Remap through Interpolation and Optimization (with application to multi-material ALE hydro)

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CASC Center for Applied Scientific Computing

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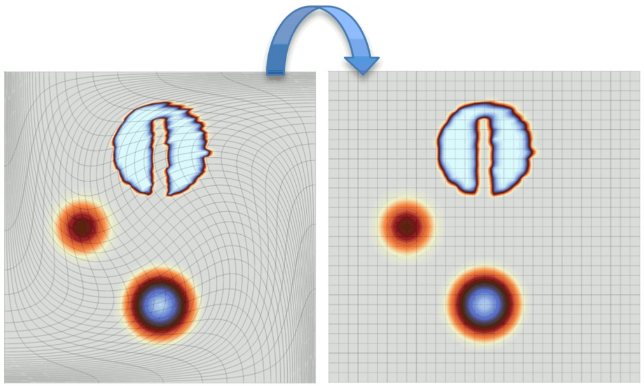
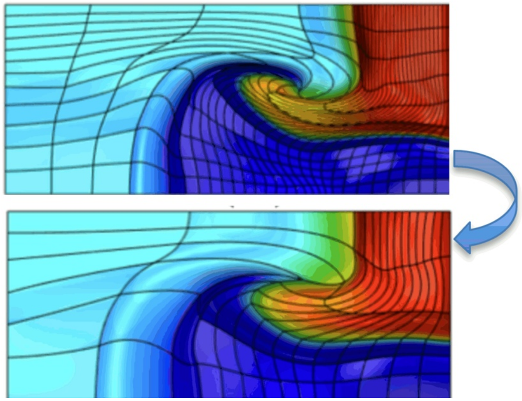
The remap problem is theoretically challenging and has high practical importance

- The remap must transfer discrete fields between computational meshes.



Advection-based remap (same topology)



Interpolation-based remap (any topology)

- Our main use case is ALE, but the usability is general.
  Ex: general data transfer between codes, projecting experimental data to a mesh, etc.

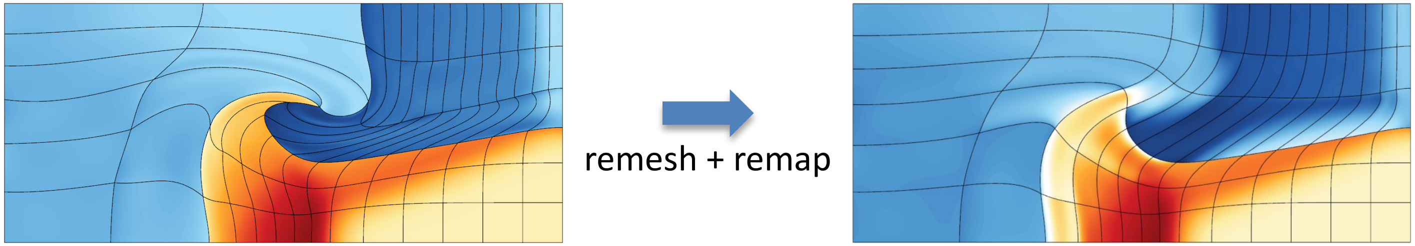
Requirements:

c1. Produce accurate and sharp fields, i.e., introduce minimal numerical diffusion.
c2. Conserve momentum and material volume / mass / total energy.
c3. Preserve the local min and max bounds of all remapped fields.
c4. Maintain consistent material coupling, i.e., volume fractions must sum to one.

- Two major approaches – advection (solve PDEs) and interpolation (geometric).

Advection-based remap methods struggle to meet all requirements

- Most remap methods rely on the advection approach.
  - Solving a PDE in pseudotime, defining "physical" motion of quantities (flux form).



Lagrange-only

Lagrange + 1 remesh/remap step

- [c2] Gives direct conservation of advected quantities by design.
- [c3] Bounds preservation requires nonlinear limiters.
- [c1] Sharpness requires nonlinear flux steepening (difficult).
- [c4] Material consistency requires tradeoffs (very difficult).
- The remap step is the primary source of errors in simulations that involve it.

The problem structure includes many local/global nonlinear constraints and coupling across materials

- Variables of the multi-material system (hydrodynamics case):
  material indicators, densities, internal energies (per material) & velocity.

  $$(\eta_k, \rho_k, e_k, v), \text{where } k \text{ is material index}$$

- [c1] Sharpness: minimize the difference between (η_k, ρ_k, e_k, v) and $(\eta_k^0, \rho_k^0, e_k^0, v^0)$.

- [c2] Conservation: linear & nonlinear equalities, global, few of them, coupled.

  $$\int_\Omega \eta_k = \int_{\Omega^0} \eta_k^0 \qquad \int_\Omega \eta_k \rho_k = \int_{\Omega^0} \eta_k^0 \rho_k^0 \qquad \int_\Omega \sum \eta_k \rho_k v = \int_{\Omega^0} \sum \eta_k^0 \rho_k^0 v^0$$

  $$\int_\Omega \eta_k \rho_k e_k + \frac{1}{2} \eta_k \rho_k v^2 = \int_{\Omega^0} \eta_k^0 \rho_k^0 e_k^0 + \frac{1}{2} \eta_k^0 \rho_k^0 (v^0)^2$$

- [c3] Bounds: two linear inequalities per DOF, local, uncoupled.

  $$\eta_k(x)^{\min} \leq \eta_k(x) \leq \eta_k(x)^{\max} \qquad \rho_k(x)^{\min} \leq \rho_k(x) \leq \rho_k(x)^{\max}$$

  $$e_k(x)^{\min} \leq e_k(x) \leq e_k(x)^{\max} \qquad v_c(x)^{\min} \leq v_c(x) \leq v_c(x)^{\max}$$

- [c4] Material coupling: one linear equality per DOF, local, coupled. $\sum_k \eta_k(x) = 1$

We use a 2-step approach that relies on solving a constrained optimization problem

1. Get a sharp initial guess through GSLIB interpolation (no conservation).

   $$(\eta_k^0, \rho_k^0, e_k^0, v^0) \rightarrow (\eta_k^*, \rho_k^*, e_k^*, v^*)$$

2. Improve the guess (through optimization) to recover all physical properties.

   $$\min_x \left(F(x) = ||x - x^*||\right), \text{subject to all constraints; } x = (\eta_k, \rho_k, e_k, v)$$

- Utilize state-of-art optimization methods developed by LLNL & collaborators.
  - Interior point methods with HiOp.
  - Latent Variable Proximal Point (LVPP) method.
  - Main difference: handling bounds constraints.

- Performed as a one-step sweep (no time stepping, no intermediate stages).

Step 1: sharp and bounded initial guess is obtained through GSLIB interpolation

- Existing MFEM capability that has been tested extensively.
  - MFEM already contains a miniapp for FE interpolation performed through GSLIB.

- GSLIB can provide a map between physical point locations.

