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Gradient-Augmented Level Set Methods and Interface Tracking with Subgrid Resolution

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Interface Tracking

Many two-phase fluid flow simulations (e.g. immersed boundary method [6], ghost fluid method [2]) use fractional steps, i.e. in each time step:

1. Update velocity field $\vec{v}(\vec{x})$ by a Navier-Stokes step;
2. Move interface by the velocity field $\vec{v}(\vec{x})$.

Fundamental problem: Represent and move the interface accurately.

Level Set Approach [5]

- Represent interface as the zero contour of a level set function $\phi : \mathbb{R}^p \to \mathbb{R}$.
- Moving interface with velocity field $\vec{v}$ translates to evolving ϕ by the PDE

$$\phi_t + \vec{v} \cdot \nabla\phi = 0 \,. \qquad (1)$$

- Solve (1) by high accuracy schemes (e.g. WENO [3]).
- Preserve $|\nabla\phi(x)| = 1$ by reinitialization [9] equation $\phi_\tau = \mathrm{sign}(\phi_0)(1 - |\nabla\phi|)$.
- Reconstruct interface by bi-/tri-linear interpolation on grid cells.

Advantages:

- Can define ϕ on regular grid; uniform resolution.
- Simple in 3D; automatic treatment of topology changes.
- More potential due to knowledge of *all* contours.
- Can obtain normals $\vec{n} = \frac{\nabla\phi}{|\nabla\phi|}$ and curvature $\kappa = \nabla \cdot \vec{n}$ from ϕ.

Problems and difficulties:

- Small structures vanish once below grid resolution.
- Wide WENO stencils are difficult to deal with near boundaries and with AMR.
- Inaccuracies with curvature approximation near boundaries and with reinitialization.

Goal: Address these problems in a simple, Eulerian fashion.
Idea: Augment the level set function by gradient information.

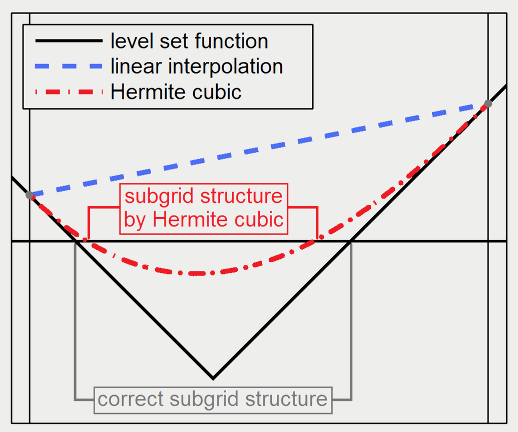
Gradient-Augmented Level Set Method and Advection Scheme

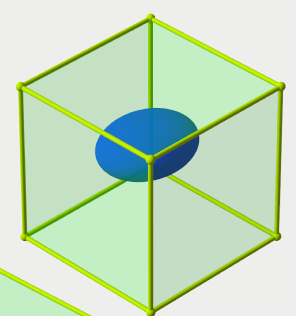
Philosophy:
Store function values ϕ and gradients $\vec{\psi} = \nabla\phi$ as independent quantities. Update both in a coupled fashion, by a scheme that uses characteristics and Hermite interpolation [4].

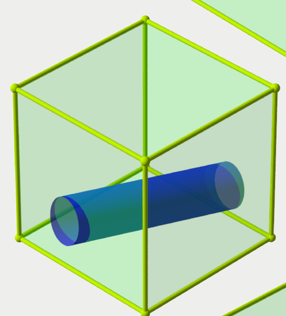
Research in the past:

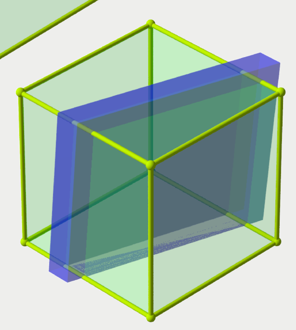
- Courant et al.: use characteristics and interpolation, but no gradients → CIR method [1]
- van Leer: use gradients for higher order, but reconstruct from ϕ [11]
- Takewaki et al.: idea to track gradients as independent quantity → CIP method [10]
- Raessi et al.: advect normal vectors, but in a decoupled fashion [7]

Motivation:
If function values ϕ and gradients $\nabla\phi$ are known at grid points, then subgrid structures can be represented.




subgrid bubble


subgrid jet


subgrid film

Hermite interpolation:
Here: p-cubic; simple tensor-product on rectangular cell.

