# Transported Probability Density Function (PDF) Methods for Multiscale and Uncertainty Problems - Part I


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# Motivation for PDF Modeling

- interested in statistical description
- joint PDF's are arbitrary
- non-linear terms in fine-scale equations
- spatial and temporal correlations

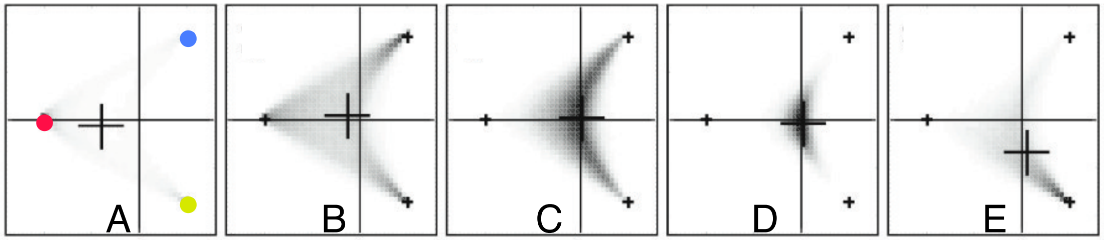
<u>Examples:</u>

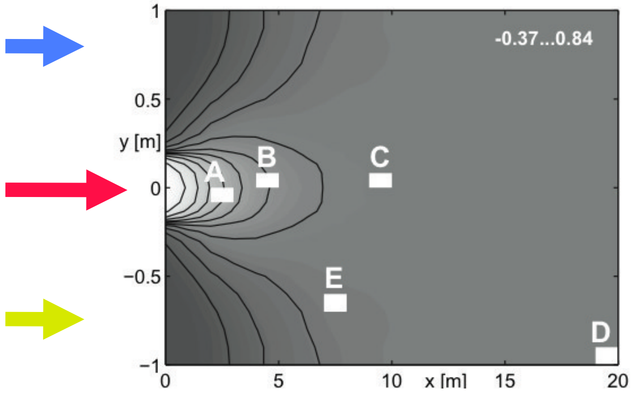
- turbulent combustion
- multi-phase flow
  - turbulent sprays
  - miscible and immiscible transport in porous media
- uncertainty assessment of contaminant transport
- non-equilibrium gas flow
- light scattering
- ...

# Motivation for PDF Modeling

## Example: Turbulence and Mixing

(D. W. Meyer, P. Jenny)




one motivation was the integration of non-linear source terms:

$$\langle Q(Y_1, Y_2, ..., Y_n, T)\rangle \neq Q(\langle Y_1\rangle, ..., \langle Y_n\rangle, \langle T\rangle)$$

$$\langle Q(Y_1, Y_2, ..., Y_n, T)\rangle = \int dY \int dT \{Q(Y_1, Y_2, ..., Y_n, T) f\}$$

# Motivation for PDF Modeling

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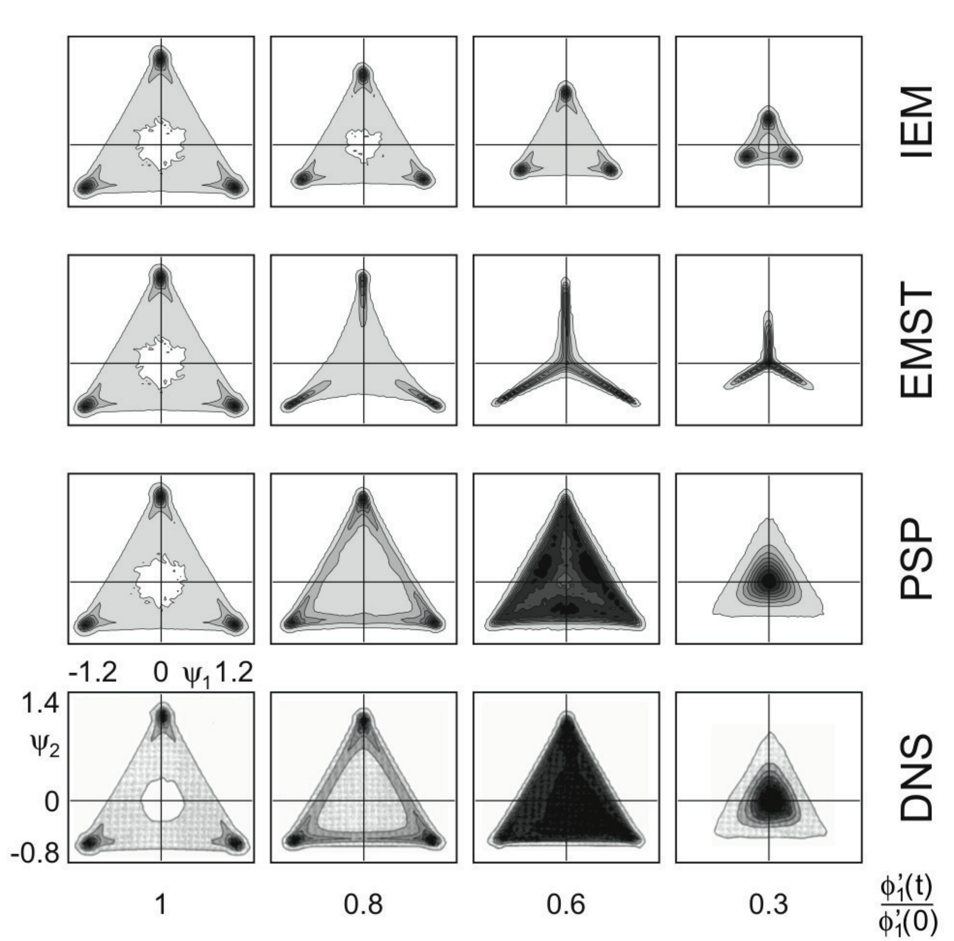
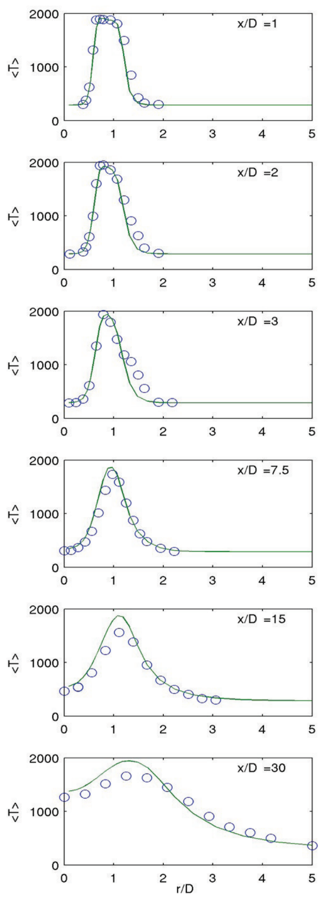