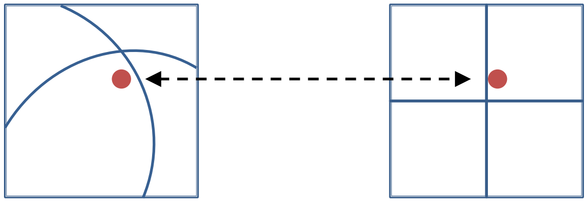
- GSLIB handles the function evaluation and the required MPI communication.

- The interpolation is sharp [c1].
  - Propagation is limited to at most one element.

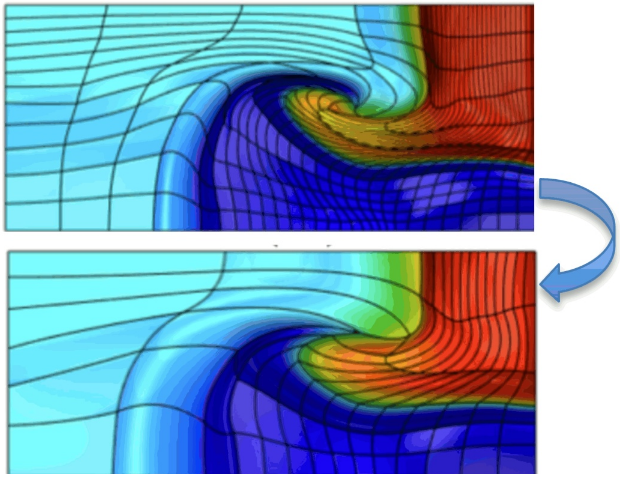
- The interpolation is not conservative ~~[c2]~~.

- The bounds are preserved [c3].

- Material consistency is preserved [c4].

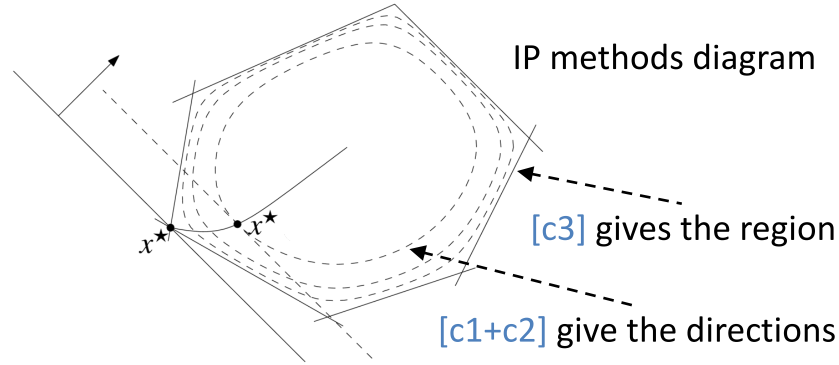


Deformed mesh   Optimized mesh



GSLIB interpolation example from MFEM

Step 2: tackle the optimization problem with HiOp's interior point methods



- Established optimization library developed by C. Petra at LLNL.

- Conservation constraints [c2] enter as Lagrange multipliers (few of them).

- Bounds constraints [c3] enter as weighted log-barriers.

$$\min_x \max_\lambda \left(\overset{\text{[c1]}}{F(x)} + \lambda \left[\int_\Omega \eta - \overset{\text{[c2]}}{\int_{\Omega^0} \eta^0} \right] + \cdots + \mu \sum_i \log(x_i - x_i^{\min}) + \overset{\text{[c3]}}{\mu \sum_i \log(x_i^{\max} - x_i)} \right)$$

Equalities are admitted as $\mu \to 0$.

- Material coupling constraint [c4] is a major challenge.

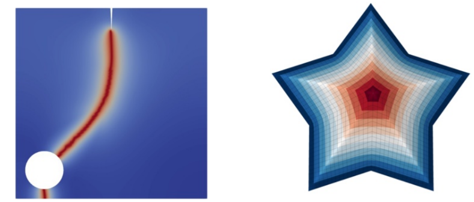
$$\sum_k \eta_k(x) = 1$$

  — Alternating projection / augmented Lagrangian type of methods. (decouple the materials / solve each / combine)
  Slack variables could be used to keep the solution in the admissible domain.

  — Keep all materials coupled, and rely on linear algebra-based decomposition. How to compute the Newton step (linearization, Hessian action)?

Step 2: tackle the optimization problem with the Latent Variable Proximal Point method

- Novel approach based on research of B. Keith.
  - Feasibility has been demonstrated simpler problems.
- Conservation constraints [c2] enter as Lagrange multipliers (few of them).



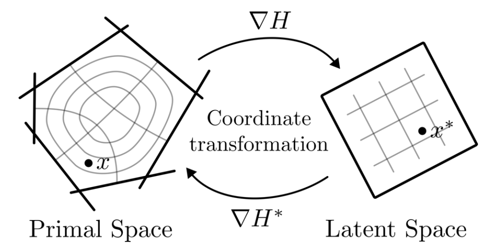
LVPP tests in MFEM: Fracture, Eikonal solver

- Bounds constraints [c3] enter as entropy regularization terms.

$$\min_x \max_\lambda \Big(\overset{[c1]}{F(x)} + \lambda \Big[\overset{[c2]}{\int_\Omega \eta - \int_{\Omega^0} \eta^0} \Big] + \dots + \frac{1}{\mu} \overset{[c3]}{H(x)} \Big), \; H(x) = \int_\Omega (x_i - x_i^{\min}) \log(x_i - x_i^{\min}) + \int_\Omega (x_i^{\max} - x_i) \log(x_i^{\max} - x_i)$$

  - Form a sequence of solutions (equivalent formulation):

$$x_k = \operatorname*{argmin}_x \Big(F(x) + \lambda \Big[\int_\Omega \eta - \int_{\Omega^0} \eta^0 \Big] + \dots + \frac{1}{\mu} D_H(x, x_{k-1}) \Big)$$



  - The trick: solve for a latent variable, eliminating [c3]: $x^* = \nabla H(x) \in (-\infty, \infty)$
  - Inner Newton iteration for x_k: no bounds constraints, mass-matrix dominated.
  - Outer iteration for the Lagrange multipliers λ.
- Material coupling constraint [c4]: enforced on the latent variable x^*. Any correction will be in bounds due to the transform.

