Optimization-Based Remap

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in collaboration with

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SIAM Conference on Computational Science and Engineering
February 28, 2011

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Outline

- Introduction to Remap
- Formulation of Optimization-Based Remap (OBR)
- Theoretical Properties of OBR
  - Mesh motion conditions for exact recovery of linear functions
  - Connection with Flux-Corrected Remap (FCR)
- Algorithms
- Three Instructive Examples
- Computational Studies
Introduction to Remap
Remap = Constrained Interpolation

**Given:** Discrete representation $f_A^h$ of function $f$ on mesh $A$.

**Find:** Accurate discrete representation $f_B^h$ of $f$ on mesh $B$, subject to physical constraints:

- conservation of mass, energy, etc.
- preservation of monotonicity
- physically meaningful ranges for variables: density $\geq 0$, concentration $\in [0, 1]$

- Uses: transport algorithms, mesh rezone/repair, mesh tying.
- One flavor: Incremental remap $\rightarrow$ Mesh $A$ is “close to” mesh $B$.
- Arbitrary Lagrangian-Eulerian (ALE) and Particle-In-Cell (PIC) methods depend on robust remap algorithms.

Challenge: Competing objectives and constraints!
Motivation for Optimization-Based Remap (OBR)

- balancing of desired mathematical features and physical constraints: accuracy vs. mass conservation, monotonicity, bounds on variables
- generality with respect to discretization: applicable to finite element, finite volume and finite difference schemes as well as particle methods; suitable for arbitrary polyhedral grids!


We have developed a new mathematical framework for the solution of incremental remap problems, based on a globally constrained optimization strategy.
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We have developed a new mathematical framework for the solution of incremental remap problems, based on a globally constrained optimization strategy.

We show that the global optimization formulation can have significant theoretical and practical advantages, at little or no added computational cost!
Problem Setup for Incremental Remap

Notation:

- $\kappa_i$ – cell in old grid, $\tilde{\kappa}_i$ – cell in new grid; $K$ is the number of cells
- $N(\kappa_i)$ – neighborhood of $\kappa_i$ in old grid; $\mathcal{I}(N(\kappa_i))$ – neighbor indices
- locality assumption: $\tilde{\kappa}_i \subset N(\kappa_i)$ for all $i = 1, \ldots, K$
- mean values of density on old mesh: $\rho_i = \int_{\kappa_i} \rho(x) \, dV / V(\kappa_i)$
- masses: $m_i = \int_{\kappa_i} \rho(x) \, dV$ or $m_i = \rho_i V(\kappa_i)$; total mass $M = \sum_{i=1}^{K} m_i$
- trivial observation: $\rho_i^{\text{min}} \leq \rho_i \leq \rho_i^{\text{max}} \iff \rho_i^{\text{min}} V(\kappa_i) \leq m_i \leq \rho_i^{\text{max}} V(\kappa_i)$, where $\rho_i^{\text{min}}$ and $\rho_i^{\text{max}}$ are the neighborhood minima and maxima
Problem Statement: Remap of Mass-Density

Given mean density values $\rho_i$ on the old grid cells $\kappa_i$, find representations $\tilde{m}_i$ for the masses on the new grid cells $\tilde{\kappa}_i$,

$$\tilde{m}_i \approx \tilde{m}_i^{ex} = \int_{\tilde{\kappa}_i} \rho(x) dV ; \quad i = 1, \ldots, K,$$

subject to the following requirements:

- **Mass conservation:** $\sum_{i=1}^{K} \tilde{m}_i = \sum_{i=1}^{K} m_i = M$.

- **‘Accuracy’:** For a globally linear density $\rho(x)$, the remapped masses are exact in the following sense:

$$\tilde{m}_i = \tilde{m}_i^{ex} = \int_{\tilde{\kappa}_i} \rho(x) dV ; \quad i = 1, \ldots, K.$$

- **Preservation of local bounds (implies monotonicity):**

$$\rho_i^{\text{min}} \leq \tilde{\rho}_i \leq \rho_i^{\text{max}} \quad \text{i.e.} \quad \rho_i^{\text{min}} V(\tilde{\kappa}_i) = \tilde{m}_i^{\text{min}} \leq \tilde{m}_i \leq \tilde{m}_i^{\text{max}} = \rho_i^{\text{max}} V(\tilde{\kappa}_i).$$
Formulation of OBR
Optimization-Based Remap

- Express new masses via flux exchanges between old and new cells:

\[ \tilde{m}_i^{\text{ex}} = m_i + \sum_{j \in \mathcal{I}(N(\kappa_i))} F_{ij}^{\text{ex}}, \]

where \( F_{ij}^{\text{ex}} = \int_{\kappa_i \cap \kappa_j} \rho(x) dV - \int_{\kappa_i \cap \tilde{\kappa}_j} \rho(x) dV. \)

