

JAX-DIPS: Differentiable Inverse PDE Solver

Pouria A. Mistani^{* †,a}, Samira Pakravan^{†,b}, Rajesh Ilango^a, Frederic G. Gibou^b

^aNVIDIA Corporation, Santa Clara, CA 95051, USA

^bUniversity of California, Santa Barbara, CA 93106-5070, USA

Abstract

We present an end-to-end differentiable PDE solver supporting free boundary problems using the level-set method. We implemented this framework using JAX, extending support for CPU/GPU/TPU platforms. Algorithmically, our proposed framework builds on the blended inverse PDE solver architecture (BiPDE) that authors have proposed earlier [3]. JAX-DIPS is an open-source software package published under MIT license and is available at <https://github.com/JAX-DIPS/JAX-DIPS>.

Keywords: level-set method, free boundary problems, inverse problems, jump conditions, differentiable programming

1. Introduction

Differentiable programming ...

2. Numerical Scheme for Free Boundary Problems

Consider a closed irregular interface (Γ) that partitions the computational domain (Ω) into interior (Ω^-) and exterior (Ω^+) subdomains; *i.e.*, $\Omega = \Omega^- \cup \Gamma \cup \Omega^+$. We are interested in the solutions $u^\pm \in \Omega^\pm$ to the following class of linear elliptic problems in $\mathbf{x} \in \Omega^\pm$:

$$\begin{aligned} k^\pm u^\pm - \nabla \cdot (\mu^\pm \nabla u^\pm) &= f^\pm, & \mathbf{x} \in \Omega^\pm \\ [u] &= \alpha, & \mathbf{x} \in \Gamma \\ [\mu \partial_{\mathbf{n}} u] &= \beta, & \mathbf{x} \in \Gamma \end{aligned}$$

Here $f^\pm = f(\mathbf{x} \in \Omega^\pm)$ is the spatially varying source term, $\mu^\pm = \mu(\mathbf{x} \in \Omega^\pm)$ are the diffusion coefficients, and k^\pm are the reaction coefficients in the two domains. We consider Dirichlet boundary conditions in a cubic domain $\Omega = [-L/2, L/2]^3$.

2.1. The level-set method

2.2. Finite discretization method

For spatial discretizations at the presence of jump conditions we employ the numerical algorithm proposed by Bochkov and Gibou (2020) [1] (BG20) on Cartesian grids. BG20 produces second-order accurate solutions and first-order accurate gradients in the L^∞ -norm, while having a compact stencil that makes it a good candidate for parallelization. Moreover, treatment of the interface jump conditions do not introduce any augmented variables, this preserves the homogeneous structure of the linear system.

Here we use a finite volume discretization equation uniformly for all grid points. At grid points where the finite volumes are crossed by Γ we have

^{*}Corresponding author: p.a.mistani@gmail.com

[†]These authors contributed equally to this work

In two dimensions and on uniform grids, the gradient operator at the grid cell (i, j) that is crossed by an interface is estimated by a least squares solution given by

$$(\nabla u^\pm)_{i,j} = \mathbf{D}_{i,j}^\pm \begin{bmatrix} u_{i-1,j-1} - u_{i,j}^\pm \\ u_{i,j-1} - u_{i,j}^\pm \\ \vdots \\ u_{i+1,j+1} - u_{i,j}^\pm \end{bmatrix} \quad \mathbf{D}_{i,j}^\pm = (X_{i,j}^T W_{i,j}^\pm X_{i,j})^{-1} (W_{i,j}^\pm X_{i,j})^T$$

and

$$W_{i,j}^\pm = \begin{bmatrix} \omega_{i,j}^\pm(-1, -1) & & & \\ & \omega_{i,j}^\pm(0, -1) & & \\ & & \ddots & \\ & & & \omega_{i,j}^\pm(1, 1) \end{bmatrix} \quad X_{i,j} = \begin{bmatrix} -h_x & -h_y \\ 0 & -h_y \\ h_x & -h_y \\ -h_x & 0 \\ 0 & 0 \\ h_x & 0 \\ -h_x & h_y \\ 0 & h_y \\ h_x & h_y \end{bmatrix}$$

and

$$\omega_{i,j}^\pm(p, q) = \begin{cases} 1 & (p, q) \in N_{i,j}^\pm \\ 0 & \text{else} \end{cases} \quad (1)$$

