathbf{u}, c) d\mathbf{x} dt \quad (3)$$

and

$$J = \int_{\Omega} j(\mathbf{u}_\infty, c) d\mathbf{x} \quad (4)$$

with respect to the control c , using the time-dependent and the steady state solutions respectively. Notice that j can depend explicitly on c , while u depends implicitly on c .

3.2 Examples of optimization constrained by gray-box simulation

We provide two examples to illustrate conservation laws with unknown fluxes. The first example is a 1-D two-phase flow in porous media [6]. The governing equation can be written as

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} F(u) = c \quad (5)$$

where $x \in [0, 1]$ is the space domain; $u = u(t, x)$, $0 \leq u \leq 1$, is the saturation of phase I (e.g. water), and $1 - u$ is the saturation of phase II (e.g. oil); $c = c(t, x)$ is the design variable. $c > 0$ models the injection of phase I replacing phase II; and $c < 0$ represents the opposite. F is an unknown flux that depends on the properties of the porous media and the fluids.

The second example is a 2-D Navier-Stokes flow for a fluid with an unknown state equation. Let ρ , u , v , E , and p denote the density, Cartesian velocity components, total energy, and pressure. The

governing equation is

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho u \\ \rho u^2 + p - \sigma_{xx} \\ \rho uv - \sigma_{xy} \\ u(E\rho + p) - \sigma_{xx}u - \sigma_{xy}v \end{pmatrix} + \frac{\partial}{\partial y} \begin{pmatrix} \rho v \\ \rho uv - \sigma_{xy} \\ \rho v^2 + p - \sigma_{yy} \\ v(E\rho + p) - \sigma_{xy}u - \sigma_{yy}v \end{pmatrix} = \mathbf{0} \quad (6)$$

where

$$\begin{aligned} \sigma_{xx} &= \mu \left(2 \frac{\partial u}{\partial x} - \frac{2}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right) \\ \sigma_{yy} &= \mu \left(2 \frac{\partial v}{\partial y} - \frac{2}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right) \\ \sigma_{xy} &= \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \end{aligned} \quad (7)$$

The pressure is governed by an unknown state equation

$$p = p(U, \rho) \quad (8)$$

where U denotes the internal energy per volume,

$$U = \rho \left(E - \frac{1}{2}(u^2 + v^2) \right). \quad (9)$$

The state equation depends on the property of the fluid.

4 Infer conservation laws by the space-time solution

Because Eqns. (1) or (2) have an unknown flux, the adjoint method cannot be applied to evaluate $\frac{dJ}{dc}$.

To enable the adjoint method in such a scenario, we will infer the unknown flux.

We use the space-time solution of the gray-box simulations to infer the flux. There are several benefits by using the space-time solution [7, 8]. Firstly, in conservation law simulations, the flow quantities only depend on the flow quantities in a previous time inside a domain of dependence. When the timestep is small, the domain of dependence can be small, as well. For example, for scalar conservation laws without exogenous control, we can view solving the conservation law for one timestep Δt at a spatial location as a mapping $\mathbb{R}^{\omega_{\Delta t}} \rightarrow \mathbb{R}$, where $\omega_{\Delta t} \in \Omega$ is the domain of dependence. By applying such mapping repeatedly to all $x \in \Omega$ and $t \in [0, T]$ (in addition to the boundary and initial conditions), we perform

a space-time simulation of the conservation law. Generally, the size of $\omega_{\Delta t}$ is small. Therefore, in the discretized simulation of conservation laws, the number of discretized flow variables involved in $\omega_{\Delta t}$ is small, as well, making it feasible to infer the mapping.

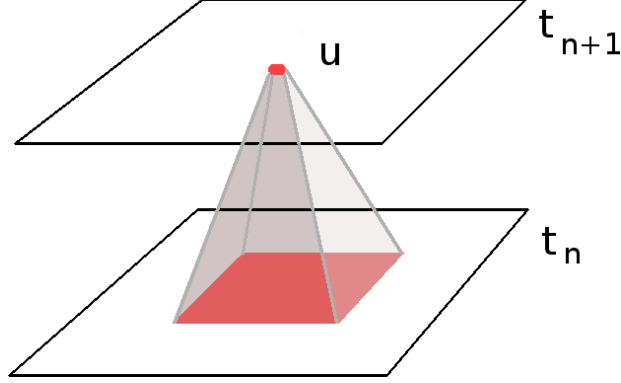


Figure 1: Domain of dependence: in conservation law simulations, the flow quantities at a given location depend on the flow quantities at an older time only within its domain of dependence. The two planes in this figure indicates the spatial solution at two adjacent timesteps. The domain of dependence can be much smaller than the overall spatial domain when the timestep is reasonably small.

Secondly, the space-time solution at almost every space-time grid point can be viewed as a sample for the mapping $\mathbb{R}^\omega \rightarrow \mathbb{R}$. Because the number of space-time grid points in gray-box simulations is generally large, we have a large number of samples to infer the mapping. In Eqn.(1) and (2), such a mapping is determined by the flux. Therefore, we will have a large number of samples to infer the flux, making the inference potentially accurate.

Thirdly, in many optimization problems, the design space is high dimensional only because the design is space- and/or time-dependent. In order to parameterize the space-time dependent design, a large number of design variables will be employed. However, the flow quantities only depend on the design variables in the domain of dependence. Therefore, even if the overall number of design variables is high, the number of design variables involved in the mapping is limited, making the inference problem

potentially immune to the design space dimensionality.

Therefore, we propose to infer the flux in Eqn.(1) or (2). The inferred PDE should yield a solution, $\tilde{\mathbf{u}}$, that matches the solution of the gray-box simulation, \mathbf{u} . A simulator of the inferred PDE is called the twin model.

5 Twin model inference as an optimization problem

Conventionally, we have a given PDE, and want to compute its space-time solution. However, in a twin model, we want to infer the PDE to match a given space-time solution. Finding a suitable PDE, specifically a suitable flux function, can be viewed as an inverse problem, which can be solved by optimization. We define a metric for the mismatch of the space-time solutions. Given the same inputs (design variables, initial conditions, and boundary conditions), a twin model should yield a space-time solution $\tilde{\mathbf{u}}$ such that $\tilde{\mathbf{u}}$ is close to \mathbf{u} . Let the space-time solution to the gray-box PDE and twin model PDE be u and \tilde{u} . Suppose that the twin model and the primal model use the same discretization; we use the following expression to quantify the mismatch:

$$\mathcal{M} = \frac{1}{T} \int_0^T \int_{\Omega} (\tilde{u} - u)^2 d\Omega \approx \frac{1}{T} \sum_{i=1}^N \sum_{k=1}^M (\tilde{\mathbf{u}}_{ik} - \mathbf{u}_{ik})^2 \Delta t_k |\Delta \mathbf{x}_i| \quad (10)$$

where $|\Delta \mathbf{x}_i|$ indicates the lengths (1-D), areas (2-D), or volumes (3-D) of the grid. If the space- and/or time-grids are different, then a mapping P from u to \tilde{u} is required. In this case, the mismatch can be approximated by

$$\mathcal{M} \approx \frac{1}{T} \sum_{i=1}^N \sum_{k=1}^M (\tilde{\mathbf{u}}_{ik} - P(\mathbf{u})_{ik})^2 \Delta t_k |\Delta \mathbf{x}_i| \quad (11)$$

For the present examples, we assume that the grids are the same for the purpose of simplicity.

We parameterize the flux function and infer the parameterization that minimizes \mathcal{M} . Let the parameterized flux function be $G(\tilde{\mathbf{u}}, \xi)$, where ξ values are the parameters. The inference problem is stated as follows:

Solve

$$\xi^* = \arg \min_{\xi} \{\mathcal{M} + \lambda \|\xi\|^p\} \quad (12)$$

where $\tilde{\mathbf{u}}$ is the discretized space-time solution of

$$\dot{\tilde{\mathbf{u}}} + \nabla \cdot G(\tilde{\mathbf{u}}, \xi) = \mathbf{q}(\tilde{\mathbf{u}}, c) \quad (13)$$

$\lambda \|\xi\|^p$ is an L_p norm regularization, and $\lambda > 0$. The space-time discretization of Eqn.(13) is the same as the gray-box simulator.

Similarly, if we are interested in the steady state solution, we have

$$\mathcal{M} = \frac{1}{T} \sum_{i=1}^N (\tilde{\mathbf{u}}_i - \mathbf{u}_i)^2 |\Delta \mathbf{x}_i| \quad (14)$$

The inference problem is stated as follows:

Solve

$$\xi^* = \arg \min_{\xi} \{\mathcal{M} + \lambda \|\xi\|^p\} \quad (15)$$

where u is the discretized spatial solution of the gray-box simulation, and \tilde{u} is the discretized spatial solution of

$$\nabla \cdot G(\tilde{\mathbf{u}}, \xi) = \mathbf{q}(\tilde{\mathbf{u}}, c) \quad (16)$$

The match of space-time solutions does not ensure the match of flux functions. The problem can be ill-posed to infer F on a domain not covered by the gray-box solution u . In other words, the basis for modeling the flux may be over-complete. We will call a domain of u “excited” if inferring F is well-posed on that domain. The ill-posedness can be alleviated by basis selection. It has been shown that basis selection can be performed by Lasso regularization corresponding to $p = 1$ [16]. We will set $p = 1$ in this article.