- Exact mass fluxes are antisymmetric: \( F_{ij}^{\text{ex}} = -F_{ji}^{\text{ex}} \rightarrow F_{ij} = -F_{ji} \)

- Using these fluxes yields the approximation of the new cell masses

\[ \tilde{m}_i = m_i + \sum_{j \in \mathcal{I}(N(\kappa_i))} F_{ij} \Rightarrow \text{mass conservation} \]

- Assume that for every old cell \( \kappa_i \) there is a density reconstruction \( \rho_i^H \) that is exact for linear functions. Define target fluxes according to

\[ F_{ij}^H = \int_{\kappa_i \cap \kappa_j} \rho_i^H(x) dV - \int_{\kappa_i \cap \tilde{\kappa}_j} \rho_i^H(x) dV. \]
Optimization-Based Remap

Reconcile preservation of linearity, mass and local bounds:

\[ \min_{F_{ij}} \sum_{i=1}^{K} \sum_{j \in I(N(\kappa_i))} (F_{ij} - F_{ij}^H)^2 \quad \text{subject to} \]

\[ F_{ij} = -F_{ji} \quad i = 1, \ldots, K, \; j \in I(N(\kappa_i)) \]

\[ \tilde{m}_i^{\text{min}} \leq m_i + \sum_{j \in I(N(\kappa_i))} F_{ij} \leq \tilde{m}_i^{\text{max}} \quad i = 1, \ldots, K. \]

Enforce antisymmetry constraint by using only \( F_{pq} \) with \( p < q \):

\[ \min_{F_{ij}} \sum_{i=1}^{K} \sum_{\substack{j \in I(N(\kappa_i)) \atop i < j}} (F_{ij} - F_{ij}^H)^2 \quad \text{subject to} \]

\[ \tilde{m}_i^{\text{min}} \leq m_i + \sum_{\substack{j \in I(N(\kappa_i)) \atop i < j}} F_{ij} - \sum_{\substack{j \in I(N(\kappa_i)) \atop i > j}} F_{ji} \leq \tilde{m}_i^{\text{max}} \quad i = 1, \ldots, K. \]
Optimization-Based Remap

Reconcile preservation of linearity, mass and local bounds:

\[
\min_{F_{ij}} \sum_{i=1}^{K} \sum_{j \in \mathcal{I}(N(\kappa_i))} (F_{ij} - F^H_{ij})^2 \quad \text{subject to}
\]

\[
F_{ij} = -F_{ji} \quad i = 1, \ldots, K, \quad j \in \mathcal{I}(N(\kappa_i))
\]

\[
\bar{m}^\text{min}_i \leq m_i + \sum_{j \in \mathcal{I}(N(\kappa_i))} F_{ij} \leq \bar{m}^\text{max}_i \quad i = 1, \ldots, K.
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Enforce antisymmetry constraint by using only \( F_{pq} \) with \( p < q \):

\[
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\]
A Taste of OBR

- low-order ‘donor-cell’ remap
- unconstrained remap (target flux $F_{ij}^H$ only)
- constrained remap
Theoretical Properties of OBR
Immediate Properties

\[
\min \sum_{i=1}^{K} \sum_{j \in I(N(\kappa_i))} (F_{ij} - F_{ij}^H)^2 \quad \text{subject to}
\]

\[
\tilde{m}_i^{\min} \leq m_i + \sum_{j \in I(N(\kappa_j))} F_{ij} - \sum_{j \in I(N(\kappa_j))} F_{ji} \leq \tilde{m}_i^{\max} \quad i = 1, \ldots, K.
\]

- Convex quadratic program.

- **Bound preservation (monotonicity)** is explicit as long as the feasible set defined by the inequalities is nonempty.

- **Theorem.** The feasible set of OBR is nonempty.

- Optimally accurate with respect to a set norm and a set target flux.
- Independent of dimension, cell topology and discretization.
- Separation of **accuracy** and **monotonicity**!
- Permits additional physical bounds.
- Extendible to compatible remap of systems.

- Mathematically "clean" formulation: **No flux limiting!**
**Theorem.** A **sufficient** condition for OBR to recover linear densities **exactly** is that the centroid of any **new** cell remain in the **convex hull** of the centroids of its **old** neighbors.

**Theorem.** FCR can be formulated as a global optimization problem.

1. The FCR cost function is equivalent to the OBR cost function.
2. The FCR feasible set is always a subset of the OBR feasible set.