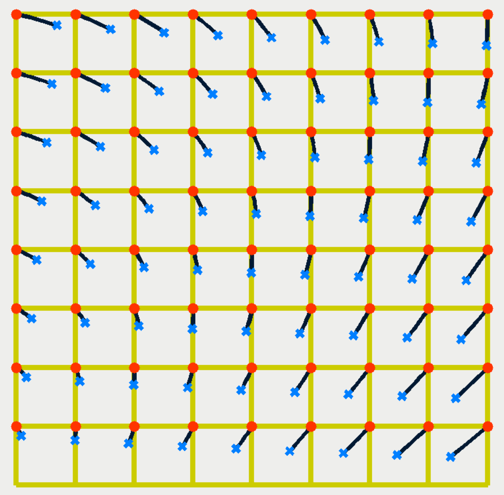
p	given on 2^p vertices	→ construct approx. to	→ interpolant
1	ϕ, ϕ_x		→ cubic
2	ϕ, ϕ_x, ϕ_y	→ ϕ_{xy}	→ bi-cubic
3	$\phi, \phi_x, \phi_y, \phi_z$	→ $\phi_{xy}, \phi_{xz}, \phi_{yz}, \phi_{xyz}$	→ tri-cubic

Thm.: The p-cubic approximates smooth functions with 4^{th} order accuracy. Gradients are 3^{rd} order accurate. Curvature can be obtained everywhere with 2^{nd} order accuracy.

Semi-Lagrangian Advection Scheme

Characteristic form of (1)

$$\begin{cases} \dot{\vec{x}} = \vec{v}(\vec{x}) \\ \dot{\phi} = 0 \\ \dot{\vec{\psi}} = -\nabla\vec{v} \cdot \vec{\psi} \end{cases} \qquad (2)$$



1. For each grid point, solve $\dot{\vec{x}} = \vec{v}(\vec{x})$ backwards to find starting point of characteristic $\mathring{\vec{x}}$ (e.g. by one RK3 step).
2. Obtain $\phi(\mathring{\vec{x}})$ and $\vec{\psi}(\mathring{\vec{x}})$ from Hermite interpolant.
3. Solve $\dot{\phi} = 0$ (trivial) and $\dot{\vec{\psi}} = -\nabla\vec{v} \cdot \vec{\psi}$ forward (e.g. RK2).

Numerical Analysis of Gradient-Augmented Schemes

Introduce concept of "superconsistency" to analyze scheme in function space setting:

- Rewrite (1) as $\phi_t = L\phi$, where $L = -\vec{v} \cdot \nabla$.
- Exact advection operator $S(t) = e^{tL}$.
- Approximate operator $A(t) \approx S(t)$, where $A(k)$ is one Runge-Kutta step of $\dot{\vec{x}} = \vec{v}(\vec{x})$.

Def.: A gradient-augmented scheme is called superconsistent, if the numerical approximation of $\dot{\vec{\psi}} = -\nabla\vec{v} \cdot \vec{\psi}$ equals $\nabla(A(t)\phi)$.

Update rule for gradients is inherited from ODE solver for characteristic curves.

