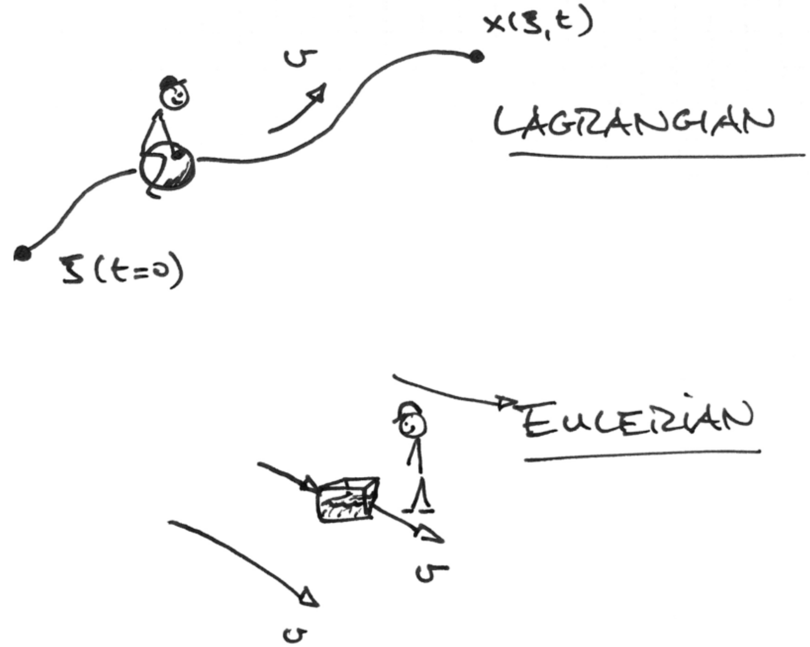
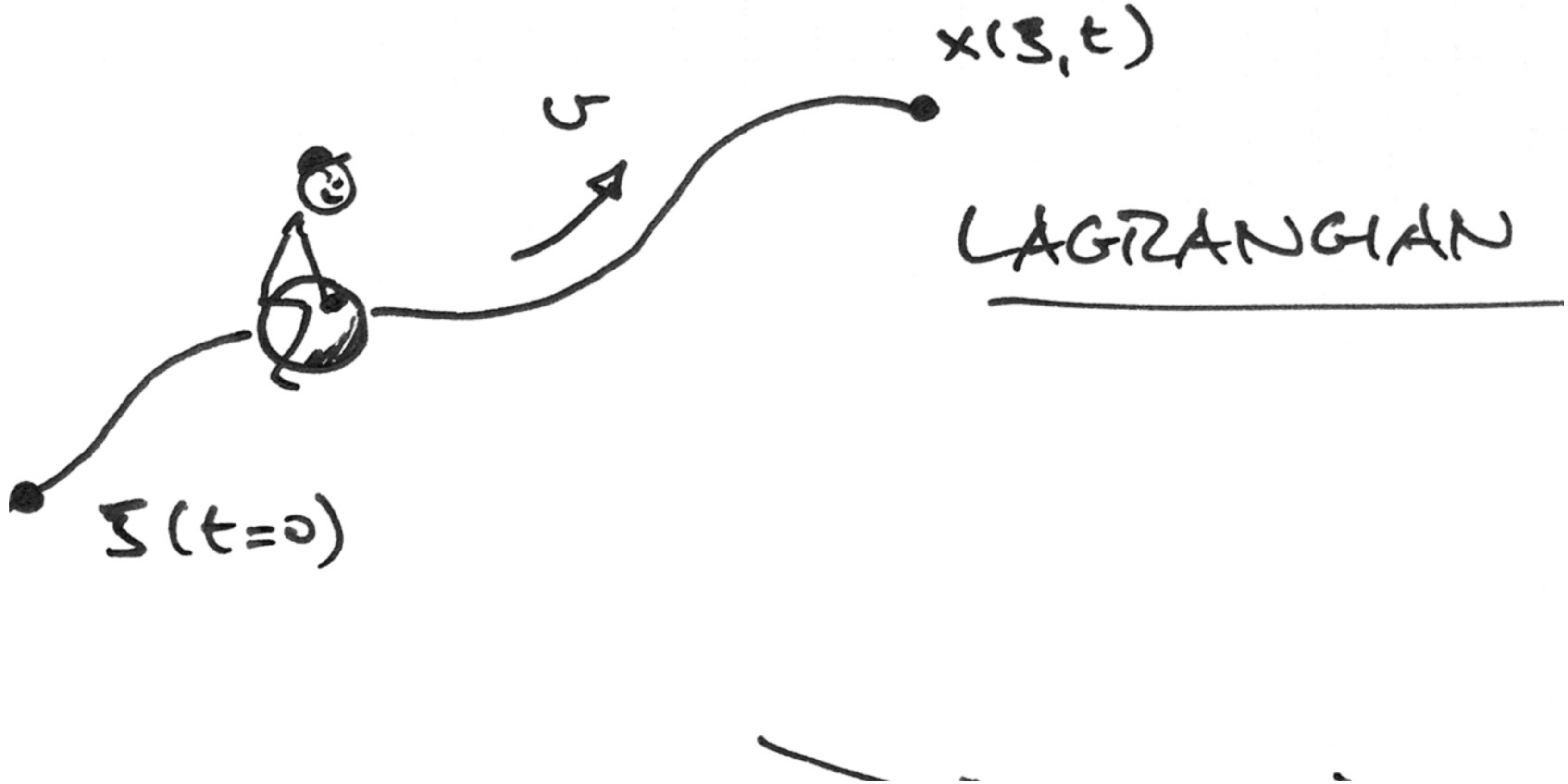
Differential Equations II