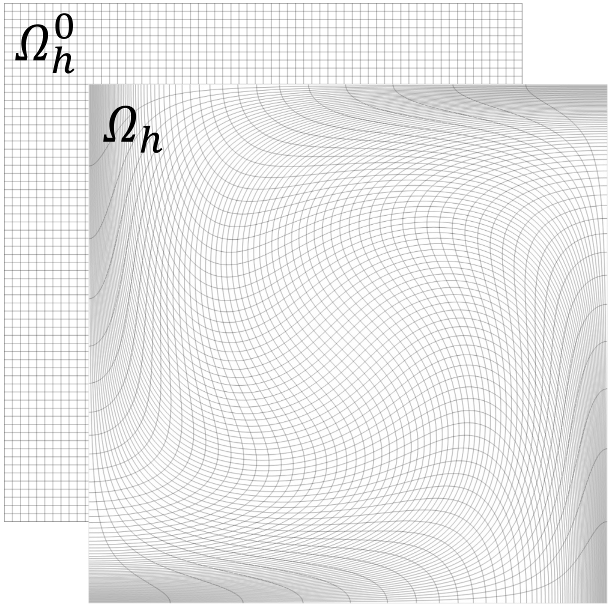
$$\sum_k \eta_k(x) = 1$$

Remap of scalar L2 GridFunctions

$$\min_{\eta} \; ||\eta - \eta^*||_{L^2}, \text{ subject to}$$

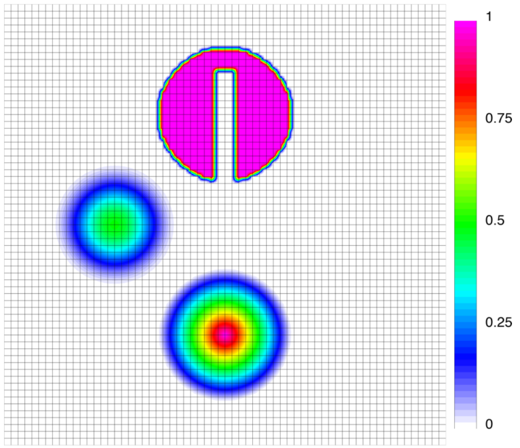
$$\int_{\Omega_h} \eta = \int_{\Omega_h^0} \eta^0,$$

$$0 \leq \eta_i^{\min} \leq \eta_i \leq \eta_i^{\max} \leq 1, \; i = 1 \ldots N$$

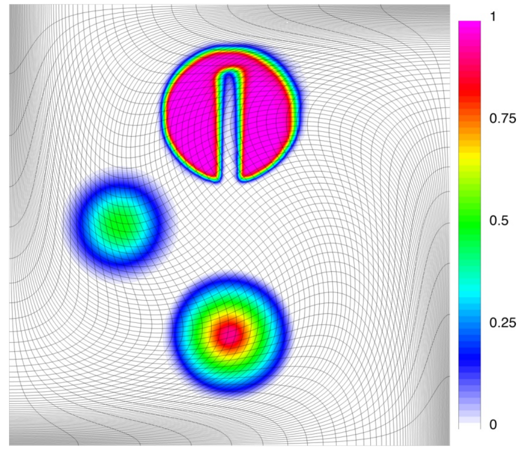


- The initial guess η^* is obtained through interpolation in physical space (*GSLIB*). (interpolated directly at support nodes of the DOFs)
- The min and max in an element K are taken from the elements in intersects.
- Solution existence: $$\int_{\Omega_h} \eta^{min} \, dx \leq \int_{\Omega_h^0} \eta^0 \, dx \leq \int_{\Omega_h} \eta^{max} \, dx$$

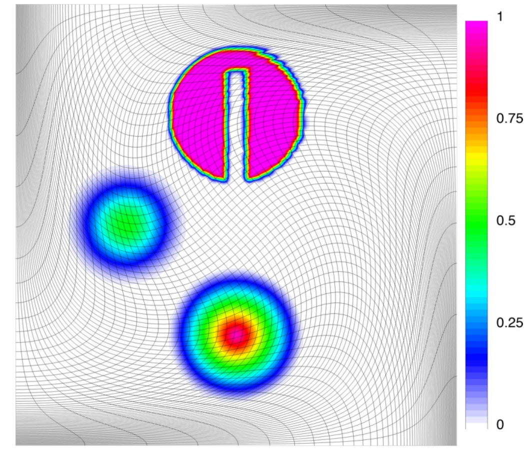
Remap of scalar L2 GridFunctions (2D result)



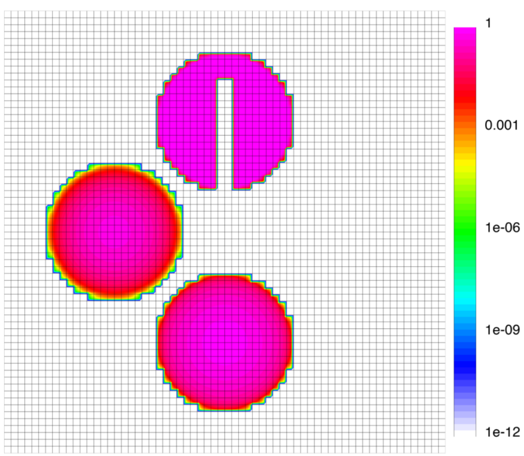
Initial condition



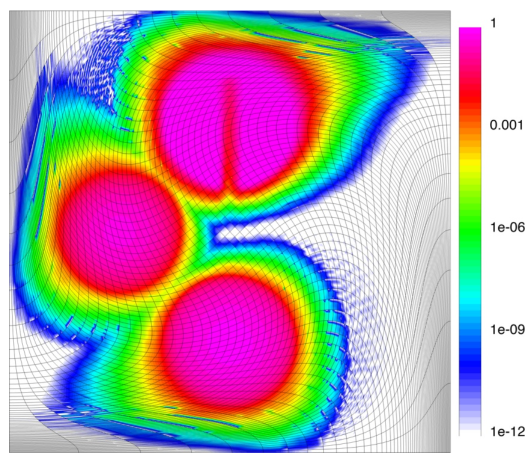
Advection solution (256 RK3)
46s, 9.8e-9 mass error



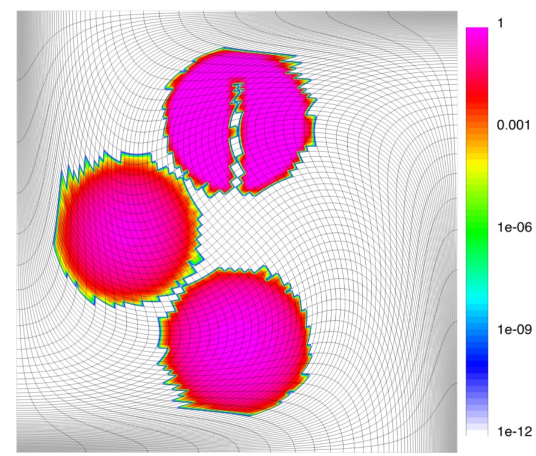
HiOp solution
1.4s, 2.5e-14 mass error



Initial condition (log)

