

LA-UR-22-28343

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Title: Applying an Oriented Divergence Theorem to Swept Face Remap

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Intended for: LANL internal presentation

Issued: 2022-08-09



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Applying an Oriented Divergence Theorem to Swept Face Remap

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CNLS Conference Room

August 11, 2022

LA-UR-YY-NNNNN



Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA.

8/11/2022

Outline

Introduction

Theoretical Results

- Swept region divergence
- Parameterized divergence
- Independence of τ

Numerical Results

Implementation Strategies and Generalizations

Conclusions

ALE hydrodynamics

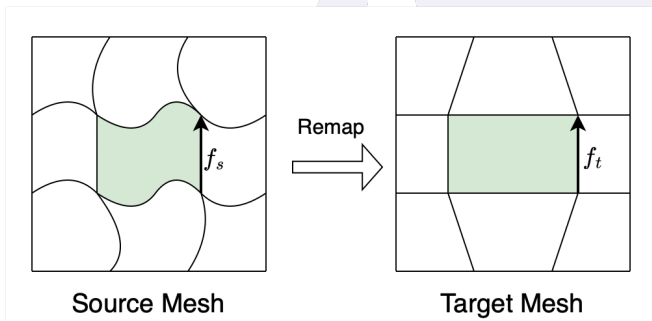
In arbitrary Lagrangian-Eulerian hydrodynamics, we compute the physical behavior of a fluid over time with three phases:

1. The **Lagrangian phase**: the mesh distorts along with the fluid. May result in a tangled, unresolved mesh, so we pause at a geometrically valid source mesh.
2. The **rezone phase**: define a compatible, geometrically valid target mesh.
3. The **remap phase**: port the physical solution computed in the Lagrangian phase from the source mesh to the target mesh.

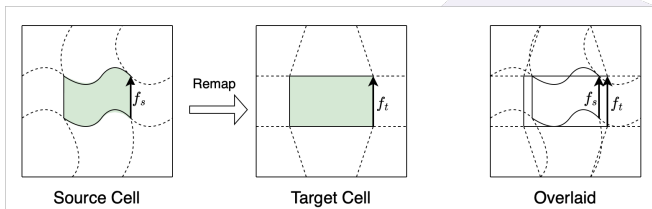
We will focus on the remap phase. Our domain is compact $\Omega \subset \mathbb{R}^n$, and we describe our physical solution with a scalar density function $\rho : \Omega \rightarrow \mathbb{R}$.

Swept remap

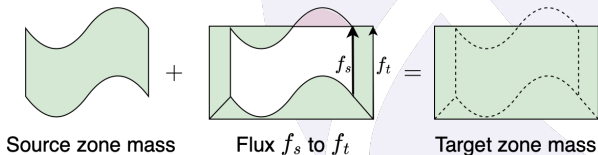
In swept remap, the source and target mesh have the same topology. Each source zone corresponds to a target zone, and each source face corresponds to a target face.



Swept remap

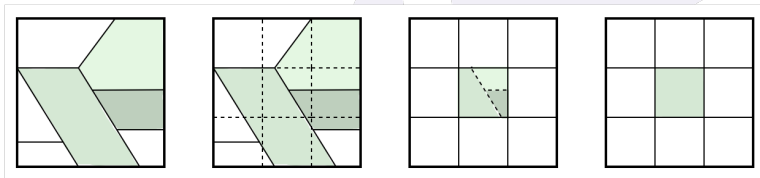


We compute the mass of the target zone using the mass of the source zone, and the change in mass through each source face sweeping to a target face.



Other types of remap

- **Intersection:** the source and target mesh may have different topologies, and the change in mass is computed by intersecting all source and target zones. This is challenging for curved meshes.



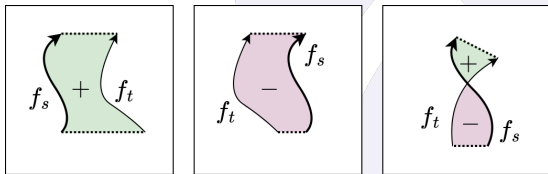
- **Dynamic process:** formulates remap as a dynamic process governed by a transport equation. The source and target mesh have the same topology, and we compute a pseudo velocity between them. Does not preserve solutions which are globally polynomials.

Swept region

We assume that our faces are described with explicit, compatible parameterizations f_s and f_t . Then we describe the swept region with a parameterization $\tau : [0, 1]^n \rightarrow \mathbb{R}^n$.

$$\begin{aligned}\tau(t_1, \dots, t_n) &: [0, 1]^n \rightarrow \mathbb{R}^n \\ \tau(t_1, \dots, t_{n-1}, 0) &= f_s(t_1, \dots, t_{n-1}) \\ \tau(t_1, \dots, t_{n-1}, 1) &= f_t(t_1, \dots, t_{n-1}).\end{aligned}$$

We assume that τ is continuous and piecewise differentiable (C^1). However, τ may not be injective or orientation-preserving, so it may overlap itself in complicated ways.