Numerical Solution of the Transport Equation:
Lagrangian and Semi-Lagrangian Methods

Lagrangian Perspective




x(ξ, t)
v
ξ (t=0)
LAGRANGIAN

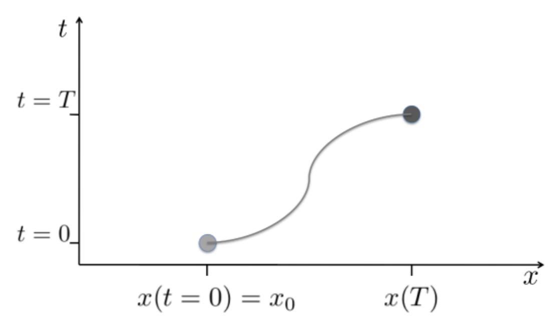
Formalization

- Position: $x = x(t)$.
- Velocity: $v = v(x, t)$.

Particle position can be computed by

$$\dot{x} = \frac{dx}{dt} = v(x, t)$$

With initial condition $x(t = 0) = x_0$

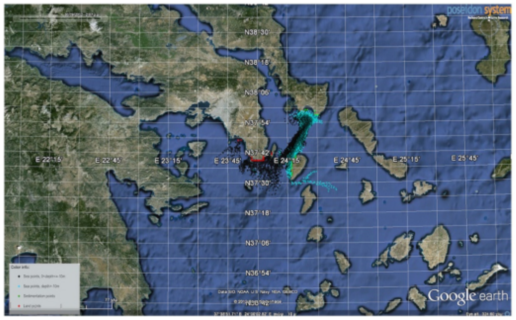


Lagrangian Transport with Source

The equation is given by

$$\frac{d\rho}{dt} = s(x,t)$$

where $\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \cdot \frac{dx}{dt}$



http://www.medess4ms.eu/oil-spill-models

Remark: With $\dot{x} = v(x,t)$ we have that

$$\frac{d}{dt} = \rho_t + v\rho_x = s(x,t).$$

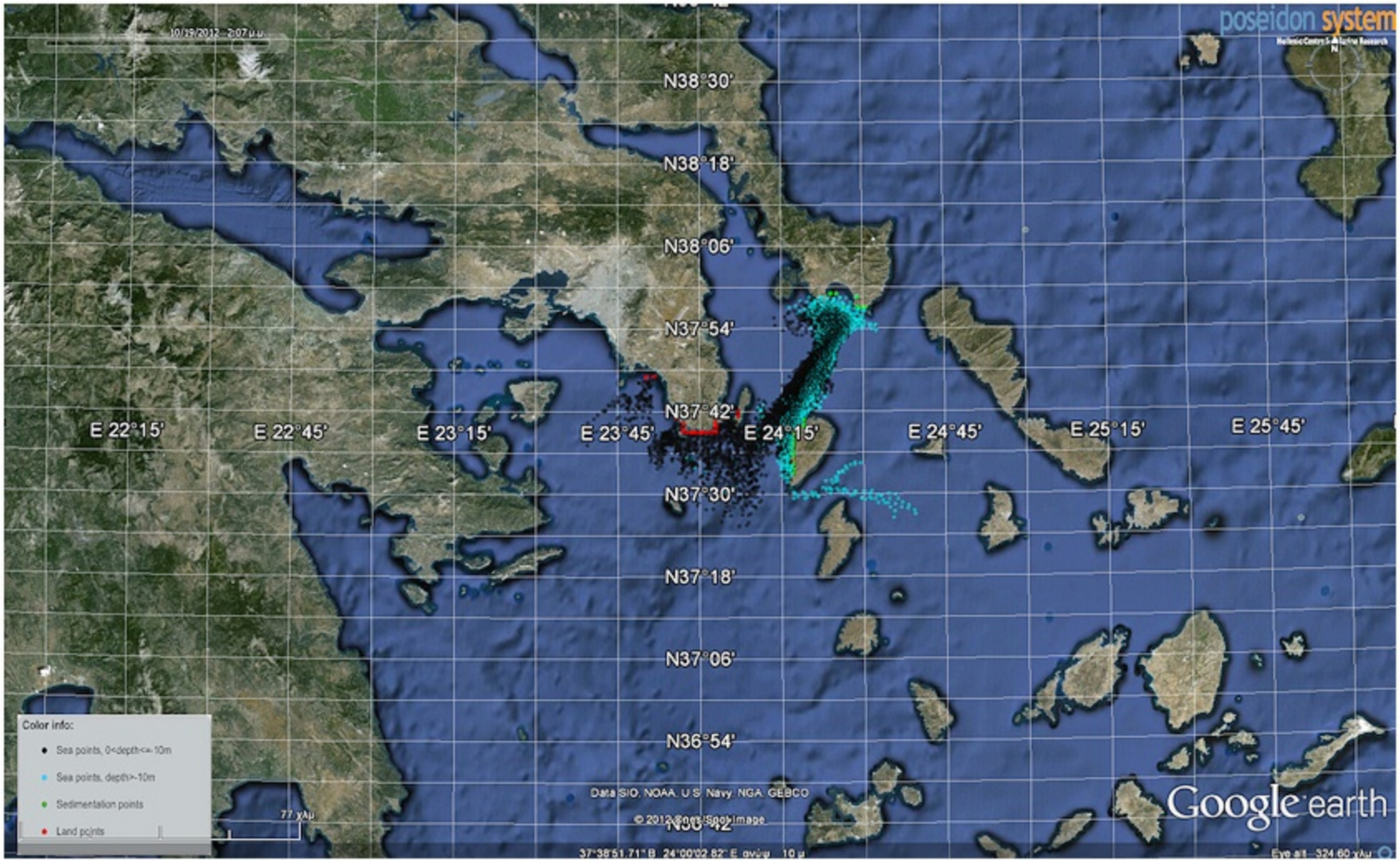
Summary: We need to solve two ODEs:

$$\begin{aligned} \dot{x} &= v(x,t), \quad x(0) = x_0, \\ \dot{\rho} &= s(\rho,x,t), \quad \rho(x,0) = \rho_0(x). \end{aligned}$$

Remark: Usually many particles are used for real applications!
Remark: Homogeneous advection, where $s \equiv 0$, yields:

$$\dot{\rho} = 0 \quad \Rightarrow \quad \rho(\cdot,t) \equiv \text{const.} = \rho_0(\cdot).$$

Since $x = x(t)$, the particle position is implied: $\rho(x,t) = \rho(x(t),t))$.



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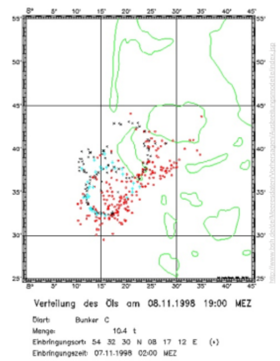
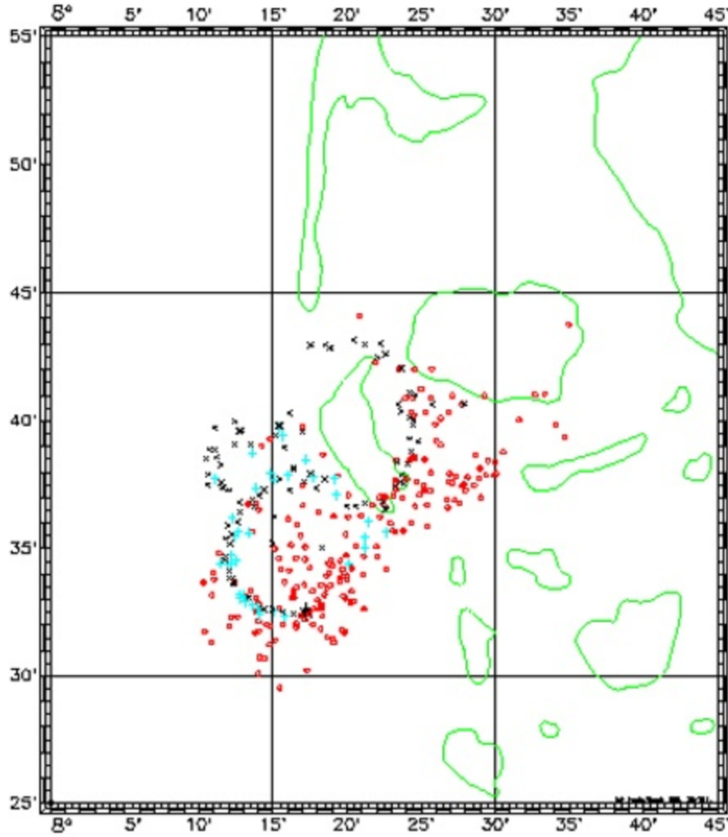
Problems of purely Lagrangian Methods

- Distribution of particles will eventually become very irregular.
- Interaction between particles is difficult to simulate (diffusive processes).
- Density distribution fields with spatial coverage hard to reconstruct.





Verteilung des Öls am 08.11.1998 19:00 MEZ

Ölart: Bunker C

Menge: 10.4 t

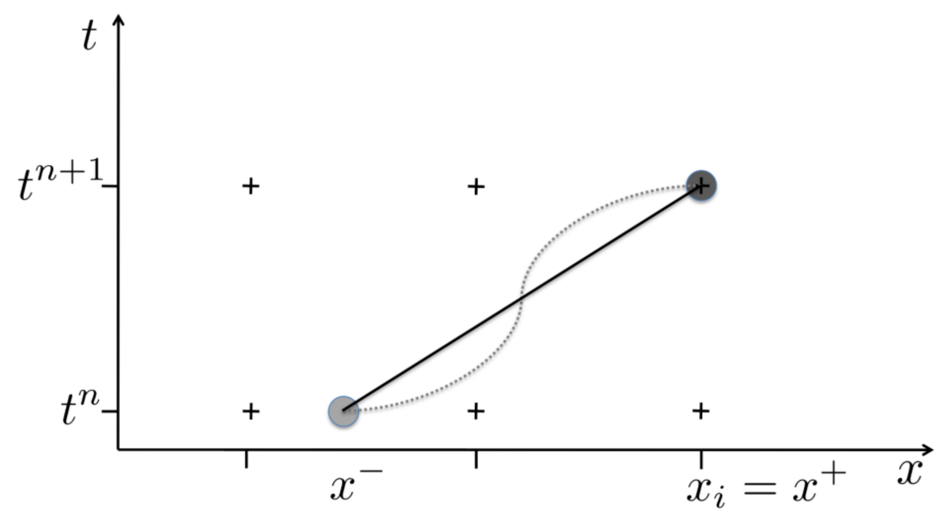
Einbringungsort: 54 32 30 N 08 17 12 E (+)

