Optimization-based modeling

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Numerical Analysis and Applications

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Outline

- **What is optimization-based modeling (OBM)?**
- **Application to transport and remap**
  - Optimization-based monotone remap (OBR)
  - Optimization-based monotone transport (OBT)
- **Flexibility of the OBM approach**
  - OBR/OBT with reduced dissipation

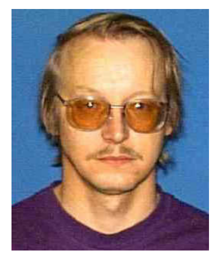
Key Collaborators

K. Peterson
SNL

D. Ridzal
SNL

G. Scovazzi
SNL

J. Young
SNL



M. Shashkov
LANL

Goal: Physically Correct Discrete Models

Challenges:

$$\partial_t u = Lu$$

Typically, constraints are not preserved automatically under discertization, even with stabilization/regularization

$$\partial_t u^h = L^h u^h$$

$$\underline{C} \le Cu \le \overline{C}$$

In multiphysics codes this solution is input for another physics component

$$\cancel{\underline{C} \le Cu^h \le \overline{C}}$$

$$Bu = b$$

$$\ldots\ldots\ldots\ldots\ldots$$

Automatic preservation of maximum principle, local and global bounds, is required for robust, predictive simulations

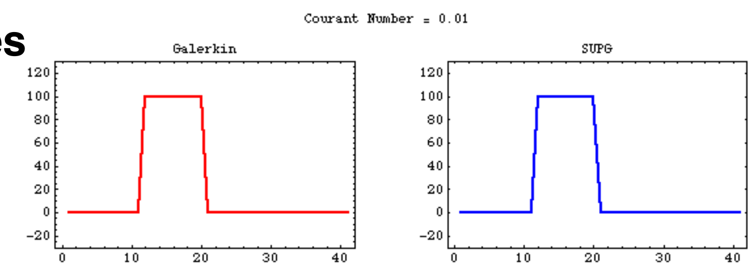
$$\cancel{Bu^h = b}$$

$$\ldots\ldots\ldots\ldots\ldots$$

Trying to deal with these challenges **directly couples constraints** with **accuracy** considerations:

$\Rightarrow$ increase **fragility** due to ad hoc "fixes"

$\Rightarrow$ reduced **functionality** due to grid restrictions



A "non-standard" strategy: Optimization-based modeling (OBM)

Motivation:

As our models become more sophisticated, continuing reliance on direct approaches will lead to **increased complexity** of resulting algorithms, accompanied by **decrease in robustness, efficiency and flexibility**.

Our approach:

Use **optimization and control ideas** to **manage externally** those objectives that are **difficult** (or impractical) to handle **directly** in the discretization process via grid and/or space manipulation.

Potential payoffs

- ➪ **Elimination of limiters**: lifts the associated restrictions on cell types & accuracy
- ➪ **Balancing of constraints**: accuracy, mass conservation, monotonicity, variable bounds…
- ➪ **Generality with respect to problem discretization**: applicable to FE, FV and FD
- ➪ **Generality with respect to problem type:** elliptic, hyperbolic, …
- ➪ **Enable efficient reuse of existing codes:** solvers, optimization tools,…

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OBM in a nutshell

Generic optimization "harness"

minimize	$J(u)+\frac{\varepsilon}{2}\|\theta\|^2$	objective	$\rightarrow$	u (state)
		regularization	$\rightarrow$	θ (control)
subject to	$Lu=\theta$	equality	$\rightarrow$	constraints
	$\underline{C}\le Cu\le\overline{C}$	inequality		

Key question: how to reformulate (map) a given problem into an optimization problem?

3 basic steps ➔

(1) identify **states**;
(2) identify **objective**;
(3) identify **constraints:**

- "*Flux-corrected remap*", M. Shashkov et al, 2010 - using local optimization strategy; FCT inspired
- "*Enforcing discrete maximum principle*", M. Shashkov et al, 2007 - using constrained optimization
- "*Enforcement of constraints & max. principle in VMS*", T. Hughes, 2009 - applies Shashkov's idea to VMS

Specialization to preservation of properties

Objective	Constraints
Match a discrete target solution having the best possible accuracy	**Enforce** lost physical properties

$$\partial_t u = Lu$$

$$\underline{C} \le Cu \le \overline{C}$$

....

$$\text{minimize} \quad \frac{1}{2}\left\| u^h - u_T^h \right\|^2$$

$$\text{subject to} \quad \begin{cases} \underline{C} \le Cu^h \le \overline{C} \\ \partial_t u_T^h = L^h u_T^h \end{cases}$$

← **Match** target field

← Enforce constraints

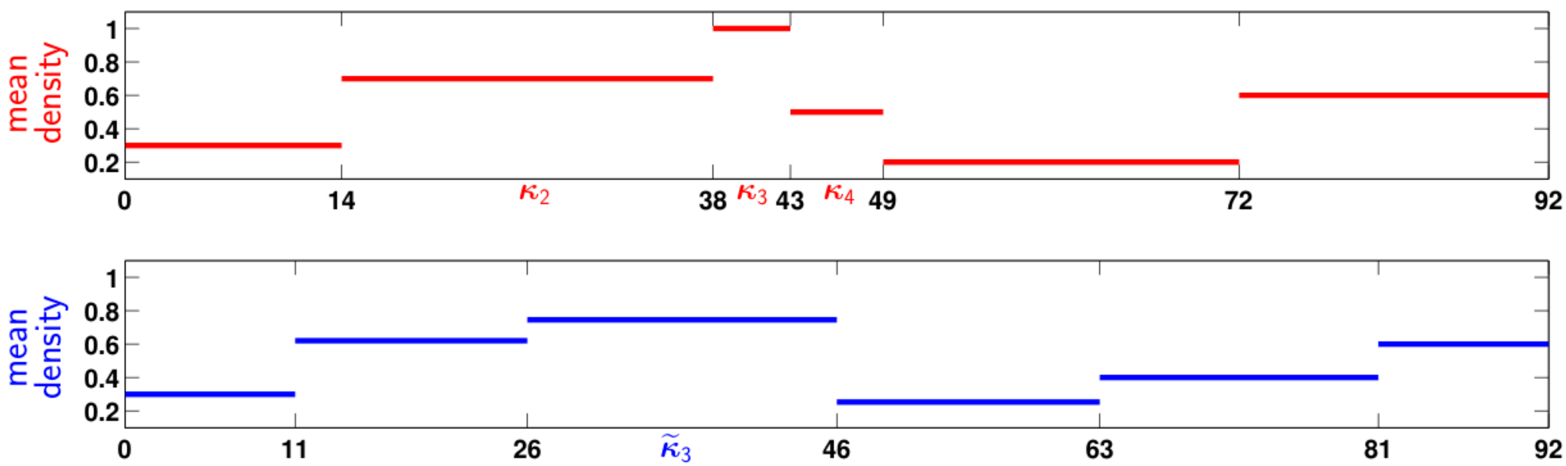
← Define target field

Focus on remap and transport algorithms

- "*Optimization based remap",* Bochev, Ridzal, Scovazzi, Shashkov JCP, 2011
- "*Optimization-based transport*", Parts 1-3, Bochev, Peterson, Ridzal, Young, LNCS 2012