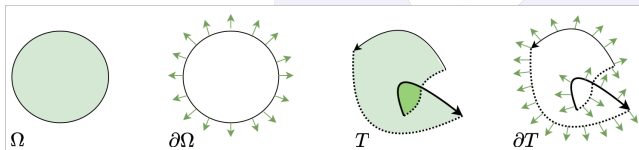


Divergence theorem

Theorem (Divergence)

Let $\Omega \subset \mathbb{R}^n$ a compact subset with piecewise smooth boundary $\partial\Omega$. Let $\mathbf{v} \in H_{\text{div}}(\Omega)$ a vector field such that $\rho = \nabla \cdot \mathbf{v}$. Then

$$\mathcal{F}_\rho(\Omega) \equiv \int_\Omega \rho dv = \oint_{\partial\Omega} \mathbf{v} \cdot d\mathbf{s}.$$



Our swept region T may not fulfill the assumptions for Ω .

Novelty and roadmap

Though divergence theorem does not formally apply to swept regions, M. Shashkov and others have used it for swept remap. This project creates a solid theoretical foundation for this usage.

- We provide an explicit mathematical description for a swept region.
- We provide several characterizations of the flux through the swept region. The most practical of these is a volume integral of the unit cube, which makes use of a change of variables:

$$\mathcal{F}_\rho(T) = \int_{[0,1]^n} (\rho \circ \tau) j_\tau dt.$$

- We validate the theoretical results numerically.
- We discuss implementation strategies for swept remap, and extend the results to polygonal mesh topologies.

We gain remap methods which preserve globally polynomial solutions.

A large, stylized atomic symbol in the background, consisting of three overlapping elliptical orbits in a light purple color and a central white nucleus with a small white circle. The text "Theoretical Results" is centered over the middle of the symbol.

Theoretical Results

Parameterizing our swept region

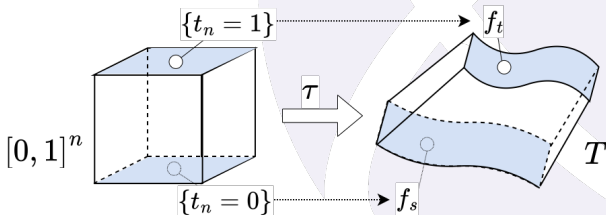
We choose a continuous, piecewise differentiable parameterization map from the n -cube:

$$\tau : [0, 1]^n \rightarrow \mathbb{R}^n.$$

To relate τ to remap, we want it to sweep between our source and target faces:

$$f_s(t_1, \dots, t_{n-1}) = \tau(t_1, \dots, t_{n-1}, 0)$$

$$f_t(t_1, \dots, t_{n-1}) = \tau(t_1, \dots, t_{n-1}, 1).$$



Parameterizing our swept region (notation)

We also use the following conventions for component functions and coordinates:

$$\boldsymbol{\tau} = (\tau_1, \dots, \tau_n)$$

$$\mathbf{x} = (x_1, \dots, x_n) \in \mathbb{R}^n$$

$$\mathbf{t} = (t_1, \dots, t_n) \in [0, 1]^n.$$

Since $\boldsymbol{\tau}$ is piecewise differentiable, we may define the Jacobian determinant $j_{\boldsymbol{\tau}}$ almost everywhere on $[0, 1]^n$ using the partial derivatives of component functions τ_i :

$$j_{\boldsymbol{\tau}} = \det \left(\frac{\partial \tau_i}{\partial t_j} \right)_{ij}.$$

We use $d\mathbf{x}$ and $d\mathbf{t}$ for both volume (dim n) and area (dim $n-1$) integrals.

Features of swept regions

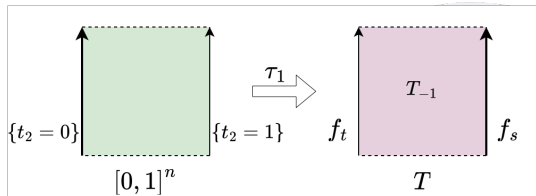
The parameterizations are continuous and piecewise differentiable, but not injective or orientation-preserving.

We consider the following features of their images:

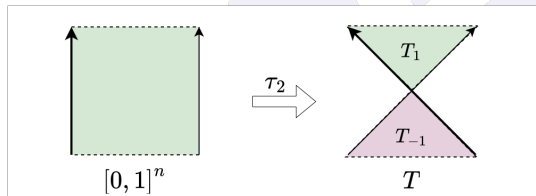
- **Orientation:** positive if $j_\tau > 0$, and negative if $j_\tau < 0$.
- **Overlaps:** constructive if they have the same orientation, and destructive if they have opposite orientations.

We define a swept region as the **signed, multiset image of τ** with an integer-valued characteristic function which has value k on component sets T_k .

