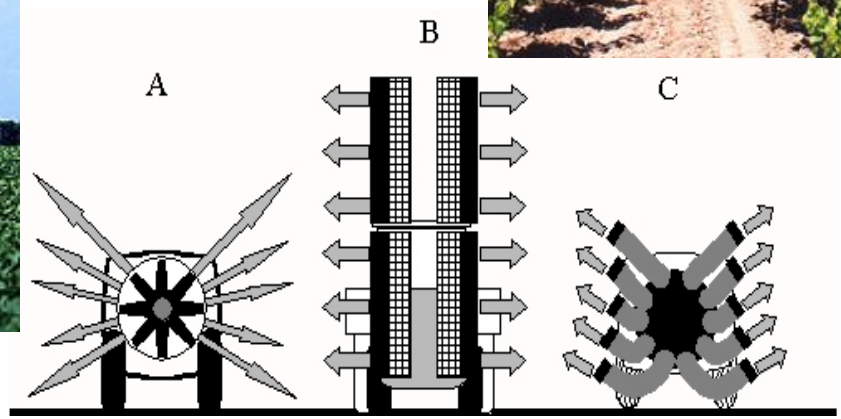
Low-complexity transport models

for environmental studies

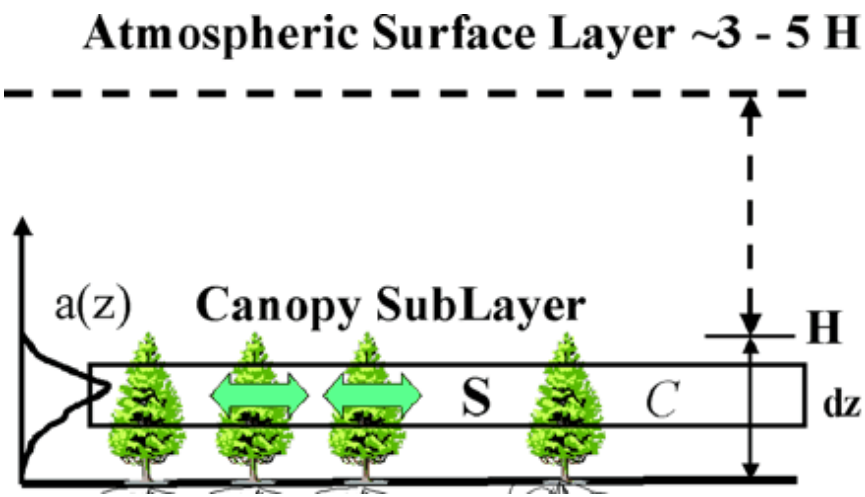
Some applications

- Risk analysis
- Optimize treatments wrt. weather conditions
- Optimize measurement devices location
- Complete partial measurements
- Aid to decision for topography modifications
- Identification of sources of observed pollution

Some devices



Experimental studies



Ingredients

- Multi-level modelling: local (row level), semi-local (vineyard), global (water-capture basin)

  Aim: define an adequate solution space for each level
- Ground level and weather conditions assimilation
- Mesh free approach
- Point-based information : no need for global solution calculation
- LCM solutions need be solution of direct model (DM): divergence free wind, conservation, linearity of transport, positive solution,…

Background

- h-methods (FE, FV, FD,…) : low regularity for functional search space, needs mesh adaptation.
- p-methods (spectral, …) : high accuracy, need definition of the ‘spectral’ search space, difficult visualization.

In these approaches, no a priori information is introduced on the solution.

- Reduced order methods (Modal, POD, LCM,…) : adapt the search space or consider a reduced complexity model easier to solve.

LCM

Consider a dependency chain :

$$p,\ U(p),\ J(U(p))$$

Reduced dependency :

$$p,\ u(p),\ J(u(p))$$

$u(p)$ either by LCM or from projection on $S(W_N)$

N small, where W_N from snapshots of $U(p)$ or LCM

See also incomplete sensitivity

Data assimilation & Modelling

Simulation model parameters obtained minimizing

$$J(p)=\| u(p) - u_{obs} \| + \| c(p,u(p)) - c_{obs} \|$$

c_{obs} and u_{obs} not observed at the same points.

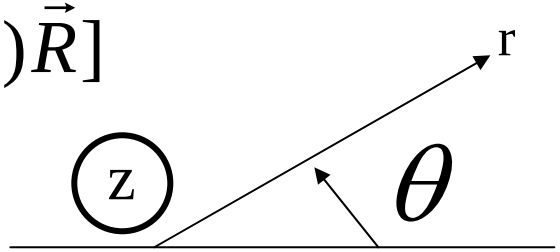
Modelling 'near-field'

Reducing the solution space

- Near-field in a radial local frame, z in the direction of treatment

$$u_{loc} = f_1(r)g_1(\theta)[h_1(z)\vec{z} + (1 - h_1(z))\vec{R}]$$

$$c_{loc} = f_2(r)g_2(\theta)h_2(z)$$



f_i : by assimilation of experimental data after rows

g_i : characteristics of injection devices (observed)

h_i : characteristics of vegetation (h_1 *in [-1,1]* odd positive monotonic increasing, h_2Gaussian distribution)

