Lagrangian modelling of reactive contaminant transport in marine environment.

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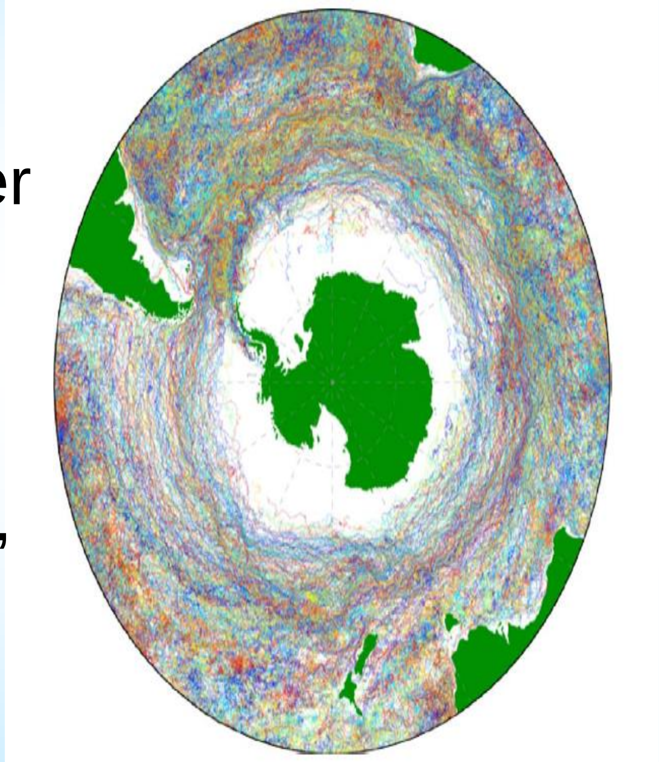
Particles methods for ocean research

- Interpretation of measurement results (trajectory analysis, estimation of velocities, temperature, salinity, turbulence, trajectories of moving water masses, finding special points, migration of biological objects)
- Modeling for forecasting and analysis of the state of the environment (pollution distribution, risk assessment, statistics of possible scenarios, finding sources, finding stagnant zones)



Near 100 papers per year titled «Lagrangian ocean modelling»   Van Sebille, 2018

Solution of transport problem by Lagrangian method

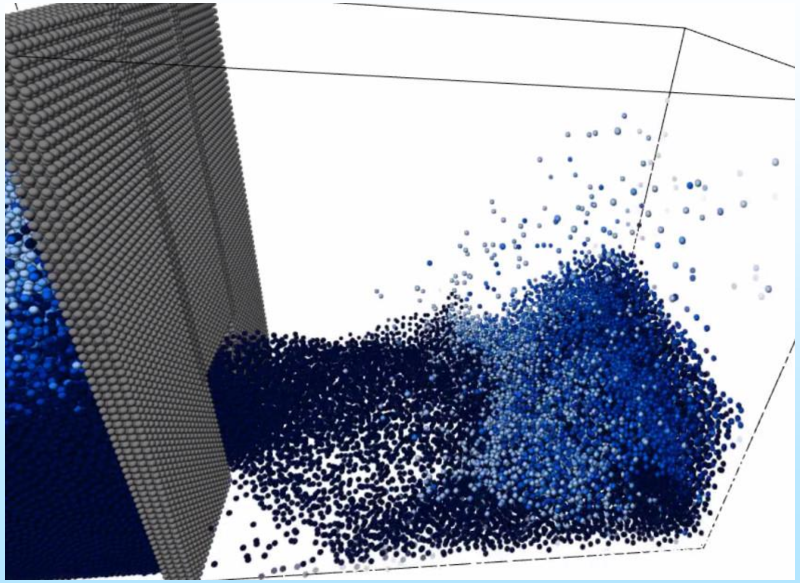
$$\frac{d\vec{x}}{dt} = \vec{u}_c(x,t)$$

-equation for the particle trajectory

- The Lagrangian approach is more natural because it describes the motion of a continuous medium as the movement of individual material particles
- Lagrangian methods allow us to describe multiple-scale processes
- Lagrangian methods are conservative by definition.
- Lagrangian methods make it possible to track the trajectory of each particle
- Simple and effective parallelization

Issues:

- Smoothness
- Visualization
- Phase transitions
- Boundary conditions
- Stochastic methods



Equation of advection-diffusion-reaction

$$\frac{dC_i}{dt} = -\nabla \cdot (\vec{u}_i C_i) + \nabla \cdot (\mathrm{D}\nabla \mathrm{C}_i) + \sum_{j=1}^{n} \alpha_{ij} C_j + R_i$$

advection diffusion reaction sorces

C_i - concentration of material i

$\vec{u}_i$ - flow velocity

$D = (D_x, D_y, D_z)$ – diffusion coefficient

α_{ij} - kinetic transfer coefficients or reaction, sorption, decay.

R_i - sources/sinks

Advection of particles

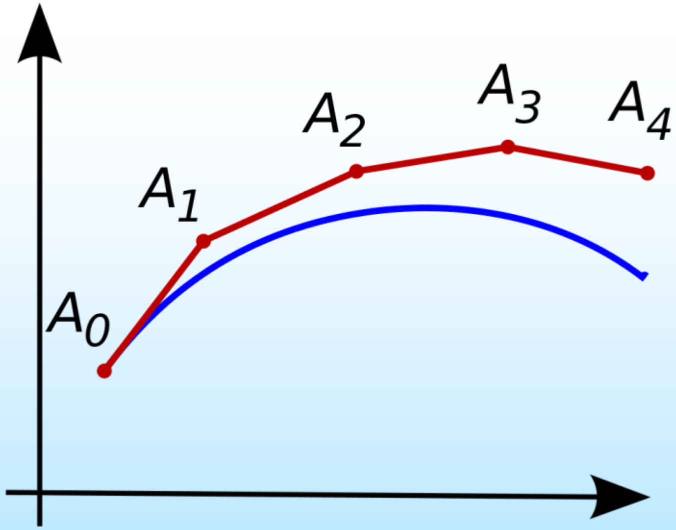
$$\frac{dC}{dt} = -\nabla \cdot (\vec{u}C)$$ - eulerian equation

