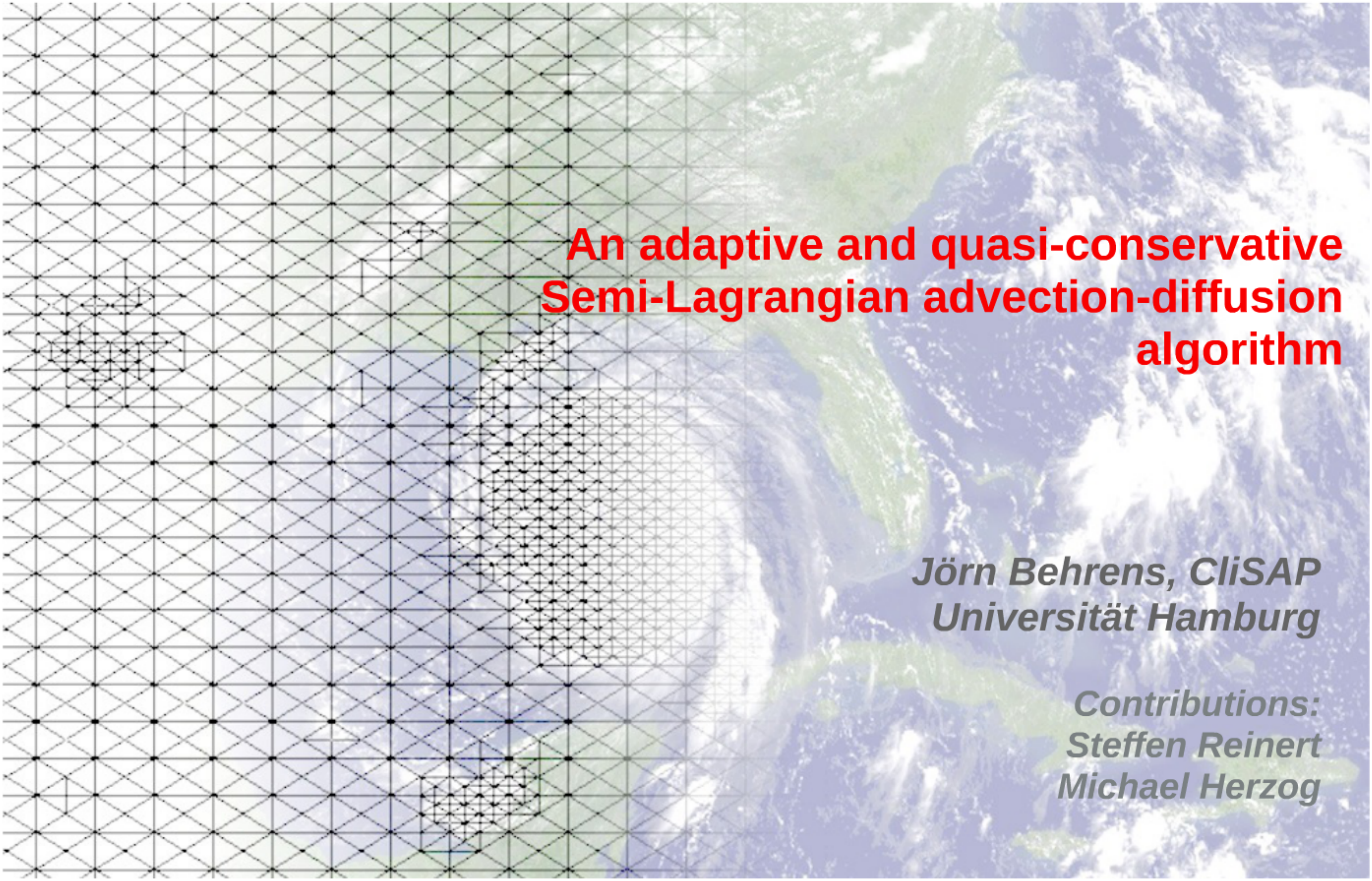
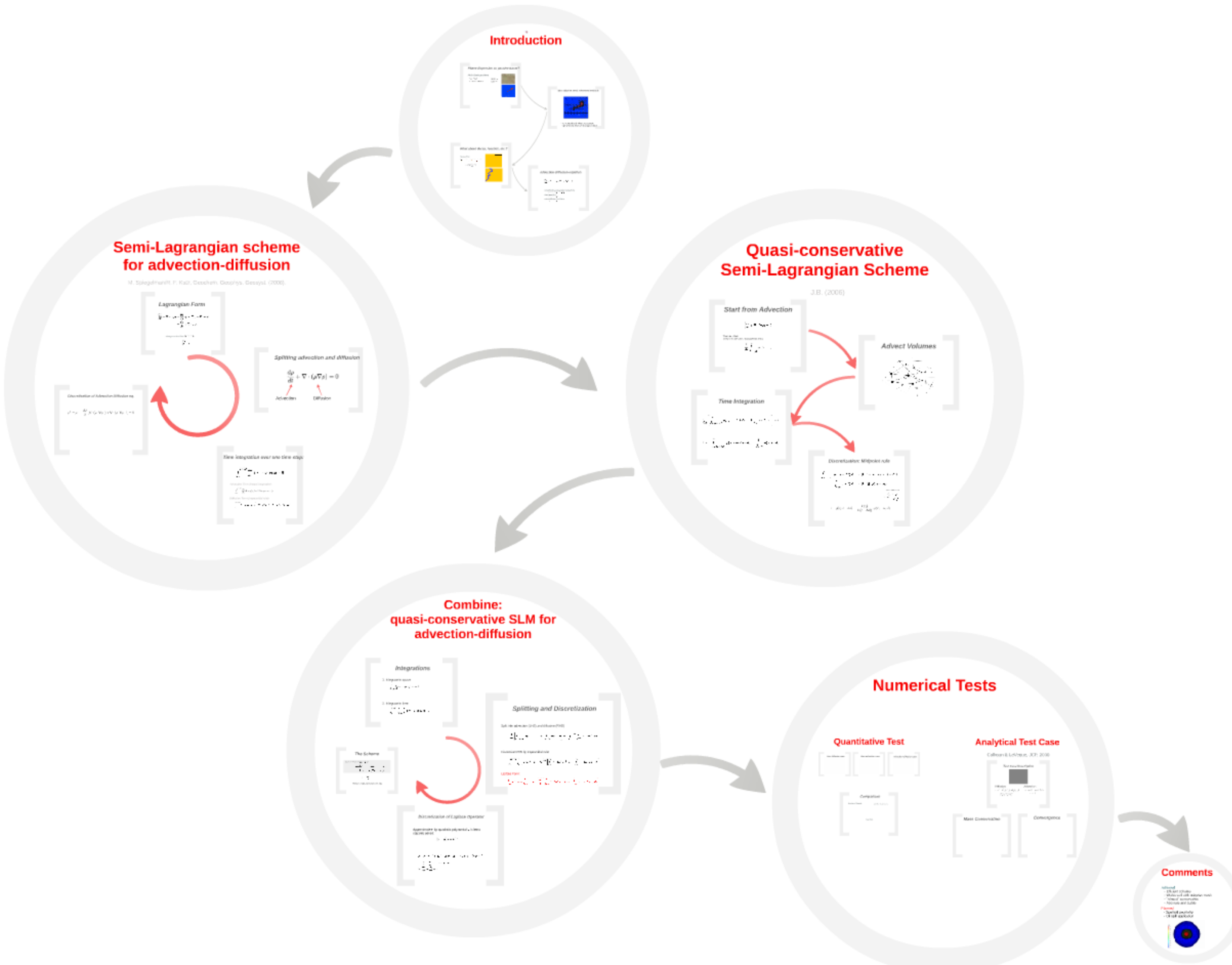


An adaptive and quasi-conservative Semi-Lagrangian advection-diffusion algorithm

Jörn Behrens, CliSAP
Universität Hamburg

Contributions:
Steffen Reinert
Michael Herzog

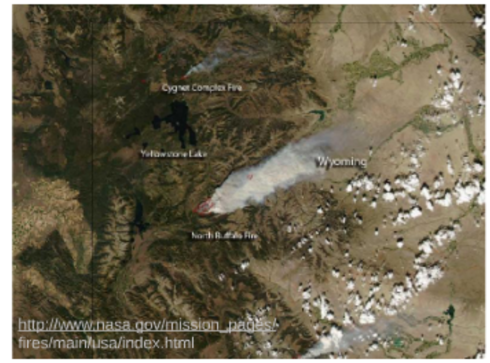

Introduction
Semi-Lagrangian scheme for advection-diffusion
Lagrangian Form
Splitting advection and diffusion
Advection
Diffusion
Time integration over one time step
Quasi-conservative Semi-Lagrangian Scheme
J.B. (2006)
Start from Advection
Advect Volumes
Time Integration
Discretization: Midpoint rule
Combine: quasi-conservative SLM for advection-diffusion
Integrations
Splitting and Discretization
The Scheme
Discretization of Laplace Operator
Numerical Tests
Quantitative Test
Analytical Test Case
Comparison
Mass Conservation
Convergence
Comments

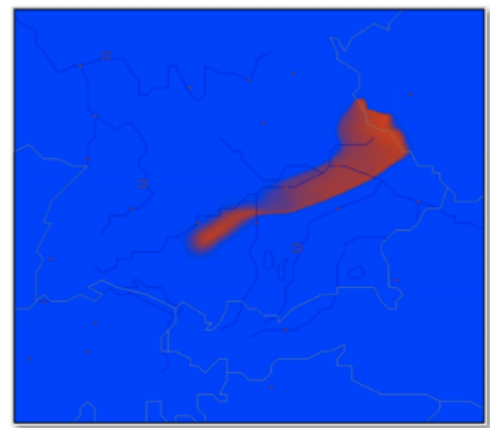
Plume dispersion as passive tracer?