Because the twin model is an open-box system, Eqns.(12) and (15) can be solved by adjoint gradient-based methods. The parameterization of the twin model flux G will be problem-dependent. We will discuss this topic in Section 7.

5.1 Selecting the flux basis

two issues. 1. Range of flux function being defined. Excited domain definition. Select a region that include the gray solution 2.

Next, we consider choosing an appropriate basis library g . Many basis can be used, such as polynomial basis, Fourier basis, and wavelet basis. For the example of inferring the 1D conservation law, we are interested in inferring the flux. The addition of a constant to the flux function does not change the conservation law, therefore we are actually interested in inferring the derivative of the flux. We will use sigmoid functions as the basis, because the derivative of sigmoid functions is almost zero except at the region close to its center.

Although the objective is to minimize $\sum_{i=1}^N \sum_{k=1}^T (\tilde{u}_{ik} - u_{ik})^2 \Delta t_k |\Delta \mathbf{x}_i|$, we will not use it as the objective function directly and perform optimization in one shot. If $\tilde{F}(u)$ deviates from $F(u)$ a lot, then $\tilde{u}(x, t)$ can deviate from $u(x, t)$ significantly even at a small t . Therefore, solving the twin model and its adjoint in $t = [0, T]$ without an educated $\tilde{F}(u)$ can be a waste of computation resources. To improve efficiency, we propose a progressive optimization procedure:

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 $\xi^* = \mathbf{0};$ 

Set integers  $2 = i_1 < \dots < i_M = T$ ;

for  $I = i_1, \dots, i_M$  do
    Optimize
        
$$\xi^* \leftarrow \arg \min_{\xi} \sum_{i=1}^N \sum_{k=1}^I (\tilde{u}_{ik} - u_{ik})^2 \Delta t_k |\Delta \mathbf{x}_i|$$

        with initial guess  $\xi^*$ .
end

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Algorithm 1: Progressive optimization procedure

Notice $k = 1$ corresponds to the initial condition. Since the twin model uses the same initial condition as the black-box model, $\tilde{u}_{i1} - u_{i1}$ is always zero. Choosing the integer sequence i_1, \dots, i_M can be problem dependent. Our experience shows the sequence should be denser at small i , and sparser at larger i . The tolerance of each sub-optimization problem does not need to be tight, except for the last iteration where $I = T$. In our problem, we use $i_l = \min \{1 + 2^l, T\}$, a relative tolerance of 10%, and maximum 10

iterations for the sub-optimization problems.

6 Excited domain and basis selection

The basis for modelling the flux or the source term may be over-complete. In other words, the inference may be ill-posed and not has a unique solution. A twin model with a basis selection scheme should be able to adaptively refine its basis on-the-fly during fitting the basis coefficients ξ . For example, in the Buckley-Leverett equation example, the value of $u(t, x)$, $t \in [0, T]$, $x \in [0, 1]$ is bounded, i.e. $0 < u_{\min} \leq u(t, x) \leq u_{\max} < 1$; therefore as long as $\nabla \tilde{F}(u) = \nabla F(u)$ for $u \in [u_{\min}, u_{\max}]$, we will have $\tilde{u}(t, x) = u(t, x)$ for $t \in [0, T]$ and $x \in [0, 1]$. In other words, in the numerical example, $\nabla \tilde{F}(u) = \nabla F(u)$ for $u \in [0, 1]$ is a sufficient but not necessary condition for $\tilde{u}(t, x) = u(t, x)$. Intuitively, for some domains u , $\nabla \tilde{F}(u)$ has to approximate $\nabla F(u)$ accurately in order to give a good space-time solution match. We will call such domains *excited domain*, written as \mathcal{E} . Notice the excited domain is not a domain of space or time. Clearly \mathcal{E} depends on $u(t, x)$. For u not inside \mathcal{E} , $\nabla \tilde{F}(u)$ will have little or no effect on the solution match; therefore we may not certify $\nabla \tilde{F}(u)$'s accuracy outside \mathcal{E} no matter how closely the solutions match. Basis selections should only be navigated to \mathcal{E} .

Consider a twin model solving

$$\frac{\partial \tilde{u}(t, x)}{\partial t} + \nabla \cdot \tilde{F}(\mathcal{D}\tilde{u}, \kappa) = q(\tilde{u}, c(t, x)), \quad \tilde{u}(t, x) \in \mathbb{R}^n, \quad (17)$$

We define the excited domain \mathcal{E} by its complement $\bar{\mathcal{E}}$:

Definition 1. *Given a primal model, its discretized solution of $u(t, x)$, and a twin model Eqn(17), the excited domain \mathcal{E} is a domain of $\tilde{F}(\cdot)$. Let the complement of \mathcal{E} be $\bar{\mathcal{E}}$. Consider a perturbed twin model flux $\tilde{F}_\delta(\cdot) = F(\cdot) + \delta(\cdot)$. The perturbed twin model gives the discretized solution \tilde{u}_δ .*

A set $e \subseteq \bar{\mathcal{E}}$ if and only if

$$\frac{1}{T} \sum_{i=1}^N \sum_{k=1}^T (\tilde{u}_{\delta, ik} - u_{ik})^2 \Delta t_k |\Delta \mathbf{x}_i|$$

is a constant for any δ with $\text{support}[\delta] = e$.

This definition requires F a priori, therefore it is not directly implementable. The definition also requires enumeration of all possible δ to validate \mathcal{E} . In practice, we can only validate a finite set of δ , for example the basis function library g .

Basis selection may be performed by regularization [16, ?]. For example, it has been shown that basis selection can be performed by having a Lasso regularization term in the solution mismatch. In our problem, the metric of solution mismatch with Lasso regularization would be

$$\frac{1}{T} \sum_{i=1}^N \sum_{k=1}^T (\tilde{u}_{\epsilon\delta,ik} - u_{ik})^2 \Delta t_k |\Delta \mathbf{x}_i| + \lambda \|\xi\|_1, \quad (18)$$

where $\|\cdot\|_1$ is the L_1 norm.

7 Numerical examples

In this section, we demonstrate the twin model with two numerical examples.

7.1 Gradient estimation for a 1-D porous media flow

Consider a 1-D PDE

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = c \quad x \in [0, 1] \quad t \in [0, 1] \quad (19)$$

with periodic boundary condition

$$u(x=0) = u(x=1) \quad (20)$$

and initial condition

$$u(t=0) = u_0 \quad (21)$$

Eqn.(19) can be used to model 1-D, two-phase, porous media flow, where u denotes the saturation of one phase. $0 \leq u \leq 1$. $c = c(t, x)$ is a space-time dependent exogenous control. The flux function $F(u)$ depends on the properties of the porous media and the fluids. For example, the Buckley-Leverett

equation models the flow driven by capillary pressure and Darcy's law [6], whose flux is

$$F(u) = \frac{u^2}{1 + A(1 - u)^2} \quad (22)$$

where A is a constant. In the following we assume the graybox simulation solves Eqn.(19) and (22) with $A = 2$.

Assuming that $F(u)$ is unknown, we will fit a twin model using the graybox simulation. We parameterize the twin model according to Eqn.(13)

$$\frac{\partial \tilde{u}}{\partial t} + \frac{\partial}{\partial x} \left(\sum_{k=1}^m \xi_k g_k(\tilde{u}) \right) = c \quad (23)$$

with the same initial condition, boundary conditions, and exogenous control.

Generally, the flux F is a monotonic increasing function. To respect this fact, we choose g values as a family of sigmoid functions

$$g_k(\tilde{u}) = \left(\tanh \left(\frac{\tilde{u} - \eta_k}{\sigma} \right) + 1 \right) / 2 \quad (24)$$

where η_k and σ are constants. Therefore, we just need to set $\xi \geq 0$ to enforce the monotonicity of the flux. We will use a second-order finite volume discretization and Crank-Nicolson time integration scheme in the twin model.

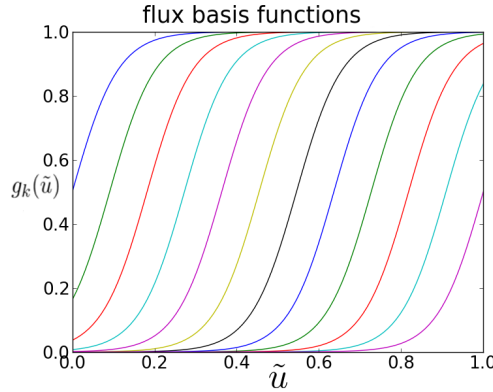


Figure 2: An example of the flux basis functions $g_k(\tilde{u})$. These basis functions are distinguished by different colors.