$$\frac{d\vec{x}}{dt} = \vec{u}$$ Equivivalent lagrangian trajectory equation

Euler 1st order numerical method:

$$\frac{x(t_0+\Delta t) - x(t_0)}{\Delta t} = u(t_0)$$

$$x(t_0+\Delta t) = x(t_0) + u(t_0)\Delta t$$



Derivation:

$$x(t) = x(t_0) + x'(t_0)\Delta t + \frac{1}{2}x''(t_0)\Delta t^2 + \ldots$$ Taylor expansion

Diffusion modelling

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

1D diffusion equation

$$\frac{\partial p}{\partial t} = D\frac{\partial^2 p}{\partial x^2}$$

1D Fokker-Plank equation for the probability distribution

$$dx = \sqrt{2D}dW$$

-stochastic process equivalent to the Fokker-Plank equation

W -Wiener process

$$\Delta x = x(t+\Delta t) - x(t) = R\sqrt{2D\Delta t}$$

-numerical algorithm of random walk

$R = N(0,1)$ -normally distributed random number with zero mean and unit standard deviation

Particles phase transformations (reaction)

- Adsorption-desorption
- Decay
- Chemical reaction
- Boundary conditions
- …..

Solving the Kolmogorov equation

$$\frac{dC_i}{dt} = \sum_{j=1}^{n} \alpha_{ij} C_j \quad \Longrightarrow \quad \frac{dp_i}{dt} = \sum_{j=1}^{n} \alpha_{i,j} p_j$$

Kolmogorov equation for probabilities of each possible state:

Let the system be in state i $\Rightarrow p_i(0) = 1, \quad p_j(0) = 0, \quad i \neq j$

$$p_{i,j}(\Delta t) = p_j(\Delta t)$$
$$p_{i,i}(\Delta t) = p_i(\Delta t)$$

-general solution for transition probabilities

$$p_{i,j}(\Delta t) = p_j(\Delta t) = \alpha_{i,j}\Delta t$$
$$p_{i,i}(\Delta t) = p_i(\Delta t) = 1 - \alpha_{i,i}\Delta t$$

Linear numerical scheme

Modelling of decay process using particles

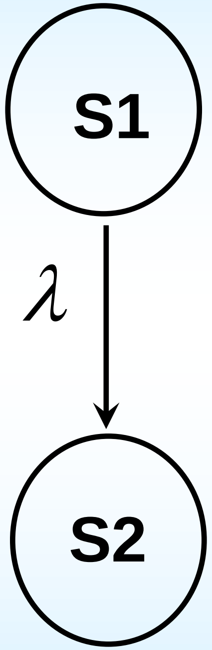
$$\frac{\partial C}{\partial t} = -\lambda C$$

Decay equation

$$\lambda = 0.693 / T_{1/2}$$

$$\begin{cases} \dfrac{\partial p_1}{\partial t} = -\lambda p_1, & p_1(0) = 1 \\ \dfrac{\partial p_2}{\partial t} = \lambda p_1, & p_2(0) = 0 \end{cases}$$

Kolmogorov equation



Graph
of decay

$$p_1(t) = e^{-\lambda t}$$

$$p_2(t) = 1 - e^{-\lambda t}$$

Solution of the Kolmogorov equation

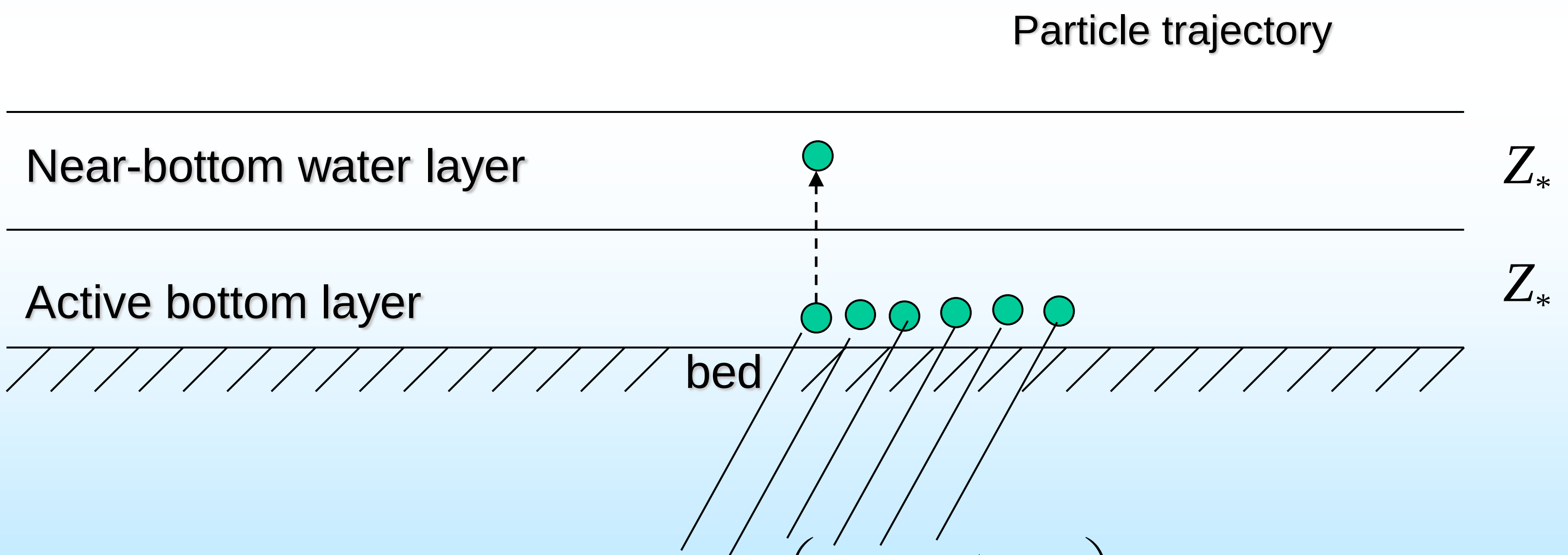
$$p_{1,2} = p_2(\Delta t) = 1 - e^{-\lambda \Delta t}$$