Projection operator P in function space: (1) evaluate ϕ and $\nabla\phi$ on grid points; (2) construct new function by Hermite interpolation on each cell. Thus one step of scheme:

$$\underbrace{PA(k)}_{\text{num. scheme}} \approx PS(k) \approx \underbrace{S(k)}_{\text{exact evolution}}$$

Example: superconsistent Shu-Osher [8] scheme

$$\begin{aligned}
\vec{x}_1 &= \vec{x} - k\,\vec{v}(\vec{x}, t+k) \\
\nabla\vec{x}_1 &= I - k\,\nabla\vec{v}(\vec{x}, t+k) \\
\vec{x}_2 &= \vec{x} - k(\tfrac{1}{4}\vec{v}(\vec{x}, t+k) + \tfrac{1}{4}\vec{v}(\vec{x}_1, t)) \\
\nabla\vec{x}_2 &= I - k(\tfrac{1}{4}\nabla\vec{v}(\vec{x}, t+k) + \tfrac{1}{4}\nabla\vec{x}_1 \cdot \nabla\vec{v}(\vec{x}_1, t)) \\
\mathring{\vec{x}} &= \vec{x} - k(\tfrac{1}{6}\vec{v}(\vec{x}, t+k) + \tfrac{1}{6}\vec{v}(\vec{x}_1, t) + \tfrac{2}{3}\vec{v}(\vec{x}_2, t+\tfrac{1}{2}k)) \\
\nabla\mathring{\vec{x}} &= I - k(\tfrac{1}{6}\nabla\vec{v}(\vec{x}, t+k) + \tfrac{1}{6}\nabla\vec{x}_1 \cdot \nabla\vec{v}(\vec{x}_1, t) + \tfrac{2}{3}\nabla\vec{x}_2 \cdot \nabla\vec{v}(\vec{x}_2, t+\tfrac{1}{2}k)) \\
\phi(\vec{x}, t+k) &= \phi(\mathring{\vec{x}}, t) \\
\vec{\psi}(\vec{x}, t+k) &= \nabla\mathring{\vec{x}} \cdot \vec{\psi}(\mathring{\vec{x}}, t)
\end{aligned}$$

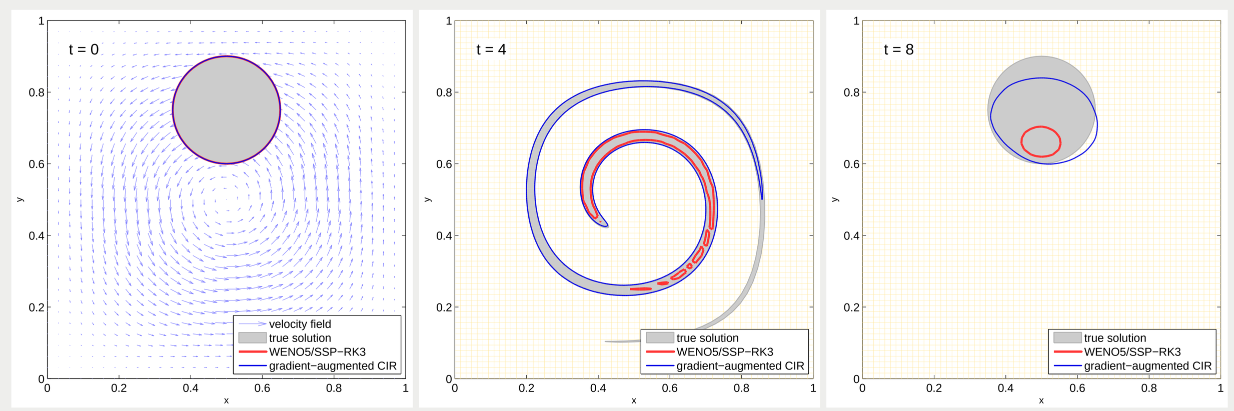
Accuracy:
Projection P fourth order accurate. Use locally fourth order accurate ODE solver for $\dot{\vec{x}} = \vec{v}(\vec{x})$. Then the scheme is locally fourth order accurate, globally third order.

Stability:
1D constant coefficients: Hermite cubic minimizes $F(u) = \int u_{xx}^2 \,\mathrm{d}x$;
hence $F(PA(k)\phi) \le F(A(k)\phi) = F(S(k)\phi) = F(\phi)$.