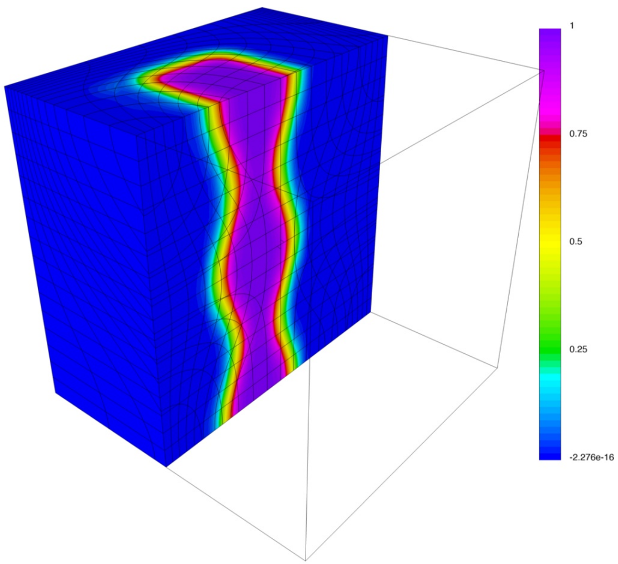


Advection solution (log)

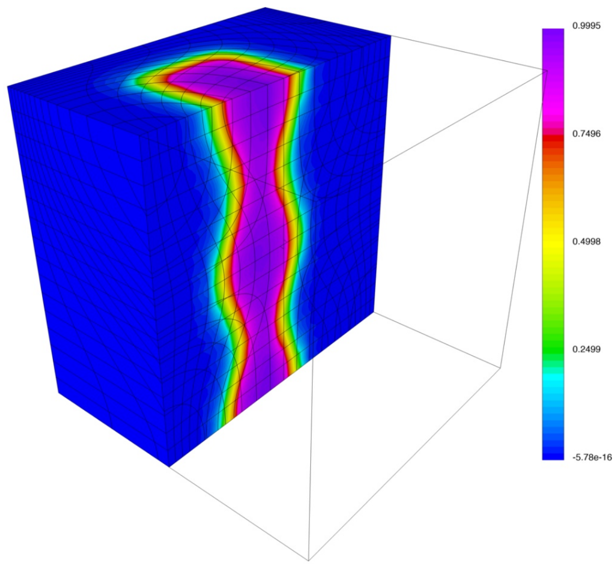


HiOp solution (log)

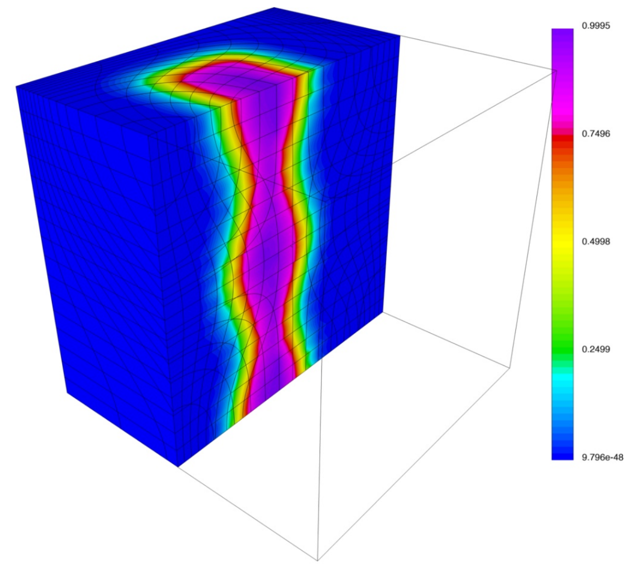
Remap of scalar L2 GridFunctions (3D result)



advection solution
mass error: 3.93e-5
time: 68s



HiOp solution
mass error: 2.35e-16
time: 1.9s



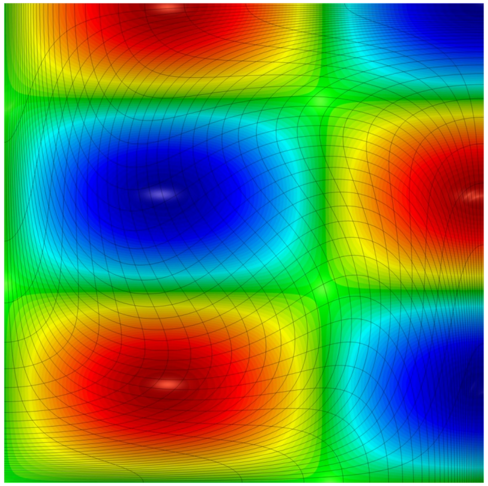
LVPP solution
mass error: 1.52e-16
time: 1.2s

Remap of a scalar smooth function: HO convergence + exact mass + correct bounds!

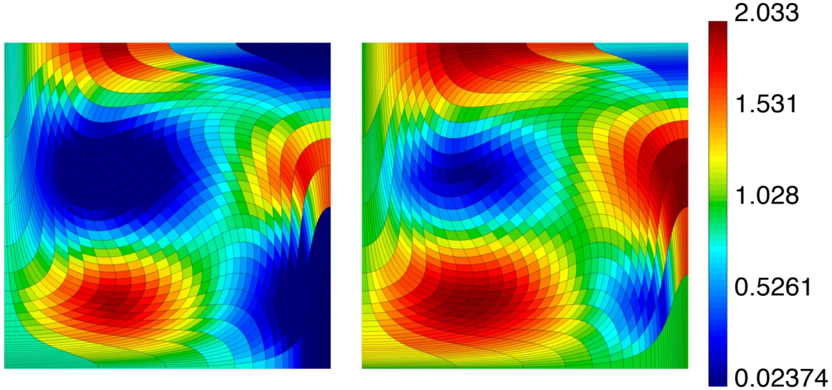
1. Interpolation on the final mesh.
   (interpolated solution has wrong mass).
2. Bounds computation.
   (interpolated solution is always in bounds).
3. Mass correction.
   (optimization – fix mass, preserve bounds).

	Q2 - interp			Q2 - opt		
ref	L1 error	rate	mass error	L1 error	rate	mass error
1	2.29E-02		3.10E-04	2.29E-02		6.70E-16
2	4.16E-03	2.46	4.92E-06	4.16E-03	2.46	7.20E-13
3	5.74E-04	2.86	2.13E-07	5.74E-04	2.86	5.77E-15
4	9.16E-05	2.65	4.44E-09	9.16E-05	2.65	5.98E-13
5	1.16E-05	2.98	7.71E-11	1.16E-05	2.98	1.39E-14
6	1.48E-06	2.97	1.25E-12	1.48E-06	2.97	2.04E-14

	Q3 - interp			Q3 - opt		
ref	L1 error	rate	mass error	L1 error	rate	mass error
1	5.54E-03		4.19E-04	5.60E-03		8.30E-14
2	6.38E-04	3.12	1.29E-05	6.39E-04	3.13	3.33E-15
3	8.32E-05	2.94	1.22E-07	8.32E-05	2.94	2.60E-13
4	5.17E-06	4.01	3.40E-09	5.17E-06	4.01	3.33E-15
5	3.29E-07	3.97	6.07E-11	3.29E-07	3.97	6.70E-16
6	2.09E-08	3.98	1.00E-12	2.09E-08	3.98	9.68E-13