In this case, $D_{i,j}^\pm$ is a 2×9 matrix and we denote each of its 2×1 columns with $d_{i,j,p,q}^\pm$

$$\mathbf{D}_{i,j}^\pm = [\quad d_{i,j,-1,-1}^\pm \quad d_{i,j,0,-1}^\pm \quad d_{i,j,1,-1}^\pm \quad d_{i,j,-1,0}^\pm \quad d_{i,j,0,0}^\pm \quad d_{i,j,1,0}^\pm \quad d_{i,j,-1,1}^\pm \quad d_{i,j,0,1}^\pm \quad d_{i,j,1,1}^\pm]$$

The least square coefficients are then obtained by dot product of normal vector with these columns

$$c_{i,j,p,q}^\pm = \mathbf{n}_{i,j}^T d_{i,j,p,q}^\pm$$

At this point we can define a few intermediate variables at each grid point to simplify the presentation of the method,

$$\begin{aligned} \zeta_{i,j,p,q}^\pm &:= \delta_{i,j} \frac{[\mu]}{\mu^\mp} c_{i,j,p,q}^\pm & \zeta_{i,j}^\pm &:= - \sum_{(p,q) \in N_{i,j}^\pm} \zeta_{i,j,p,q}^\pm \\ \gamma_{i,j,p,q}^\pm &:= \frac{\zeta_{i,j,p,q}^\pm}{1 \pm \zeta_{i,j}^\pm} & \gamma_{i,j}^\pm &:= - \sum_{(p,q) \in N_{i,j}^\pm} \gamma_{i,j,p,q}^\pm \end{aligned}$$

where the set of neighboring grid points are

$$N_{i,j}^\pm = \{(p, q) : \quad p = -1, 0, 1, \quad q = -1, 0, 1, \quad (p, q) \neq (0, 0), \quad \mathbf{x}_{i+p,j+q} \in \Omega^\pm\}$$

and $\delta_{i,j}$ is the signed distance from $\mathbf{x}_{i,j}$ that is computed from the level-set function $\phi(\mathbf{x})$

$$\delta_{i,j} = \frac{\phi(\mathbf{x}_{i,j})}{|\nabla \phi(\mathbf{x}_{i,j})|}$$

- Rules based on approximating $\partial_{\mathbf{n}} u^+(\mathbf{r}_{i,j}^{pr})$:

$$u_{i,j}^- = \begin{cases} u_{i,j} & \mathbf{x}_{i,j} \in \Omega^- \\ u_{i,j}(1 - \gamma_{i,j}^-) - \sum_{(p,q) \in N_{i,j}^-} \gamma_{i,j,p,q}^- u_{i+p,j+q} - (\alpha + \frac{\delta_{i,j}\beta}{\mu^\mp})(1 - \gamma_{i,j}^-) & \mathbf{x}_{i,j} \in \Omega^+ \end{cases} \quad (2)$$

$$u_{i,j}^+ = \begin{cases} u_{i,j}(1 - \zeta_{i,j}^-) - \sum_{(p,q) \in N_{i,j}^-} \zeta_{i,j,p,q}^- u_{i+p,j+q} + \alpha + \delta_{i,j} \frac{\beta}{\mu^+} & \mathbf{x}_{i,j} \in \Omega^- \\ u_{i,j} & \mathbf{x}_{i,j} \in \Omega^+ \end{cases} \quad (3)$$