---

**OBR**

\[
\min_{\{a_{ij}\}} \sum_{i=1}^{K} \sum_{j \in I(N(\kappa_i)) \atop i < j} (1 - a_{ij})^2 (dF_{ij})^2 \quad \text{subject to}
\]

\[
\tilde{Q}_{i}\min \leq \sum_{j \in I(E(\kappa_i)) \atop i < j} a_{ij} dF_{ij} - \sum_{j \in I(E(\kappa_i)) \atop i > j} a_{ji} dF_{ji} \leq \tilde{Q}_{i}\max
\]

Admits a larger feasible set!

**FCR**

\[
\min_{\{a_{ij}\}} \sum_{i=1}^{K} \sum_{j \in I(N(\kappa_i)) \atop i < j} (1 - a_{ij})^2 (dF_{ij})^2 \quad \text{subject to}
\]

\[
\begin{align*}
(a) \quad & D_i^- dF_{ij} \leq a_{ij} dF_{ij} \leq 0 & \text{for } i < j, dF_{ij} \leq 0 \\
& D_i^- dF_{ij} \geq a_{ij} dF_{ij} \geq 0 & \text{for } i > j, dF_{ij} \geq 0 \\
(b) & 0 \leq a_{ij} dF_{ij} \leq D_i^+ dF_{ij} & \text{for } i < j, dF_{ij} \geq 0 \\
& 0 \geq a_{ij} dF_{ij} \geq D_i^+ dF_{ij} & \text{for } i > j, dF_{ij} \leq 0
\end{align*}
\]
Algorithms
The Swept-Region Approximation

- OBR (and FCR) can be implemented using exact cell intersections.
- In 1D, we use exact cell intersections.
- In 2D, in order to avoid expensive geometric computations, we use the concept of swept regions (Margolin, Shashkov, JCP 2002).
- **OBR**: The swept-region flux approximation of $F_{ij}^H$ is exact for linears.
- **FCR**: Blends $F_{ij}^H$ and a monotone (provided exact cell intersections!) low-order reconstruction $F_{ij}^L$. **Problem**: The swept-region approx. of $F_{ij}^L$ is monotone only under additional assumptions on mesh motion.

Margolin, Shashkov
Optimization Techniques

Primal OBR quadratic program:

\[
\begin{align*}
\min_{\vec{F}} \quad & \frac{1}{2} (\vec{F} - \vec{F}^H)^T (\vec{F} - \vec{F}^H) \\
\text{subject to} \quad & \vec{b}_{\min} \leq A\vec{F} \leq \vec{b}_{\max}
\end{align*}
\]

Dual OBR quadratic program:

\[
\begin{align*}
\min_{\vec{\lambda}, \vec{\mu}} \quad & \frac{1}{2} \left( A^T \vec{\lambda} - A^T \vec{\mu} \right)^T \left( A^T \vec{\lambda} - A^T \vec{\mu} \right) - \vec{\lambda}^T \left( \vec{b}_{\min} - A\vec{F}^H \right) - \vec{\mu}^T \left( -\vec{b}_{\max} + A\vec{F}^H \right) \\
\text{subject to} \quad & \vec{\lambda} \geq 0, \quad \vec{\mu} \geq 0
\end{align*}
\]

- **Strong duality**, etc. imply \( \vec{F}_* = A^T \vec{\lambda}_* - A^T \vec{\mu}_* + \vec{F}^H \).
- Use **reflective Newton method** by Coleman and Li (SIAM J. Opt. 1996): Newton iteration applied to a piecewise differentiable system that results from the first order optimality conditions for the dual problem.
- The quadratic term in the dual is governed by a symmetric positive semidefinite matrix; the computational cost of each Newton iteration is dominated by the solution of a well-structured sparse symmetric positive definite linear system (fast Cholesky factorizations) \( \mathcal{O}(K) \) algorithm.
Three Instructive Examples

OBR preserves shape when FCR does not.

OBR preserves linear densities when FCR does not.

OBR preserves monotonicity when FCR does not.
OBR preserves shape when FCR does not.

Compressive Mesh Motion

OBR Feasible Set (Cartoon)

FCR Feasible Set (Cartoon)

Original

After a single OBR step

After a single FCR step
OBR preserves shape when FCR does not.

Figure: Level sets of the objective functional and the feasible sets for \( \Delta_1 = \Delta_2 = 0.14, \rho_1 = 80, \rho_2 = 100, \rho_3 = 0, \) and \( \rho_1^b = \rho_3^b = 0 \). The red region gives the OBR feasible set which contains the point \((1, 1)\). The feasible set of FCR is given by the solid horizontal segment (black) and does not contain the point \((1, 1)\). The right pane shows a zoom of the OBR and FCR feasible sets.
OBR preserves linear densities when FCR does not.