OBM Framework for Remap and Transport

Remap Nomenclature



κ_i → Lagrangian (old) cell

$\tilde{\kappa}_i$ → Rezoned (new) cell

$E(\tilde{\kappa}_i)$ → Neighbors of old cell

$V(\kappa_i) = \int_{\kappa_i} dV$ → (old) cell volume

$m_i = \int_{\kappa_i} \rho(x) dV$ → (old) cell mass

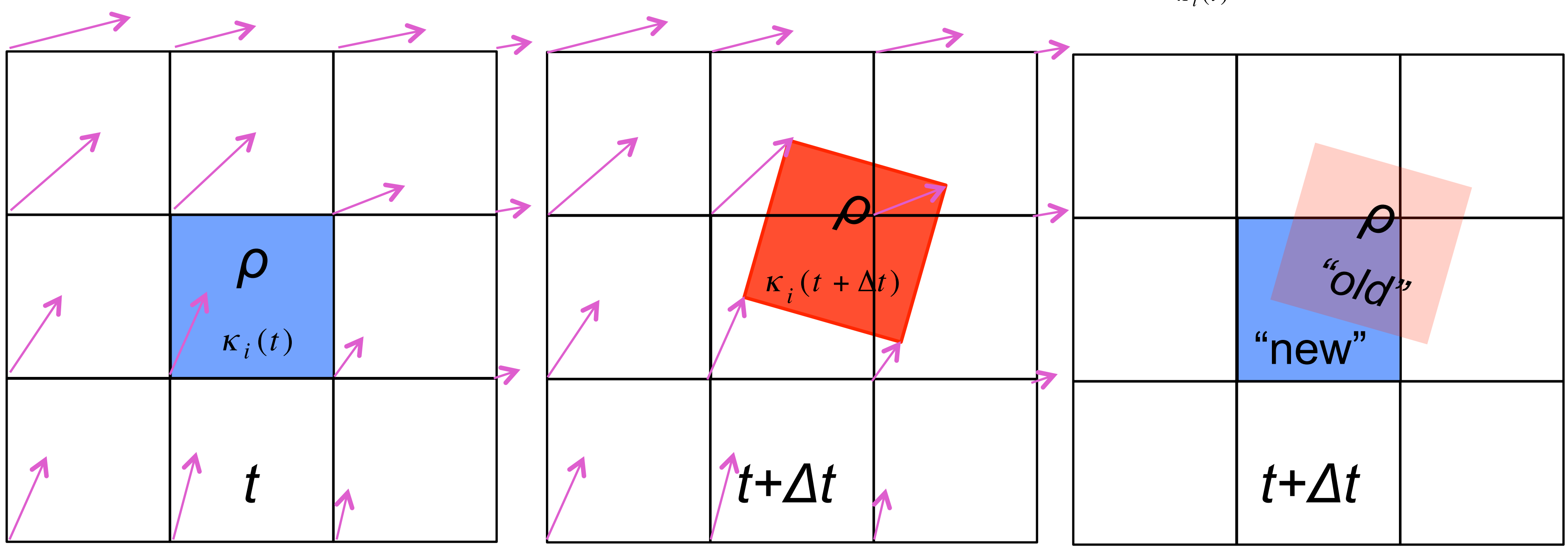
Local bounds

$$\rho_i = \frac{m_i}{V(\kappa_i)} \quad \Longrightarrow \quad \rho_i^{\min} \le \rho_i \le \rho_i^{\max} \quad \Longrightarrow \quad \rho_i^{\min} V(\kappa_i) \le m_i \le \rho_i^{\max} V(\kappa_i)$$

Optimization-based monotone transport (OBT)

Transport = incremental remap (Dukowicz and Baumgardner, JCP 2000)

Mass is conserved in Lagrangian volumes: $\frac{d}{dt} m_i(t) = \frac{d}{dt} \int_{\kappa_i(t)} \rho(x) dV = 0$



$m_i(t) = \int_{\kappa_i(t)} \rho(x) dV$

$m_i(t+\Delta t) = m_i(t)$

Remap

Optimization-based Remap (OBR) ⇒ OBT algorithm

Statement of the remap problem

Given: Mean density values ρ_i on the old grid cells κ_i

Find: Accurate approximations $\tilde{m}_i$ for the masses of the new cells $\tilde{\kappa}_i$:

$$\tilde{m}_i \approx m_i^{EX} = \int_{\tilde{\kappa}_i} \rho(x)dV; \quad i = 1,\dots,i_N$$

Subject to: **Total mass conservation**

C1: $$\sum_i \tilde{m}_i = \sum_i m_i = M$$

Linearity preservation

C2: $$\rho(x) = \mathbf{c}_0 + \mathbf{c}^T\mathbf{x} \quad \Rightarrow \quad \tilde{m}_i = m_i^{EX} = \int_{\tilde{\kappa}_i} \rho(x)dV; \quad i = 1,\dots,i_N$$

Bounds preservation

C3: $$\rho_i^{\min} \le \tilde{\rho}_i \le \rho_i^{\max} \quad \longrightarrow \quad \rho_i^{\min} V(\tilde{\kappa}_i) \le \tilde{m}_i \le \rho_i^{\max} V(\tilde{\kappa}_i)$$

This begins to look like an optimization problem

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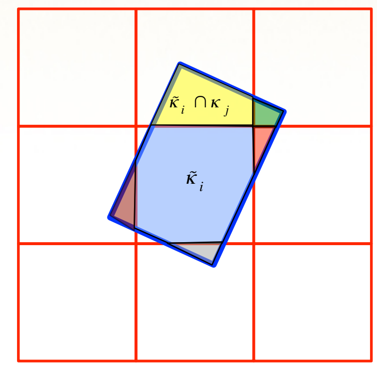
Optimization-based remap (OBR): setup



The exact mass on new cell $\tilde{\kappa}_i$ can be expressed in mass-flux form:

$$\tilde{m}_i^{EX} = m_i^{EX} + \sum_{E(\tilde{\kappa}_i)} F_{ij}^{EX}; \quad F_{ij}^{EX} = \int_{\tilde{\kappa}_i \cap \kappa_j} \rho(x)dV - \int_{\kappa_i \cap \tilde{\kappa}_j} \rho(x)dV$$

Therefore, the mass on the new cell $\tilde{\kappa}_i$ can be approximated by

$$\tilde{m}_i^h = m_i^h + \sum_{E(\tilde{\kappa}_i)} F_{ij}^h, \quad \text{where} \quad F_{ij}^h = \int_{\tilde{\kappa}_i \cap \kappa_j} \rho_i^h(x)dV - \int_{\kappa_i \cap \tilde{\kappa}_j} \rho_i^h(x)dV \approx F_{ij}^{EX}$$