Einbringungszeit: 07-11-1998 02:00 MEZ

Idea

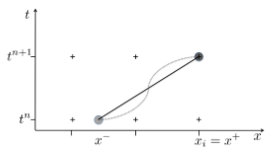
Combine Lagrangian and Eulerian Methods

Idea of the Semi-Lagrangian Method



Formalization

Problem: Passive advection ($s \equiv 0$):



$$\frac{dx}{dt} = v(x,t), \quad x(0) = x_0,$$
$$\frac{d\rho}{dt} = 0, \quad \rho(x,0) = \rho_0(x).$$

Strategy:

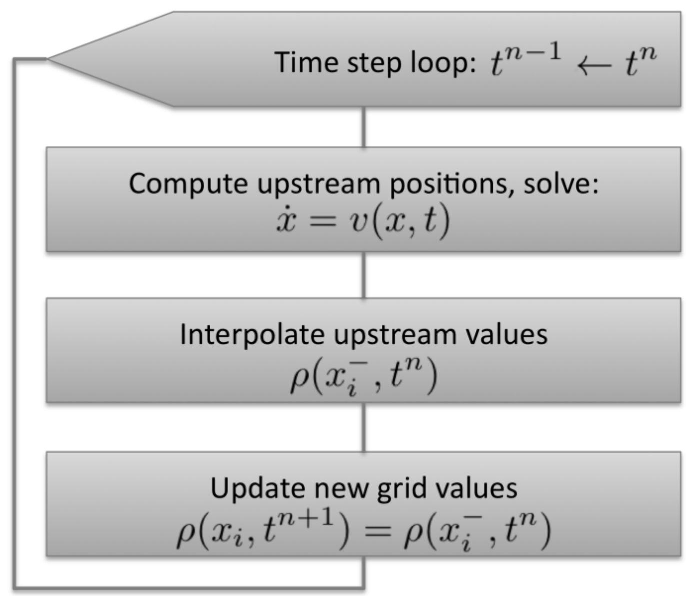
- Solve $\frac{dx}{dt} = v$ by any ODE solver,
- Solve $\frac{d\rho}{dt} = 0$ by finite difference.

$$\frac{d\rho}{dt} \approx \frac{\rho(x_i, t^{n+1} - \rho(x_i^-, t^n)}{\Delta t} = 0$$

$$\Rightarrow \rho^+ = \rho^-.$$

x_i, $i = 1 : N$ grid points, t^n, $n = 1 : M$ time steps.

Algorithm


Time step loop: $t^{n-1} \leftarrow t^n$
Compute upstream positions, solve:
$\dot{x} = v(x, t)$
Interpolate upstream values
$\rho(x_i^-, t^n)$
Update new grid values
$\rho(x_i, t^{n+1}) = \rho(x_i^-, t^n)$

Stability and Consistency

Von Neumann Stability Analysis:
Assume linear interpolation of upstream points and exact wind, i.e.

$$\rho_i^{n+1} = (1-\nu)\rho_{k_i}^n + \nu\rho_{k_i-1}^n$$

- $[x_{k_{i-1}}, x_{k_i}]$ interval containting upstream point x_i^-,
- $\nu = \frac{x_k - x^-}{\Delta x}$.

Then using $z_n e^{ik(jh)}$ we have:

$$\begin{aligned} z_{n+1} e^{ik(jh)} &= (1-\nu) z_n e^{ik(k_i h)} + \nu z_n e^{ik(k_i - 1h)}, \\ &= z_n \left[1 - \nu(1 - e^{-ik(h)})\right] e^{ik(k_i - j)h} e^{ik(jh)}; \\ \Rightarrow \xi = & \quad \left[1 - \nu(1 - e^{-ik(h)})\right] e^{ik(k_i - j)h}; \\ \Rightarrow |\xi|^2 &= 1 - 2\nu(1-\nu)(1 - \cos(kh)). \end{aligned}$$

Stability follows for: $0 \leq \nu \leq 1$, i.e. always!

Remark (Order of Consistency):
It can be shown the the semi-Lagrangian advection scheme retains the consistency order of the discretization schemes involved:

$$\left.\begin{array}{l} \dot{x} = v \text{ order } p \\ \dot{\rho} = 0 \text{ order } p \end{array}\right\} \Rightarrow \text{SLM order } p.$$

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Advection with Source

Recall:
$\rho_t + v\rho_x = s.$

Lagrangian:
$\dot{x} = v; \dot{\rho} = s.$

For one particle we solve:

$$\begin{aligned} \dot{x} &= v(x,t), \quad x(0) = x_0, \\ \dot{\rho} &= s(\rho, x, t), \quad \rho(x,0) = \rho_0(x). \end{aligned}$$