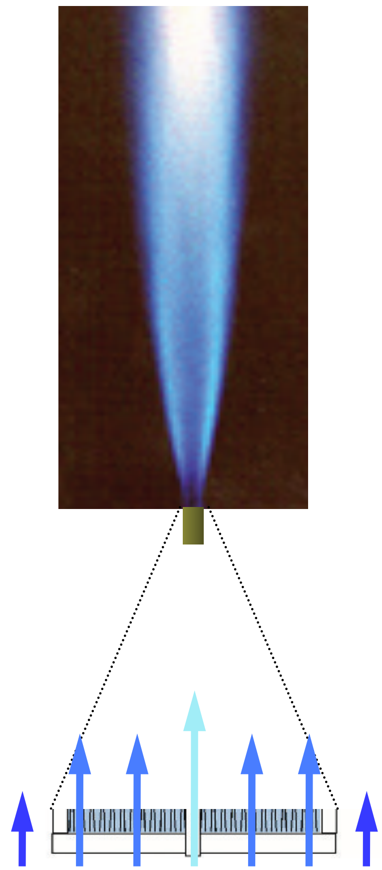
# Motivation for PDF Modeling

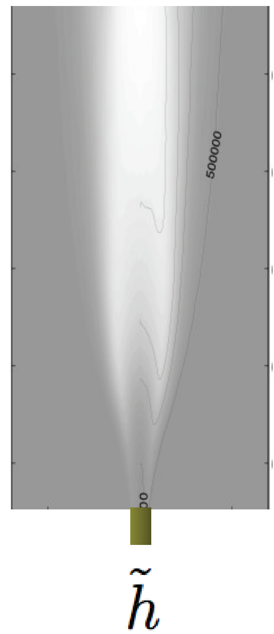
## Example: Turbulent Combustion

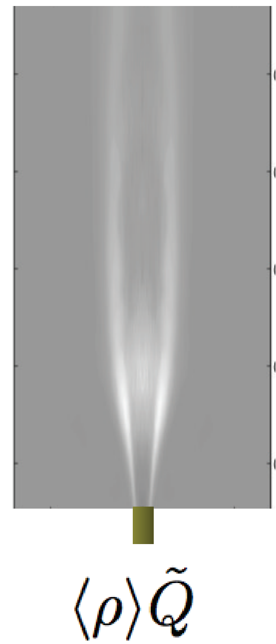
(M. Hegetschweiler, P. Jenny)