C1: Mass conservation. Guaranteed if discrete fluxes are antisymmetric:

$$F_{ij}^h = -F_{ij}^h \quad \Rightarrow \quad \sum_{Cell} \tilde{m}_i^h = M$$

C2: Linearity preservation. Guaranteed if ρ_i^h is exact for linear functions on all κ_i:

$$F_{ij}^T = \int_{\tilde{\kappa}_i \cap \kappa_j} \rho_i^h(x)dV - \int_{\kappa_i \cap \tilde{\kappa}_j} \rho_i^h(x)dV \longrightarrow$$

Target (**high-order**) mass fluxes

Optimization-based remap (OBR): formulation

Constrained optimization formulation of remap

$$\underset{F_{ij}^h}{\text{minimize}} \quad \sum_{Cell} \sum_{Flux} \left(F_{ij}^h - F_{ij}^T\right)^2 \quad \text{subject to}$$

$$\tilde{m}_i^{\min} \le m_i + \sum_{i<j} F_{ij}^h - \sum_{i>j} F_{ji}^h \le \tilde{m}_i^{\max} \qquad i = 1,\ldots,N$$

- **Objective** = **minimize distance** between **discrete** and **target** fluxes
- **Constraint** = **C3: Local bounds preservation**
- **Accuracy** (high-order target) is completely **separated** from **bounds** enforcement
  - ⇒ Allows extension of OBR to arbitrary cells, e.g., polygons and polyhedra
  - ⇒ Local bounds and linearity preservation impervious to cell shapes!
  - ⇒ Allows extension of OBR to higher than 2nd order using appropriate reconstruction ρ_i^h
- OBR can be extended to **systems/coupled** transport
- Motivated in part by the **Flux-corrected remap** (FCR) (Liska, Shashkov, et al JCP 2010)

OBR is provably accurate

Theorem. (Preservation of linearity)

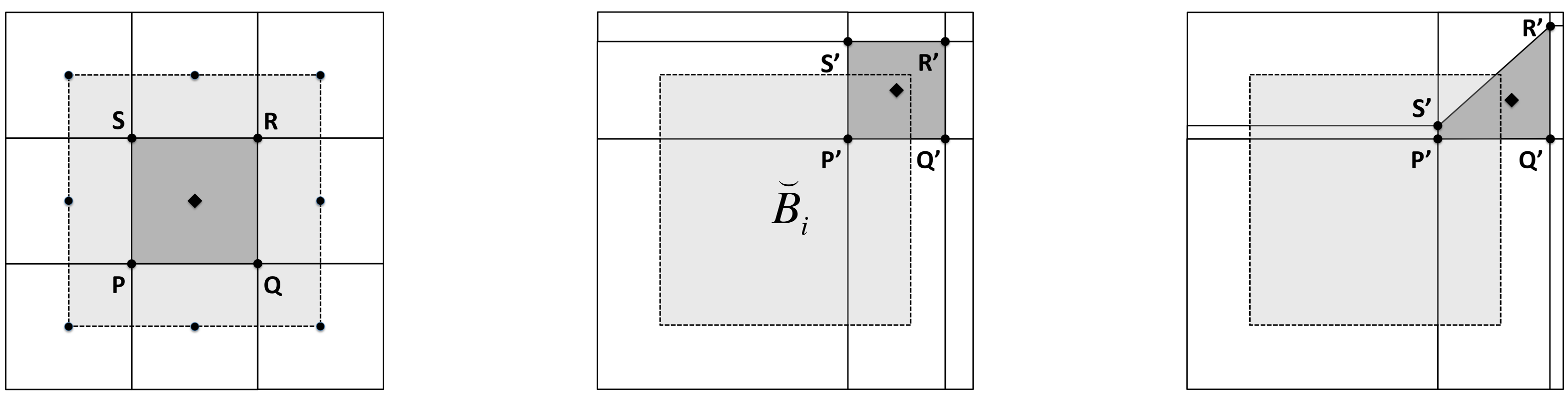
Let B_i denote the set of barycenters (centroids) $\mathbf{b}_j$ of the old cells in the neighborhood of a new cell $\tilde{\kappa}_i$:

$$B_i = \left\{ \mathbf{b}_j \,\middle|\, \kappa_j \in E(\tilde{\kappa}_j) \right\}$$

A sufficient condition for the target fluxes F_{ij}^T to be in the feasible set, i.e. for the optimization based remap to preserve linear functions, is

$$\tilde{\mathbf{b}}_i \in \breve{B}_i \quad \text{for all} \quad i = 1, \ldots, N$$

where $\tilde{\mathbf{b}}_i$ is the barycenter of $\tilde{\kappa}_i$ and $\breve{B}_i$ is the convex hull of B_i .



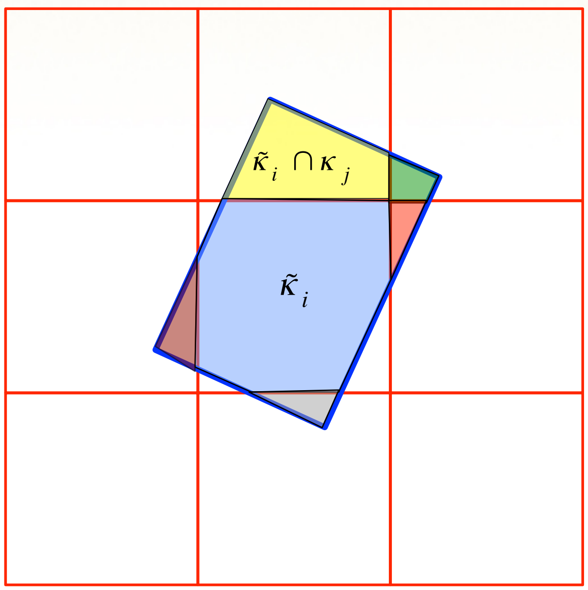
1) Less restrictive than similar condition for Van Leer (B. Swartz, JCP 1999)

2) Result independent of cell shape (arbitrary polyhedral grids are OK).

OBR in two-dimensions

Exact cell intersections

Dukowicz, 1984

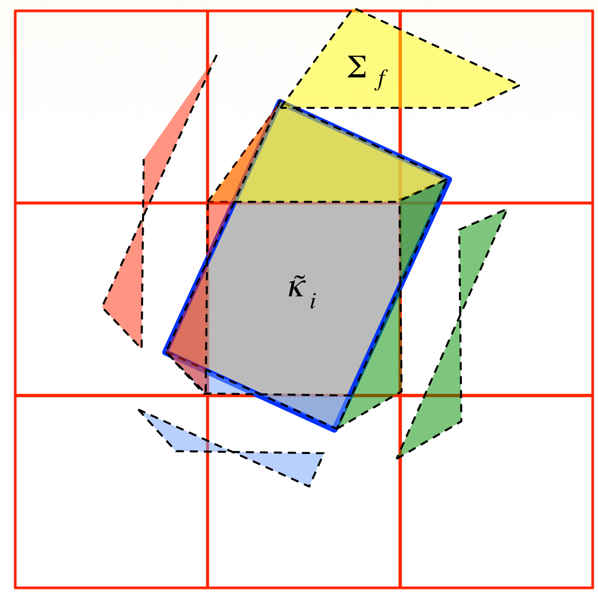


$$F_{ij}^h = \int_{\tilde{\kappa}_i \cap \kappa_j} \rho_i^h(x)dV - \int_{\kappa_i \cap \tilde{\kappa}_j} \rho_i^h(x)dV$$

$$\tilde{m}_i^h = m_i^h + \sum_{E(\tilde{\kappa}_i)} F_{ij}^h$$

Swept region (SR) approximation

Margolin, Shashkov, 2003



$$F_{ij}^h = \int_{\Sigma_f} \rho_i^h(x)dV$$

SRs are completely determined by the coordinates of old and new cells ⇒ **efficiency**

SRs give exact cell masses for linear density ⇒ **accuracy**

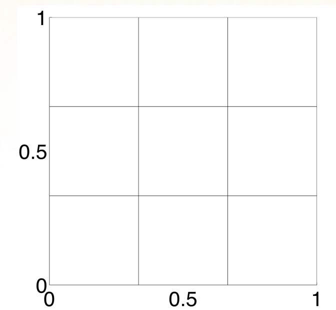
Exact cell intersections guarantee that low order fluxes in FCR are monotone. However, this is not true for SR without additional restrictions on mesh motion.