To infer the coefficients ξ , we minimize

$$\int_0^1 \int_0^1 (u - \tilde{u})^2 dx dt + \lambda \sum_{k=1}^m |\xi_k| \quad (25)$$

We use the low-memory Broyden-Fletcher-Goldfarb-Shannon (BFGS) algorithm [15] for the minimization. L-BFGS approximates the Hessian using only the gradients at newer previous iterations, and inverses the approximated Hessian efficiently using the Sherman-Morrison formula. The gradient, $\frac{dJ}{d\xi_k}, k = 1, \dots, m$, is computed by an automatic differentiation module *numpad*

[Q. Wang, <https://github.com/qiqi/numpad.git>.]

We set $c = 0$, and test the quality of the twin model given several initial conditions. These initial conditions are shown in Fig. 3. For different initial conditions, the excited domain will be different. Let $u_{\max} = \max_{t,x} u(t, x)$ and $u_{\min} = \min_{t,x} u(t, x)$, we expect the inferred flux to match the true flux within $[u_{\min}, u_{\max}]$.

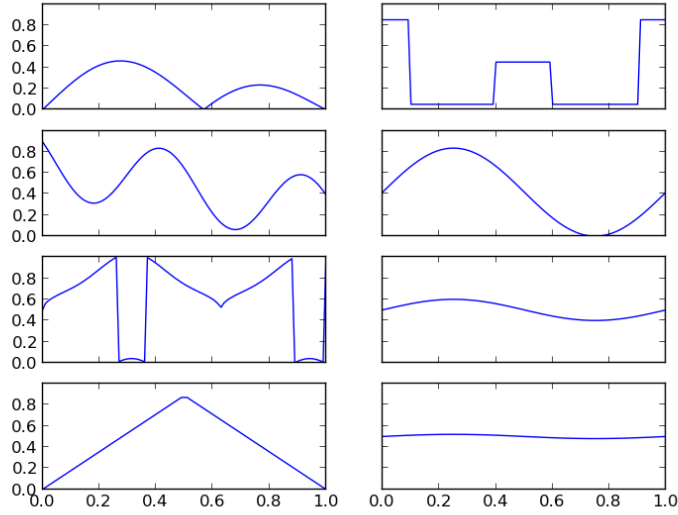
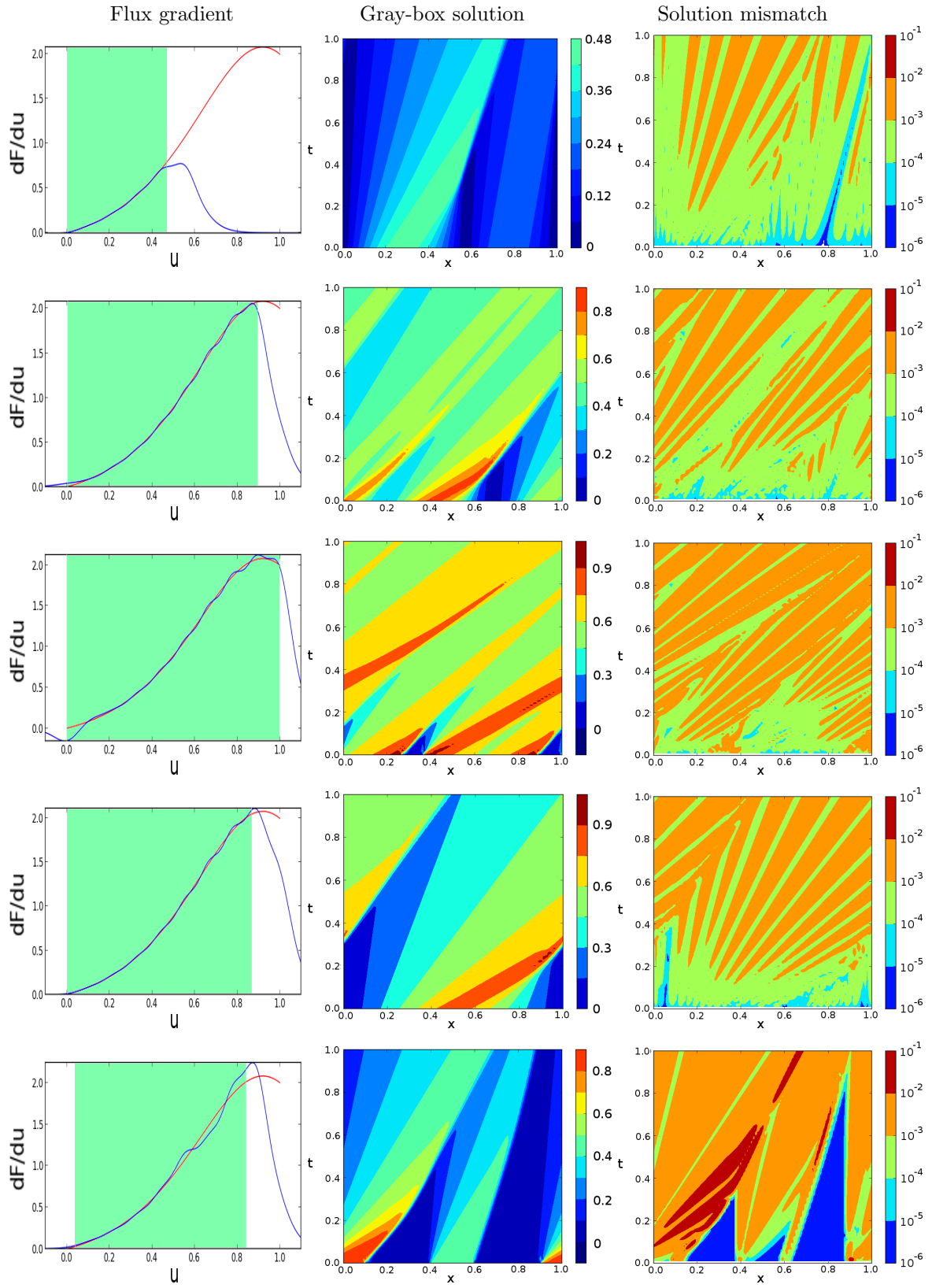


Figure 3: Initial condition $u_0(x)$. We choose a diverse set of initial conditions to test the twin model method.

In Eqn.(1), we can add a constant to the flux while yielding the same solution u . Therefore, we compare $\frac{dF}{du}$ with $\frac{d\tilde{F}}{du}$, instead of comparing F with \tilde{F} . We also show the space-time solution of the gray-box simulation, as well as the solution mismatch, for these initial conditions.