Probability to die during time step

Bottom boundary conditions: Resuspension of particulated particles

$$\begin{cases} \dfrac{\partial C_s}{\partial t} = \dfrac{C_b E}{Z_*} \\ \dfrac{\partial C_b Z_*}{\partial t} = -\dfrac{C_b E}{\rho_s (1-\varepsilon)} \end{cases}$$

$$p = 1 - \exp\left(-\frac{E \Delta t}{\rho (1-\varepsilon) Z_1} \right)$$

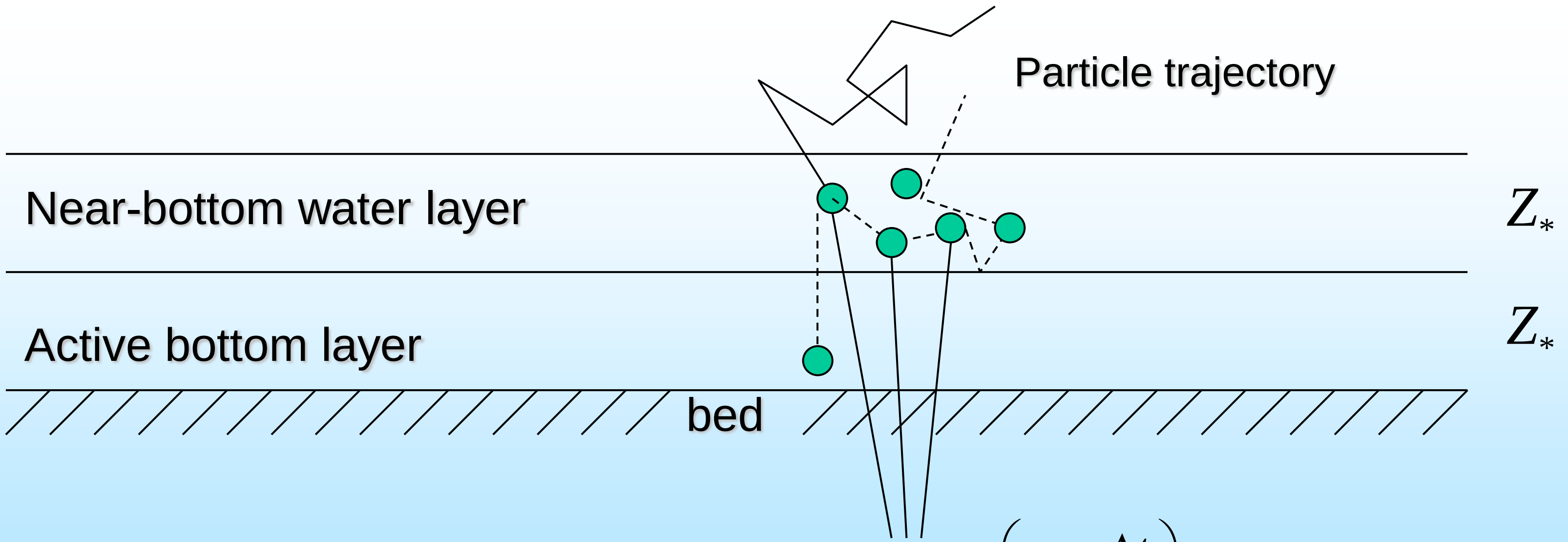


$$p = 1 - \exp\left(-\frac{E \Delta t}{\rho (1-\varepsilon) Z_1} \right)$$

Settling algorithm

$$\frac{\partial C_w}{\partial t} = -\frac{w_s C_w}{Z_*} \quad \Rightarrow \quad p = 1 - \exp\left(-\frac{w_s \Delta t}{Z_1}\right)$$

probability of settling



$$p = 1 - \exp\left(-\frac{w_s \Delta t}{Z_1}\right)$$

Oil transport and fate model OILTOX

OILTOX is Lagrangian model to simulate oil transport and fate in four interacted phases:
oil-on-surface, oil-in-water, oil-on-bottom, oil-at-shoreline