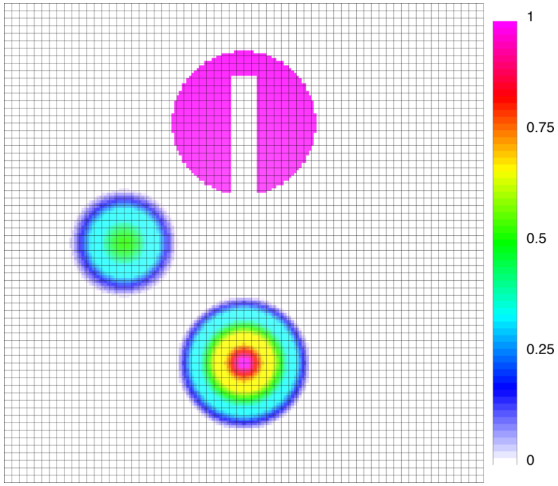
Smooth solution on the final mesh



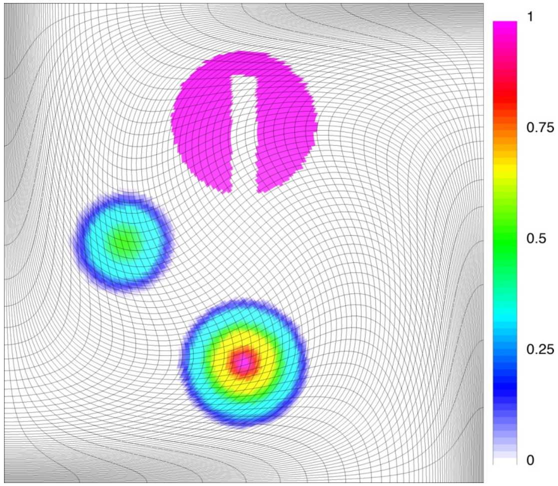
Min and Max bounds

Remap of scalar QuadratureFunctions

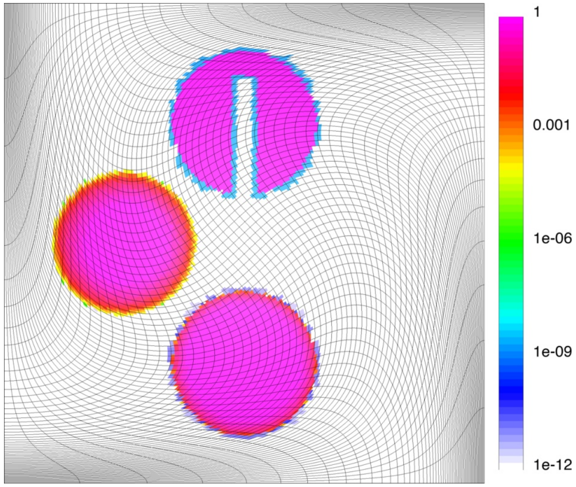
- There is no advection capability to remap Q-functions directly. (done through FE projections).
- Same interpolation / optimization method, but for the quadrature points / values.
- Intuitive control over small values / sub-element diffusion.



Initial condition



LVPP solution, zero mass error



LVPP solution (log)

Remap of the (η, ρ, e) coupled system

- Material indicator η is a Q-function.
- Material density ρ is a Q-function.
- Specific internal energy e is an L2 GridFunction.
- Don't form any product fields.
- Bounds are imposed directly on the primal (η, ρ, e) variables (simple).
- The coupling is in the *global* integrals.

$$
\begin{aligned}
&\min_{\eta,\rho,e} \; J(\eta, \rho, e)\,, \\
&\int_{\Omega_h} \eta = \int_{\Omega_h^0} \eta^0, \\
&\int_{\Omega_h} \eta\rho = \int_{\Omega_h^0} \eta^0 \rho^0, \\
&\int_{\Omega_h} \eta\rho e = \int \eta^0 \rho^0 e^0, \\
&0 \le \eta_i^{\min} \le \eta_i \le \eta_i^{\max} \le 1, \\
&e_i^{\min} \le e_i \le e_i^{\max}, \\
&\rho_i^{\min} \le \rho_i \le \rho_i^{\max}.
\end{aligned}
$$

Remap of the (η, ρ, e) coupled system: all requirements are satisfied on toy benchmarks

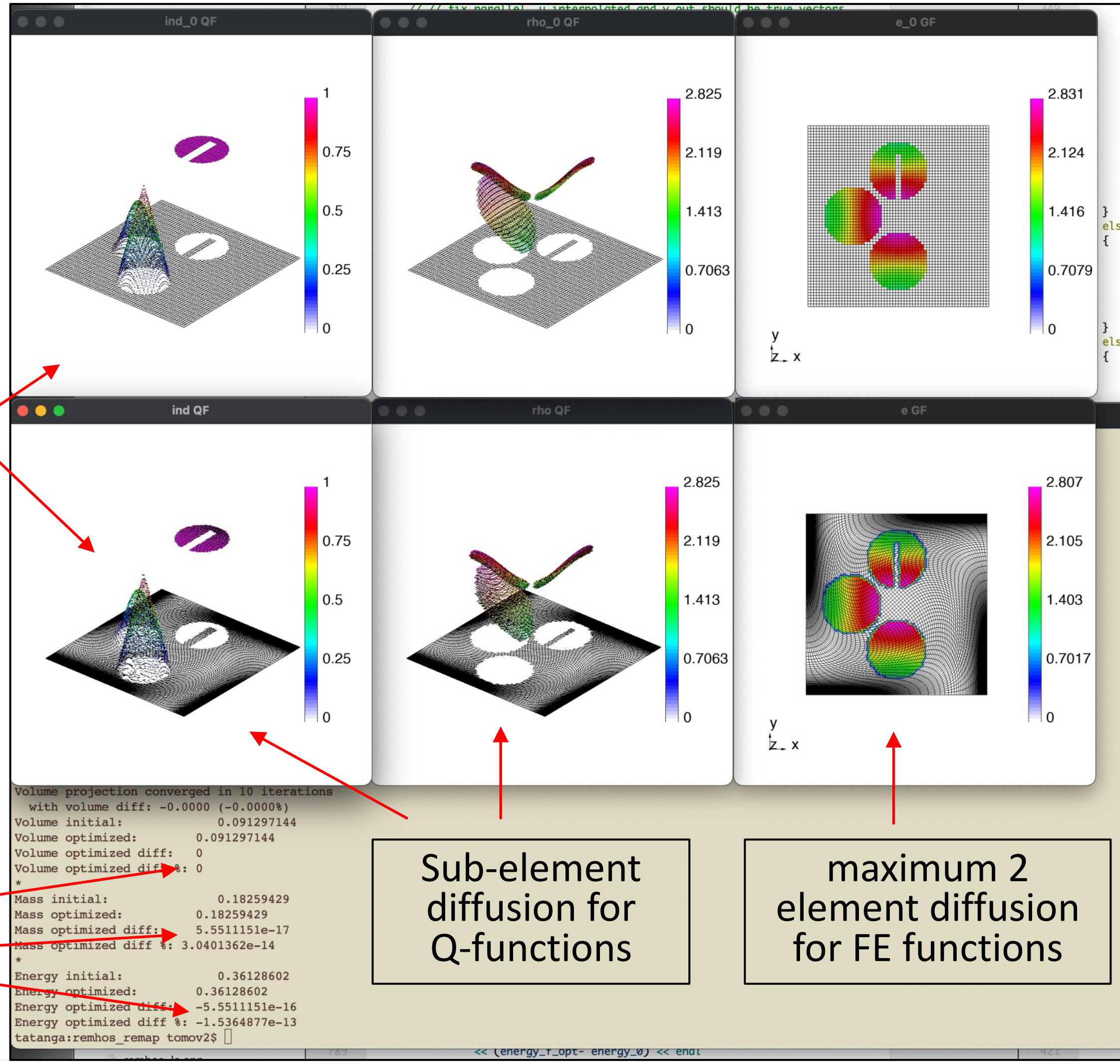
Supports indicator+density+energy coupled remap