2D examples: τ_1 and T_2

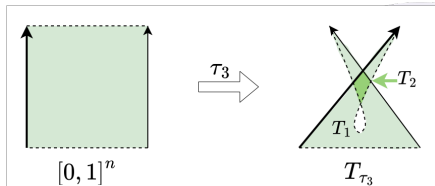


$$\tau_1(t_1, t_2) = (t_1, -t_2)$$

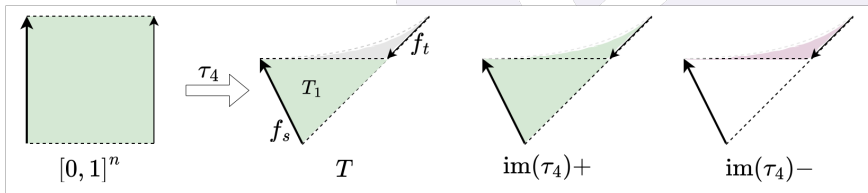


$$\tau_2(t_1, t_2) = (1 + t_1, 0 - t_1 - t_2 - 2t_1 t_2)$$

2D examples: τ_3 and τ_4



$$\tau_3(t_1, t_2) = (2.5t_2 - 9t_1t_2 + 9t_1^2t_2, 3t_1 + 2.8t_2 - 13t_1t_2 + 23t_1^2t_2 - 16t_1^3t_2)$$



$$\tau_4(t_1, t_2) = (t_2 - 2t_1t_2, -2t_1 + t_2)$$

Swept region

Definition

The **swept region** T is a compact, oriented multiset with characteristic function

$$\begin{aligned}\chi_T : \mathbb{R}^n &\rightarrow \mathbb{Z} \\ \chi_T(\mathbf{x}) &= \sum_{\mathbf{t} \in \tau^{-1}(\mathbf{x})} \text{sgn} \circ j_\tau(\mathbf{t}).\end{aligned}$$

As sets, the $\text{supp}(\chi_T) \subset \text{im}(\tau)$, but the subset may be strict.

Flux through a swept region

We define component sets $T_k \subset \mathbb{R}^n$ using the level sets of χ_T :

$$T_k = \chi_T^{-1}(k) \text{ for all } k \in \mathbb{Z}.$$

Each T_k is pre-compact with compact, piecewise differentiable boundary ∂T_k .

Definition

For a swept region T and a scalar function $\rho : \mathbb{R}^n \rightarrow \mathbb{R}$, the **flux of ρ through T** is

$$\mathcal{F}_\rho(T) \equiv \sum_{k \in \mathbb{Z}} k \int_{T_k} \rho(\mathbf{x}) d\mathbf{x} = \int_{\text{supp}(\chi_T)} \chi_T(\mathbf{x}) \rho(\mathbf{x}) d\mathbf{x}.$$

Swept region boundary

Definition

For a swept region T determined by τ , the **boundary of T** is

$$\partial T \equiv \tau(\partial[0, 1]^n) \supset \bigcup_{k \in \mathbb{Z}} \partial T_k.$$

The containment follows from the continuity of τ and the compactness of its domain. Only interfaces between distinct component sets will contribute to our contour integrals. However, ∂T may not contain the boundary of the footprint $\text{im}(\tau)$.

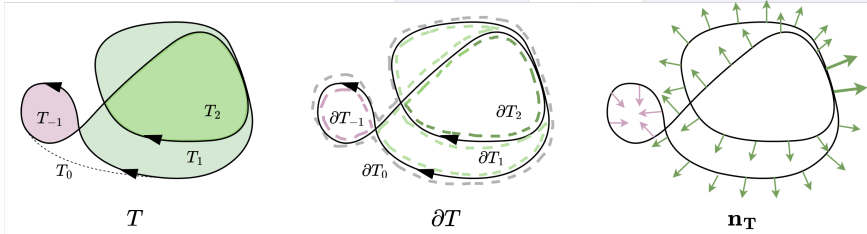
Outward normal

Definition

The **outward normal vector field** \mathbf{n}_T on ∂T is given by

$$\mathbf{n}_T(\mathbf{x}) = \sum_{k \in \mathbb{Z}} k \mathbf{n}_k(\mathbf{x}) \text{ for } \mathbf{x} \in \partial T.$$

We use the outward normals \mathbf{n}_k of the component sets T_k .



Contour integral on ∂T

We demonstrate that \mathbf{n}_T aligns with T almost everywhere. More explicitly, it points from tangent component sets T_i to T_j with magnitude $i - j$ when $i < j$.

Then we may compute contour integrals around ∂T :

$$\oint_{\partial T} \mathbf{v} \cdot \mathbf{n}_T d\mathbf{x} = \sum_{k \in \mathbb{Z}} k \oint_{\partial T_k} \mathbf{v} \cdot \mathbf{n}_k d\mathbf{x}.$$

We want to show that divergence theorem applies to these swept regions.