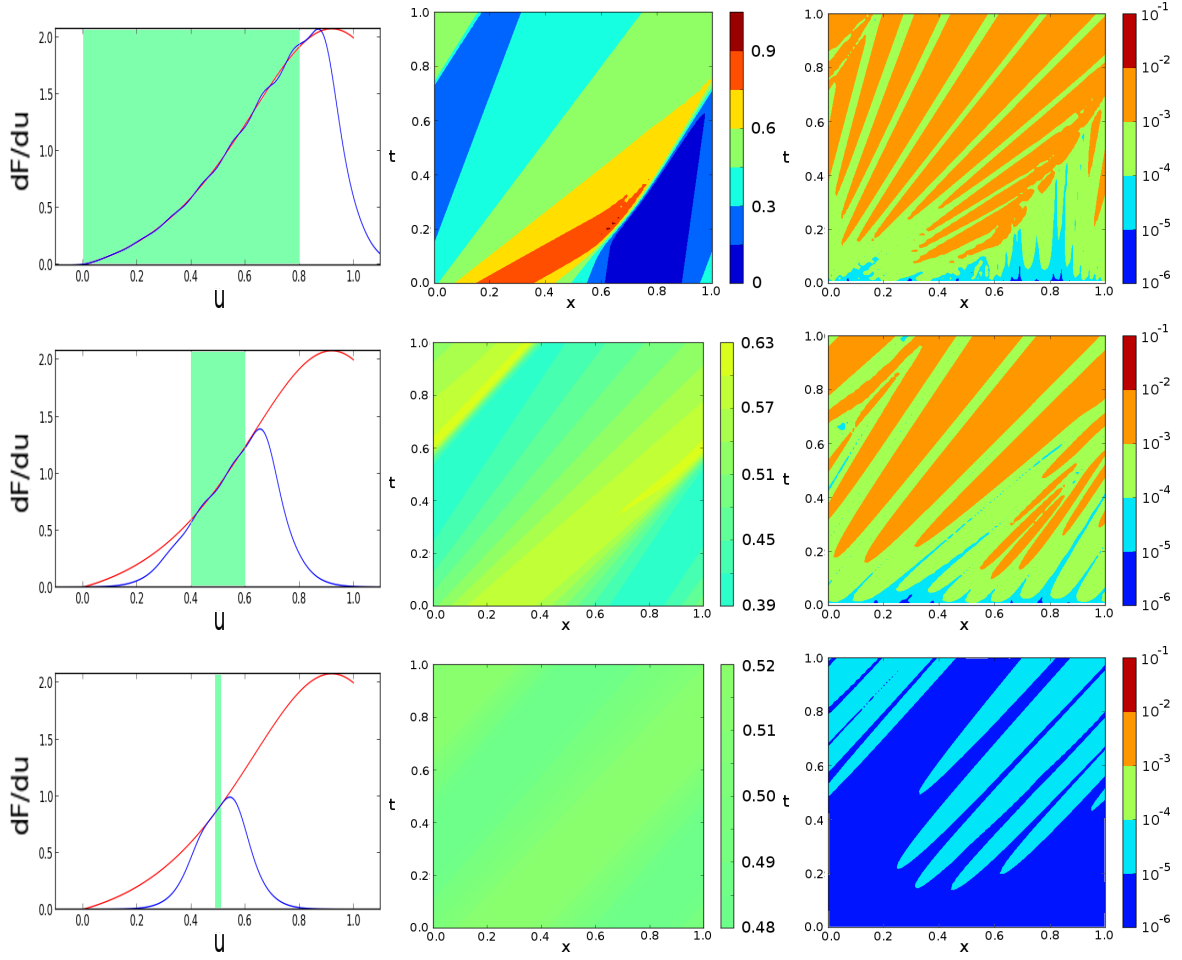


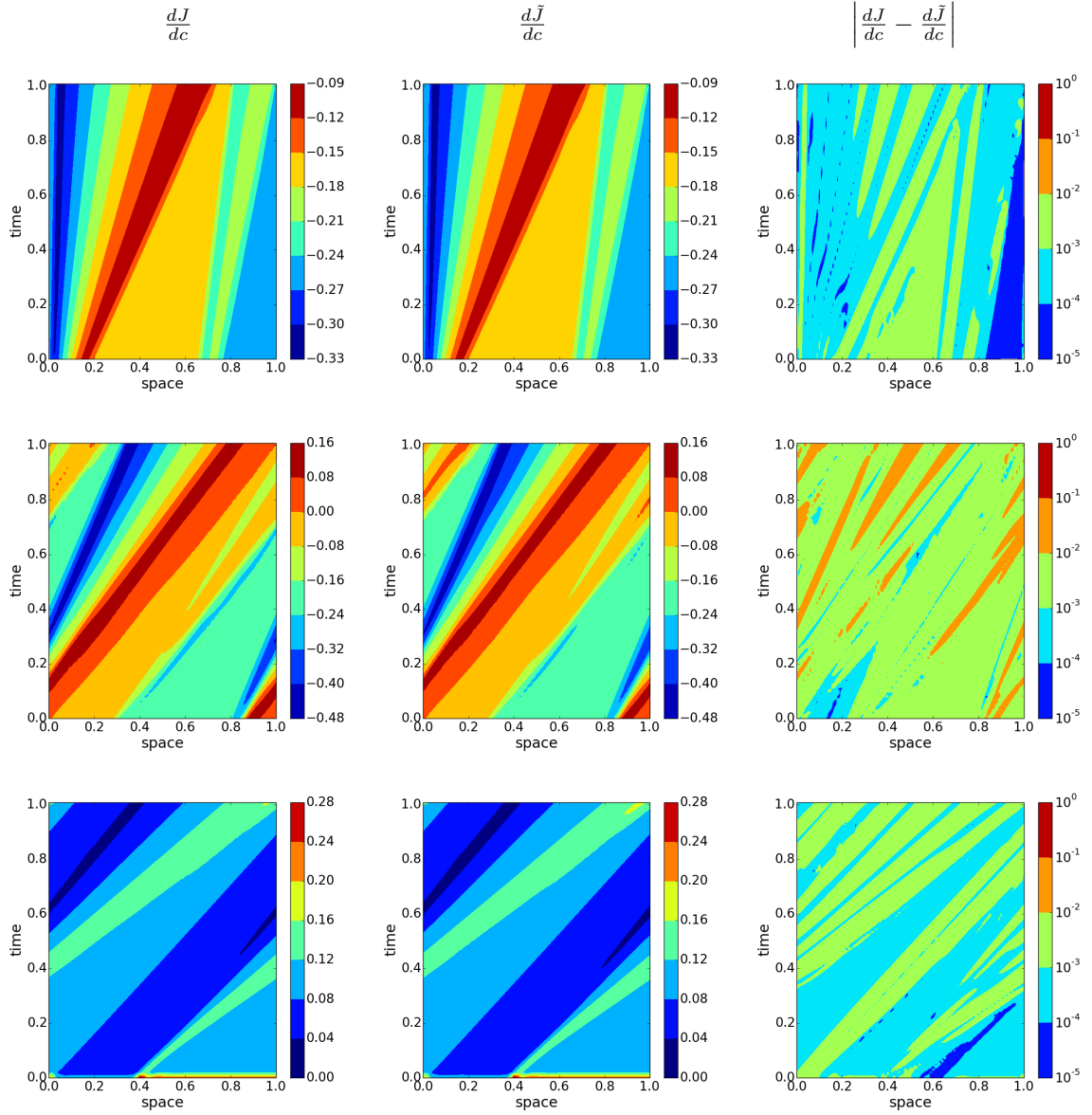
Figure 4: The left column shows the gradient of F (red line) with the gradient of \tilde{F} (blue line). The middle column shows the space-time solutions of the gray-box model. The right column shows the solution mismatch $|u - \tilde{u}|$. Each row corresponds to an initial condition. The excited domain, $[u_{\min}, u_{\max}]$, is indicated by the green region in the left column. When the excited domain is large, the twin model's flux approximates the gray-box model's flux in a large range of u , but the solution mismatch tends to be less accurate in the excited domain. When the excited domain is small, the twin model's flux approximates the gray-box model's flux in a small range of u , but the flux approximation tends to be more accurate in the excited domain.

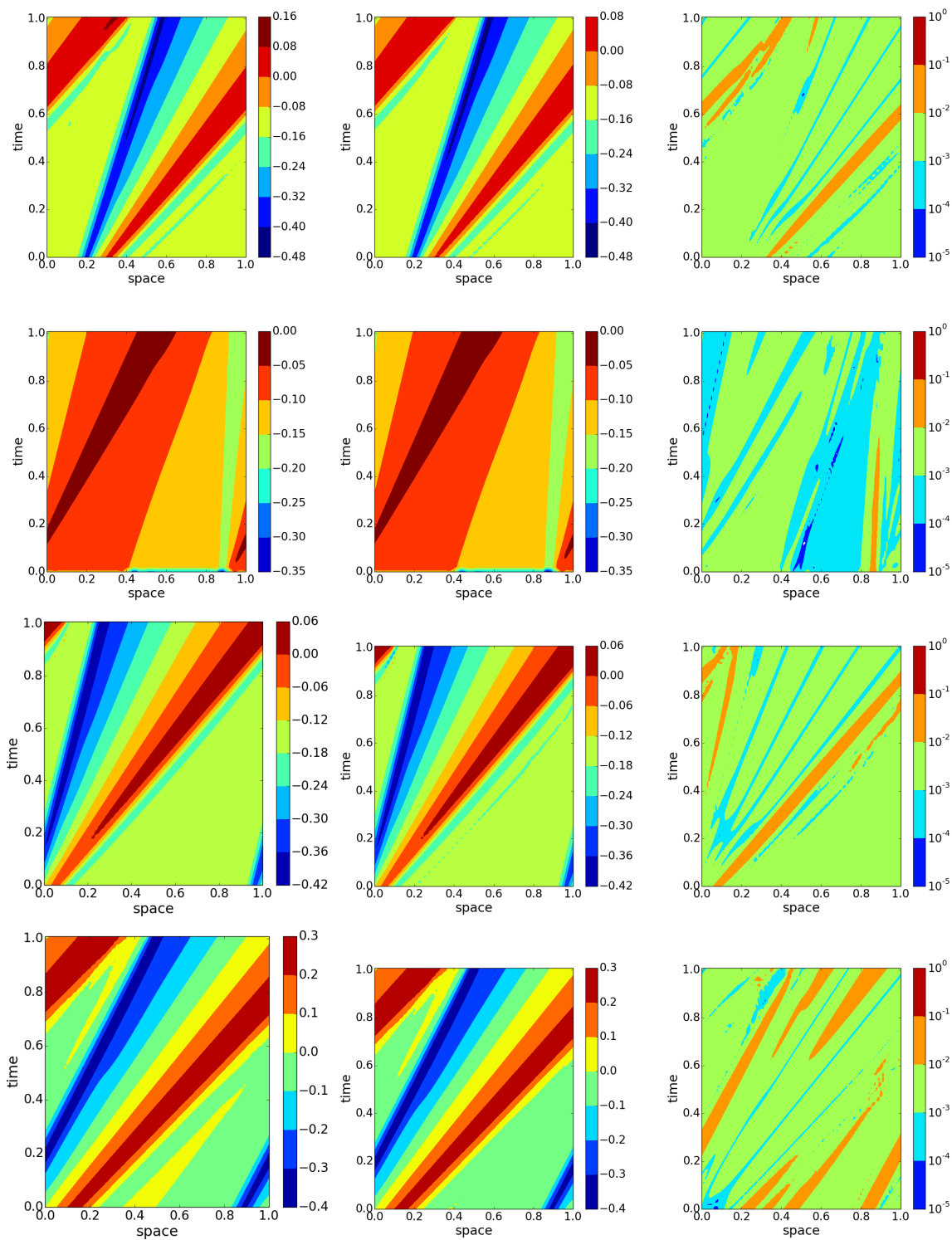
Using the twin model, we can estimate the objective's gradient by applying the adjoint method to

the twin model, i.e. we approximate $\frac{\partial J}{\partial u}$ with $\frac{\partial \tilde{J}}{\partial u}$. Suppose the gray-box model solves