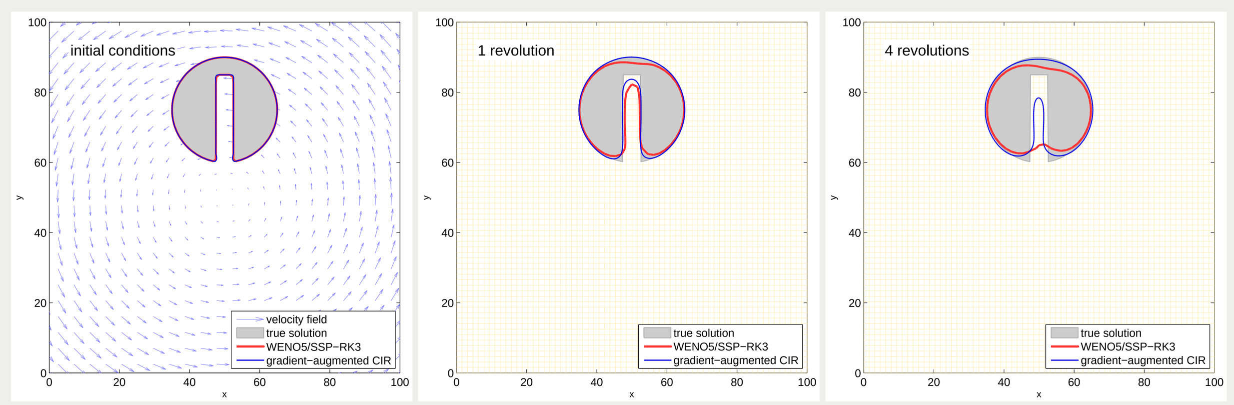
Convergence:
Linear scheme, thus convergence due to the Lax equivalence theorem.

Numerical Benchmark Tests

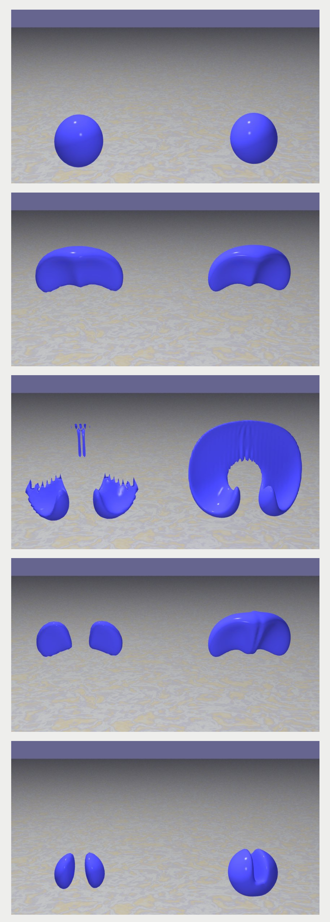
2D deformation field



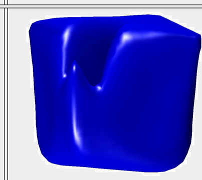
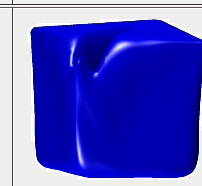
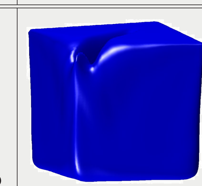
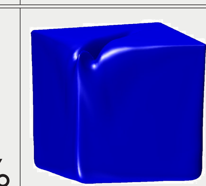
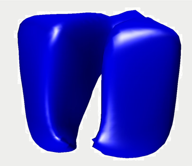
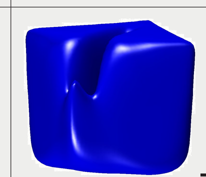
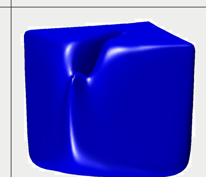
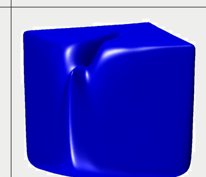
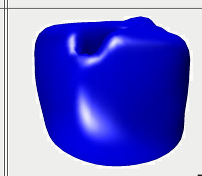
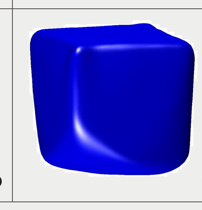
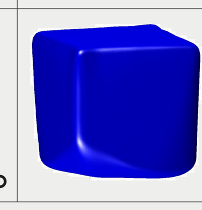
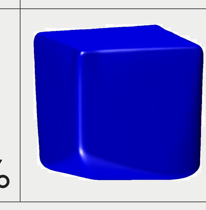
2D Zalesak circle