Swept region divergence theorem

Theorem (Swept region divergence)

- Let $\tau : [0, 1]^n \rightarrow \mathbb{R}^n$ a continuous, piecewise differentiable function.
- Let T the compact swept region determined by τ .
- Let ∂T be the boundary of T with outward normal \mathbf{n}_T .
- Let $\mathbf{v} \in H_{div}(\Omega)$ a vector field with divergence $\rho = \nabla \cdot \mathbf{v}$.

$$\text{Then } \mathcal{F}_\rho(T) = \oint_{\partial T} \mathbf{v} \cdot \mathbf{n}_T da.$$

Sketch of proof

We first state our definition of flux of ρ through T :

$$\mathcal{F}_\rho(T) = \sum_{k \in \mathbb{Z}} k \int_{T_k} \rho(\mathbf{x}) d\mathbf{x}.$$

Then we apply divergence theorem to each component set T_k and its boundary ∂T_k :

$$\mathcal{F}_\rho(T) = \sum_{k \in \mathbb{Z}} k \oint_{\partial T_k} \mathbf{v} \cdot \mathbf{n}_k da.$$

Finally, we apply our definition for the contour integral of \mathbf{V} around ∂T :

$$\mathcal{F}_\rho(T) = \oint_{\partial T} \mathbf{v} \cdot \mathbf{n}_T da.$$

Change of variables

Assumption: τ is an orientation-preserving diffeomorphism.

For volume integrals, we precompose ρ with τ and multiply by j_τ to account for the change in volume:

$$\mathcal{F}_\rho(T) = \int_T \rho d\mathbf{x} = \int_{[0,1]^n} (\rho \circ \tau) j_\tau dt.$$

For contour integrals, we precompose \mathbf{v} with τ , but we need to account for both a change in outward direction and a change in area.

Cross-product and pushforward

We use the **generalized cross-product** to compute an orthogonal vector from $n - 1$ independent vectors $\mathbf{v}, \dots, \mathbf{w}$.

$$\mathbf{n} = \begin{vmatrix} \mathbf{x}_1 & \dots & \mathbf{x}_n \\ v_1 & \dots & v_n \\ \dots & \dots & \dots \\ w_1 & \dots & w_n \end{vmatrix}.$$

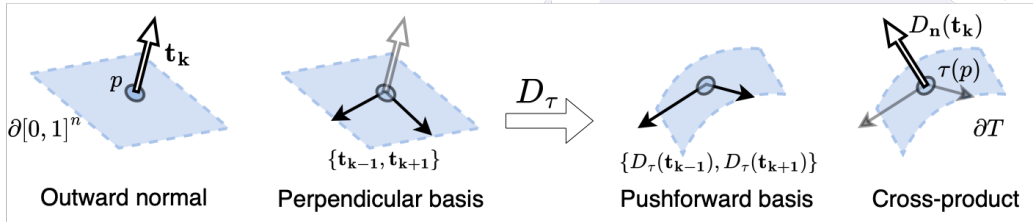
We use the **pushforward** D_τ to transport vectors along τ . For a unit vector \mathbf{t}_k at $p \in [0, 1]^n$, then

$$D_\tau(p, \mathbf{t}_k) = \left(\frac{\partial \tau_1}{\partial t_k}(p), \dots, \frac{\partial \tau_n}{\partial t_k}(p) \right).$$

The pushforward is linear but does not maintain orthogonality.

Contour integral change of variables

We compute an outward normal \mathbf{N}_τ along τ . Its magnitude will be the change in area.



Finally, we complete our contour integral change of variables:

$$\mathcal{F}_\rho(T) = \oint_{\partial T} \mathbf{v} \cdot \mathbf{n} dx = \oint_{\partial[0, 1]^n} (\mathbf{v} \circ \tau) \cdot \mathbf{N}_\tau dt.$$

Revisiting assumptions: more general τ

Piecewise differentiable: No change.

Orientation-reversing: For volume integrals, j_τ will be negative:

$$\mathcal{F}_\rho(T) = - \int_T \rho d\mathbf{x} = \int_{[0,1]^n} (\rho \circ \tau) j_\tau d\mathbf{t}.$$

For contour integrals, \mathbf{N}_τ will point inward with respect to $\text{im}(\tau)$:

$$\mathcal{F}_\rho(T) = - \oint_{\partial T} \mathbf{v} \cdot \mathbf{n} d\mathbf{x} = \oint_{\partial[0,1]^n} (\mathbf{v} \circ \tau) \cdot \mathbf{N}_\tau d\mathbf{t}.$$

Degenerate: If $j_\tau = 0$ or $\mathbf{N}_\tau = 0$, then the corresponding integral is zero.

