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ÉCOLE DOCTORALE 162

Inverse modelling for source characterization in complex industrial sites: Development of the adjoint state method applied to a Lagrangian stochastic dispersion model

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H22-065
June 13th, 2024

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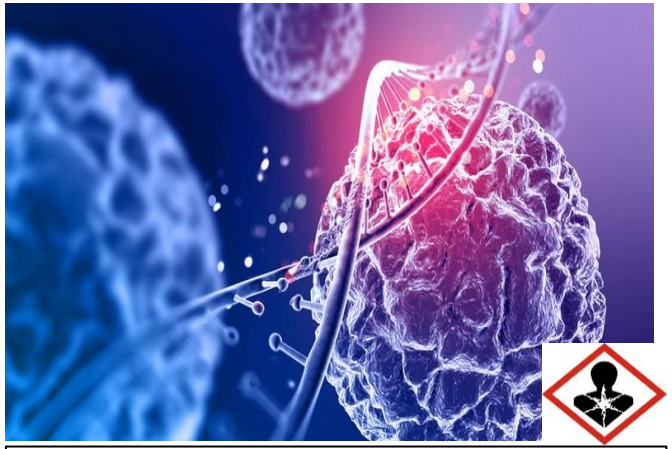
INTRODUCTION

ATMOSPHERIC POLLUTION

- **Health risks (cancers, …)**



Cancer cell

- **Environmental risks (global warming, contamination, …)**

Water pollution contamination with mercury, New Idria, USA, 2004

Nuclear radioactive contamination risk

- **Security risks (flammability, explosion, …)**

Refinery fire, Indonesia, 2021 (©AGUS SIPUR / AFP)

- **Need for atmospheric pollutant source identification & quantification in complex industrial sites**

Real-time constraint
Important for industrial companies !

⇨ To improve on-site safety & to evaluate environmental impact

INTRODUCTION

HOW TO QUANTIFY EMISSIONS ?

- Direct measurements of pollutant in atmosphere

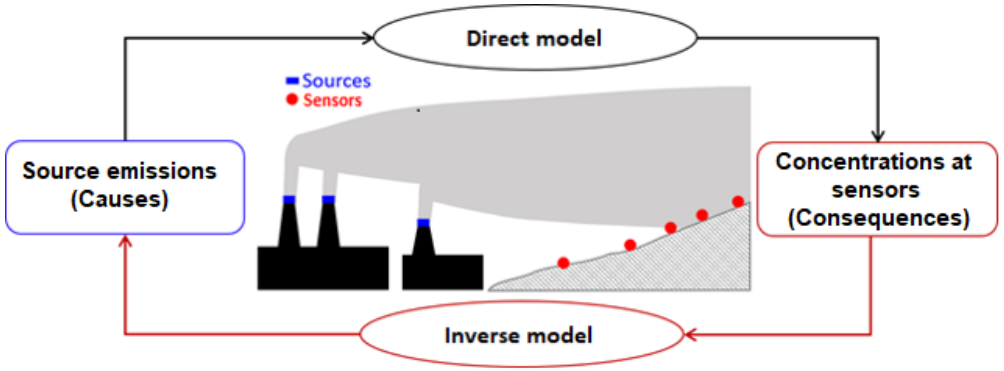
Process: **Source** ⇨ Pollutant transport ⇨ Sensor

Drone AUSEA on a TotalEnergies site (©TotalEnergies)

✗ Leaks & diffuse emissions difficult to characterize, especially in real-time

- **Inverse modelling**: Dispersion prediction & recovery of source characteristics

Process: **Source** ⇦ Pollutant transport ⇦ Sensor



✓ Quality & accuracy of results

- Different approaches exist for inverse modelling:
  - Grid search “brute force” methods (*Ben Salem et al., 2014*)
  - **Minimization problem** (*Gill et al., 1981*)

    Requires cost function Jacobian matrix computation

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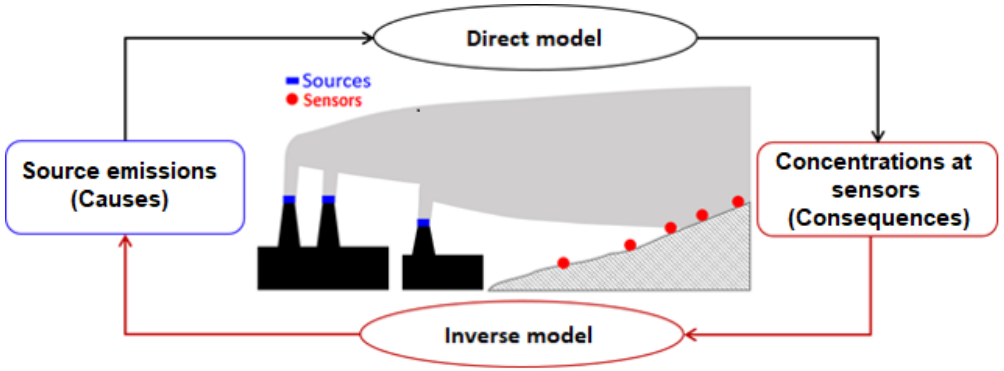

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Time-consuming techniques !
Need to find an alternative:
<u>the adjoint state method</u> (*Chavent, 1974*)

OUTLINE

- Adjoint state method for inverse problem solving
- Application to a Lagrangian stochastic particle dispersion model
- Application results on a numerical test case
- Conclusion

ADJOINT STATE METHOD FOR INVERSE PROBLEM SOLVING
Forward model definition

- **State equation** - generally implicit (*Plessix, 2006*):

$$\underbrace{F_s}_{n_F \times 1}\left(\underbrace{u_s}_{n_u \times 1}, \underbrace{m_s}_{n_m \times 1}\right) = \underbrace{0}_{n_F \times 1}$$

F_s numerical forward model
m_s model parameters
u_s state (output) variable

- If an explicit relationship f_s exists between u_s and m_s, F_s:

$$F_s(u_s, m_s) = u_s - f_s(m_s) = 0$$

- In atmospheric dispersion context:
  - F_s forward transport and dispersion model of pollutants, originating from a source s
  - u_s concentration vector
  - m_s source parameter vector

- m_s: **Source position** $x_s(x_s, y_s, z_s)$ & **flow rate** $q_s \Rightarrow n_m = 4$

ADJOINT STATE METHOD FOR INVERSE PROBLEM SOLVING
Methodology for inverse problem solving

- No explicit analytical inversion of the state equation generally !

- Inverse problem must be considered as a **minimization problem**

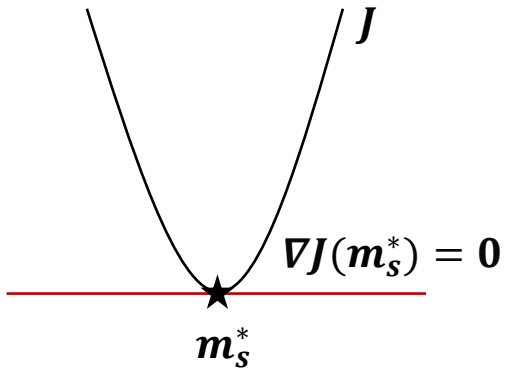
⇨ To minimize the **<u>difference</u>** between **the observation data d** & **the model output data u_s** provided by F_s

1. Define a cost function J depending on model parameters m_s to optimize

$$\underbrace{J}_{1\times 1}\ (\underbrace{m_s}_{n_m\times 1}) = \underbrace{E}_{1\times 1}\ (\underbrace{u_s}_{n_u\times 1}\ ,\ \underbrace{m_s}_{n_m\times 1})$$

with E the error functional of the difference

2. Compute ∇J as $m_s^* = \min_{m_s} J(m_s) \Longrightarrow \nabla J(m_s^*) = 0$



3. Solving of the minimization problem, iteratively, to recover m_s

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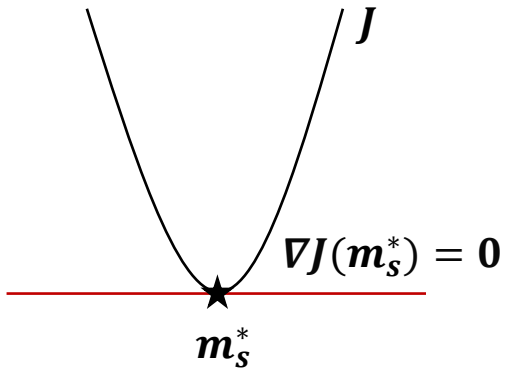

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ADJOINT STATE METHOD FOR INVERSE PROBLEM SOLVING
Introduction of the adjoint state equation to compute the gradient