Multi-Scale problem:

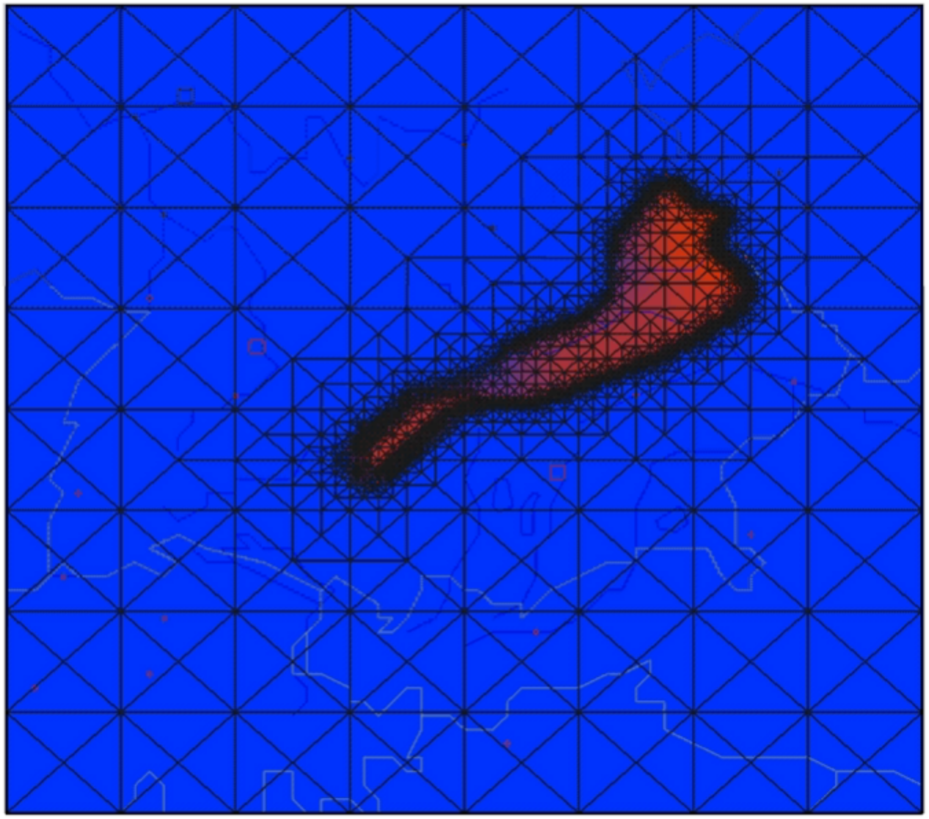
Total Extent $\mathcal{O}(10^5 m^2)$

Local concentrations $\mathcal{O}(10^2 m^2)$





Idea: adaptive mesh refinement methods



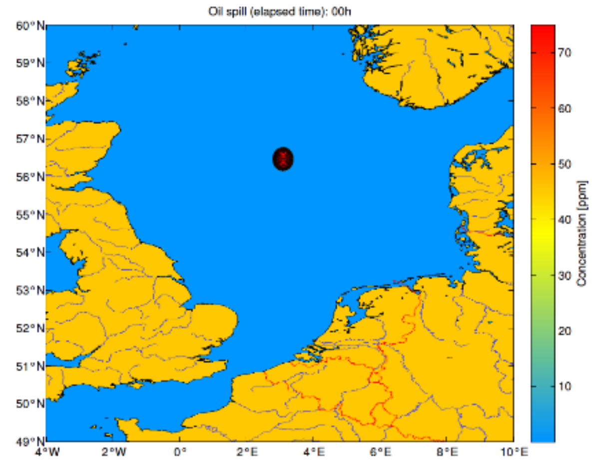
- refinement only where necessary
- dynamically adaptive during run-time

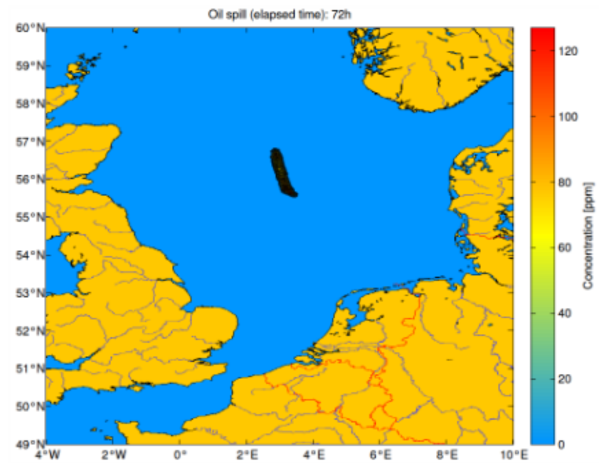
What about decay, reaction, etc.?

Spreading:

$$\frac{\partial K_{oil}}{\partial t} + \vec{u} \cdot \vec{\nabla} K_{oil} - \vec{\nabla} \cdot \left(k_d \vec{\nabla} K_{oil} \right) = \frac{R}{\rho_{oil}}$$

$$k_d = \frac{g h_{oil}^2 \rho_{oil} \left(\rho_w - \rho_{oil} \right)}{\rho_w k_f}$$





Advection-Diffusion equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{v}\rho) + \nabla \cdot (\mu \nabla \rho) = 0$$

Constituent (possibly multi-component)

$$\rho : \Omega \times T \to \mathbb{R}^m, \quad \Omega \subset \mathbb{R}^d$$

Given wind field

$$\mathbf{v} : \Omega \times T \to \mathbb{R}^d$$

Given diffusion coefficient

$$\mu : \Omega \times T \to \mathbb{R}$$

Semi-Lagrangian scheme for advection-diffusion

M. Spiegelman/R. F. Katz, Geochem. Geophys. Geosyst. (2006).

Lagrangian Form

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\mathbf{v}\rho) = \frac{\partial\rho}{\partial t} + \mathbf{v}\cdot\nabla\rho + \nabla\cdot\mathbf{v}\ \rho$$
$$= \frac{d\rho}{dt} + \nabla\cdot\mathbf{v}\ \rho.$$

Divergence-free flow: $\nabla\cdot\mathbf{v} = 0$

$$\frac{d\rho}{dt} = 0$$

Splitting advection and diffusion

$$\frac{d\rho}{dt} + \nabla\cdot(\mu\nabla\rho) = 0$$

Advection Diffusion

Time integration over one time step:

$$\int_t^{t+\Delta t} \frac{d\rho}{dt} + \nabla\cdot(\mu\nabla\rho)\ dt = 0$$

Advection Term (exact integration):

$$\int_t^{t+\Delta t} \frac{d\rho}{dt}\, dt = \rho(x, t+\Delta t) - \rho(x-\alpha, t)$$

Diffusion Term (trapezoidal rule):

$$\int_t^{t+\Delta t} \nabla\cdot(\mu\nabla\rho)\, dt \approx \frac{1}{2}\left[\nabla\cdot(\mu^+\nabla\rho^+) + \nabla\cdot(\mu^-\nabla\rho^-)\right]\Delta t$$

Discretization of Advection-Diffusion eq.

$$\rho^+ - \rho^- - \frac{\Delta t}{2}\left[\nabla\cdot(\mu^+\nabla\rho^+) + \nabla\cdot(\mu^-\nabla\rho^-)\right] = 0$$

Lagrangian Form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{v}\rho) = \frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \nabla \rho + \nabla \cdot \mathbf{v} \;\; \rho$$
$$= \frac{d\rho}{dt} + \nabla \cdot \mathbf{v} \;\; \rho.$$

Divergence-free flow: $\nabla \cdot \mathbf{v} = 0$

$$\frac{d\rho}{dt} = 0$$

Splitting advection and diffusion

$$\frac{d\rho}{dt} + \nabla \cdot (\mu \nabla \rho) = 0$$

Advection

Diffusion

Time integration over one time step:

$$\int_t^{t+\Delta t} \frac{d\rho}{dt} + \nabla \cdot (\mu \nabla \rho)\; dt = 0$$