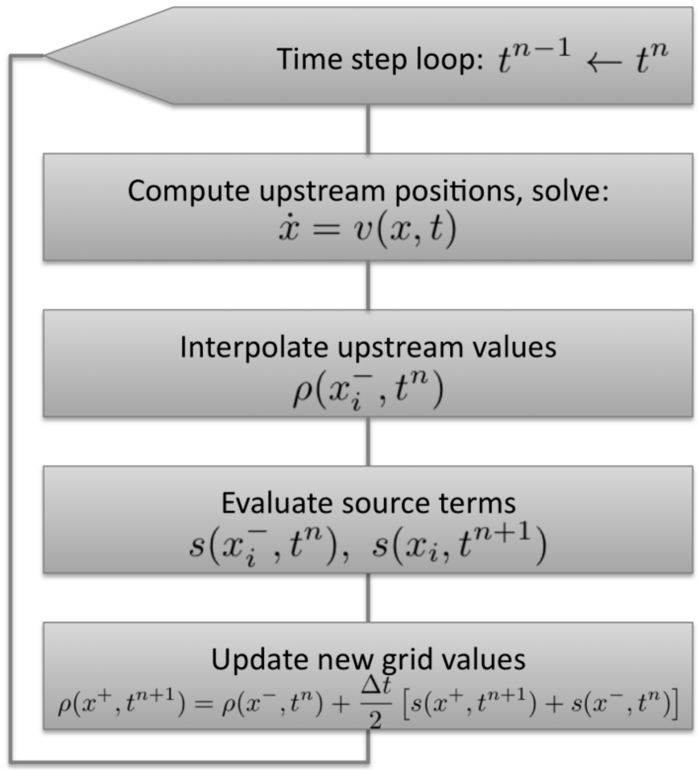
Assume $s = s(x,t)$, use trapezoidal rule:

$$\frac{\rho(x^+, t^{n+1}) - \rho(x^-, t^n)}{\Delta t} = \frac{1}{2}\left[s(x^+, t^{n+1}) + s(x^-, t^n)\right]$$

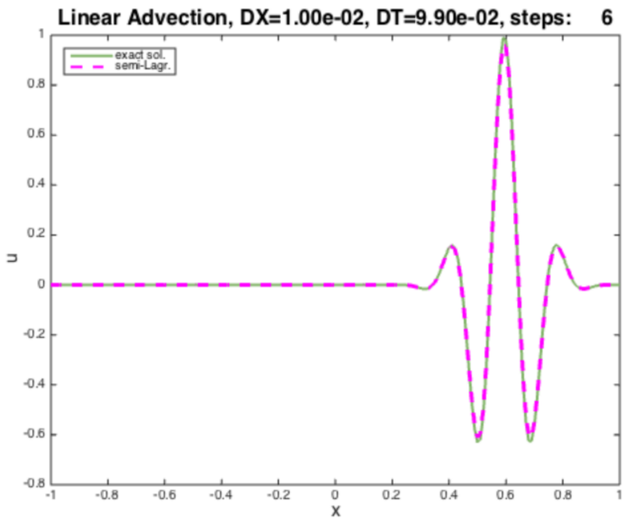
Or even simpler:

$$\frac{\rho(x^+, t^{n+1}) - \rho(x^-, t^n)}{\Delta t} = s(x^0, t^{n+1/2})$$

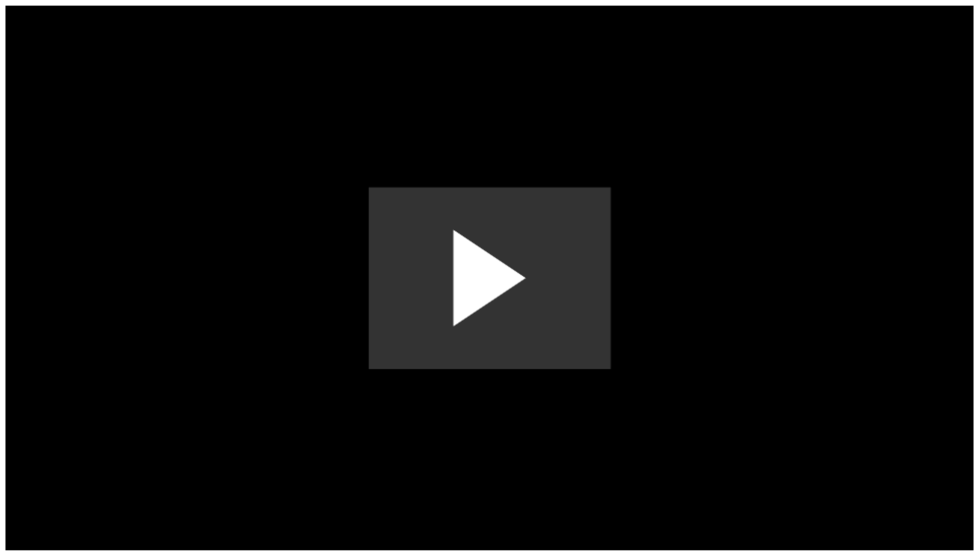
Algorithm with Source



Semi-Lagrangian Algorithm Result



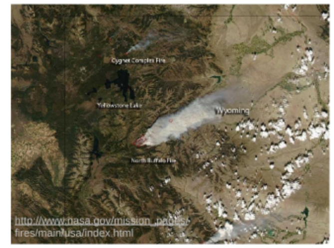
Now 2D

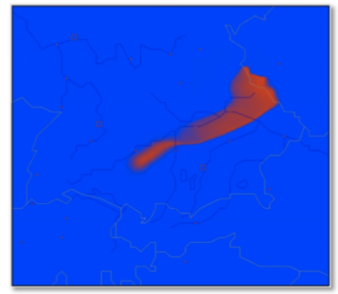


Plume dispersion as passive tracer?