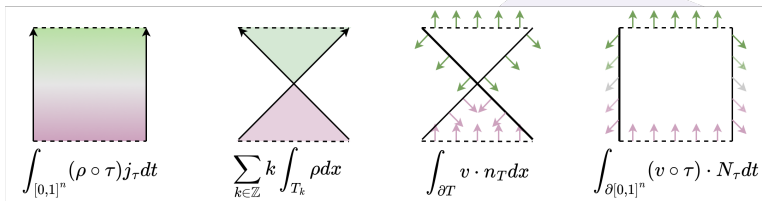
Parameterized divergence theorem

Theorem (Parameterized divergence)

- Let $\tau : [0, 1]^n \rightarrow \mathbb{R}^n$ a continuous, piecewise differentiable function.
- Let T the compact swept region determined by τ .
- Let $\mathbf{v} \in H_{div}(\Omega)$ a vector field with divergence $\rho = \nabla \cdot \mathbf{v}$.

$$\text{Then } \mathcal{F}_\rho(T) = \int_{[0,1]^n} (\rho \circ \tau) j_\tau dt = \oint_{\partial[0,1]} (\mathbf{v} \circ \tau) \cdot \mathbf{N}_\tau dt.$$

Sketch of proof



We use the behavior of injective τ to generalize to non-injective τ .

- Partition $[0, 1]^n$ into injective domains with a positive orientation U_i and injective domains with negative orientation V_j . We may ignore degenerate regions W_k .
- Since τ is continuous from a compact domain, then there are finitely many U_i and V_j , so we can break up our integral.
- Using injectivity, we perform a change of variables in these restricted domains.
- Combine like domains in \mathbb{R}^n to recover χ_T or \mathbf{n}_T .

Independence of parameterization

Theorem

Let $\tau, \omega : [0, 1]^n \rightarrow \mathbb{R}^n$ continuous, piecewise differentiable functions which agree for all $\mathbf{t} \in \partial[0, 1]^n$. Let T, Ω the compact swept regions determined by τ, ω respectively.

Then $T = \Omega$.

Theorem

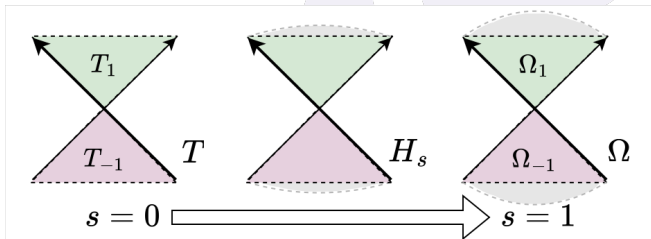
Let T the swept region determined by τ .

Suppose $\sigma : [0, 1]^n \rightarrow [0, 1]^n$ a diffeomorphism which fixes the vertices of $[0, 1]^n$. Let T_σ the swept region determined by $\tau \circ \sigma$.

Then $T = T_\sigma$.

Sketch of proofs

- Define a map h_s which sweeps between τ and ω with respect to s , and is constant along the boundary. It determines intermediate swept regions H_s .
- Since the boundary cannot move, then $\chi_{H_s}(\mathbf{x})$ must be constant along s .



Since σ is a diffeomorphism which fixes vertices, then it preserves orientation. So then precomposing with σ does not change the image of τ or the orientation of τ .

Summary of theoretical results

- Define a swept region T as a signed multiset. Define the flux of ρ through T , and contour integrals around ∂T .
- **Swept region divergence:** Compute the flux with a contour integral.
- Define notation to change variables from T to $[0, 1]^n$.
- **Parameterized divergence:** Compute the flux with a change of variables.
- **Independence of τ :** Our swept regions are an oriented, geometric object rather than an artifact of parameterization.

Numerical Results

2D numerical models

We use the same parameterizations τ_1, \dots, τ_4 from earlier. We choose ρ a polynomial with the same degree, and take antiderivatives to determine a vector field \mathbf{v} explicitly. We compute the flux of ρ through T using numerical approximations of

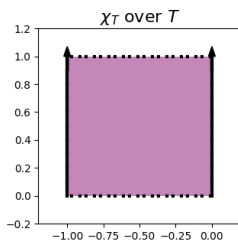
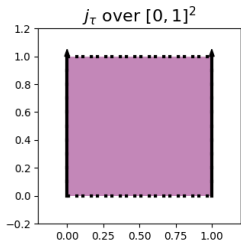
the area integral (A) and contour integral (C):

$$A = (res)^2 \sum_{\text{squares in } [0,1]^2} \sum (\rho \circ \tau)(j_\tau)(t_{\text{center}})$$
$$C = (res) \sum_{\text{segments in } \partial[0,1]^2} (\mathbf{v} \circ \tau)(\mathbf{N}_\tau)(t_{\text{center}}).$$

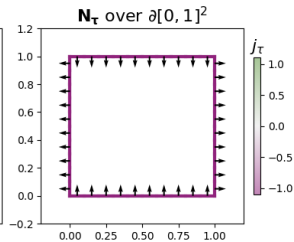
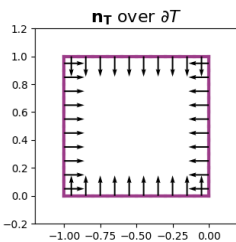
We use resolutions $res = 0.1, 0.01, \text{ and } 0.001$.