- Classically, calculating $\boldsymbol{\nabla J}$ requires the computation of the whole Jacobian matrix

$$\underbrace{\boldsymbol{\nabla J}}_{\boldsymbol{n_m \times 1}} := \left(\frac{\boldsymbol{dJ}}{\boldsymbol{dm_s}}\right)^{\boldsymbol{T}} = \left(\frac{\boldsymbol{\partial E}}{\boldsymbol{\partial u_s}}\frac{\boldsymbol{du_s}}{\boldsymbol{dm_s}} + \frac{\boldsymbol{\partial E}}{\boldsymbol{\partial m_s}}\right)^{\boldsymbol{T}} = \underbrace{\left(\frac{\boldsymbol{du_s}}{\boldsymbol{dm_s}}\right)^{\boldsymbol{T}}}_{\boldsymbol{n_m \times n_u}} \underbrace{\left(\frac{\boldsymbol{\partial E}}{\boldsymbol{\partial u_s}}\right)^{\boldsymbol{T}}}_{\boldsymbol{n_u \times 1}} + \underbrace{\left(\frac{\boldsymbol{\partial E}}{\boldsymbol{\partial m_s}}\right)^{\boldsymbol{T}}}_{\boldsymbol{n_m \times 1}}$$

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- Matrix $\frac{\boldsymbol{du_s}}{\boldsymbol{dm_s}}$ is the bottleneck term
  - $\boldsymbol{u_s}$ does not depend generally explicitly on $\boldsymbol{m_s}$ ⇨ **Impossible to differentiate $\boldsymbol{u_s}$!**
  - $\frac{\boldsymbol{du_s}}{\boldsymbol{dm_s}}$ must be computed for each perturbation $\boldsymbol{dm_s}$, typically on each grid point.
    ⇨ **Can exceed many thousands at industrial scale, leading to large computation cost !**

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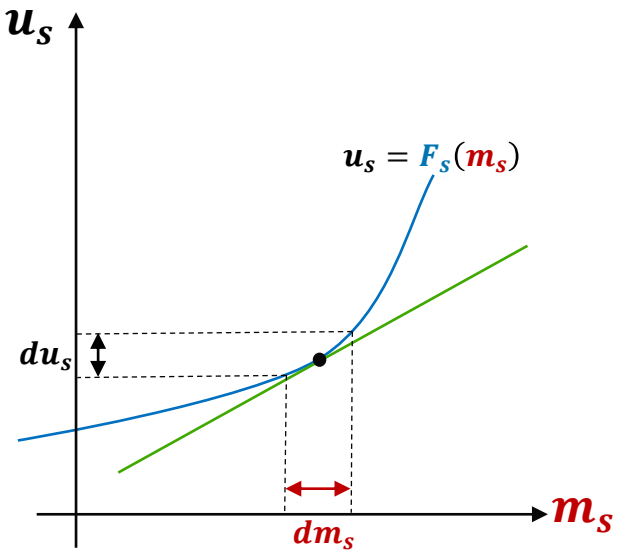
- **Adjoint state method**: alternate way to efficiently compute ∇J

  - Formally derives adjoint equations from transport models (*Pudykiewicz, 1998*) providing sensitivity of model output u_s to input variables m_s

  - Instead of computing $\frac{du_s}{dm_s}$, solving of a linear system, **the adjoint state equation**, specifying the adjoint state λ_s:

$$\underbrace{\left(\frac{\partial F_s}{\partial u_s}\right)^T}_{n_u \times n_F}\underbrace{\lambda_s}_{n_F \times 1} = \underbrace{\left(\frac{\partial E}{\partial u_s}\right)^T}_{n_u \times 1}$$



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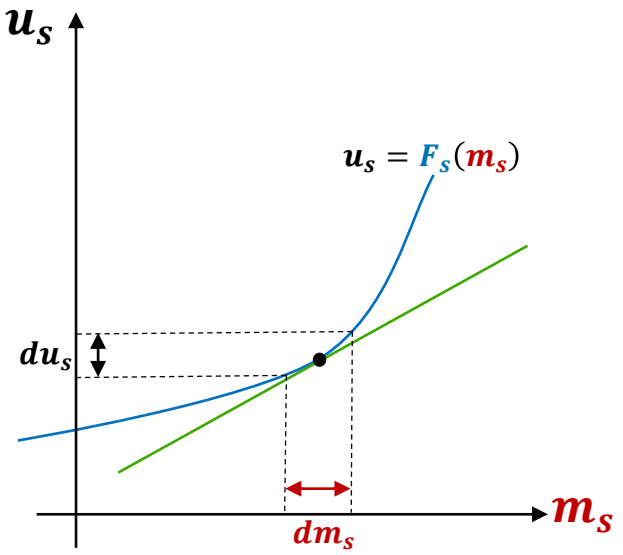

- ∇J becomes:

$$\underbrace{\nabla J}_{n_m \times 1} := \left(\frac{\mathrm{d}J}{\mathrm{d}m_s}\right)^T = -\underbrace{\left(\frac{\partial F_s}{\partial m_s}\right)^T}_{n_m \times n_F}\underbrace{\lambda_s}_{n_F \times 1} + \underbrace{\left(\frac{\partial E}{\partial m_s}\right)^T}_{n_m \times 1}$$

- **λ_s is a vector, independent of the optimization parameter number, reducing computation time !**

ADJOINT STATE METHOD FOR INVERSE PROBLEM SOLVING
Extension to a Markovian explicit iterative model with least-square misfit

- **Adjoint method** widely used in atmospheric dispersion field

  - Applications to Gaussian and Eulerian models (*Pudykiewicz, 1998; Giering, 2000*)

  - Not known application to forward Lagrangian Stochastic (LS) models
    BUT:
    - ✓ Suitable for modelling turbulent dispersion in complex environment
    - ✓ Reasonable computational cost

    ⇨ **Objective:** Application to a Lagrangian Stochastic model

- **Case definition**:
  Explicit
  Iterative
  Markov process
  Least-square error functional

ADJOINT STATE METHOD FOR INVERSE PROBLEM SOLVING
Extension to a Markovian explicit iterative model with least-square misfit

- Under these assumptions + observations only at final N^{th} iteration, **linear adjoint system** becomes iterative
- Computation of ∇J, using λ_s^1 found solving iteratively the **adjoint state equation**

$$\underbrace{\nabla J}_{n_m \times 1} = \underbrace{\left(\frac{\partial f_s^1}{\partial m_s}\right)^T}_{n_m \times n_1} \underbrace{\prod_{j=1}^{N-1}\left(\frac{\partial f_s^{j+1}}{\partial u_s^j}\right)^T}_{n_1 \times n_N} \underbrace{\left[\frac{u_s^N - d^N}{\overline{d^N} * \overline{d^N}}\right]}_{n_N \times 1}$$

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- Efficient way to compute ∇J (chain rule)
- ∇J obtained computing only a product iteratively
- A priori knowledge of u_s^N, d^N & N not necessary

APPLICATION TO A LAGRANGIAN STOCHASTIC PARTICLE DISPERSION MODEL

- Simplified LS model ⇨ Gaussian steady isotropic homogeneous turbulence and diagonal Reynolds stresses

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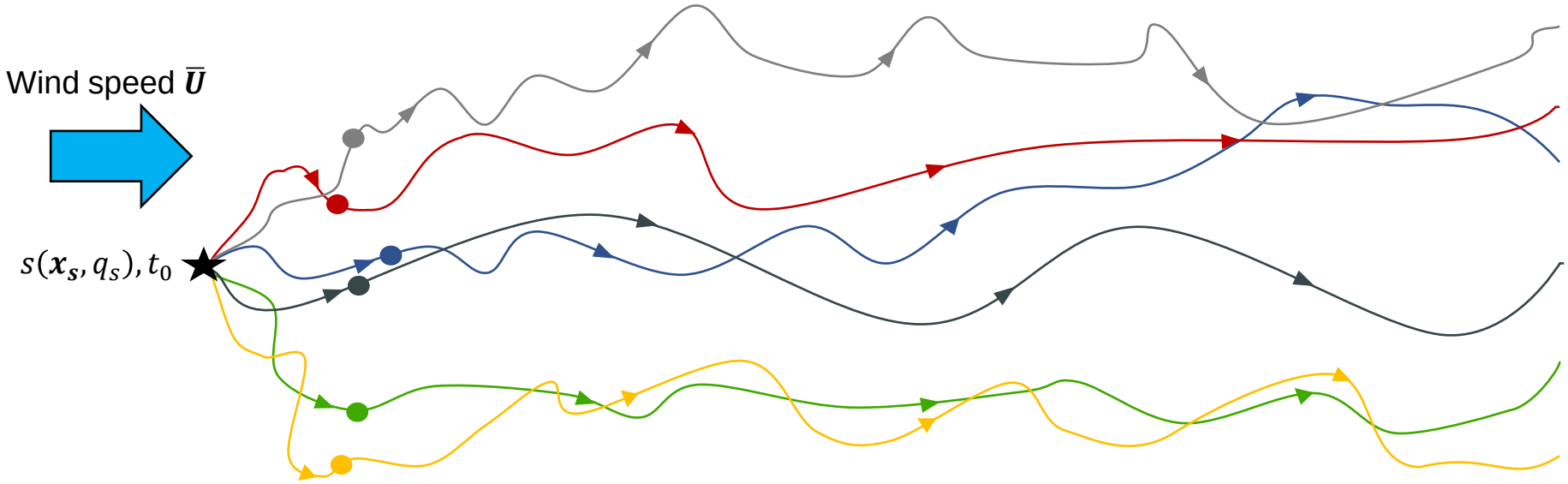
- **3D/CFD Lagrangian models**: Describes the turbulent pathway simulation of thousands of particles, through a stochastic process