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} (F(u)) = c \quad (26)$$

for $c = 0$, with $F(u)$ given by Eqn.(22) with $A = 2$. We have trained a twin model Eqn.(23) using the space-time solution. We are interested in the approximation quality of the twin model's gradient at $c = 0$. c is space-time dependent, therefore $\frac{dJ}{dc}$ is space-time dependent too. We compare $\frac{dJ}{dc}$ with $\frac{d\tilde{J}}{dc}$ in Fig. 5.





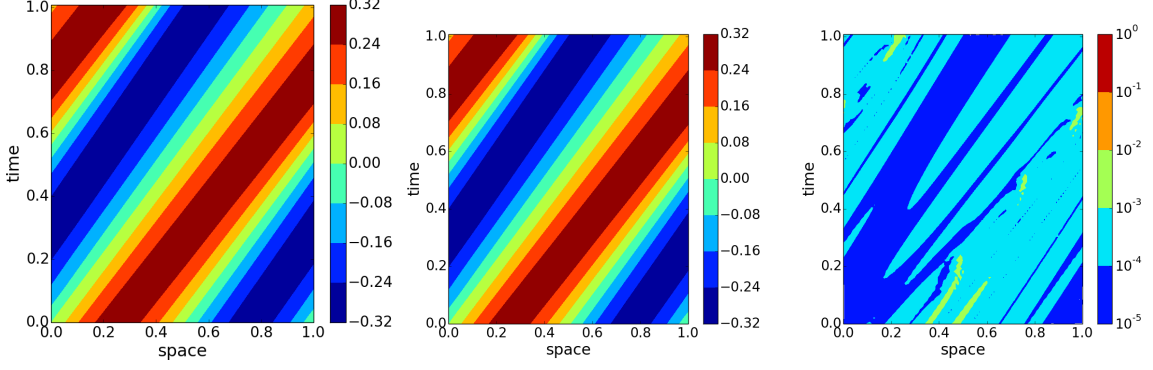


Figure 5: The left column shows $\frac{dJ}{dc}$ which is evaluated by the gray-box model. The middle column shows $\frac{d\tilde{J}}{dc}$ which is evaluated by the trained twin model. The right column shows $\left| \frac{dJ}{dc} - \frac{d\tilde{J}}{dc} \right|$. We observe that the gradient is more accurate when the excited domain is smaller.

The result is encouraging, as the gradient computed by the twin model provides a good approximation of the gradient of the primal model. We reiterate that the good approximation quality benefits from the matching of the space-time solution.

7.2 Gradient estimation of Navier-Stokes flows

In the second numerical test case, we consider a compressible internal flow in a 2-D return bend channel. The flow is driven by the pressure difference between the inlet and the outlet. The flow is governed by Navier-Stokes equations, Eqn.(6). Navier-Stokes equations require an additional state equation, Eqn.(8), for closure. Many models of the state equations have been developed, including the ideal gas equation, the van der Waals equation, and the Redlich-Kwong equation [17].

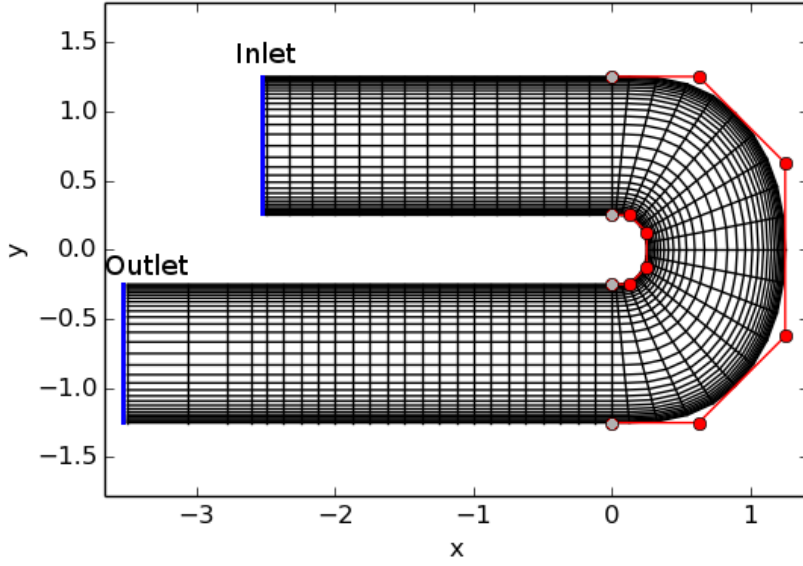


Figure 6: The return bend geometry and the mesh for simulation. The return bend is bounded by no-slip walls. The values of pressure are fixed at the inlet and at the outlet. The inner and outer boundaries of the bend are generated by the control points using quadratic B-spline. We estimate the gradient of the steady state mass flux to the red control points' coordinates.

The inner and outer boundaries at the bending section are each generated by 6 control points using quadratic B-spline. The control points are shown by the red and gray dots in Fig. 6. The gray control points are fixed on the straight sections. The spanwise grid is generated by geometric grading. The streamwise grid at the straight and the bending section are each generated by uniform grading, except at the sponge region. The pressure at the outlet is set to be a constant p_{out} while the total pressure at the inlet is set to be a constant $p_{t,in}$. Let ρ_∞ be the steady state density, and $\mathbf{u}_\infty = (u_\infty, v_\infty)$ be the steady state Cartesian velocity. The steady state mass flux is

$$J = - \int_{\text{outlet}} \rho_\infty u_\infty|_{\text{outlet}} dy = \int_{\text{inlet}} \rho_\infty u_\infty|_{\text{inlet}} dy \quad (27)$$

We want to estimate the gradient of the steady state mass flux to the red control points' coordinates.

When the state equation of the fluid is unknown, the adjoint method cannot be applied directly to

estimate the gradient. We use the proposed twin model to infer the state equation from the steady state solution of the gray-box simulation. Assume that the gray-box simulation provides ρ_∞ , \mathbf{u}_∞ , and E_∞ .

Fig. 7 shows an example of the solution.

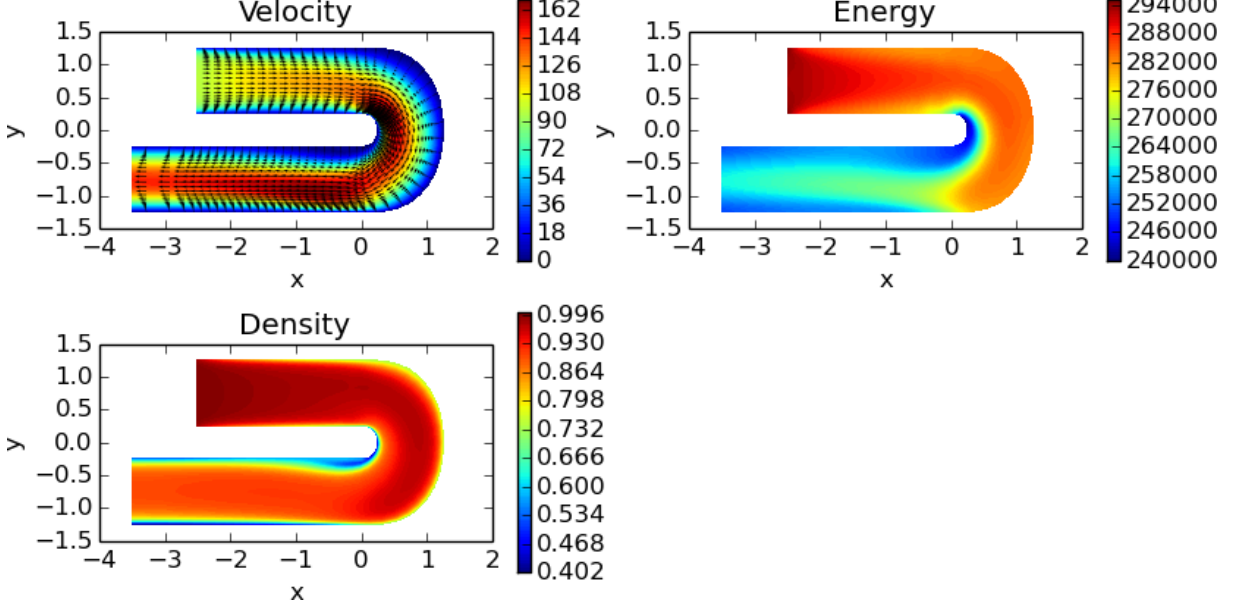


Figure 7: An example of the steady state velocity, energy, and density provided by the gray-box simulation. In the velocity subplot, the magnitude of the velocity is overlaid with the velocity vectors.