+ include constraint from direct model

Modelling ‘near-field’

Constraint from governing equations

$$\nabla . u_{loc} = 0$$

$$\nabla . (c_{loc} u_{loc}) = 0$$

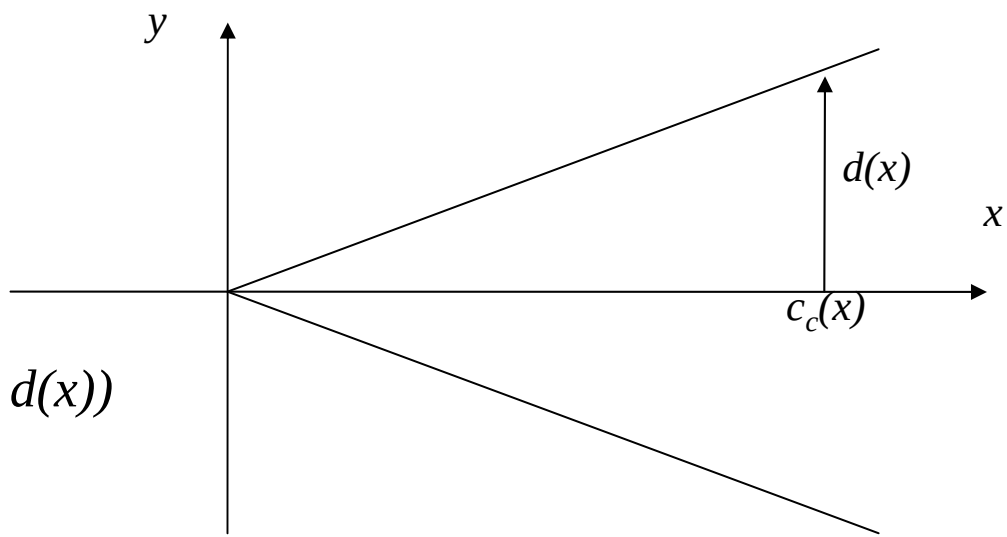
$$\int_{R^3} c_{loc} = given$$

- Linearity of transport equation
- Accumulation in time
- Evaluate *c+ = c max(0,Uz)* for transport over large distances

Modelling : ‘transport over large distances’

- Wind & topography assimilation by ‘compatible & incremental’ interpolation (divergence free wind …)
- Inlet condition c^+ provided by previous ‘local’ model
- Use transport solution in Euclidean *(x,y)* frame in a non symmetric geometry based on transport time
- No characteristics evaluation
- Mesh free calculation
- Point to point solution without global calculation