It is useful to cast this in the form of matrix operations through defining intermediate tensors:

$$\mathbf{\Gamma}_{i,j} := \begin{bmatrix} \gamma_{i-1,j+1}^- & \gamma_{i,j+1}^- & \gamma_{i+1,j+1}^- \\ \gamma_{i-1,j}^- & \gamma_{i,j}^- & \gamma_{i+1,j}^- \\ \gamma_{i-1,j-1}^- & \gamma_{i,j-1}^- & \gamma_{i+1,j-1}^- \end{bmatrix}, \quad \mathbf{\zeta}_{i,j} := \begin{bmatrix} \zeta_{i-1,j+1}^- & \zeta_{i,j+1}^- & \zeta_{i+1,j+1}^- \\ \zeta_{i-1,j}^- & \zeta_{i,j}^- & \zeta_{i+1,j}^- \\ \zeta_{i-1,j-1}^- & \zeta_{i,j-1}^- & \zeta_{i+1,j-1}^- \end{bmatrix}$$

$$\mathbf{U}_{i,j} := \begin{bmatrix} u_{i-1,j+1} & u_{i,j+1} & u_{i+1,j+1} \\ u_{i-1,j} & u_{i,j} & u_{i+1,j} \\ u_{i-1,j-1} & u_{i,j-1} & u_{i+1,j-1} \end{bmatrix}, \quad \mathbf{N}_{i,j}^\pm := \begin{bmatrix} \omega_{i,j}^\pm(-1,1) & \omega_{i,j}^\pm(0,1) & \omega_{i,j}^\pm(1,1) \\ \omega_{i,j}^\pm(-1,0) & 0 & \omega_{i,j}^\pm(1,0) \\ \omega_{i,j}^\pm(-1,-1) & \omega_{i,j}^\pm(0,-1) & \omega_{i,j}^\pm(1,-1) \end{bmatrix}$$

where \mathbf{N}^- is a masking filter that passes the values in the negative neighborhood of node (i, j) .

We also introduce the Hadamard product \odot between two identical matrices that creates another identical matrix with each entry being elementwise products. Moreover, double contraction of two tensors A and B is defined by $A : B = \sum A \odot B$ which is a scalar value and equals the sum of all entries of the Hadamard product of the tensors; *i.e.*, note $A : A$ is square of Frobenius norm of A . Using these notations, the substitution rules read

$$u_{i,j}^- = \begin{cases} u_{i,j} & \mathbf{x}_{i,j} \in \Omega^- \\ (1 + \mathbf{\Gamma}_{i,j}^- : \mathbf{N}_{i,j}^-) u_{i,j} - (\mathbf{\Gamma}_{i,j}^- \odot \mathbf{N}_{i,j}^-) : \mathbf{U}_{i,j} - (\alpha + \delta_{i,j} \frac{\beta}{\mu^+})(1 + \mathbf{\Gamma}_{i,j}^- : \mathbf{N}_{i,j}^-) & \mathbf{x}_{i,j} \in \Omega^+ \end{cases} \quad (4)$$

$$u_{i,j}^+ = \begin{cases} (1 + \mathbf{\zeta}_{i,j}^- : \mathbf{N}_{i,j}^-) u_{i,j} - (\mathbf{\zeta}_{i,j}^- \odot \mathbf{N}_{i,j}^-) : \mathbf{U}_{i,j} + \alpha + \delta_{i,j} \frac{\beta}{\mu^+} & \mathbf{x}_{i,j} \in \Omega^- \\ u_{i,j} & \mathbf{x}_{i,j} \in \Omega^+ \end{cases} \quad (5)$$