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Diffusion Term (trapezoidal rule):

$$\int_t^{t+\Delta t} \nabla \cdot (\mu \nabla \rho)\; dt \approx \frac{1}{2}\left[\nabla \cdot (\mu^+ \nabla \rho^+) + \nabla \cdot (\mu^- \nabla \rho^-)\right] \cdot \Delta t$$

Discretization of Advection-Diffusion eq.

$$\rho^+ = \rho^- - \frac{\Delta t}{2}\left[\nabla \cdot (\mu^+ \nabla \rho^+) + \nabla \cdot (\mu^- \nabla \rho^-)\right] = 0$$

Quasi-conservative Semi-Lagrangian Scheme

J.B. (2006)

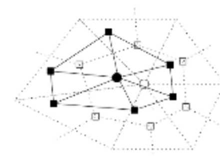
Start from Advection

$$\frac{\partial \rho}{\partial t} - \nabla \cdot (\mathbf{v}\rho) = 0$$

Then we obtain
(integrate over area, transport theorem):

$$\frac{d}{dt} \int_{V(t)} \rho \, dx = 0$$

Advect Volumes



Time Integration

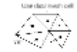
$$\frac{1}{\Delta t}\left[\int_{V(t+\Delta t)} \rho(x, t+\Delta t)\, dx - \int_{V(t)} \rho(x,t)\, dx\right] = 0$$

$$\Rightarrow \quad \int_{V(t+\Delta t)} \rho(x, t+\Delta t)\, dx = \int_{v(t)} \rho(x,t)\, dx$$

Discretization: Midpoint rule

$$\int_{V(t+\Delta t)} \rho(x, t+\Delta t)\, dx \approx |V(t+\Delta t)| \cdot \rho(x_i, t-\Delta t)$$

$$\int_{V(t)} \rho(x,t)\, dx \approx |V(t)| \cdot \rho(x_i - \alpha_i, t)$$



$$\Rightarrow \quad \rho(x_i, t+\Delta t) = \frac{|V(t)|}{|V(t+\Delta t)|} \cdot \rho(x_i - \alpha_i, t)$$

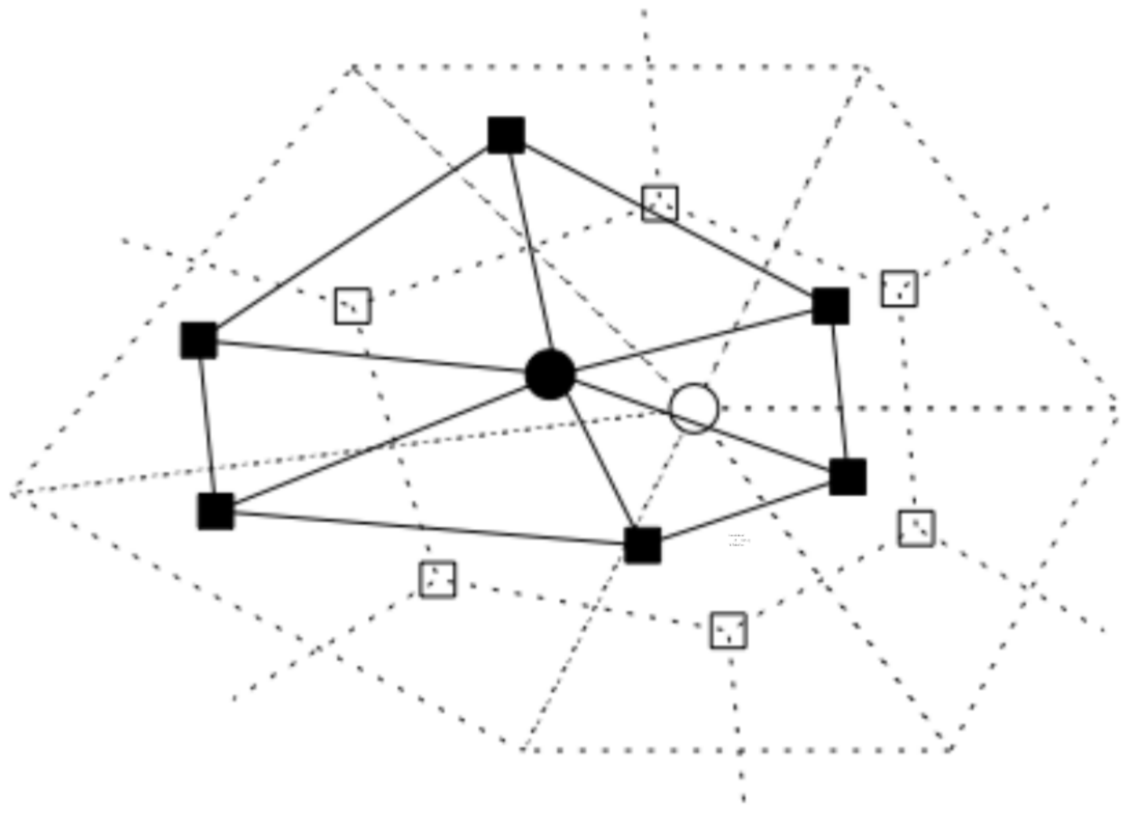
Start from Advection

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{v}\rho) = 0$$

Then we obtain
(integrate over area, transport theorem):

$$\frac{d}{dt}\int_{V(t)} \rho \; dx = 0$$

Advect Volumes



Use solution of

$$\dot{x} = \mathbf{v}(x, t)$$

for trajectories.

Time Integration

$$\frac{1}{\Delta t}\left[\int_{V(t+\Delta t)} \rho(x, t+\Delta t)\ dx - \int_{V(t)} \rho(x,t)\ dx\right] = 0$$

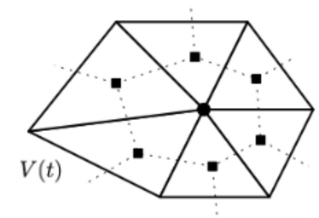
$$\Rightarrow \quad \int_{V(t+\Delta t)} \rho(x, t+\Delta t)\ dx = \int_{v(t)} \rho(x,t)\ dx$$

Discretization: Midpoint rule

$$\int_{V(t+\Delta t)} \rho(x, t+\Delta t)\; dx \;\approx\; |V(t+\Delta t)| \cdot \rho(x_i, t+\Delta t)$$

$$\int_{V(t)} \rho(x, t)\; dx \;\approx\; |V(t)| \cdot \rho(x_i - \alpha_i, t)$$

Use dual mesh cell



$$\Rightarrow \quad \rho(x_i, t+\Delta t) = \frac{|V(t)|}{|V(t+\Delta t)|} \cdot \rho(x_i - \alpha_i, t)$$

Combine: quasi-conservative SLM for advection-diffusion

Integrations

1. Integrate in space

$$\int_{V(t)} \frac{d\rho}{dt} + \nabla\cdot(\mu\nabla\rho)\, dx = 0$$

2. Integrate in time

$$\int_t^{t+\Delta t}\int_{V(t)} \frac{d\rho}{dt} + \nabla\cdot(\mu\nabla\rho)\, dx\, dt = 0$$

Splitting and Discretization

Split into advection (LHS) and diffusion (RHS)

$$\frac{1}{\Delta t}\left[\int_{V(t+\Delta t)} \rho(x,t+\Delta t)\, dx - \int_{V(t)} \rho(x,t)\, dx\right] = -\int_t^{t+\Delta t}\int_{V(t)} \nabla\cdot(\mu\nabla\rho)\, dx\, dt$$

Discretize RHS by trapezoidal rule:

$$\int_t^{t+\Delta t}\int_{V(t)} \nabla\cdot(\mu\nabla\rho)\, dx\, dt \approx \frac{\Delta t}{2}\left[\int_{V^+} \nabla\cdot(\mu^+\nabla\rho^+)\, dx + \int_{V^-} \nabla\cdot(\mu^-\nabla\rho^-)\, dx\right]$$

Update Form:

$$\int_{V^+} \rho^+\, dx - \int_{V^-} \rho^-\, dx = \frac{\Delta t^2}{2}\left[\int_{V^+} \nabla\cdot(\mu^+\nabla\rho^+)\, dx + \int_{V^-} \nabla\cdot(\mu^-\nabla\rho^-)\, dx\right]$$

The Scheme

[illegible]

[illegible]

Remark: Apply Godunov Splitting

Discretization of Laplace Operator

Approximate ρ by quadratic polynomial q in least squares sense:

$$\|\rho - q\|_2 = \min$$

$$q(x,y) = q_1x^2 + q_2y^2 + q_3xy + q_4x + q_5y + q_6, \quad (x,y)\in\Omega$$

$$\frac{\partial\rho}{\partial x} \approx \frac{\partial q}{\partial x} = 2q_1x + q_3y + q_4$$

$$\Rightarrow \frac{\partial^2\rho}{\partial x^2} \approx \frac{\partial^2 q}{\partial x^2} = 2q_1$$