***Temperature***

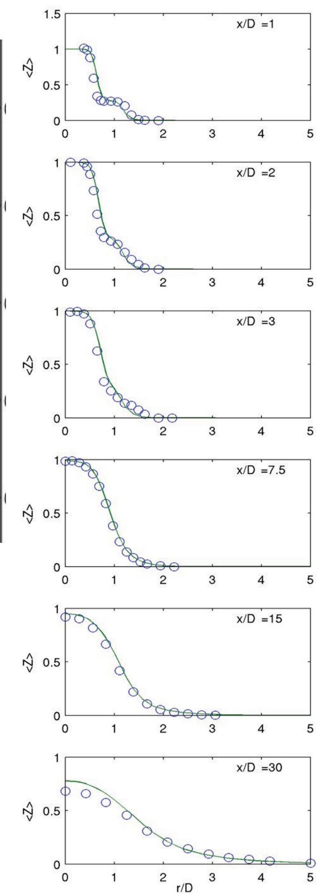




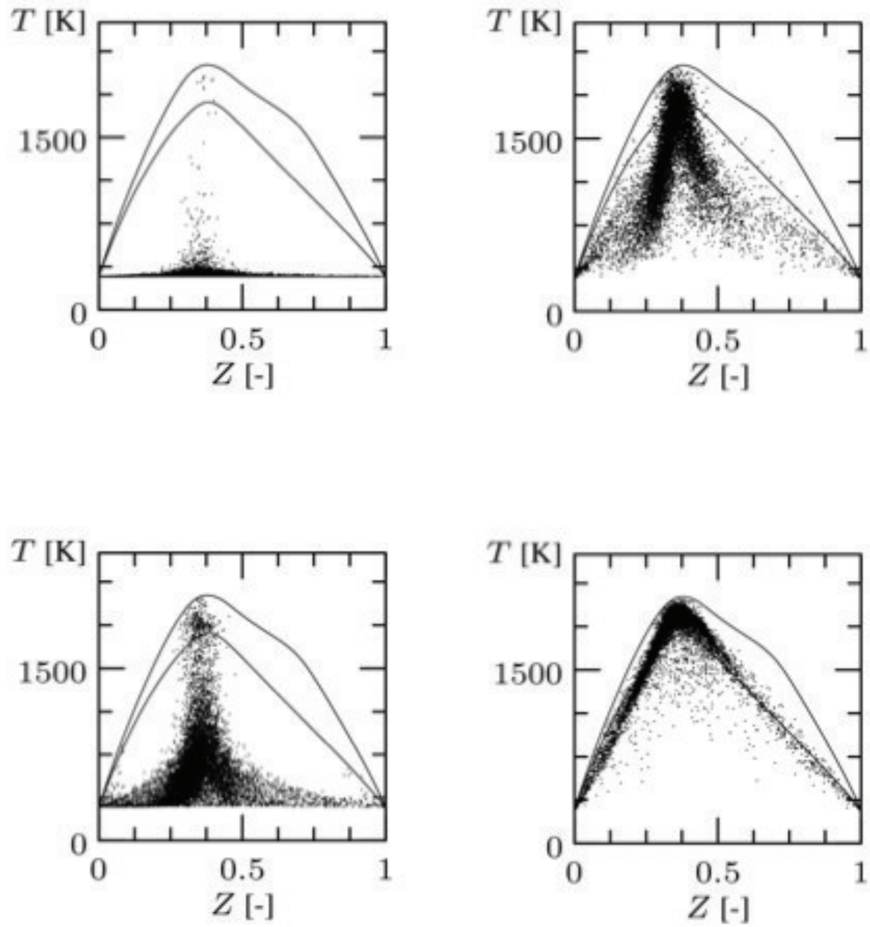

***Mixture fraction***



# Motivation for PDF Modeling

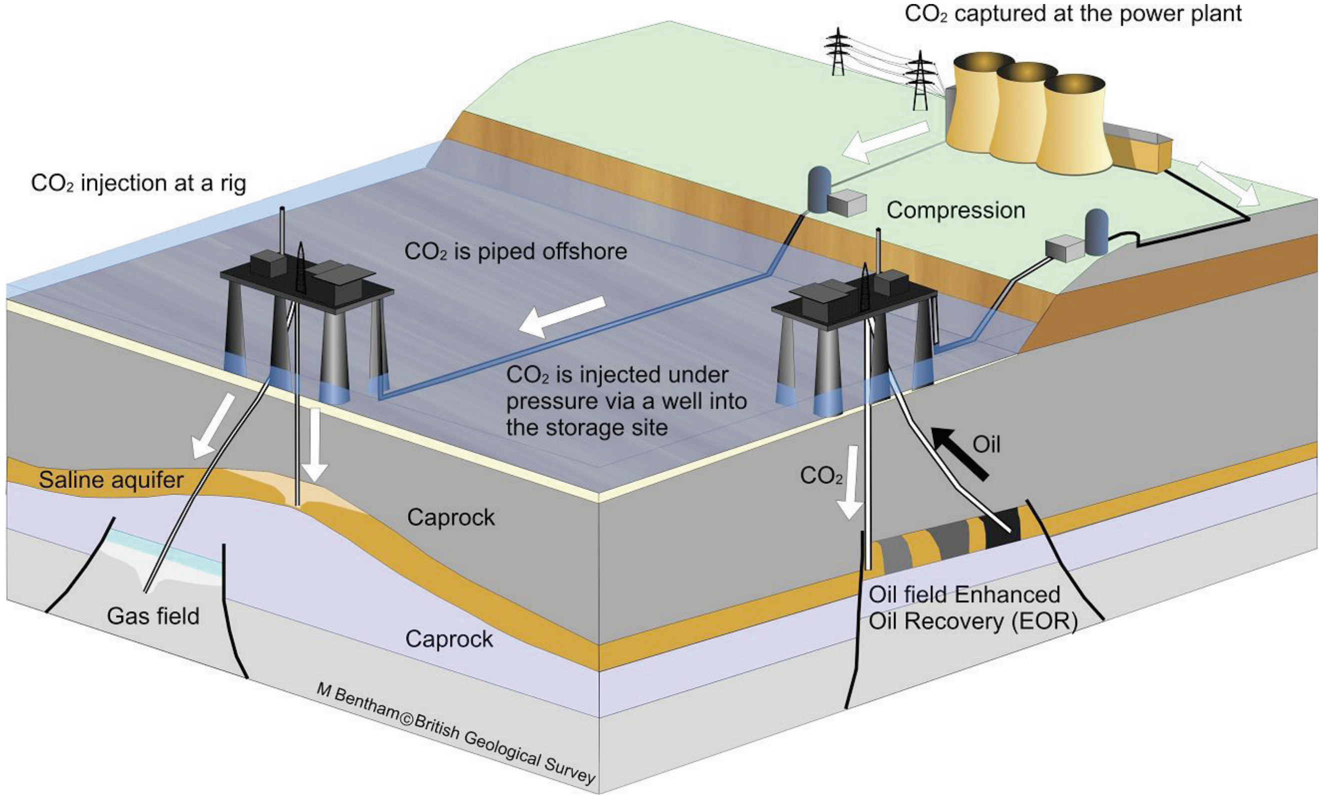
## Example: Turbulent Combustion

(B. Zoller, P. Jenny)



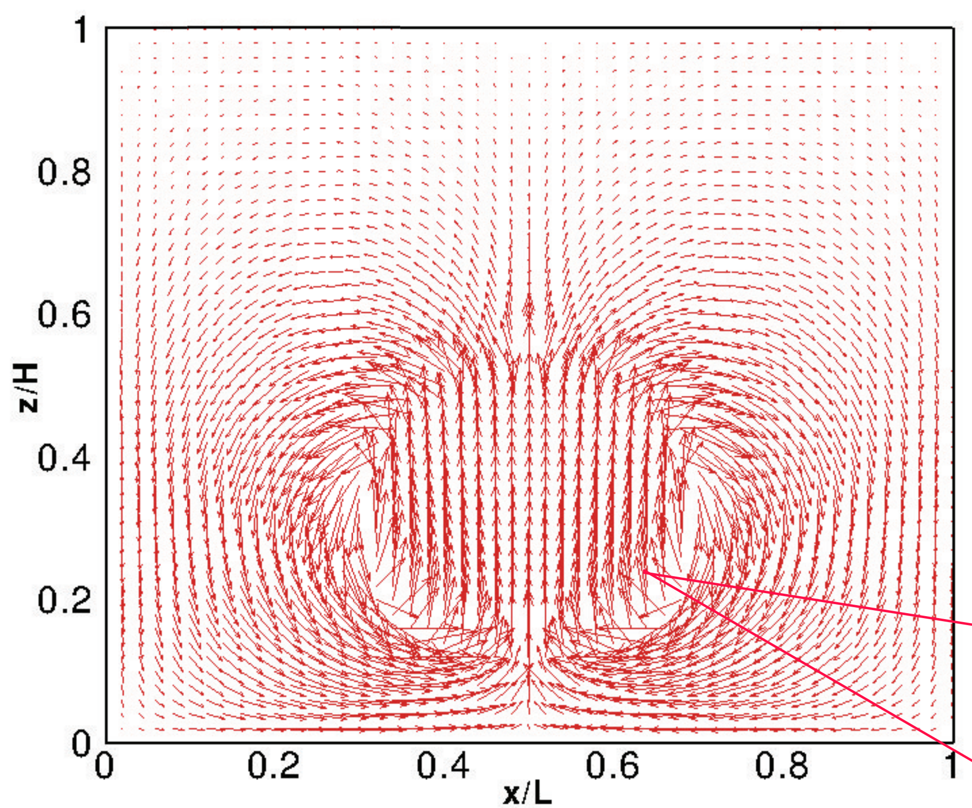
# Motivation for PDF Modeling

## Example: Multi-Phase Flow in Porous Media



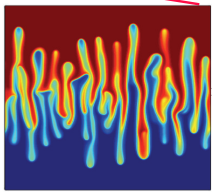
# Motivation for PDF Modeling

## Example: Multi-Phase Flow in Porous Media (M. Tyagi, P. Jenny)



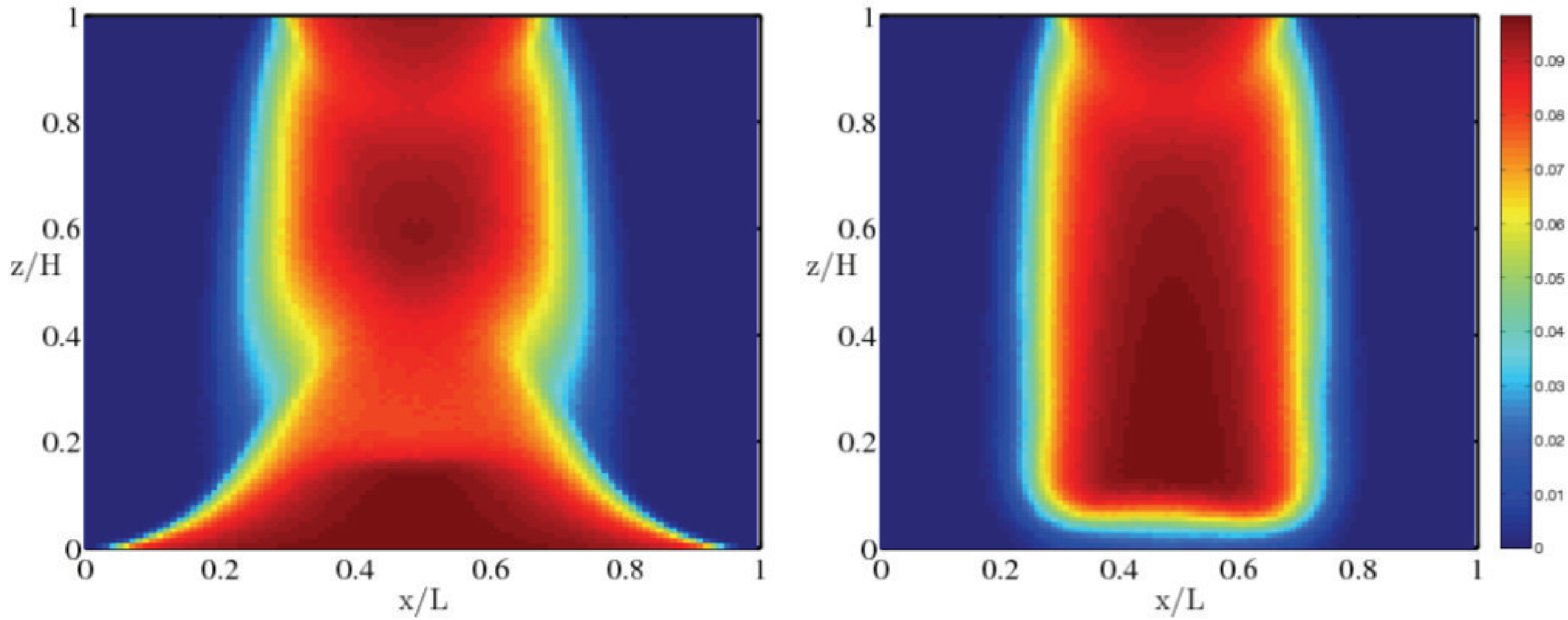

modeling difficulties:

- miscible and immiscible
- reactive
- many scales
- many dof
- instabilities + fingering
- physics
- complex joint PDFs
- non-equilibrium
- ...