Max sharpness through physical space interpolation

Direct Q-function remap (no transitions to FE) for indicators & densities

Bounds are preserved for indicators / densities / internal energies (no product fields)

Exact conservation of volume / mass / internal energy

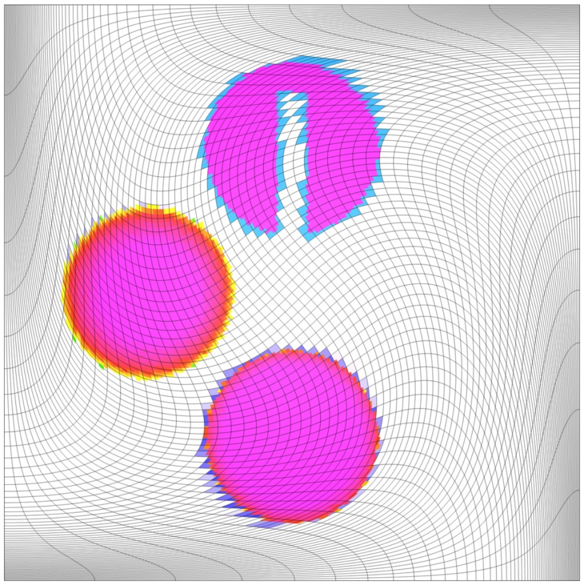


Sub-element diffusion for Q-functions

maximum 2 element diffusion for FE functions

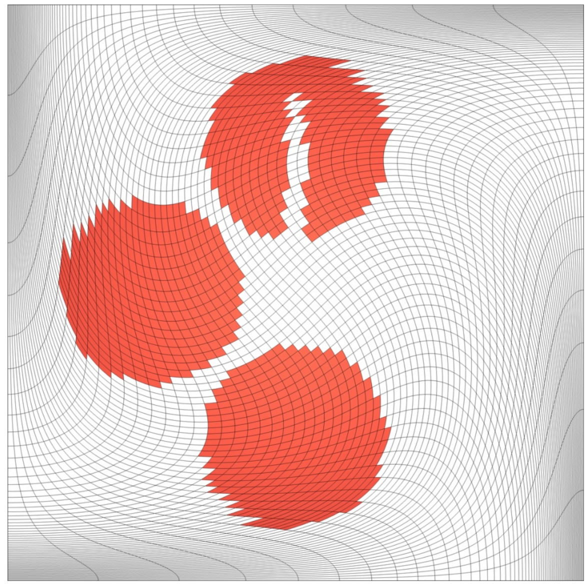
Remap of the (η, ρ, e) system: preservation of constant density and energy

$\eta \in [10^{-12}, 1]$



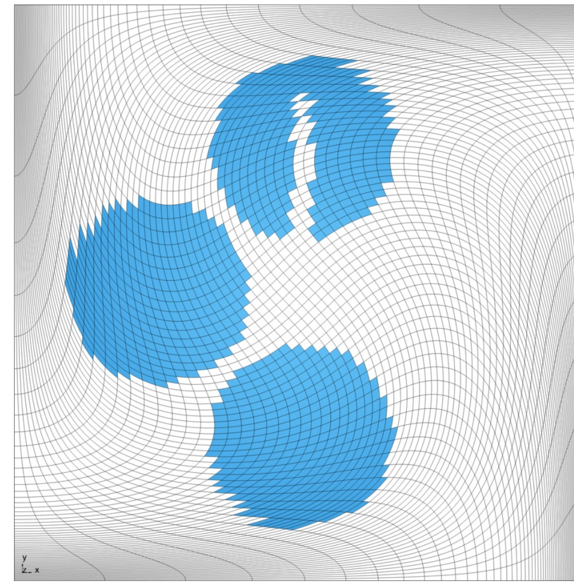
Material indicator (Q-function)
* sub-element diffusion
* volume error 1e-13