Transport in Euclidean *(x,y)* frame by a uniform flow



$$c(x,y) = c_c(x)\, f(y\,,\, d(x))$$

with

$$c_c(x) \sim \exp\,(\,-\,a(U_{inj})\,x\,)$$

$$f(\,y\,,\,d(x)\,) \sim \exp\,(\,-\,b(U_{inj}\,,\,d(x))\,y^2)$$

a(.) positive monotonic decreasing function

b(.,.) positive, monotonic increasing in U_{inj} and decreasing in *d*

Distance

Symmetric geometry

$$d(A,B) \geq 0$$

$$d(A,B) = d(B,A)$$

$$d(A,B) = 0 \Leftrightarrow A = B$$

$$d(A,B) \leq d(A,C) + d(C,B)$$

Non symmetric geometry

In symmetric geometry : *d(A,B)= d(B,A)*

but not necessarily uniform and isotropic

$$d(A,B) = \int_0^1 \left(AB\, {}^t M\, (A + tAB)\, AB \right)^{1/2} dt$$

M = I in Euclidean geometry

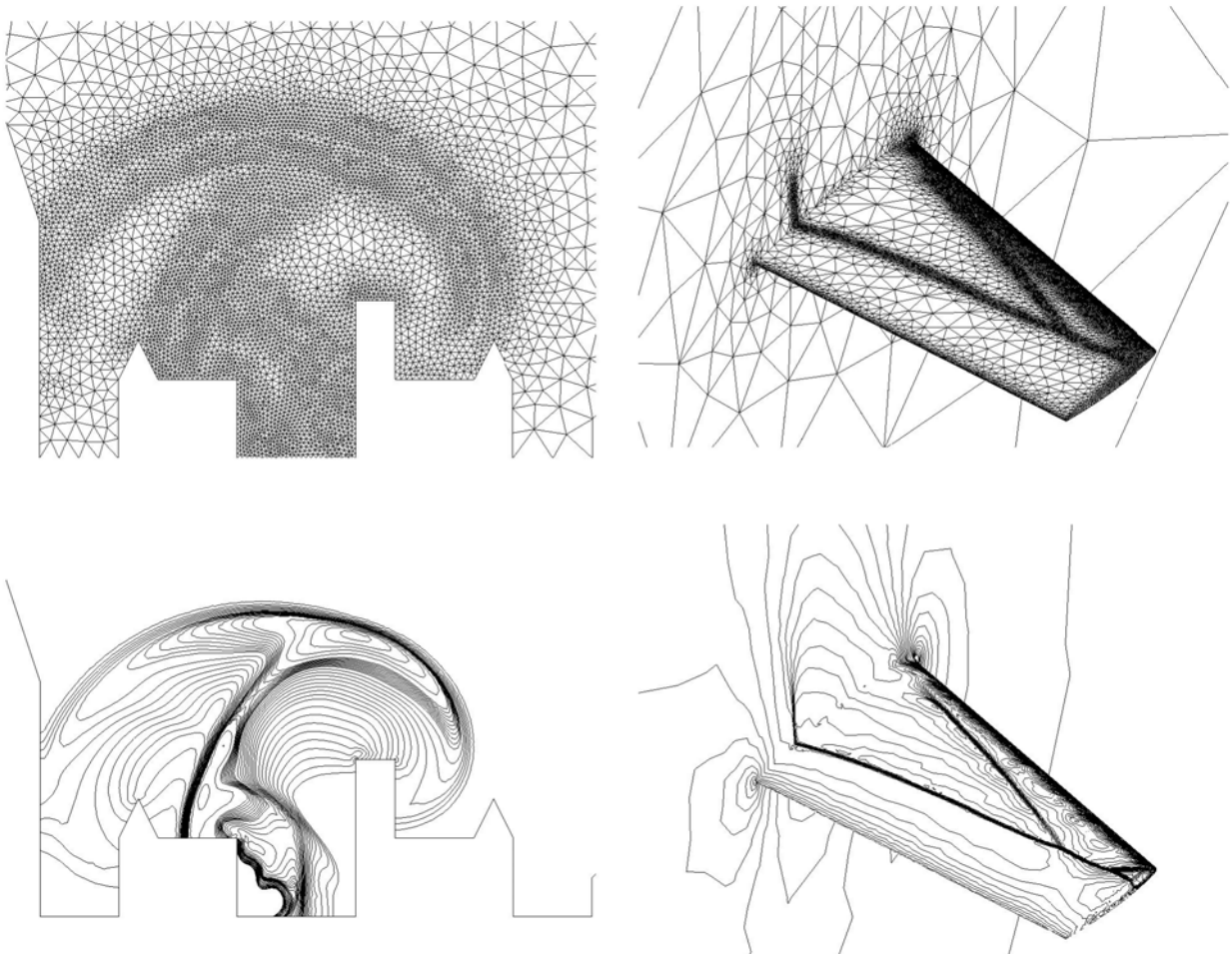
M variable in space in Riemanian geometry, including anisotropy

(unit spheres are ellipsoids)

Widely used in mesh adaptation (INRIA).

Also in '*travel time based*' maps.

Application of Riemanian metric in Delaunay mesh adaptation for time dependent and steady flows



Transport-based non-symmetric geometry

$$d(A,B) \neq d(B,A)$$

Example : d based on the migration time = min (T_{adv} , T_{diff})
If A is upstream wrt B then T_{adv} (B,A)=infinite

$$d(A,B) = T = \int_{A}^{B^{\perp}} ds / u$$

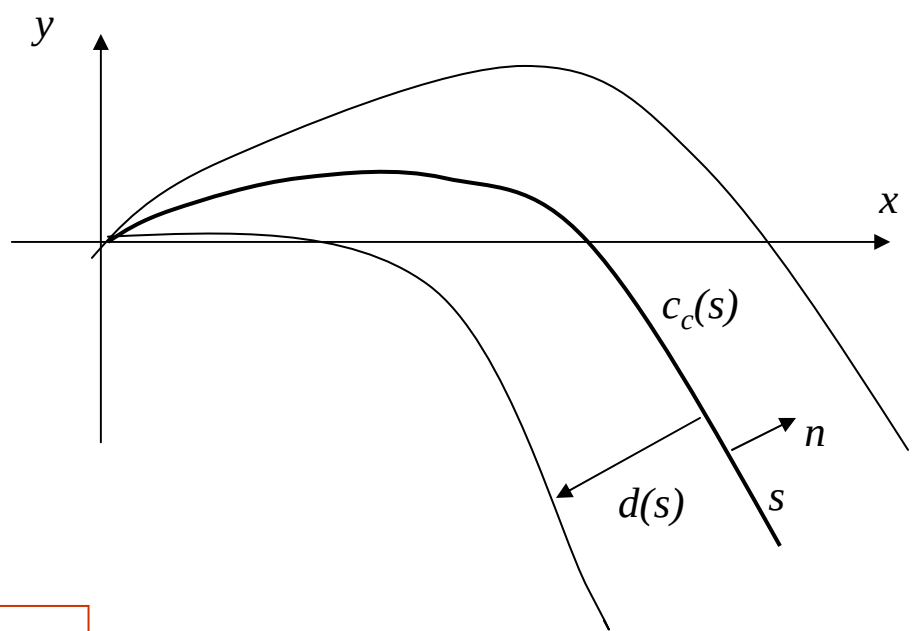
along 'the' characteristic passing by *A*
(no source or sink)

In practice : build the distance on a coarse background mesh compatible with wind information (once for all) and use interpolation.