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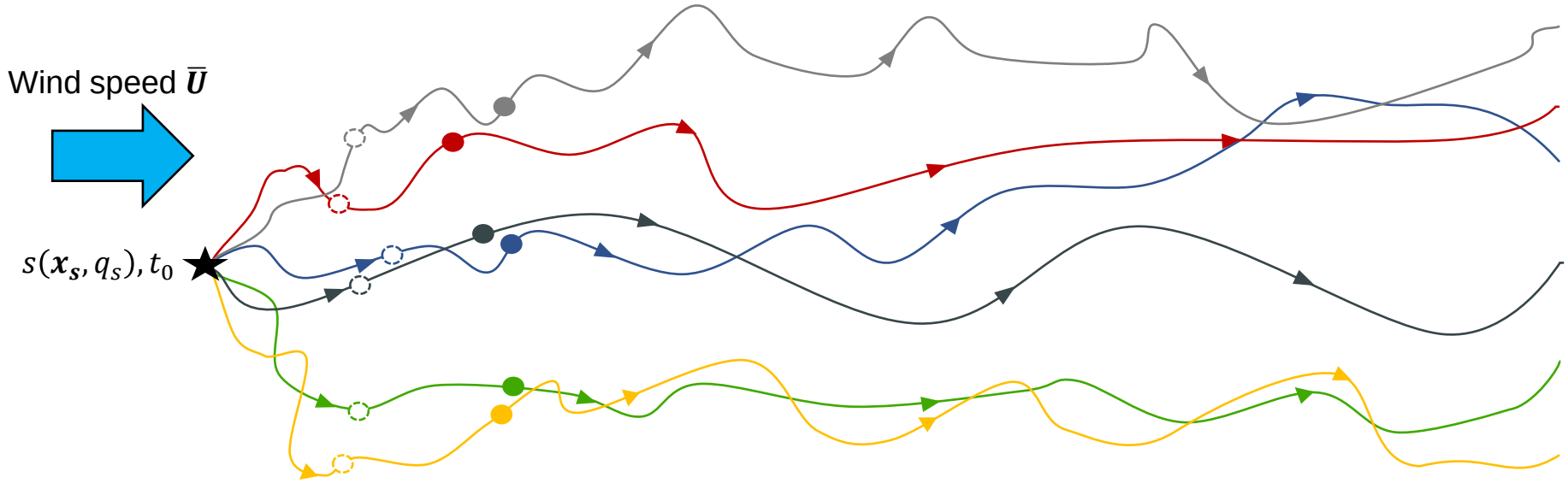

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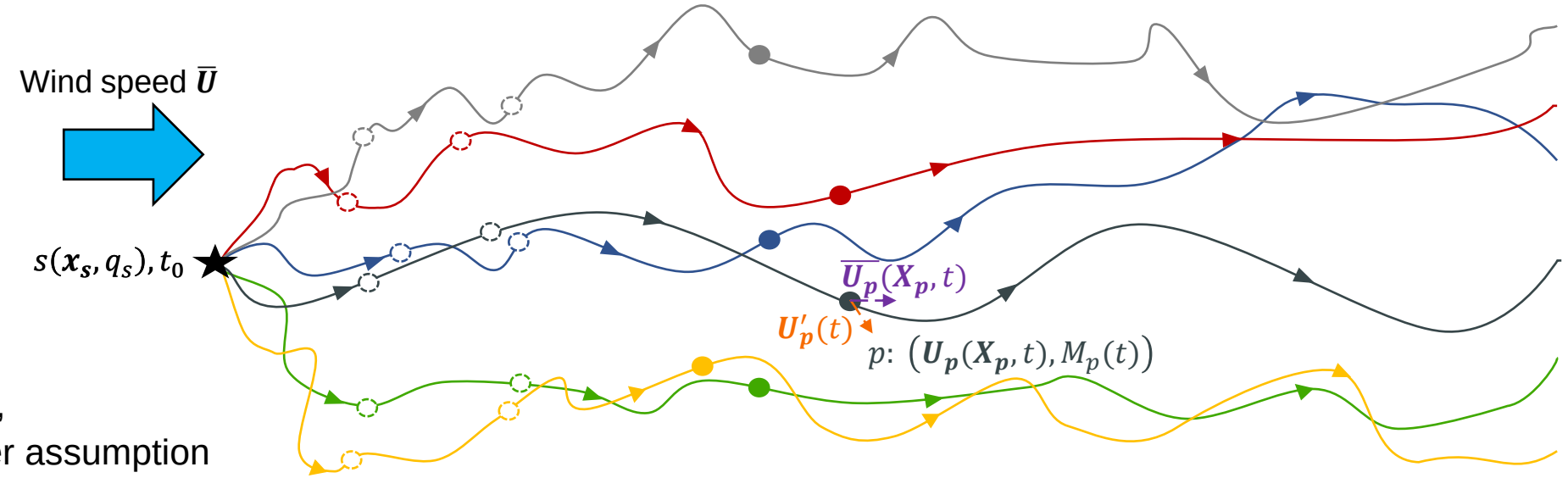
- Simplified LS model ⇨ Gaussian steady isotropic homogeneous turbulence and diagonal Reynolds stresses
- **3D/CFD Lagrangian models**: Describes the turbulent pathway simulation of thousands of particles, through a stochastic process
- At each time t, a particle p is fully described by:
  - its **fluctuating velocity** $U'_{p,i}(t)$, for the i^{th} space component
  - its **pseudo-mass** $M_p(t)$, constant over time under assumption of decay process absence



$$\begin{cases} X_{p,i}(t+\delta t) = X_{p,i}(t) + \left(\overline{u_i}(\boldsymbol{X_p}, t) + U'_{p,i}(t)\right)\ \delta t \\ U'_{p,i}(t+\delta t) = U'_{p,i}(t) + \underbrace{\delta U'_{p,i}}_{\text{Stochastic variation}} \end{cases}$$

with $X_{p,i}(t_0) = x_{s,i}$

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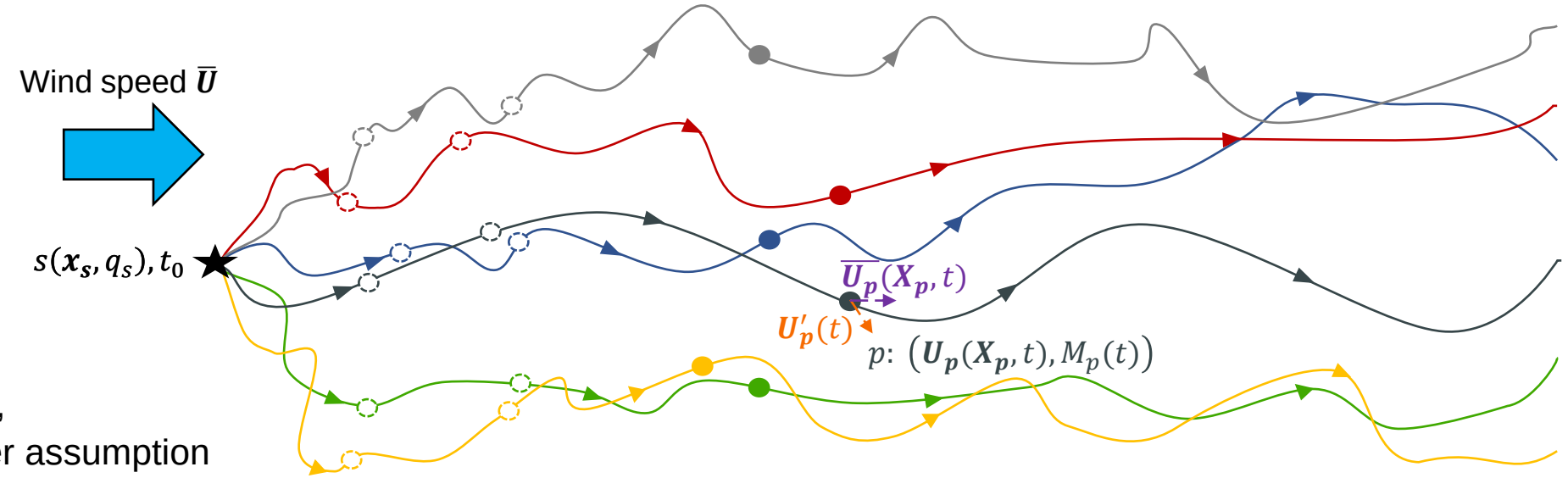

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Stochastic variation

with $X_{p,i}(t_0) = x_{s,i}$

Generalized Langevin Equation[1]

[1]Thomson, D. J. (1987). "Criteria for the selection of stochastic models of particle trajectories in turbulent flows". In: Journal of Fluid Mechanics 180.-1, pp. 529