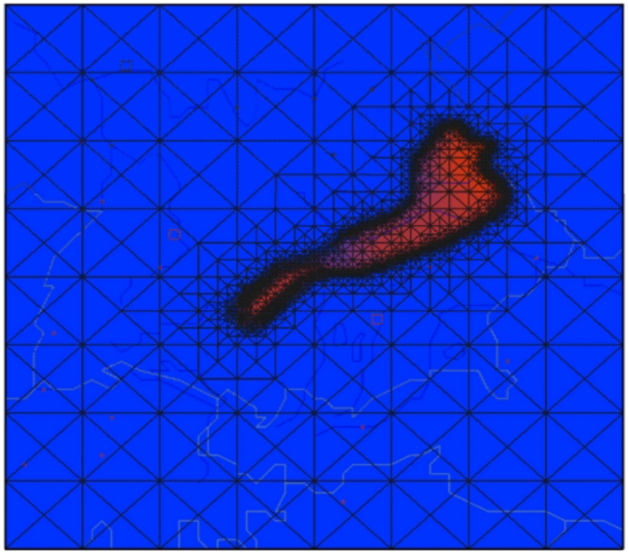
Multi-Scale problem:

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

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

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

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):

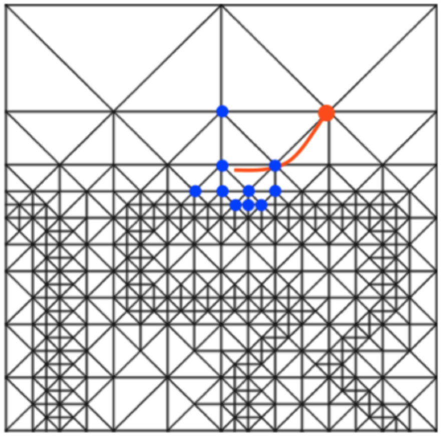
$$\int_t^{t+\Delta t} \nabla \cdot (\mu \nabla \rho)\ dt \approx \frac{1}{2}\left[\nabla \cdot (\mu^+ \nabla \rho^+) + \nabla \cdot (\mu^- \nabla \rho^-)\right] \cdot \Delta t$$

Discretization of Advection-Diffusion eq.

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

Problem with non-uniform Meshes

Semi-Lagrangian Method:



Lagrange Form: $\frac{dc}{dt} = 0$

Difference along trajectory:

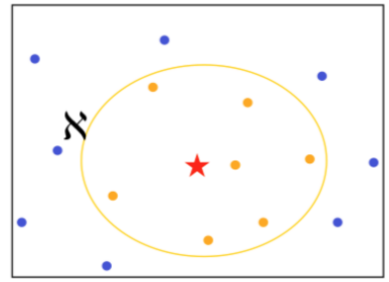
$$\frac{dc}{dt} \approx \frac{c(\vec{x}, t + \Delta t) - c(\vec{x} - 2\vec{\alpha}, t - \Delta t)}{2\Delta t}$$

$$\Rightarrow \boxed{c(\vec{x}, t + \Delta t)} = \boxed{c(\vec{x} - 2\vec{\alpha}, t - \Delta t)}$$

Interpolation with Radial Basis Functions

Interpolation Problem:

$$s:\mathbb{R}^d \to \mathbb{R} \quad \text{with} \qquad s|_{\aleph} = c(\cdot,t)|_{\aleph}.$$



ℵ set of *k* neighbors

Interpolating Function:

$$s(x) = \sum_{j=1}^{k} \lambda_j \Phi(\|x-y_j\|) + p(x), \qquad y_j \in \aleph,\ p(x) = \sum_{l=1}^{q} \mu_l p_l(x).$$

$$\begin{bmatrix} A_{\Phi,\aleph} & P \\ P & 0 \end{bmatrix} \begin{bmatrix} \lambda \\ \mu \end{bmatrix} \begin{bmatrix} c(y_j) \\ 0 \end{bmatrix}$$

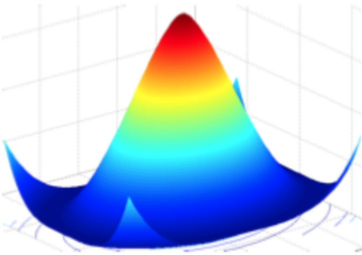
$$A_{\Phi,\aleph} = \left[\Phi(\|x_j - x_l\|)\right]_{j,l=1:k}, \qquad P = \left[p_n(x_j)\right]_{n=1:q,j=1:k}.$$

(ℵ non-degenerate)

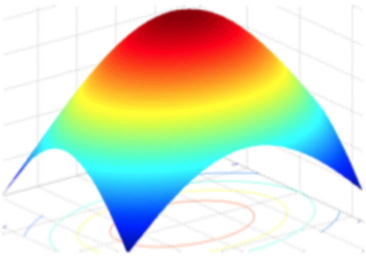
R.L. Hardy (1971), J. Duchon (1976), W.R. Madych/S.A. Nelson (1988)

Examples of Radial Basis Funktions

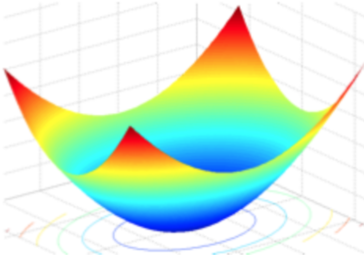
Thin Plate Spline $\Phi(r) = r^2 \log r$