We parameterize the unknown state equation by

$$p(\rho, U) = \sum_{i=1}^{N_\rho} \sum_{j=1}^{N_U} \alpha_{ij} R_i(\rho) S_j(U) + p_0 \quad (28)$$

where

$$R_i(\rho) = \exp\left(\frac{-(\rho - \rho_i)^2}{\sigma_\rho}\right), \quad i = 1, \dots, N_\rho \quad (29)$$

$$S_j(U) = \frac{1}{2} \left(\tanh\left(\frac{U - U_j}{\sigma_U}\right) + 1 \right) \quad j = 1, \dots, N_U. \quad (30)$$

R_i are radial basis functions, and S_j are sigmoid functions. Let the density of the gray-box solution be in the range of $[\rho_{\min}, \rho_{\max}]$, and let the internal energy of the gray-box solution be in the range of $[U_{\min}, U_{\max}]$. We set ρ_i , $i = 1, \dots, N_\rho$ to be equally spaced in $[\rho_{\min}, \rho_{\max}]$, and set U_j , $j = 1, \dots, N_U$ to be equally spaced in $[U_{\min}, U_{\max}]$. We constrain α values to be positive to respect the fact that pressure

monotonically increases with the internal energy. p_0 is a scalar. We set $\sigma_\rho = \frac{\rho_{\max} - \rho_{\min}}{N_\rho}$, $\sigma_U = \frac{U_{\max} - U_{\min}}{N_U}$.

We define the solution mismatch, Eqn.(14), as

$$\mathcal{M} = w_\rho \|\tilde{\rho}_\infty - \rho_\infty\|^2 + w_u \|\tilde{u}_\infty - u_\infty\|^2 + w_v \|\tilde{v}_\infty - v_\infty\|^2 + w_E \|\tilde{E}_\infty - E_\infty\|^2 \quad (31)$$

where w_ρ , w_u , w_v , and w_E are positive weight constants. $\|\cdot\|$ is the L_2 norm. To infer the state equation we solve the optimization problem:

$$\min_{\alpha, p_0} \left\{ \mathcal{M} + \lambda \sum_{i=1}^{N_\rho} \sum_{j=1}^{N_U} |\alpha_{ij}| \right\} \quad (32)$$

We need to choose suitable weights w_ρ , w_u , w_v , and w_E in Eqn.(32). To select these weights, we first set α and p_0 values to several randomly guessed values. Using these guessed state equation, we obtain $\|\tilde{\rho}_\infty - \rho_\infty\|^2$, $\|\tilde{u}_\infty - u_\infty\|^2$, $\|\tilde{v}_\infty - v_\infty\|^2$, and $\|\tilde{E}_\infty - E_\infty\|^2$. The weights are chosen to be

$$\begin{aligned} w_\rho &= \frac{1}{\langle \|\tilde{\rho}_\infty - \rho_\infty\|^2 \rangle} \\ w_u &= \frac{1}{\langle \|\tilde{u}_\infty - u_\infty\|^2 \rangle} \\ w_v &= \frac{1}{\langle \|\tilde{v}_\infty - v_\infty\|^2 \rangle} \\ w_E &= \frac{1}{\langle \|\tilde{E}_\infty - E_\infty\|^2 \rangle} \end{aligned} \quad (33)$$

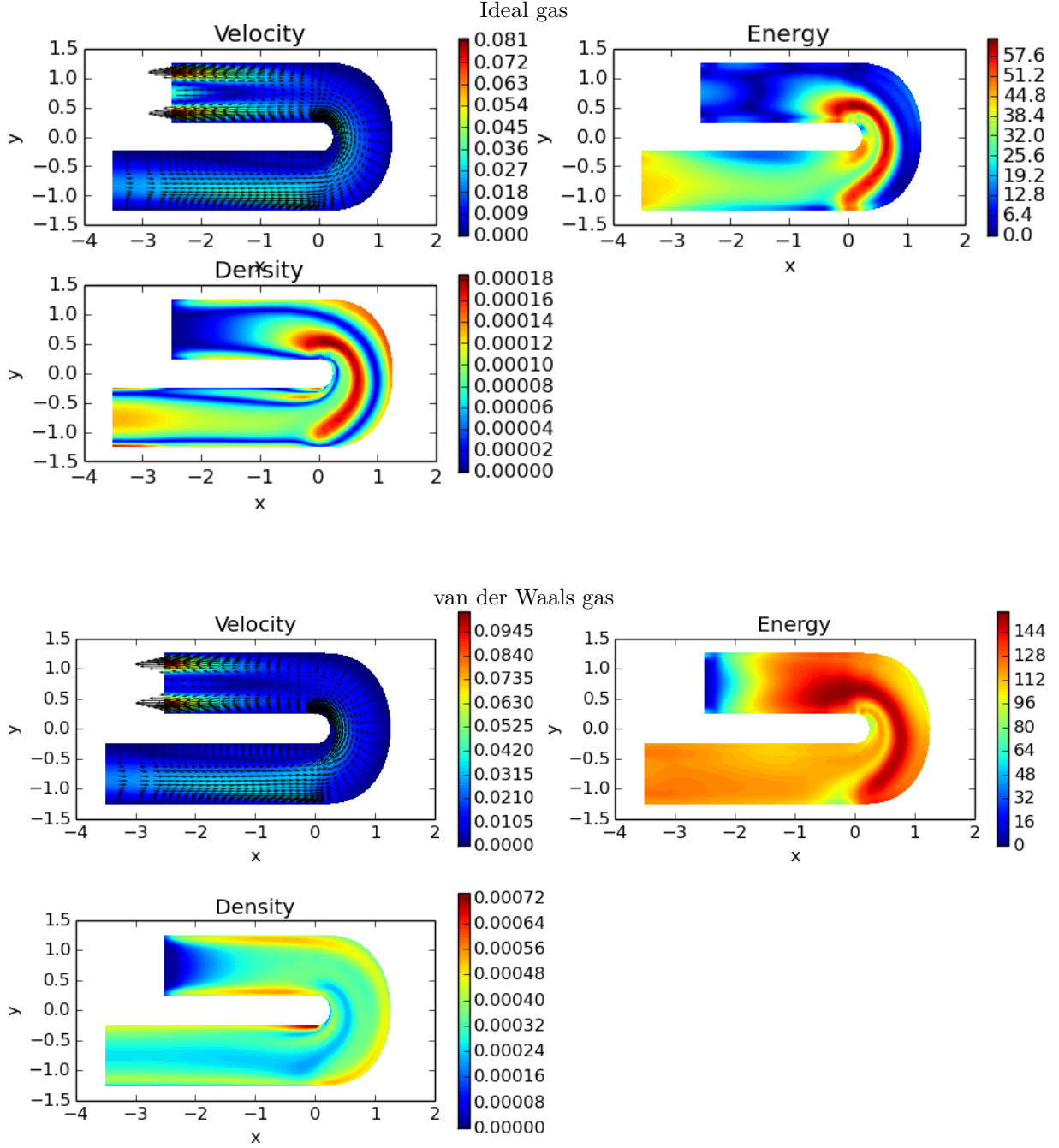
where $\langle \cdot \rangle$ denotes the sample average of the randomly-guessed state equations. In this way, $\tilde{\rho}_\infty - \rho_\infty$, $\tilde{u}_\infty - u_\infty$, $\tilde{v}_\infty - v_\infty$, and $\tilde{E}_\infty - E_\infty$ will, on average, contribute similarly to the solution mismatch for the randomly-guessed state equations.

We tested three example state equations in the graybox simulator: the ideal gas equation, the van der Waals equation, and the Redlich-Kwong equation:

$$\begin{aligned} p_{ig} &= (\gamma - 1)U \\ p_{vdw} &= \frac{(\gamma - 1)U}{1 - b_{vdw}\rho} - a_{vdw}\rho^2 \\ p_{rk} &= \frac{(\gamma - 1)U}{1 - b_{rk}\rho} - \frac{a_{rk}\rho^{5/2}}{((\gamma - 1)U)^{1/2}(1 + b_{rk}\rho)} \end{aligned} \quad (34)$$

where a_{vdw} , b_{vdw} , a_{rk} , b_{rk} are constants. In the following testcases, we choose $a_{vdw} = 10^4$, $b_{vdw} = 0.1$, $a_{rk} = 10^7$, $b_{rk} = 0.1$.