# Motivation for PDF Modeling

## Example: Multi-Phase Flow in Porous Media (M. Tyagi, P. Jenny)



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## Example: Multi-Phase Flow in Porous Media

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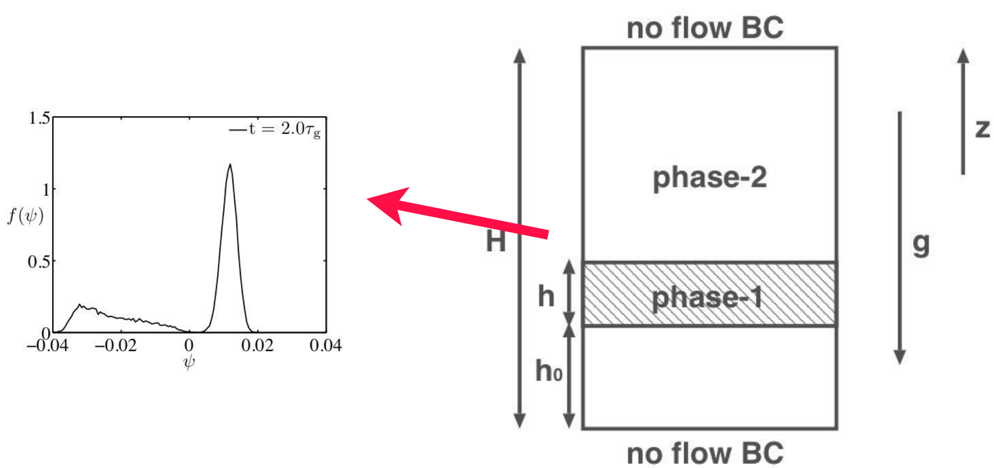
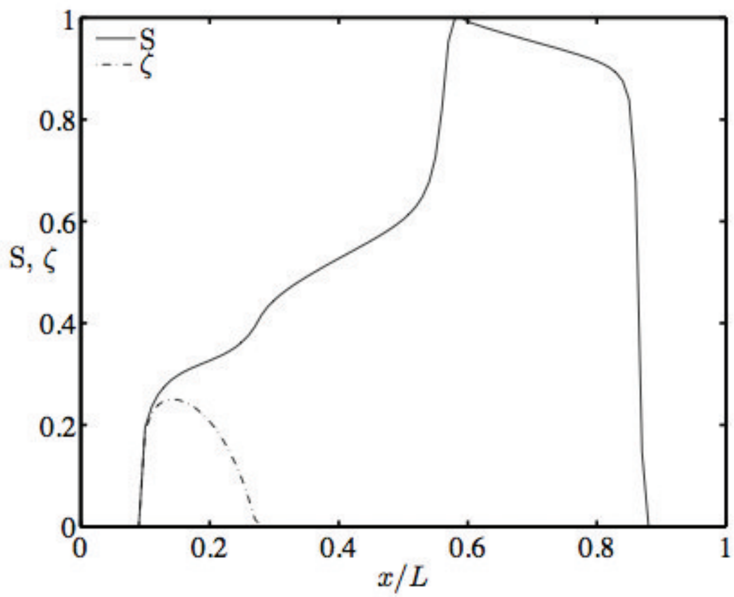
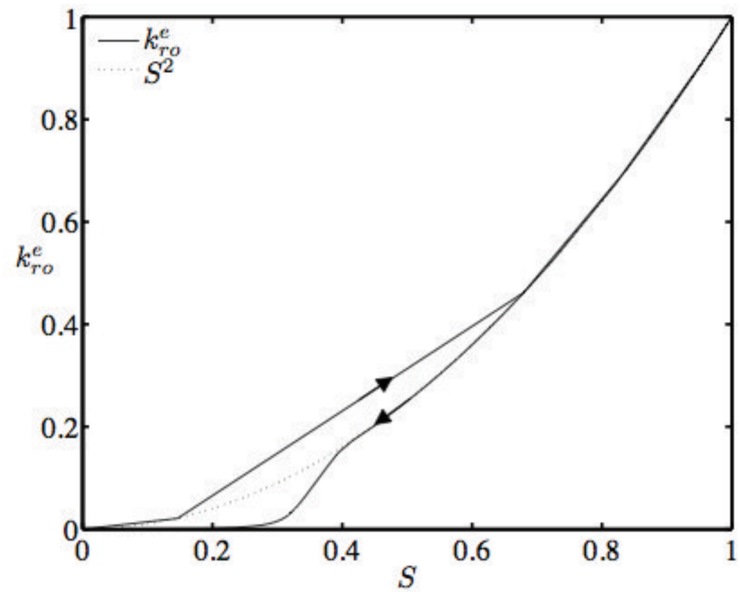