Potential issue for FCR but not for OBR, which does not use low order fluxes

Comparison of swept region implementations

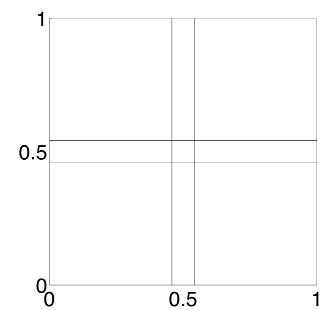
Preservation of monotonicity

	C=5	C=6	C=7	C=14	C=15	C=16	C=100
OBR	✔	✔	✔	✔	✔	✔	✔
FCR	✔	✔	✔	✗	✗	✗	✗
Donor	✔	✗	✗	✗	✗	✗	✗



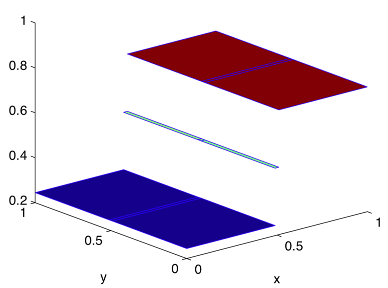
Preservation of linearity

	C=3	C=4	C=5	C=15	C=16	C=100
OBR	✔	✔	✔	✔	✔	✔
FCR	✔	✗	✗	✗	✗	✗

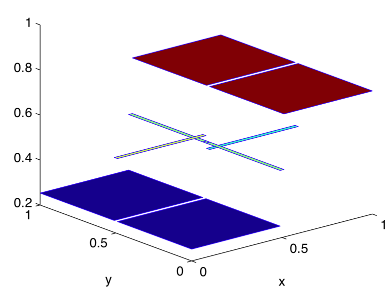


Mesh motion

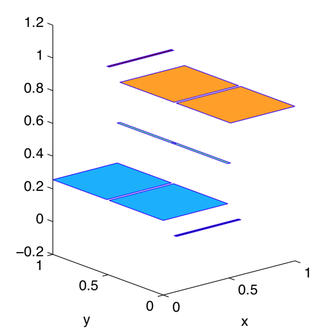
OBR



FCR



Donor



Efficiency: OBR vs. FCR in 2D

***Matlab* wall-clock times on a single Intel Xeon X5680 3.33 GHz processor**

“Sine” density

Cells	Remaps	FCR (sec)	OBR (sec)	Ratio
64x64	320	4.2	7.3	**1.7**
128x128	640	25.4	49.5	**1.9**
256x256	1280	176.5	390.6	**2.2**
512x512	2560	1812.5	3663.8	**2.0**

“Peak” density

Cells	Remaps	FCR (sec)	OBR (sec)	Ratio
64x64	320	4.9	8.4	**1.7**
128x128	640	28.5	57.8	**2.0**
256x256	1280	183.8	418.6	**2.3**
512x512	2560	1832.9	4528.6	**2.5**

OBT applied to a standard 2D test case

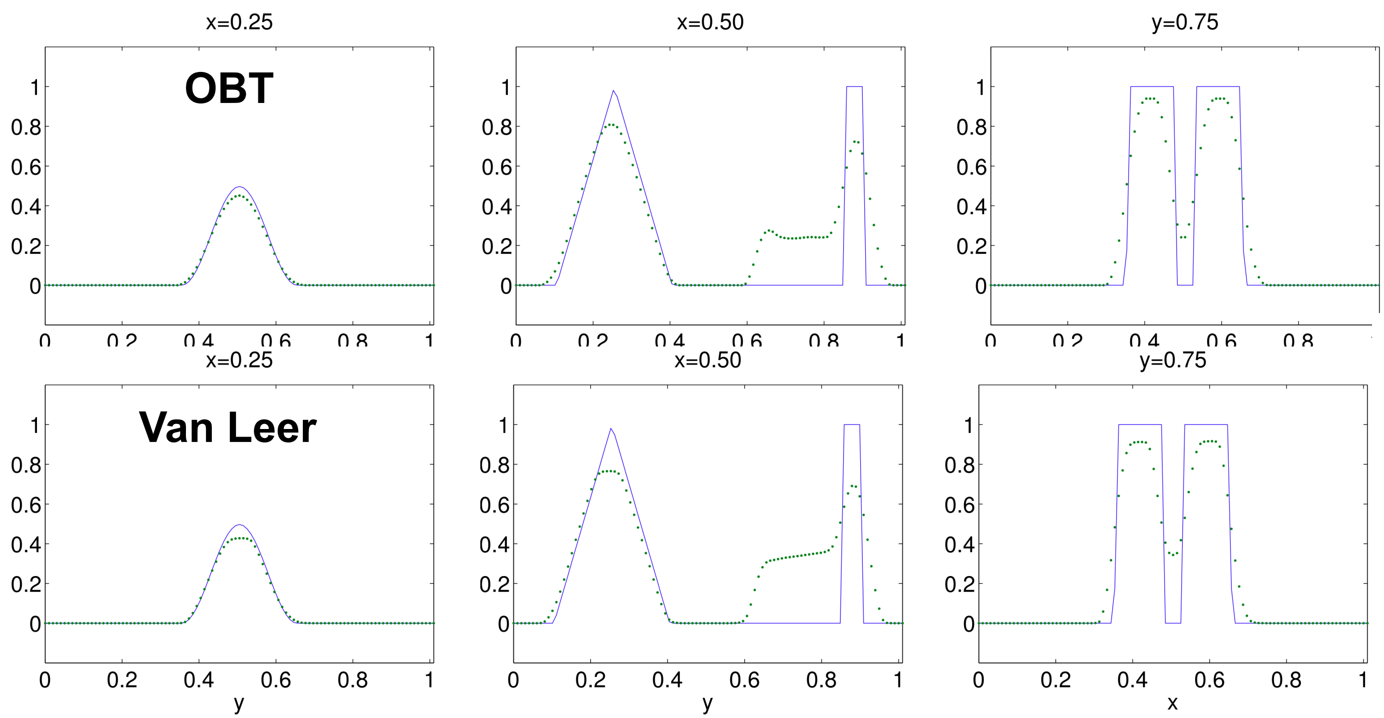
Rotating flow example (LeVeque, SINUM 33, 1996)