Transport solution written in a transport-based frame

$$c(x,y) = c_c(s)\, f(n\ ,\ d(s))$$

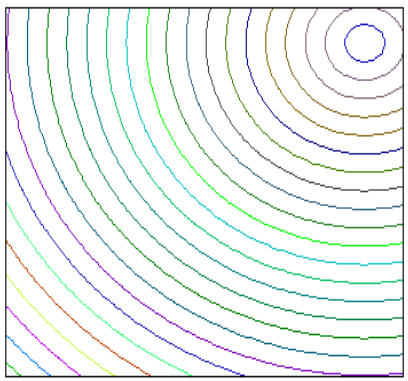
(s,n) local coordinate along the characteristic

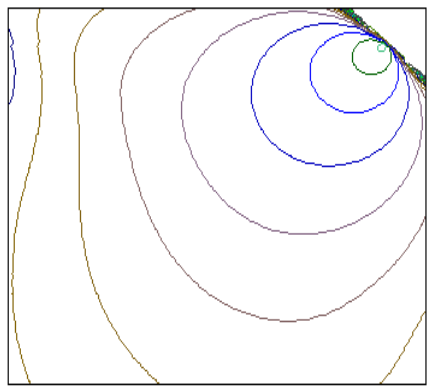


Calculation becomes point to point : no need for global solution of transport equation to find the solution in one point.