Model numerical features

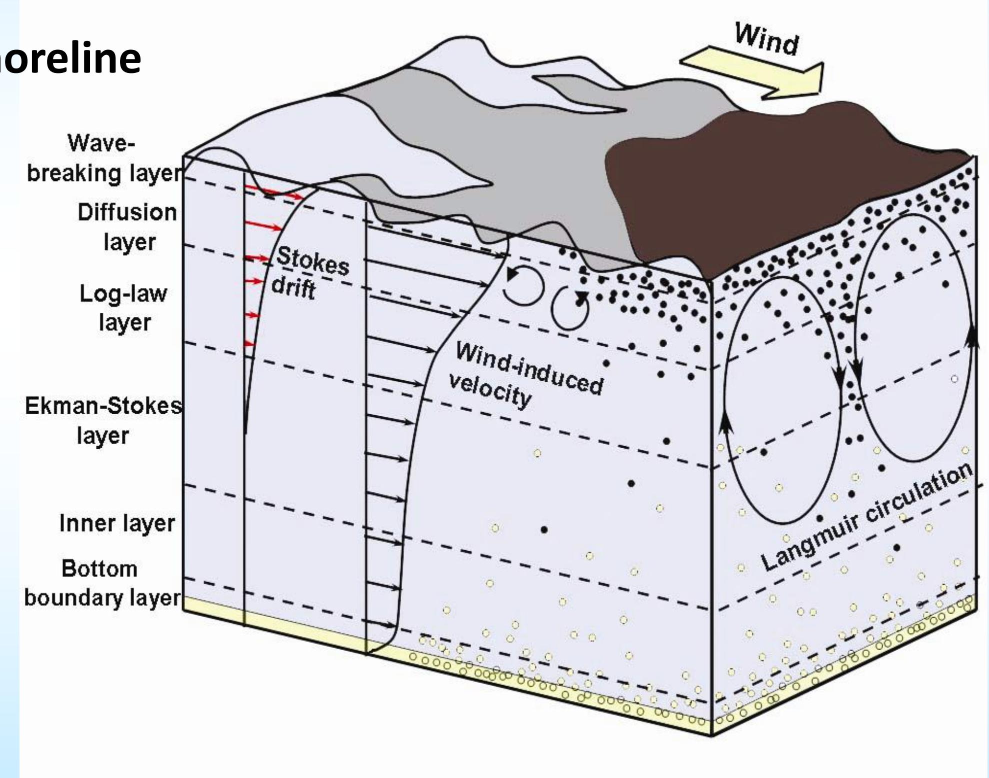
-Lagrangian algorithm for particle tracking
-3D Random Walk method for turbulent diffusion of oil droplets
-2D SPH method for solving shallow water equation for the gravitational spreading of surface oil slick
-Solves Kolmogorov equation for the probability of particle evaporation

Transport processes

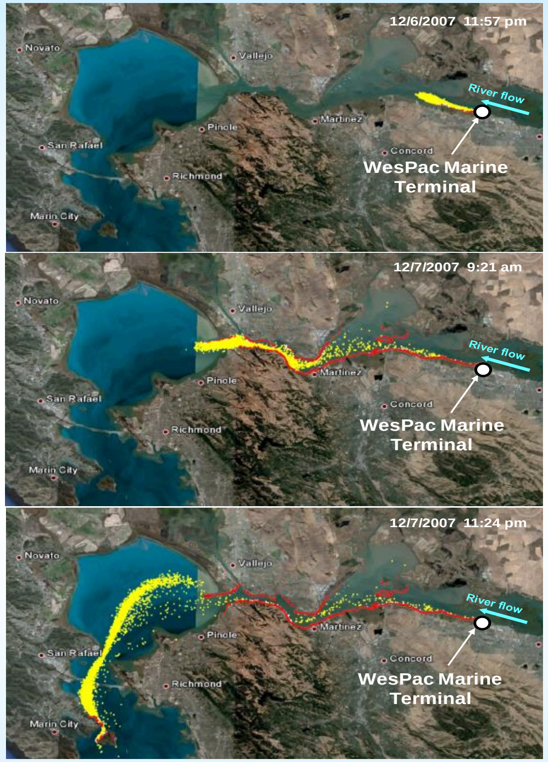
- Spreading
- Advection
- Horizontal and vertical turbulent dispersion
- Oil-shore interaction

Weathering processes

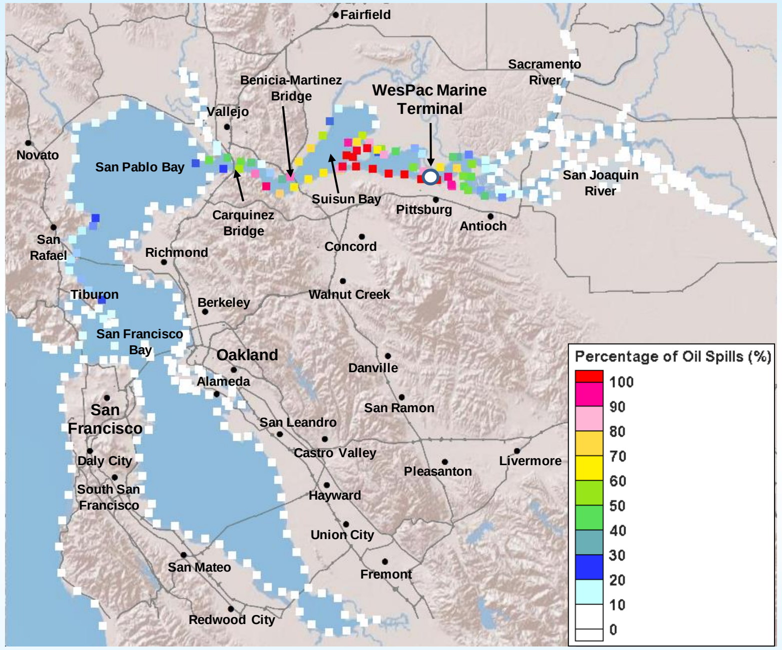
- Evaporation
- Entrainment in water
- Emulsification
- Dissolution
- Sedimentation



Oil Spill Analysis WesPac Pittsburg Energy Infrastructure (San-Francisco bay)