APPLICATION TO A LAGRANGIAN STOCHASTIC PARTICLE DISPERSION MODEL
Generalized Langevin equation

- Stochastic variation $\delta U'_{\mathrm{p},i}$, for the i^{th} space component, described by the **Generalized Langevin Equation**[1], **for Gaussian steady isotropic homogeneous turbulence and diagonal Reynolds stress tensor**:

$$\delta U'_{p,i} = \left[-\frac{1}{T_L} U'_{p,i}\right] \delta t + \sigma_u \sqrt{\frac{2}{T_L}} \sqrt{\delta t} \xi_{p,u_i}$$

  - T_L Lagrangian correlation time of the considered particle
  - σ_u velocity amplitude fluctuation

- **Describes Brownian motion of small dimension particle in a fluid ⇨ Markov process**
- Allows to reproduce some statistics on correlation time between particles

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Simplification of the real atmosphere

For the rest of this presentation, work has been done under these assumptions, for understanding of the adjoint state method approach

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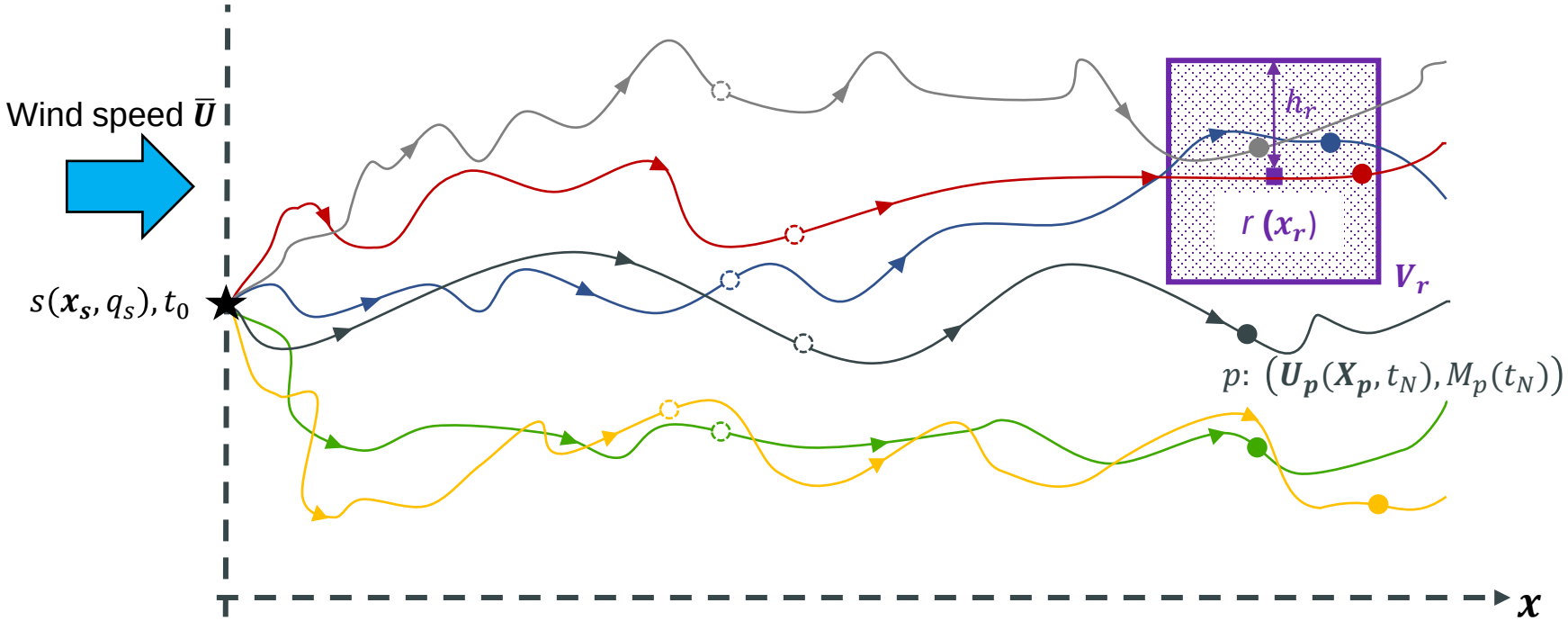
APPLICATION TO A LAGRANGIAN STOCHASTIC PARTICLE DISPERSION MODEL
Concentration computation

- **Objective**: Compute average concentration $\overline{C_s}(\boldsymbol{x_r}, t_N)$ over volume $\boldsymbol{V_r}$ centred on sensor position $\boldsymbol{x_r}$ for t_N



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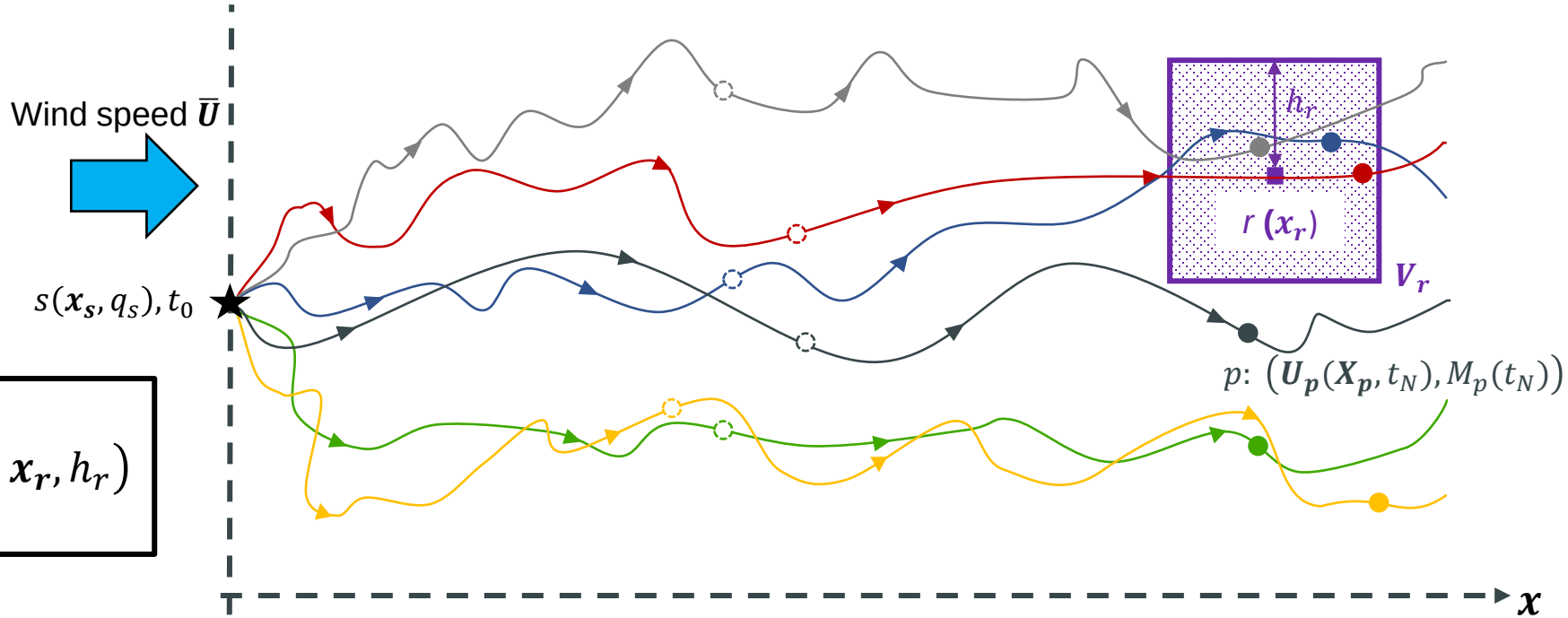

- **Density kernel approach**[2]:

$$\overline{C_s}(\boldsymbol{x_r}, t_N) = \sum_{p=1}^{N_p} M_p(t_N)\, K\left(\boldsymbol{X_p}(t_N) - \boldsymbol{x_r}, h_r\right)$$

- K a kernel function, modelling the detector response function of sensor r
- h_r smoothing radius

[2]Lorimer, G. S. (1986). "The kernel method for air quality modelling-I. Mathematical foundation". In: Atmospheric Environment 20-7, pp. 1447-14520