$\rho \in \{0,7\}$



Constant density (Q-function)
* constant over bool quads
* mass error 1e-12

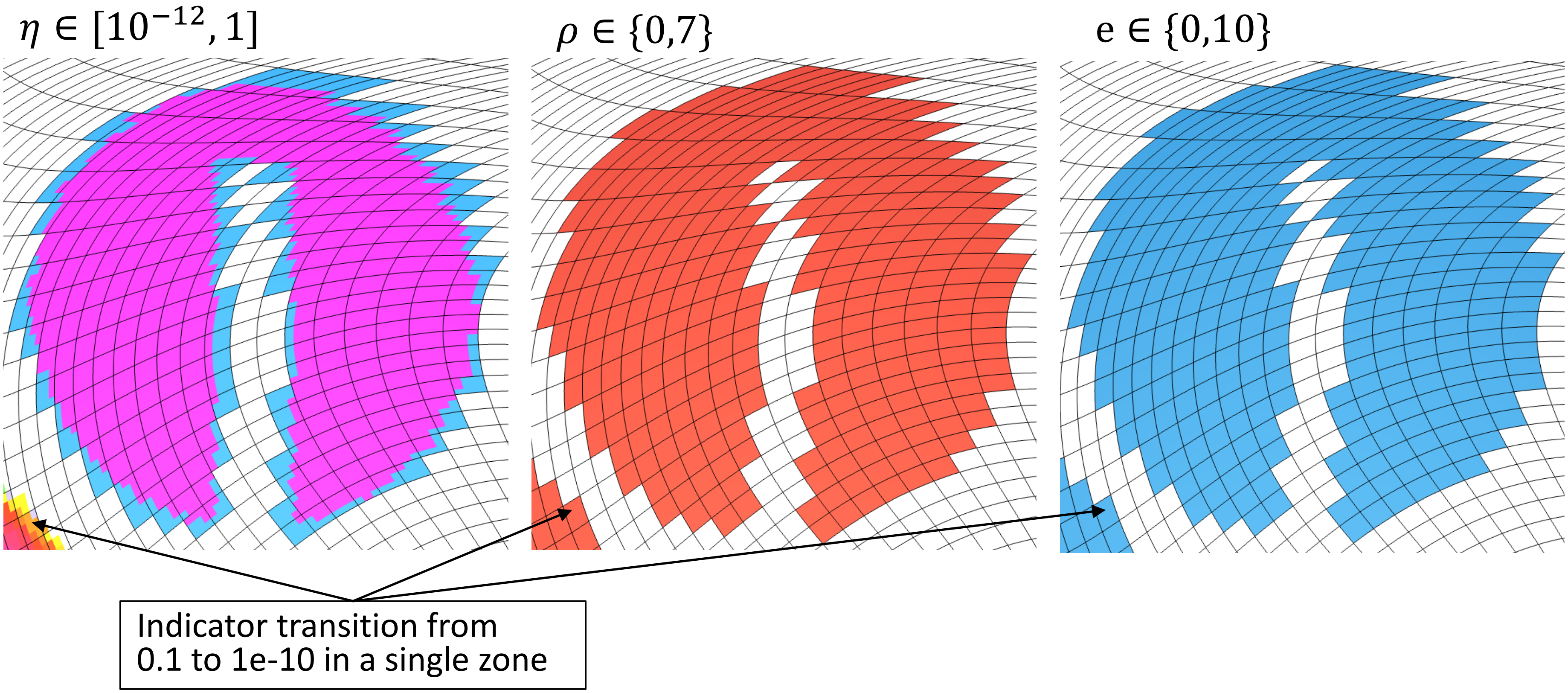
$e \in \{0,10\}$



Constant energy (FE function)
* constant over bool elements
* energy error 1e-11

- Constants are preserved exactly ($\rho = 7, e = 10$).
- Much better intuitive control of tiny volume fractions.

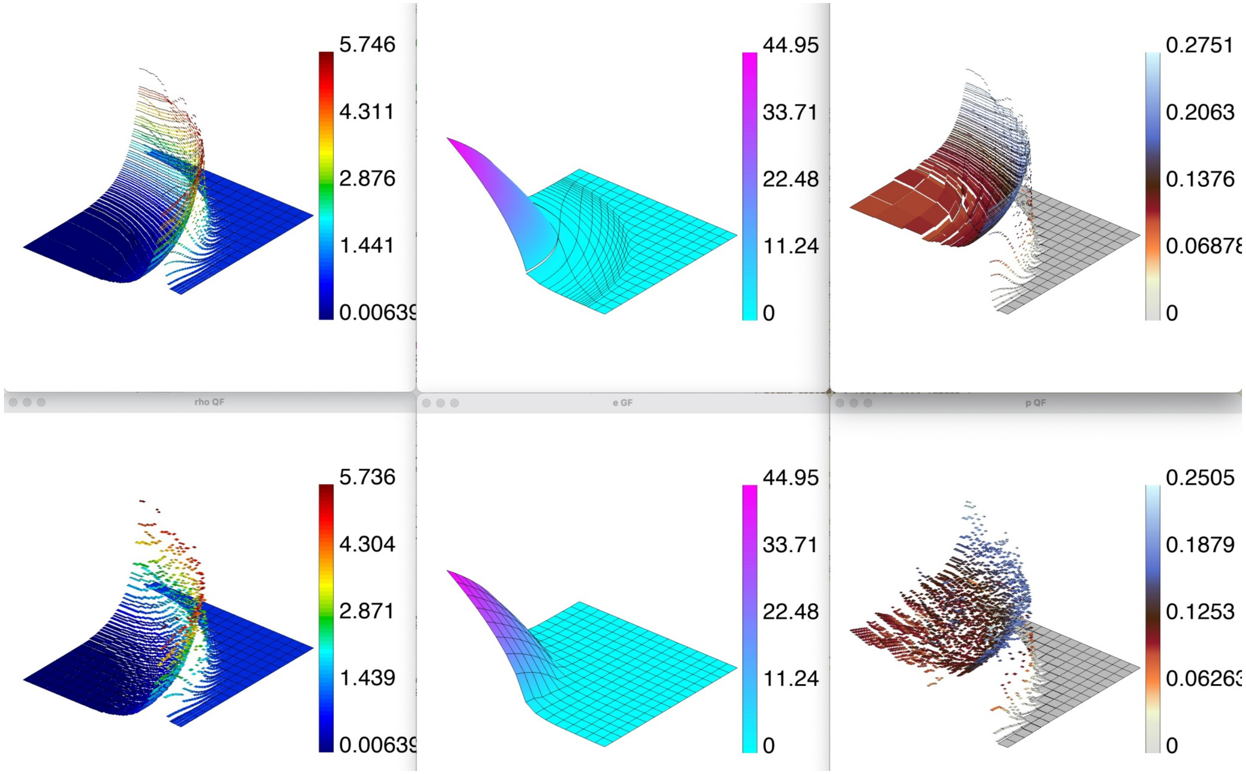
Remap of the (η, ρ, e) system: preservation of constant density and energy



- Matching spatial support for volume / mass /energy.
  (Difficult with sharp nonlinear advection methods, especially with tiny indicators)

Remap of the (η, ρ, e) system: pressure control (control over derived fields)

- Pressure $p(\rho, e)$ is a derived (nonlinear) field controlling the physical velocity.
- Additional requirement: avoid numerical oscillations in derived fields.