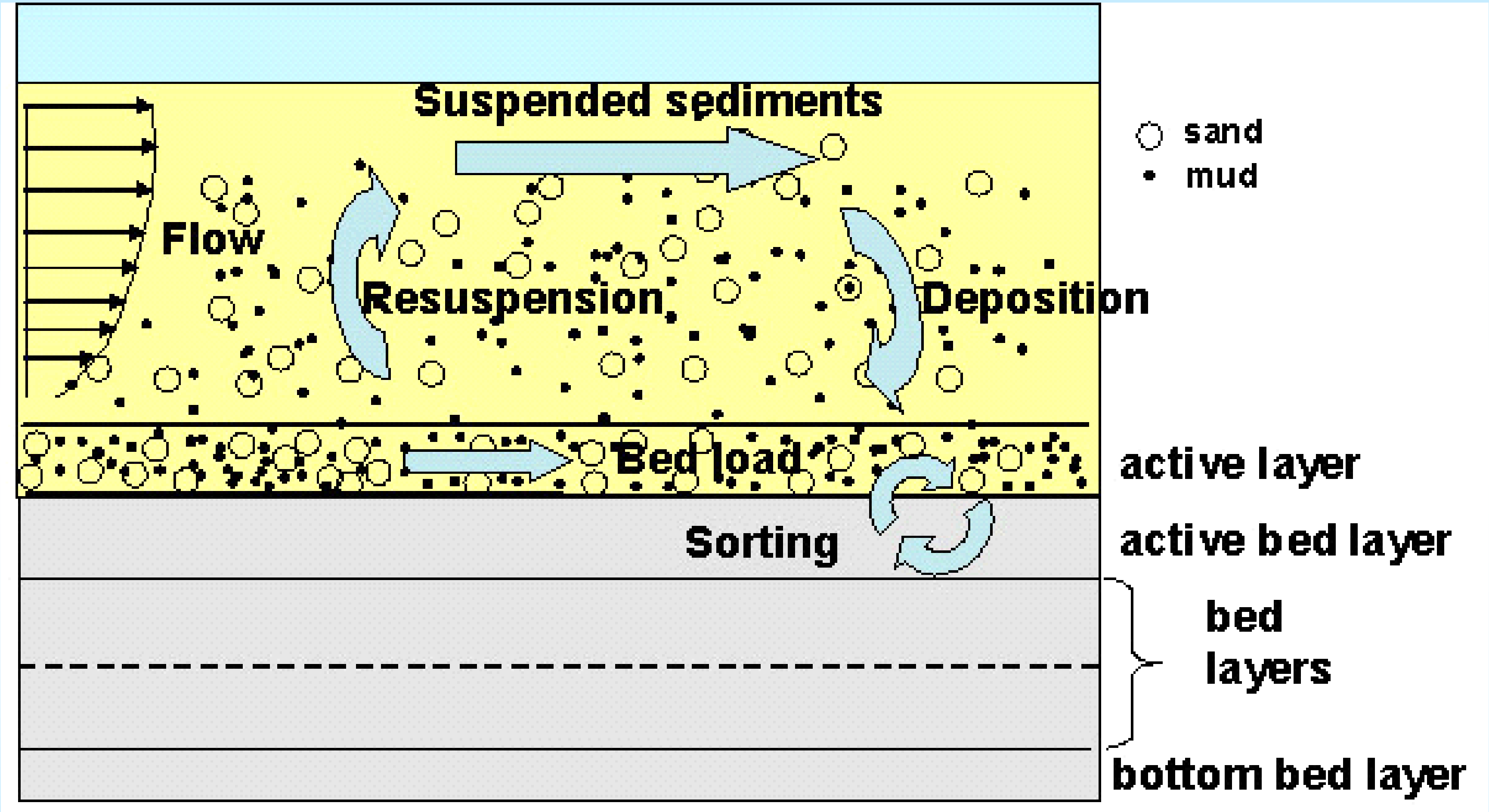


Example spill trajectory for a winter OILTOX simulation at three different times

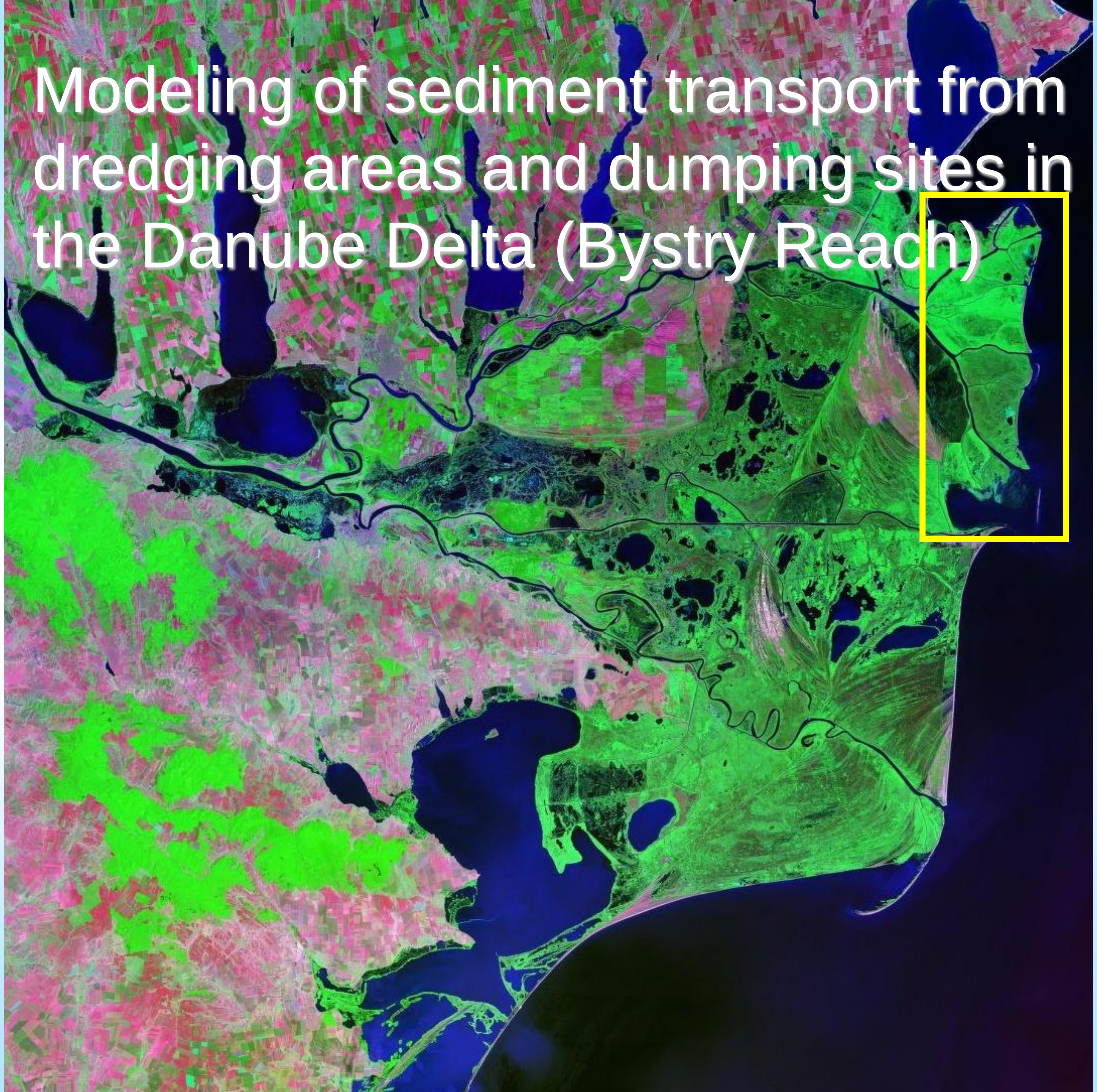


For each of the 12 modeling scenarios, 100 individual oil spills occurring during winter and 100 individual oil spills