By solving Eqn (32), we obtain the solution mismatch for the state equations. The solution mismatch, $|\tilde{\rho} - \rho|$, $|\tilde{\mathbf{u}} - \mathbf{u}|$, and $|\tilde{E} - E|$, between the inferred twin model's solution and the graybox solution is shown in Fig. 8.



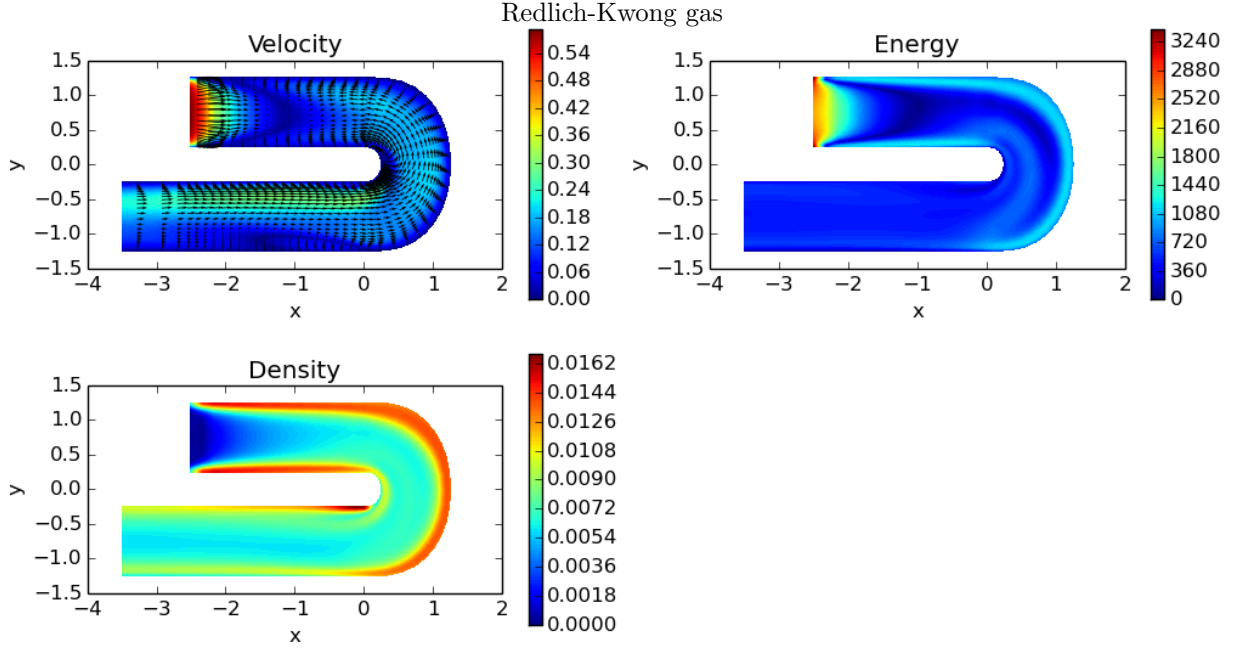
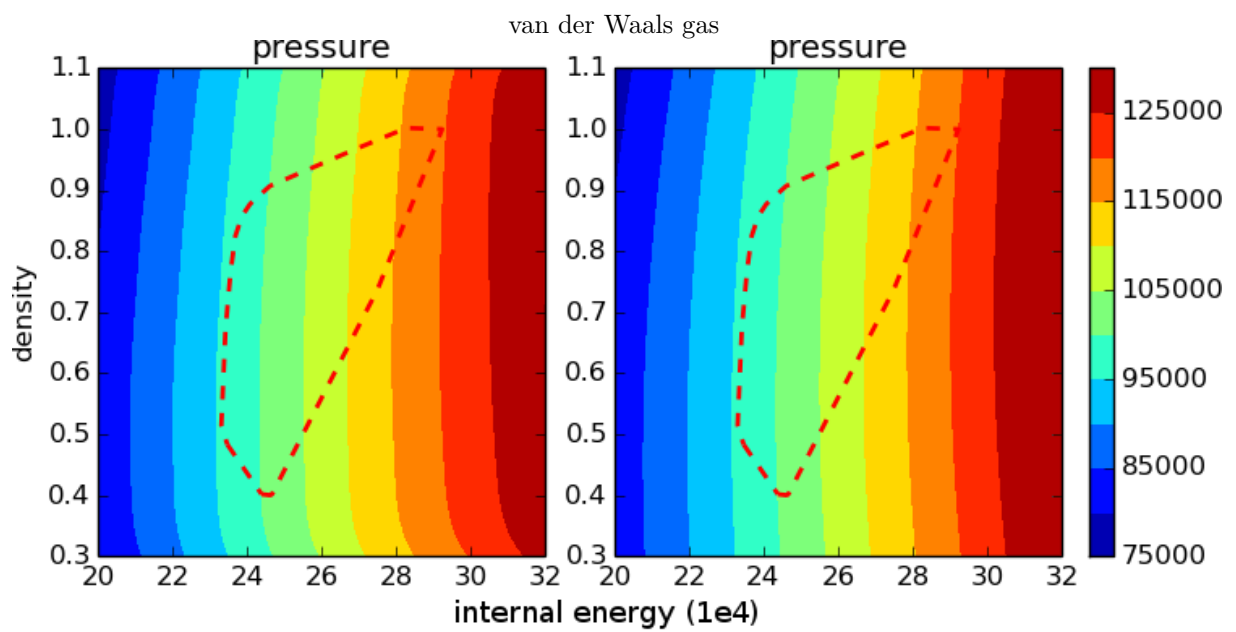
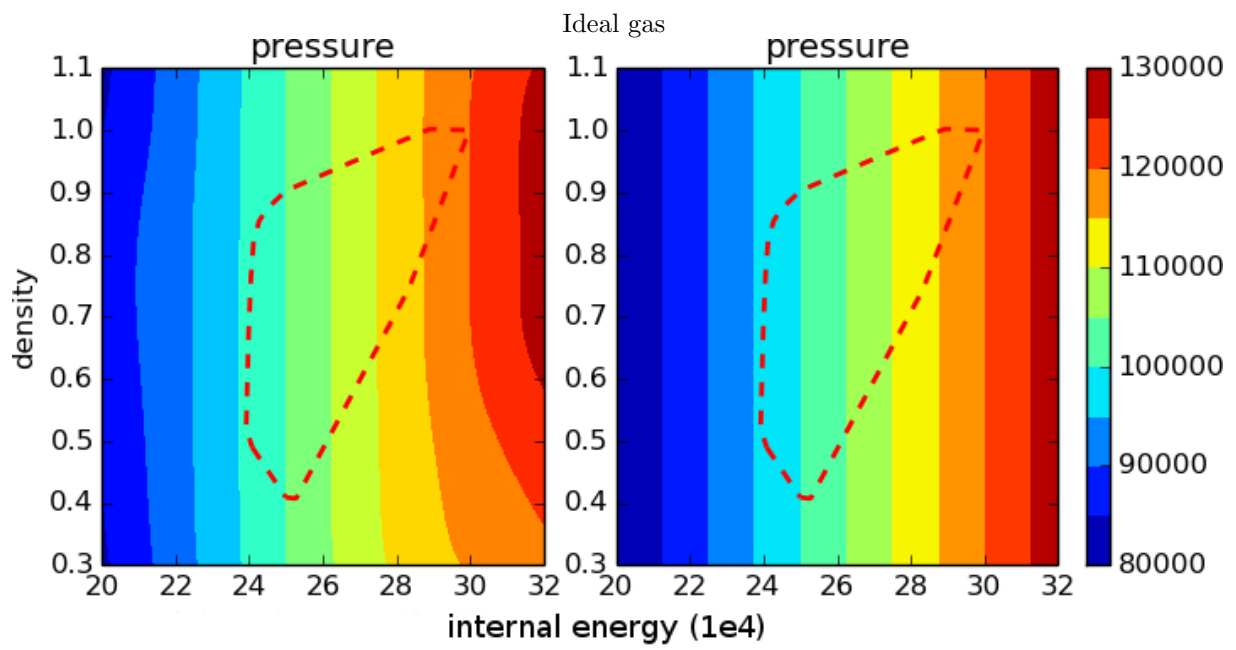


Figure 8: The solution mismatch between the twin model's solution and the graybox solution for the ideal gas equation, the van der Waals equation, and the Redlich-Kwong equation. The first group of images is for the ideal gas, the second group of images is for the van der Waals gas, and the third group of images is for the Redlich-Kwong gas. For each gas, we show the solution mismatch of velocity, energy, and density. For all three test cases, the relative error of the velocity, energy, and density is small.

Let the (ρ, U) be the gray-box steady state solution's density and internal energy at all the spatial gridpoint, and let $H(\rho, U)$ be its convex hull. We expect the the estimated state equation to be more accurate inside $H(\rho, U)$ than outside $H(\rho, U)$. The inferred state equation, $p = p(\rho, U)$, is shown in Fig. 9.