Integrations

1. Integrate in space

$$\int_{V(t)} \frac{d\rho}{dt} + \nabla \cdot (\mu \nabla \rho) \; dx = 0$$

2. Integrate in time

$$\int_{t}^{t+\Delta t} \int_{V(t)} \frac{d\rho}{dt} + \nabla \cdot (\mu \nabla \rho) \; dx \; dt = 0$$

Splitting and Discretization

Split into advection (LHS) and diffusion (RHS)

$$\frac{1}{\Delta t}\left[\int_{V(t+\Delta t)} \rho(x, t+\Delta t)\ dx - \int_{V(t)} \rho(x,t)\ dx\right] = -\int_t^{t+\Delta t}\int_{V(t)} \nabla\cdot(\mu\nabla\rho)\ dx\ dt$$

Discretize RHS by trapezoidal rule:

$$\int_t^{t+\Delta t}\int_{V(t)} \nabla\cdot(\mu\nabla\rho)\ dx\ dt \approx \frac{\Delta t}{2}\left[\int_{V+} \nabla\cdot(\mu^+\nabla\rho^+)\ dx + \int_{V-} \nabla\cdot(\mu^-\nabla\rho^-)\ dx\right]$$

Update Form:

$$\int_{V+} \rho^+\ dx = \int_{V-} \rho^-\ dx - \frac{\Delta t^2}{2}\left[\int_{V+} \nabla\cdot(\mu^+\nabla\rho^+)\ dx + \int_{V-} \nabla\cdot(\mu^-\nabla\rho^-)\ dx\right]$$

Discretization of Laplace Operator

Approximate ρ by quadratic polynomial q in least squares sense:

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$$\frac{\partial \rho}{\partial x} \approx \frac{\partial q}{\partial x} = 2q_1 x + q_3 y + q4$$

$$\Rightarrow \frac{\partial^2 \rho}{\partial x^2} \approx \frac{\partial^2 q}{\partial x^2} = 2q_1$$

The Scheme

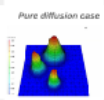
$$\begin{aligned}\rho(x,t+\Delta t) = {} & \chi\rho(x_i-\alpha_i,t) \\ & -\frac{\Delta t^2}{2}\left[\nabla\cdot(\mu(x,t+\Delta t)\nabla\bar{\rho}(x,t+\Delta t))\right. \\ & \left.+\chi\nabla\cdot(\mu(x-\alpha,t)\nabla\rho((x-\alpha,t))\right]\end{aligned}$$

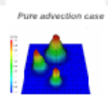
$$\chi = \frac{|V(t)|}{|V(t+\Delta t)|}$$

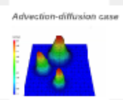
Remark: Apply Godunov Splitting

Numerical Tests

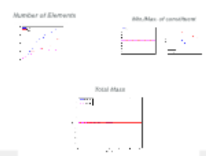
Quantitative Test







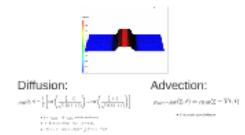
Comparison



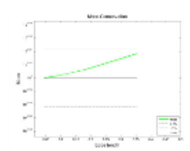
Analytical Test Case

Calhoun & LeVeque, JCP, 2000

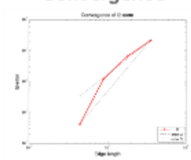
Test Case Description



Mass Conservation



Convergence



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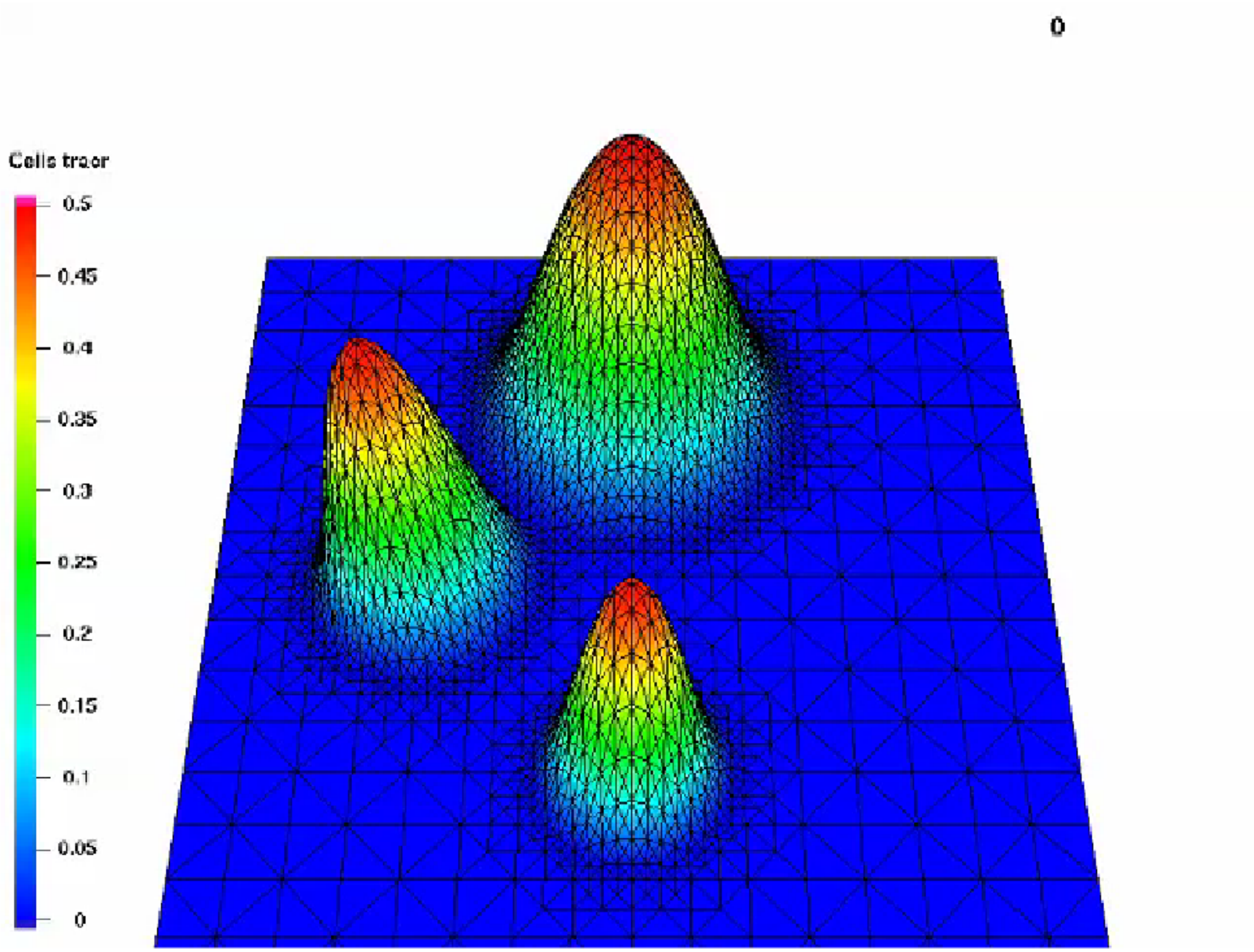
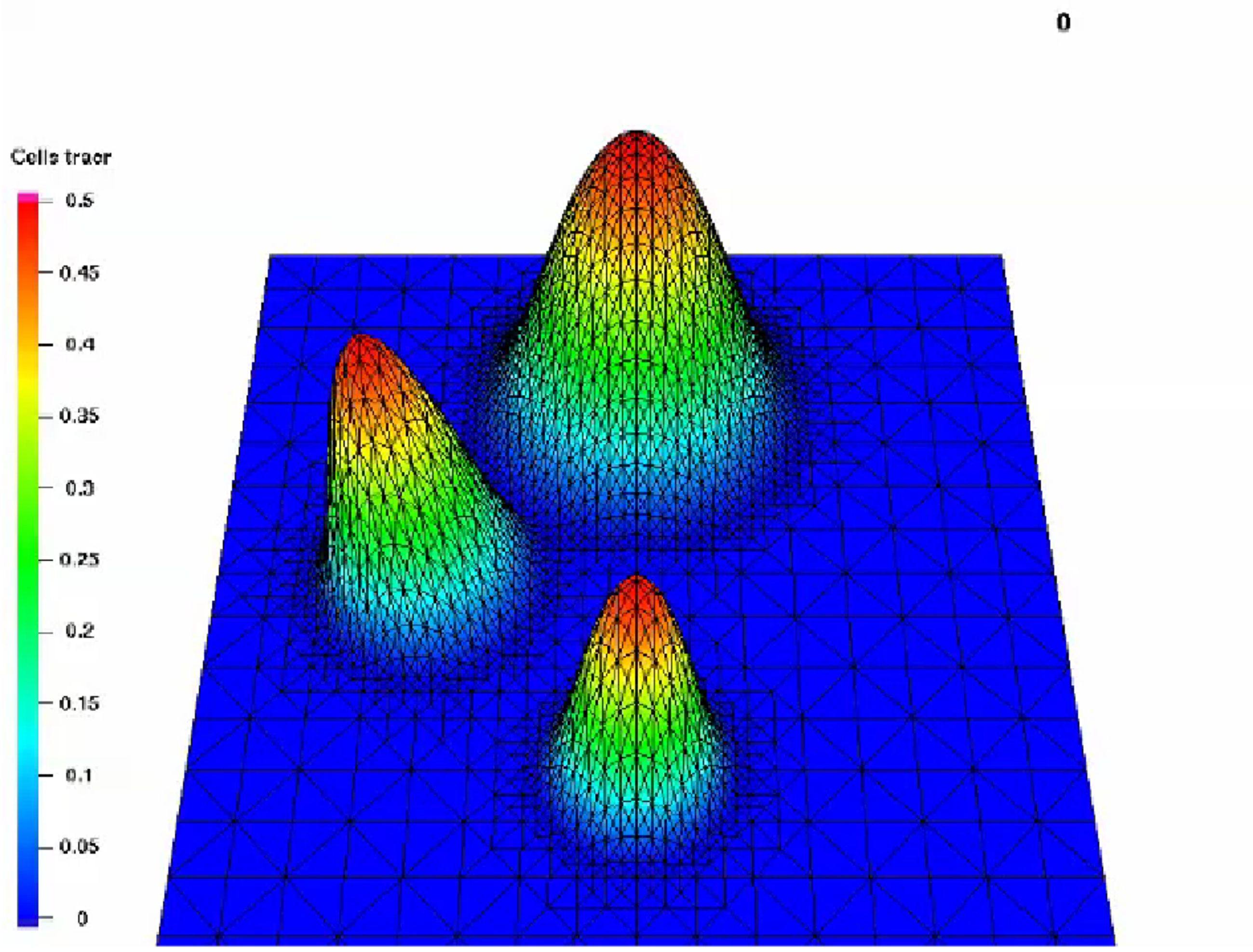
- Acc