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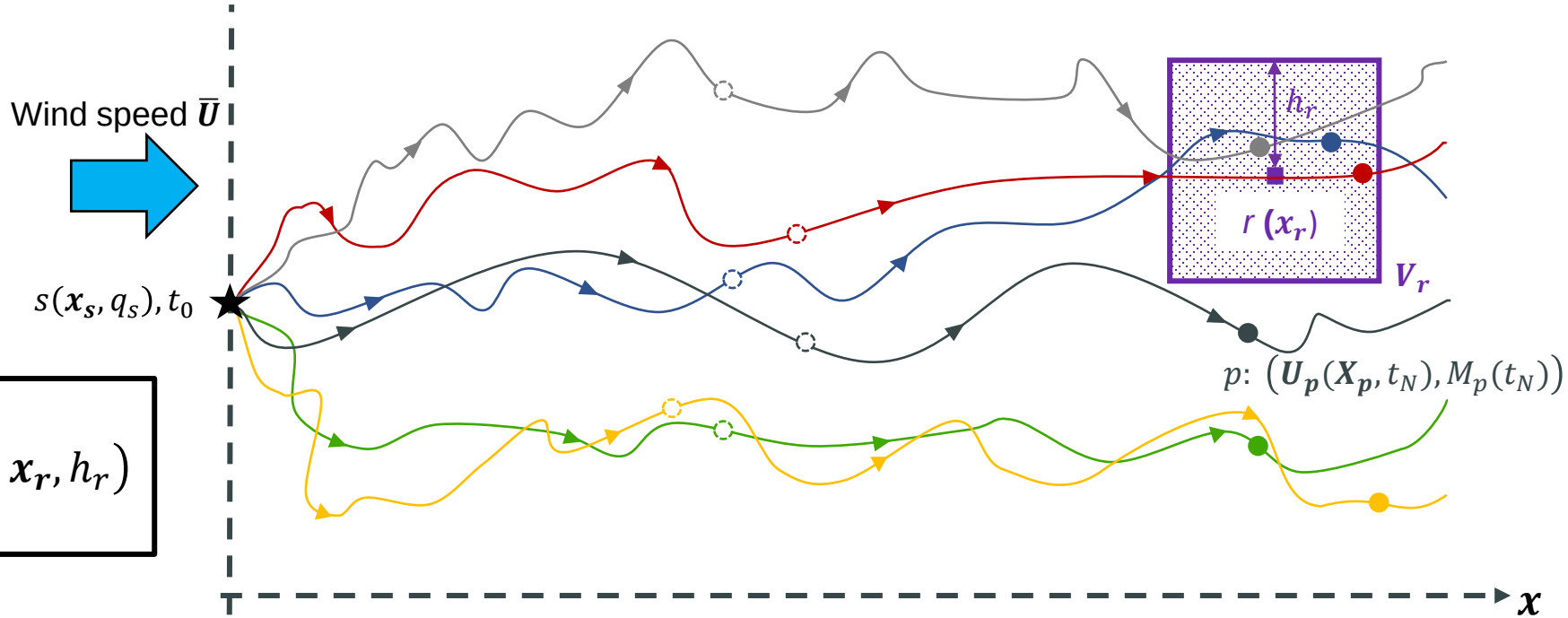

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- $\overline{C_s}$ considered as particle density function, affected by M_p, over $\boldsymbol{V_r}$:
  the density of particles inside $\mathbf{V_r}$ which have been transported forward in time from source s.

[2]Lorimer, G. S. (1986). "The kernel method for air quality modelling-I. Mathematical foundation". In: Atmospheric Environment 20-7, pp. 1447-14520

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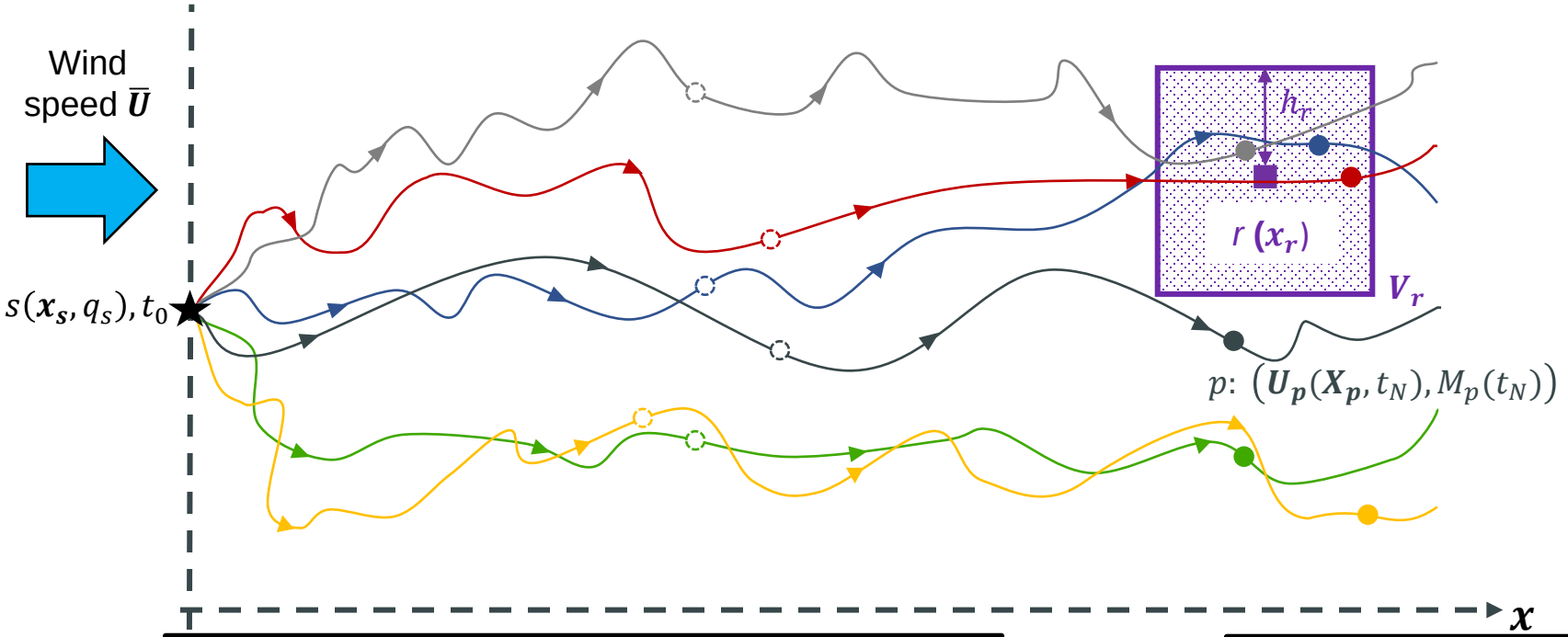
Adjoint computation



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$$\underbrace{\nabla J}_{n_m \times 1} = \underbrace{\left(\sum_{t=1}^{N} \sum_{p=1}^{N_p} O_{p,s}\right)}_{n_m \times n_N} \underbrace{\left[\frac{u_s^N - d^N}{\overline{d^N} * \overline{d^N}}\right]}_{n_N \times 1}$$

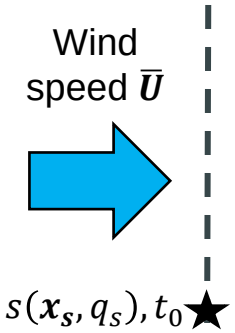
with

$$O_{p,s} = \underbrace{P_{p,s}^T \left[\prod_{j=1}^{N-2} Q_{p,s}^{j+1\,T}\right] R_{p,s}^T}_{n_m \times n_N}$$

APPLICATION TO A LAGRANGIAN STOCHASTIC PARTICLE DISPERSION MODEL

Adjoint computation-Disaggregation step

Disaggregation: Instant emission of N_p particles from source s, at t_0



$$\underbrace{\left(\frac{\partial f_s^1}{\partial m_s}\right)^T}_{n_m \times 1} = \left[\underbrace{P_{1,s}^T}_{n_m \times 7} \cdots \underbrace{P_{p,s}^T}_{n_m \times 7} \cdots \underbrace{P_{N_p,s}^T}_{n_m \times 7}\right]$$

$P_{p,s}^T$ sensitivity matrix of p characteristics (X_p, U'_p and M_p) w.r.t. m_s at t_0

$$\underbrace{\nabla J}_{n_m \times 1} = \underbrace{\left(\frac{\partial f_s^1}{\partial m_s}\right)^T}_{n_m \times n_1} \underbrace{\prod_{j=1}^{N-1}\left(\frac{\partial f_s^{j+1}}{\partial u_s^j}\right)^T}_{n_1 \times n_N} \underbrace{\left[\frac{u_s^N - d^N}{\overline{d^N} * \overline{d^N}}\right]}_{n_N \times 1}$$