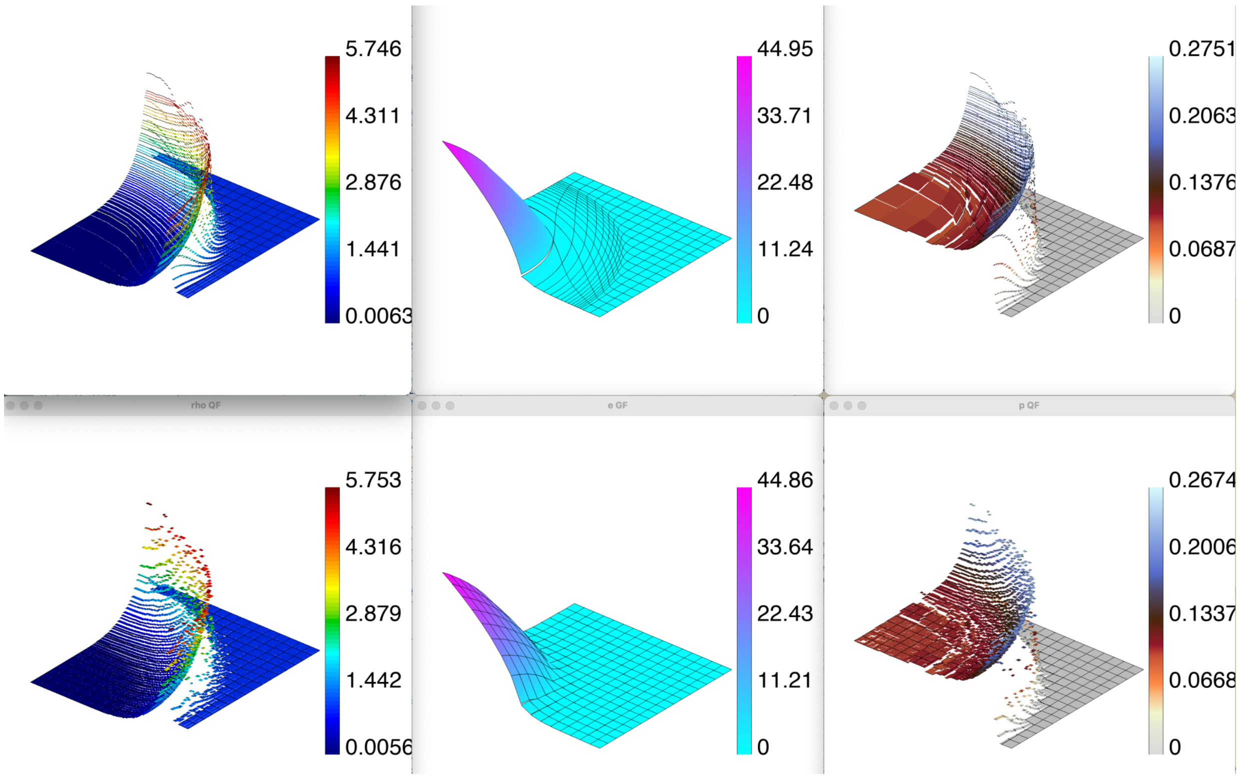


Density Internal Energy Pressure

Remap of the (η, ρ, e) system: pressure control (control over derived fields)

- Approach: interpolate $p_0 \to p^*$ and include it in the objective.

$$\min_{\eta,\rho,e} \left(J(\eta, \rho, e) + ||p - p^*||_{L^2} \right)$$



Density Internal Energy Pressure

Remap of the full (η, ρ, e, v) coupled system.

- Material indicator η is a Q-function.
- Material density ρ is a Q-function.
- Specific energy e is an L2 GridFunction.
- Velocity v is an H1 vector GridFunction.

$$
\begin{aligned}
\min_{\eta,\rho,e,v} \quad & J(\eta,\rho,e,v) \\
& \int_{\Omega_h} \eta = \int_{\Omega_h^0} \eta^0, \\
& \int_{\Omega_h} \eta\rho = \int_{\Omega_h^0} \eta^0\rho^0 \\
& \int_{\Omega_h} \eta\rho v = \int \eta^0\rho^0 v^0 \\
& \int_{\Omega_h} \eta\rho e + \frac{1}{2}\eta\rho v^2 = \int_{\Omega_h^0} \eta^0\rho^0 e^0 + \frac{1}{2}\eta^0\rho^0\left(v^0\right)^2 \\
& 0 \le \eta_i^{\min} \le \eta_i \le \eta_i^{\max} \le 1, \\
& e_i^{\min} \le e_i \le e_i^{\max} \\
& \rho_i^{\min} \le \rho_i \le \rho_i^{\max} \\
& v_{i,c}^{\min} \le v_{i,c} \le v_{i,c}^{\max}
\end{aligned}
$$

- Don't form any product fields.
- Bounds are imposed directly on the primal (η, ρ, e, v) variables (simple).
- The coupling is in the *global* integrals.

Remap of the full hydro (η, ρ, e, v) system.

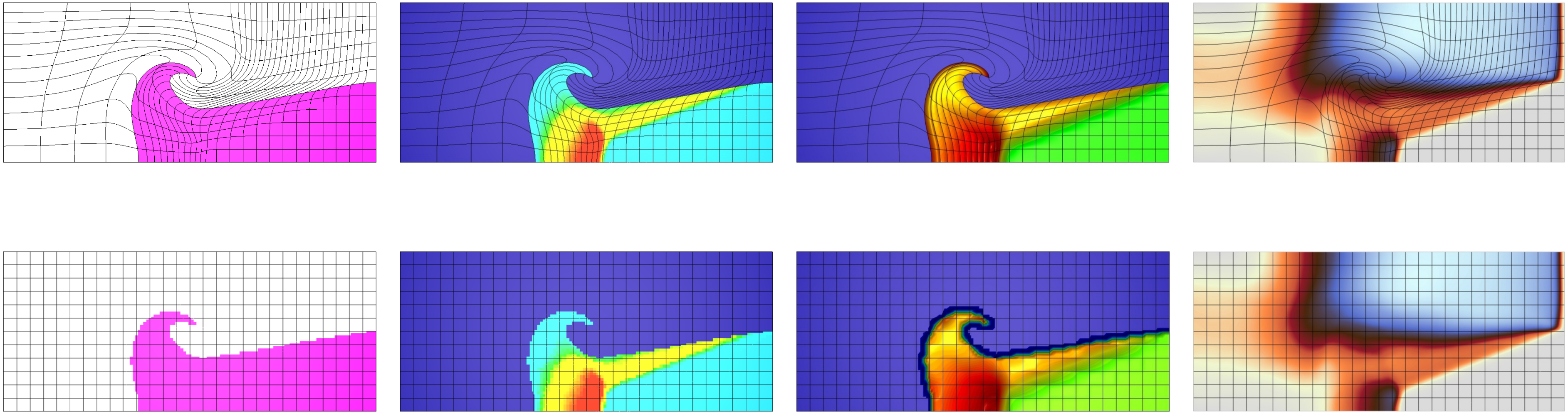
```
Volume interpolated diff: 1.6e-03
Volume optimized diff:    4.4e-15

Mass interpolated diff:   6.2e-03
Mass optimized diff:     -8.9e-15
```

```
Momentum (1) interpolated diff: 1.4e-03
Momentum (1) optimized diff:    1.1e-15

Total energy interpolated diff: 1.1e-01
Total energy optimized diff:    1.9e-12
```

```
Triple Point Q3Q2, single ALE step to uniform mesh at t = 3.5:
```



Material Indicator Mass Internal Energy Velocity Magnitude

Conclusions

- The optimization approach achieves all requirements.
- Optimization based formulations speeds up the remap process significantly.
- The artificial diffusion is decreased to a single cell.
- The optimization is scalable and easily parallelizable.
- Future work: formulations and algorithms for sum-to-one.

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