- Rules based on approximating $\partial_{\mathbf{n}} u^-(\mathbf{r}_{i,j}^{pr})$:

$$u_{i,j}^- = \begin{cases} u_{i,j} & \mathbf{x}_{i,j} \in \Omega^- \\ u_{i,j}(1 - \zeta_{i,j}^+) - \sum_{(p,q) \in N_{i,j}^+} \zeta_{i,j,p,q}^+ u_{i+p,j+q} - \alpha - \delta_{i,j} \frac{\beta}{\mu^-} & \mathbf{x}_{i,j} \in \Omega^+ \end{cases} \quad (6)$$

$$u_{i,j}^+ = \begin{cases} u_{i,j}(1 - \gamma_{i,j}^+) - \sum_{(p,q) \in N_{i,j}^+} \gamma_{i,j,p,q}^+ u_{i+p,j+q} + (\alpha + \delta_{i,j} \frac{\beta}{\mu^-})(1 - \gamma_{i,j}^+) & \mathbf{x}_{i,j} \in \Omega^- \\ u_{i,j} & \mathbf{x}_{i,j} \in \Omega^+ \end{cases} \quad (7)$$

in matrix notation we have

$$u_{i,j}^- = \begin{cases} u_{i,j} & \mathbf{x}_{i,j} \in \Omega^- \\ (1 + \mathbf{\zeta}_{i,j}^+ : \mathbf{N}_{i,j}^+) u_{i,j} - (\mathbf{\zeta}_{i,j}^+ \odot \mathbf{N}_{i,j}^+) : \mathbf{U}_{i,j} - \alpha - \delta_{i,j} \frac{\beta}{\mu^-} & \mathbf{x}_{i,j} \in \Omega^+ \end{cases} \quad (8)$$

$$u_{i,j}^+ = \begin{cases} (1 + \mathbf{\Gamma}_{i,j}^+ : \mathbf{N}_{i,j}^+) u_{i,j} - (\mathbf{\Gamma}_{i,j}^+ \odot \mathbf{N}_{i,j}^+) : \mathbf{U}_{i,j} + (\alpha + \delta_{i,j} \frac{\beta}{\mu^-})(1 + \mathbf{\Gamma}_{i,j}^+ : \mathbf{N}_{i,j}^+) & \mathbf{x}_{i,j} \in \Omega^- \\ u_{i,j} & \mathbf{x}_{i,j} \in \Omega^+ \end{cases} \quad (9)$$

2.3. 3D geometric integrations

We use uniform Cartesian grids. For computational cells that are crossed by the interface, *i.e.* $\mathcal{V}_{i,j,k} \cap \Gamma \neq \emptyset$, we use the geometric integrations proposed by Min & Gibou (2007) [2]. In this scheme each grid cell is decomposed into five tetrahedra by the middle-cut triangulation [4] where