$$u = -(y - 0.5) \qquad v = (x - 0.5)$$

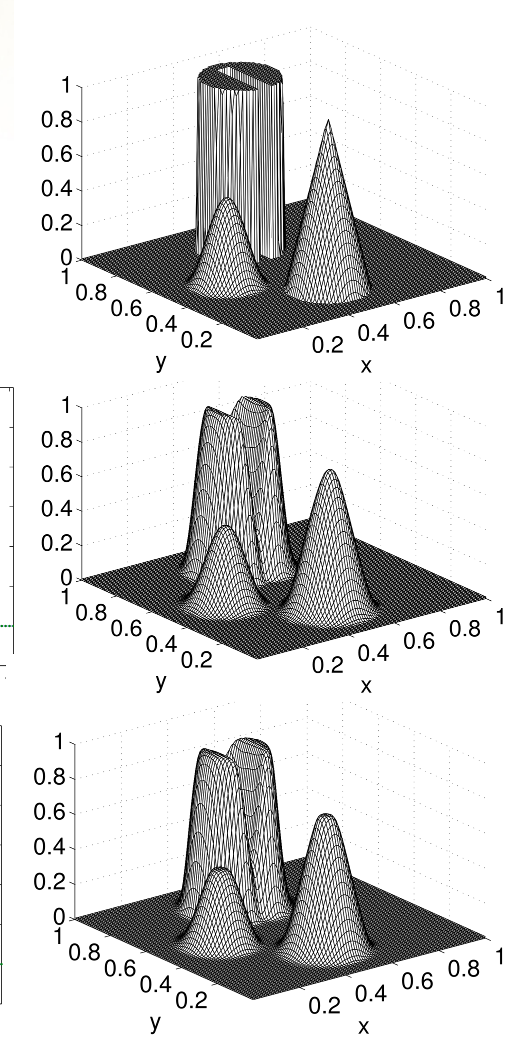
Grid size: *NxN*, ***N*=100**

Time steps: $2\pi N$ **628**

CFL < 1



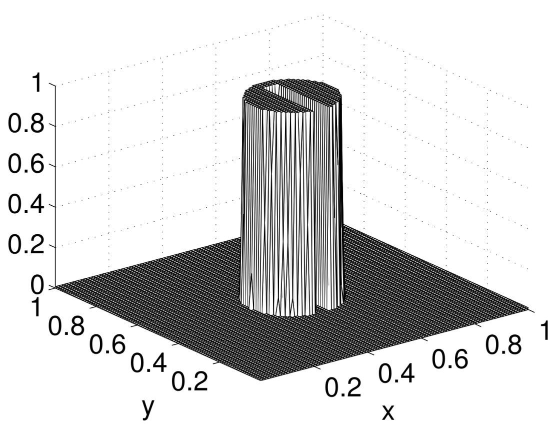
Initial



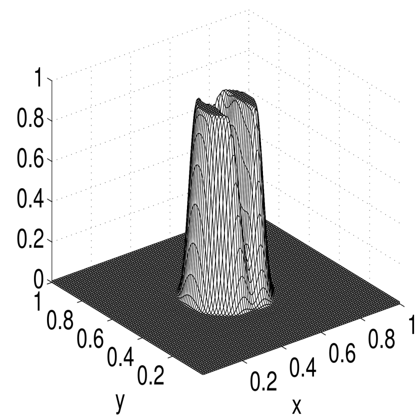
OBT inherits the robustness of OBR

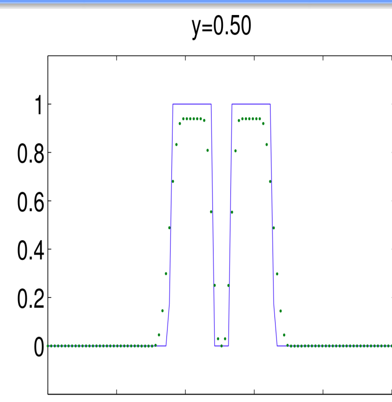
Zalesak cylinder: rotation

L1 Error	CFL=1	CFL=1.60	CFL=1.62	CFL=2.20	CFL=2.25	CFL=5.21	CFL=5.50
OBT	2.14E-02	2.37E-02	2.38E-02	2.60E-02	2.62E-02	4.02E-02	4.36E-02
FCRT	1.97E-02	2.19E-02	2.21E-02	3.00E-02	**6.00E+06**	**9.45E+38**	**1.83E+40**
VLT	2.14E-02	2.36E-02	8.15E-01	**3.47E+54**	**2.85E+56**	**2.83E+79**	**6.23E+77**

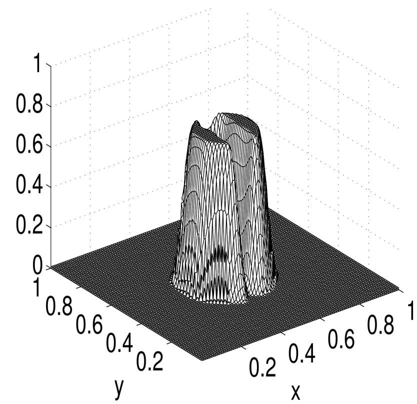


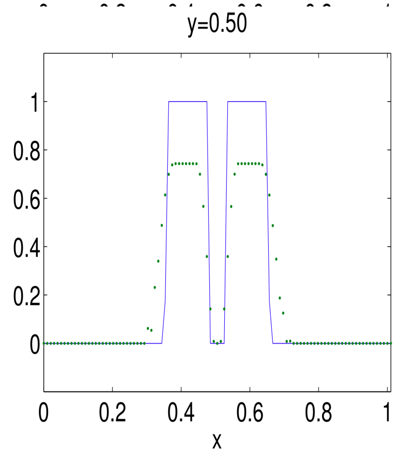
Initial density





OBR: CFL=1.0





OBR: CFL=4.7

OBT inherits the accuracy of OBR

Cumulative convergence rate (CR): smooth cone

Grid	$1/\Delta t$	L_∞ OBT	L_∞ FCRT	L_∞ VLT	CR-OBR	CR-FCRT	CR-VLT
100^2	5026	3.76E-02	3.66E-02	5.08E-02	1.88	1.76	1.66
120^2	6031	2.60E-02	2.57E-02	3.78E-02	1.94	1.84	1.64
140^2	7037	1.98E-02	1.98E-02	2.97E-02	1.91	1.82	1.62