Planne
- Spe
- Oil

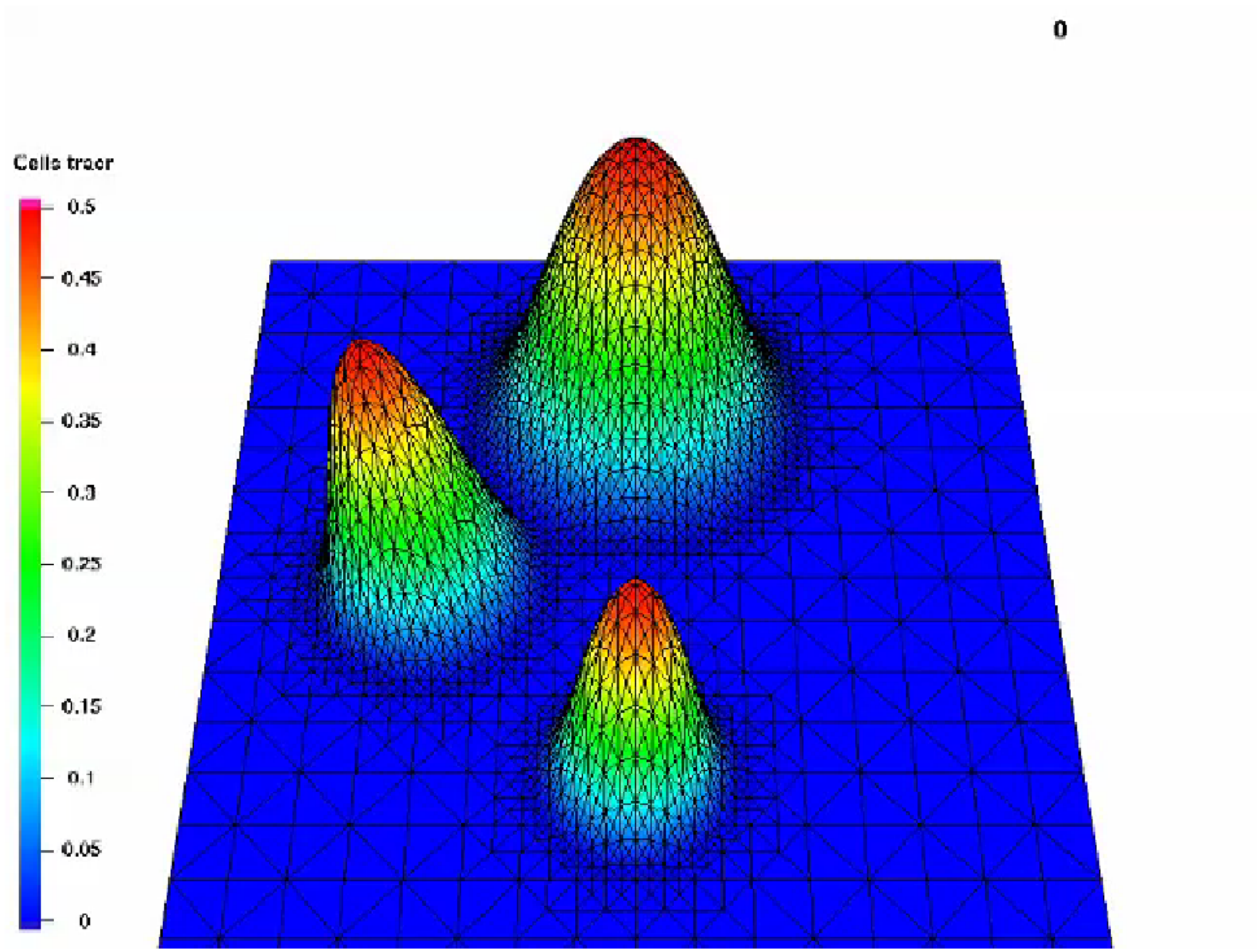
Pure diffusion case



Pure advection case

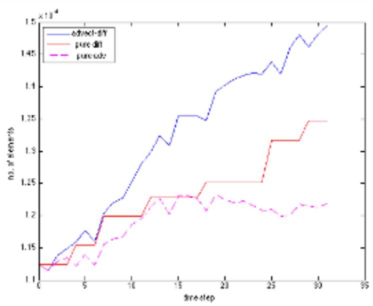


Advection-diffusion case

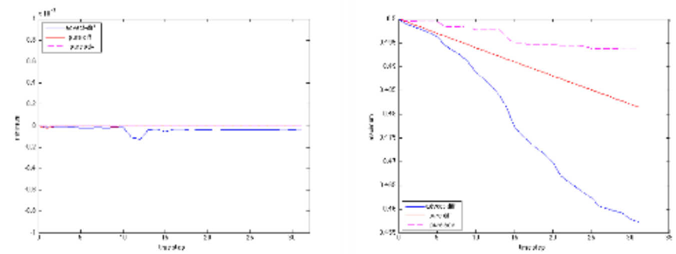


Comparison

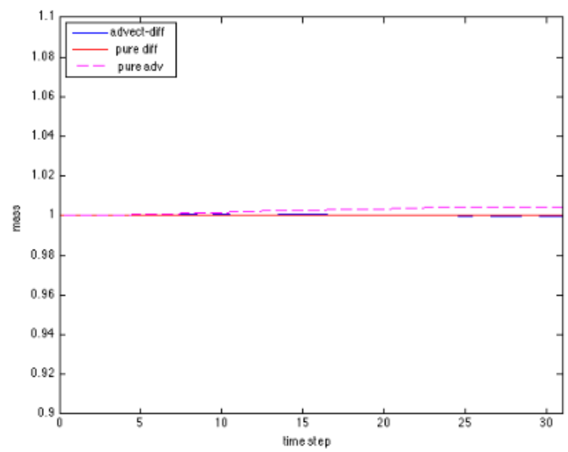
Number of Elements



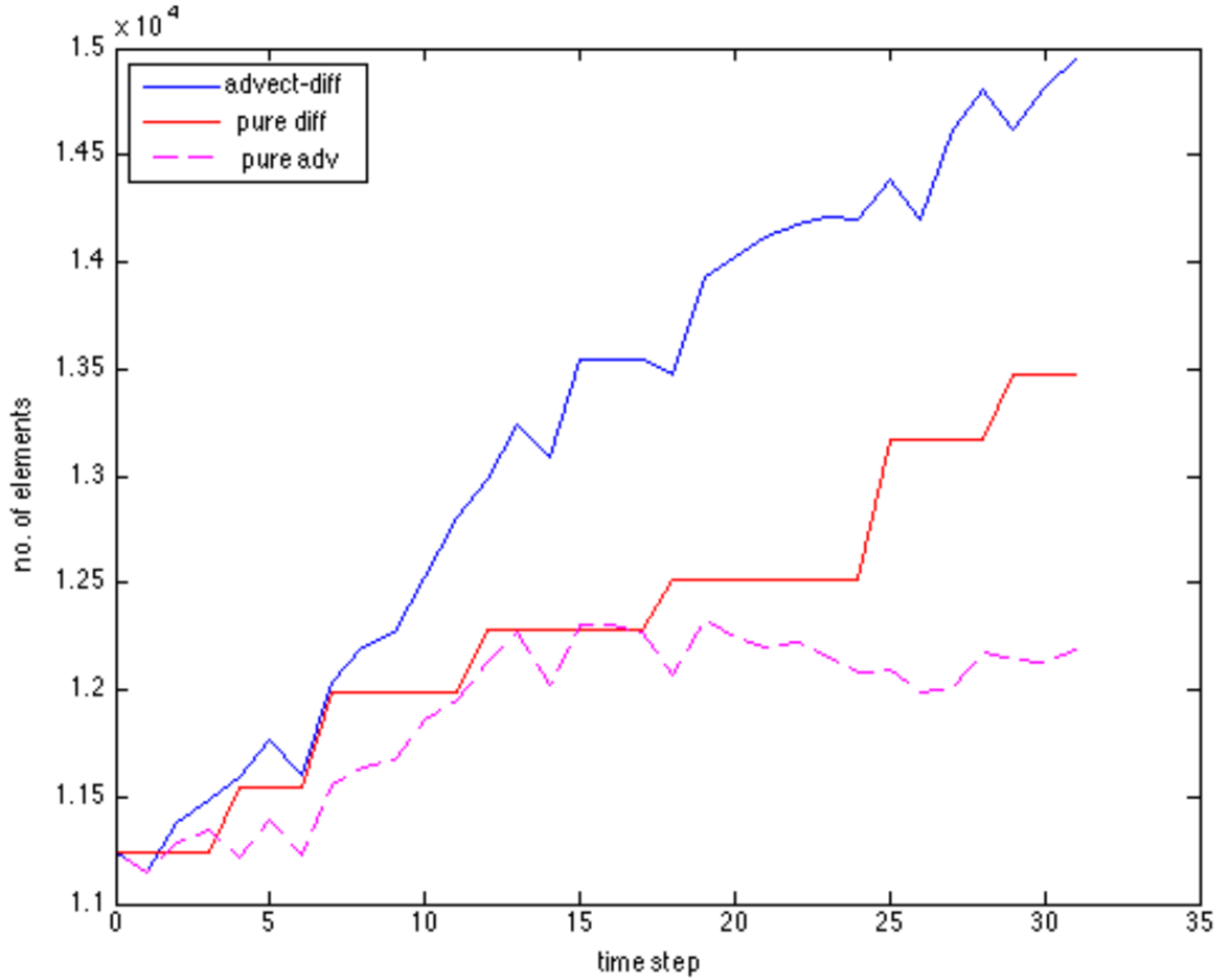
Min./Max. of constituent



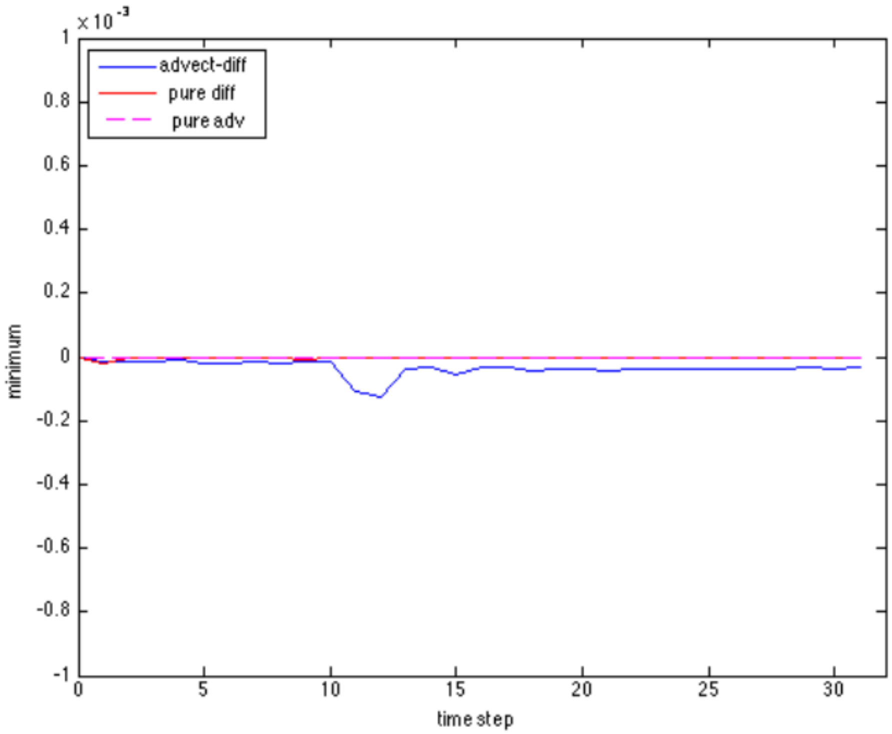
Total Mass

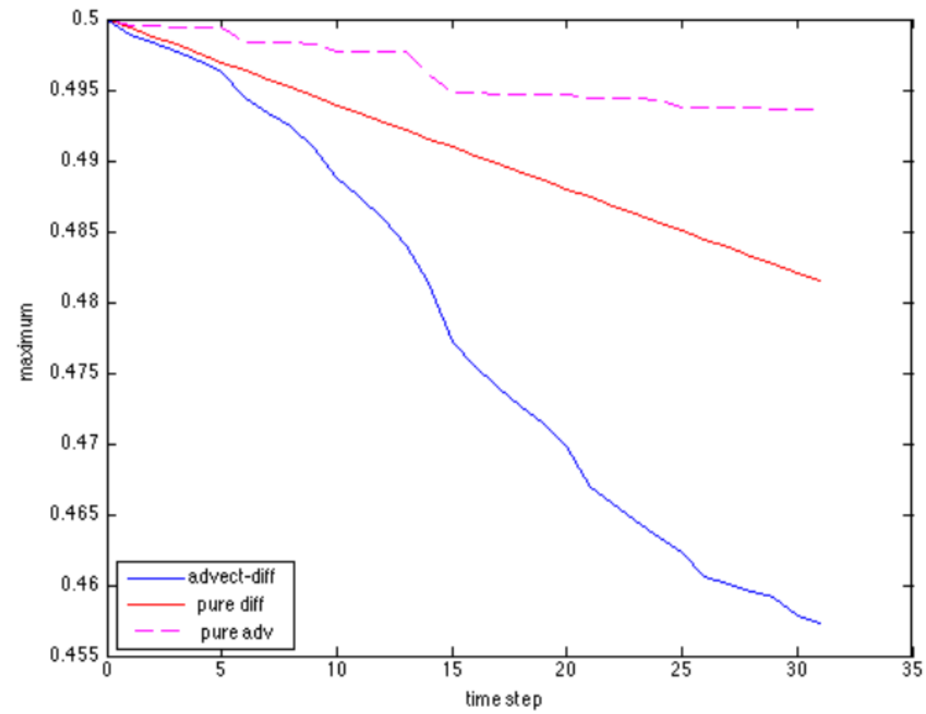


Number of Elements

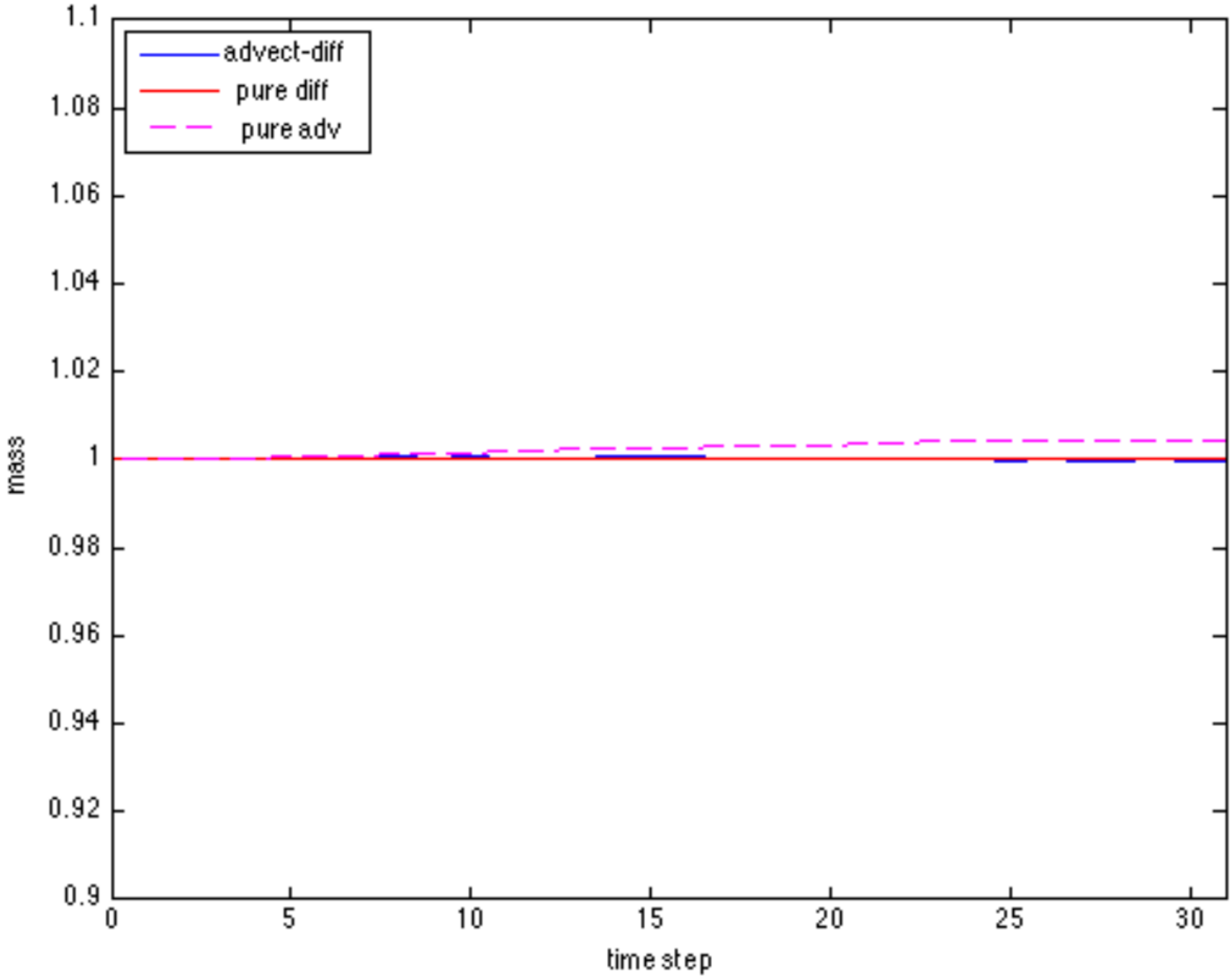


Min./Max. of constituent



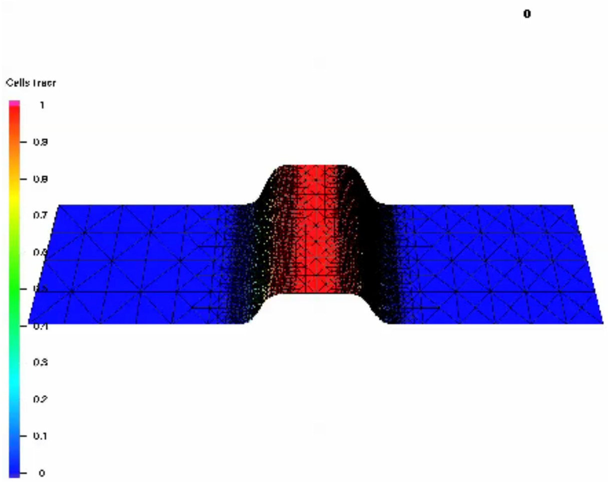


Total Mass



advect-diff
pure diff
pure adv
mass
time step
1.1
1.08
1.06
1.04
1.02
1
0.98
0.96
0.94
0.92
0.9
0
5
10
15
20
25
30

Test Case Description



Diffusion:

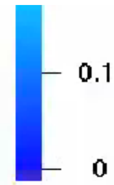
$$\rho_{\text{diff}}(\xi,t) = \frac{1}{2}\left[\text{erf}\left(\frac{\frac{3}{4}-\xi}{\sqrt{4D(1+t)}}\right) + \text{erf}\left(\frac{\frac{3}{4}+\xi}{\sqrt{4D(1+t)}}\right)\right]$$

- $\xi = |x_{\text{center}} - x|$, x_{center} half channel length,
- D diffusion coefficient (here: $D = 0.01$),
- erf the error function $\text{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x \exp(-r^2)\, dr$.

Advection:

$$\rho_{\text{adv-diff}}(\xi,t) = \rho_{\text{diff}}(\xi - Vt, t)$$

- V constant zonal velocity.



Diffusion:

$$\rho_{\text{diff}}(\xi, t) = \frac{1}{2}\left[\operatorname{erf}\left(\frac{\frac{3}{4} - \xi}{\sqrt{4D(1+t)}}\right) + \operatorname{erf}\left(\frac{\frac{3}{4} + \xi}{\sqrt{4D(1+t)}}\right)\right]$$

- $\xi = |x_{\text{center}} - x|$, x_{center} half channel length,
- D diffusion coefficient (here: $D = 0.01$),
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Advection:

$$\rho_{\mathrm{adv-diff}}(\xi, t) = \rho_{\mathrm{diff}}(\xi - Vt, t)$$

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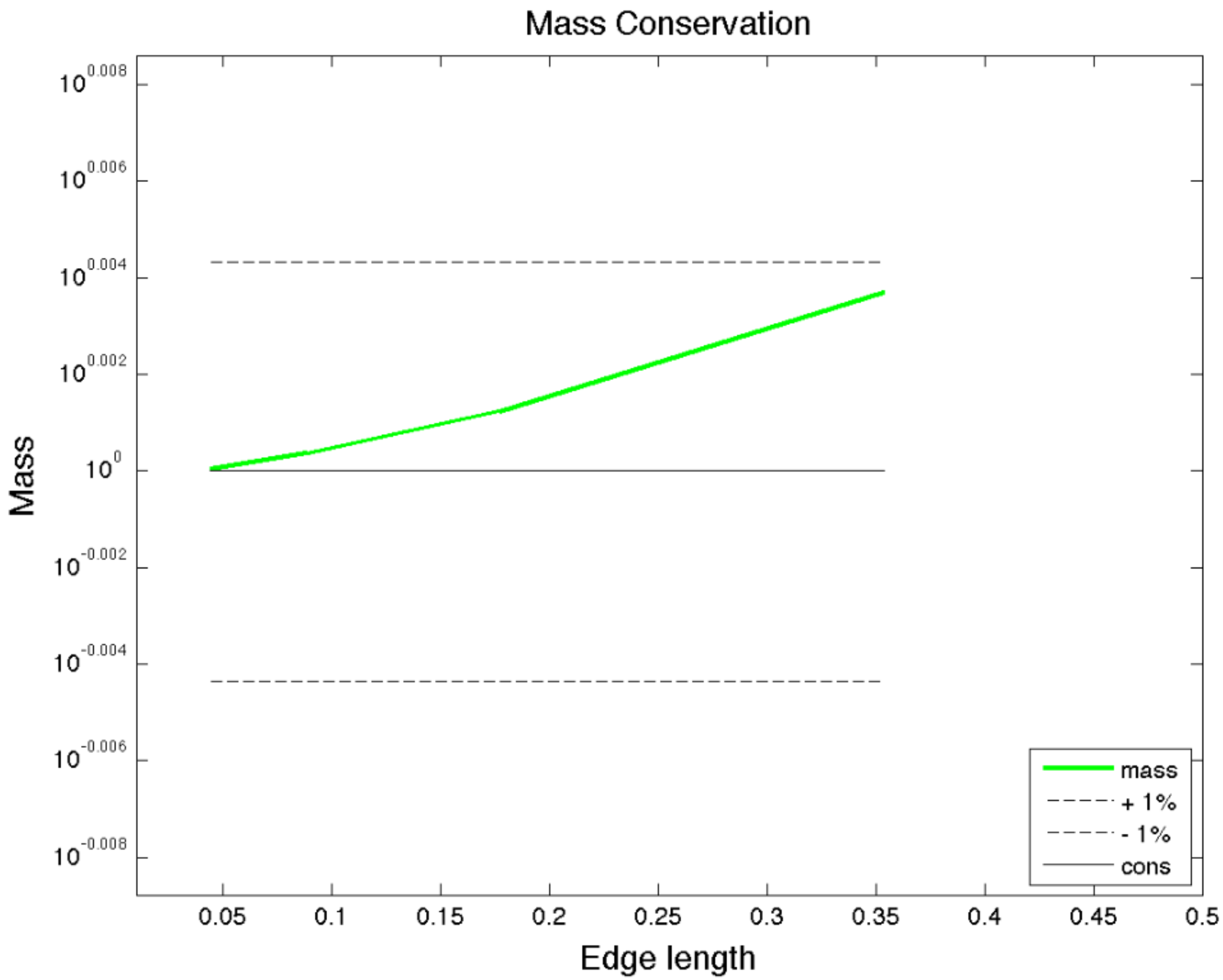
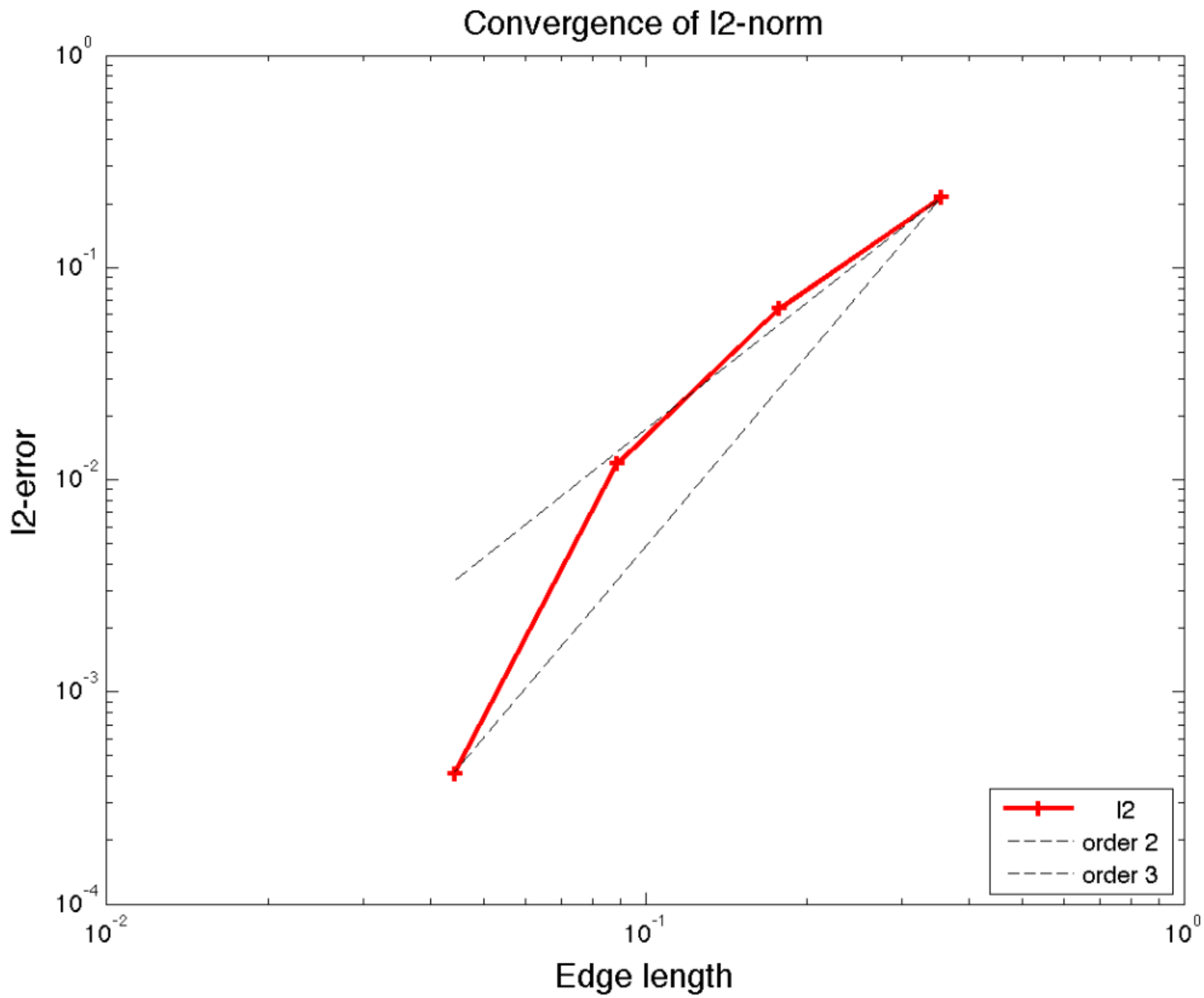
Mass Conservation



Convergence



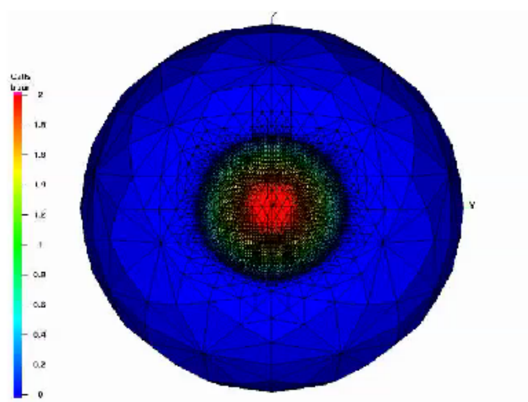
Comments