occurring during summer were simulated with the OILTOX model, for a total of 2,400 oil spill modeling runs

Sediment transport modelling



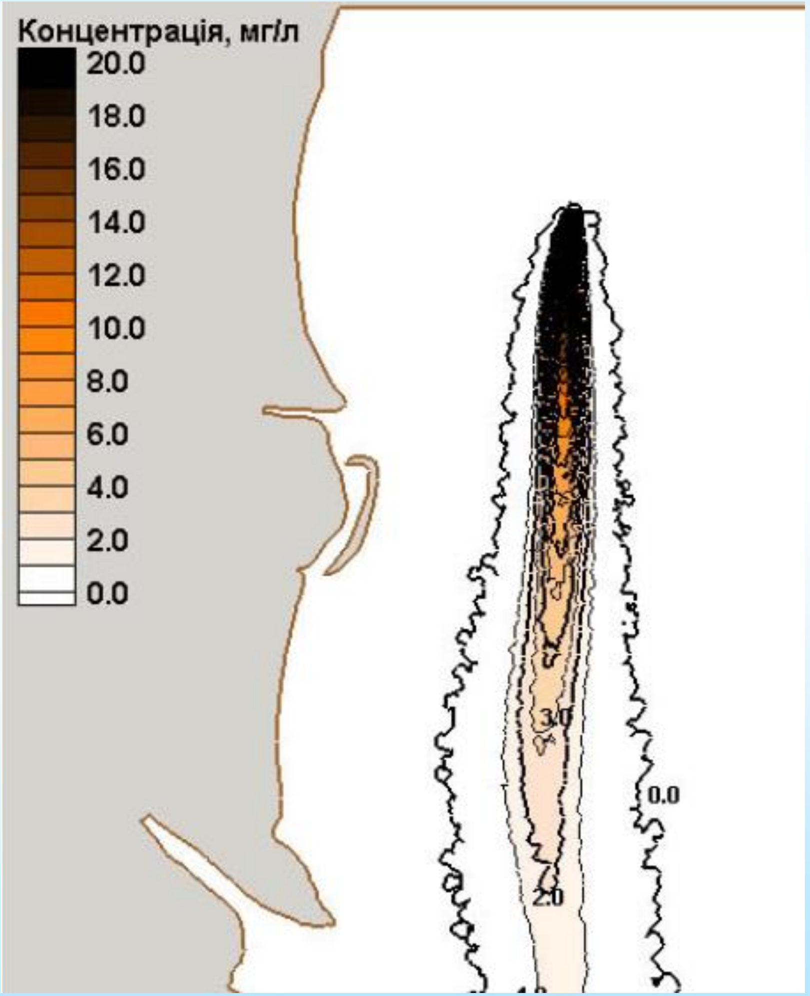
Modeling of sediment transport from dredging areas and dumping sites in the Danube Delta (Bystry Reach)