# Motivation for PDF Modeling

## Example: Multi-Phase Flow in Porous Media (M. Tyagi, P. Jenny)



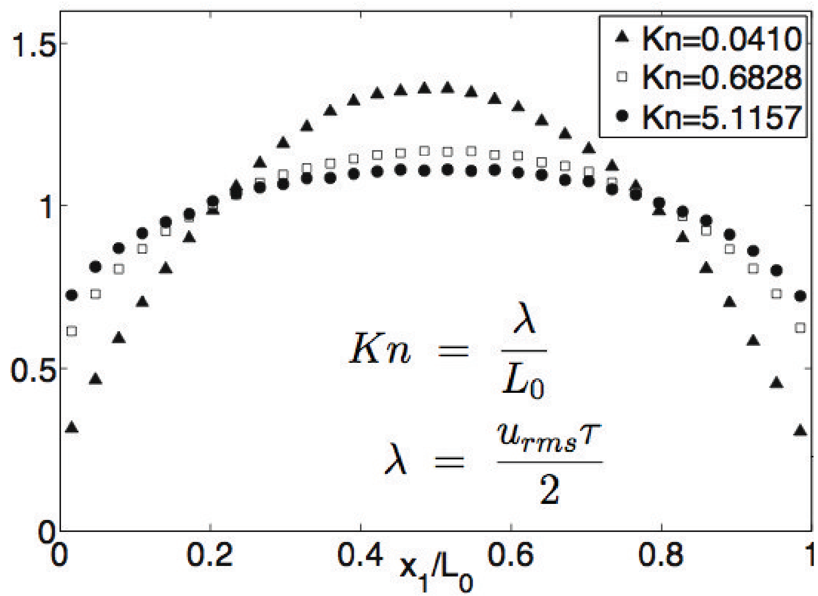



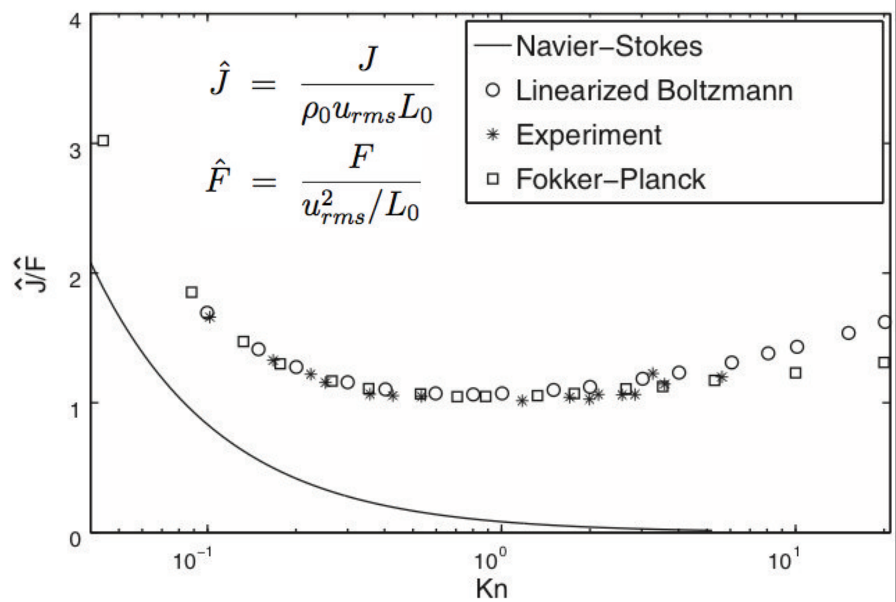

$$t = 0.25\tau_x$$

# Motivation for PDF Modeling

## Example: Knudsen Paradox

(P. Jenny, M. Torrilhon, S. Heinz)



# Motivation for PDF Modeling

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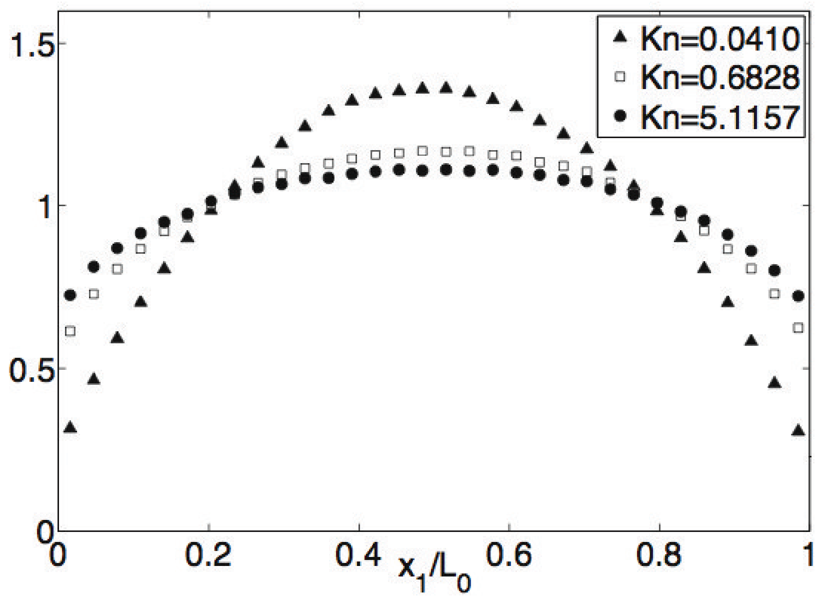
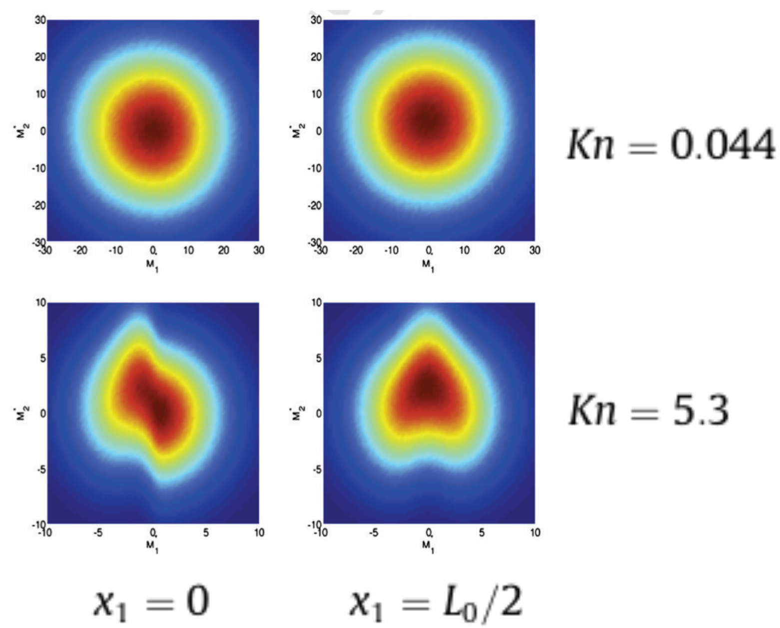


# Basic Background

## First Illustrative Example: Brownian Motion

Particle evolves according to Brownian motion:

$$dX_i = (2\Gamma)^{1/2} dW_i, \tag{1}$$

where $W_i(t)$ is a Wiener process with $dW_i = W_i(t+dt) - W_i(t)$ being independent normal distributed random variables with

$$\langle dW_i \rangle \equiv 0 \quad \text{and} \quad \langle dW_i dW_j \rangle = dt\delta_{ij}. \tag{2}$$

A statistically exact integration of the position is achieved with

$$\Delta X_i = (2\Gamma\Delta t)^{1/2} \xi_i, \tag{3}$$

where $\xi_i$ are independent normal distributed random variables and $\Delta t$ is the time step size.

Question: how dies the probability density finction (PDF) $f_{\boldsymbol{X}}$ of the particle position $\boldsymbol{X}$ evolve?

# Basic Background

Answer:

$$\frac{\partial f_{\boldsymbol{X}}}{\partial t} = \frac{\partial^2}{\partial x_i \partial x_i} (\Gamma f_{\boldsymbol{X}}) , \tag{4}$$

where $x_i$ is the sample space coordinate of the stochastic variable $X_i$.