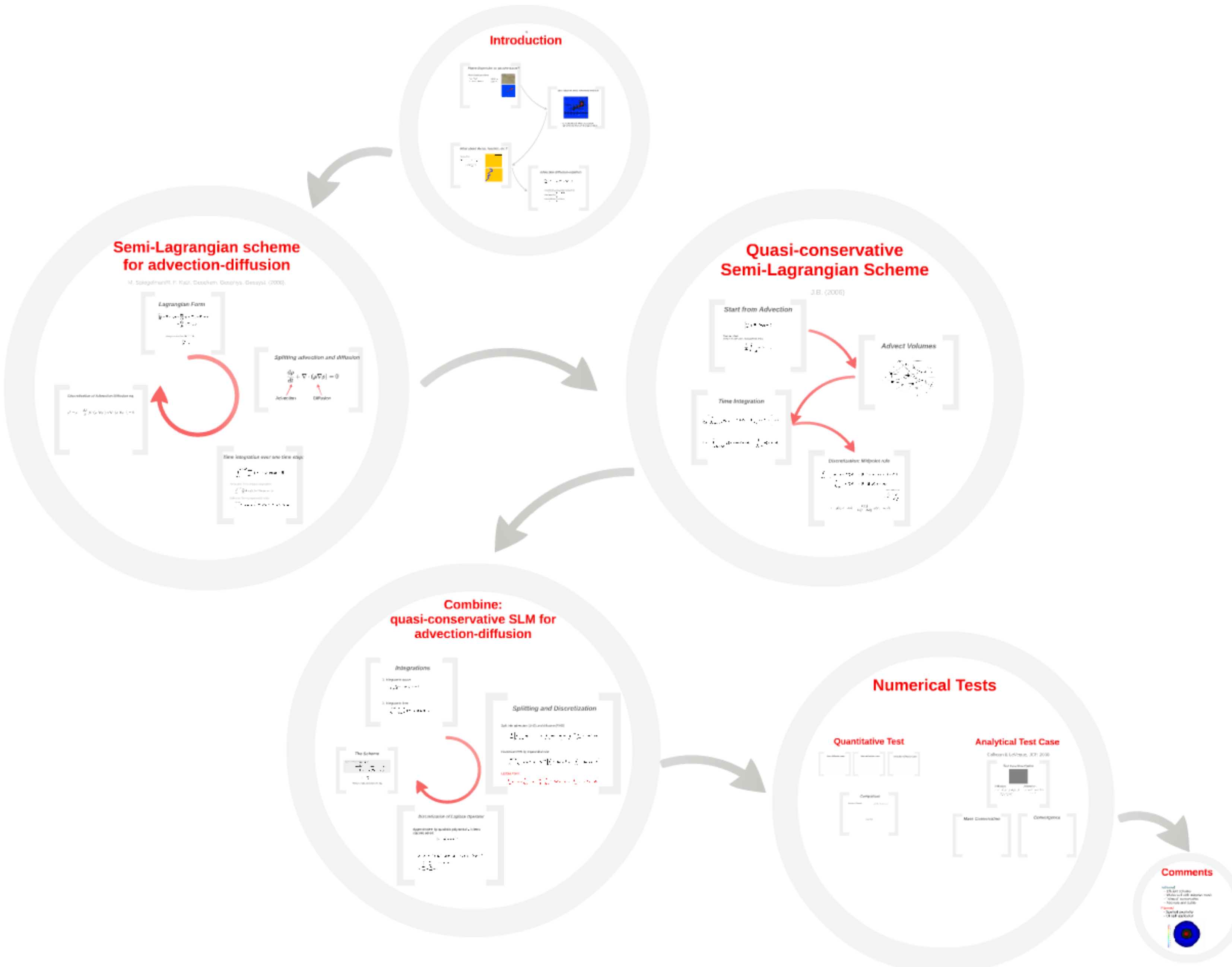
Achieved

- Efficient scheme
- Works well with adaptive mesh
- "Almost" conservative
- Accurate and stable

Planned

- Sperical geometry
- Oil spill application

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Analytical Test Case
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