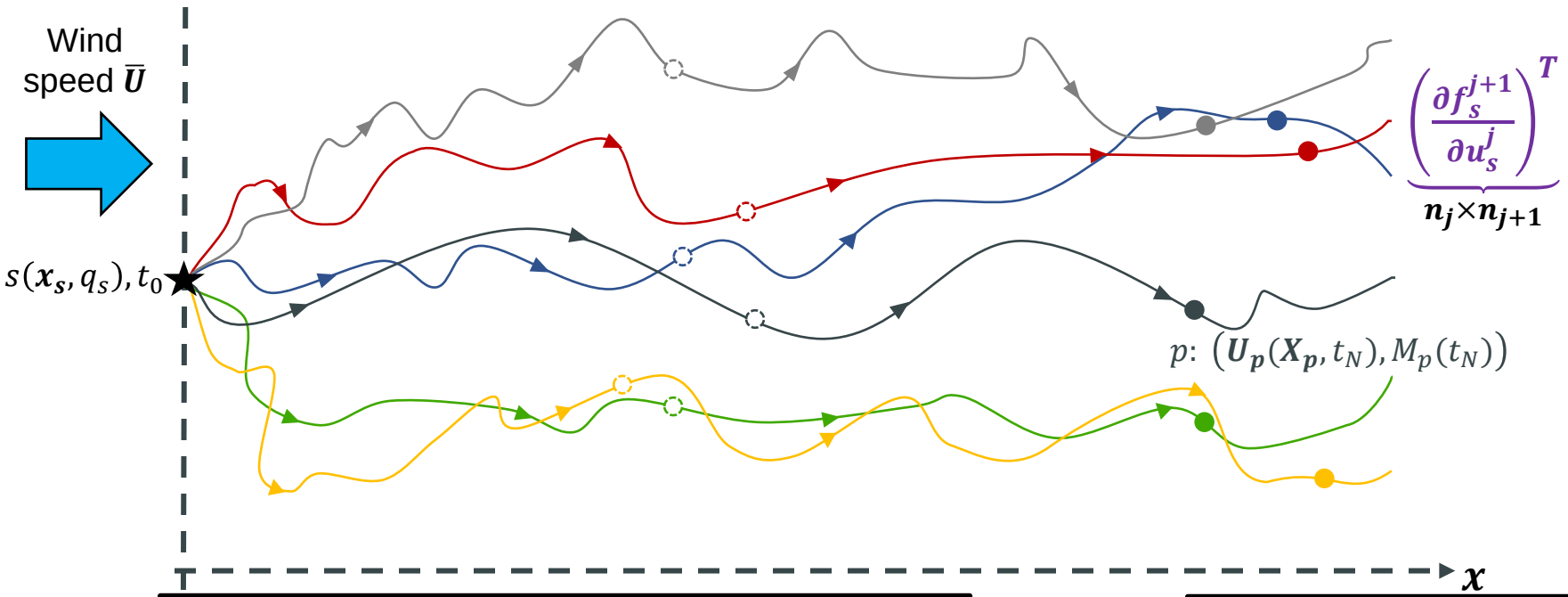
$$\underbrace{\nabla J}_{n_m \times 1} = \underbrace{\left(\sum_{t=1}^{N}\sum_{p=1}^{N_p} O_{p,s}\right)}_{n_m \times n_N} \underbrace{\left[\frac{u_s^N - d^N}{\overline{d^N} * \overline{d^N}}\right]}_{n_N \times 1}$$

with $$O_{p,s} = \underbrace{P_{p,s}^T \left[\prod_{j=1}^{N-2} Q_{p,s}^{j+1\,T}\right] R_{p,s}^T}_{n_m \times n_N}$$

APPLICATION TO A LAGRANGIAN STOCHASTIC PARTICLE DISPERSION MODEL

Adjoint computation-Transport step

Transport / Advection: Advection of particles at each time step δt, for N iterations (Lagrangian stochastic path)



$$\underbrace{\left(\frac{\partial f_s^{j+1}}{\partial u_s^j}\right)^T}_{n_j \times n_{j+1}} = diag\left(\underbrace{Q_{1,s}^{j+1\,T}}_{7\times7}, \cdots, \underbrace{Q_{p,s}^{j+1\,T}}_{7\times7}, \cdots, \underbrace{Q_{N_p,s}^{j+1\,T}}_{7\times7}\right)$$

$Q_{p,s}^{j+1\,T}$ sensitivity matrix of p characteristics at $(j+1)^{th}$ iteration w.r.t. j^{th} one

$$\underbrace{\nabla J}_{n_m\times1} = \underbrace{\left(\frac{\partial f_s^1}{\partial m_s}\right)^T}_{n_m\times n_1} \underbrace{\prod_{j=1}^{N-1}\left(\frac{\partial f_s^{j+1}}{\partial u_s^j}\right)^T}_{n_1\times n_N} \underbrace{\left[\frac{u_s^N - d^N}{\overline{d^N} * \overline{d^N}}\right]}_{n_N\times1}$$

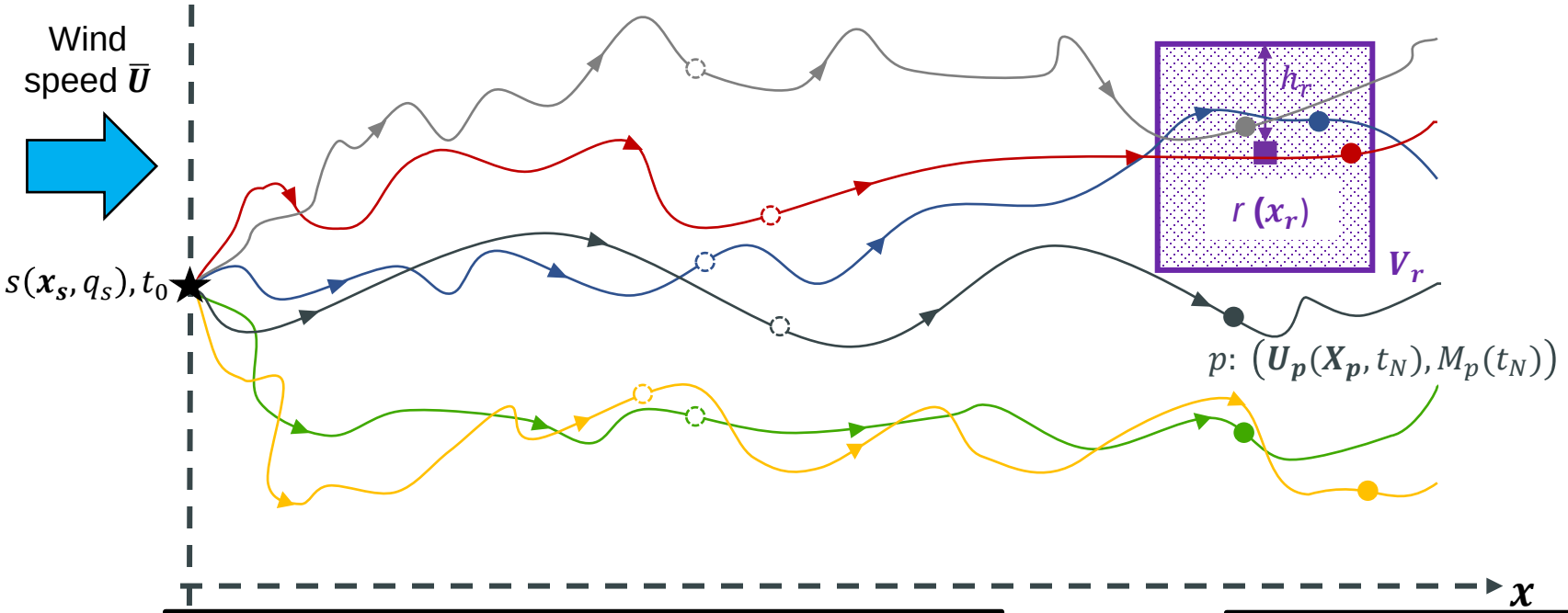
$$\underbrace{\nabla J}_{n_m\times1} = \underbrace{\left(\sum_{t=1}^{N}\sum_{p=1}^{N_p} O_{p,s}\right)}_{n_m\times n_N} \underbrace{\left[\frac{u_s^N - d^N}{\overline{d^N} * \overline{d^N}}\right]}_{n_N\times1}$$

with $$\underbrace{O_{p,s} = P_{p,s}^T \left[\prod_{j=1}^{N-2} Q_{p,s}^{j+1\,T}\right] R_{p,s}^T}_{n_m\times n_N}$$

APPLICATION TO A LAGRANGIAN STOCHASTIC PARTICLE DISPERSION MODEL

Adjoint computation-Aggregation step

Aggregation: Concentration computation at receiver r, after N iterations



$$\underbrace{\left(\frac{\partial f_s^N}{\partial u_s^{N-1}}\right)^T}_{n_{N-1}\times n_N} = \left[\underbrace{R_{1,s}}_{n_N\times 7} \cdots \underbrace{R_{p,s}}_{n_N\times 7} \cdots \underbrace{R_{N_p,s}}_{n_N\times 7}\right]^T$$

$R_{p,s}^T$ sensitivity matrix of concentration of particles at sensor r w.r.t. p characteristics at N^{th} iteration

$$\underbrace{\nabla J}_{n_m\times 1} = \underbrace{\left(\frac{\partial f_s^1}{\partial m_s}\right)^T}_{n_m\times n_1} \underbrace{\prod_{j=1}^{N-1}\left(\frac{\partial f_s^{j+1}}{\partial u_s^j}\right)^T}_{n_1\times n_N} \underbrace{\left[\frac{u_s^N - d^N}{\overline{d^N} * \overline{d^N}}\right]}_{n_N\times 1}$$