Example of transport-based distance

Euclidean distance



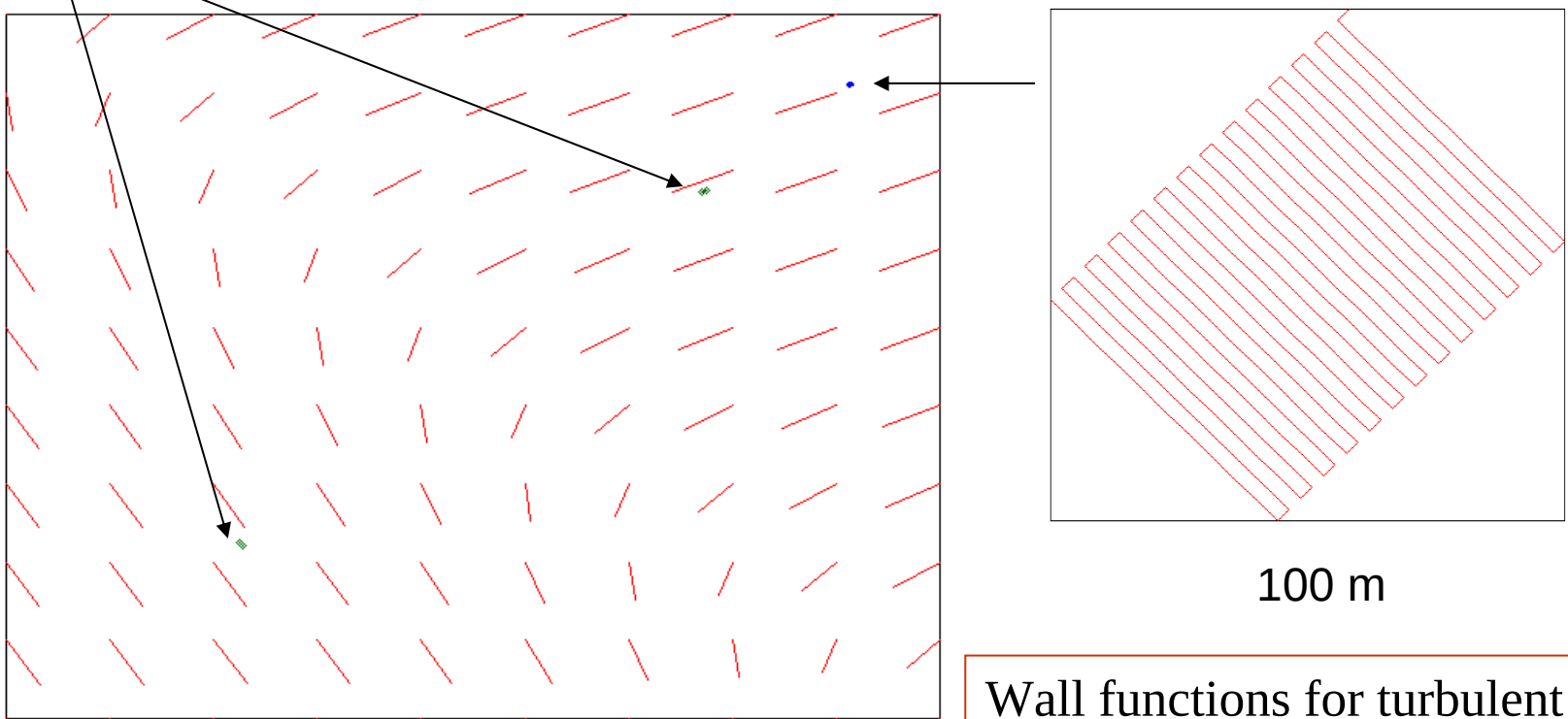


Travel time based distance

Example of simulation configuration

Wind measurement locations

Vineyard and source trajectory



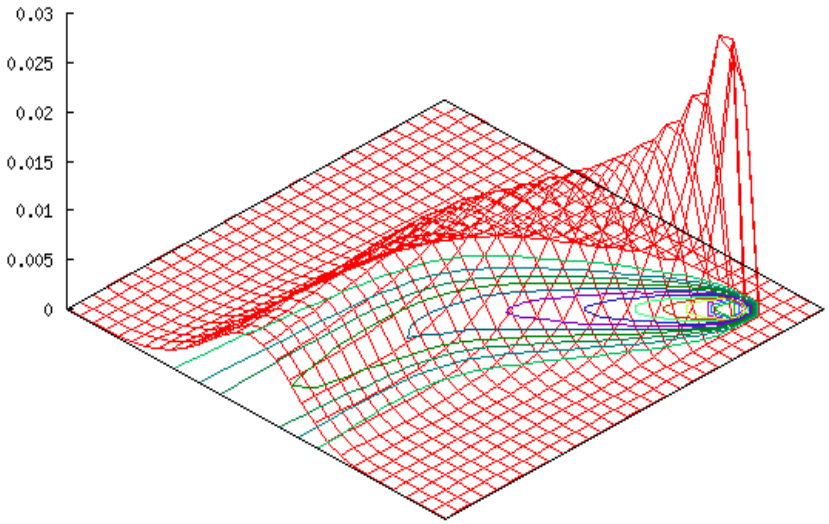
20 km

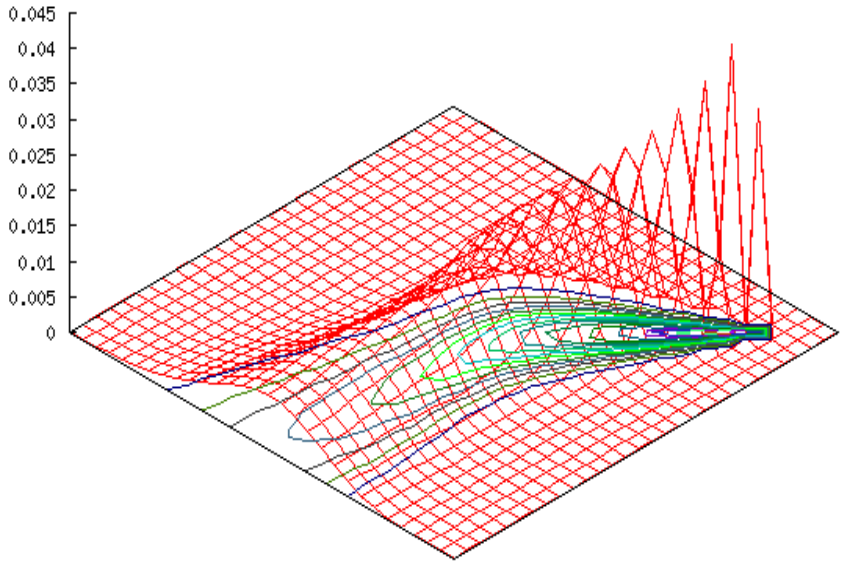
100 m

Wall functions for turbulent flows for extension in z:

$$u+=f(z+)$$

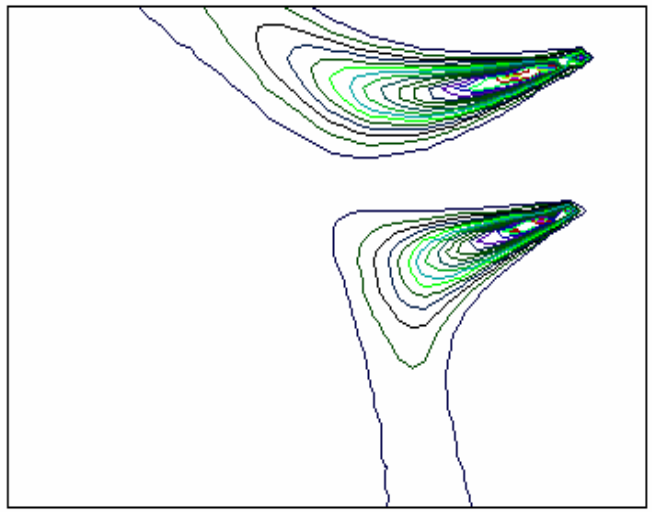
Simulation in transport-based metric vs. governing equations