Table: \( L_2 \) errors in the OBR and FCR remap of a linear density function in one dimension, for different compression ratios \( \ell : 1 \) of the middle cell.
OBR preserves monotonicity when FCR does not.

Figure: A 3×3 uniform initial grid (left pane) and the “compressed” grid (right pane) with a 4×4-fold compression of the middle cell.

Figure: Linear density $\rho(x, y) = x$ remapped from the uniform 3 × 3 grid to the compressed “torture” grid with $\ell = 16$. Left to right: the donor-cell method, FCR, OBR. It is clear that OBR gives the best density approximation.
Computational Studies

Cyclic grids with small cell displacements.

Cyclic grids with large cell displacements.

Computational cost.
## Small cell displacements

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**Table:** OBR and FCR errors and convergence rate estimates for the *sine* density using 4 tensor-product cyclic grids. The $L_2$ and $L_\infty$ rates for OBR are slightly better than those for FCR.
Small cell displacements

Table: OBR and FCR errors and convergence rate estimates for the shock density using 4 tensor-product cyclic grids. For this classical example, the convergence rates of OBR and M-OBR (FCR) are virtually identical.

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Large cell displacements

Figure: Grid deformation due to local compression (left pane) and the ‘repaired’ uniform grid (right pane).
## Large cell displacements

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**Table:** OBR and FCR errors and convergence rate estimates for the sine density using 4 cyclic repeated-repair grids. Rates expected of a second-order scheme are highlighted. It is evident that OBR delivers second-order accuracy, while FCR exhibits a trend toward a first-order scheme.
Large cell displacements

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<td>4.06e-06</td>
<td>1.53e-05</td>
<td>1.97e-03</td>
<td>6.48e-03</td>
</tr>
<tr>
<td>FCR</td>
<td>1.32e-13</td>
<td>5.32e-08</td>
<td>1.10e-06</td>
<td>2.26e-03</td>
<td>2.35e-03</td>
<td>2.44e-03</td>
<td>5.73e+04</td>
<td>8.50e+11</td>
</tr>
</tbody>
</table>

**Table:** $L_1$ errors in the OBR and FCR remap of a linear density function on the 64×64 tensor-product grid, for different values of the pseudo-time step $1/R$. Errors smaller than 1e-8 are highlighted. OBR fails to preserve linear densities at $R = 154$, while FCR fails at $R = 212$, resulting in a pseudo-time step advantage for OBR of $212/154 \approx 1.4$. Beyond this point, OBR exhibits a graceful loss of accuracy; FCR becomes numerically unstable.

<table>
<thead>
<tr>
<th></th>
<th>R = 25</th>
<th>R = 24</th>
<th>R = 23</th>
<th>R = 16</th>
<th>R = 15</th>
<th>R = 14</th>
<th>R = 10</th>
<th>R = 5</th>
</tr>
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<tbody>
<tr>
<td>OBR</td>
<td>2.32e-14</td>
<td>4.49e-14</td>
<td>2.15e-13</td>
<td>4.52e-10</td>
<td>4.14e-05</td>
<td>5.13e-04</td>
<td>1.16e-03</td>
<td>2.45e-03</td>
</tr>
<tr>
<td>FCR</td>
<td>2.32e-14</td>
<td>3.63e-07</td>
<td>1.67e-06</td>
<td>8.60e-04</td>
<td>1.16e-03</td>
<td>1.69e-03</td>
<td>5.74e-03</td>
<td>1.09e-02</td>
</tr>
</tbody>
</table>

**Table:** $L_1$ errors in the OBR and FCR remap of a linear density function on the 64×64 smooth nonorthogonal grid, for different values of the pseudo-time step $1/R$. Errors smaller than 1e-8 are highlighted. OBR fails to preserve linear densities at $R = 15$, while FCR fails at $R = 24$, resulting in a pseudo-time step advantage for OBR of $24/15 \approx 1.6$. 
# Table: Comparison of the computational costs of FCR and OBR, as measured by Matlab™ wall-clock times on a single Intel Xeon X5680 3.33GHz processor, for density functions sine, peak and shock and the tensor-product cyclic grid. The cost of OBR is proportional, up to a modest constant, to the cost of FCR. The average cost ratio is only 2.1.
Conclusions

- OBR is **monotone, conservative** and **linearity preserving** — and otherwise **optimally accurate** for a *fixed* norm and target flux.
- Independent of dimension, cell topology and discretization.
- OBR fully separates considerations of **accuracy** and **monotonicity**!
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- Extendible to **compatible remap of systems**.
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- **Future:** remap of systems, various objective functions (norms and targets), remap of vector fields, use in ALE transport, use with nodal flux discretizations (Scovazzi), comparison with iterated FCR.