3D deformation

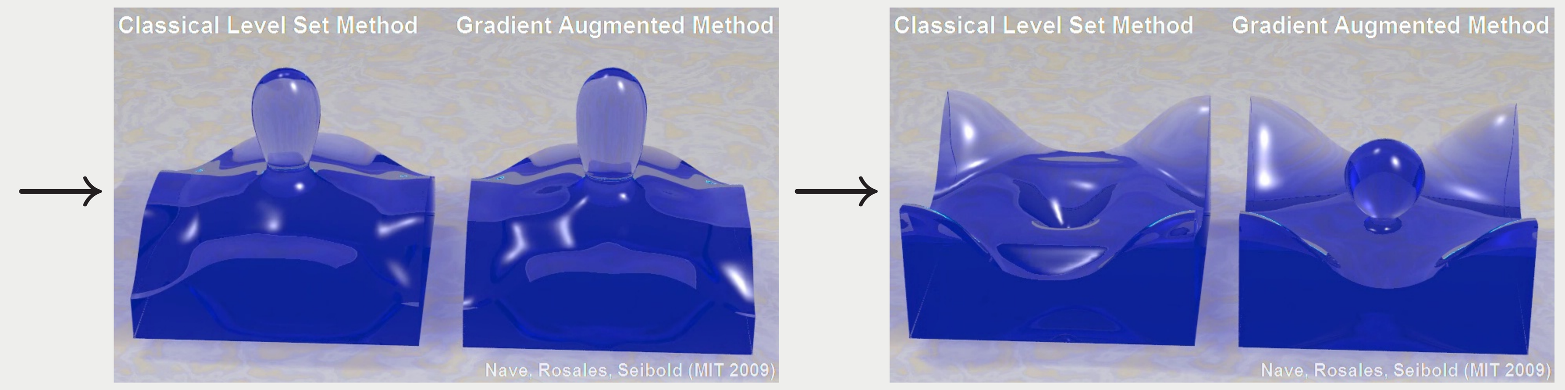


Loss of Volume

resolution	50 × 50 × 50	100 × 100 × 100	150 × 150 × 150	200 × 200 × 200
GA-CIR	 -5.4%	 -3.3%	 -1.6%	 -0.9%
WENO5-TVD3	 -54.5%	 -15.8%	 -9.6%	 -6.5%
WENO5 reinit.	 -35.4%	 -11.2%	 -7.1%	 -5.0%

Evolution of a cube in a 3D deformation field. Lowest volume loss with the new approach.

Fluid Flow Simulation (Using Ghost Fluid Method [2])



The gradient-augmented approach for interface evolution yields a more accurate resolution of partial coalescence events. The ability to resolve small structures pays off.

Conclusions and Outlook

Advantages of gradient-augmented level set approaches:

- Representation of subgrid structures.
- Optimal locality: each point uses only information in a single cell. Great benefit for AMR.
- Accurate approximation to $\vec{n}$ and κ everywhere (directly from interpolation).
- Characteristics yield a natural treatment of boundary conditions.
- Robust implementation: use interpolation for everything.

Current research:

- Analysis: extend concept of TVD to gradient-augmented setting.
- Extension: use other Hermite interpolations than p-cubics.
- Extension: track higher derivatives.
- Extension: nonlinear Hamilton-Jacobi equations (such as the reinitialization equation).

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