If a huge number $M$ of particles is considered, then the local particle number density $C$ represents $M f_{\boldsymbol{X}}$, i.e. for constant $M$ on obtains

$$\frac{\partial C}{\partial t} = \frac{\partial^2}{\partial x_i \partial x_i} (\Gamma C) . \tag{5}$$

# Basic Background

## General PDF Evolution Equations

Next: we derive the general form of an evolution equation for $f_X(x;t)$, where $x \in \mathbb{R}$:

$$
\begin{aligned}
f_X(x;t) &= \langle \delta(X(t)-x) \rangle \\
f_X(x;t+\Delta t) &= \langle \delta(X(t)-x+\Delta X) \rangle \\
&= f_X(x;t) + \sum_{k=1}^{\infty} \frac{1}{k!} \left\langle \left(-\frac{\partial}{\partial x}\right)^k \delta(X(t)-x)\, \Delta X^k \right\rangle \\
&= f_X(x;t) + \sum_{k=1}^{\infty} \left(-\frac{\partial}{\partial x}\right)^k \left\{ \frac{\langle \Delta X^k | x;t \rangle}{k!} f_X(x;t) \right\} \qquad (6)
\end{aligned}
$$

from which follows the Kramers Moyal equation:

$$
\frac{\partial f_X(x;t)}{\partial t} = \sum_{k=1}^{\infty} \left(-\frac{\partial}{\partial x}\right)^k \left\{ \underbrace{\lim_{\Delta t \to 0} \frac{\langle \Delta X^k | x;t \rangle}{k! \Delta t}}_{D^{(k)}} f_X(x;t) \right\}. \qquad (7)
$$

# Basic Background

## Kramers-Moyal Equation

Problem: $\infty$ many terms!

Next: show that only two terms ($k = 1, 2$) are required, if $\lim_{\Delta t \to 0} \Delta x / \Delta t$ is bounded

# Basic Background

## Theorem of Pawula

**Theorem 1** *If* $\exists m > 1 : D^{(2m)} = 0$*, then* $\forall k > 2 : D^{(k)} = 0$.

**Proof 1** *Consider the two random variables* $\alpha = \Delta X^a$ *and* $\beta = \Delta X^b$ *with* $a, b \in \mathbb{N} \wedge a, b \geq 1$.
*Schwarz inequality* $\Rightarrow$

$$\begin{aligned} \langle \alpha\beta | x; t\rangle^2 &\leq \langle \alpha^2 | x; t\rangle \langle \beta^2 | x; t\rangle \\ \langle \Delta X^{a+b} | x; t\rangle^2 &\leq \langle \Delta X^{2a} | x; t\rangle \langle \Delta X^{2b} | x; t\rangle \end{aligned}$$

$$\boxed{\underbrace{\lim_{\Delta t \to 0} \frac{\langle \Delta X^k | x; t\rangle}{k! \Delta t}}_{D^{(k)}}}$$

$\Delta t \to 0 \wedge b = a + k \Rightarrow$

$$\left((2a+k)! D^{(2a+k)}\right)^2 \leq (2a)!(2a+2k)! D^{(2a)} D^{(2a+2k)} \tag{8}$$

$$\begin{aligned} &\textit{If} \quad D^{(2a)} = 0 \quad &\Rightarrow \quad D^{(2a+k)} = 0 \quad \forall k \geq 1 \\ &\textit{If} \quad D^{(2a+2k)} = 0 \quad &\Rightarrow \quad D^{(2a+k)} = 0 \quad \forall k \geq 1 \end{aligned}$$

$\Rightarrow$ *if* $\exists m > 1 : D^{(2m)} = 0$*, then* $\forall k > 2 : D^{(k)} = 0$.
$\square$

# Basic Background

## Kramers-Moyal Equation

$$\frac{\partial f_X(x;t)}{\partial t} = \sum_{k=1}^{\infty} \left(-\frac{\partial}{\partial x}\right)^k \left\{ \underbrace{\lim_{\Delta t \to 0} \frac{\langle \Delta X^k | x; t\rangle}{k! \Delta t}}_{D^{(k)}} f_X(x;t) \right\}$$

There exist two possibilities:

1. only $D^{(1)}$ and $D^{(2)}$ are unequal zero, or
2. $D^{(2k)} \neq 0$ for all $k \geq 1$.

Gradiner showed that option one is true, if $\lim_{\Delta t \to 0} \Delta X / \Delta t$ is bounded.

# Basic Background

## Fokker-Planck Equation

From the theorem of Pawula it follows that the Fokker-Planck equation

$$\frac{\partial f_X(x;t)}{\partial t} = -\frac{\partial D^{(1)} f_X(x;t)}{\partial x} + \frac{\partial^2 D^{(2)} f_X(x;t)}{\partial x^2} \tag{9}$$

with

$$D^{(1)} = \lim_{\Delta t \to 0} \frac{\langle \Delta X | x; t \rangle}{\Delta t}$$

$$D^{(2)} = \lim_{\Delta t \to 0} \frac{\langle \Delta X^2 | x; t \rangle}{2\Delta t}$$

describes the evolution of PDF's based on continuous processes. Note that the PDF equation allows to "link" stochastic processes (or rules) with a deterministic description.

# Basic Background

## Fokker-Planck Equation

More general for high dimensional probability (sample) spaces with $\boldsymbol{X}(t)$ being a realization in the $\boldsymbol{x}$-space at time $t$:

$$\frac{\partial f_{\boldsymbol{X}}(\boldsymbol{x};t)}{\partial t} = -\frac{\partial D_i^{(1)} f_{\boldsymbol{X}}(\boldsymbol{x};t)}{\partial x_i} + \frac{\partial^2 D_{ij}^{(2)} f_{\boldsymbol{X}}(\boldsymbol{x};t)}{\partial x_i \partial x_j} \tag{10}$$

with with

$$\begin{aligned} D_i^{(1)} &= \lim_{\Delta t \to 0} \frac{\langle \Delta X_i | \boldsymbol{x}; t \rangle}{\Delta t} \\ D_{ij}^{(2)} &= \lim_{\Delta t \to 0} \frac{\langle \Delta X_i \Delta X_j | \boldsymbol{x}; t \rangle}{2 \Delta t}. \end{aligned}$$

# Basic Background

## Fokker-Planck Equation

Remember Brownian motion example with

$$\Delta X_i = (2\Gamma\Delta t)^{1/2}\xi_i \tag{11}$$

from which follows that

$$\begin{aligned} D_i^{(1)} &= \lim_{\Delta t\to 0} \tfrac{1}{\Delta t}(2\Gamma\Delta t)^{1/2}\langle\xi_i\rangle &&= 0 \\ \text{and} \quad D_{ij}^{(2)} &= \lim_{\Delta t\to 0} \tfrac{1}{2\Delta t}2\Gamma\Delta t\langle\xi_i\xi_j\rangle &&= \Gamma\delta_{ij}. \end{aligned}$$

and therefore

$$\frac{\partial f}{\partial t} = \frac{\partial^2 \Gamma f}{\partial x_i \partial x_i} \tag{12}$$

as presented earlier.