Preliminary cost studies with a *Matlab*™ prototype show

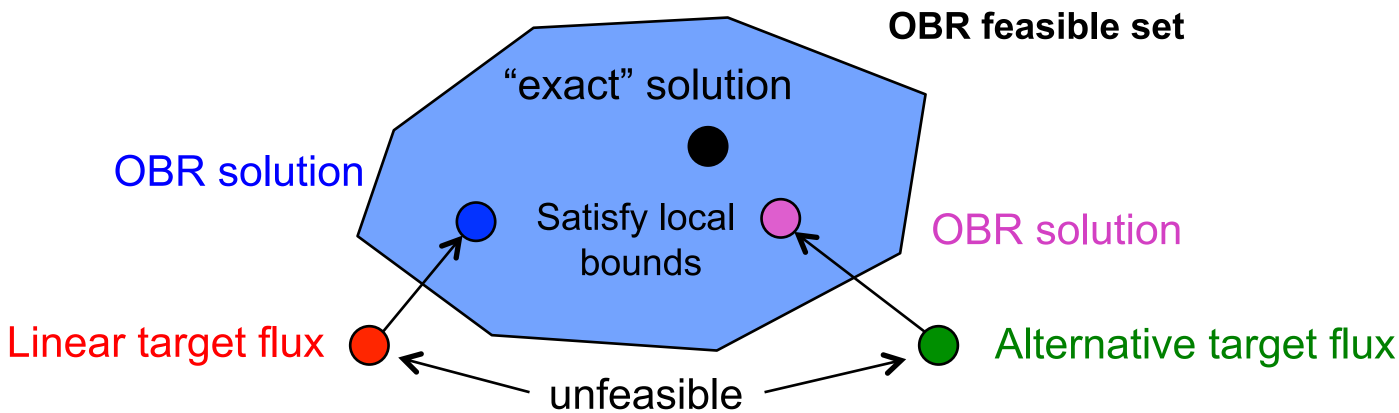
- Linear *O(N)* cost for OBR and OBT (same as local approaches)
- OBR/OBT more expensive by a factor of ~ 2.1 than local methods

OBR/OBT With Reduced Dissipation

Key observations

- OBR/OBT feasible set always contains the “exact solution”
- Linear reconstruction yields one possible set of target fluxes
- In OBR/OBT reconstruction and bounds enforcement are **completely separated**

  ⇒ reconstruction can be adjusted to problem features without concern for the bounds, the latter will be imposed by the inequality constraints

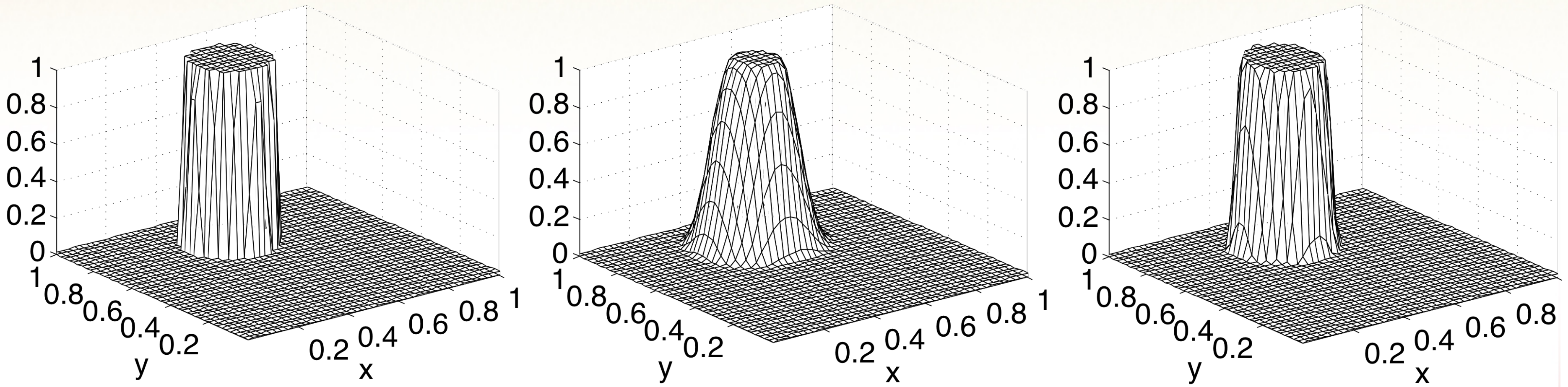


Our approach

Modify the linear reconstruction process using residual information.

The corresponding fluxes capture better salient solution features.