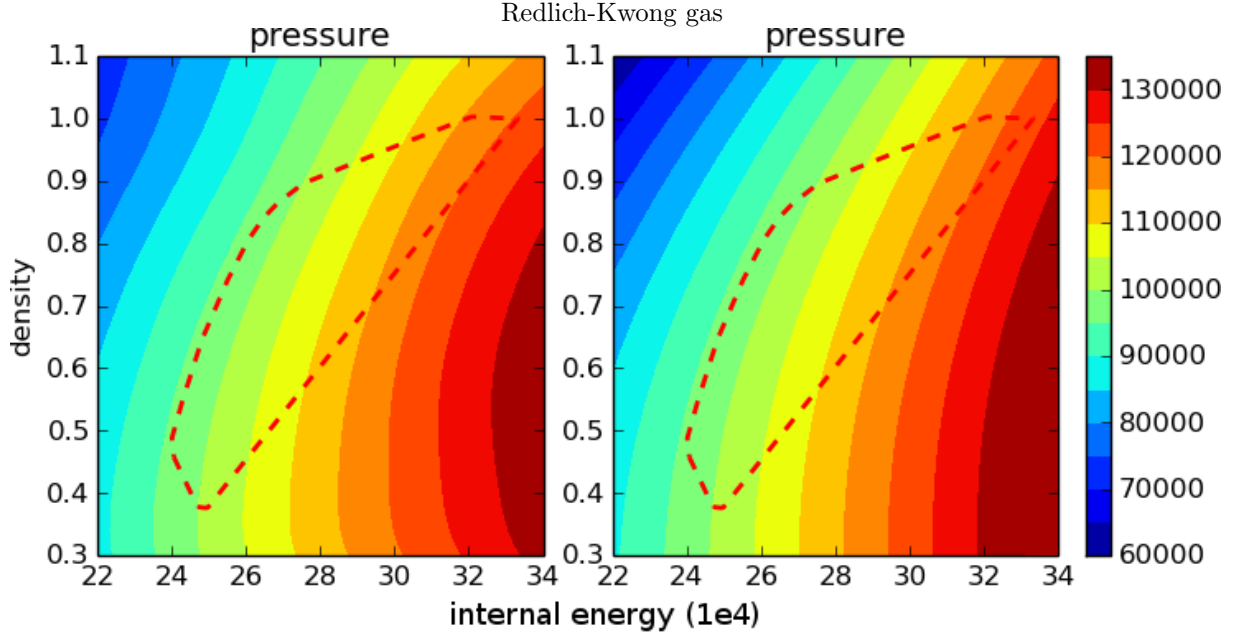


Figure 9: The inferred state equation and the gray-box state equation for the three gases.

The left column shows the inferred state equation, and the right column shows the gray-box state equation. In all the three test cases, the inferred state equation approximates the gray-box state equation accurately inside $H(\rho, U)$ indicated by the dashed line.

Using the inferred state equation, we are able to compute the gradient of the mass flux to the control points at the bending section. For example, the gradient and the perturbed boundary for the ideal gas are shown in Fig. 10. For all the three gases, the difference between the gray-box gradient and the twin model gradient is hardly visible.

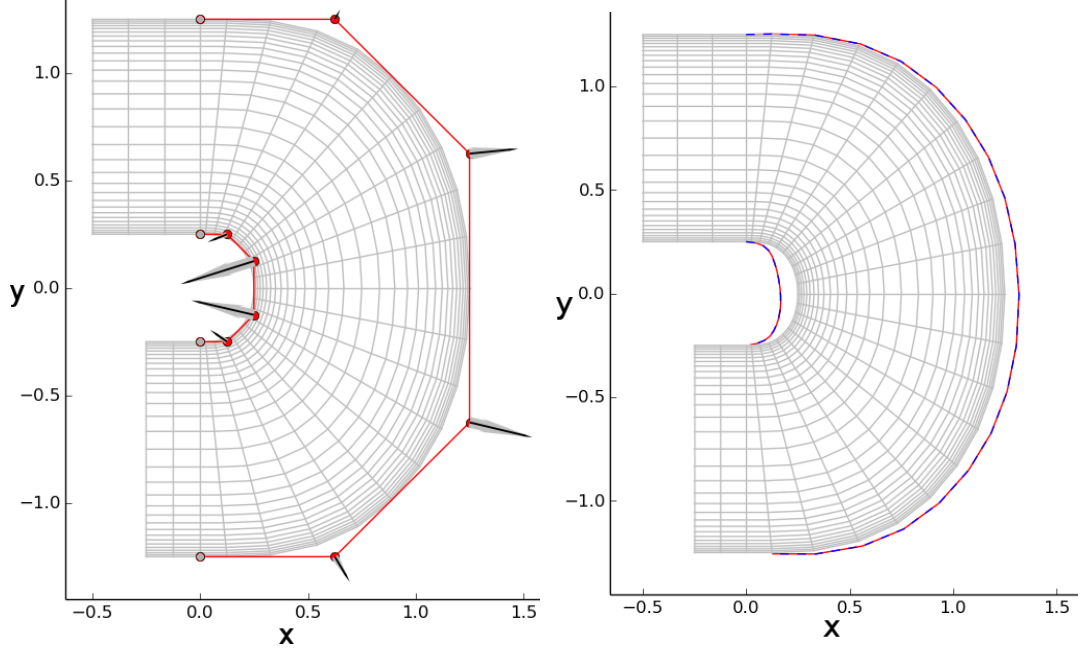


Figure 10: The left column shows the gradient of the outflux to the control points for the ideal gas. The wide gray arrow is the gradient evaluated by the gray-box model, while the thin black arrow is the gradient evaluated by the twin model. The right column shows a perturbed boundary according to the gradient. The blue dashed line is computed by the gray-box model's gradient, while the red dashed line is computed by the twin model's gradient.

We summarized the estimated gradient computed by the twin model in Table 2, which is compared with the gradient computed by the gray-box model. For each gas, we compare the x-component and the y-component of the gradients. Twin model demonstrates to estimate the gradients accurately.

Table 2: The gradient of the mass flux to the control points' coordinates

Ideal gas		gradient at inner boundary				gradient at outer boundary			
x	Graybox	-2.407	-9.079	-7.727	-2.085	0.661	6.013	7.756	1.843
	Twin model	-2.406	-9.071	-7.722	-2.084	0.661	6.008	7.751	1.841
y	Graybox	-0.971	-2.852	1.792	1.472	1.190	0.596	-1.854	-3.097
	Twin model	-0.972	-2.849	1.792	1.473	1.189	0.595	-1.853	-3.094
VDW gas		gradient at inner boundary				gradient at outer boundary			
x	Graybox	-2.389	-9.091	-7.736	-2.073	0.660	6.003	7.756	1.846
	Twin model	-2.392	-9.085	-7.739	-2.078	0.659	6.006	7.759	1.846
y	Graybox	-0.942	-2.848	1.785	1.443	1.192	0.593	-1.858	-3.105
	Twin model	-0.948	-2.846	1.789	1.452	1.188	0.593	-1.858	-3.104
RK gas		gradient at inner boundary				gradient at outer boundary			
x	Graybox	-2.429	-9.064	-7.749	-2.122	0.663	6.045	7.773	1.837
	Twin model	-2.412	-9.039	-7.702	-2.092	0.660	6.000	7.731	1.832
y	Graybox	-1.010	-2.848	1.820	1.536	1.183	0.603	-1.851	-3.081
	Twin model	-0.995	-2.844	1.812	1.519	1.190	0.596	-1.845	-3.076

8 Conclusion

We propose a method to estimate the objective’s gradient when the simulator is a gray-box conservation law simulator and does not implement the adjoint method. The proposed method uses the space-time or spatial solution of the gray-box simulation to infer a twin model. There are several benefits to use the space-time or spatial solution. Firstly, in many conservation law simulations, flow quantities have a small domain of dependence. Secondly, the space-time or spatial solution from a single simulation provides a large number of samples for the inference. Thirdly, in many high-dimensional design problems, the design variables are space-time or spatially distributed, so the inference’s input dimension does not scale up with the design dimension. The twin model method enables adjoint computation. We use the gradient computed by the twin model to estimate the gradient of the gray-box simulation.

The twin model method is demonstrated on a 1-D porous media flow problem and a 2-D Navier-Stokes problem. In the 1-D problem the flux function is unknown. We are able to infer the flux function in the excited domain. Using the inferred twin model, we estimate the gradient of the objective to the space-time dependent control. In the 2-D problem, the state equation is unknown. We are able to infer the state equation using the steady state solution of the gray-box model. Using the inferred state

equation, we estimate the gradient of the mass flux to the coordinates of the control points. Our research shows that gradient can be efficiently estimated by adjoint method even if the simulator is gray-box.

The twin model enables adjoint computation for gray-box simulations. In the future, we plan to apply the twin model to high-dimensional optimization problems.

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