2D graphs: τ_1

Area integral of τ_1 and $\rho = 1$



Contour integral of τ_1 and $\rho = 1$

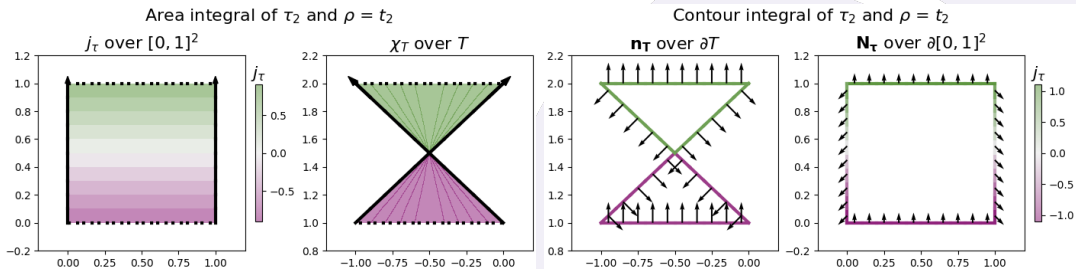


$$\tau_1(t_1, t_2) = (t_1, -t_2)$$

$$\rho(x_1, x_2) = 1$$

$$\mathbf{v}(x_1, x_2) = \left(\frac{1}{2}x_1, \frac{1}{2}x_2\right)$$

2D graphs: τ_2

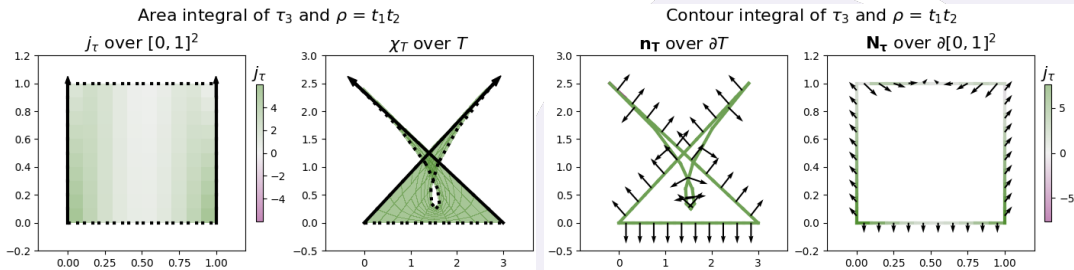


$$\tau_2(t_1, t_2) = (1 + t_1, 0 - t_1 - t_2 - 2t_1 t_2)$$

$$\rho(x_1, x_2) = x_2$$

$$\mathbf{v}(x_1, x_2) = \left(\frac{1}{2} x_1 x_2, \frac{1}{4} x_2^2 \right)$$

2D graphs: τ_3

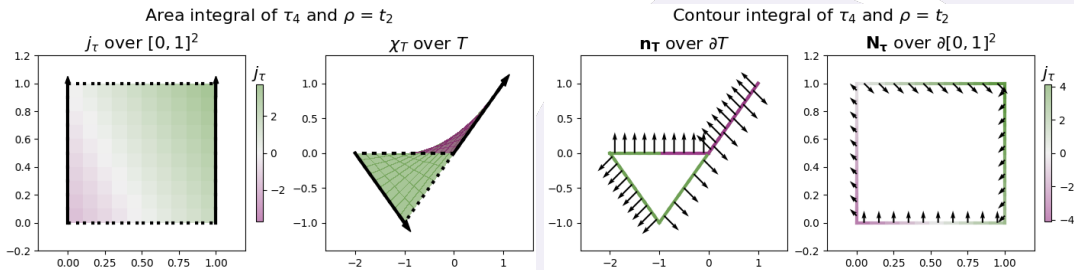


$$\tau_3(t_1, t_2) = (2.5t_2 - 9t_1 t_2 + 9t_1^2 t_2, 3t_1 + 2.8t_2 - 13t_1 t_2 + 23t_1^2 t_2 - 16t_1^3 t_2)$$

$$\rho(x_1, x_2) = x_1 x_2$$

$$\mathbf{v}(x_1, x_2) = \left(\frac{1}{4} x_1^2 x_2, \frac{1}{4} x_1 x_2^2 \right)$$

2D graphs: τ_4



$$\tau_4(t_1, t_2) = (t_2 - 2t_1 t_2, -2t_1 + t_2)$$

$$\rho(x_1, x_2) = x_2$$

$$\mathbf{v}(x_1, x_2) = \left(\frac{1}{2} x_1 x_2, \frac{1}{4} x_2^2 \right)$$

2D convergence

We measure the discrepancy between area integral A and contour integral C with their difference $|C - A|$.

The discrepancy decreases by **two orders of magnitude** for each increase in resolution. The values A and C converge linearly.