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1: procedure BIAS SLOW
2:   if  $\Gamma \cap \mathcal{C}_{i,j} = \emptyset$  then
3:      $B_{i,j}^\pm = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ ;  $r_{i,j}^\pm = 0$ 
4:   else
5:     if  $\mu_{i,j}^- > \mu_{i,j}^+$  then
6:       if  $\phi_{i,j} \geq 0$  then
7:          $B_{i,j}^+ = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ ;  $r_{i,j}^+ = 0$ 
8:          $B_{i,j}^- = \begin{bmatrix} -\gamma_{i,j,-1,1} & -\gamma_{i,j,0,1} & -\gamma_{i,j,1,1} \\ -\gamma_{i,j,-1,0} & 1 - \gamma_{i,j} & -\gamma_{i,j,1,0} \\ -\gamma_{i,j,-1,-1} & -\gamma_{i,j,0,-1} & -\gamma_{i,j,1,-1} \end{bmatrix}$ ;  $r_{i,j}^- = -(\alpha_{i,j}^{proj} + \delta_{i,j} \frac{\beta_{i,j}^{proj}}{\mu_{i,j}^+})(1 - \gamma_{i,j}^-)$ 
9:       else
10:         $B_{i,j}^+ = \begin{bmatrix} -\zeta_{i,j,-1,1} & -\zeta_{i,j,0,1} & -\zeta_{i,j,1,1} \\ -\zeta_{i,j,-1,0} & 1 - \zeta_{i,j} & -\zeta_{i,j,1,0} \\ -\zeta_{i,j,-1,-1} & -\zeta_{i,j,0,-1} & -\zeta_{i,j,1,-1} \end{bmatrix}$ ;  $r_{i,j}^+ = \alpha_{i,j}^{proj} + \delta_{i,j} \frac{\beta_{i,j}^{proj}}{\mu_{i,j}^+}$ 
11:         $B_{i,j}^- = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ ;  $r_{i,j}^- = 0$ 
12:      else
13:        if  $\phi_{i,j} \geq 0$  then
14:           $B_{i,j}^+ = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ ;  $r_{i,j}^+ = 0$ 
15:           $B_{i,j}^- = \begin{bmatrix} -\zeta_{i,j,-1,1}^+ & -\zeta_{i,j,0,1}^+ & -\zeta_{i,j,1,1}^+ \\ -\zeta_{i,j,-1,0}^+ & 1 - \zeta_{i,j}^+ & -\zeta_{i,j,1,0}^+ \\ -\zeta_{i,j,-1,-1}^+ & -\zeta_{i,j,0,-1}^+ & -\zeta_{i,j,1,-1}^+ \end{bmatrix}$ ;  $r_{i,j}^- = \alpha_{i,j}^{proj} + \delta_{i,j} \frac{\beta_{i,j}^{proj}}{\mu_{i,j}^-}$ 
16:        else
17:           $B_{i,j}^+ = \begin{bmatrix} -\gamma_{i,j,-1,1}^+ & -\gamma_{i,j,0,1}^+ & -\gamma_{i,j,1,1}^+ \\ -\gamma_{i,j,-1,0}^+ & 1 - \gamma_{i,j}^+ & -\gamma_{i,j,1,0}^+ \\ -\gamma_{i,j,-1,-1}^+ & -\gamma_{i,j,0,-1}^+ & -\gamma_{i,j,1,-1}^+ \end{bmatrix}$ ;  $r_{i,j}^+ = (\alpha_{i,j}^{proj} + \delta_{i,j} \frac{\beta_{i,j}^{proj}}{\mu_{i,j}^-})(1 - \gamma_{i,j}^+)$ 
18:           $B_{i,j}^- = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ ;  $r_{i,j}^- = 0$ 

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Algorithm 1: Bias Slow approximation of the non-existing solution value on a grid point based on existing solution values in its neighborhood. The notation is used for $u_{i,j}^\pm = B_{i,j}^\pm : \mathbf{U}_{i,j} + r_{i,j}^\pm$.

each grid cell crossed by the interface is decomposed to five tetrahedra given by (each cell is rescaled to $[0, 1]^3$):

$T_1 \equiv \text{conv}(P_{000}; P_{100}; P_{010}; P_{001})$	x = 0 face, y = 0 face, z = 0 face
$T_2 \equiv \text{conv}(P_{110}; P_{100}; P_{010}; P_{111})$	x = 1 face, y = 1 face, z = 0 face
$T_3 \equiv \text{conv}(P_{101}; P_{100}; P_{111}; P_{001})$	x = 1 face, y = 0 face, z = 1 face
$T_4 \equiv \text{conv}(P_{011}; P_{111}; P_{010}; P_{001})$	x = 0 face, y = 1 face, z = 1 face
$T_5 \equiv \text{conv}(P_{111}; P_{100}; P_{010}; P_{001})$	no face exposure

3. Numerical Examples

3.1. Stationary linear case

$$\begin{aligned}
 k^\pm u^\pm - \nabla \cdot (\mu^\pm \nabla u^\pm) &= f^\pm, & \mathbf{x} \in \Omega^\pm \\
 [u] &= \alpha, & \mathbf{x} \in \Gamma \\
 [\mu \partial_{\mathbf{n}} u] &= \beta, & \mathbf{x} \in \Gamma
 \end{aligned}$$

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