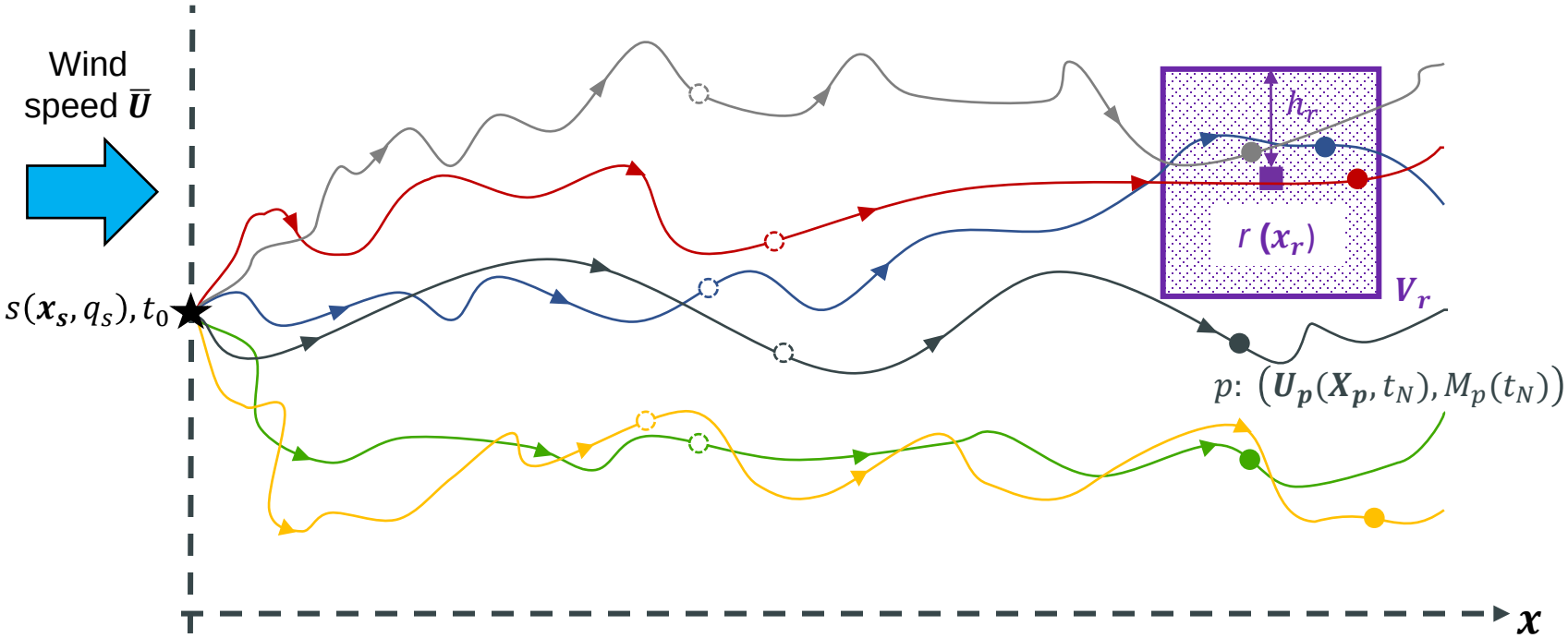
$$\underbrace{\nabla J}_{n_m\times 1} = \underbrace{\left(\sum_{t=1}^{N}\sum_{p=1}^{N_p} O_{p,s}\right)}_{n_m\times n_N} \underbrace{\left[\frac{u_s^N - d^N}{\overline{d^N} * \overline{d^N}}\right]}_{n_N\times 1}$$

with

$$O_{p,s} = \underbrace{P_{p,s}^T\left[\prod_{j=1}^{N-2} Q_{p,s}^{j+1\,T}\right] R_{p,s}^T}_{n_m\times n_N}$$

APPLICATION TO A LAGRANGIAN STOCHASTIC PARTICLE DISPERSION MODEL

Adjoint computation



$$\underbrace{\nabla J}_{n_m \times 1} = \underbrace{\left(\sum_{t=1}^{N} \sum_{p=1}^{N_p} O_{p,s} \right)}_{n_m \times n_N} \underbrace{\left[\frac{u_s^N - d^N}{\overline{d^N} * \overline{d^N}} \right]}_{n_N \times 1}$$

- $O_{p,s}$ (size $4 * n_N$) computed independently for each particle

⇨ **Allows parallelization, reducing restitution time**

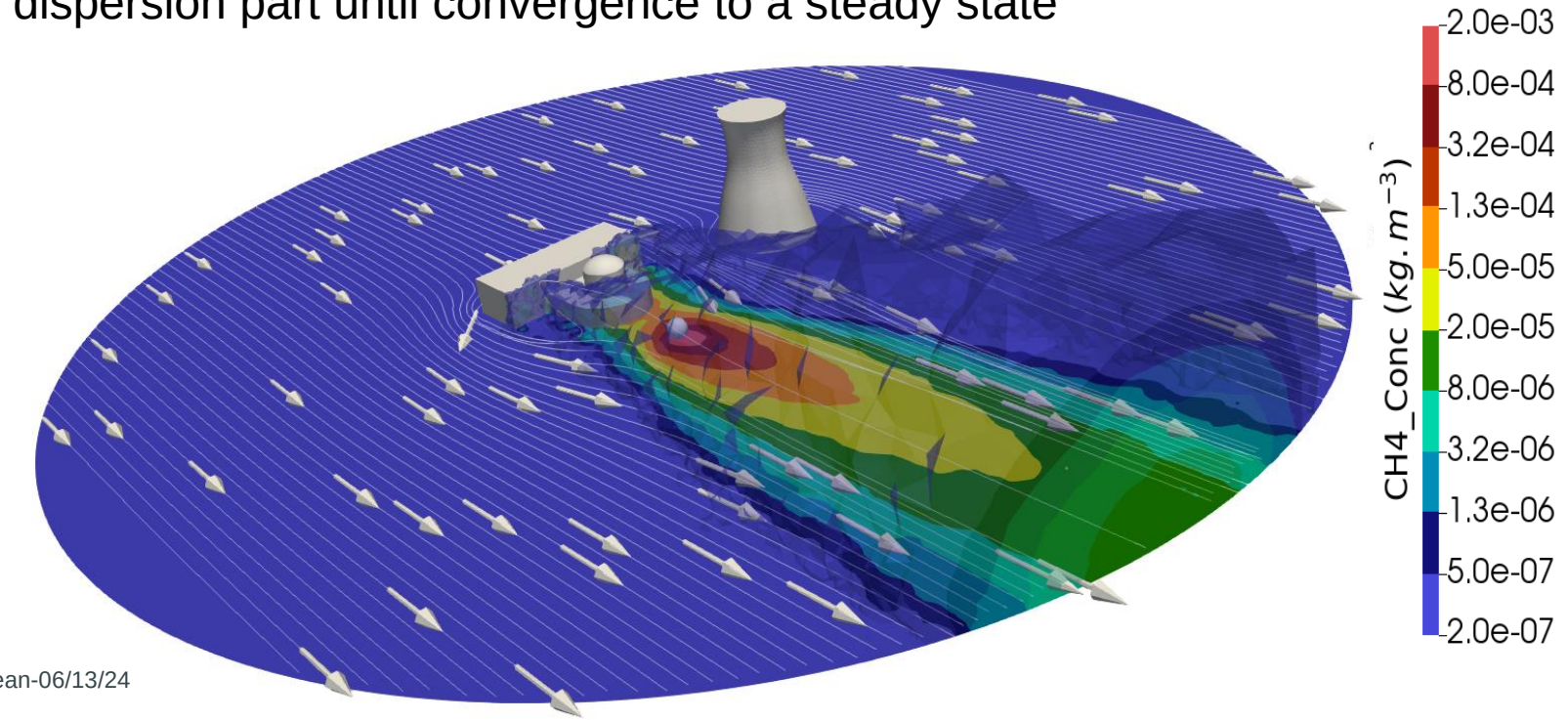
- Product calculated iteratively while forward model running

⇨ **Avoids particle data storage at each time step and excessive memory use**

- Easy adaptation of $O_{p,s}$ for more general cases, by summing equivalent terms corresponding to these cases.