τ	ρ	A	C	A	C	C-A		
	<i>res</i>	0.1		0.001		0.1	0.01	0.001
τ_1	1	-1.0	-1.0	-1.0	-1.0	0.0	0.0	0.0
τ_2	x_2	0.165	0.162	0.167	0.167	2.6e-3	1.4e-5	1.2e-7
τ_3	$x_1 x_2$	1.722	1.674	1.712	1.712	4.8e-2	5.2e-4	5.2e-6
τ_4	x_2	-0.330	-0.335	-0.333	-0.333	5.0e-3	5.0e-5	5.0e-7

3D numerical models

We choose polynomial parameterizations τ_5, τ_6, τ_7 , then choose polynomial ρ with the same degree and compute \mathbf{v} explicitly. We compute the flux of ρ through T using

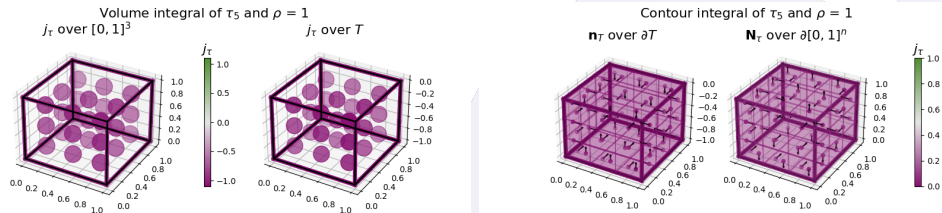
numerical approximations of the volume integral (V) and contour integral (C):

$$V = (res)^3 \sum_{\text{cubes in } [0,1]^3} \sum \sum (\rho \circ \tau)(j_\tau)(t_{\text{center}})$$

$$C = (res)^2 \sum_{\text{squares in } \partial[0,1]^3} \sum (\mathbf{v} \circ \tau)(\mathbf{N}_\tau)(t_{\text{center}}).$$

We use resolutions $res = 0.33, 0.033, \text{ and } 0.0033$.

3D graphs: τ_5

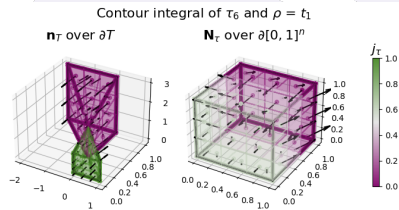
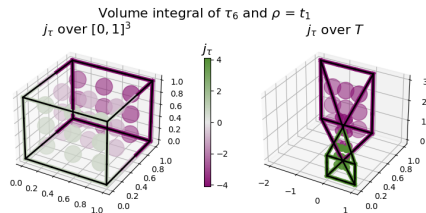


$$t_5(t_1, t_2, t_3) = (t_1, t_2, t_3)$$

$$\rho(x_1, x_2, x_3) = 1$$

$$\mathbf{v}(x_1, x_2, x_3) = \frac{1}{3}(x_1, x_2, x_3)$$

3D graphs: τ_6

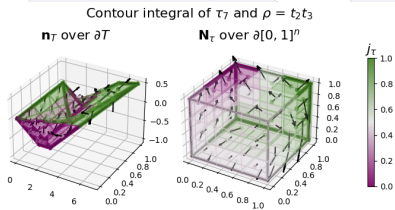
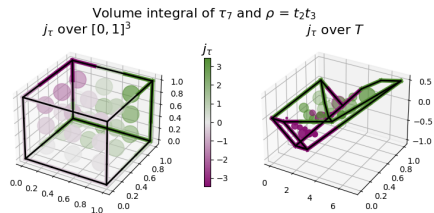


$$t_6(t_1, t_2, t_3) = (t_1 - 3t_1t_2, t_2, t_3 + 2t_2t_3)$$

$$\rho(x_1, x_2, x_3) = x_1$$

$$\mathbf{v}(x_1, x_2, x_3) = \frac{1}{3} \left(\frac{1}{2}x_1^2, x_1x_2, x_1x_3 \right)$$

3D graphs: τ_7



$$t_7(t_1, t_2, t_3) = (t_1 + 2t_3 + 4t_1 t_2 t_3, t_2, -2t_1 t_2 + t_1^2 t_2 - 0.5t_3 + 4t_1 t_2 t_3 - 2t_1^2 t_2 t_3)$$

$$\rho(x_1, x_2, x_3) = x_2 x_3$$

$$\mathbf{v}(x_1, x_2, x_3) = \frac{1}{3} \left(x_1 x_2 x_3, \frac{1}{2} x_2^2 x_3, \frac{1}{2} x_2 x_3^2 \right)$$

3D convergence

We measure the discrepancy between volume integral V and contour integral C with their difference $|C - V|$.

The discrepancy decreases by two orders of magnitude for each increase in resolution. The values V and C converge.