# Example Non-Fickian Dispersion with Reactions

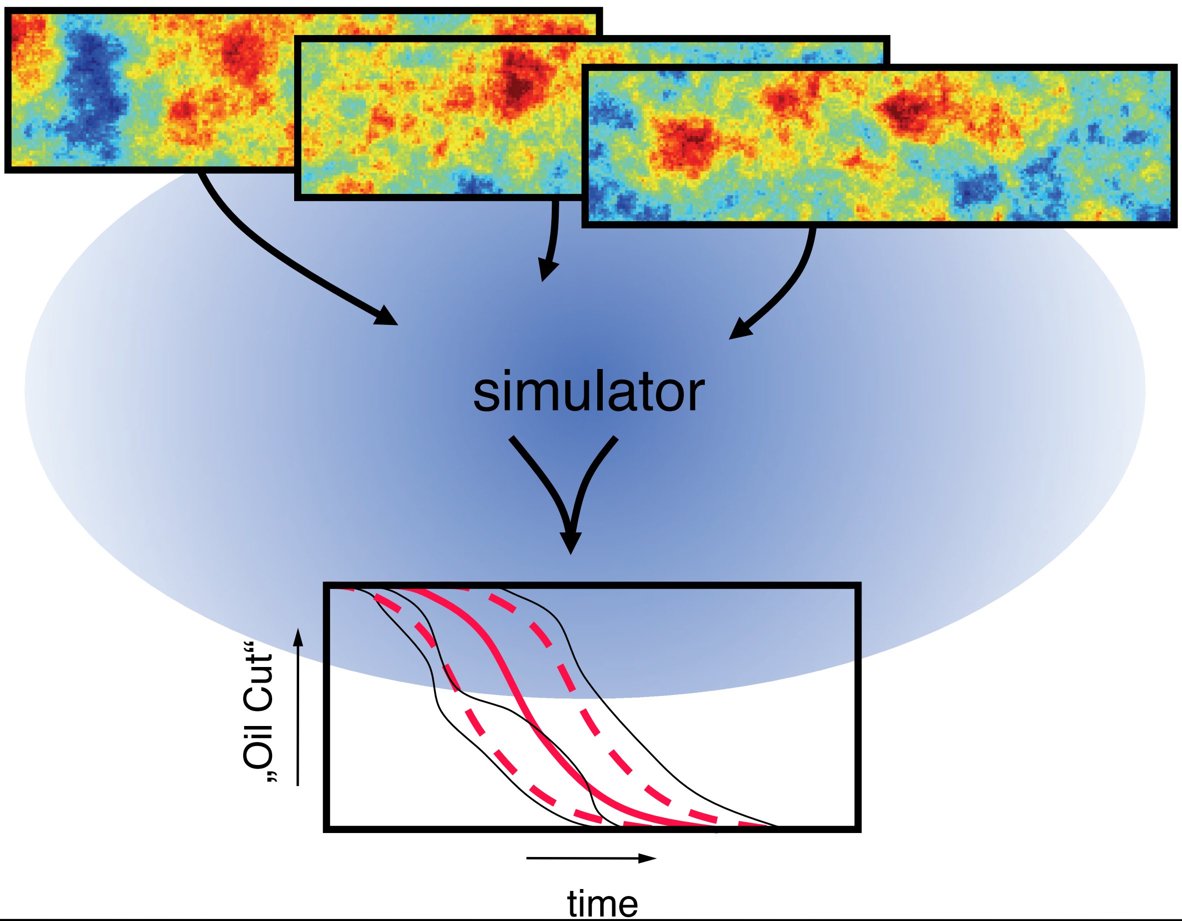
Consider reactive single phase flow in a porous medium. The incompressible fluid is composed of the components $\alpha \in \{1, ..., n_c\}$ with mass fractions $\Phi_\alpha$. Each fluid element of mass $m$ has a position $\boldsymbol{X}(t) \in \mathbb{R}^3$, a velocity $\boldsymbol{U}(t) \in \mathbb{R}^3$ and a composition vector $\boldsymbol{\Phi}(t) \in \mathbb{R}^{n_c}$, which are modeled as

$$\begin{aligned} dX_i &= U_i dt \\ dU_i &= -|\boldsymbol{U}|/L_U(U_i - \langle U_i \rangle)dt \ + \ (2\sigma^2|\boldsymbol{U}|/L_U)^{1/2} dW_i \ + \ F_i dt \\ d\Phi_\alpha &= -|\boldsymbol{U}|/L_\Phi(\Phi_\alpha - \langle \Phi_\alpha \rangle)dt \ + \ S_\alpha(\boldsymbol{\Phi})dt. \end{aligned}$$

Extracted: $\langle \boldsymbol{\Phi} \rangle$
Specified: $\langle \boldsymbol{U} \rangle$, $\sigma^2$, $L_U$, $L_\Phi$ and $\boldsymbol{S}(\boldsymbol{\Phi})$

# Example Non-Fickian Dispersion with Reactions

Monte Carlo:



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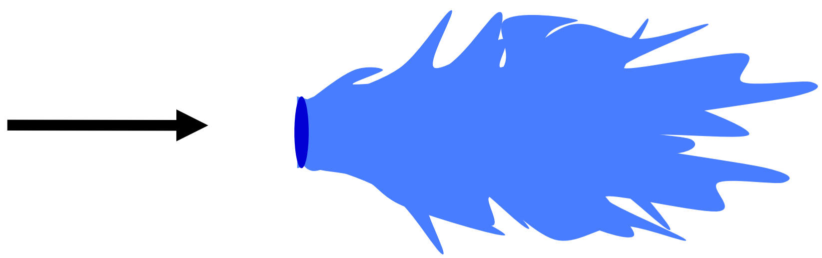
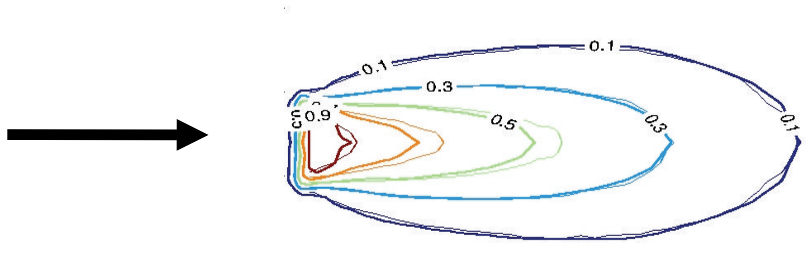


transport of tracer particles

# Example Non-Fickian Dispersion with Reactions 

Monte Carlo:




transport of tracer particles

# Example Non-Fickian Dispersion with Reactions

$$
\begin{aligned}
dX_i &= U_i dt \\
dU_i &= -|\boldsymbol{U}|/L_U(U_i - \langle U_i \rangle)dt \;+\; (2\sigma^2|\boldsymbol{U}|/L_U)^{1/2}dW_i \;+\; F_i dt \\
d\Phi_\alpha &= -|\boldsymbol{U}|/L_\Phi(\Phi_\alpha - \langle \Phi_\alpha \rangle)dt \;+\; S_\alpha(\boldsymbol{\Phi})dt.
\end{aligned}
$$

From this follows for joint PDF $f(\boldsymbol{V}, \boldsymbol{\Psi}, \boldsymbol{x}; t)$:

$$
\begin{aligned}
\frac{\partial f}{\partial t} + V_i \frac{\partial f}{\partial x_i} &+ \frac{\partial}{\partial V_i}\left\{\left(\frac{|\boldsymbol{V}|(\langle U_i \rangle - V_i)}{L_U} + F_i\right) f\right\} \\
&+ \frac{\partial}{\partial \Psi_\alpha}\left\{\left(\frac{|\boldsymbol{V}|(\langle \Phi_\alpha \rangle - \Psi_\alpha)}{L_\Phi} + S_\alpha(\boldsymbol{\Psi})\right) f\right\} \\
&= \frac{\partial^2}{\partial V_i \partial V_i}\left\{\frac{|\boldsymbol{V}|\sigma^2}{L_U} f\right\}. \qquad (13)
\end{aligned}
$$