APPLICATION RESULTS ON A NUMERICAL TEST CASE
Case description

- Computational domain: test case power plant at the centre of a 600-meter radius disk
- Continuous release from a point source located 10 meters above the ground
  - Steady configuration with Gaussian isotropic homogeneous turbulence and diagonal Reynolds stresses
  - Neutral atmosphere
- LS model runs dispersion part until convergence to a steady state



APPLICATION RESULTS ON A NUMERICAL TEST CASE
Adjoint concentration fields

- Direct concentration field and its adjoint ones to compute ground sensitivities
- **Gradients**: opposite directions of source displacement reducing difference between model and observations

⇨ **Allows to approach source true characteristics**

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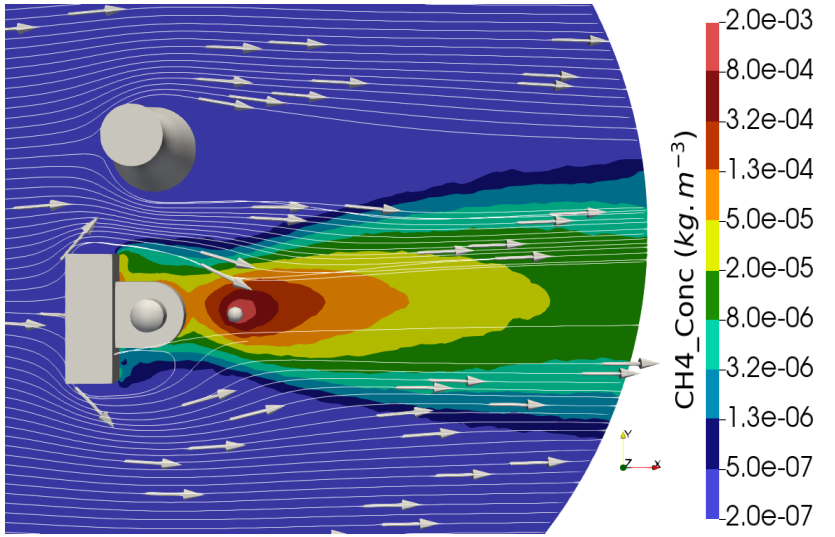

Figure 1 - Concentration field with wind flow (log-scale)

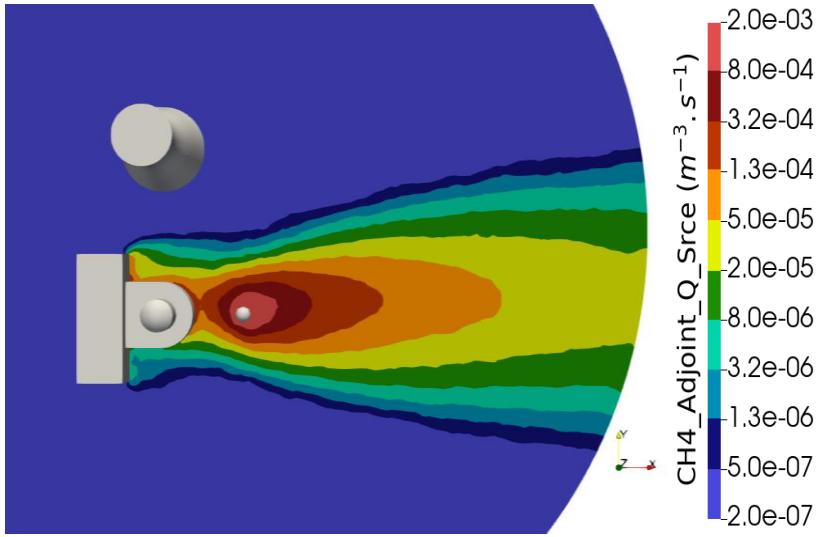

Figure 2 - Concentration variation for a unit increase of source flow rate (log-scale)

$$\underbrace{\nabla J}_{n_m \times 1} = \underbrace{\left(\sum_{t=1}^{N} \sum_{p=1}^{N_p} O_{p,s} \right)}_{n_m \times n_N} \underbrace{\left[\frac{u_s^N - d^N}{\overline{d^N} * \overline{d^N}} \right]}_{n_N \times 1} = 1$$

APPLICATION RESULTS ON A NUMERICAL TEST CASE
Adjoint concentration fields

- Direct concentration field and its adjoint ones to compute ground sensitivities
- **Gradients**: opposite directions of source displacement reducing difference between model and observations

⇨ **Allows to approach source true characteristics**

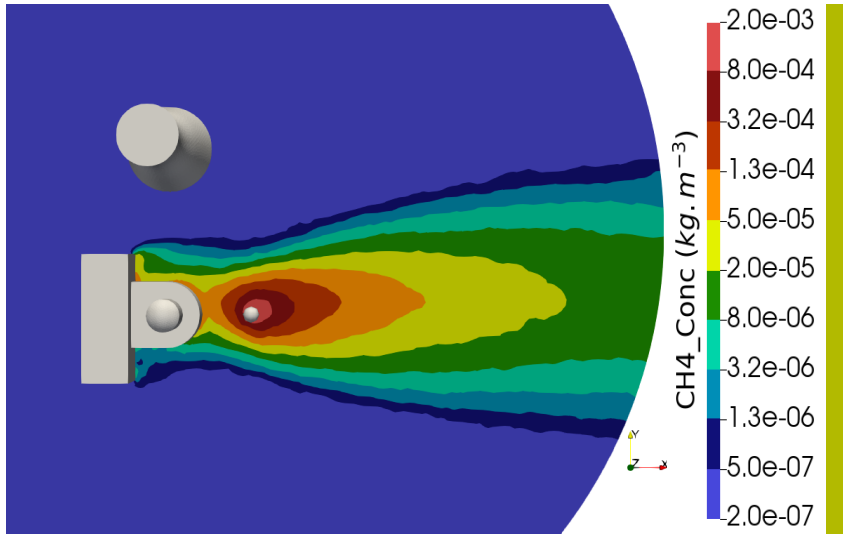

Figure 1 - Concentration field (log-scale)

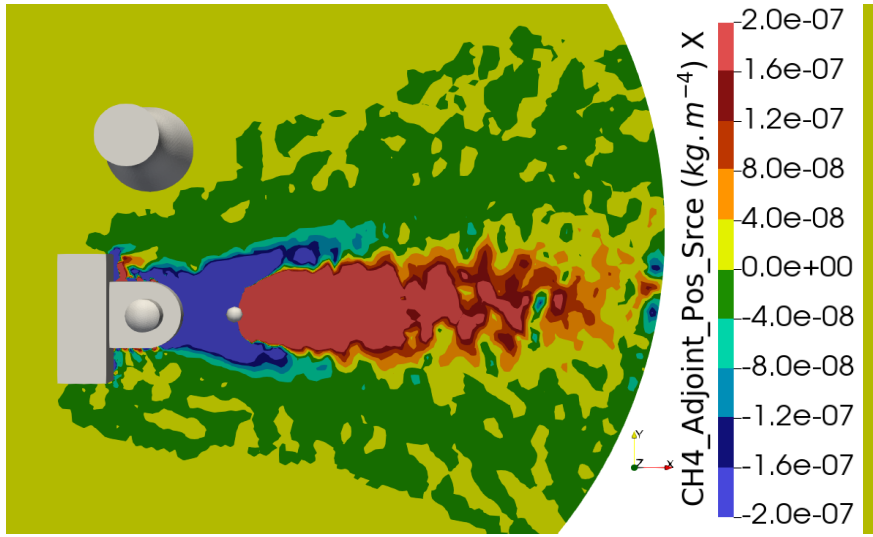

Figure 3 - Concentration variation for a unit increase of source X-coordinate (linear scale)

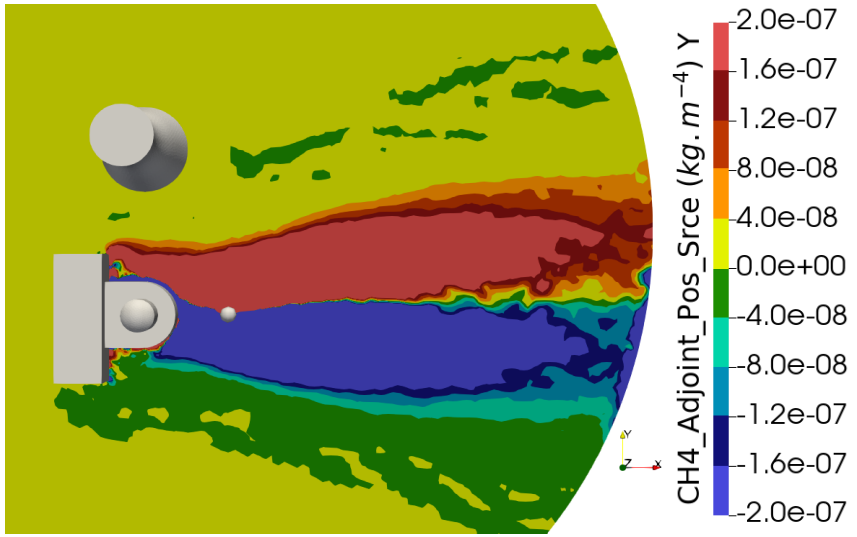

Figure 4 - Concentration variation for a unit increase of source Y-coordinate (linear scale)

CONCLUSION

- Use of the **adjoint state method** to solve the minimization problem avoids:
  - Computation of the whole Jacobian matrix
  - Dependence on the number of optimization parameters

⇨ **Save significant computation time !**

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- Use of the **adjoint state method** to solve the minimization problem avoids:
  - Computation of the whole Jacobian matrix
  - Dependence on the number of optimization parameters

⇨ **Save significant computation time !**

- New application of the adjoint state method, for a LS model (Markovian explicit iterative model)

⇨ **Combined use of the adjoint method with a LS model is well suited to source characterization with real time constraint in complex industrial sites**

THANK YOU !