Gaussians $\Phi(r) = e^{-r^2}$

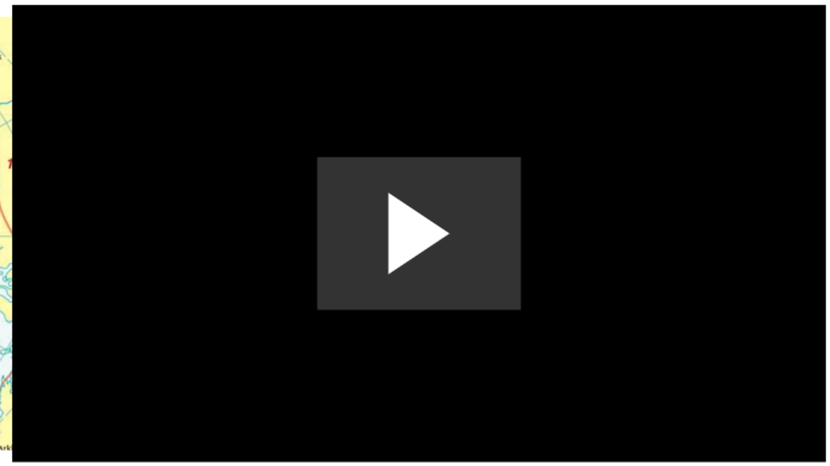


Multiquadrics $\Phi(r) = \sqrt{r^2 + 1}$



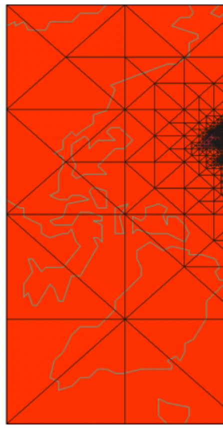
Application: Tracer Transport

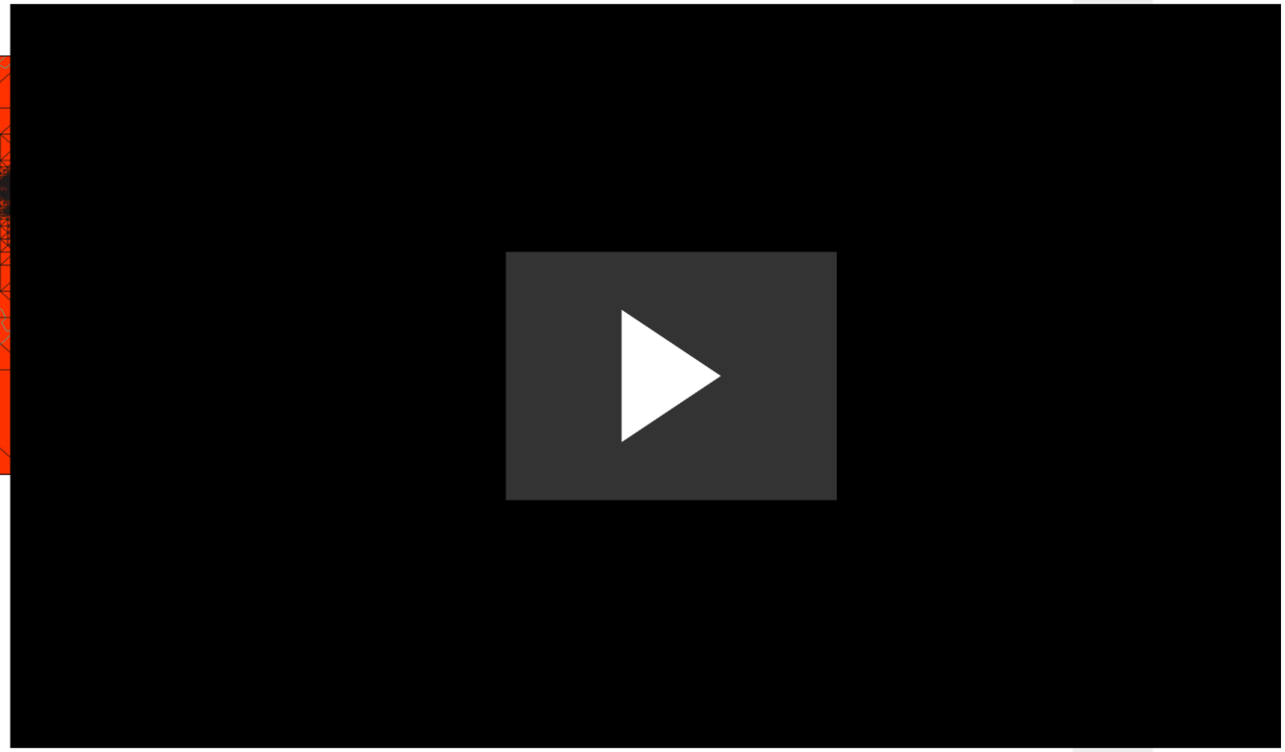
Given: Wind Data