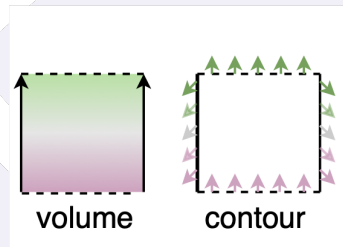
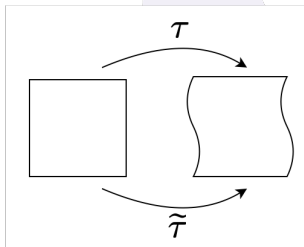
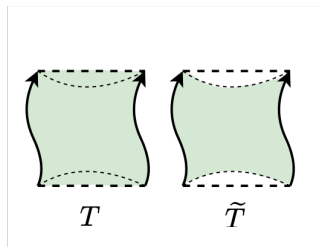
τ	ρ	V	C	V	C	$ C-V $		
	<i>res</i>	0.33		0.0033		0.33	0.033	0.0033
τ_5	1	-1.0	-1.0	-1.0	-1.0	0.0	0.0	0.0
τ_6	x_1	1.139	1.291	1.250	1.250	1.5e-1	1.5e-3	1.5e-5
τ_7	$x_2 x_3$	-0.135	-0.148	-0.135	-0.135	1.3e-2	1.3e-4	1.3e-6

Implementation Strategies and Generalizations

Implementation Choices

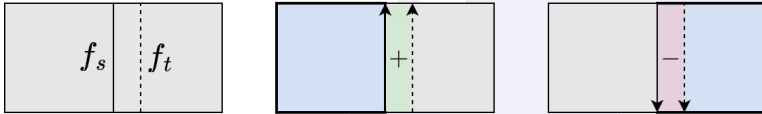
To compute the flux through the region swept between a source and target face, we make several intermediate choices.

1. Between a source and target face, there are many possible swept regions.
2. For a given swept region, we have many possible parameterizations.
3. Finally, given a swept region and parameterization, we may compute the flux in several equivalent ways.

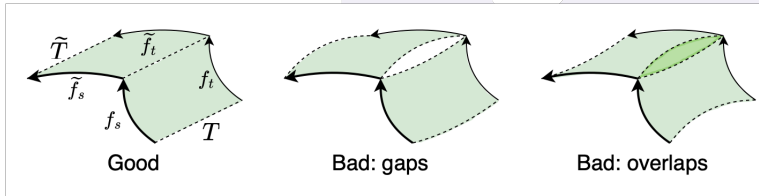


Neighboring swept regions

The swept regions associated with a shared face should be computed once with opposite sign.



Neighboring swept regions must be contiguous without overlaps or gaps.

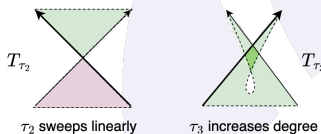


An efficient implementation strategy

Choose a consistent mesh parameterization, then linearly sweep between f_s and f_t .

$$\tau(t_1, \dots, t_n) = f_s(t_1, \dots, t_{n-1}) + t_n(f_t - f_s)(t_1, \dots, t_{n-1}).$$

For computing numerical integrals, this adds only one degree to polynomial faces, and eliminates gaps and overlaps between neighboring zones.

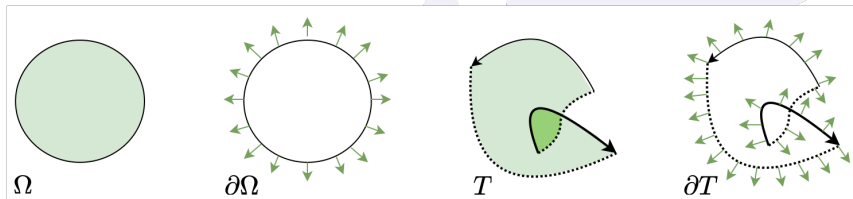


To compute the flux, we recommend the parameterized volume integral:

$$\mathcal{F}_\rho(T) = \int_{[0,1]^n} (\rho \circ \tau) j_\tau dt.$$

Extensions to non-rectangular topologies

Our parameterization $\tau : [0, 1]^n \rightarrow \mathbb{R}^n$ maps from the unit cube. However, we could have used $\tau : \Omega \rightarrow \mathbb{R}^n$ where $\Omega \subset \mathbb{R}^n$ compact with piecewise differentiable boundary.



This gives us additional flexibility to non-rectangular mesh geometries. However, rectangular meshes are particularly convenient to parameterize, since we can use a map from a unit grid.



Conclusions

Summary of results and novelty

- We described our swept region mathematically, and provide several characterizations of the flux.
- We validate the theoretical results with numerical modeling.
- We discuss efficient strategies for parameterizing our swept regions and computing the flux.
- We consider non-rectangular mesh geometries.

This method for remap preserves globally polynomial solutions. It is continuous in that an unchanged mesh means no change in zone masses.

Next steps

- If our physical solution ρ is defined on source zones, how do we compute the flux without reconstructing a global ρ ?
- How do we construct an efficient global mesh parameterization?
- How robust is this method to uncertainty in our measurements?
- Considering higher-order remap, can we create a flux integral directly from moments, rather than explicitly giving a parameterization?

Acknowledgments

- This project was supported by the National Nuclear Security Administration and the DOE.
- Thanks to my GRA mentors Konstantin Lipnikov and Angela Herring for their support.
- Thanks to Misha Shashkov for the problem motivation, and for feedback.
- Thanks to Rao Garimella for abstract feedback, and to the Portage team for including me this summer.

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