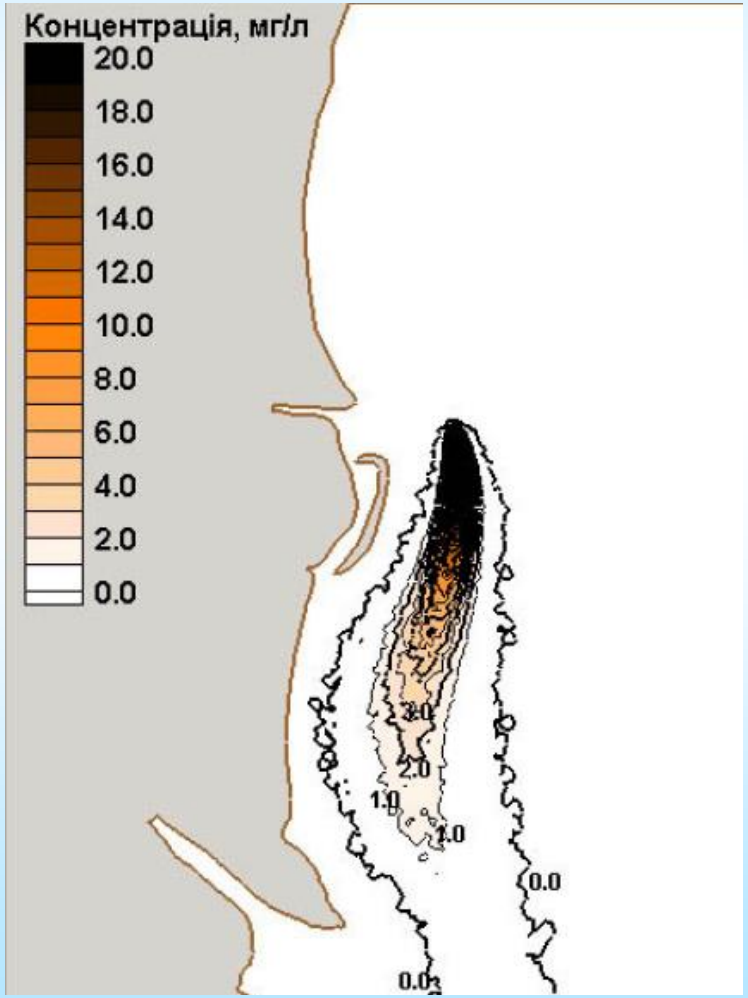


Sediment transport from dredging area in the Danube delta

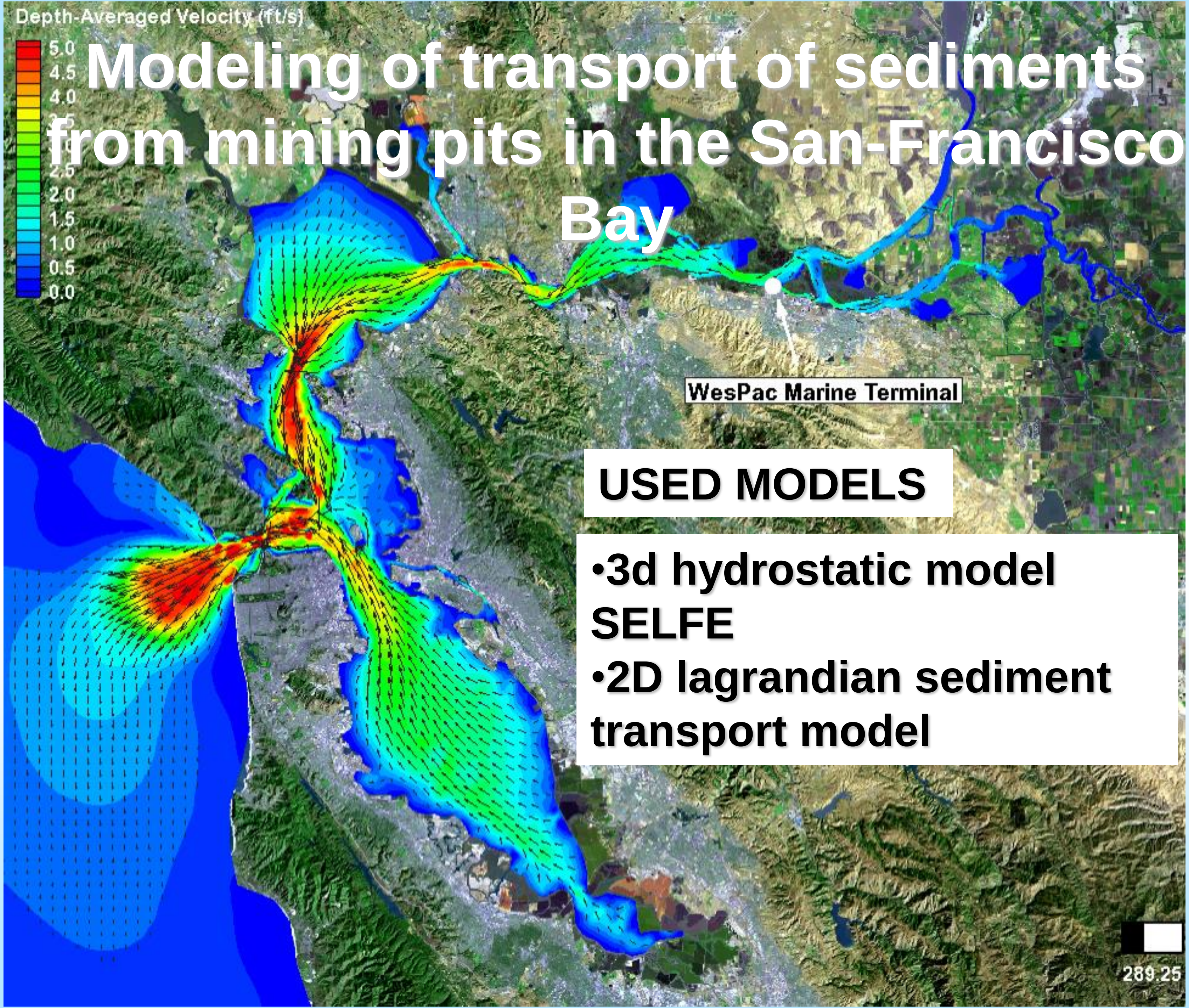
sand fraction **mud fraction**

Modelling allows to optimize place and intensity of dumping to satisfy restrictions on the transboundary transport of sediments





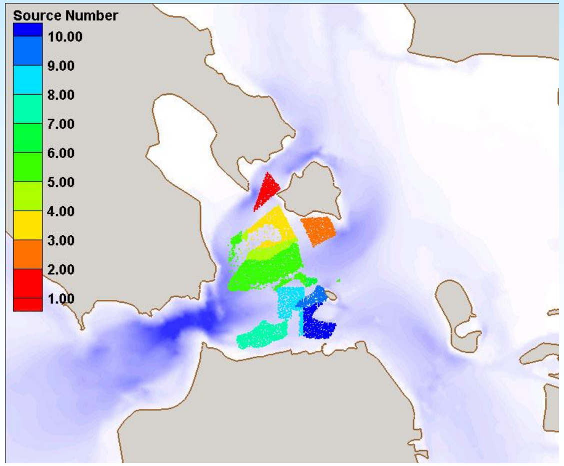
Modeling of transport of sediments from mining pits in the San-Francisco Bay