OBT with reduced dissipation



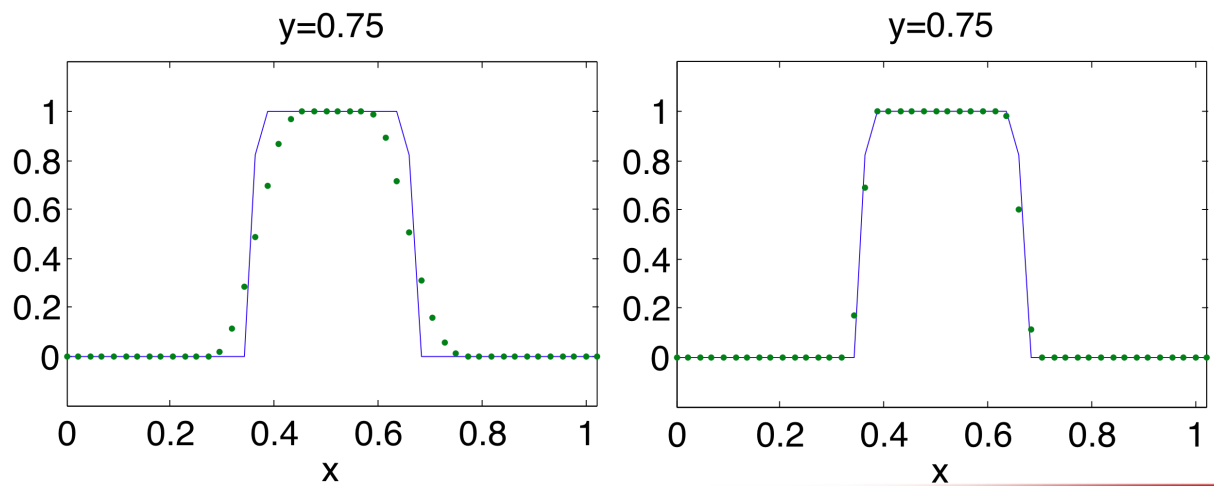
Initial **OBT** **OBT-RD**

Rotating cylinder

$$u = -(y - 0.5) \qquad v = (x - 0.5)$$

Grid size: *N*x*N*, ***N*=45**

Time steps: $2\pi N$ **282**



OBT with reduced dissipation: fine grid

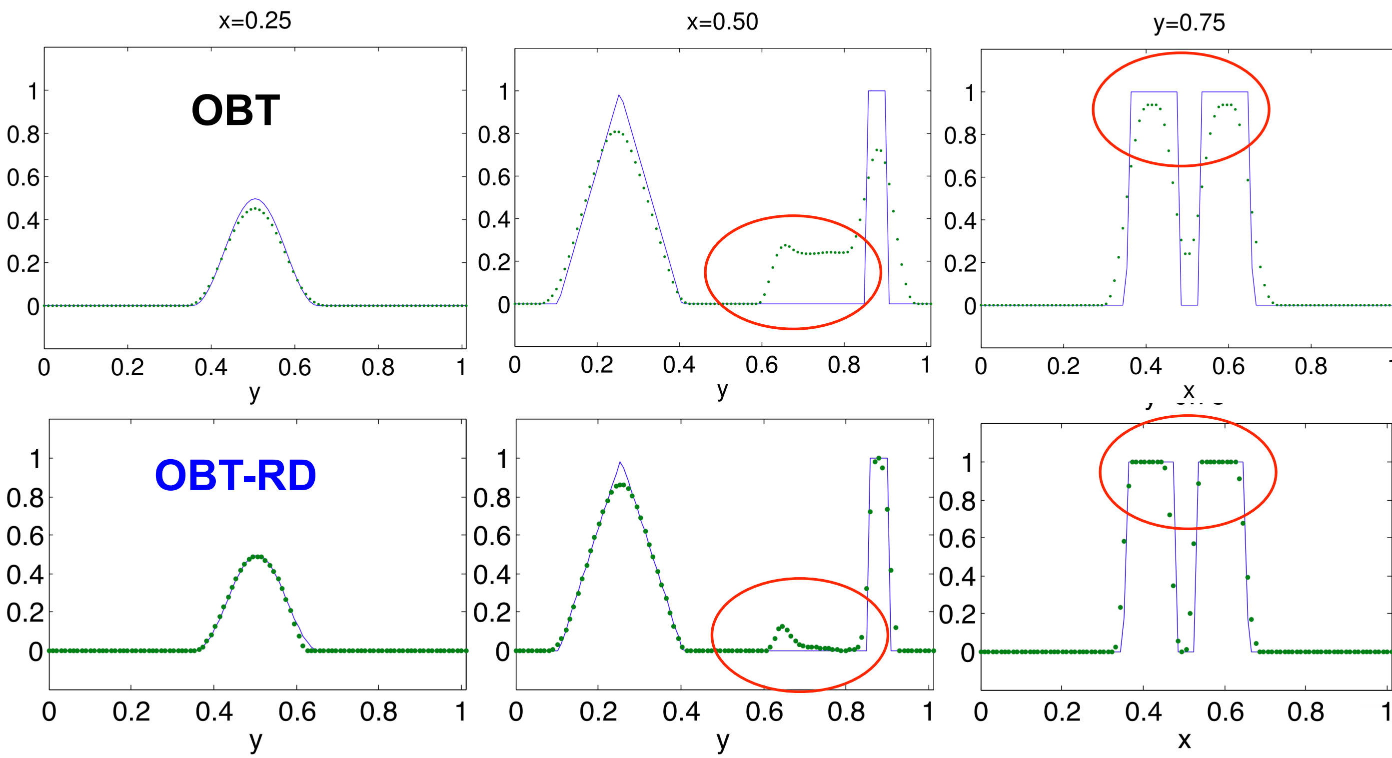
Rotating flow example (LeVeque, SINUM 33, 1996)

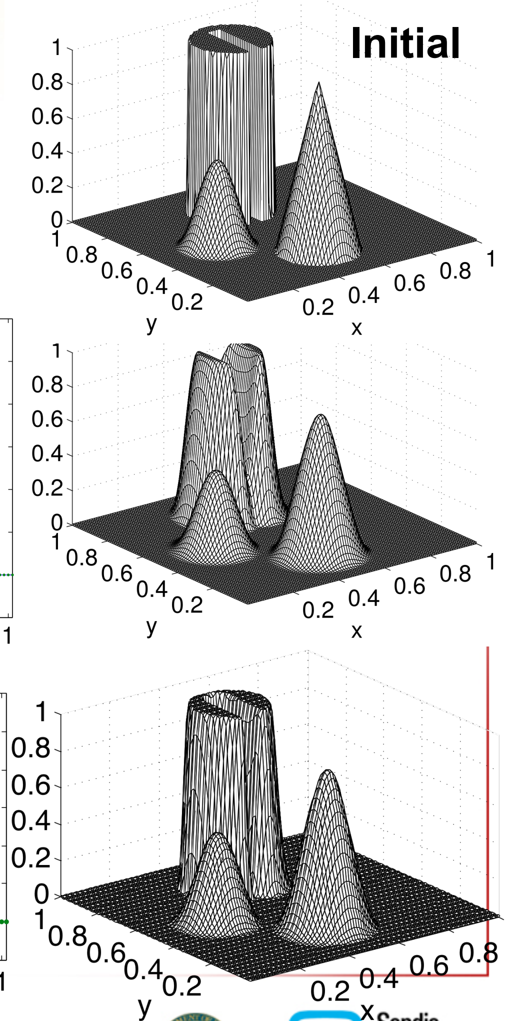
$$u = -(y - 0.5) \qquad v = (x - 0.5)$$

Grid size: *N*x*N*, ***N*=100**

Time steps: $2\pi N$ **628**

CFL < 1





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OBT with reduced dissipation: coarse grid

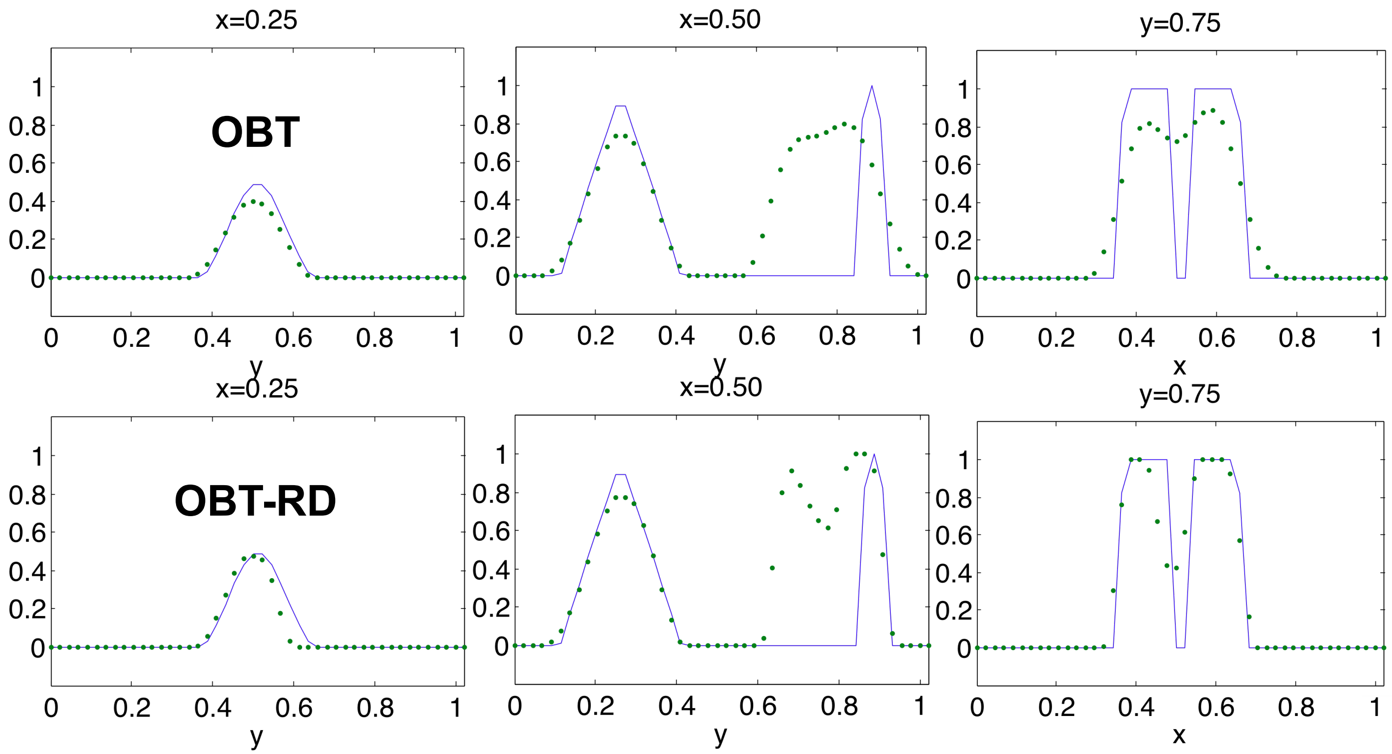
Rotating flow example (LeVeque, SINUM 33, 1996)