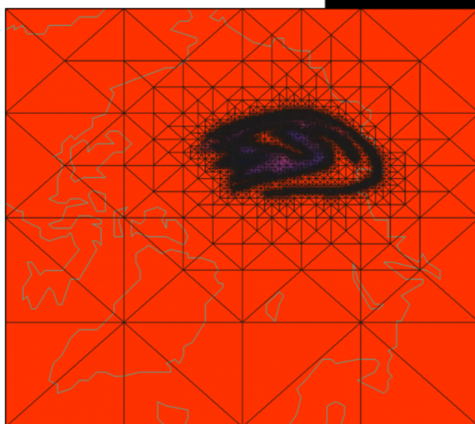
http://www.lib.utexas.edu/maps

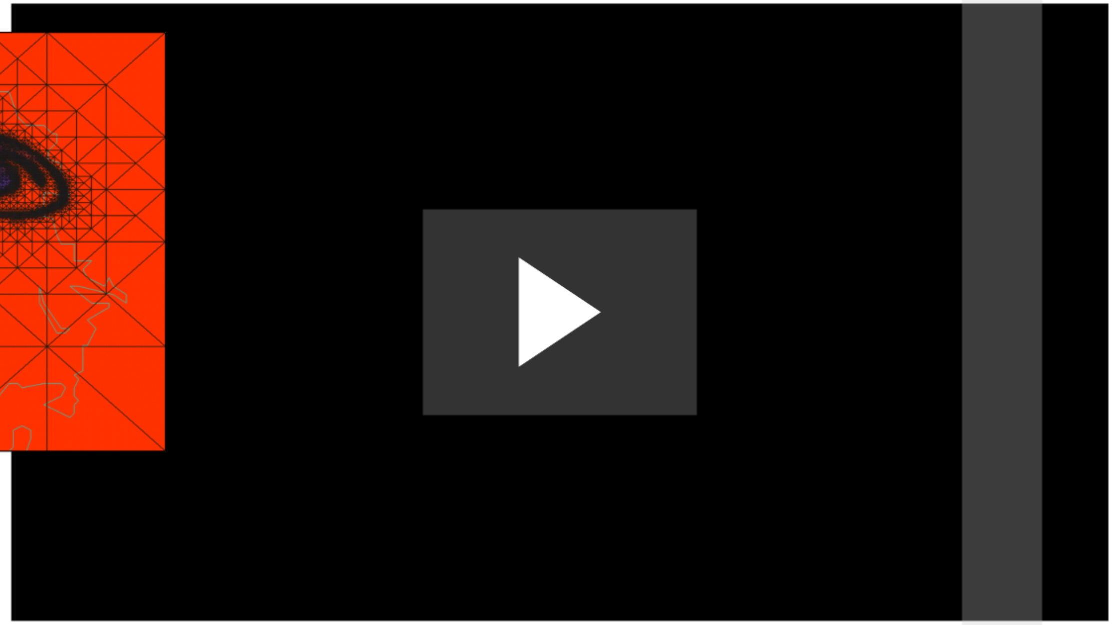
Tracer Transport (Adaptive Mesh)

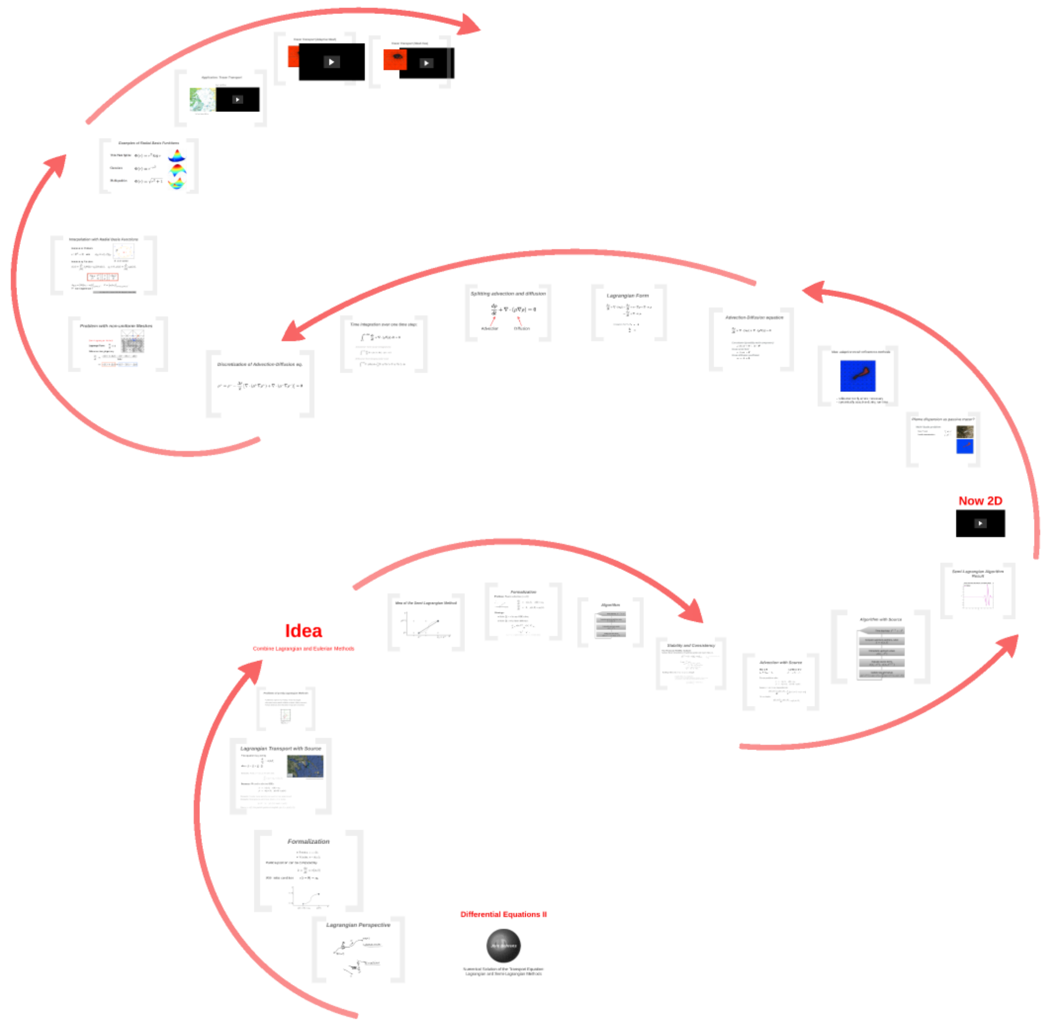




Tracer Transport (Mesh-free)







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