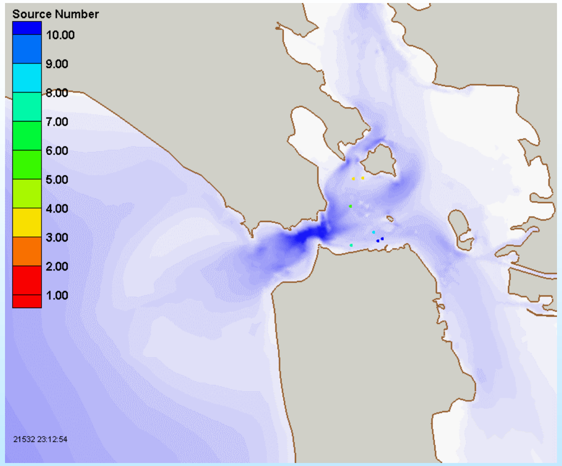


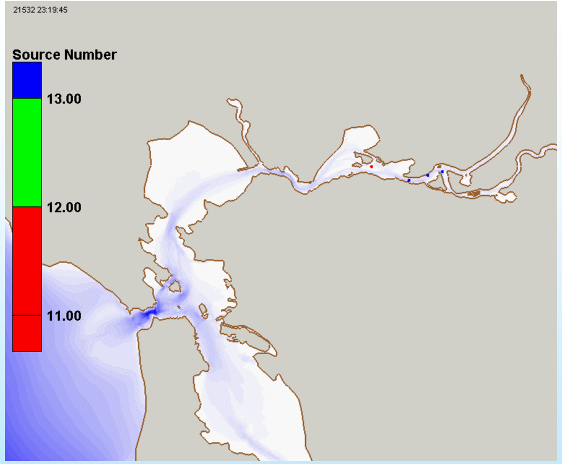
USED MODELS

- **3d hydrostatic model SELFE**
- **2D lagrandian sediment transport model**

Modeling of transport of sediments from sand mining pits in the San-Francisco Bay

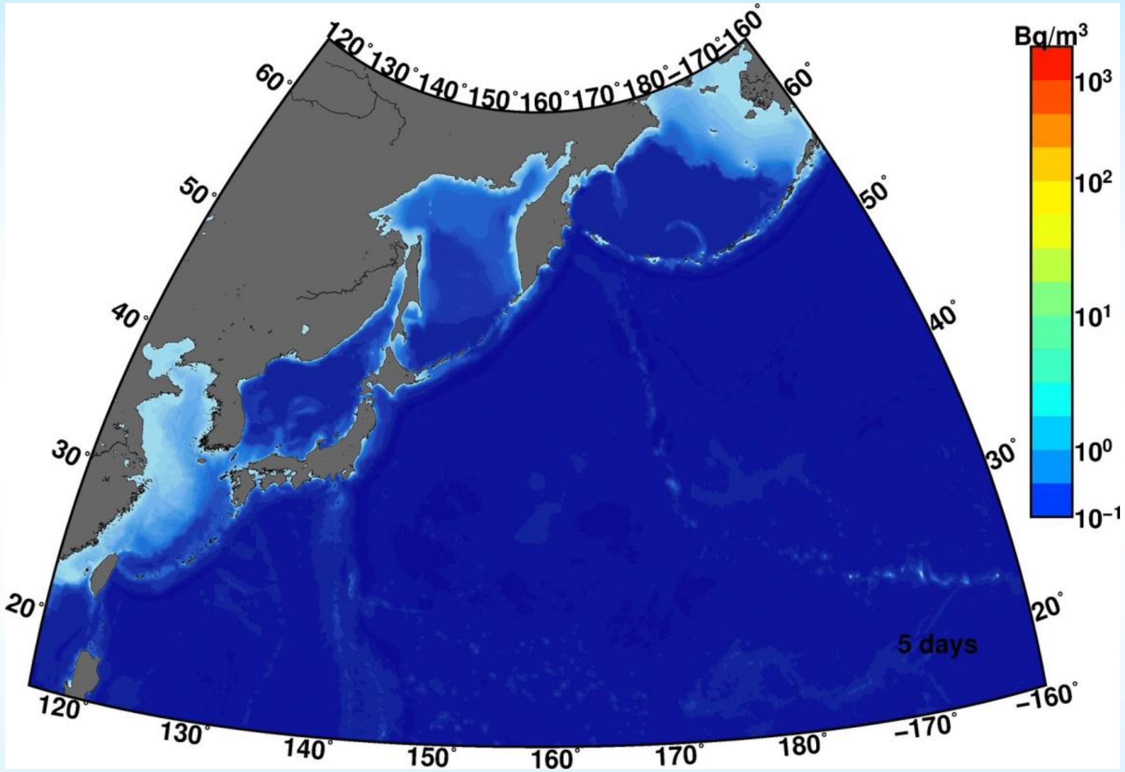






Colored particles originate from different mining areas

Large scale lagrangian modelling of ^{137}Cs concentration after the Fukushima accident



3D lagrangian random walk algorithm
Radioactive decay
Atmospheric deposition and direct release of 137Cs
Parallel algorithm, 300M particles

Conclusions

- Lagrangian methods is powerful tool to analyse the output of ocean circulation models
- A generalized probabilistic approach was developed to simulate transitions of particles between different states (e.g. radioactive decay, adsorption. Interaction with surface or bottom, droplets breakup)
- Lagrangian models of oil spill transport, sediments and radionuclide transport were developed verified and applied for a number of problems