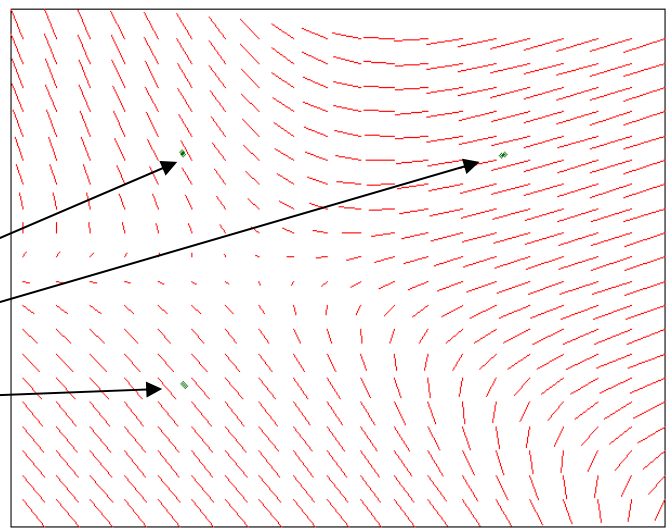


Multi-source configurations

Linearity of transport



3 pts wind measurements

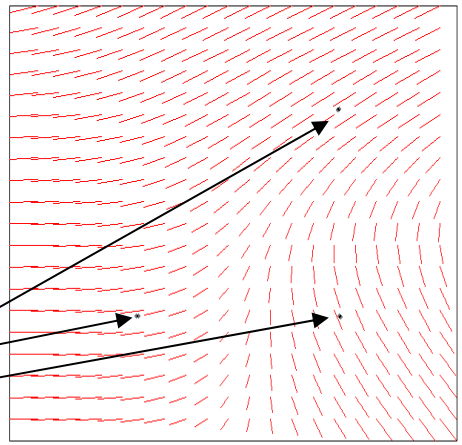


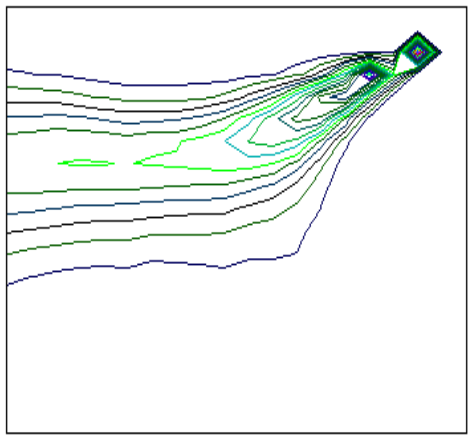
Some interesting features :

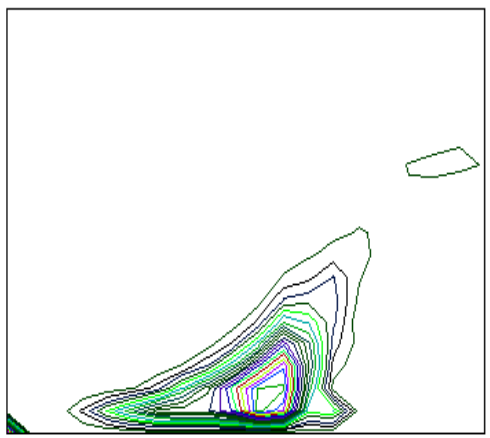
- Sensitivity analysis
- Source identification

Sensitivity evaluation & source identification

3 pts wind measurements





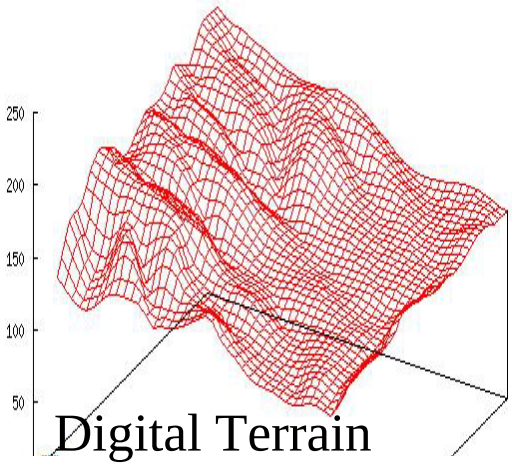


Sensitivity analysis

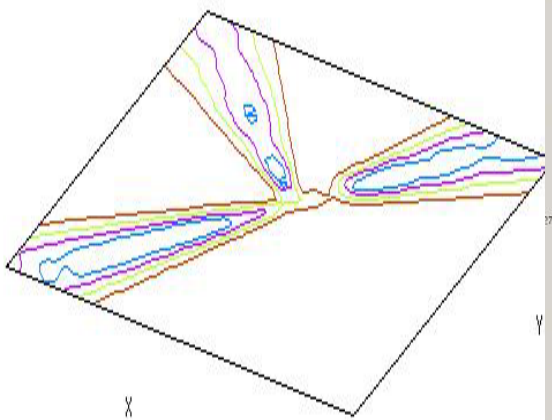
$J(p) = (c(p,u(p)) - c_{obs})^2$

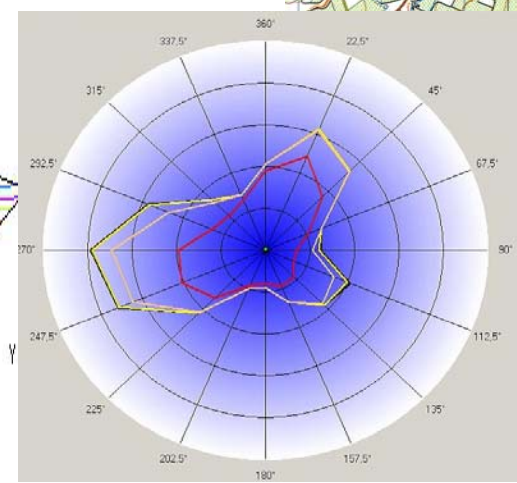
Risk evaluation and localizing measurement devices