# Example Non-Fickian Dispersion with Reactions

The total mass is $M$ and $\langle \rho \rangle(\boldsymbol{x};t) = M \int_{\mathbb{R}^{3+n_c}} f d\boldsymbol{V} d\boldsymbol{\Psi}$ is the mean fluid density, which is constant here (equal $\rho$), since incompressible. Multiplying the PDF equation with $(1, V_j, \Psi_\beta)^T$ and integrating over the $\boldsymbol{V}$-$\boldsymbol{\Psi}$-space leads to

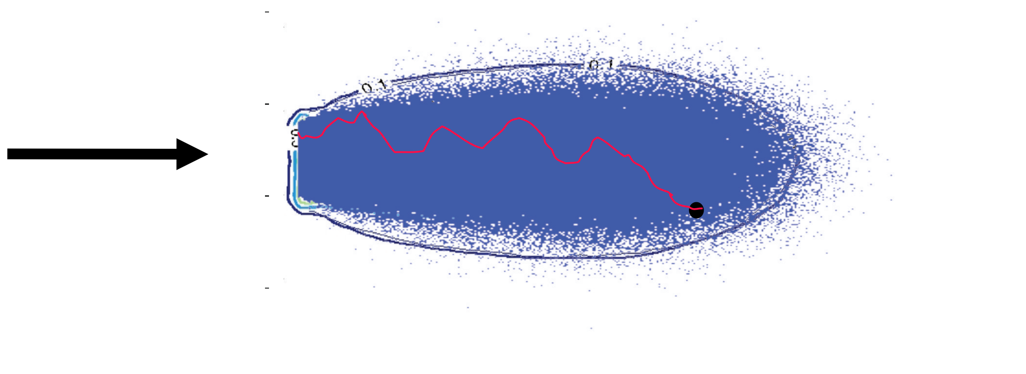
$$\begin{aligned}
\frac{\partial \langle U_i \rangle}{\partial x_i} &= 0 \\
\frac{\partial \langle U_j \rangle}{\partial t} + \frac{\partial \langle U_i \rangle \langle U_j \rangle}{\partial x_i} &= -\frac{\partial \langle u_i' u_j' \rangle}{\partial x_i} - \frac{1}{L_U} \langle |\boldsymbol{U}| u_j' \rangle + F_j \\
\frac{\partial \langle \Phi_\beta \rangle}{\partial t} + \frac{\partial \langle U_i \rangle \langle \Phi_\beta \rangle}{\partial x_i} &= -\underbrace{\frac{\partial \langle u_i' \Phi_\beta' \rangle}{\partial x_i}}_{\text{unclosed}} - \underbrace{\frac{1}{L_\Phi} \langle |\boldsymbol{U}| \Phi_\beta' \rangle}_{\text{unclosed}} + \underbrace{\langle S_\beta(\boldsymbol{\Phi}) \rangle}_{\text{unclosed}},
\end{aligned}$$

where $\boldsymbol{U} = \langle \boldsymbol{U} \rangle + \boldsymbol{u}'$ and $\boldsymbol{\Phi} = \langle \boldsymbol{\Phi} \rangle + \boldsymbol{\Phi}'$. Note that $\boldsymbol{F} = \langle |\boldsymbol{U}| \boldsymbol{u}' \rangle / L_U$ if homogeneous.

# Example Non-Fickian Dispersion with Reactions



PDF method:



transport of tracer particles

# Example Non-Fickian Dispersion with Reactions

Conclusions:

- Moment equations can be derived from PDF equation, but typically new closure problems arise. Tradeoff: high dimensional scalar PDF equation without closure problems vs. system of low dimensional moment equations with closure problems.
- Presumed PDF approach can be a good compromise: parametrization of PDF leads to closed set of moment equations.
- General approach: due to high dimensionality evolve many particles and extract desired statistics *Rightarrow* computational challenges.
- Note: here the reactive dispersive transport problem is closed, if Lagrangian velocity statistics can be specified (stochastic rules).
- For these stochastic small scale rules one can derive deterministic (but typically unclosed) large scale moment equations.

# Turbulent Reactive Flows

## Basic Equations: Compressible Navier-Stokes

$$\text{Continuity:} \quad \frac{\partial \rho}{\partial t} + \frac{\partial \rho U_i}{\partial x_i} = 0$$

$$\text{Momentum:} \quad \underbrace{\frac{\partial U_j}{\partial t} + U_i \frac{\partial U_j}{\partial x_i}}_{\frac{dU_j}{dt}} = \frac{1}{\rho}\left(-\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i}\right) + F_j$$

$$\text{Composition:} \quad \underbrace{\frac{\partial \Phi_\beta}{\partial t} + U_i \frac{\partial \Phi_\beta}{\partial x_i}}_{d\Phi_\beta} = -\frac{1}{\rho}\frac{\partial J_{\beta_i}}{\partial x_i} + S_\beta$$

Note: for low Mach numbers $\delta p \ll p \Rightarrow \rho(\boldsymbol{\Phi}) \wedge T(\boldsymbol{\Phi})$ and the enthalpy $h$ can be treated as a component, e.g. $h = \Phi_1$, $\boldsymbol{J}_1 = -\lambda \boldsymbol{\nabla} T$ and $S_1$ =heat release due to reactions.

# Turbulent Reactive Flows

## Basic Equations: Compressible Navier-Stokes

$$\text{Continuity:} \quad \frac{\partial \rho}{\partial t} + \frac{\partial \rho U_i}{\partial x_i} = 0$$

$$\text{Momentum:} \quad \underbrace{\frac{\partial U_j}{\partial t} + U_i \frac{\partial U_j}{\partial x_i}}_{\frac{dU_j}{dt}} = \frac{1}{\rho}\left(-\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i}\right) + F_j$$

$$\text{Composition:} \quad \underbrace{\frac{\partial \Phi_\beta}{\partial t} + U_i \frac{\partial \Phi_\beta}{\partial x_i}}_{\frac{d\Phi_\beta}{dt}} = -\frac{1}{\rho}\frac{\partial J_{\beta_i}}{\partial x_i} + S_\beta$$

Reynolds averaging:

$$\frac{\partial \langle\rho\rangle}{\partial t} + \frac{\partial \langle\rho\rangle \widetilde{U}_i}{\partial x_i} = 0$$

$$\frac{\partial \widetilde{U}_j}{\partial t} + \widetilde{U}_i \frac{\partial \widetilde{U}_j}{\partial x_i} = \frac{1}{\langle\rho\rangle}\left(-\frac{\partial \langle p\rangle}{\partial x_j} + \frac{\partial \langle\tau_{ij}\rangle}{\partial x_i} - \frac{\partial \langle\rho\rangle \widetilde{u_i'' u_j''}}{\partial x_i}\right) + F_j$$

$$\frac{\partial \widetilde{\Phi}_\beta}{\partial t} + \widetilde{U}_i \frac{\partial \widetilde{\Phi}_\beta}{\partial x_i} = \frac{1}{\langle\rho\rangle}\left(-\frac{\partial \langle J_{\beta_i}\rangle}{\partial x_i} - \frac{\partial \langle\rho\rangle \widetilde{u_i'' \Phi_\beta''}}{\partial x_i}\right) + \widetilde{S}_\beta$$