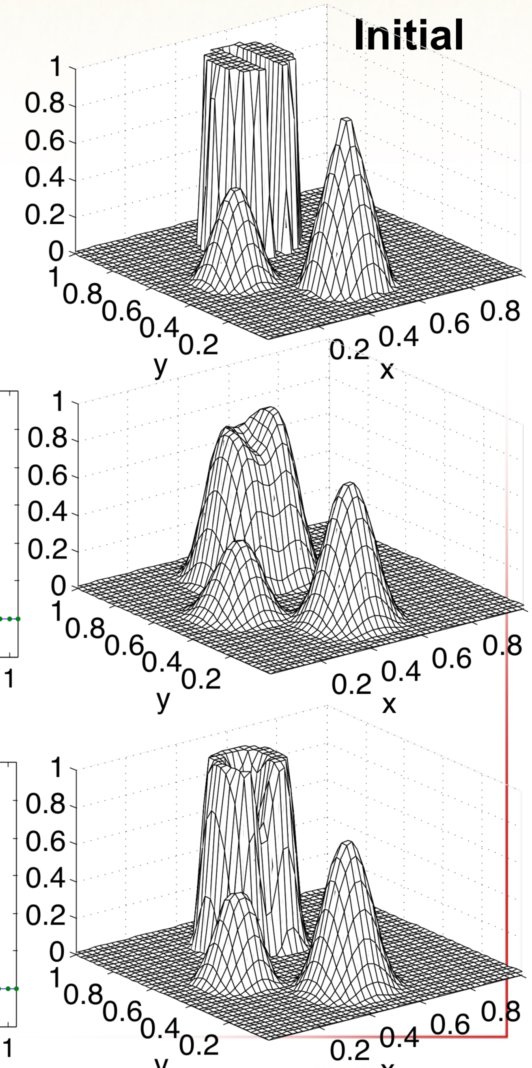
$$u = -(y - 0.5) \qquad v = (x - 0.5)$$

Grid size: *NxN*, ***N*=45**

Time steps: $2\pi N$ **282**

CFL < 1





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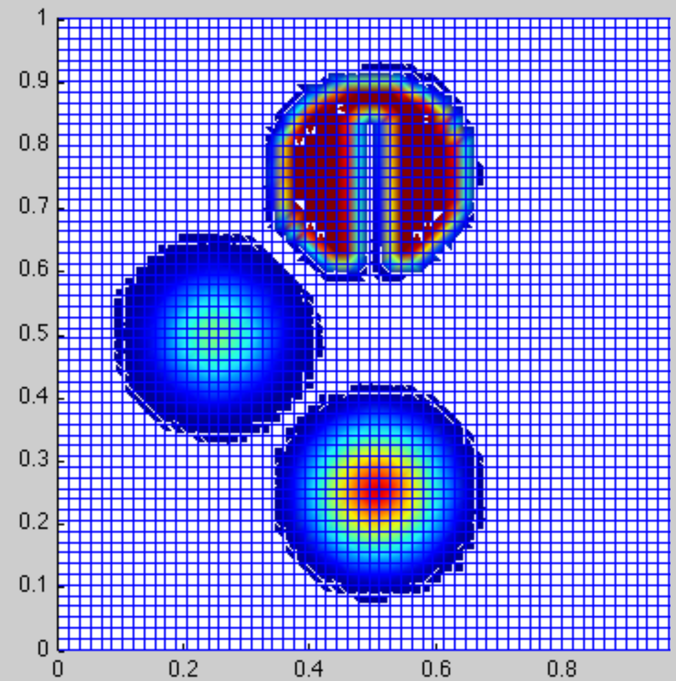

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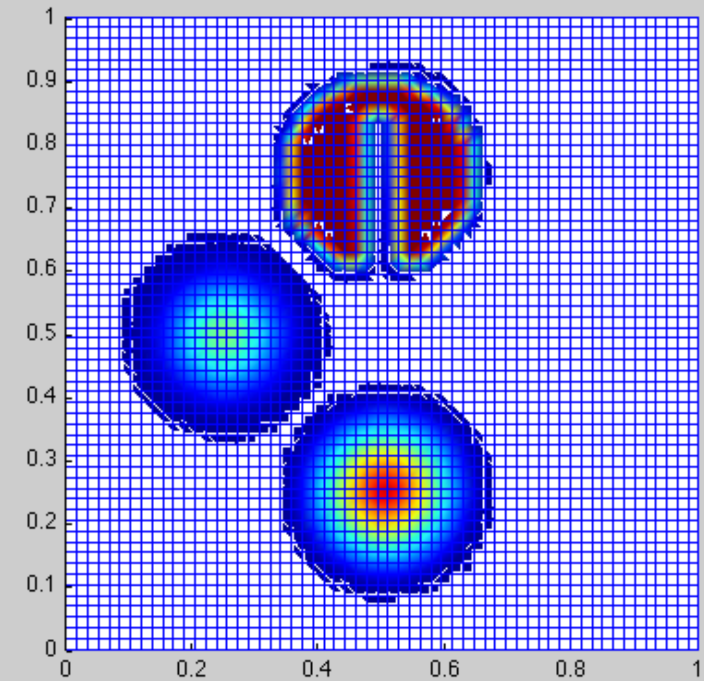
0.8

OBT-RD



1
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0.4
0.6
0.8
1

OBT

Summary: OBM is a non-standard strategy for improved predictiveness with significant potential payoffs

We apply optimization and control tools to automatically manage discretization tasks that are difficult to accomplish directly:

— Reconcile solutions from constituent components of multi-physics problems
— Reconcile different representations of the same field in physically consistent manner
— Impose physical constraints that were lost during discretization

Advantages

— Expand scope of methods to, e.g., unstructured grids and arbitrary cells
— Remove order limitations (reformulation yields **equivalent** problems)
— Rigorous mathematical foundations inherited from rich optimization theory
— Reuse of software components

Target Applications

— Climate models involve large number of transport equations on different grids: OBM can provide a unified approach to handle these equations

— Compatible data transfer (remap) of scalar, vector and tensor fields for
  - code to code coupling (Euler + Lagrange); overset methods
  - conservative, bounds preserving remap for ALE methods

— Constrained transport of vector fields, e.g., magnetic advection

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