- Aim : define where to measure pesticides in air & identify possible pollution sources
- Drass, Cemagref, Air LR, chambre d'agriculture



Digital Terrain Model (MNT)





Minimization problem :

$$\min_x J(x,q,U), \quad F(x,q,U)=0, \quad x \in \mathcal{O} \subset \mathbf{R}^n$$

$$x \to q(x) \to U(q(x)) \to J(x,q(x),U(q(x))).$$

Minimization algorithm : $x^{n+1} = x^n - \rho \frac{dJ}{dx^n}$.

Gradient : $\frac{dJ}{dx} = \frac{\partial J}{\partial x} + \frac{\partial J}{\partial q}\frac{\partial q}{\partial x} + \frac{\partial J}{\partial U}\frac{\partial U}{\partial q}\frac{\partial q}{\partial x}$.

Adjoint Method : v solution of : $v^T(\frac{\partial F}{\partial U}) = \frac{\partial J}{\partial U}$.

$$\frac{dJ}{dx} = \frac{\partial J}{\partial x} + \frac{\partial J}{\partial q}\frac{\partial q}{\partial x} + v^T\frac{\partial F}{\partial x}.$$

- **Use automatic differentiation for adjoint code derivation from the LCM solver.**
- **Application to source identification, data assimilation,…**
- **Use the LCM for sensitivity evaluation for the direct model.**

Sensitivity evaluation

- Low-complexity sensitivity and incomplete gradients:
  - gradient modeling (as for the state)
  - $\tilde{J}'(n, h, x) \rightarrow J'(\infty, 0, x) = J'(x)$ incomplete evaluation
  - Projection operator in admissible space for regularity control, preconditionning, smoothing
- Incomplete linesearch. Rotation and smoothing operator on the admissible unit sphere

Incomplete sensitivity and low-complexity models

From:

$$x \to q(x) \to U(q(x)) \to J(x, q(x), U(q(x))).$$

To:

$$x \to q(x) \to \tilde{U}(q(x))(\frac{U}{\tilde{U}}),$$

where $\tilde{U} \sim U$ is obtained using a simple model.

Incomplete sensitivity can be improved by:

$$\frac{dJ}{dx} \sim \frac{\partial J(U)}{\partial x} + \frac{\partial J(U)}{\partial q}\frac{\partial q}{\partial x} + \frac{\partial J(U)}{\partial U}\frac{\partial \tilde{U}}{\partial q}\frac{\partial q}{\partial x}\frac{U}{\tilde{U}}.$$

$\tilde{U}$ never used, only $\partial \tilde{U}/\partial q$.

Low-complexity model needs to be only locally valid.

Example of a low-complexity model

Suppose $U = \log(1+x)$ and $J = U^2$

$J' = 2UU' = 2\log(1+x)/(1+x)$

$\sim 2\log(1+x)(1-x+x^2...)$

Consider $\tilde{U} = x$ valid around $x = 0$

$J' \sim 2U\tilde{U}' = 2\log(1+x)$

On the other hand, after normalizing

$J' \sim 2U\tilde{U}'(U/\tilde{U})$

$= 2\log(1+x)(\log(1+x)/x)$

$\sim 2\log(1+x)(1-x/2+x^2/3...)$

which is a better approximation of the gradient.

Summary

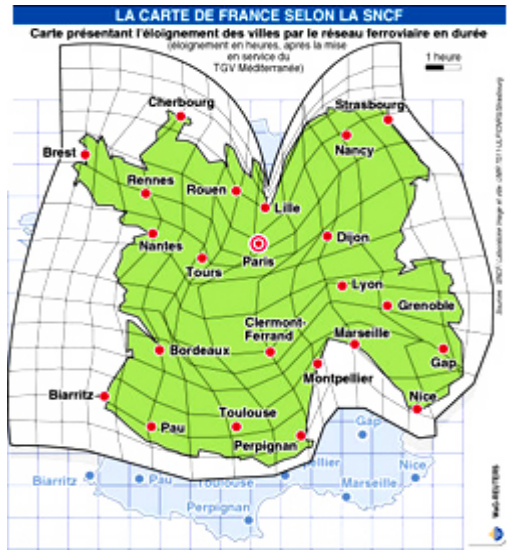
- Low-complexity multi-level modelling
- Data assimilation for wind conditions and topography by ‘compatible’ interpolation
- Model parameters definition by data assimilation
- Similarity solution of transport in non symmetric transport time based geometry

Ingredients…

- Low-complexity models (LCM) in sensitivity evaluation: risk analysis & source identification
- Statistical deviation analysis for wind and topography characteristics & other parameters
- LCM evaluation (less than 1 second) for Monte Carlo analysis
- LCM solutions need be solution of direct model (DM): divergence free wind, conservation, linearity of transport, positive solution,…
- Dissociate the analysis of the flow field and dispersion
- Remove the difficulty of atmospheric turbulence modelling

MODELE :

- Modèle à complexité réduite, de la dispersion et de la dérive des pesticides en cours de développement au Cemagref (DRIFTX).
- Principes :
  - Multi-échelle.
  - Assimilation des données.
  - Utilisation de la méthode des caractéristiques avec un géométrie basée sur les temps de migration prenant en compte topo et météo.
- Avantage : le problème inverse est peu coûteux en temps de calcul.



Exemple de géométrie basée sur les temps de parcours SNCF. Contraction des distances réelles.

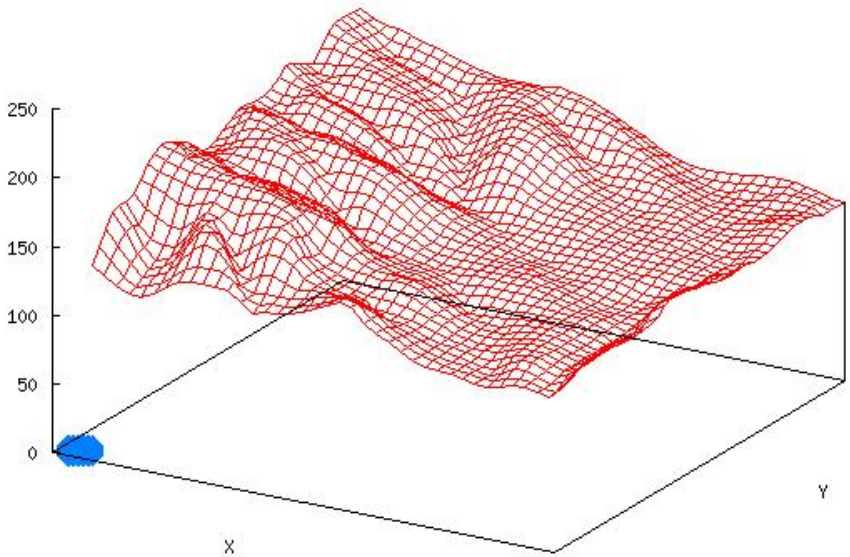
PROBLEME

- Etude conduite avec les principaux acteurs du domaine (SRPV/DRAF, DIREN, Cémagref, Air LR, Drass, chambre régionale d'agriculture) :
  - Estimer l'exposition de la population aux pesticides dans l'air, en procédant à des mesures de pesticides dans l'air. Prélèvement sur 4 sites représentatifs :
    - Claret/Pic St Loup,
    - St Gély,
    - Grabels/Mas de Piquet,
    - Montpellier/Cévennes
- But : déterminer les secteurs dans lesquels seront réalisées les enquêtes en délimitant les zones d'étude autour des quatre sites de mesures :
  - identification des zones sources de pollution / localisation des zones à risques : application du problème inverse

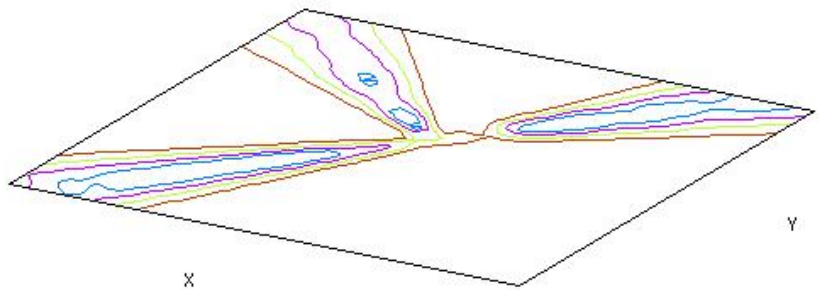
EXEMPLE/APPLICATION

- Site d'étude : St Gély
- Données météo et topo
  - Sélection d’un rayon d'action de 2km autour du site de prélèvements, mesures topo : une vingtaine de points représentatifs de la topographie, coordonnées en (x,y,z) sous forme de fichier MNT.
  - Sélection des directions de vents dominants (deux à trois configurations les plus probables), pondérés par leur amplitude. Météo assimilée à celle des Cévennes :
    - Vent de sud-sud-ouest (le Garbi dans la région de Montpellier)
    - Vent de nord-est (le Mistral)
    - Vent du sud-sud-est (marin)

RESULTATS NUMERIQUES



Données topographiques MNT correspondant au site de St Gély du Fesc. La zone représente un carré de 2km centrée sur le sit de prélèvement.



Représentation des isovaleurs signifiant la provenance des polluants pour les 3 configurations de vent dominant sélectionnées :

Vent de N-E à 7 m/s
Vent de S-S-O à 5 m/s
Vent de S-S-E à 2 m/s

Le Nord est orienté suivant l'axe Y.

EN COURS (Perspectives)

- Echantillonner angles de la rose des vents (rq : vent est constant et la topo plane, alors les isovaleurs sont des cercles)
- Superposition des résultats avec scan IGN
- Élargissement zone autour sites de mesure (de 2km à 5km)